



# Full wwPDB X-ray Structure Validation Report ⓘ

May 4, 2024 – 03:03 pm BST

PDB ID : 5ON6  
Title : Crystal structure of haemanthamine bound to the 80S ribosome  
Authors : Pellegrino, S.; Meyer, M.; Yusupova, G.; Yusupov, M.  
Deposited on : 2017-08-03  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

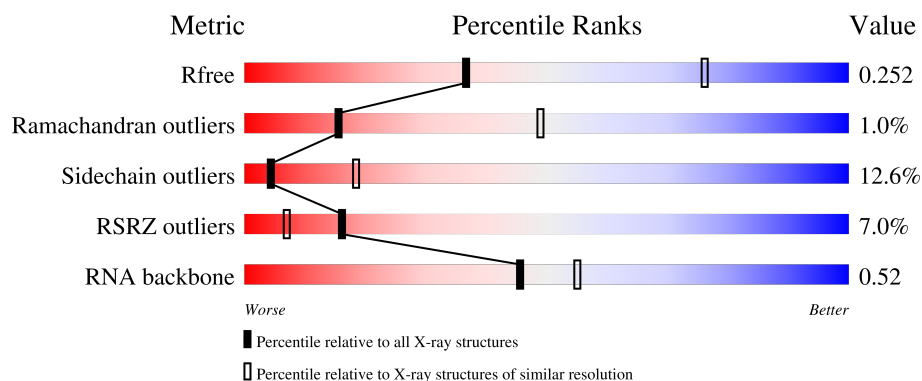
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	3396	<div> <div>3%</div> <div>75%</div> <div>17%</div> <div>7%</div> </div>
1	AR	3396	<div> <div>3%</div> <div>74%</div> <div>18%</div> <div>7%</div> </div>
2	3	121	<div> <div>89%</div> <div>11%</div> </div>
2	AS	121	<div> <div>%</div> <div>88%</div> <div>11%</div> </div>
3	4	158	<div> <div>3%</div> <div>78%</div> <div>22%</div> </div>














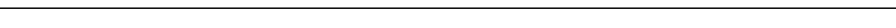

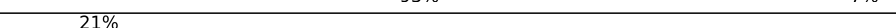

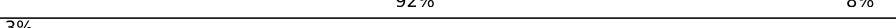



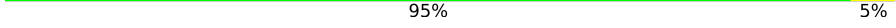



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Mol	Chain	Length	Quality of chain
3	AT	158	<div> <div>4%</div> <div>82%</div> <div>18%</div> <div>.</div> </div>
4	CD	252	<div> <div>%</div> <div>90%</div> <div>10%</div> </div>
4	j	252	<div> <div>89%</div> <div>11%</div> </div>
5	CE	386	<div> <div>87%</div> <div>13%</div> <div>.</div> </div>
5	k	386	<div> <div>%</div> <div>87%</div> <div>13%</div> </div>
6	CF	361	<div> <div>90%</div> <div>10%</div> </div>
6	l	361	<div> <div>89%</div> <div>10%</div> <div>.</div> </div>
7	CG	296	<div> <div>4%</div> <div>86%</div> <div>14%</div> </div>
7	m	296	<div> <div>6%</div> <div>90%</div> <div>10%</div> </div>
8	CH	175	<div> <div>2%</div> <div>78%</div> <div>11%</div> <div>11%</div> </div>
8	n	175	<div> <div>%</div> <div>81%</div> <div>7%</div> <div>11%</div> </div>
9	CI	222	<div> <div>%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
9	o	222	<div> <div>2%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
10	CJ	233	<div> <div>14%</div> <div>92%</div> <div>8%</div> </div>
10	p	233	<div> <div>6%</div> <div>91%</div> <div>9%</div> </div>
11	CK	191	<div> <div>2%</div> <div>85%</div> <div>15%</div> </div>
11	q	191	<div> <div>87%</div> <div>13%</div> </div>
12	CL	220	<div> <div>6%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>
12	r	220	<div> <div>%</div> <div>82%</div> <div>14%</div> <div>.</div> </div>
13	CM	169	<div> <div>%</div> <div>85%</div> <div>15%</div> <div>.</div> </div>
13	s	169	<div> <div>2%</div> <div>85%</div> <div>14%</div> <div>..</div> </div>
14	CN	193	<div> <div>8%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
14	t	193	<div> <div>86%</div> <div>13%</div> <div>.</div> </div>
15	CO	136	<div> <div>%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
15	u	136	<div> <div>2%</div> <div>85%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
16	CP	203	 92% 8%
16	v	203	 90% 10%
17	CQ	197	 2% 90% 9%
17	w	197	 88% 11%
18	CR	183	 16% 87% 13%
18	x	183	 11% 87% 12%
19	CS	185	 87% 13%
19	y	185	 89% 10%
20	CT	188	 5% 89% 11%
20	z	188	 4% 93% 7%
21	0	172	 85% 14%
21	CU	172	 85% 15%
22	2	159	 86% 14%
22	CV	159	 84% 16%
23	5	100	 12% 93% 7%
23	CW	100	 21% 89% 11%
24	CX	136	 92% 8%
24	lR	136	 3% 89% 11%
25	6	1800	 6% 77% 22%
25	A	1800	 7% 74% 24%
26	7	98	 30% 95% 5%
26	CY	98	 11% 88% 11%
27	8	121	 89% 11%
27	CZ	121	 3% 88% 12%
28	9	126	 5% 89% 11%







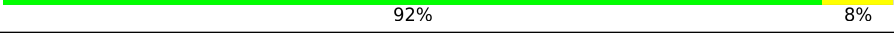

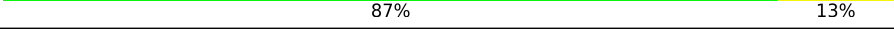

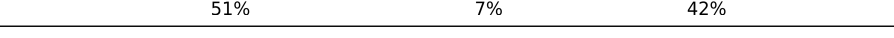
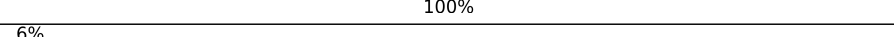
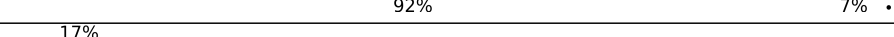
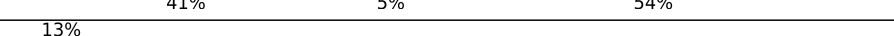


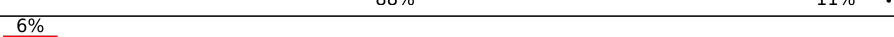

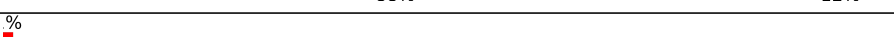






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Mol	Chain	Length	Quality of chain
28	DA	126	
29	AA	135	
29	DB	135	
30	AB	148	
30	DC	148	
31	AC	58	
31	DD	58	
32	AD	97	
32	DE	97	
33	AE	109	
33	DF	109	
34	AF	127	
34	DG	127	
35	AG	106	
35	DH	106	
36	AH	112	
36	DI	112	
37	AI	119	
37	DJ	119	
38	AJ	99	
38	DK	99	
39	AK	87	
39	DL	87	
40	AL	77	
40	DM	77	

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Mol	Chain	Length	Quality of chain
41	AM	50	
41	DN	50	
42	AN	52	
42	DO	52	
43	AO	25	
43	DP	25	
44	AP	105	
44	DQ	105	
45	AQ	91	
45	DR	91	
46	i	272	
47	m2	150	
48	sM	104	
49	p0	311	
50	B	206	
50	s0	206	
51	C	216	
51	s1	216	
52	D	217	
52	s2	217	
53	E	223	
53	s3	223	
54	F	260	
54	s4	260	
55	G	206	

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Mol	Chain	Length	Quality of chain
55	s5	206	<div> <div>17%</div> <div>91%</div> <div>9%</div> </div>
56	H	226	<div> <div>17%</div> <div>87%</div> <div>13%</div> </div>
56	s6	226	<div> <div>12%</div> <div>85%</div> <div>11%</div> <div>.</div> </div>
57	I	186	<div> <div>16%</div> <div>87%</div> <div>12%</div> <div>..</div> </div>
57	s7	186	<div> <div>17%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
58	J	199	<div> <div>5%</div> <div>87%</div> <div>6%</div> <div>.</div> <div>6%</div> </div>
58	s8	199	<div> <div>7%</div> <div>88%</div> <div>6%</div> <div>.</div> <div>6%</div> </div>
59	K	185	<div> <div>18%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
59	s9	185	<div> <div>8%</div> <div>84%</div> <div>16%</div> </div>
60	L	105	<div> <div>15%</div> <div>82%</div> <div>9%</div> <div>.</div> <div>9%</div> </div>
60	c0	105	<div> <div>52%</div> <div>78%</div> <div>10%</div> <div>.</div> <div>9%</div> </div>
61	M	155	<div> <div>10%</div> <div>92%</div> <div>8%</div> </div>
61	c1	155	<div> <div>5%</div> <div>84%</div> <div>10%</div> <div>.</div> <div>6%</div> </div>
62	N	124	<div> <div>52%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
62	c2	124	<div> <div>70%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
63	O	150	<div> <div>6%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
63	c3	150	<div> <div>3%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
64	P	128	<div> <div>28%</div> <div>90%</div> <div>9%</div> <div>..</div> </div>
64	c4	128	<div> <div>9%</div> <div>89%</div> <div>11%</div> </div>
65	Q	141	<div> <div>5%</div> <div>79%</div> <div>8%</div> <div>.</div> <div>12%</div> </div>
65	c5	141	<div> <div>11%</div> <div>82%</div> <div>12%</div> <div>..</div> </div>
66	R	142	<div> <div>18%</div> <div>87%</div> <div>12%</div> <div>..</div> </div>
66	c6	142	<div> <div>11%</div> <div>82%</div> <div>18%</div> </div>
67	S	125	<div> <div>11%</div> <div>84%</div> <div>11%</div> <div>..</div> </div>
67	c7	125	<div> <div>5%</div> <div>82%</div> <div>11%</div> <div>.</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
68	T	145	
68	c8	145	
69	U	143	
69	c9	143	
70	V	110	
70	d0	110	
71	W	87	
71	d1	87	
72	X	129	
72	d2	129	
73	Y	144	
73	d3	144	
74	Z	134	
74	d4	134	
75	a	70	
75	d5	70	
76	b	97	
76	d6	97	
77	c	81	
77	d7	81	
78	d	63	
78	d8	63	
79	d9	53	
79	e	53	
80	e0	62	

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Mol	Chain	Length	Quality of chain
80	f	62	
81	g	71	
82	h	318	
82	sR	318	
83	e1	51	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	AR	3737	-	-	-	X
85	MG	1	3744	-	-	-	X
85	MG	1	3800	-	-	-	X
85	MG	1	3801	-	-	-	X
85	MG	1	3820	-	-	-	X
85	MG	1	3930	-	-	-	X
85	MG	1	3941	-	-	-	X
85	MG	1	3965	-	-	-	X
85	MG	1	3983	-	-	-	X
85	MG	1	4001	-	-	-	X
85	MG	1	4012	-	-	-	X
85	MG	1	4023	-	-	-	X
85	MG	1	4053	-	-	-	X
85	MG	1	4092	-	-	-	X
85	MG	1	4101	-	-	-	X
85	MG	1	4104	-	-	-	X
85	MG	1	4129	-	-	-	X
85	MG	1	4152	-	-	-	X
85	MG	1	4158	-	-	-	X
85	MG	1	4190	-	-	-	X
85	MG	4	221	-	-	-	X
85	MG	4	229	-	-	-	X
85	MG	4	235	-	-	-	X
85	MG	6	2076	-	-	-	X
85	MG	6	2083	-	-	-	X
85	MG	6	2092	-	-	-	X
85	MG	6	2133	-	-	-	X
85	MG	6	2154	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	6	2158	-	-	-	X
85	MG	6	2163	-	-	-	X
85	MG	6	2167	-	-	-	X
85	MG	6	2174	-	-	-	X
85	MG	6	2176	-	-	-	X
85	MG	6	2180	-	-	-	X
85	MG	6	2183	-	-	-	X
85	MG	6	2185	-	-	-	X
85	MG	6	2188	-	-	-	X
85	MG	6	2191	-	-	-	X
85	MG	6	2192	-	-	-	X
85	MG	6	2193	-	-	-	X
85	MG	6	2197	-	-	-	X
85	MG	A	2045	-	-	-	X
85	MG	A	2062	-	-	-	X
85	MG	A	2099	-	-	-	X
85	MG	A	2103	-	-	-	X
85	MG	A	2116	-	-	-	X
85	MG	A	2118	-	-	-	X
85	MG	A	2128	-	-	-	X
85	MG	A	2130	-	-	-	X
85	MG	A	2131	-	-	-	X
85	MG	A	2135	-	-	-	X
85	MG	A	2136	-	-	-	X
85	MG	A	2151	-	-	-	X
85	MG	A	2155	-	-	-	X
85	MG	AR	3803	-	-	-	X
85	MG	AR	3890	-	-	-	X
85	MG	AR	3971	-	-	-	X
85	MG	AR	3976	-	-	-	X
85	MG	AR	3998	-	-	-	X
85	MG	AR	4003	-	-	-	X
85	MG	AR	4005	-	-	-	X
85	MG	AR	4022	-	-	-	X
85	MG	AR	4024	-	-	-	X
85	MG	AR	4030	-	-	-	X
85	MG	AR	4034	-	-	-	X
85	MG	AR	4085	-	-	-	X
85	MG	AR	4097	-	-	-	X
85	MG	AR	4102	-	-	-	X
85	MG	AR	4110	-	-	-	X
85	MG	AR	4156	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	AR	4174	-	-	-	X
85	MG	AR	4196	-	-	-	X
85	MG	AR	4255	-	-	-	X
85	MG	AS	228	-	-	-	X
85	MG	CD	302	-	-	-	X
85	MG	V	201	-	-	-	X
85	MG	b	101	-	-	-	X
85	MG	l	403	-	-	-	X
85	MG	x	206	-	-	-	X
87	GOL	6	2199	-	-	-	X
88	ZN	d7	101	-	-	-	X

## 2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 410383 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
1	AR	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
2	AS	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
3	AT	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	j	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
4	CD	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	k	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
5	CE	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	l	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
6	CF	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	m	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
7	CG	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	n	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
8	CH	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	o	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
9	CI	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	p	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	q	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
11	CK	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	r	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			
12	CL	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	s	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
13	CM	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	t	193	Total	C	N	O	0	0	0
			1543	962	315	266			
14	CN	193	Total	C	N	O	0	0	0
			1543	962	315	266			

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	u	136	Total	C	N	O	0	0	0
			1053	675	199	177			
15	CO	136	Total	C	N	O	0	0	0
			1053	675	199	177			

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	v	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
16	CP	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	w	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
17	CQ	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	x	183	Total	C	N	O		0	0	0
			1420	882	281	257				
18	CR	183	Total	C	N	O		0	0	0
			1420	882	281	257				

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	y	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
19	CS	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	z	188	Total	C	N	O		0	0	0
			1521	935	326	260				
20	CT	188	Total	C	N	O		0	0	0
			1521	935	326	260				

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
21	CU	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	2	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
22	CV	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	5	100	Total	C	N	O		0	0	0
			796	516	131	149				
23	CW	100	Total	C	N	O		0	0	0
			796	516	131	149				

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	IR	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
24	CX	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 25 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	6	1783	Total	C	N	O	P	0	0	0
			37990	16984	6723	12500	1783			
25	A	1781	Total	C	N	O	P	0	0	0
			37948	16965	6715	12487	1781			

- Molecule 26 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	7	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	CY	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			

- Molecule 27 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	8	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
27	CZ	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			

- Molecule 28 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	9	126	Total	C	N	O		0	0	0
			993	625	192	176				
28	DA	126	Total	C	N	O		0	0	0
			993	625	192	176				

- Molecule 29 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	AA	135	Total	C	N	O		0	0	0
			1092	710	202	180				
29	DB	135	Total	C	N	O		0	0	0
			1092	710	202	180				

- Molecule 30 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AB	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
30	DC	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AC	58	Total	C	N	O		0	0	0
			462	289	100	73				
31	DD	58	Total	C	N	O		0	0	0
			462	289	100	73				

- Molecule 32 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AD	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
32	DE	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			

- Molecule 33 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AE	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
33	DF	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			

- Molecule 34 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	AF	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
34	DG	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	AG	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
35	DH	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 36 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	AH	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
36	DI	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

- Molecule 37 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AI	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
37	DJ	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			

- Molecule 38 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	AJ	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
38	DK	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			

- Molecule 39 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	AK	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
39	DL	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	AL	77	Total	C	N	O	0	0	0
			612	391	115	106			
40	DM	77	Total	C	N	O	0	0	0
			612	391	115	106			

- Molecule 41 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	AM	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
41	DN	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	AN	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DO	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 43 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AO	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
43	DP	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 44 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	AP	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
44	DQ	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 45 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	AQ	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
45	DR	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

- Molecule 46 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	i	159	Total	C	N	O	0	0	0
			1104	652	221	231			

- Molecule 47 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	m2	150	Total	C	N	O	0	0	0
			750	450	150	150			

- Molecule 48 is a protein called Suppressor protein STM1,Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	sM	104	Total	C	N	O			
			680	403	140	137	0	0	0

- Molecule 49 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	p0	143	Total	C	N	O	S			
			1076	686	192	195	3	0	0	0

- Molecule 50 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B	206	Total	C	N	O	S			
			1577	1014	278	283	2	0	0	0
50	s0	206	Total	C	N	O	S			
			1583	1017	281	283	2	0	0	0

- Molecule 51 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	C	214	Total	C	N	O	S			
			1709	1084	310	311	4	0	0	0
51	s1	216	Total	C	N	O	S			
			1722	1091	312	315	4	0	0	0

- Molecule 52 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	D	217	Total	C	N	O	S			
			1635	1047	289	297	2	0	0	0
52	s2	217	Total	C	N	O	S			
			1635	1047	289	297	2	0	0	0

- Molecule 53 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	E	223	Total	C	N	O	S			
			1734	1101	313	314	6	0	0	0
53	s3	223	Total	C	N	O	S			
			1734	1101	313	314	6	0	0	0

- Molecule 54 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	F	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
54	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 55 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	G	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
55	s5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

- Molecule 56 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	H	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
56	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 57 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
57	I	184	Total	C	N	O	0	0	0
			1481	951	265	265			
57	s7	186	Total	C	N	O	0	0	0
			1491	957	267	267			

- Molecule 58 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	J	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			
58	s8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

- Molecule 59 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	K	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 60 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	L	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
60	c0	96	Total	C	N	O	S	0	0	0
			760	489	125	144	2			

- Molecule 61 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	M	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
61	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 62 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	N	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			
62	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- Molecule 63 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	O	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
63	c3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

- Molecule 64 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	P	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
64	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 65 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
65	Q	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
65	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 66 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	R	141	Total	C	N	O		0	0	0
			1105	708	203	194				
66	c6	142	Total	C	N	O		0	0	0
			1111	711	204	196				

- Molecule 67 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	S	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
67	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 68 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	T	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
68	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 69 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	U	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			
69	c9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

- Molecule 70 is a protein called 40S ribosomal protein S20.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	V	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
70	d0	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

- Molecule 71 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	W	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
71	d1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

- Molecule 72 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	X	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
72	d2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

- Molecule 73 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	Y	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
73	d3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

- Molecule 74 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	Z	134	Total	C	N	O	0	0	0
			1073	676	208	189			
74	d4	134	Total	C	N	O	0	0	0
			1073	676	208	189			

- Molecule 75 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
75	a	70	Total	C	N	O	0	0	0
			563	360	104	99			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
75	d5	69	Total	C	N	O	0	0	0
			558	357	103	98			

- Molecule 76 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	b	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
76	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

- Molecule 77 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	c	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
77	d7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

- Molecule 78 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	d	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
78	d8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

- Molecule 79 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	e	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
79	d9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

- Molecule 80 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	f	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
80	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 81 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	g	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			

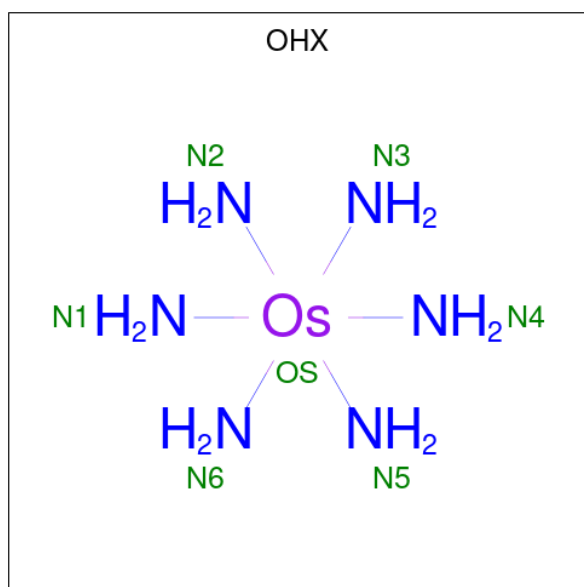
- Molecule 82 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	h	318	Total	C	N	O	S	0	0	0
			2441	1544	419	470	8			
82	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 83 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	e1	51	Total	C	N	O	S	0	0	0
			397	249	73	71	4			

- Molecule 84 is osmium (III) hexammine (three-letter code: OHX) (formula:  $\text{H}_{12}\text{N}_6\text{Os}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
			7	6	1		
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
			7	6	1		
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			7	6	1		
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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84	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	1	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	4	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	Total	N	Os	0	0
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
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84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AR	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AS	1	Total	N	Os	0	0
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84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
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84	AS	1	Total	N	Os	0	0
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84	AS	1	Total	N	Os	0	0
			7	6	1		
84	AS	1	Total	N	Os	0	0
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84	AT	1	Total	N	Os	0	0
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84	AT	1	Total	N	Os	0	0
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84	AT	1	Total	N	Os	0	0
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			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	AT	1	Total	N	Os	0	0
			7	6	1		
84	CE	1	Total	N	Os	0	0
			7	6	1		
84	CE	1	Total	N	Os	0	0
			7	6	1		
84	CF	1	Total	N	Os	0	0
			7	6	1		
84	CF	1	Total	N	Os	0	0
			7	6	1		
84	CG	1	Total	N	Os	0	0
			7	6	1		
84	CG	1	Total	N	Os	0	0
			7	6	1		
84	CK	1	Total	N	Os	0	0
			7	6	1		
84	CL	1	Total	N	Os	0	0
			7	6	1		
84	CM	1	Total	N	Os	0	0
			7	6	1		
84	CP	1	Total	N	Os	0	0
			7	6	1		
84	CV	1	Total	N	Os	0	0
			7	6	1		
84	CX	1	Total	N	Os	0	0
			7	6	1		
84	CX	1	Total	N	Os	0	0
			7	6	1		
84	DD	1	Total	N	Os	0	0
			7	6	1		
84	DH	1	Total	N	Os	0	0
			7	6	1		
84	DQ	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
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84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
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84	A	1	Total	N	Os	0	0
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84	A	1	Total	N	Os	0	0
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84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
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84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	A	1	Total	N	Os	0	0
			7	6	1		
84	J	1	Total	N	Os	0	0
			7	6	1		
84	K	1	Total	N	Os	0	0
			7	6	1		
84	M	1	Total	N	Os	0	0
			7	6	1		
84	O	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	Q	1	Total	N	Os	0	0
			7	6	1		
84	T	1	Total	N	Os	0	0
			7	6	1		
84	e	1	Total	N	Os	0	0
			7	6	1		
84	h	1	Total	N	Os	0	0
			7	6	1		
84	s8	1	Total	N	Os	0	0
			7	6	1		
84	c1	1	Total	N	Os	0	0
			7	6	1		
84	c3	1	Total	N	Os	0	0
			7	6	1		
84	c4	1	Total	N	Os	0	0
			7	6	1		
84	c5	1	Total	N	Os	0	0
			7	6	1		
84	c8	1	Total	N	Os	0	0
			7	6	1		
84	d9	1	Total	N	Os	0	0
			7	6	1		
84	sR	1	Total	N	Os	0	0
			7	6	1		

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	1	498	Total	Mg	0	0
			498	498		
85	3	13	Total	Mg	0	0
			13	13		
85	4	25	Total	Mg	0	0
			25	25		
85	j	2	Total	Mg	0	0
			2	2		
85	k	3	Total	Mg	0	0
			3	3		
85	l	3	Total	Mg	0	0
			3	3		
85	n	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	o	2	Total 2	Mg 2	0	0
85	r	1	Total 1	Mg 1	0	0
85	s	1	Total 1	Mg 1	0	0
85	t	3	Total 3	Mg 3	0	0
85	v	3	Total 3	Mg 3	0	0
85	w	2	Total 2	Mg 2	0	0
85	x	7	Total 7	Mg 7	0	0
85	z	1	Total 1	Mg 1	0	0
85	lR	1	Total 1	Mg 1	0	0
85	6	146	Total 146	Mg 146	0	0
85	AB	7	Total 7	Mg 7	0	0
85	AF	2	Total 2	Mg 2	0	0
85	AG	1	Total 1	Mg 1	0	0
85	AH	1	Total 1	Mg 1	0	0
85	AK	1	Total 1	Mg 1	0	0
85	AP	1	Total 1	Mg 1	0	0
85	AR	515	Total 515	Mg 515	0	0
85	AS	20	Total 20	Mg 20	0	0
85	AT	14	Total 14	Mg 14	0	0
85	CD	2	Total 2	Mg 2	0	0
85	CE	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	CF	1	Total 1	Mg 1	0	0
85	CG	2	Total 2	Mg 2	0	0
85	CI	1	Total 1	Mg 1	0	0
85	CJ	1	Total 1	Mg 1	0	0
85	CK	1	Total 1	Mg 1	0	0
85	CL	1	Total 1	Mg 1	0	0
85	CM	2	Total 2	Mg 2	0	0
85	CO	1	Total 1	Mg 1	0	0
85	CP	4	Total 4	Mg 4	0	0
85	CQ	4	Total 4	Mg 4	0	0
85	CR	5	Total 5	Mg 5	0	0
85	CU	1	Total 1	Mg 1	0	0
85	CX	2	Total 2	Mg 2	0	0
85	DA	2	Total 2	Mg 2	0	0
85	DC	4	Total 4	Mg 4	0	0
85	DE	1	Total 1	Mg 1	0	0
85	DH	2	Total 2	Mg 2	0	0
85	DI	2	Total 2	Mg 2	0	0
85	DL	1	Total 1	Mg 1	0	0
85	DO	1	Total 1	Mg 1	0	0
85	DQ	2	Total 2	Mg 2	0	0

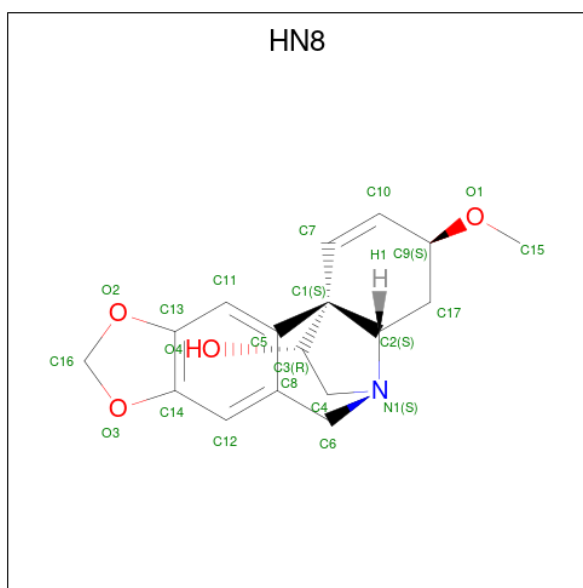
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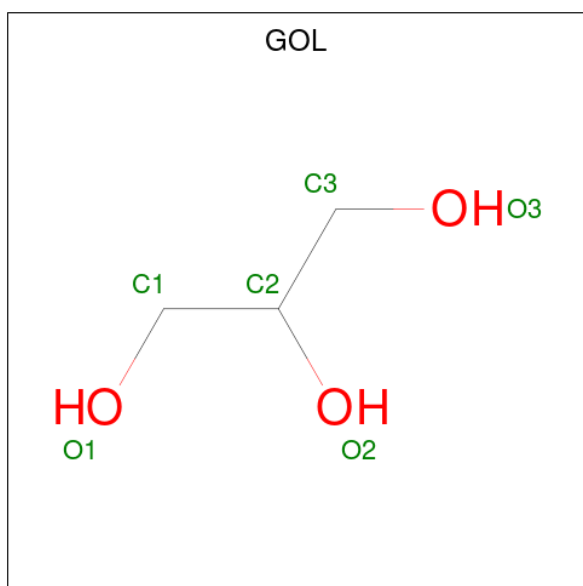
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	sM	2	Total 2	Mg 2	0	0
85	A	116	Total 116	Mg 116	0	0
85	D	1	Total 1	Mg 1	0	0
85	F	1	Total 1	Mg 1	0	0
85	H	1	Total 1	Mg 1	0	0
85	T	1	Total 1	Mg 1	0	0
85	U	1	Total 1	Mg 1	0	0
85	V	1	Total 1	Mg 1	0	0
85	Y	1	Total 1	Mg 1	0	0
85	b	1	Total 1	Mg 1	0	0
85	s4	1	Total 1	Mg 1	0	0
85	s6	1	Total 1	Mg 1	0	0
85	s8	1	Total 1	Mg 1	0	0
85	c1	1	Total 1	Mg 1	0	0
85	c6	1	Total 1	Mg 1	0	0
85	c8	1	Total 1	Mg 1	0	0
85	c9	1	Total 1	Mg 1	0	0
85	d3	2	Total 2	Mg 2	0	0
85	d4	1	Total 1	Mg 1	0	0
85	d5	1	Total 1	Mg 1	0	0
85	d6	2	Total 2	Mg 2	0	0

- Molecule 86 is Haemanthamine (three-letter code: HN8) (formula:  $C_{17}H_{19}NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
86	1	1	Total	C	N	O	0	0
			22	17	1	4		
86	AR	1	Total	C	N	O	0	0
			22	17	1	4		

- Molecule 87 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	v	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
87	6	1	Total	C	O	0	0
			6	3	3		
87	AR	1	Total	C	O	0	0
			6	3	3		
87	AR	1	Total	C	O	0	0
			6	3	3		
87	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	AK	1	Total	Zn	0	0
			1	1		
88	AN	1	Total	Zn	0	0
			1	1		
88	AP	1	Total	Zn	0	0
			1	1		
88	AQ	1	Total	Zn	0	0
			1	1		
88	DL	1	Total	Zn	0	0
			1	1		
88	DO	1	Total	Zn	0	0
			1	1		
88	DQ	1	Total	Zn	0	0
			1	1		
88	DR	1	Total	Zn	0	0
			1	1		
88	b	1	Total	Zn	0	0
			1	1		
88	c	1	Total	Zn	0	0
			1	1		
88	e	1	Total	Zn	0	0
			1	1		
88	g	1	Total	Zn	0	0
			1	1		
88	d6	1	Total	Zn	0	0
			1	1		
88	d7	1	Total	Zn	0	0
			1	1		
88	d9	1	Total	Zn	0	0
			1	1		

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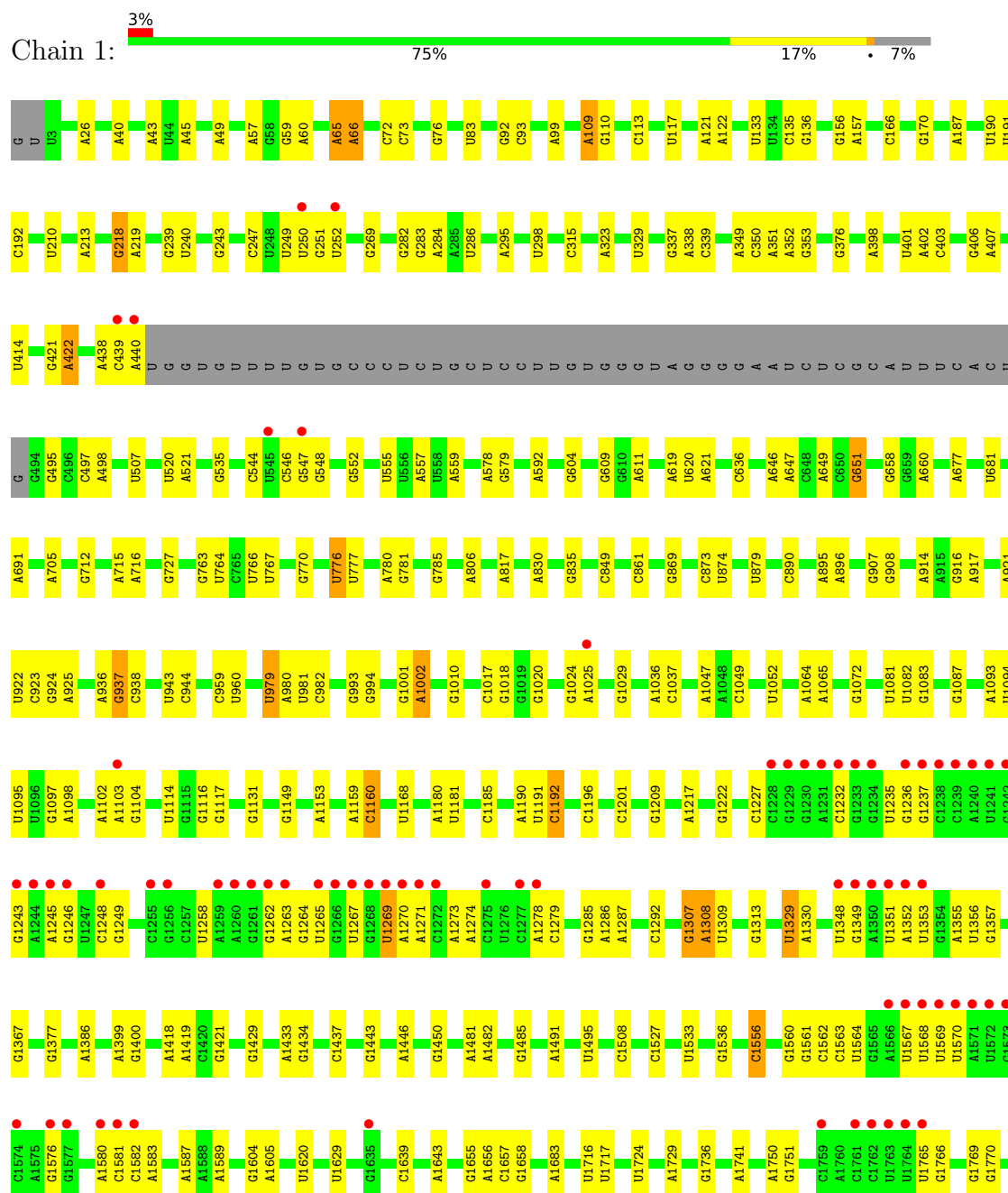
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
88	e1	1	Total	Zn	0	0
			1	1		

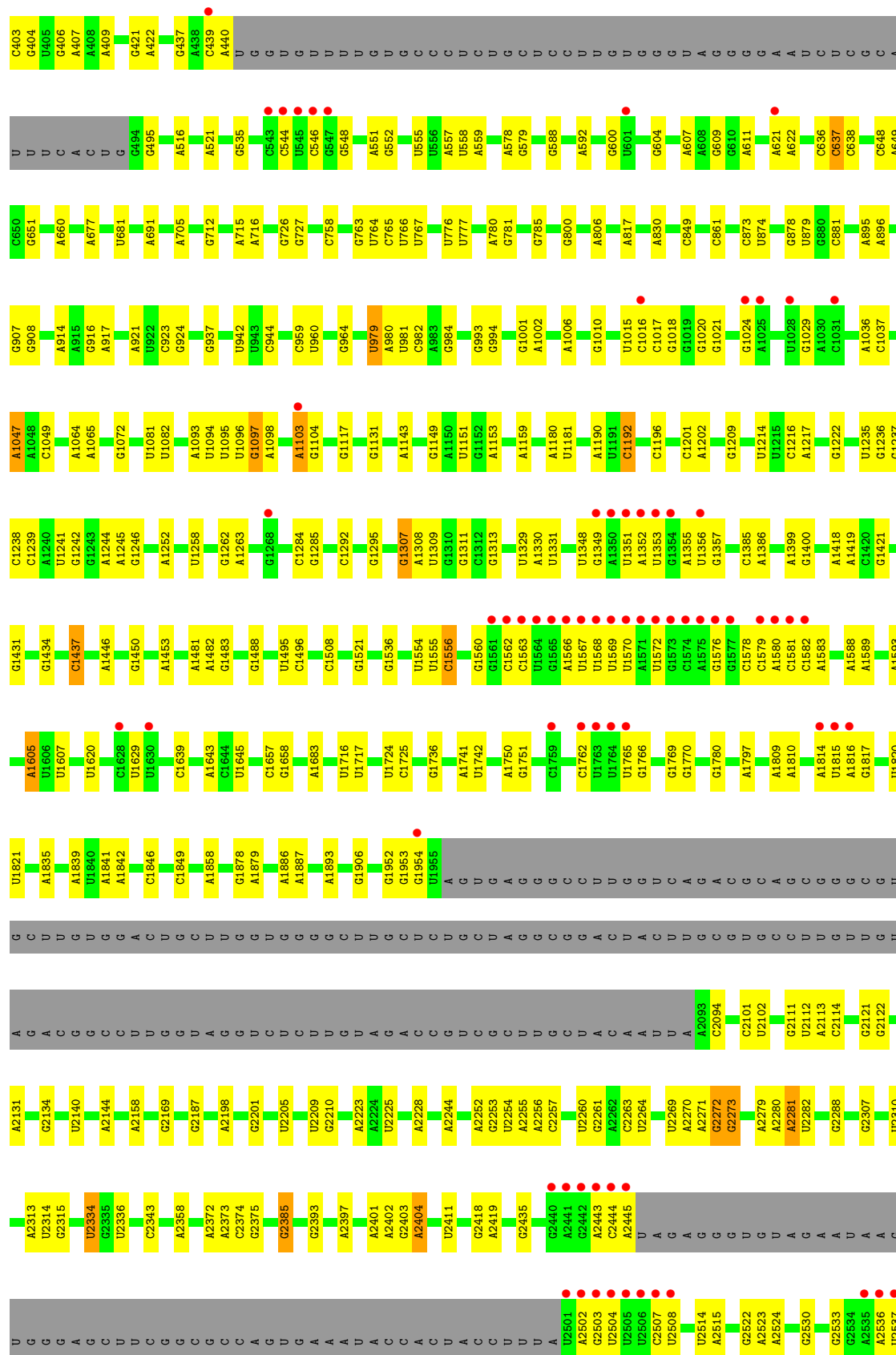
### 3 Residue-property plots

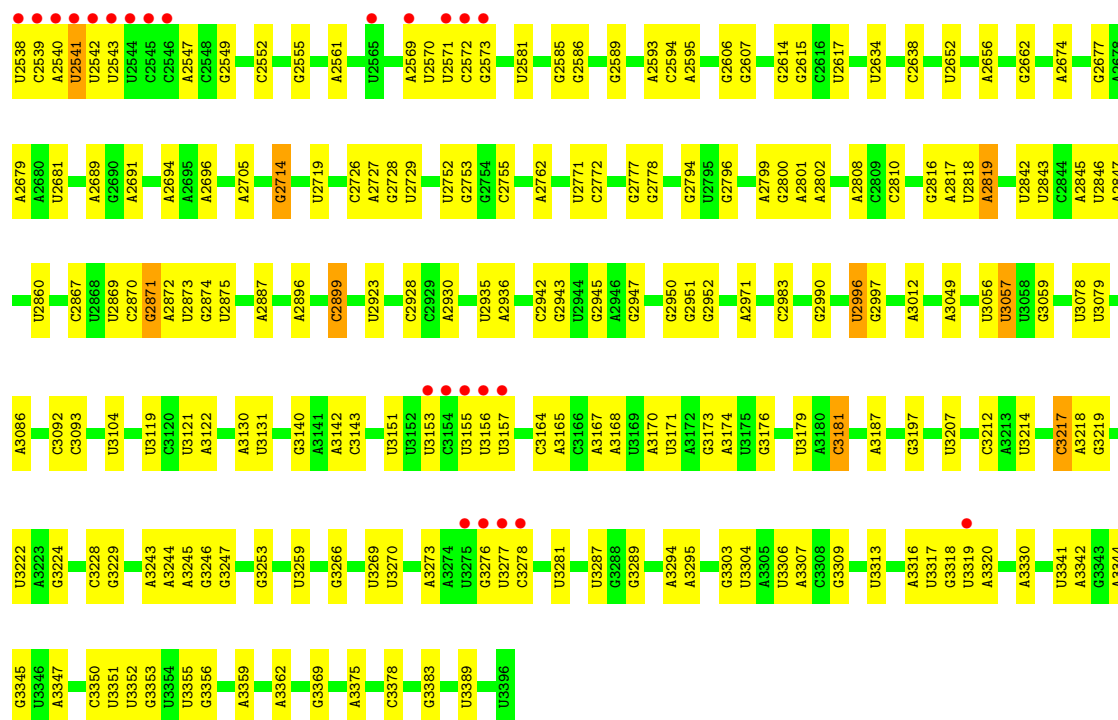
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 25S ribosomal RNA

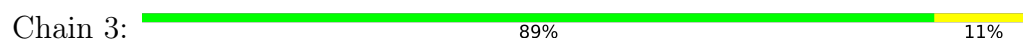




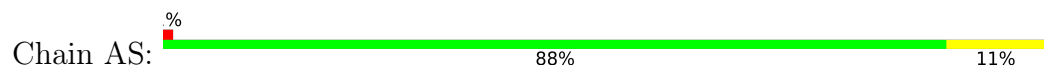




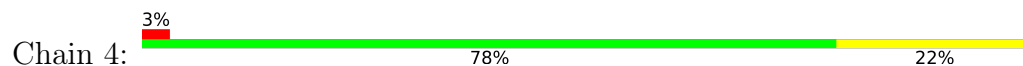
- Molecule 2: 5S ribosomal RNA



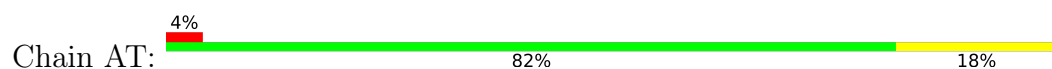
- Molecule 2: 5S ribosomal RNA



- Molecule 3: 5.8S ribosomal RNA




- Molecule 3: 5.8S ribosomal RNA



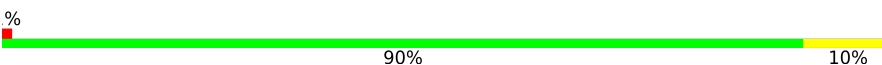


- Molecule 4: 60S ribosomal protein L2-A

Chain j:  89% 11%




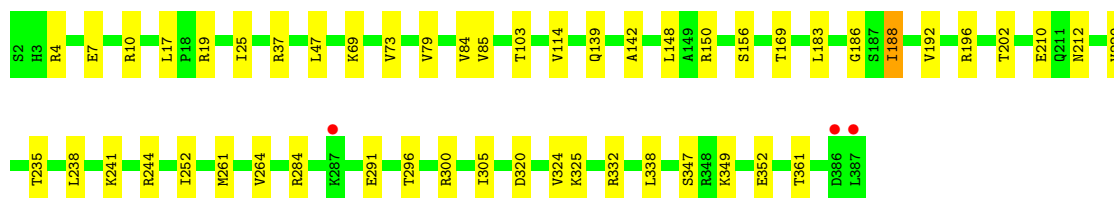
- Molecule 4: 60S ribosomal protein L2-A

Chain CD:  90% 10%




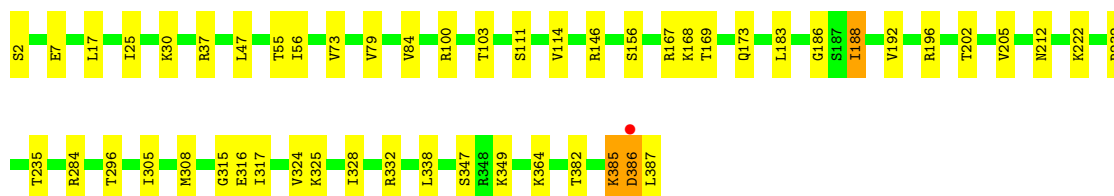
- Molecule 5: 60S ribosomal protein L3

Chain k:  87% 13%




- Molecule 5: 60S ribosomal protein L3

Chain CE:  87% 13%



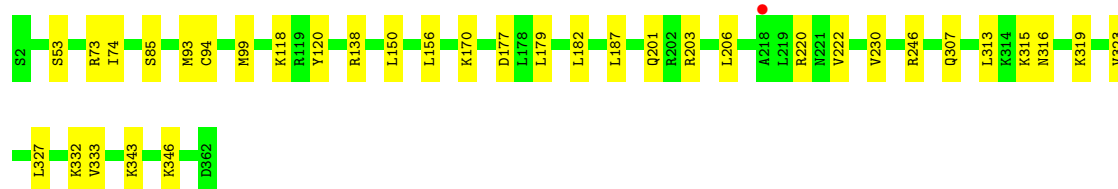
- Molecule 6: 60S ribosomal protein L4-A

Chain l:  89% 10%

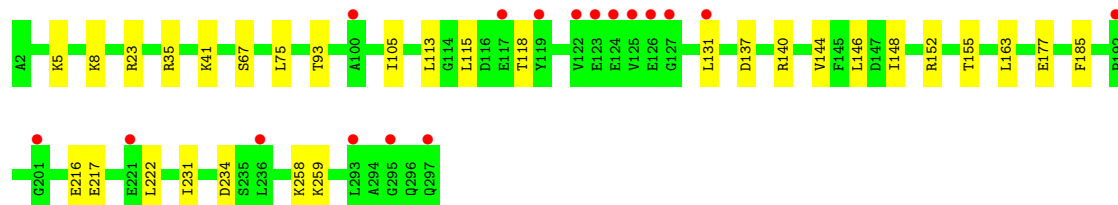
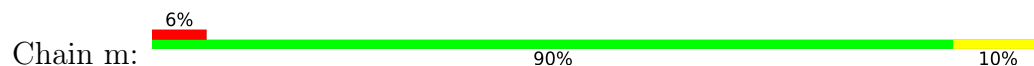


- Molecule 6: 60S ribosomal protein L4-A

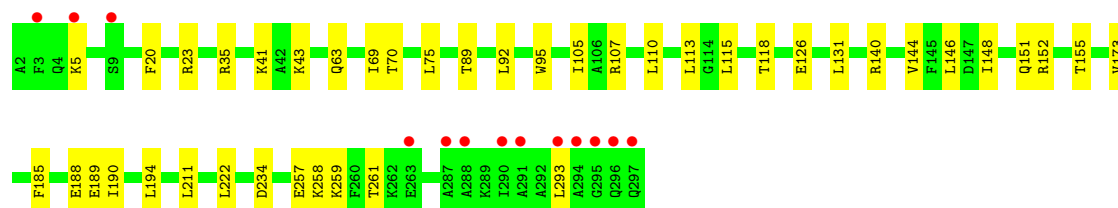
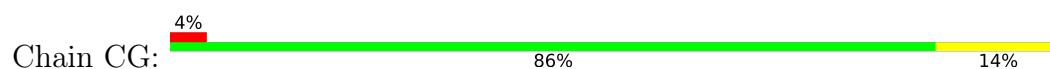
Chain CF:  90% 10%



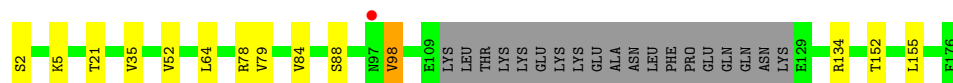
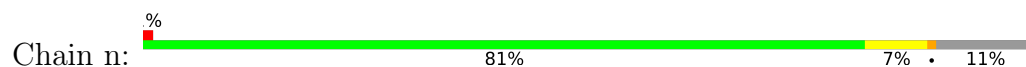
• Molecule 7: 60S ribosomal protein L5



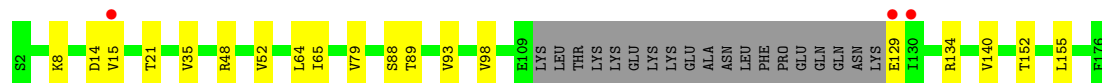
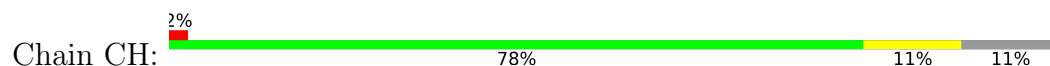
• Molecule 7: 60S ribosomal protein L5



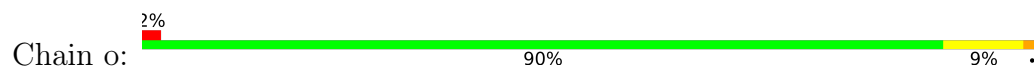
• Molecule 8: 60S ribosomal protein L6-A



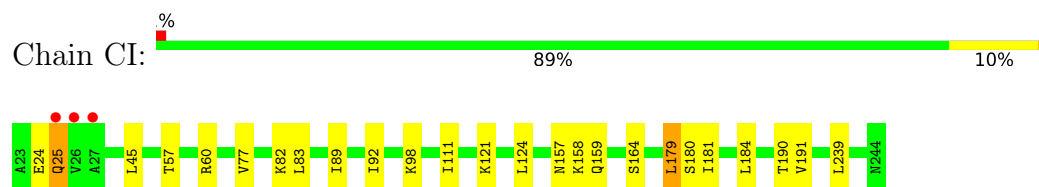
• Molecule 8: 60S ribosomal protein L6-A



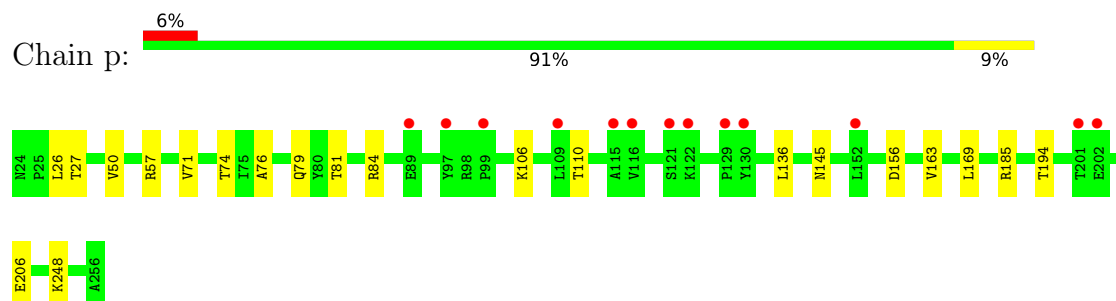
• Molecule 9: 60S ribosomal protein L7-A



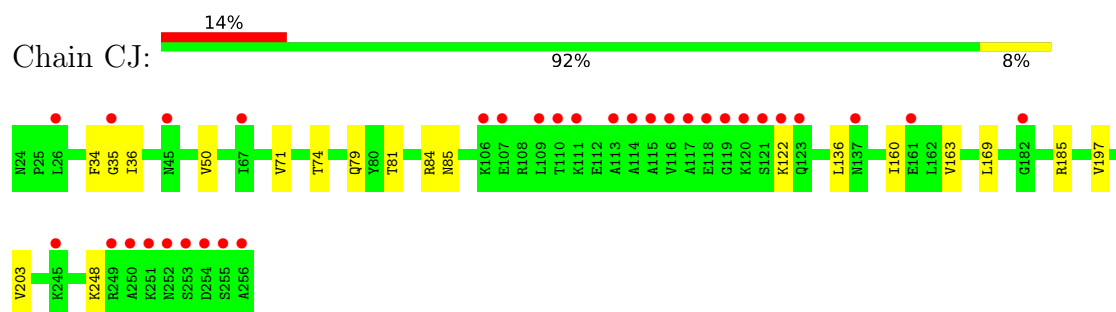
- Molecule 9: 60S ribosomal protein L7-A



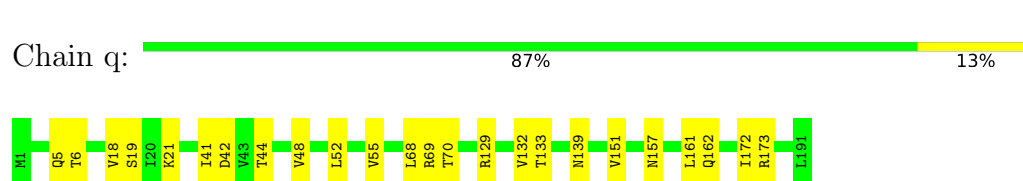
- Molecule 10: 60S ribosomal protein L8-A



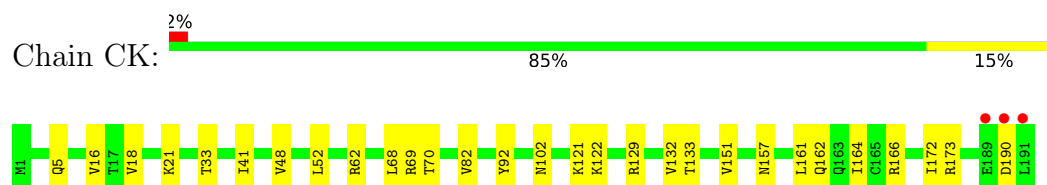
- Molecule 10: 60S ribosomal protein L8-A



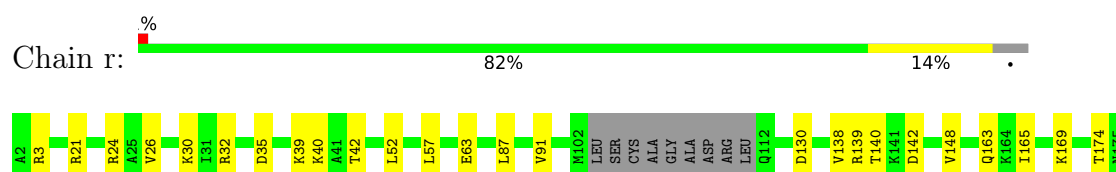
- Molecule 11: 60S ribosomal protein L9-A

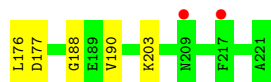


- Molecule 11: 60S ribosomal protein L9-A

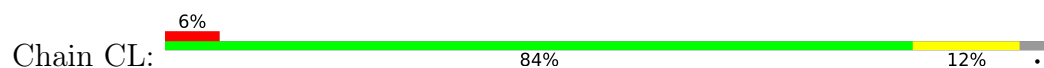


- Molecule 12: 60S ribosomal protein L10

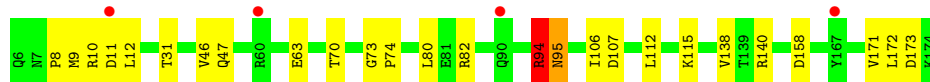
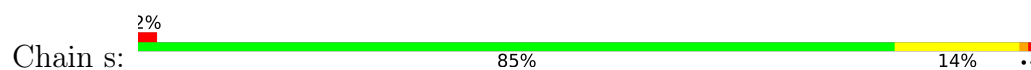




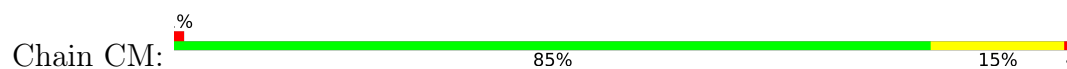
- Molecule 12: 60S ribosomal protein L10



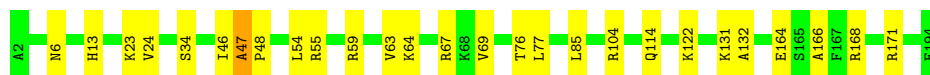
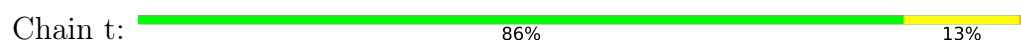
- Molecule 13: 60S ribosomal protein L11-B



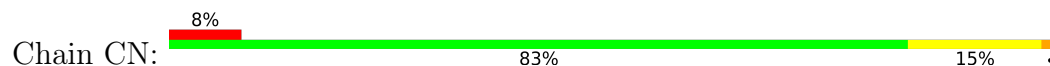
- Molecule 13: 60S ribosomal protein L11-B



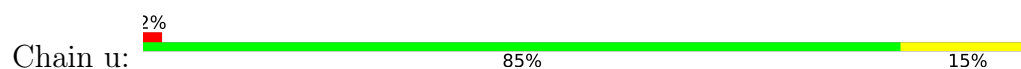
- Molecule 14: 60S ribosomal protein L13-A



- Molecule 14: 60S ribosomal protein L13-A

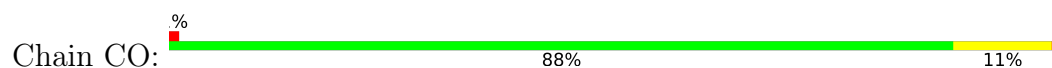


- Molecule 15: 60S ribosomal protein L14-A





- Molecule 15: 60S ribosomal protein L14-A



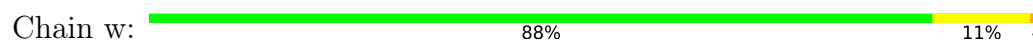
- Molecule 16: 60S ribosomal protein L15-A



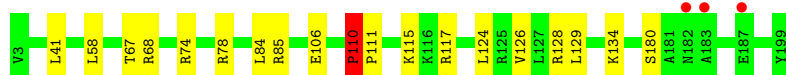
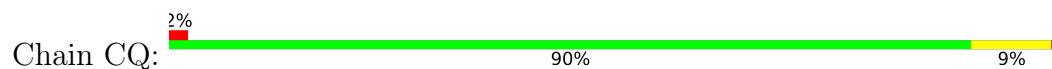
- Molecule 16: 60S ribosomal protein L15-A



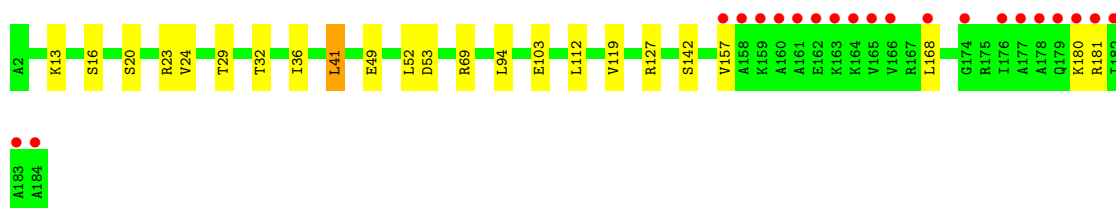
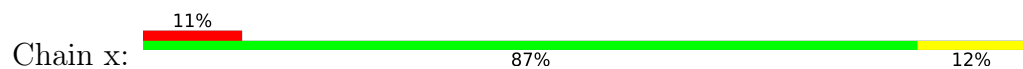
- Molecule 17: 60S ribosomal protein L16-A



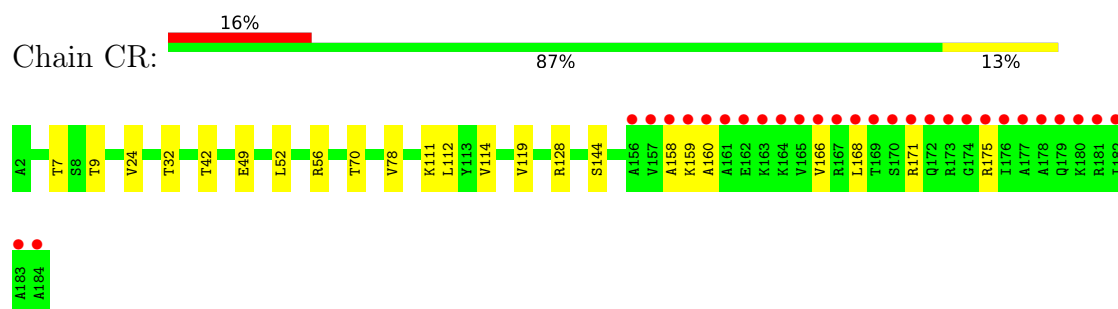
- Molecule 17: 60S ribosomal protein L16-A



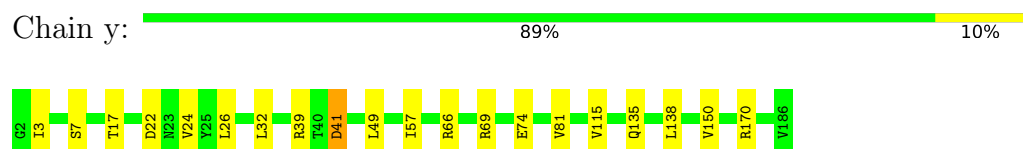
- Molecule 18: 60S ribosomal protein L17-A



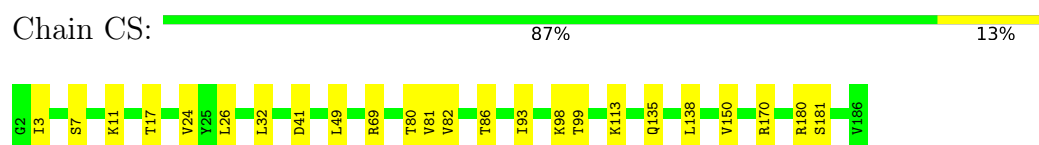
- Molecule 18: 60S ribosomal protein L17-A



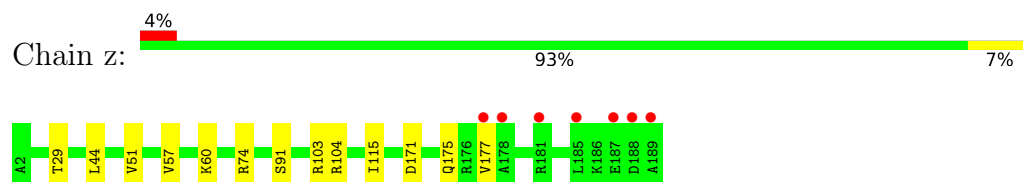
- Molecule 19: 60S ribosomal protein L18-A



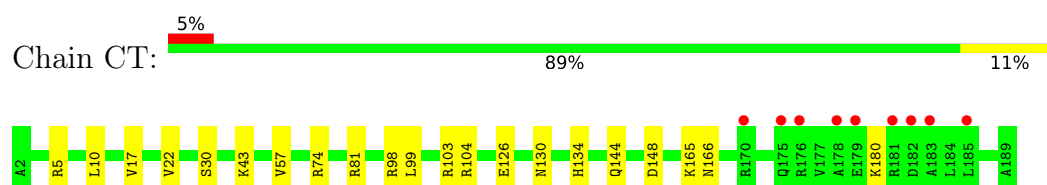
- Molecule 19: 60S ribosomal protein L18-A



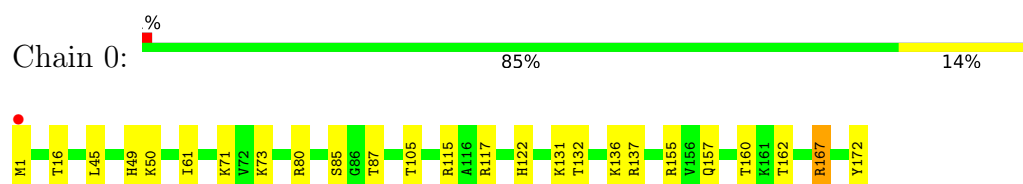
- Molecule 20: 60S ribosomal protein L19-A




- Molecule 20: 60S ribosomal protein L19-A



- Molecule 21: 60S ribosomal protein L20-A




- Molecule 21: 60S ribosomal protein L20-A

Chain CU:  85% 15%




- Molecule 22: 60S ribosomal protein L21-A

Chain 2:  86% 14%

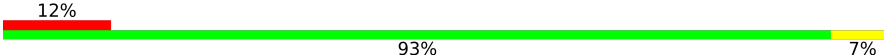


- Molecule 22: 60S ribosomal protein L21-A

Chain CV:  84% 16%




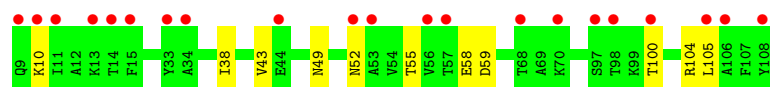
- Molecule 23: 60S ribosomal protein L22-A

Chain 5:  12% 93% 7%




- Molecule 23: 60S ribosomal protein L22-A

Chain CW:  21% 89% 11%



- Molecule 24: 60S ribosomal protein L23-A

Chain LR:  3% 89% 11%

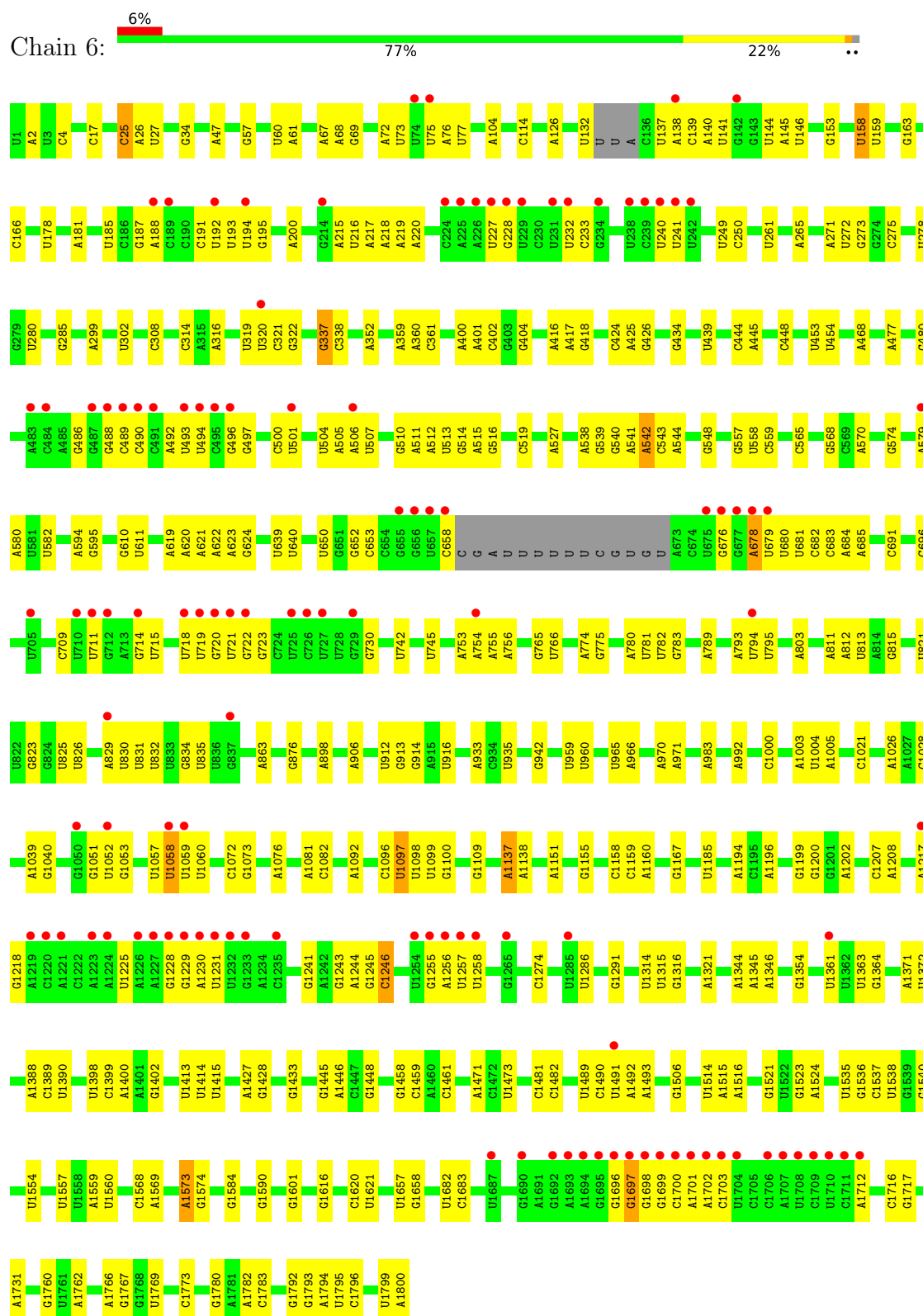


- Molecule 24: 60S ribosomal protein L23-A

Chain CX:  92% 8%



- Molecule 25: 18S ribosomal RNA

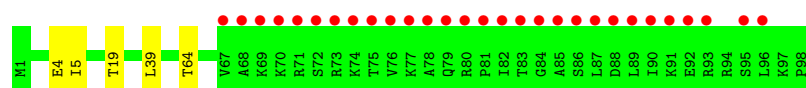


• Molecule 25: 18S ribosomal RNA

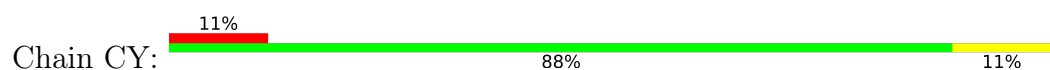




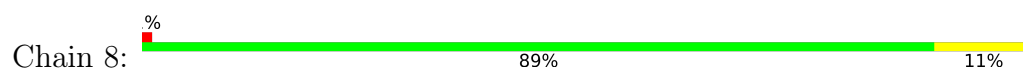




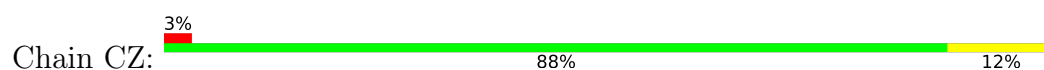
- Molecule 26: 60S ribosomal protein L24-A



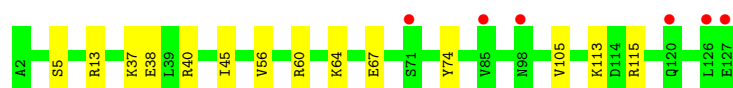
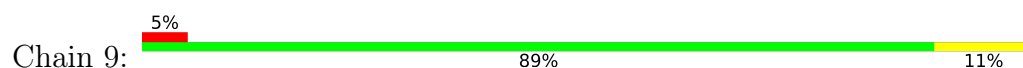
- Molecule 27: 60S ribosomal protein L25



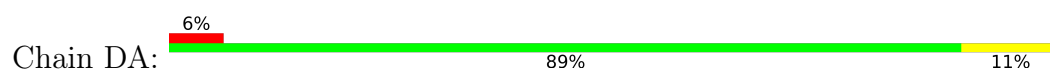
- Molecule 27: 60S ribosomal protein L25



- Molecule 28: 60S ribosomal protein L26-A

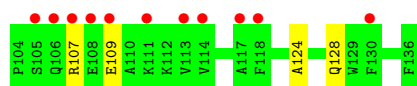


- Molecule 28: 60S ribosomal protein L26-A

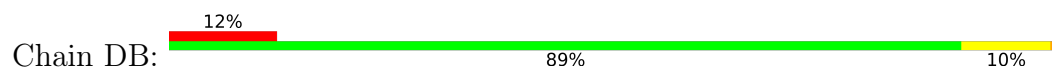


- Molecule 29: 60S ribosomal protein L27-A

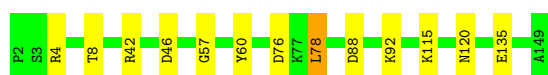




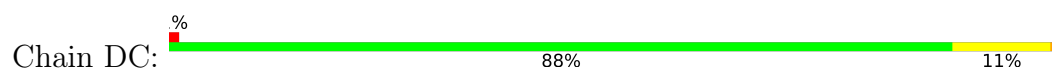
- Molecule 29: 60S ribosomal protein L27-A



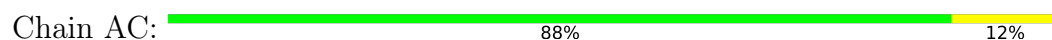
- Molecule 30: 60S ribosomal protein L28



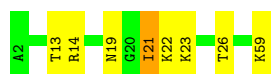
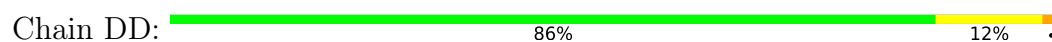
- Molecule 30: 60S ribosomal protein L28



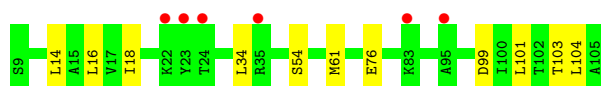
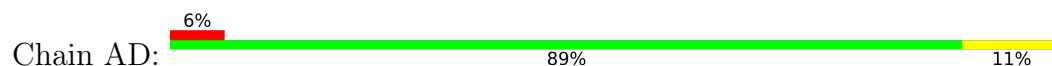
- Molecule 31: 60S ribosomal protein L29



- Molecule 31: 60S ribosomal protein L29

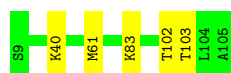


- Molecule 32: 60S ribosomal protein L30

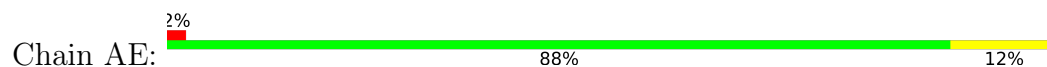


- Molecule 32: 60S ribosomal protein L30

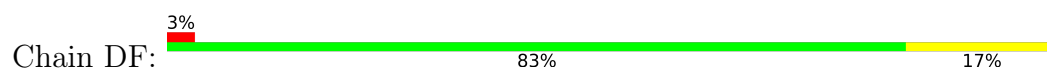




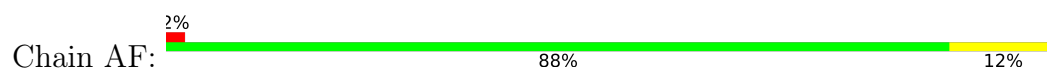
- Molecule 33: 60S ribosomal protein L31-A



- Molecule 33: 60S ribosomal protein L31-A



- Molecule 34: 60S ribosomal protein L32



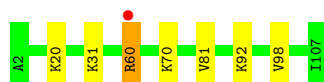
- Molecule 34: 60S ribosomal protein L32



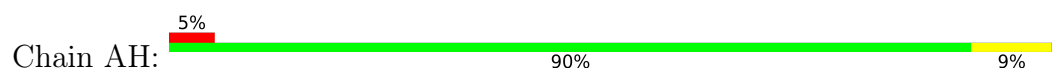
- Molecule 35: 60S ribosomal protein L33-A



- Molecule 35: 60S ribosomal protein L33-A



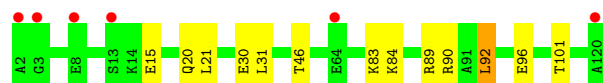
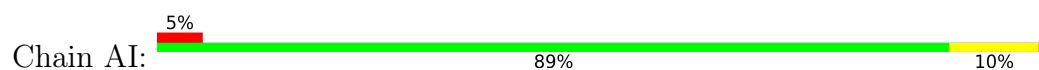
- Molecule 36: 60S ribosomal protein L34-A



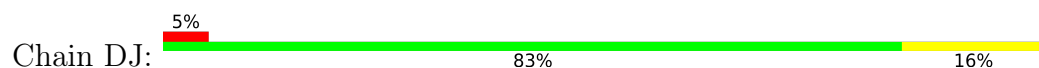
- Molecule 36: 60S ribosomal protein L34-A



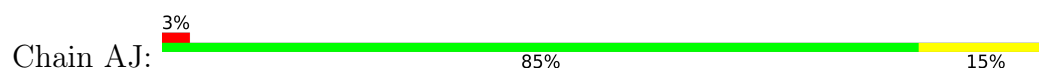
- Molecule 37: 60S ribosomal protein L35-A



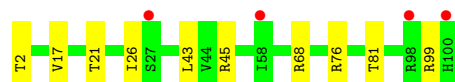
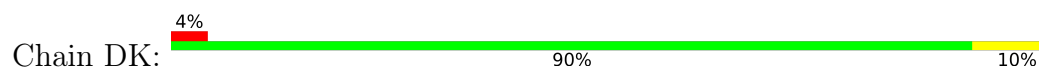
- Molecule 37: 60S ribosomal protein L35-A



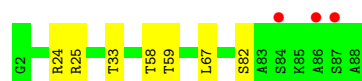
- Molecule 38: 60S ribosomal protein L36-A



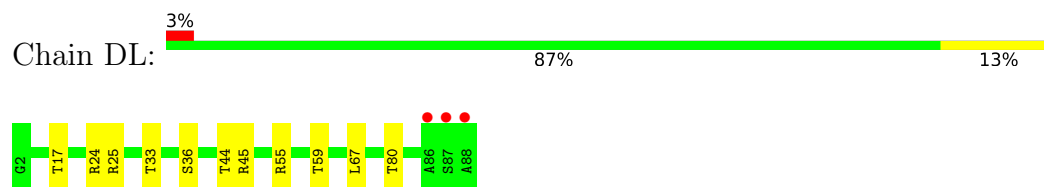
- Molecule 38: 60S ribosomal protein L36-A



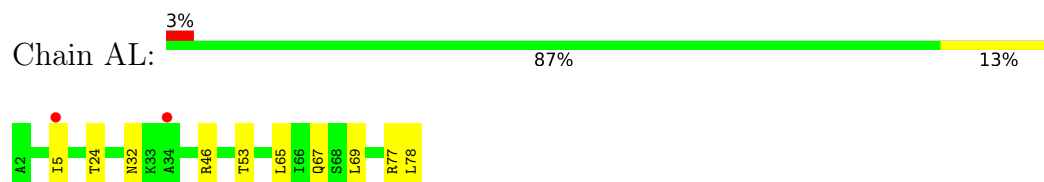
- Molecule 39: 60S ribosomal protein L37-A



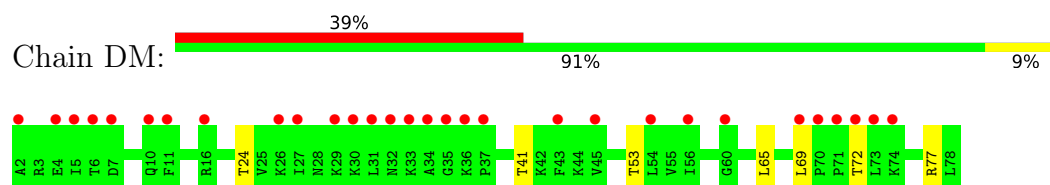
- Molecule 39: 60S ribosomal protein L37-A



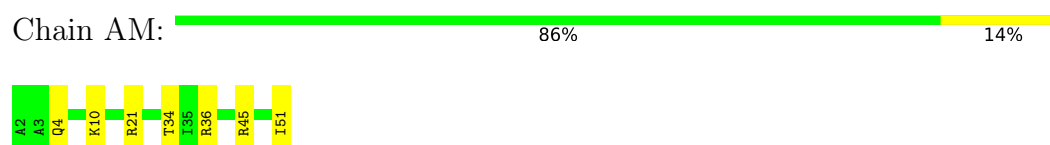
- Molecule 40: 60S ribosomal protein L38



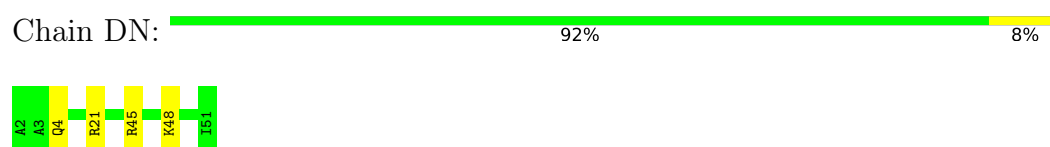
- Molecule 40: 60S ribosomal protein L38



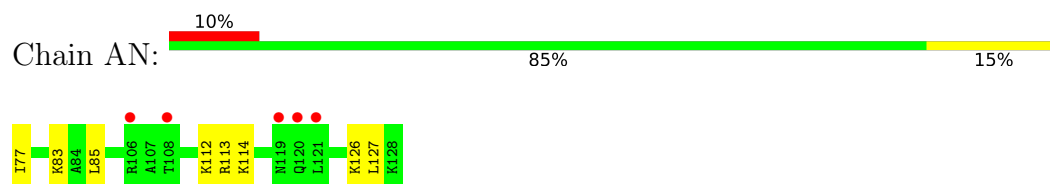
- Molecule 41: 60S ribosomal protein L39



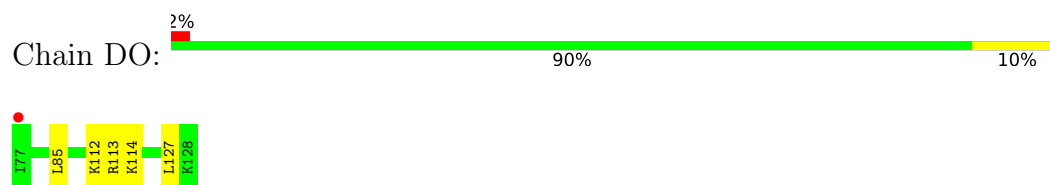
- Molecule 41: 60S ribosomal protein L39



- Molecule 42: Ubiquitin-60S ribosomal protein L40



- Molecule 42: Ubiquitin-60S ribosomal protein L40




- Molecule 43: 60S ribosomal protein L41-B

Chain AO:  88% 12%

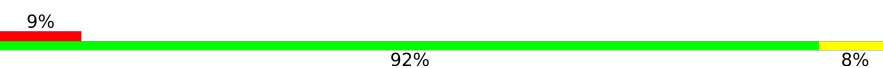


- Molecule 43: 60S ribosomal protein L41-B

Chain DP:  84% 16%



- Molecule 44: 60S ribosomal protein L42-A

Chain AP:  9% 92% 8%




- Molecule 44: 60S ribosomal protein L42-A

Chain DQ:  91% 9%



- Molecule 45: 60S ribosomal protein L43-A

Chain AQ:  87% 13%



- Molecule 45: 60S ribosomal protein L43-A

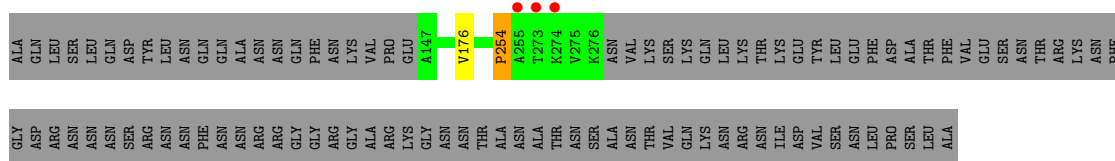
Chain DR:  91% 9%



- Molecule 46: Suppressor protein STM1

Chain i:  7% 51% 7% 42%





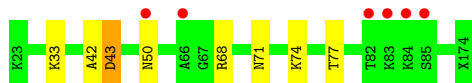
- Molecule 47: 60S ribosomal protein L12

Chain m2: 100%

There are no outlier residues recorded for this chain.

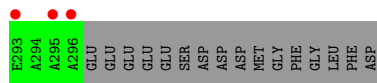
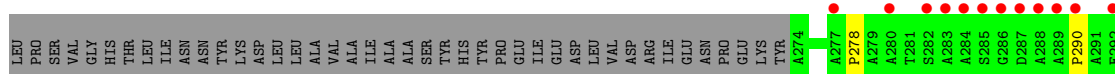
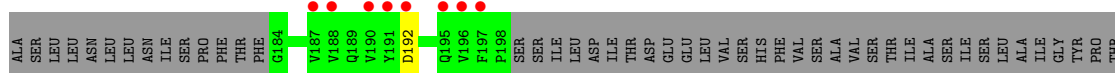
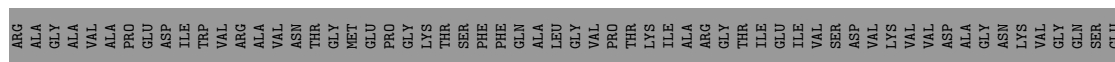
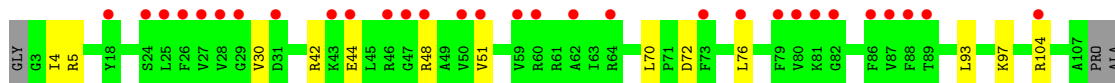
- Molecule 48: Suppressor protein STM1, Suppressor protein STM1

Chain sM: 6% 92% 7%



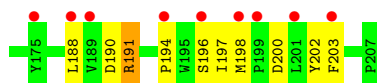
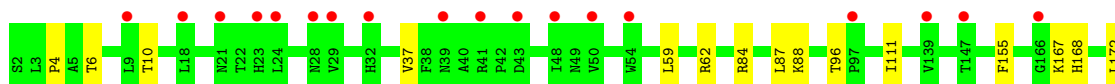
- Molecule 49: 60S acidic ribosomal protein P0

Chain p0: 17% 41% 5% 54%



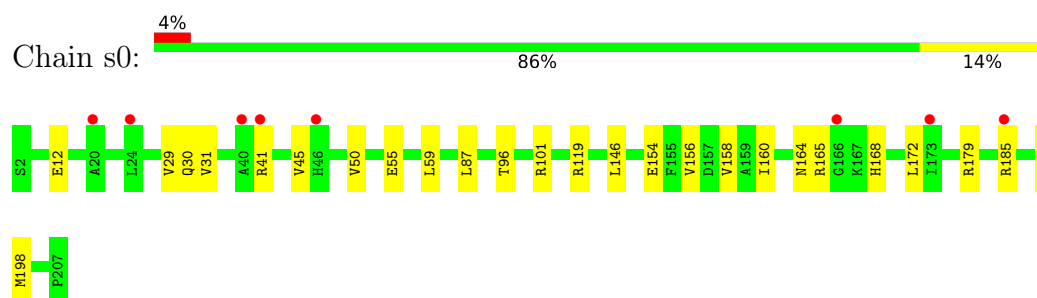
- Molecule 50: 40S ribosomal protein S0-A

Chain B: 13% 88% 12%

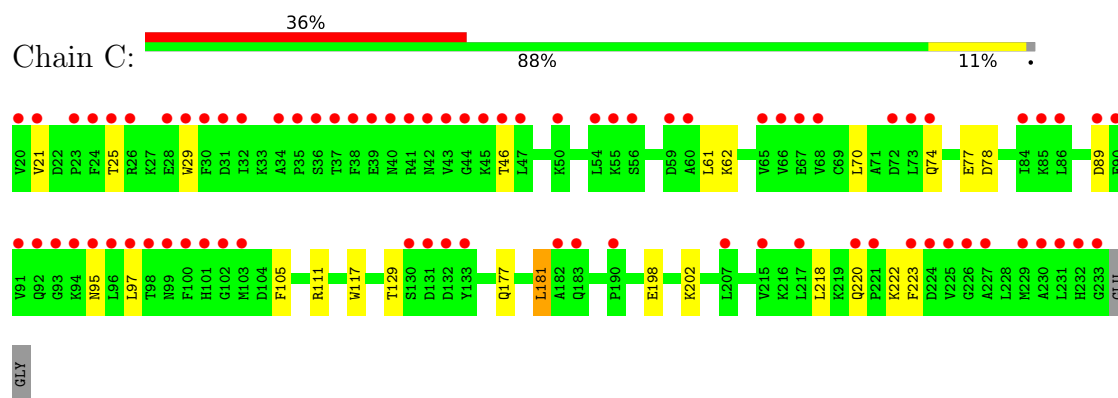




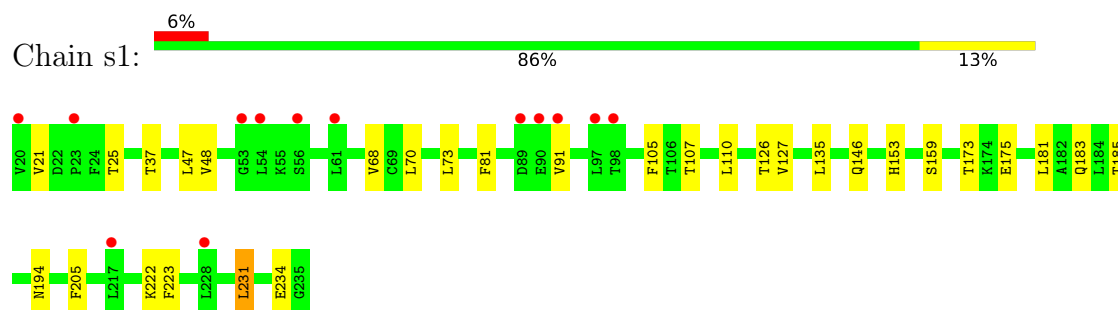
- Molecule 50: 40S ribosomal protein S0-A



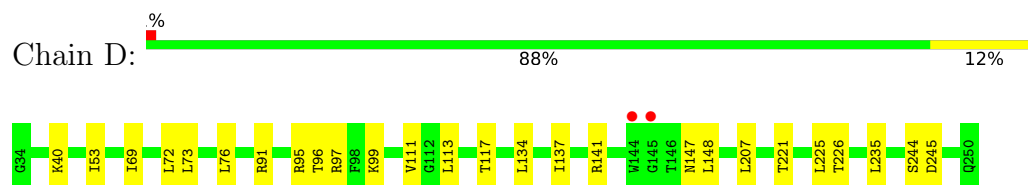
- Molecule 51: 40S ribosomal protein S1-A



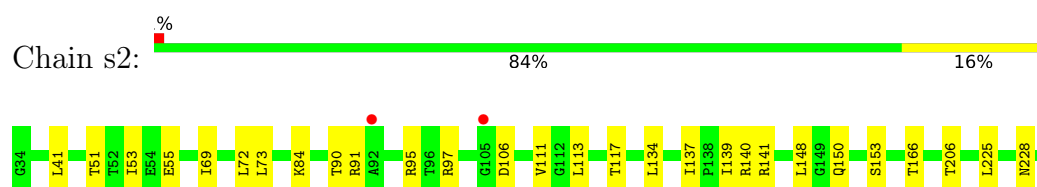
- Molecule 51: 40S ribosomal protein S1-A



- Molecule 52: 40S ribosomal protein S2

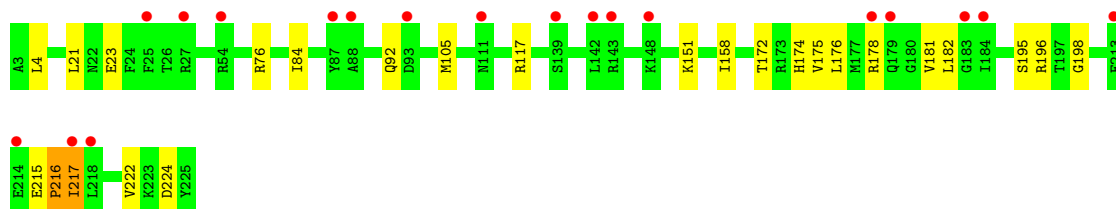
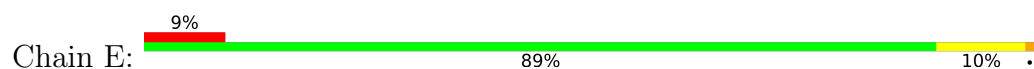


- Molecule 52: 40S ribosomal protein S2

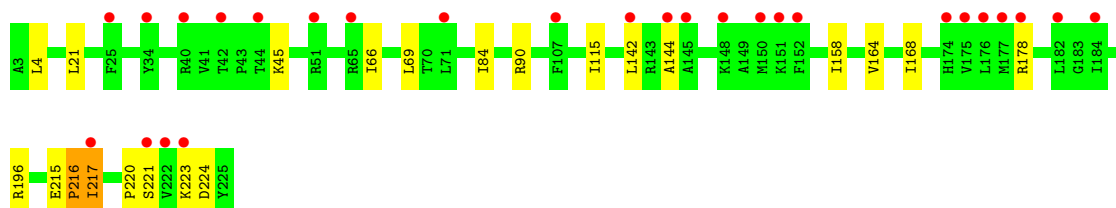




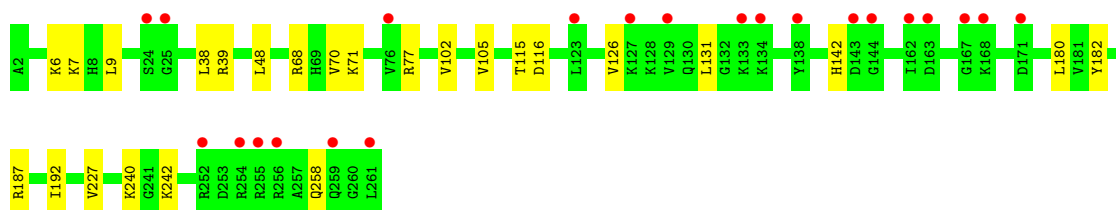
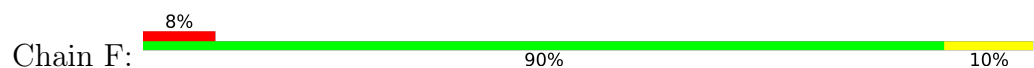
- Molecule 53: 40S ribosomal protein S3



- Molecule 53: 40S ribosomal protein S3



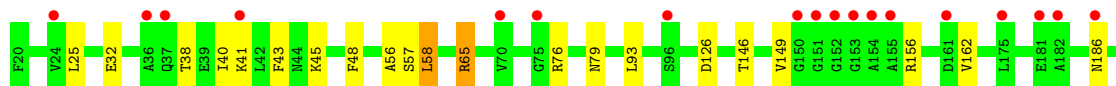
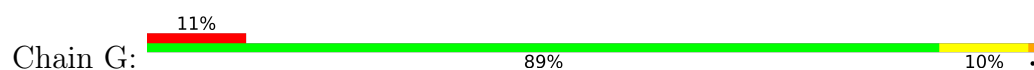
- Molecule 54: 40S ribosomal protein S4-A



- Molecule 54: 40S ribosomal protein S4-A

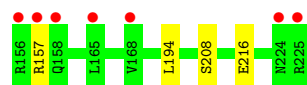
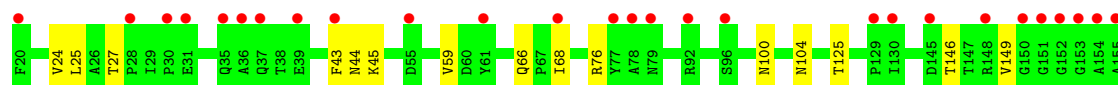


- Molecule 55: 40S ribosomal protein S5

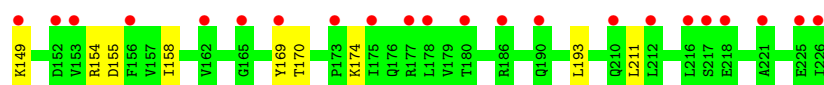
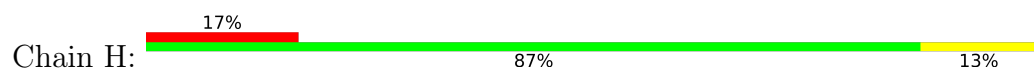




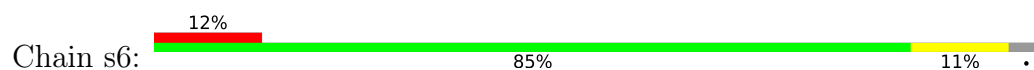
- Molecule 55: 40S ribosomal protein S5



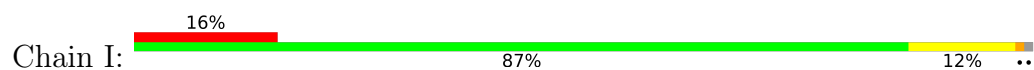
- Molecule 56: 40S ribosomal protein S6-A



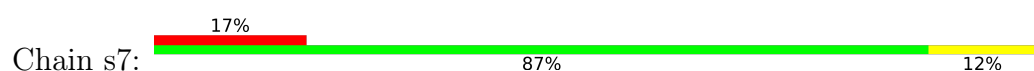
- Molecule 56: 40S ribosomal protein S6-A

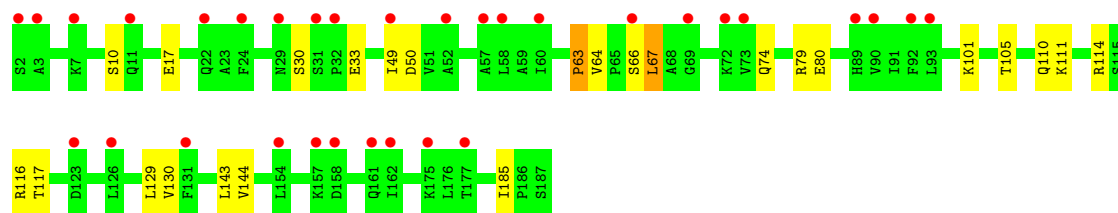


- Molecule 57: 40S ribosomal protein S7-A

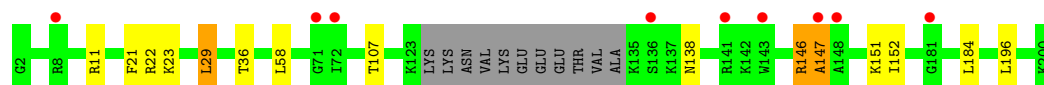
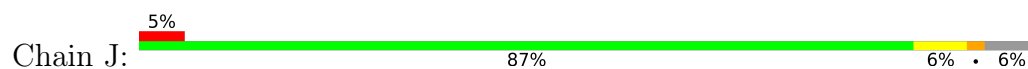


- Molecule 57: 40S ribosomal protein S7-A

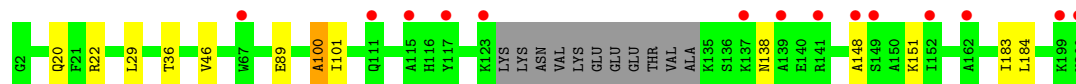
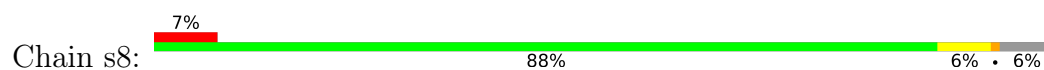




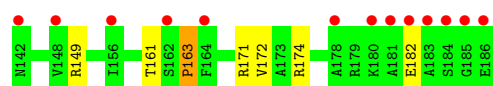
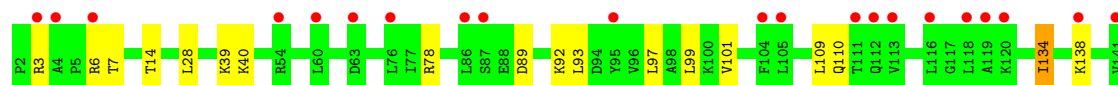
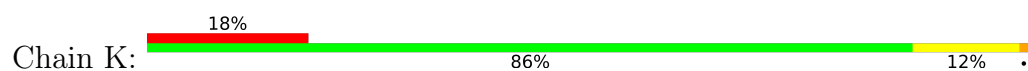
- Molecule 58: 40S ribosomal protein S8-A



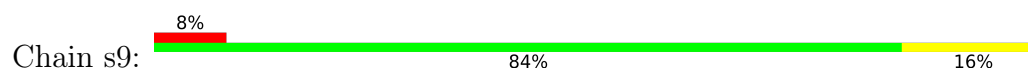
- Molecule 58: 40S ribosomal protein S8-A



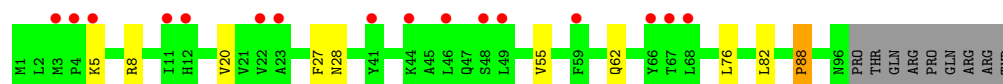
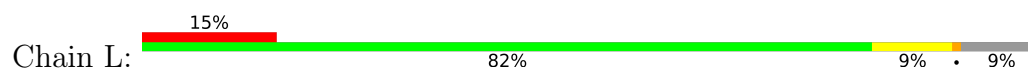
- Molecule 59: 40S ribosomal protein S9-A



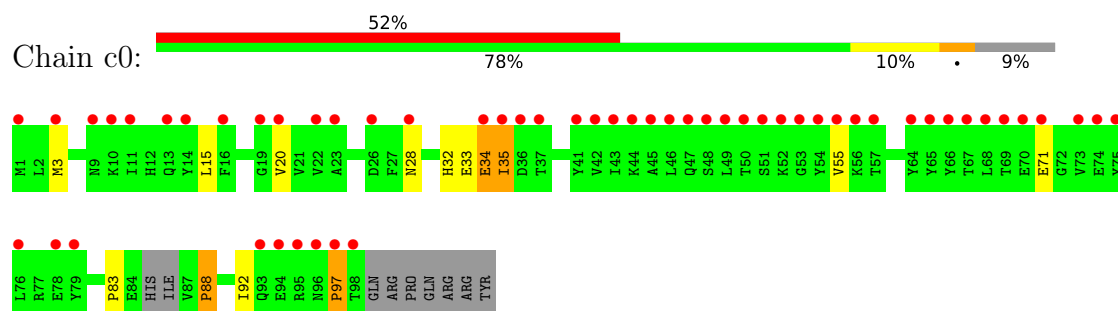
- Molecule 59: 40S ribosomal protein S9-A



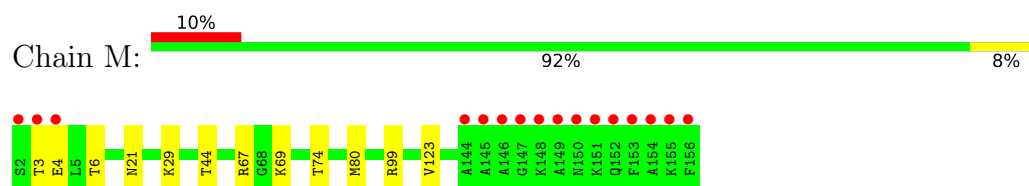
- Molecule 60: 40S ribosomal protein S10-A



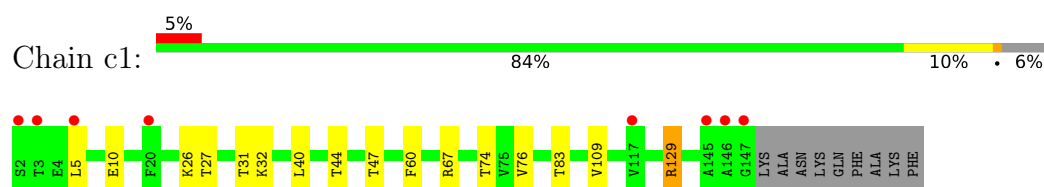
- Molecule 60: 40S ribosomal protein S10-A



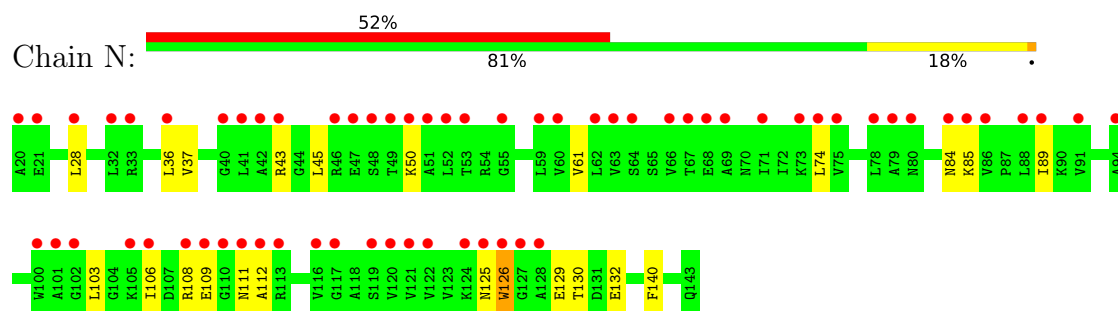
- Molecule 61: 40S ribosomal protein S11-A



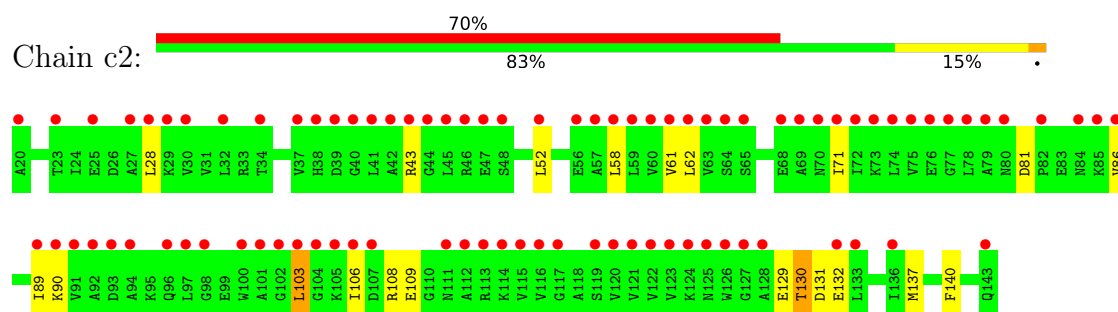
- Molecule 61: 40S ribosomal protein S11-A



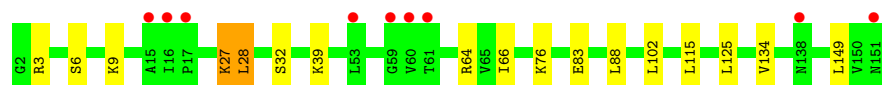
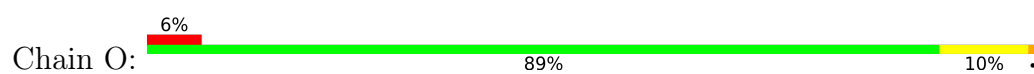
- Molecule 62: 40S ribosomal protein S12



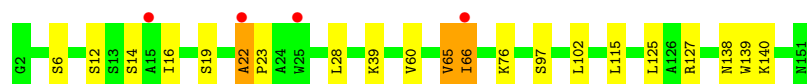
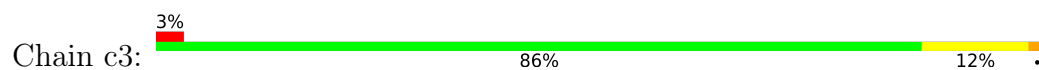
- Molecule 62: 40S ribosomal protein S12



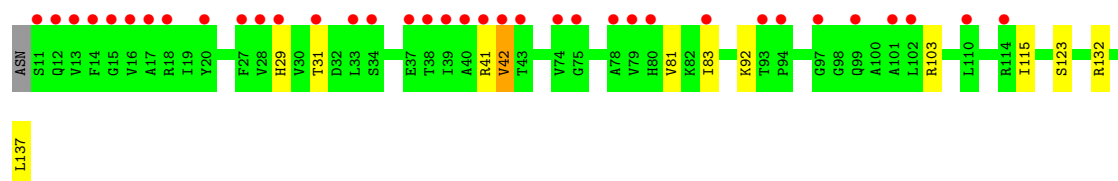
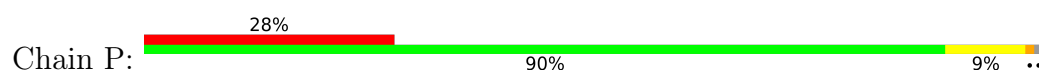
- Molecule 63: 40S ribosomal protein S13



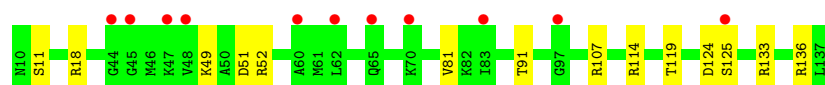
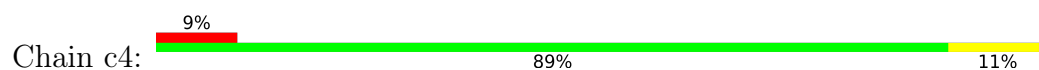
- Molecule 63: 40S ribosomal protein S13



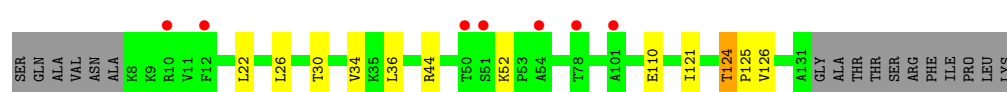
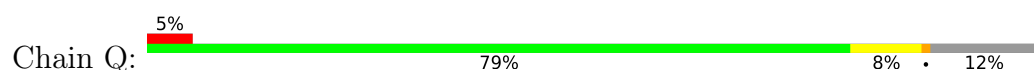
- Molecule 64: 40S ribosomal protein S14-B



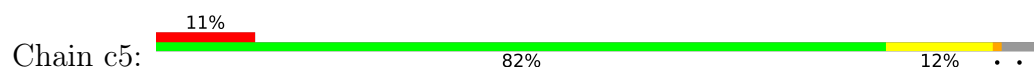
- Molecule 64: 40S ribosomal protein S14-B



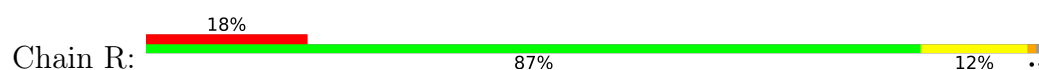
- Molecule 65: 40S ribosomal protein S15

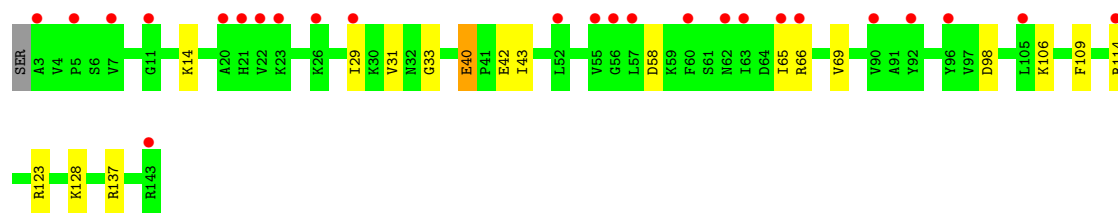


- Molecule 65: 40S ribosomal protein S15

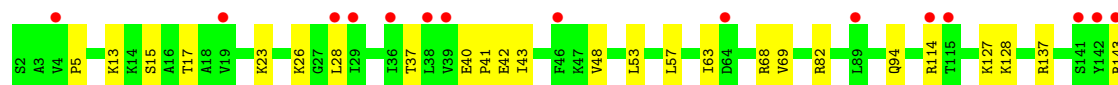
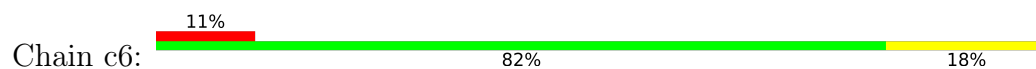


- Molecule 66: 40S ribosomal protein S16-A

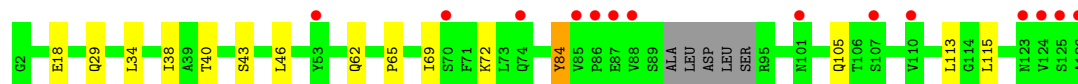
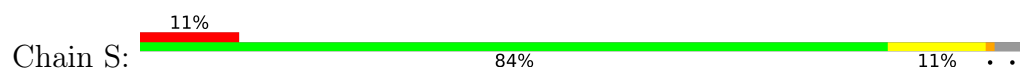




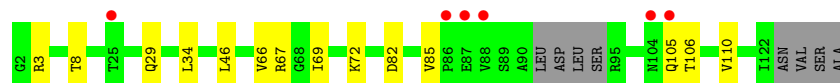
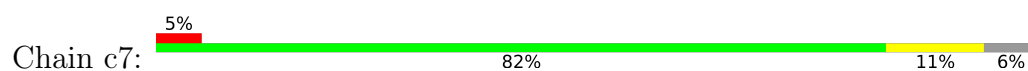
- Molecule 66: 40S ribosomal protein S16-A



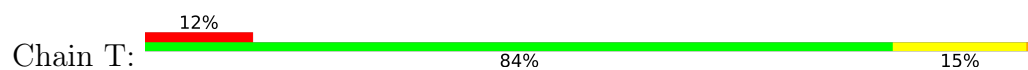
- Molecule 67: 40S ribosomal protein S17-A



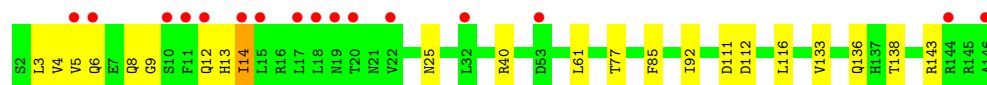
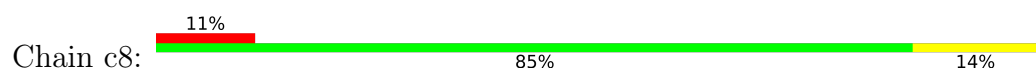
- Molecule 67: 40S ribosomal protein S17-A



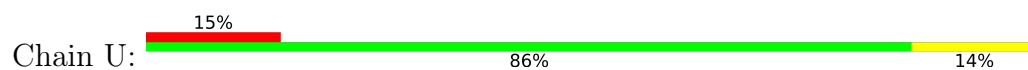
- Molecule 68: 40S ribosomal protein S18-A

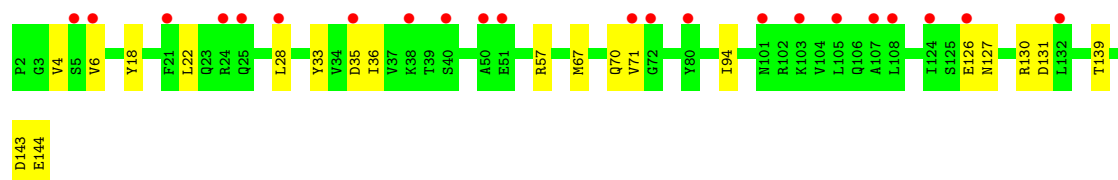


- Molecule 68: 40S ribosomal protein S18-A

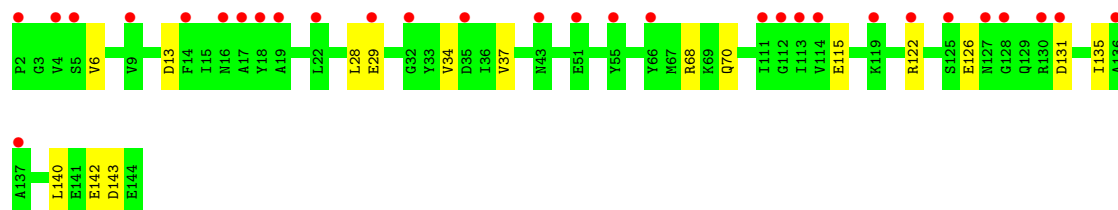
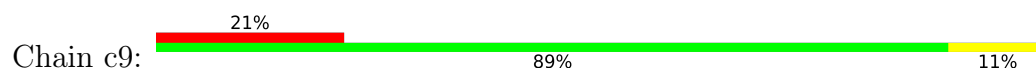


- Molecule 69: 40S ribosomal protein S19-A

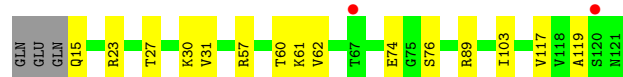
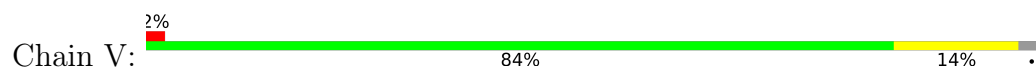




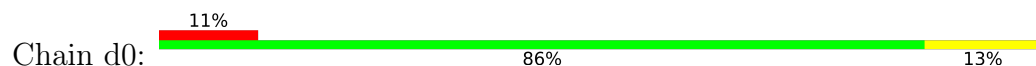
- Molecule 69: 40S ribosomal protein S19-A



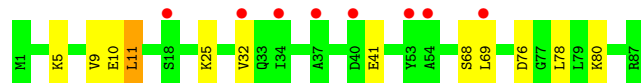
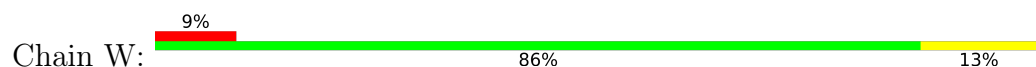
- Molecule 70: 40S ribosomal protein S20



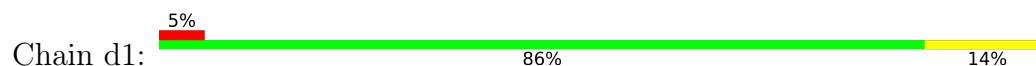
- Molecule 70: 40S ribosomal protein S20



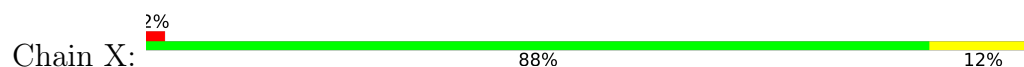
- Molecule 71: 40S ribosomal protein S21-A



- Molecule 71: 40S ribosomal protein S21-A



- Molecule 72: 40S ribosomal protein S22-A



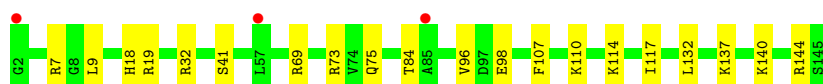
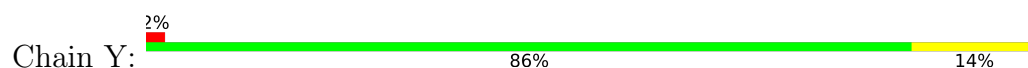




- Molecule 72: 40S ribosomal protein S22-A



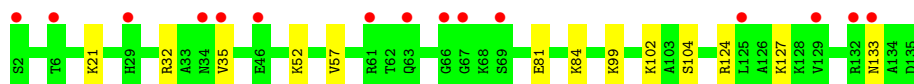
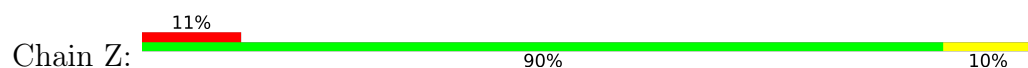
- Molecule 73: 40S ribosomal protein S23-A



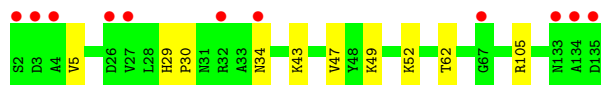
- Molecule 73: 40S ribosomal protein S23-A



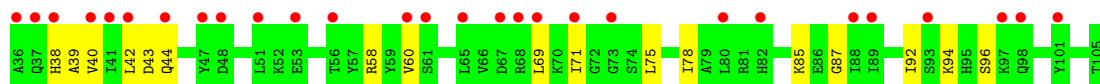
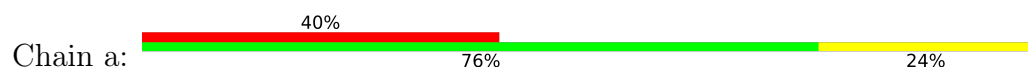
- Molecule 74: 40S ribosomal protein S24-A



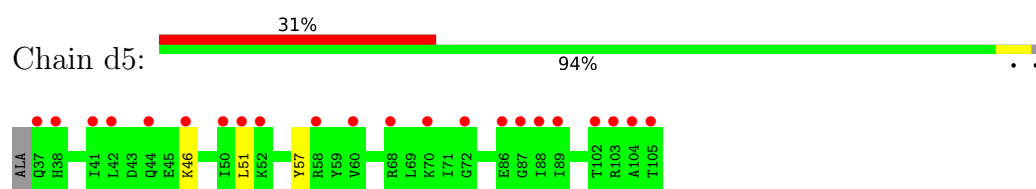
- Molecule 74: 40S ribosomal protein S24-A



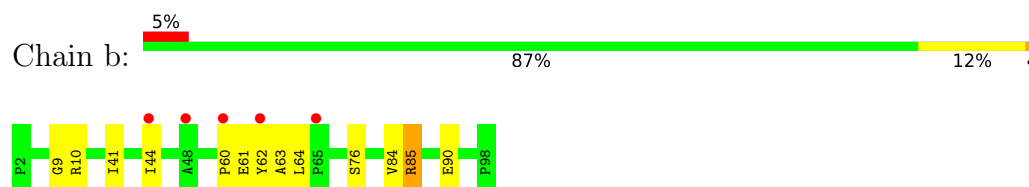
- Molecule 75: 40S ribosomal protein S25-A



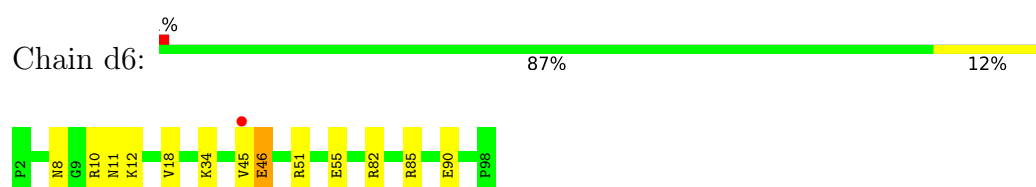
- Molecule 75: 40S ribosomal protein S25-A



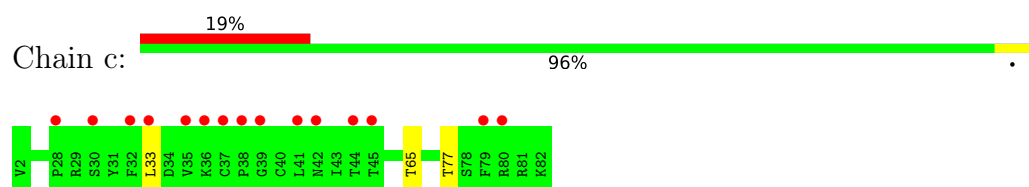
- Molecule 76: 40S ribosomal protein S26-B



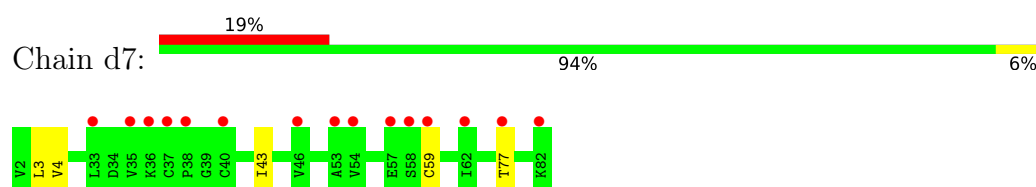
- Molecule 76: 40S ribosomal protein S26-B



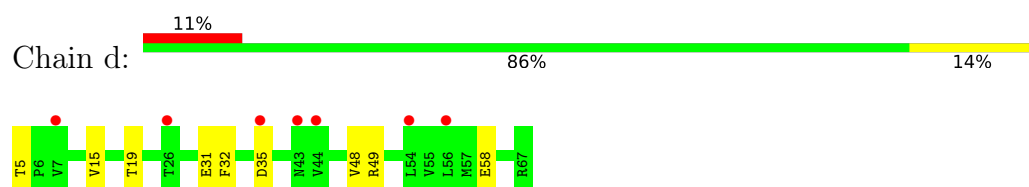
- Molecule 77: 40S ribosomal protein S27-A



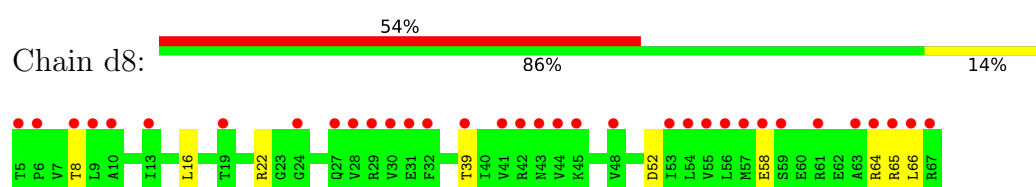
- Molecule 77: 40S ribosomal protein S27-A



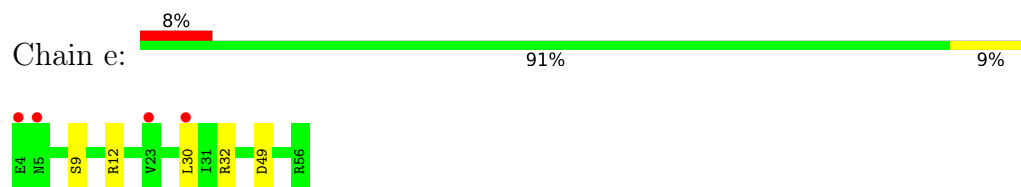
- Molecule 78: 40S ribosomal protein S28-A



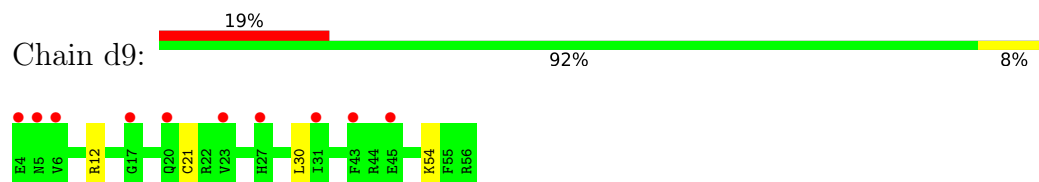
- Molecule 78: 40S ribosomal protein S28-A



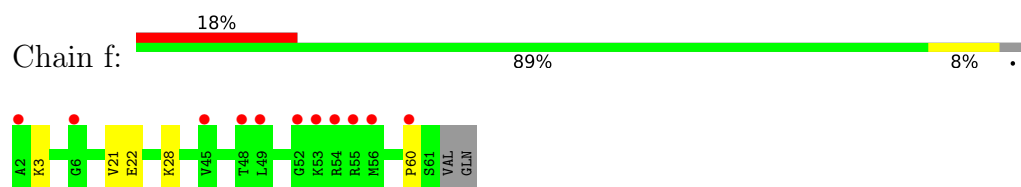
- Molecule 79: 40S ribosomal protein S29-A



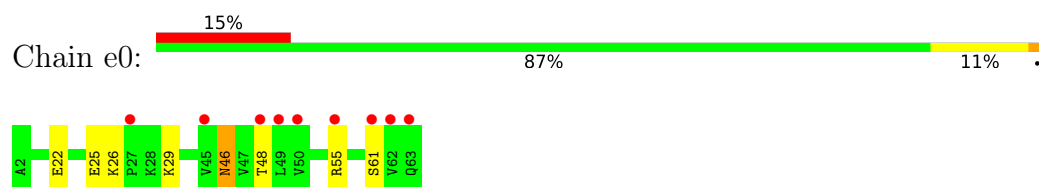
- Molecule 79: 40S ribosomal protein S29-A



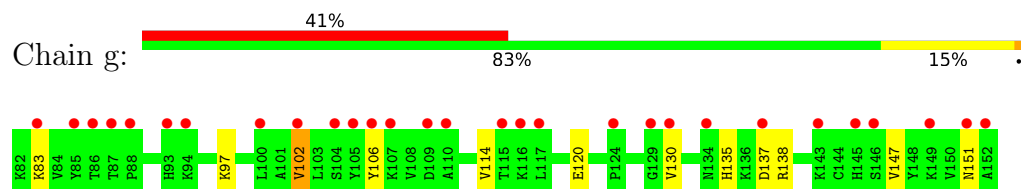
- Molecule 80: 40S ribosomal protein S30-A



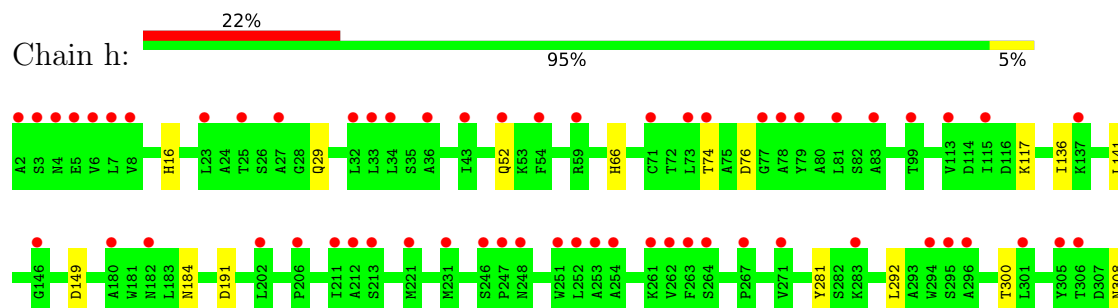
- Molecule 80: 40S ribosomal protein S30-A

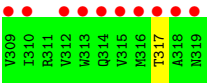


- Molecule 81: Ubiquitin-40S ribosomal protein S31

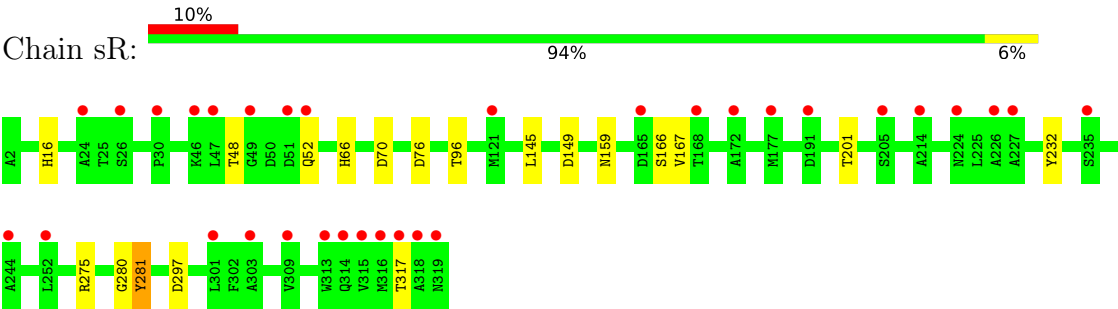


- Molecule 82: Guanine nucleotide-binding protein subunit beta-like protein

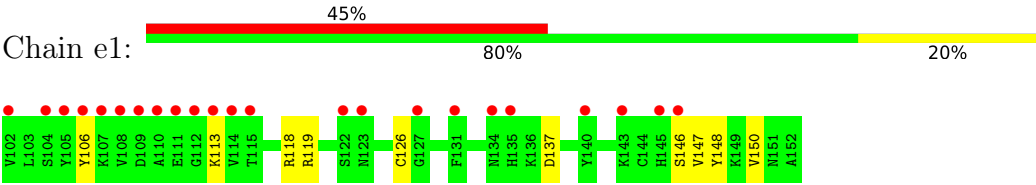




● Molecule 82: Guanine nucleotide-binding protein subunit beta-like protein



● Molecule 83: Ubiquitin-40S ribosomal protein S31



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	303.13Å 286.50Å 435.66Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	99.84 – 3.10 99.94 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (99.84-3.10) 99.5 (99.94-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 3.13Å)	Xtriage
Refinement program	PHENIX dev_2450	Depositor
R, $R_{free}$	0.222 , 0.252 0.222 , 0.252	Depositor DCC
$R_{free}$ test set	26196 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.3	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 69.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	410383	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, HN8, ZN, OHX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.60	1/75394 (0.0%)	1.02	117/117545 (0.1%)
1	AR	0.61	0/75394	1.03	127/117545 (0.1%)
2	3	0.51	0/2883	0.88	0/4491
2	AS	0.57	0/2883	0.97	1/4491 (0.0%)
3	4	0.57	0/3746	0.97	0/5832
3	AT	0.50	0/3746	0.90	2/5832 (0.0%)
4	CD	0.36	0/1948	0.55	0/2617
4	j	0.39	0/1948	0.60	0/2617
5	CE	0.44	1/3146 (0.0%)	0.61	0/4228
5	k	0.39	0/3146	0.58	0/4228
6	CF	0.40	1/2800 (0.0%)	0.62	2/3790 (0.1%)
6	l	0.41	0/2800	0.62	2/3790 (0.1%)
7	CG	0.40	0/2425	0.55	0/3271
7	m	0.34	0/2425	0.53	0/3271
8	CH	0.41	0/1260	0.56	0/1694
8	n	0.39	0/1260	0.53	0/1694
9	CI	0.44	0/1821	0.61	1/2451 (0.0%)
9	o	0.43	0/1821	0.60	1/2451 (0.0%)
10	CJ	0.32	0/1836	0.48	0/2481
10	p	0.32	0/1836	0.49	0/2481
11	CK	0.40	0/1539	0.57	0/2073
11	q	0.39	0/1539	0.56	0/2073
12	CL	0.42	0/1741	0.57	1/2335 (0.0%)
12	r	0.42	0/1741	0.57	1/2335 (0.0%)
13	CM	0.41	1/1374 (0.1%)	0.60	1/1842 (0.1%)
13	s	0.33	0/1374	0.56	0/1842
14	CN	0.39	1/1568 (0.1%)	0.58	1/2106 (0.0%)
14	t	0.42	1/1568 (0.1%)	0.57	0/2106
15	CO	0.40	0/1068	0.59	1/1438 (0.1%)
15	u	0.40	0/1068	0.55	0/1438
16	CP	0.35	0/1757	0.53	0/2354
16	v	0.39	0/1757	0.58	0/2354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	CQ	0.51	0/1585	0.61	2/2128 (0.1%)
17	w	0.46	0/1585	0.59	0/2128
18	CR	0.45	0/1443	0.61	0/1944
18	x	0.42	0/1443	0.61	1/1944 (0.1%)
19	CS	0.41	0/1465	0.58	0/1965
19	y	0.40	0/1465	0.60	1/1965 (0.1%)
20	CT	0.34	0/1538	0.49	0/2050
20	z	0.32	0/1538	0.47	0/2050
21	0	0.40	0/1481	0.58	0/1990
21	CU	0.44	0/1481	0.59	0/1990
22	2	0.40	0/1300	0.57	0/1743
22	CV	0.46	0/1300	0.58	0/1743
23	5	0.30	0/812	0.47	0/1099
23	CW	0.35	0/812	0.51	0/1099
24	CX	0.46	0/1018	0.59	0/1369
24	lR	0.41	0/1018	0.58	0/1369
25	6	0.43	0/42490	0.88	37/66207 (0.1%)
25	A	0.39	0/42443	0.87	34/66134 (0.1%)
26	7	0.35	0/712	0.50	0/958
26	CY	0.38	0/712	0.54	0/958
27	8	0.35	0/979	0.55	0/1321
27	CZ	0.35	0/979	0.52	0/1321
28	9	0.37	0/1004	0.58	0/1341
28	DA	0.38	0/1004	0.55	0/1341
29	AA	0.36	0/1118	0.50	0/1497
29	DB	0.47	1/1118 (0.1%)	0.48	0/1497
30	AB	0.43	0/1204	0.64	0/1612
30	DC	0.39	0/1204	0.62	0/1612
31	AC	0.34	0/473	0.54	0/629
31	DD	0.39	0/473	0.57	0/629
32	AD	0.30	0/751	0.48	0/1008
32	DE	0.30	0/751	0.47	0/1008
33	AE	0.39	0/890	0.54	0/1196
33	DF	0.37	0/890	0.55	0/1196
34	AF	0.42	0/1041	0.59	0/1394
34	DG	0.42	0/1041	0.57	0/1394
35	AG	0.47	0/868	0.57	0/1168
35	DH	0.46	0/868	0.62	0/1168
36	AH	0.36	0/890	0.57	1/1189 (0.1%)
36	DI	0.35	0/890	0.54	0/1189
37	AI	0.37	0/978	0.53	0/1301
37	DJ	0.35	0/978	0.52	1/1301 (0.1%)
38	AJ	0.33	0/778	0.52	0/1034

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DK	0.32	0/778	0.51	0/1034
39	AK	0.39	0/696	0.60	0/923
39	DL	0.39	0/696	0.58	0/923
40	AL	0.34	0/618	0.50	0/826
40	DM	0.32	0/618	0.49	0/826
41	AM	0.40	0/443	0.59	0/588
41	DN	0.36	0/443	0.59	0/588
42	AN	0.44	0/423	0.56	0/562
42	DO	0.43	0/423	0.60	0/562
43	AO	0.36	0/234	0.62	0/300
43	DP	0.39	0/234	0.51	0/300
44	AP	0.41	0/860	0.59	0/1136
44	DQ	0.41	0/860	0.59	0/1136
45	AQ	0.40	0/701	0.56	0/934
45	DR	0.39	0/701	0.58	0/934
46	i	0.31	0/1113	0.54	1/1502 (0.1%)
48	sM	0.34	0/480	0.58	0/642
49	p0	0.30	0/1091	0.53	2/1472 (0.1%)
50	B	0.29	0/1617	0.51	0/2215
50	s0	0.36	1/1623 (0.1%)	0.49	0/2222
51	C	0.27	0/1735	0.54	0/2335
51	s1	0.30	0/1748	0.55	1/2352 (0.0%)
52	D	0.30	0/1665	0.50	0/2263
52	s2	0.31	0/1665	0.52	0/2263
53	E	0.30	0/1759	0.51	0/2368
53	s3	0.28	0/1759	0.50	0/2368
54	F	0.31	0/2109	0.53	0/2839
54	s4	0.36	1/2109 (0.0%)	0.52	0/2839
55	G	0.27	0/1629	0.50	0/2202
55	s5	0.29	0/1629	0.47	0/2202
56	H	0.32	0/1823	0.51	1/2439 (0.0%)
56	s6	0.32	0/1779	0.53	0/2379
57	I	0.30	0/1506	0.52	0/2028
57	s7	0.30	0/1516	0.51	0/2043
58	J	0.31	0/1514	0.57	1/2021 (0.0%)
58	s8	0.33	0/1514	0.53	0/2021
59	K	0.29	0/1519	0.49	0/2035
59	s9	0.30	0/1519	0.49	0/2035
60	L	0.29	0/789	0.57	1/1067 (0.1%)
60	c0	0.27	0/775	0.62	3/1045 (0.3%)
61	M	0.33	0/1239	0.52	0/1673
61	c1	0.34	0/1194	0.52	0/1610
62	N	0.30	0/898	0.62	0/1220



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
62	c2	0.35	1/898 (0.1%)	0.62	1/1220 (0.1%)
63	O	0.31	0/1215	0.49	0/1638
63	c3	0.32	0/1215	0.53	0/1638
64	P	0.28	0/901	0.54	0/1217
64	c4	0.32	0/960	0.55	0/1290
65	Q	0.31	0/998	0.49	0/1341
65	c5	0.29	0/1060	0.60	0/1426
66	R	0.29	0/1125	0.55	0/1510
66	c6	0.29	0/1131	0.54	0/1518
67	S	0.29	0/935	0.52	0/1254
67	c7	0.28	0/914	0.48	0/1224
68	T	0.29	0/1211	0.50	0/1628
68	c8	0.29	0/1211	0.50	0/1628
69	U	0.29	0/1130	0.46	0/1517
69	c9	0.29	0/1130	0.46	0/1517
70	V	0.27	0/865	0.51	0/1169
70	d0	0.29	0/892	0.52	0/1205
71	W	0.31	0/693	0.50	0/935
71	d1	0.30	0/693	0.51	0/935
72	X	0.30	0/1038	0.55	0/1395
72	d2	0.31	0/1038	0.52	0/1395
73	Y	0.33	0/1139	0.55	0/1518
73	d3	0.35	0/1139	0.54	0/1518
74	Z	0.31	0/1087	0.49	0/1449
74	d4	0.32	0/1087	0.54	0/1449
75	a	0.29	0/571	0.53	0/768
75	d5	0.27	0/566	0.46	0/761
76	b	0.34	0/782	0.61	0/1047
76	d6	0.33	0/782	0.60	0/1047
77	c	0.27	0/620	0.54	0/838
77	d7	0.28	0/620	0.54	0/838
78	d	0.43	1/499 (0.2%)	0.53	0/670
78	d8	0.28	0/499	0.62	0/670
79	d9	0.33	0/452	0.51	0/600
79	e	0.30	0/452	0.50	0/600
80	e0	0.32	0/499	0.49	0/665
80	f	0.29	0/483	0.48	0/643
81	g	0.29	0/577	0.58	0/770
82	h	0.26	0/2494	0.49	0/3393
82	sR	0.27	0/2495	0.50	0/3395
83	e1	0.27	0/404	0.56	0/542
All	All	0.47	11/429967 (0.0%)	0.83	346/631328 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	CE	0	3
5	k	0	2
6	l	0	2
7	CG	0	3
7	m	0	1
9	CI	0	2
9	o	0	2
10	CJ	0	2
10	p	0	1
11	CK	0	1
11	q	0	1
12	CL	0	1
13	CM	0	2
13	s	0	2
14	CN	0	1
14	t	0	2
15	CO	0	1
15	u	0	1
16	CP	0	1
17	CQ	0	1
17	w	0	1
18	x	0	1
19	CS	0	1
21	CU	0	2
26	CY	0	1
29	AA	0	2
30	DC	0	2
31	AC	0	1
31	DD	0	1
37	AI	0	1
37	DJ	0	1
50	B	0	1
51	s1	0	1
53	E	0	2
53	s3	0	2
55	G	0	3
55	s5	0	1
56	H	0	2
57	I	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
57	s7	0	2
58	J	0	2
58	s8	0	2
59	K	0	1
60	c0	0	1
61	M	0	1
62	N	0	1
62	c2	0	2
63	c3	0	2
64	P	0	1
64	c4	0	2
65	Q	0	1
65	c5	0	2
66	R	0	2
66	c6	0	4
67	S	0	1
67	c7	0	2
68	T	0	3
68	c8	0	1
70	d0	0	1
74	d4	0	1
75	a	0	2
76	b	0	2
80	e0	0	1
81	g	0	1
82	sR	0	1
83	e1	0	1
All	All	0	103

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	DB	36	HIS	C-N	11.46	1.56	1.34
54	s4	82	TYR	C-N	-8.48	1.18	1.34
14	t	132	ALA	C-N	8.06	1.49	1.34
50	s0	160	ILE	C-N	-7.98	1.19	1.34
78	d	5	THR	C-N	7.62	1.48	1.34
62	c2	81	ASP	C-N	6.82	1.47	1.34
5	CE	168	LYS	C-N	-6.50	1.19	1.34
13	CM	43	GLN	C-N	6.35	1.48	1.34
6	CF	94	CYS	CB-SG	-5.58	1.72	1.81
14	CN	49	ARG	C-N	5.20	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1308	A	N7-C5	-5.02	1.36	1.39

All (346) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3278	C	N1-C2-O2	10.14	124.98	118.90
1	1	2373	A	O5'-P-OP1	-9.82	96.86	105.70
1	1	1308	A	C8-N9-C4	-8.98	102.21	105.80
1	AR	2846	U	N3-C2-O2	-8.79	116.05	122.20
1	AR	2714	G	N3-C4-C5	8.71	132.95	128.60
1	AR	2870	C	C2-N1-C1'	-8.67	109.26	118.80
1	1	3278	C	N3-C2-O2	-8.64	115.86	121.90
1	1	2870	C	C2-N1-C1'	-8.61	109.33	118.80
1	AR	1307	G	P-O3'-C3'	8.57	129.98	119.70
1	AR	3217	C	N1-C2-O2	8.51	124.01	118.90
1	AR	3344	A	N7-C8-N9	8.48	118.04	113.80
1	AR	2726	C	C6-N1-C2	-8.34	116.96	120.30
1	1	3217	C	C2-N1-C1'	8.29	127.91	118.80
1	1	1308	A	N7-C8-N9	8.01	117.81	113.80
1	1	1192	C	N1-C2-O2	8.00	123.70	118.90
1	1	1495	U	C5-C6-N1	-7.96	118.72	122.70
25	6	453	U	N1-C2-O2	7.92	128.34	122.80
1	AR	2714	G	N3-C4-N9	-7.89	121.27	126.00
1	1	406	G	O4'-C1'-N9	7.88	114.51	108.20
1	AR	2846	U	C5-C4-O4	7.85	130.61	125.90
1	1	3217	C	N3-C2-O2	-7.85	116.41	121.90
1	1	1495	U	N1-C2-O2	-7.85	117.31	122.80
1	AR	2404	A	N1-C6-N6	7.82	123.29	118.60
1	AR	3344	A	C8-N9-C4	-7.77	102.69	105.80
1	1	2870	C	C6-N1-C1'	7.60	129.92	120.80
1	1	3217	C	N1-C2-O2	7.53	123.42	118.90
1	AR	1149	G	N1-C6-O6	7.53	124.42	119.90
1	AR	2871	G	O5'-P-OP2	-7.52	98.93	105.70
1	1	3278	C	C2-N1-C1'	7.51	127.06	118.80
1	1	3306	U	C5-C4-O4	7.47	130.38	125.90
1	AR	2870	C	C6-N1-C1'	7.43	129.71	120.80
1	AR	1495	U	C5-C6-N1	-7.36	119.02	122.70
25	6	453	U	C2-N1-C1'	7.32	126.48	117.70
1	AR	3217	C	C2-N1-C1'	7.27	126.79	118.80
1	AR	3306	U	N3-C2-O2	-7.22	117.14	122.20
25	6	163	G	N3-C4-N9	-7.20	121.68	126.00
25	6	453	U	N3-C2-O2	-7.19	117.17	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2846	U	N3-C2-O2	-7.18	117.17	122.20
1	1	1858	A	C2-N3-C4	7.11	114.15	110.60
51	s1	231	LEU	CA-CB-CG	6.98	131.35	115.30
60	c0	97	PRO	N-CA-CB	6.97	111.67	103.30
1	AR	3057	U	C5-C4-O4	6.95	130.07	125.90
25	A	553	G	N1-C6-O6	6.95	124.07	119.90
25	A	507	U	C2-N1-C1'	6.91	125.99	117.70
1	1	3306	U	N3-C2-O2	-6.91	117.37	122.20
1	AR	3217	C	N3-C2-O2	-6.87	117.09	121.90
1	1	937	G	C5-C6-O6	-6.86	124.48	128.60
1	1	1269	U	C2-N1-C1'	6.84	125.91	117.70
25	6	1274	C	N1-C2-O2	6.75	122.95	118.90
1	AR	2263	C	C4-C5-C6	-6.73	114.04	117.40
1	AR	3093	C	N1-C2-O2	-6.71	114.87	118.90
1	1	2726	C	C6-N1-C2	-6.69	117.62	120.30
1	1	1849	C	O5'-P-OP1	-6.68	99.69	105.70
60	c0	88	PRO	N-CA-CB	6.67	111.30	103.30
1	AR	2726	C	N3-C2-O2	-6.65	117.24	121.90
25	6	1274	C	C2-N1-C1'	6.65	126.11	118.80
1	AR	2819	A	O5'-P-OP2	-6.64	99.72	105.70
25	A	577	G	N1-C6-O6	6.62	123.87	119.90
1	AR	2808	A	C8-N9-C4	6.59	108.44	105.80
1	1	3217	C	C6-N1-C2	-6.58	117.67	120.30
1	1	1307	G	P-O3'-C3'	6.57	127.58	119.70
1	AR	2617	U	C4-C5-C6	6.57	123.64	119.70
1	1	407	A	N1-C6-N6	6.56	122.54	118.60
1	AR	2257	C	C2-N1-C1'	6.55	126.00	118.80
1	AR	2404	A	N7-C8-N9	6.55	117.07	113.80
6	1	327	LEU	CA-CB-CG	6.50	130.26	115.30
25	A	553	G	C5-C6-O6	-6.49	124.71	128.60
25	A	728	U	C2-N1-C1'	6.47	125.46	117.70
1	1	2726	C	C5-C4-N4	6.45	124.72	120.20
25	A	577	G	C5-C6-O6	-6.45	124.73	128.60
1	AR	1495	U	C5-C4-O4	6.43	129.76	125.90
1	AR	2272	G	O4'-C1'-N9	6.43	113.35	108.20
1	1	2620	G	N1-C6-O6	6.42	123.75	119.90
25	A	639	U	N3-C2-O2	-6.41	117.71	122.20
1	1	3306	U	N3-C4-O4	-6.40	114.92	119.40
25	6	813	U	N1-C2-O2	6.40	127.28	122.80
1	AR	3344	A	C5-N7-C8	-6.38	100.71	103.90
1	1	1192	C	C2-N1-C1'	6.38	125.81	118.80
1	AR	2870	C	N3-C4-C5	6.37	124.45	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1160	C	C6-N1-C2	6.37	122.85	120.30
1	1	2827	U	C5-C6-N1	-6.37	119.52	122.70
25	A	507	U	N1-C2-O2	6.34	127.24	122.80
49	p0	278	PRO	N-CA-CB	6.33	110.89	103.30
1	1	1556	C	N1-C2-O2	6.32	122.69	118.90
25	A	507	U	N3-C2-O2	-6.31	117.78	122.20
1	1	2870	C	N1-C2-O2	-6.31	115.12	118.90
1	1	65	A	P-O3'-C3'	6.29	127.25	119.70
60	L	88	PRO	N-CA-CB	6.26	110.81	103.30
25	6	813	U	C2-N1-C1'	6.25	125.21	117.70
1	1	1495	U	N1-C2-N3	6.25	118.65	114.90
1	1	3278	C	C6-N1-C2	-6.22	117.81	120.30
1	AR	1311	G	O5'-P-OP2	-6.21	100.11	105.70
56	H	69	LEU	CA-CB-CG	6.20	129.56	115.30
6	CF	182	LEU	CA-CB-CG	6.20	129.56	115.30
1	1	3181	C	N3-C2-O2	-6.17	117.58	121.90
1	1	1495	U	C2-N1-C1'	-6.16	110.31	117.70
1	1	353	G	C5-C6-O6	-6.15	124.91	128.60
1	AR	2257	C	C6-N1-C2	-6.14	117.84	120.30
25	A	959	U	C2-N1-C1'	6.14	125.07	117.70
1	AR	3309	G	N3-C4-N9	6.14	129.68	126.00
1	AR	3057	U	N3-C2-O2	-6.13	117.91	122.20
12	r	57	LEU	CA-CB-CG	6.12	129.37	115.30
1	1	2281	A	O4'-C1'-N9	6.09	113.07	108.20
1	AR	3309	G	C4-N9-C1'	6.09	134.41	126.50
1	AR	2899	C	C6-N1-C2	-6.08	117.87	120.30
46	i	254	PRO	N-CA-CB	6.07	110.58	103.30
1	AR	637	C	C6-N1-C2	-6.06	117.88	120.30
25	A	1389	C	C2-N1-C1'	6.06	125.46	118.80
1	AR	1495	U	C4-C5-C6	6.04	123.33	119.70
14	CN	46	ILE	C-N-CA	6.04	136.81	121.70
1	AR	3057	U	N3-C4-O4	-6.04	115.17	119.40
1	1	2257	C	C2-N1-C1'	6.03	125.43	118.80
1	AR	2950	G	O4'-C1'-N9	6.03	113.02	108.20
25	6	1389	C	C2-N1-C1'	6.02	125.42	118.80
1	AR	637	C	C2-N1-C1'	6.02	125.42	118.80
1	1	1329	U	C2-N1-C1'	6.01	124.91	117.70
1	1	3344	A	N7-C8-N9	5.99	116.79	113.80
1	AR	1103	A	O4'-C1'-N9	5.98	112.98	108.20
1	AR	2726	C	C5-C4-N4	5.96	124.37	120.20
1	1	2355	G	N1-C6-O6	5.95	123.47	119.90
1	1	1820	U	P-O3'-C3'	5.95	126.84	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	2343	C	C6-N1-C2	5.94	122.68	120.30
1	AR	437	G	N7-C8-N9	5.94	116.07	113.10
1	AR	2846	U	N3-C4-O4	-5.93	115.25	119.40
1	AR	2714	G	C2-N3-C4	-5.91	108.94	111.90
25	A	1274	C	C6-N1-C2	-5.91	117.94	120.30
1	AR	2404	A	C5-N7-C8	-5.90	100.95	103.90
1	1	1269	U	N1-C2-O2	5.90	126.93	122.80
25	A	1560	U	N3-C2-O2	-5.90	118.07	122.20
25	6	163	G	N3-C4-C5	5.89	131.54	128.60
1	AR	2996	U	N1-C2-O2	5.88	126.92	122.80
1	1	1858	A	C8-N9-C4	-5.87	103.45	105.80
49	p0	290	PRO	N-CA-CB	5.84	110.31	103.30
25	A	728	U	N1-C2-O2	5.82	126.88	122.80
1	1	835	G	O4'-C1'-N9	5.82	112.86	108.20
17	CQ	68	ARG	NE-CZ-NH1	-5.81	117.40	120.30
1	AR	3309	G	C6-C5-N7	-5.80	126.92	130.40
1	AR	637	C	P-O3'-C3'	5.79	126.65	119.70
1	AR	2899	C	N3-C2-O2	-5.79	117.85	121.90
1	1	3214	U	N3-C2-O2	-5.79	118.15	122.20
1	AR	2385	G	N3-C4-C5	5.79	131.49	128.60
1	1	1858	A	N3-C4-C5	-5.78	122.76	126.80
1	AR	2404	A	C6-C5-N7	-5.77	128.26	132.30
25	6	795	U	N3-C2-O2	-5.76	118.17	122.20
25	A	720	G	OP1-P-O3'	5.76	117.86	105.20
1	1	895	A	N1-C6-N6	5.75	122.05	118.60
1	1	2714	G	N3-C4-C5	5.75	131.47	128.60
1	AR	637	C	C5-C6-N1	5.74	123.87	121.00
25	A	959	U	N3-C2-O2	-5.72	118.19	122.20
1	1	1556	C	N3-C2-O2	-5.72	117.90	121.90
1	AR	407	A	N1-C6-N6	5.71	122.03	118.60
25	6	965	U	N1-C2-O2	5.70	126.79	122.80
1	AR	1556	C	C2-N1-C1'	5.70	125.07	118.80
1	AR	1149	G	C5-C6-O6	-5.70	125.18	128.60
1	1	1581	C	N1-C2-O2	5.69	122.32	118.90
1	AR	2662	G	N1-C6-O6	-5.69	116.49	119.90
1	1	895	A	C6-C5-N7	-5.68	128.32	132.30
1	1	2871	G	O5'-P-OP2	-5.68	100.58	105.70
25	A	453	U	C2-N1-C1'	5.68	124.52	117.70
25	A	959	U	N1-C2-O2	5.68	126.78	122.80
1	1	2169	G	N1-C6-O6	-5.67	116.50	119.90
1	AR	3344	A	O4'-C1'-N9	5.67	112.73	108.20
1	1	2808	A	N1-C6-N6	5.66	122.00	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1456	C	C2-N1-C1'	5.66	125.03	118.80
1	1	3344	A	O4'-C1'-N9	5.66	112.73	108.20
15	CO	72	LEU	CA-CB-CG	5.65	128.29	115.30
1	1	218	G	O5'-P-OP2	-5.64	100.62	105.70
25	A	639	U	N1-C2-O2	5.64	126.75	122.80
25	A	1698	G	P-O3'-C3'	5.62	126.44	119.70
1	AR	1103	A	P-O3'-C3'	5.62	126.44	119.70
1	AR	2617	U	C5-C6-N1	-5.62	119.89	122.70
1	1	2314	U	C5-C4-O4	-5.59	122.55	125.90
1	1	1149	G	N1-C6-O6	5.58	123.25	119.90
25	A	1039	A	O4'-C1'-N9	5.57	112.66	108.20
1	1	2899	C	C6-N1-C2	-5.57	118.07	120.30
25	A	75	U	N1-C2-O2	5.56	126.69	122.80
1	1	2726	C	N3-C2-O2	-5.55	118.01	121.90
1	1	770	G	O4'-C1'-N9	5.55	112.64	108.20
1	AR	2808	A	N9-C4-C5	-5.54	103.58	105.80
1	1	1377	G	C5-C6-O6	-5.53	125.28	128.60
1	AR	2714	G	C5-N7-C8	-5.53	101.53	104.30
1	AR	2334	U	N3-C2-O2	-5.53	118.33	122.20
1	AR	3309	G	C8-N9-C1'	-5.51	119.84	127.00
25	6	337	G	C4-N9-C1'	5.50	133.66	126.50
1	AR	2358	A	C8-N9-C4	5.50	108.00	105.80
1	1	2627	C	C6-N1-C2	5.49	122.50	120.30
1	AR	3212	C	N1-C2-O2	-5.49	115.61	118.90
1	AR	2870	C	N1-C2-O2	-5.48	115.61	118.90
1	1	979	U	P-O3'-C3'	5.48	126.27	119.70
25	6	1473	U	C2-N1-C1'	5.47	124.27	117.70
25	6	1473	U	N1-C2-O2	5.47	126.63	122.80
1	AR	3217	C	C6-N1-C1'	-5.46	114.24	120.80
1	AR	3181	C	N3-C2-O2	-5.46	118.08	121.90
1	AR	2281	A	O4'-C1'-N9	5.46	112.56	108.20
1	AR	1588	A	N1-C6-N6	-5.45	115.33	118.60
25	6	1097	U	P-O3'-C3'	5.45	126.24	119.70
60	c0	83	PRO	N-CA-CB	5.45	109.84	103.30
1	1	2550	U	N1-C2-O2	5.45	126.61	122.80
1	1	2944	U	C5-C4-O4	-5.45	122.63	125.90
1	AR	979	U	P-O3'-C3'	5.45	126.23	119.70
25	6	1473	U	N3-C2-O2	-5.44	118.39	122.20
1	AR	1605	A	O4'-C1'-N9	5.44	112.55	108.20
1	1	2286	U	O5'-P-OP2	-5.44	100.81	105.70
1	AR	2617	U	N3-C2-O2	-5.44	118.39	122.20
25	A	1761	U	P-O3'-C3'	5.44	126.22	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3057	U	N3-C2-O2	-5.43	118.40	122.20
1	AR	2263	C	N3-C4-C5	5.43	124.07	121.90
1	1	646	A	O5'-P-OP2	-5.43	100.82	105.70
25	6	610	G	C4-N9-C1'	5.42	133.55	126.50
25	6	1000	C	C2-N1-C1'	5.42	124.77	118.80
25	6	1389	C	N1-C2-O2	5.42	122.16	118.90
1	AR	2816	G	C8-N9-C4	5.42	108.57	106.40
17	CQ	84	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	AR	881	C	N1-C2-O2	5.42	122.15	118.90
1	1	2374	C	N3-C2-O2	-5.41	118.11	121.90
25	A	1241	G	O4'-C1'-N9	5.41	112.53	108.20
25	A	1370	U	P-O3'-C3'	5.41	126.19	119.70
25	6	25	C	P-O3'-C3'	5.41	126.19	119.70
1	1	776	U	C4-C5-C6	5.40	122.94	119.70
1	1	1556	C	C2-N1-C1'	5.40	124.74	118.80
1	AR	895	A	C6-C5-N7	-5.40	128.52	132.30
1	1	937	G	N1-C6-O6	5.40	123.14	119.90
1	1	66	A	O5'-P-OP1	-5.39	100.85	105.70
1	1	1604	G	C4-N9-C1'	5.39	133.51	126.50
1	AR	65	A	P-O3'-C3'	5.39	126.17	119.70
1	AR	3057	U	N1-C2-N3	5.39	118.14	114.90
25	6	1560	U	C2-N1-C1'	5.39	124.16	117.70
1	AR	2541	U	P-O3'-C3'	5.38	126.16	119.70
1	AR	406	G	O4'-C1'-N9	5.38	112.50	108.20
1	AR	1097	G	P-O3'-C3'	5.38	126.16	119.70
25	A	610	G	C4-N9-C1'	5.38	133.49	126.50
1	1	3217	C	C6-N1-C1'	-5.37	114.35	120.80
1	AR	3344	A	C6-C5-N7	-5.37	128.54	132.30
1	1	1367	G	N1-C6-O6	5.36	123.12	119.90
9	o	179	LEU	CA-CB-CG	5.35	127.61	115.30
1	AR	1495	U	N1-C2-N3	5.35	118.11	114.90
25	A	158	U	P-O3'-C3'	5.35	126.12	119.70
25	6	158	U	P-O3'-C3'	5.35	126.12	119.70
36	AH	51	LEU	CA-CB-CG	5.35	127.60	115.30
1	AR	1192	C	N1-C2-O2	5.34	122.10	118.90
1	AR	1886	A	O5'-P-OP2	-5.34	100.89	105.70
1	1	1269	U	N3-C2-O2	-5.33	118.47	122.20
1	AR	2273	G	C8-N9-C4	5.33	108.53	106.40
1	1	353	G	N1-C6-O6	5.33	123.10	119.90
1	AR	437	G	C8-N9-C4	-5.33	104.27	106.40
1	1	1114	U	N1-C2-O2	5.32	126.52	122.80
25	6	1773	C	N3-C4-C5	-5.31	119.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	422	A	N1-C6-N6	-5.31	115.41	118.60
1	AR	2257	C	O4'-C1'-N1	5.30	112.44	108.20
1	1	1495	U	C4-C5-C6	5.30	122.88	119.70
25	A	1196	A	P-O3'-C3'	5.30	126.06	119.70
25	6	542	A	P-O3'-C3'	5.30	126.06	119.70
1	1	1196	C	C6-N1-C2	5.29	122.42	120.30
1	AR	1556	C	N1-C2-O2	5.29	122.07	118.90
25	6	1137	A	C8-N9-C4	5.27	107.91	105.80
1	1	497	C	N1-C2-O2	-5.27	115.74	118.90
1	AR	2679	A	C2-N3-C4	-5.27	107.97	110.60
1	1	3275	U	OP1-P-O3'	5.26	116.78	105.20
25	6	610	G	C8-N9-C1'	-5.26	120.16	127.00
13	CM	172	LEU	C-N-CA	5.26	134.85	121.70
1	AR	3309	G	N3-C4-C5	-5.26	125.97	128.60
1	1	3362	A	O4'-C1'-N9	5.25	112.40	108.20
1	1	651	G	N3-C4-N9	5.25	129.15	126.00
19	y	41	ASP	CB-CG-OD1	5.25	123.02	118.30
1	1	1897	G	C5-C6-O6	-5.25	125.45	128.60
1	AR	2899	C	N3-C4-C5	-5.24	119.80	121.90
1	1	922	U	N1-C2-O2	5.23	126.46	122.80
25	6	1058	U	OP1-P-O3'	5.23	116.70	105.20
1	AR	1149	G	C4-C5-C6	5.22	121.93	118.80
6	1	313	LEU	CA-CB-CG	5.22	127.31	115.30
1	AR	878	G	C8-N9-C4	-5.22	104.31	106.40
1	1	2550	U	N3-C2-O2	-5.22	118.55	122.20
1	1	936	A	P-O3'-C3'	5.22	125.96	119.70
1	AR	2943	G	N1-C6-O6	5.21	123.03	119.90
37	DJ	28	LEU	CA-CB-CG	5.21	127.29	115.30
25	6	1573	A	P-O3'-C3'	5.21	125.95	119.70
25	A	581	U	C2-N1-C1'	5.21	123.95	117.70
25	A	720	G	P-O3'-C3'	5.21	125.95	119.70
1	1	2358	A	N1-C6-N6	5.21	121.72	118.60
1	AR	1858	A	C4-N9-C1'	5.20	135.66	126.30
1	AR	3306	U	N3-C4-O4	-5.19	115.77	119.40
1	1	2827	U	C2-N3-C4	-5.18	123.89	127.00
1	AR	942	U	N3-C4-O4	5.18	123.03	119.40
58	J	29	LEU	CA-CB-CG	5.18	127.21	115.30
3	AT	82	U	C2-N1-C1'	5.18	123.91	117.70
1	1	2585	G	N3-C4-C5	-5.18	126.01	128.60
1	1	3344	A	C8-N9-C4	-5.17	103.73	105.80
1	AR	1521	G	N1-C6-O6	-5.17	116.80	119.90
1	1	1904	C	C6-N1-C2	-5.16	118.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AS	101	G	N1-C6-O6	5.16	122.99	119.90
1	AR	3214	U	C2-N1-C1'	5.16	123.89	117.70
62	c2	103	LEU	CA-CB-CG	5.16	127.16	115.30
1	AR	1496	C	C2-N1-C1'	5.15	124.47	118.80
1	AR	800	G	N3-C4-N9	5.15	129.09	126.00
1	1	2418	G	OP1-P-O3'	5.14	116.51	105.20
25	A	831	U	C5-C6-N1	5.14	125.27	122.70
25	6	1000	C	N3-C2-O2	-5.14	118.30	121.90
25	A	1060	U	N1-C2-O2	5.13	126.39	122.80
18	x	41	LEU	CA-CB-CG	5.13	127.10	115.30
1	1	1897	G	C6-C5-N7	-5.13	127.32	130.40
1	1	3277	U	N3-C2-O2	-5.13	118.61	122.20
1	AR	1151	U	N3-C2-O2	5.13	125.79	122.20
1	AR	2615	G	N9-C4-C5	-5.13	103.35	105.40
1	AR	1887	A	O5'-P-OP2	-5.12	101.09	105.70
3	AT	82	U	P-O3'-C3'	5.12	125.85	119.70
1	1	1002	A	N1-C6-N6	5.12	121.67	118.60
9	CI	179	LEU	CA-CB-CG	5.11	127.05	115.30
1	AR	2679	A	N1-C6-N6	5.11	121.67	118.60
1	1	2593	A	P-O3'-C3'	5.11	125.83	119.70
25	6	453	U	C6-N1-C1'	-5.11	114.05	121.20
25	6	1246	C	C2-N1-C1'	5.11	124.42	118.80
1	AR	1047	A	N1-C6-N6	5.11	121.66	118.60
1	1	2112	U	P-O3'-C3'	5.10	125.82	119.70
1	1	2400	G	N1-C6-O6	5.10	122.96	119.90
1	AR	895	A	C5-N7-C8	-5.10	101.35	103.90
1	AR	2869	U	C5-C4-O4	-5.09	122.84	125.90
25	6	795	U	C2-N1-C1'	5.08	123.80	117.70
1	AR	2679	A	O4'-C1'-N9	5.08	112.27	108.20
1	AR	3362	A	O4'-C1'-N9	5.08	112.26	108.20
1	AR	2808	A	N1-C6-N6	5.07	121.64	118.60
25	6	1274	C	N3-C2-O2	-5.07	118.35	121.90
1	1	2176	U	N3-C2-O2	-5.07	118.65	122.20
1	1	922	U	C2-N1-C1'	5.06	123.77	117.70
1	1	3209	A	N1-C6-N6	5.06	121.64	118.60
1	1	109	A	OP1-P-O3'	5.05	116.32	105.20
1	AR	2846	U	C6-N1-C2	-5.05	117.97	121.00
1	AR	3306	U	C5-C4-O4	5.05	128.93	125.90
25	A	1060	U	N3-C2-O2	-5.05	118.66	122.20
1	AR	2930	A	O4'-C1'-N9	5.05	112.24	108.20
25	6	1697	G	C4-N9-C1'	5.04	133.06	126.50
1	AR	1437	C	C2-N1-C1'	5.04	124.35	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	1483	G	O4'-C1'-N9	5.04	112.23	108.20
1	1	1495	U	C2-N3-C4	-5.04	123.98	127.00
6	CF	315	LYS	C-N-CA	-5.04	109.10	121.70
1	AR	2794	G	O4'-C1'-N9	5.04	112.23	108.20
1	AR	3278	C	C2-N1-C1'	5.04	124.34	118.80
12	CL	87	LEU	CA-CB-CG	5.04	126.88	115.30
1	AR	648	C	O5'-P-OP1	-5.03	101.17	105.70
1	1	2808	A	N9-C4-C5	-5.03	103.79	105.80
25	6	678	A	P-O3'-C3'	5.03	125.73	119.70
1	1	936	A	O4'-C1'-N9	5.02	112.21	108.20
1	1	2802	A	OP2-P-O3'	5.01	116.23	105.20
25	6	813	U	N3-C2-O2	-5.01	118.70	122.20
1	AR	2874	G	C5-C6-O6	5.00	131.60	128.60
1	1	2541	U	P-O3'-C3'	5.00	125.70	119.70
1	AR	3140	G	N1-C6-O6	5.00	122.90	119.90

There are no chirality outliers.

All (103) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	AA	102	GLU	Peptide
29	AA	124	ALA	Peptide
31	AC	19	ASN	Peptide
37	AI	83	LYS	Peptide
50	B	191	ARG	Peptide
5	CE	186	GLY	Peptide
5	CE	315	GLY	Peptide
5	CE	385	LYS	Peptide
7	CG	257	GLU	Peptide
7	CG	258	LYS	Peptide
7	CG	43	LYS	Peptide
9	CI	157	ASN	Peptide
9	CI	190	THR	Peptide
10	CJ	34	PHE	Peptide
10	CJ	35	GLY	Peptide
11	CK	21	LYS	Peptide
12	CL	218	ALA	Peptide
13	CM	172	LEU	Peptide
13	CM	73	GLY	Peptide
14	CN	4	SER	Peptide
15	CO	7	VAL	Peptide
16	CP	92	LEU	Peptide

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Mol	Chain	Res	Type	Group
17	CQ	110	PRO	Peptide
19	CS	98	LYS	Peptide
21	CU	133	ALA	Peptide
21	CU	22	PRO	Peptide
26	CY	80	ARG	Peptide
30	DC	115	LYS	Peptide
30	DC	45	MET	Peptide
31	DD	19	ASN	Peptide
37	DJ	118	ILE	Peptide
53	E	198	GLY	Peptide
53	E	216	PRO	Peptide
55	G	56	ALA	Peptide
55	G	58	LEU	Peptide
55	G	65	ARG	Peptide
56	H	148	SER	Peptide
56	H	67	VAL	Peptide
57	I	30	SER	Peptide
57	I	63	PRO	Peptide
58	J	146	ARG	Peptide
58	J	147	ALA	Peptide
59	K	163	PRO	Peptide
61	M	3	THR	Peptide
62	N	111	ASN	Peptide
64	P	41	ARG	Peptide
65	Q	124	THR	Peptide
66	R	14	LYS	Peptide
66	R	40	GLU	Peptide
67	S	84	TYR	Peptide
68	T	13	HIS	Peptide
68	T	144	ARG	Peptide
68	T	81	ILE	Peptide
75	a	87	GLY	Peptide
75	a	94	LYS	Peptide
76	b	10	ARG	Peptide
76	b	84	VAL	Peptide
60	c0	34	GLU	Peptide
62	c2	108	ARG	Peptide
62	c2	130	THR	Peptide
63	c3	22	ALA	Peptide
63	c3	65	VAL	Peptide
64	c4	11	SER	Peptide
64	c4	125	SER	Peptide

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Mol	Chain	Res	Type	Group
65	c5	134	THR	Peptide
65	c5	52	LYS	Peptide
66	c6	114	ARG	Peptide
66	c6	13	LYS	Peptide
66	c6	40	GLU	Peptide
66	c6	41	PRO	Peptide
67	c7	105	GLN	Peptide
67	c7	66	VAL	Peptide
68	c8	13	HIS	Peptide
70	d0	70	THR	Peptide
74	d4	29	HIS	Peptide
80	e0	46	ASN	Peptide
83	e1	146	SER	Peptide
81	g	102	VAL	Peptide
5	k	186	GLY	Peptide
5	k	349	LYS	Peptide
6	l	291	ASN	Peptide
6	l	338	LYS	Peptide
7	m	258	LYS	Peptide
9	o	157	ASN	Peptide
9	o	190	THR	Peptide
10	p	76	ALA	Peptide
11	q	21	LYS	Peptide
13	s	171	VAL	Peptide
13	s	94	ARG	Peptide
51	s1	146	GLN	Peptide
53	s3	144	ALA	Peptide
53	s3	216	PRO	Peptide
55	s5	44	ASN	Peptide
57	s7	130	VAL	Peptide
57	s7	63	PRO	Peptide
58	s8	100	ALA	Peptide
58	s8	148	ALA	Peptide
82	sR	280	GLY	Peptide
14	t	46	ILE	Peptide
14	t	47	ALA	Peptide
15	u	7	VAL	Peptide
17	w	110	PRO	Peptide
18	x	157	VAL	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CD	250/252 (99%)	226 (90%)	23 (9%)	1 (0%)	34	69
4	j	250/252 (99%)	230 (92%)	19 (8%)	1 (0%)	34	69
5	CE	384/386 (100%)	349 (91%)	31 (8%)	4 (1%)	15	49
5	k	384/386 (100%)	348 (91%)	33 (9%)	3 (1%)	19	54
6	CF	359/361 (99%)	326 (91%)	33 (9%)	0	100	100
6	l	359/361 (99%)	320 (89%)	37 (10%)	2 (1%)	25	59
7	CG	294/296 (99%)	254 (86%)	38 (13%)	2 (1%)	22	57
7	m	294/296 (99%)	263 (90%)	30 (10%)	1 (0%)	41	73
8	CH	152/175 (87%)	139 (91%)	12 (8%)	1 (1%)	22	57
8	n	152/175 (87%)	145 (95%)	6 (4%)	1 (1%)	22	57
9	CI	220/222 (99%)	199 (90%)	16 (7%)	5 (2%)	6	28
9	o	220/222 (99%)	204 (93%)	13 (6%)	3 (1%)	11	40
10	CJ	231/233 (99%)	201 (87%)	28 (12%)	2 (1%)	17	52
10	p	231/233 (99%)	207 (90%)	24 (10%)	0	100	100
11	CK	189/191 (99%)	176 (93%)	13 (7%)	0	100	100
11	q	189/191 (99%)	168 (89%)	21 (11%)	0	100	100
12	CL	207/220 (94%)	188 (91%)	19 (9%)	0	100	100
12	r	207/220 (94%)	189 (91%)	17 (8%)	1 (0%)	29	64
13	CM	167/169 (99%)	145 (87%)	19 (11%)	3 (2%)	8	34
13	s	167/169 (99%)	137 (82%)	23 (14%)	7 (4%)	3	16
14	CN	191/193 (99%)	168 (88%)	17 (9%)	6 (3%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	t	191/193 (99%)	171 (90%)	13 (7%)	7 (4%)	3	19
15	CO	134/136 (98%)	122 (91%)	11 (8%)	1 (1%)	22	57
15	u	134/136 (98%)	120 (90%)	13 (10%)	1 (1%)	22	57
16	CP	201/203 (99%)	188 (94%)	13 (6%)	0	100	100
16	v	201/203 (99%)	177 (88%)	23 (11%)	1 (0%)	29	64
17	CQ	195/197 (99%)	185 (95%)	8 (4%)	2 (1%)	15	49
17	w	195/197 (99%)	187 (96%)	6 (3%)	2 (1%)	15	49
18	CR	181/183 (99%)	161 (89%)	17 (9%)	3 (2%)	9	36
18	x	181/183 (99%)	164 (91%)	17 (9%)	0	100	100
19	CS	183/185 (99%)	166 (91%)	16 (9%)	1 (0%)	29	64
19	y	183/185 (99%)	167 (91%)	16 (9%)	0	100	100
20	CT	186/188 (99%)	171 (92%)	15 (8%)	0	100	100
20	z	186/188 (99%)	175 (94%)	11 (6%)	0	100	100
21	0	170/172 (99%)	158 (93%)	11 (6%)	1 (1%)	25	59
21	CU	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
22	2	157/159 (99%)	142 (90%)	13 (8%)	2 (1%)	12	42
22	CV	157/159 (99%)	146 (93%)	10 (6%)	1 (1%)	25	59
23	5	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
23	CW	98/100 (98%)	81 (83%)	16 (16%)	1 (1%)	15	49
24	CX	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
24	IR	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
26	7	96/98 (98%)	83 (86%)	13 (14%)	0	100	100
26	CY	96/98 (98%)	79 (82%)	15 (16%)	2 (2%)	7	30
27	8	119/121 (98%)	108 (91%)	11 (9%)	0	100	100
27	CZ	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
28	9	124/126 (98%)	113 (91%)	11 (9%)	0	100	100
28	DA	124/126 (98%)	119 (96%)	5 (4%)	0	100	100
29	AA	133/135 (98%)	115 (86%)	15 (11%)	3 (2%)	6	28
29	DB	133/135 (98%)	119 (90%)	10 (8%)	4 (3%)	4	23
30	AB	146/148 (99%)	125 (86%)	19 (13%)	2 (1%)	11	40
30	DC	146/148 (99%)	123 (84%)	21 (14%)	2 (1%)	11	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	AC	56/58 (97%)	48 (86%)	8 (14%)	0	100	100
31	DD	56/58 (97%)	50 (89%)	5 (9%)	1 (2%)	8	34
32	AD	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
32	DE	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
33	AE	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	17	52
33	DF	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	17	52
34	AF	125/127 (98%)	116 (93%)	9 (7%)	0	100	100
34	DG	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
35	AG	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
35	DH	104/106 (98%)	99 (95%)	4 (4%)	1 (1%)	15	49
36	AH	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
36	DI	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
37	AI	117/119 (98%)	104 (89%)	12 (10%)	1 (1%)	17	52
37	DJ	117/119 (98%)	109 (93%)	7 (6%)	1 (1%)	17	52
38	AJ	97/99 (98%)	83 (86%)	11 (11%)	3 (3%)	4	23
38	DK	97/99 (98%)	84 (87%)	13 (13%)	0	100	100
39	AK	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
39	DL	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
40	AL	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
40	DM	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
41	AM	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
41	DN	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
42	AN	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
42	DO	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
43	AO	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
43	DP	23/25 (92%)	23 (100%)	0	0	100	100
44	AP	103/105 (98%)	84 (82%)	19 (18%)	0	100	100
44	DQ	103/105 (98%)	88 (85%)	15 (15%)	0	100	100
45	AQ	89/91 (98%)	79 (89%)	10 (11%)	0	100	100
45	DR	89/91 (98%)	82 (92%)	7 (8%)	0	100	100
46	i	155/272 (57%)	121 (78%)	30 (19%)	4 (3%)	5	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	sM	61/104 (59%)	45 (74%)	14 (23%)	2 (3%)	4	21
49	p0	139/311 (45%)	131 (94%)	8 (6%)	0	100	100
50	B	204/206 (99%)	157 (77%)	40 (20%)	7 (3%)	3	21
50	s0	204/206 (99%)	172 (84%)	30 (15%)	2 (1%)	15	49
51	C	212/216 (98%)	167 (79%)	43 (20%)	2 (1%)	17	52
51	s1	214/216 (99%)	190 (89%)	23 (11%)	1 (0%)	29	64
52	D	215/217 (99%)	189 (88%)	25 (12%)	1 (0%)	29	64
52	s2	215/217 (99%)	190 (88%)	23 (11%)	2 (1%)	17	52
53	E	221/223 (99%)	200 (90%)	19 (9%)	2 (1%)	17	52
53	s3	221/223 (99%)	195 (88%)	22 (10%)	4 (2%)	8	34
54	F	258/260 (99%)	233 (90%)	25 (10%)	0	100	100
54	s4	258/260 (99%)	229 (89%)	28 (11%)	1 (0%)	34	69
55	G	204/206 (99%)	166 (81%)	36 (18%)	2 (1%)	15	49
55	s5	204/206 (99%)	168 (82%)	36 (18%)	0	100	100
56	H	224/226 (99%)	202 (90%)	19 (8%)	3 (1%)	12	42
56	s6	216/226 (96%)	199 (92%)	15 (7%)	2 (1%)	17	52
57	I	182/186 (98%)	154 (85%)	25 (14%)	3 (2%)	9	37
57	s7	184/186 (99%)	158 (86%)	21 (11%)	5 (3%)	5	25
58	J	184/199 (92%)	159 (86%)	21 (11%)	4 (2%)	6	29
58	s8	184/199 (92%)	159 (86%)	23 (12%)	2 (1%)	14	46
59	K	183/185 (99%)	160 (87%)	21 (12%)	2 (1%)	14	46
59	s9	183/185 (99%)	161 (88%)	22 (12%)	0	100	100
60	L	94/105 (90%)	70 (74%)	23 (24%)	1 (1%)	14	46
60	c0	92/105 (88%)	61 (66%)	25 (27%)	6 (6%)	1	8
61	M	153/155 (99%)	137 (90%)	14 (9%)	2 (1%)	12	42
61	c1	144/155 (93%)	128 (89%)	15 (10%)	1 (1%)	22	57
62	N	122/124 (98%)	81 (66%)	33 (27%)	8 (7%)	1	7
62	c2	122/124 (98%)	81 (66%)	37 (30%)	4 (3%)	4	21
63	O	148/150 (99%)	137 (93%)	9 (6%)	2 (1%)	11	40
63	c3	148/150 (99%)	128 (86%)	14 (10%)	6 (4%)	3	16
64	P	125/128 (98%)	103 (82%)	21 (17%)	1 (1%)	19	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	c4	126/128 (98%)	110 (87%)	16 (13%)	0	100	100
65	Q	122/141 (86%)	100 (82%)	19 (16%)	3 (2%)	5	27
65	c5	133/141 (94%)	99 (74%)	27 (20%)	7 (5%)	2	12
66	R	139/142 (98%)	122 (88%)	16 (12%)	1 (1%)	22	57
66	c6	140/142 (99%)	124 (89%)	15 (11%)	1 (1%)	22	57
67	S	116/125 (93%)	93 (80%)	22 (19%)	1 (1%)	17	52
67	c7	113/125 (90%)	91 (80%)	21 (19%)	1 (1%)	17	52
68	T	143/145 (99%)	126 (88%)	16 (11%)	1 (1%)	22	57
68	c8	143/145 (99%)	121 (85%)	19 (13%)	3 (2%)	7	30
69	U	141/143 (99%)	127 (90%)	14 (10%)	0	100	100
69	c9	141/143 (99%)	130 (92%)	11 (8%)	0	100	100
70	V	105/110 (96%)	89 (85%)	15 (14%)	1 (1%)	15	49
70	d0	108/110 (98%)	92 (85%)	14 (13%)	2 (2%)	8	33
71	W	85/87 (98%)	62 (73%)	22 (26%)	1 (1%)	13	44
71	d1	85/87 (98%)	77 (91%)	7 (8%)	1 (1%)	13	44
72	X	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	54
72	d2	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
73	Y	142/144 (99%)	115 (81%)	24 (17%)	3 (2%)	7	30
73	d3	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
74	Z	132/134 (98%)	120 (91%)	10 (8%)	2 (2%)	10	39
74	d4	132/134 (98%)	114 (86%)	16 (12%)	2 (2%)	10	39
75	a	68/70 (97%)	51 (75%)	14 (21%)	3 (4%)	2	15
75	d5	67/70 (96%)	56 (84%)	11 (16%)	0	100	100
76	b	95/97 (98%)	66 (70%)	24 (25%)	5 (5%)	2	12
76	d6	95/97 (98%)	73 (77%)	20 (21%)	2 (2%)	7	30
77	c	79/81 (98%)	65 (82%)	14 (18%)	0	100	100
77	d7	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
78	d	61/63 (97%)	51 (84%)	10 (16%)	0	100	100
78	d8	61/63 (97%)	47 (77%)	14 (23%)	0	100	100
79	d9	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
79	e	51/53 (96%)	46 (90%)	5 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	e0	60/62 (97%)	52 (87%)	8 (13%)	0	100	100
80	f	58/62 (94%)	47 (81%)	10 (17%)	1 (2%)	9	36
81	g	69/71 (97%)	38 (55%)	31 (45%)	0	100	100
82	h	316/318 (99%)	277 (88%)	39 (12%)	0	100	100
82	sR	316/318 (99%)	285 (90%)	30 (10%)	1 (0%)	41	73
83	e1	49/51 (96%)	30 (61%)	18 (37%)	1 (2%)	7	31
All	All	22260/23067 (96%)	19629 (88%)	2417 (11%)	214 (1%)	15	49

All (214) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	l	339	LEU
13	s	74	PRO
13	s	95	ASN
13	s	172	LEU
14	t	47	ALA
14	t	63	VAL
15	u	8	LYS
29	AA	128	GLN
46	i	176	VAL
46	i	254	PRO
13	CM	173	ASP
14	CN	5	LYS
14	CN	47	ALA
14	CN	48	PRO
14	CN	63	VAL
51	C	62	LYS
51	C	181	LEU
55	G	57	SER
55	G	126	ASP
56	H	68	LEU
56	H	149	LYS
57	I	63	PRO
57	I	74	GLN
58	J	147	ALA
60	L	88	PRO
62	N	106	ILE
63	O	28	LEU
74	Z	52	LYS
53	s3	220	PRO

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Mol	Chain	Res	Type
56	s6	68	LEU
57	s7	63	PRO
57	s7	67	LEU
60	c0	88	PRO
60	c0	97	PRO
62	c2	130	THR
63	c3	66	ILE
65	c5	51	SER
65	c5	128	HIS
74	d4	52	LYS
5	k	347	SER
6	l	292	SER
9	o	158	LYS
14	t	77	LEU
17	w	111	PRO
30	AB	57	GLY
30	AB	78	LEU
37	AI	92	LEU
38	AJ	35	ASN
4	CD	144	ASN
5	CE	386	ASP
7	CG	20	PHE
9	CI	158	LYS
10	CJ	36	ILE
15	CO	8	LYS
19	CS	99	THR
29	DB	60	LYS
30	DC	78	LEU
35	DH	60	ARG
50	B	4	PRO
50	B	191	ARG
50	B	196	SER
61	M	4	GLU
62	N	109	GLU
62	N	112	ALA
63	O	27	LYS
64	P	42	VAL
65	Q	30	THR
73	Y	137	LYS
75	a	39	ALA
51	s1	107	THR
52	s2	106	ASP

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Mol	Chain	Res	Type
53	s3	216	PRO
53	s3	217	ILE
57	s7	74	GLN
58	s8	100	ALA
58	s8	101	ILE
60	c0	32	HIS
60	c0	35	ILE
62	c2	106	ILE
62	c2	131	ASP
76	d6	46	GLU
82	sR	281	TYR
7	m	259	LYS
9	o	191	VAL
13	s	94	ARG
14	t	48	PRO
14	t	166	ALA
38	AJ	77	LEU
46	i	86	ASN
7	CG	259	LYS
8	CH	98	VAL
9	CI	164	SER
9	CI	191	VAL
17	CQ	110	PRO
17	CQ	111	PRO
18	CR	159	LYS
30	DC	57	GLY
37	DJ	85	THR
48	sM	42	ALA
50	B	190	ASP
52	D	40	LYS
53	E	216	PRO
58	J	11	ARG
58	J	146	ARG
61	M	6	THR
62	N	85	LYS
62	N	108	ARG
62	N	126	TRP
62	N	130	THR
65	Q	125	PRO
71	W	11	LEU
76	b	63	ALA
60	c0	34	GLU

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Mol	Chain	Res	Type
63	c3	23	PRO
63	c3	65	VAL
65	c5	68	PRO
67	c7	67	ARG
68	c8	9	GLY
71	d1	11	LEU
4	j	250	GLN
9	o	164	SER
13	s	8	PRO
13	s	73	GLY
14	t	76	THR
17	w	110	PRO
5	CE	385	LYS
13	CM	172	LEU
18	CR	158	ALA
50	B	167	LYS
50	B	202	TYR
57	I	64	VAL
58	J	23	LYS
70	V	119	ALA
73	Y	98	GLU
75	a	38	HIS
76	b	61	GLU
76	b	85	ARG
57	s7	64	VAL
57	s7	66	SER
62	c2	109	GLU
63	c3	22	ALA
63	c3	140	LYS
65	c5	125	PRO
70	d0	73	GLY
76	d6	34	LYS
5	k	142	ALA
13	s	173	ASP
14	t	6	ASN
21	0	167	ARG
22	2	125	ALA
29	AA	102	GLU
29	AA	103	GLN
38	AJ	78	GLY
9	CI	25	GLN
9	CI	159	GLN

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Mol	Chain	Res	Type
14	CN	166	ALA
18	CR	160	ALA
26	CY	25	ASP
29	DB	59	ALA
29	DB	102	GLU
29	DB	103	GLN
48	sM	43	ASP
53	E	217	ILE
68	T	60	GLU
50	s0	31	VAL
50	s0	168	HIS
65	c5	135	THR
68	c8	8	GLN
33	AE	7	VAL
46	i	87	THR
10	CJ	122	LYS
13	CM	8	PRO
23	CW	52	ASN
26	CY	81	PRO
62	N	84	ASN
66	R	33	GLY
75	a	44	GLN
53	s3	221	SER
63	c3	139	TRP
65	c5	52	LYS
70	d0	52	LYS
83	e1	118	ARG
5	k	188	ILE
8	n	98	VAL
31	DD	21	ILE
33	DF	7	VAL
50	B	194	PRO
56	H	69	LEU
59	K	134	ILE
59	K	163	PRO
65	Q	126	VAL
76	b	9	GLY
52	s2	239	PRO
22	2	124	VAL
5	CE	188	ILE
14	CN	50	PRO
67	S	65	PRO

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Mol	Chain	Res	Type
72	X	67	GLY
76	b	60	PRO
80	f	60	PRO
61	c1	129	ARG
16	v	75	VAL
22	CV	124	VAL
73	Y	41	SER
74	Z	35	VAL
68	c8	14	ILE
74	d4	30	PRO
12	r	188	GLY
5	CE	317	ILE
54	s4	90	ILE
56	s6	70	PRO
66	c6	5	PRO
60	c0	92	ILE
65	c5	126	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	193/194 (100%)	169 (88%)	24 (12%)	4	19
4	j	193/194 (100%)	166 (86%)	27 (14%)	3	15
5	CE	319/322 (99%)	272 (85%)	47 (15%)	3	13
5	k	321/322 (100%)	274 (85%)	47 (15%)	3	13
6	CF	288/288 (100%)	256 (89%)	32 (11%)	6	24
6	l	288/288 (100%)	249 (86%)	39 (14%)	4	16
7	CG	244/244 (100%)	207 (85%)	37 (15%)	3	12
7	m	244/244 (100%)	216 (88%)	28 (12%)	5	22
8	CH	134/152 (88%)	116 (87%)	18 (13%)	4	16
8	n	134/152 (88%)	120 (90%)	14 (10%)	7	27
9	CI	186/186 (100%)	167 (90%)	19 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	o	186/186 (100%)	165 (89%)	21 (11%)	6	23
10	CJ	187/191 (98%)	172 (92%)	15 (8%)	12	40
10	p	187/191 (98%)	167 (89%)	20 (11%)	6	26
11	CK	171/171 (100%)	143 (84%)	28 (16%)	2	10
11	q	171/171 (100%)	148 (86%)	23 (14%)	4	16
12	CL	177/186 (95%)	151 (85%)	26 (15%)	3	13
12	r	177/186 (95%)	149 (84%)	28 (16%)	2	11
13	CM	147/147 (100%)	125 (85%)	22 (15%)	3	12
13	s	147/147 (100%)	127 (86%)	20 (14%)	3	16
14	CN	154/154 (100%)	128 (83%)	26 (17%)	2	9
14	t	154/154 (100%)	136 (88%)	18 (12%)	5	22
15	CO	107/107 (100%)	93 (87%)	14 (13%)	4	17
15	u	107/107 (100%)	89 (83%)	18 (17%)	2	9
16	CP	175/175 (100%)	160 (91%)	15 (9%)	10	37
16	v	175/175 (100%)	155 (89%)	20 (11%)	5	23
17	CQ	160/160 (100%)	144 (90%)	16 (10%)	7	28
17	w	160/160 (100%)	139 (87%)	21 (13%)	4	17
18	CR	140/145 (97%)	120 (86%)	20 (14%)	3	14
18	x	140/145 (97%)	118 (84%)	22 (16%)	2	11
19	CS	150/150 (100%)	128 (85%)	22 (15%)	3	13
19	y	150/150 (100%)	130 (87%)	20 (13%)	4	16
20	CT	153/153 (100%)	132 (86%)	21 (14%)	3	16
20	z	153/153 (100%)	140 (92%)	13 (8%)	10	37
21	0	156/156 (100%)	131 (84%)	25 (16%)	2	11
21	CU	156/156 (100%)	133 (85%)	23 (15%)	3	13
22	2	136/136 (100%)	116 (85%)	20 (15%)	3	13
22	CV	136/136 (100%)	112 (82%)	24 (18%)	2	8
23	5	87/87 (100%)	80 (92%)	7 (8%)	12	40
23	CW	87/87 (100%)	77 (88%)	10 (12%)	5	22
24	CX	104/104 (100%)	93 (89%)	11 (11%)	6	26
24	LR	104/104 (100%)	89 (86%)	15 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	7	57/86 (66%)	52 (91%)	5 (9%)	10	36
26	CY	57/86 (66%)	47 (82%)	10 (18%)	2	8
27	8	104/105 (99%)	91 (88%)	13 (12%)	4	18
27	CZ	104/105 (99%)	90 (86%)	14 (14%)	4	16
28	9	109/109 (100%)	95 (87%)	14 (13%)	4	18
28	DA	109/109 (100%)	95 (87%)	14 (13%)	4	18
29	AA	115/115 (100%)	104 (90%)	11 (10%)	8	31
29	DB	115/115 (100%)	104 (90%)	11 (10%)	8	31
30	AB	118/118 (100%)	106 (90%)	12 (10%)	7	27
30	DC	118/118 (100%)	103 (87%)	15 (13%)	4	18
31	AC	46/46 (100%)	40 (87%)	6 (13%)	4	18
31	DD	46/46 (100%)	39 (85%)	7 (15%)	3	12
32	AD	81/81 (100%)	70 (86%)	11 (14%)	3	16
32	DE	81/81 (100%)	76 (94%)	5 (6%)	18	49
33	AE	92/96 (96%)	80 (87%)	12 (13%)	4	18
33	DF	92/96 (96%)	75 (82%)	17 (18%)	1	7
34	AF	109/109 (100%)	94 (86%)	15 (14%)	3	16
34	DG	109/109 (100%)	96 (88%)	13 (12%)	5	20
35	AG	90/90 (100%)	81 (90%)	9 (10%)	7	28
35	DH	90/90 (100%)	83 (92%)	7 (8%)	12	40
36	AH	95/95 (100%)	84 (88%)	11 (12%)	5	22
36	DI	95/95 (100%)	85 (90%)	10 (10%)	7	26
37	AI	104/104 (100%)	92 (88%)	12 (12%)	5	22
37	DJ	104/104 (100%)	86 (83%)	18 (17%)	2	9
38	AJ	81/81 (100%)	69 (85%)	12 (15%)	3	13
38	DK	81/81 (100%)	71 (88%)	10 (12%)	4	19
39	AK	70/70 (100%)	63 (90%)	7 (10%)	7	28
39	DL	70/70 (100%)	59 (84%)	11 (16%)	2	11
40	AL	68/68 (100%)	58 (85%)	10 (15%)	3	13
40	DM	68/68 (100%)	61 (90%)	7 (10%)	7	27
41	AM	45/45 (100%)	38 (84%)	7 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DN	45/45 (100%)	41 (91%)	4 (9%)	9	34
42	AN	47/47 (100%)	39 (83%)	8 (17%)	2	9
42	DO	47/47 (100%)	42 (89%)	5 (11%)	6	26
43	AO	23/23 (100%)	20 (87%)	3 (13%)	4	18
43	DP	23/23 (100%)	19 (83%)	4 (17%)	2	9
44	AP	90/90 (100%)	82 (91%)	8 (9%)	9	34
44	DQ	90/90 (100%)	81 (90%)	9 (10%)	7	28
45	AQ	71/71 (100%)	59 (83%)	12 (17%)	2	9
45	DR	71/71 (100%)	63 (89%)	8 (11%)	6	23
46	i	97/227 (43%)	82 (84%)	15 (16%)	2	11
48	sM	54/54 (100%)	47 (87%)	7 (13%)	4	18
49	p0	105/253 (42%)	91 (87%)	14 (13%)	4	16
50	B	164/173 (95%)	146 (89%)	18 (11%)	6	25
50	s0	165/173 (95%)	140 (85%)	25 (15%)	3	12
51	C	191/192 (100%)	167 (87%)	24 (13%)	4	18
51	s1	192/192 (100%)	164 (85%)	28 (15%)	3	13
52	D	176/176 (100%)	151 (86%)	25 (14%)	3	14
52	s2	176/176 (100%)	144 (82%)	32 (18%)	1	7
53	E	182/182 (100%)	159 (87%)	23 (13%)	4	18
53	s3	182/182 (100%)	164 (90%)	18 (10%)	8	29
54	F	221/221 (100%)	196 (89%)	25 (11%)	6	23
54	s4	221/221 (100%)	200 (90%)	21 (10%)	8	31
55	G	173/173 (100%)	153 (88%)	20 (12%)	5	22
55	s5	173/173 (100%)	155 (90%)	18 (10%)	7	27
56	H	188/193 (97%)	163 (87%)	25 (13%)	4	16
56	s6	187/193 (97%)	163 (87%)	24 (13%)	4	18
57	I	165/166 (99%)	146 (88%)	19 (12%)	5	22
57	s7	165/166 (99%)	145 (88%)	20 (12%)	5	20
58	J	150/160 (94%)	139 (93%)	11 (7%)	14	43
58	s8	150/160 (94%)	140 (93%)	10 (7%)	16	46
59	K	158/158 (100%)	134 (85%)	24 (15%)	3	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	s9	158/158 (100%)	129 (82%)	29 (18%)	1	7
60	L	77/98 (79%)	68 (88%)	9 (12%)	5	22
60	c0	73/98 (74%)	65 (89%)	8 (11%)	6	25
61	M	129/136 (95%)	120 (93%)	9 (7%)	15	45
61	c1	129/136 (95%)	113 (88%)	16 (12%)	4	19
62	N	88/100 (88%)	73 (83%)	15 (17%)	2	9
62	c2	88/100 (88%)	73 (83%)	15 (17%)	2	9
63	O	127/127 (100%)	110 (87%)	17 (13%)	4	16
63	c3	127/127 (100%)	111 (87%)	16 (13%)	4	18
64	P	81/97 (84%)	70 (86%)	11 (14%)	3	16
64	c4	97/97 (100%)	85 (88%)	12 (12%)	4	19
65	Q	101/117 (86%)	92 (91%)	9 (9%)	9	34
65	c5	103/117 (88%)	91 (88%)	12 (12%)	5	22
66	R	117/118 (99%)	101 (86%)	16 (14%)	3	16
66	c6	118/118 (100%)	98 (83%)	20 (17%)	2	9
67	S	94/113 (83%)	80 (85%)	14 (15%)	3	13
67	c7	92/113 (81%)	81 (88%)	11 (12%)	5	20
68	T	128/128 (100%)	108 (84%)	20 (16%)	2	11
68	c8	128/128 (100%)	109 (85%)	19 (15%)	3	13
69	U	115/115 (100%)	95 (83%)	20 (17%)	2	9
69	c9	115/115 (100%)	99 (86%)	16 (14%)	3	15
70	V	100/103 (97%)	86 (86%)	14 (14%)	3	15
70	d0	103/103 (100%)	90 (87%)	13 (13%)	4	18
71	W	74/74 (100%)	62 (84%)	12 (16%)	2	10
71	d1	74/74 (100%)	63 (85%)	11 (15%)	3	13
72	X	110/110 (100%)	95 (86%)	15 (14%)	3	16
72	d2	110/110 (100%)	103 (94%)	7 (6%)	17	48
73	Y	119/119 (100%)	102 (86%)	17 (14%)	3	14
73	d3	119/119 (100%)	104 (87%)	15 (13%)	4	18
74	Z	112/112 (100%)	101 (90%)	11 (10%)	8	29
74	d4	112/112 (100%)	105 (94%)	7 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	a	61/61 (100%)	49 (80%)	12 (20%)	1	6
75	d5	61/61 (100%)	58 (95%)	3 (5%)	25	57
76	b	83/83 (100%)	76 (92%)	7 (8%)	11	38
76	d6	83/83 (100%)	71 (86%)	12 (14%)	3	13
77	c	70/70 (100%)	67 (96%)	3 (4%)	29	62
77	d7	70/70 (100%)	65 (93%)	5 (7%)	14	44
78	d	56/56 (100%)	48 (86%)	8 (14%)	3	14
78	d8	56/56 (100%)	47 (84%)	9 (16%)	2	10
79	d9	47/47 (100%)	43 (92%)	4 (8%)	10	37
79	e	47/47 (100%)	42 (89%)	5 (11%)	6	26
80	e0	53/53 (100%)	45 (85%)	8 (15%)	3	12
80	f	51/53 (96%)	47 (92%)	4 (8%)	12	40
81	g	62/62 (100%)	50 (81%)	12 (19%)	1	6
82	h	260/261 (100%)	243 (94%)	17 (6%)	17	47
82	sR	260/261 (100%)	242 (93%)	18 (7%)	15	45
83	e1	43/43 (100%)	35 (81%)	8 (19%)	1	7
All	All	18684/19337 (97%)	16334 (87%)	2350 (13%)	4	18

All (2350) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	j	20	THR
4	j	23	ARG
4	j	32	LEU
4	j	44	ILE
4	j	45	VAL
4	j	48	ILE
4	j	49	VAL
4	j	62	VAL
4	j	72	ARG
4	j	74	GLU
4	j	84	THR
4	j	96	LEU
4	j	101	VAL
4	j	104	LEU
4	j	119	LYS

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Mol	Chain	Res	Type
4	j	157	VAL
4	j	165	VAL
4	j	179	LEU
4	j	180	LEU
4	j	202	VAL
4	j	204	MET
4	j	207	VAL
4	j	226	SER
4	j	227	ARG
4	j	230	VAL
4	j	231	SER
4	j	247	ARG
5	k	4	ARG
5	k	7	GLU
5	k	10	ARG
5	k	17	LEU
5	k	19	ARG
5	k	25	ILE
5	k	37	ARG
5	k	47	LEU
5	k	69	LYS
5	k	73	VAL
5	k	79	VAL
5	k	84	VAL
5	k	85	VAL
5	k	103	THR
5	k	114	VAL
5	k	139	GLN
5	k	148	LEU
5	k	150	ARG
5	k	156	SER
5	k	169	THR
5	k	183	LEU
5	k	188	ILE
5	k	192	VAL
5	k	196	ARG
5	k	202	THR
5	k	210	GLU
5	k	212	ASN
5	k	229	VAL
5	k	235	THR
5	k	238	LEU

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Mol	Chain	Res	Type
5	k	241	LYS
5	k	244	ARG
5	k	252	ILE
5	k	261	MET
5	k	264	VAL
5	k	284	ARG
5	k	291	GLU
5	k	296	THR
5	k	300	ARG
5	k	305	ILE
5	k	320	ASP
5	k	324	VAL
5	k	325	LYS
5	k	332	ARG
5	k	338	LEU
5	k	352	GLU
5	k	361	THR
6	l	22	LEU
6	l	71	VAL
6	l	73	ARG
6	l	74	ILE
6	l	93	MET
6	l	98	ARG
6	l	103	THR
6	l	112	LYS
6	l	120	TYR
6	l	133	SER
6	l	138	ARG
6	l	150	LEU
6	l	156	LEU
6	l	161	LYS
6	l	163	LYS
6	l	172	VAL
6	l	177	ASP
6	l	179	LEU
6	l	187	LEU
6	l	188	ARG
6	l	193	LYS
6	l	200	THR
6	l	203	ARG
6	l	206	LEU
6	l	220	ARG

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Mol	Chain	Res	Type
6	l	222	VAL
6	l	230	VAL
6	l	246	ARG
6	l	258	LEU
6	l	267	VAL
6	l	287	THR
6	l	308	LYS
6	l	313	LEU
6	l	323	VAL
6	l	327	LEU
6	l	333	VAL
6	l	338	LYS
6	l	339	LEU
6	l	349	THR
7	m	5	LYS
7	m	8	LYS
7	m	23	ARG
7	m	35	ARG
7	m	41	LYS
7	m	67	SER
7	m	75	LEU
7	m	93	THR
7	m	105	ILE
7	m	113	LEU
7	m	115	LEU
7	m	118	THR
7	m	131	LEU
7	m	137	ASP
7	m	140	ARG
7	m	144	VAL
7	m	146	LEU
7	m	148	ILE
7	m	152	ARG
7	m	155	THR
7	m	163	LEU
7	m	177	GLU
7	m	185	PHE
7	m	216	GLU
7	m	217	GLU
7	m	222	LEU
7	m	231	ILE
7	m	234	ASP

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Mol	Chain	Res	Type
8	n	2	SER
8	n	5	LYS
8	n	21	THR
8	n	35	VAL
8	n	52	VAL
8	n	64	LEU
8	n	78	ARG
8	n	79	VAL
8	n	84	VAL
8	n	88	SER
8	n	98	VAL
8	n	134	ARG
8	n	152	THR
8	n	155	LEU
9	o	24	GLU
9	o	25	GLN
9	o	26	VAL
9	o	45	LEU
9	o	60	ARG
9	o	80	GLN
9	o	82	LYS
9	o	83	LEU
9	o	88	ARG
9	o	93	ASN
9	o	101	LYS
9	o	110	ARG
9	o	121	LYS
9	o	124	LEU
9	o	157	ASN
9	o	158	LYS
9	o	164	SER
9	o	175	LYS
9	o	179	LEU
9	o	184	LEU
9	o	239	LEU
10	p	26	LEU
10	p	27	THR
10	p	50	VAL
10	p	57	ARG
10	p	71	VAL
10	p	74	THR
10	p	79	GLN

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Mol	Chain	Res	Type
10	p	81	THR
10	p	84	ARG
10	p	106	LYS
10	p	110	THR
10	p	136	LEU
10	p	145	ASN
10	p	156	ASP
10	p	163	VAL
10	p	169	LEU
10	p	185	ARG
10	p	194	THR
10	p	206	GLU
10	p	248	LYS
11	q	5	GLN
11	q	6	THR
11	q	18	VAL
11	q	19	SER
11	q	41	ILE
11	q	42	ASP
11	q	44	THR
11	q	48	VAL
11	q	52	LEU
11	q	55	VAL
11	q	68	LEU
11	q	69	ARG
11	q	70	THR
11	q	129	ARG
11	q	132	VAL
11	q	133	THR
11	q	139	ASN
11	q	151	VAL
11	q	157	ASN
11	q	161	LEU
11	q	162	GLN
11	q	172	ILE
11	q	173	ARG
12	r	3	ARG
12	r	21	ARG
12	r	24	ARG
12	r	26	VAL
12	r	30	LYS
12	r	32	ARG

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Mol	Chain	Res	Type
12	r	35	ASP
12	r	39	LYS
12	r	40	LYS
12	r	42	THR
12	r	52	LEU
12	r	63	GLU
12	r	87	LEU
12	r	91	VAL
12	r	130	ASP
12	r	138	VAL
12	r	139	ARG
12	r	140	THR
12	r	142	ASP
12	r	148	VAL
12	r	163	GLN
12	r	165	ILE
12	r	169	LYS
12	r	174	THR
12	r	176	LEU
12	r	177	ASP
12	r	190	VAL
12	r	203	LYS
13	s	9	MET
13	s	10	ARG
13	s	11	ASP
13	s	12	LEU
13	s	31	THR
13	s	46	VAL
13	s	47	GLN
13	s	63	GLU
13	s	70	THR
13	s	80	LEU
13	s	82	ARG
13	s	94	ARG
13	s	95	ASN
13	s	106	ILE
13	s	107	ASP
13	s	112	LEU
13	s	115	LYS
13	s	138	VAL
13	s	140	ARG
13	s	158	ASP

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Mol	Chain	Res	Type
14	t	13	HIS
14	t	23	LYS
14	t	24	VAL
14	t	34	SER
14	t	54	LEU
14	t	55	ARG
14	t	59	ARG
14	t	64	LYS
14	t	67	ARG
14	t	69	VAL
14	t	85	LEU
14	t	104	ARG
14	t	114	GLN
14	t	122	LYS
14	t	131	LYS
14	t	164	GLU
14	t	168	ARG
14	t	171	ARG
15	u	3	THR
15	u	5	SER
15	u	10	SER
15	u	15	VAL
15	u	27	GLN
15	u	38	ILE
15	u	50	LYS
15	u	53	VAL
15	u	58	ILE
15	u	63	VAL
15	u	66	THR
15	u	69	THR
15	u	90	VAL
15	u	91	CYS
15	u	102	LYS
15	u	107	GLU
15	u	135	LEU
15	u	137	LYS
16	v	10	LEU
16	v	15	GLN
16	v	19	LEU
16	v	22	LEU
16	v	38	ARG
16	v	49	ARG

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Mol	Chain	Res	Type
16	v	50	ARG
16	v	80	THR
16	v	85	THR
16	v	96	ARG
16	v	106	VAL
16	v	109	ARG
16	v	117	ASN
16	v	132	VAL
16	v	133	ILE
16	v	151	ILE
16	v	182	ASN
16	v	183	THR
16	v	187	ARG
16	v	201	ARG
17	w	22	VAL
17	w	34	VAL
17	w	68	ARG
17	w	78	ARG
17	w	84	LEU
17	w	85	ARG
17	w	106	GLU
17	w	116	LYS
17	w	117	ARG
17	w	122	GLN
17	w	124	LEU
17	w	126	VAL
17	w	128	ARG
17	w	129	LEU
17	w	143	THR
17	w	160	ARG
17	w	161	LYS
17	w	180	SER
17	w	184	THR
17	w	188	SER
17	w	190	VAL
18	x	13	LYS
18	x	16	SER
18	x	20	SER
18	x	23	ARG
18	x	24	VAL
18	x	29	THR
18	x	32	THR

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Mol	Chain	Res	Type
18	x	36	ILE
18	x	41	LEU
18	x	49	GLU
18	x	52	LEU
18	x	53	ASP
18	x	69	ARG
18	x	94	LEU
18	x	103	GLU
18	x	112	LEU
18	x	119	VAL
18	x	127	ARG
18	x	142	SER
18	x	168	LEU
18	x	180	LYS
18	x	181	ARG
19	y	3	ILE
19	y	7	SER
19	y	17	THR
19	y	22	ASP
19	y	24	VAL
19	y	26	LEU
19	y	32	LEU
19	y	39	ARG
19	y	41	ASP
19	y	49	LEU
19	y	57	ILE
19	y	66	ARG
19	y	69	ARG
19	y	74	GLU
19	y	81	VAL
19	y	115	VAL
19	y	135	GLN
19	y	138	LEU
19	y	150	VAL
19	y	170	ARG
20	z	29	THR
20	z	44	LEU
20	z	51	VAL
20	z	57	VAL
20	z	60	LYS
20	z	74	ARG
20	z	91	SER

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Mol	Chain	Res	Type
20	z	103	ARG
20	z	104	ARG
20	z	115	ILE
20	z	171	ASP
20	z	175	GLN
20	z	177	VAL
21	0	1	MET
21	0	16	THR
21	0	45	LEU
21	0	49	HIS
21	0	50	LYS
21	0	61	ILE
21	0	71	LYS
21	0	73	LYS
21	0	80	ARG
21	0	85	SER
21	0	87	THR
21	0	105	THR
21	0	115	ARG
21	0	117	ARG
21	0	122	HIS
21	0	131	LYS
21	0	132	THR
21	0	136	LYS
21	0	137	ARG
21	0	155	ARG
21	0	157	GLN
21	0	160	THR
21	0	162	THR
21	0	167	ARG
21	0	172	TYR
22	2	12	ARG
22	2	18	ASP
22	2	25	VAL
22	2	27	LEU
22	2	32	LYS
22	2	52	MET
22	2	75	ILE
22	2	78	LYS
22	2	79	MET
22	2	80	VAL
22	2	83	ARG

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Mol	Chain	Res	Type
22	2	88	ARG
22	2	96	ILE
22	2	103	GLN
22	2	122	GLN
22	2	126	VAL
22	2	128	LEU
22	2	139	ARG
22	2	143	THR
22	2	160	ILE
23	5	10	LYS
23	5	35	LYS
23	5	52	ASN
23	5	66	VAL
23	5	93	ILE
23	5	100	THR
23	5	104	ARG
24	1R	12	ARG
24	1R	13	ILE
24	1R	14	SER
24	1R	32	ARG
24	1R	45	ARG
24	1R	48	ARG
24	1R	63	LYS
24	1R	64	LYS
24	1R	69	LEU
24	1R	72	LYS
24	1R	83	LYS
24	1R	102	ILE
24	1R	106	LYS
24	1R	115	THR
24	1R	120	LYS
26	7	4	GLU
26	7	5	ILE
26	7	19	THR
26	7	39	LEU
26	7	64	THR
27	8	27	ARG
27	8	28	THR
27	8	36	LYS
27	8	63	ILE
27	8	92	LYS
27	8	104	GLU

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Mol	Chain	Res	Type
27	8	108	LEU
27	8	115	ARG
27	8	125	ARG
27	8	129	ASP
27	8	135	ILE
27	8	139	ILE
27	8	142	ILE
28	9	5	SER
28	9	13	ARG
28	9	37	LYS
28	9	38	GLU
28	9	40	ARG
28	9	45	ILE
28	9	56	VAL
28	9	60	ARG
28	9	64	LYS
28	9	67	GLU
28	9	74	TYR
28	9	105	VAL
28	9	113	LYS
28	9	115	ARG
29	AA	14	VAL
29	AA	24	VAL
29	AA	46	ILE
29	AA	52	LYS
29	AA	81	LEU
29	AA	83	THR
29	AA	90	GLU
29	AA	102	GLU
29	AA	103	GLN
29	AA	107	ARG
29	AA	109	GLU
30	AB	4	ARG
30	AB	8	THR
30	AB	42	ARG
30	AB	46	ASP
30	AB	60	TYR
30	AB	76	ASP
30	AB	78	LEU
30	AB	88	ASP
30	AB	92	LYS
30	AB	115	LYS

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Mol	Chain	Res	Type
30	AB	120	ASN
30	AB	135	GLU
31	AC	13	THR
31	AC	14	ARG
31	AC	25	LYS
31	AC	31	SER
31	AC	50	THR
31	AC	59	LYS
32	AD	14	LEU
32	AD	16	LEU
32	AD	18	ILE
32	AD	34	LEU
32	AD	54	SER
32	AD	61	MET
32	AD	76	GLU
32	AD	99	ASP
32	AD	101	LEU
32	AD	103	THR
32	AD	104	LEU
33	AE	8	VAL
33	AE	16	LEU
33	AE	26	LYS
33	AE	31	ARG
33	AE	55	LEU
33	AE	79	ARG
33	AE	86	LYS
33	AE	96	VAL
33	AE	100	SER
33	AE	106	THR
33	AE	107	VAL
33	AE	110	GLU
34	AF	14	THR
34	AF	16	LYS
34	AF	19	ARG
34	AF	27	ARG
34	AF	33	ARG
34	AF	44	ARG
34	AF	51	SER
34	AF	61	LYS
34	AF	62	LYS
34	AF	73	THR
34	AF	89	THR

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Mol	Chain	Res	Type
34	AF	106	VAL
34	AF	109	LEU
34	AF	111	ARG
34	AF	128	LEU
35	AG	15	SER
35	AG	20	LYS
35	AG	22	VAL
35	AG	49	ILE
35	AG	59	VAL
35	AG	70	LYS
35	AG	81	VAL
35	AG	98	VAL
35	AG	105	SER
36	AH	8	ARG
36	AH	20	ILE
36	AH	24	LYS
36	AH	29	ILE
36	AH	31	ARG
36	AH	51	LEU
36	AH	58	ARG
36	AH	65	VAL
36	AH	71	THR
36	AH	102	LYS
36	AH	104	VAL
37	AI	15	GLU
37	AI	20	GLN
37	AI	21	LEU
37	AI	30	GLU
37	AI	31	LEU
37	AI	46	THR
37	AI	84	LYS
37	AI	89	ARG
37	AI	90	ARG
37	AI	92	LEU
37	AI	96	GLU
37	AI	101	THR
38	AJ	11	LEU
38	AJ	18	THR
38	AJ	25	LYS
38	AJ	26	ILE
38	AJ	34	SER
38	AJ	45	ARG

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Mol	Chain	Res	Type
38	AJ	57	LEU
38	AJ	60	LEU
38	AJ	62	ARG
38	AJ	68	ARG
38	AJ	88	GLU
38	AJ	90	MET
39	AK	24	ARG
39	AK	25	ARG
39	AK	33	THR
39	AK	58	THR
39	AK	59	THR
39	AK	67	LEU
39	AK	82	SER
40	AL	5	ILE
40	AL	24	THR
40	AL	32	ASN
40	AL	46	ARG
40	AL	53	THR
40	AL	65	LEU
40	AL	67	GLN
40	AL	69	LEU
40	AL	77	ARG
40	AL	78	LEU
41	AM	4	GLN
41	AM	10	LYS
41	AM	21	ARG
41	AM	34	THR
41	AM	36	ARG
41	AM	45	ARG
41	AM	51	ILE
42	AN	77	ILE
42	AN	83	LYS
42	AN	85	LEU
42	AN	112	LYS
42	AN	113	ARG
42	AN	114	LYS
42	AN	126	LYS
42	AN	127	LEU
43	AO	2	ARG
43	AO	11	ARG
43	AO	13	LEU
44	AP	2	VAL

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Mol	Chain	Res	Type
44	AP	8	ARG
44	AP	26	THR
44	AP	35	LEU
44	AP	78	LYS
44	AP	83	LEU
44	AP	84	THR
44	AP	104	LEU
45	AQ	11	THR
45	AQ	16	VAL
45	AQ	25	GLN
45	AQ	45	LYS
45	AQ	46	THR
45	AQ	49	ARG
45	AQ	56	THR
45	AQ	59	CYS
45	AQ	60	CYS
45	AQ	84	ARG
45	AQ	90	VAL
45	AQ	91	GLU
46	i	34	LYS
46	i	46	LYS
46	i	68	ARG
46	i	75	ASP
46	i	77	THR
46	i	84	LYS
46	i	91	THR
46	i	96	ARG
46	i	97	THR
46	i	100	THR
46	i	102	THR
46	i	116	GLU
46	i	130	GLU
46	i	131	ILE
46	i	134	ASP
4	CD	10	LYS
4	CD	19	HIS
4	CD	20	THR
4	CD	32	LEU
4	CD	44	ILE
4	CD	45	VAL
4	CD	48	ILE
4	CD	62	VAL

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Mol	Chain	Res	Type
4	CD	64	ARG
4	CD	70	ARG
4	CD	82	VAL
4	CD	96	LEU
4	CD	101	VAL
4	CD	137	ILE
4	CD	142	ASP
4	CD	149	ARG
4	CD	179	LEU
4	CD	180	LEU
4	CD	204	MET
4	CD	207	VAL
4	CD	227	ARG
4	CD	230	VAL
4	CD	250	GLN
4	CD	252	THR
5	CE	2	SER
5	CE	7	GLU
5	CE	17	LEU
5	CE	25	ILE
5	CE	30	LYS
5	CE	37	ARG
5	CE	47	LEU
5	CE	55	THR
5	CE	56	ILE
5	CE	73	VAL
5	CE	79	VAL
5	CE	84	VAL
5	CE	100	ARG
5	CE	103	THR
5	CE	111	SER
5	CE	114	VAL
5	CE	146	ARG
5	CE	156	SER
5	CE	167	ARG
5	CE	169	THR
5	CE	173	GLN
5	CE	183	LEU
5	CE	188	ILE
5	CE	192	VAL
5	CE	196	ARG
5	CE	202	THR

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Mol	Chain	Res	Type
5	CE	205	VAL
5	CE	212	ASN
5	CE	222	LYS
5	CE	232	ARG
5	CE	235	THR
5	CE	284	ARG
5	CE	296	THR
5	CE	305	ILE
5	CE	308	MET
5	CE	316	GLU
5	CE	324	VAL
5	CE	325	LYS
5	CE	328	ILE
5	CE	332	ARG
5	CE	338	LEU
5	CE	347	SER
5	CE	349	LYS
5	CE	364	LYS
5	CE	382	THR
5	CE	386	ASP
5	CE	387	LEU
6	CF	53	SER
6	CF	73	ARG
6	CF	74	ILE
6	CF	85	SER
6	CF	93	MET
6	CF	99	MET
6	CF	118	LYS
6	CF	120	TYR
6	CF	138	ARG
6	CF	150	LEU
6	CF	156	LEU
6	CF	170	LYS
6	CF	177	ASP
6	CF	179	LEU
6	CF	187	LEU
6	CF	201	GLN
6	CF	203	ARG
6	CF	206	LEU
6	CF	220	ARG
6	CF	222	VAL
6	CF	230	VAL

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Mol	Chain	Res	Type
6	CF	246	ARG
6	CF	307	GLN
6	CF	313	LEU
6	CF	316	ASN
6	CF	319	LYS
6	CF	323	VAL
6	CF	327	LEU
6	CF	332	LYS
6	CF	333	VAL
6	CF	343	LYS
6	CF	346	LYS
7	CG	5	LYS
7	CG	23	ARG
7	CG	35	ARG
7	CG	41	LYS
7	CG	63	GLN
7	CG	69	ILE
7	CG	70	THR
7	CG	75	LEU
7	CG	89	THR
7	CG	92	LEU
7	CG	95	TRP
7	CG	105	ILE
7	CG	107	ARG
7	CG	110	LEU
7	CG	113	LEU
7	CG	115	LEU
7	CG	118	THR
7	CG	126	GLU
7	CG	131	LEU
7	CG	140	ARG
7	CG	144	VAL
7	CG	146	LEU
7	CG	148	ILE
7	CG	151	GLN
7	CG	152	ARG
7	CG	155	THR
7	CG	173	VAL
7	CG	185	PHE
7	CG	188	GLU
7	CG	189	GLU
7	CG	190	ILE

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Mol	Chain	Res	Type
7	CG	194	LEU
7	CG	211	LEU
7	CG	222	LEU
7	CG	234	ASP
7	CG	261	THR
7	CG	293	LEU
8	CH	8	LYS
8	CH	14	ASP
8	CH	15	VAL
8	CH	21	THR
8	CH	35	VAL
8	CH	48	ARG
8	CH	52	VAL
8	CH	64	LEU
8	CH	65	ILE
8	CH	79	VAL
8	CH	88	SER
8	CH	89	THR
8	CH	93	VAL
8	CH	129	GLU
8	CH	134	ARG
8	CH	140	VAL
8	CH	152	THR
8	CH	155	LEU
9	CI	24	GLU
9	CI	25	GLN
9	CI	45	LEU
9	CI	57	THR
9	CI	60	ARG
9	CI	77	VAL
9	CI	82	LYS
9	CI	83	LEU
9	CI	89	ILE
9	CI	92	ILE
9	CI	98	LYS
9	CI	111	ILE
9	CI	121	LYS
9	CI	124	LEU
9	CI	179	LEU
9	CI	180	SER
9	CI	181	ILE
9	CI	184	LEU

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Mol	Chain	Res	Type
9	CI	239	LEU
10	CJ	50	VAL
10	CJ	71	VAL
10	CJ	74	THR
10	CJ	79	GLN
10	CJ	81	THR
10	CJ	84	ARG
10	CJ	85	ASN
10	CJ	136	LEU
10	CJ	160	ILE
10	CJ	163	VAL
10	CJ	169	LEU
10	CJ	185	ARG
10	CJ	197	VAL
10	CJ	203	VAL
10	CJ	248	LYS
11	CK	5	GLN
11	CK	16	VAL
11	CK	18	VAL
11	CK	33	THR
11	CK	41	ILE
11	CK	48	VAL
11	CK	52	LEU
11	CK	62	ARG
11	CK	68	LEU
11	CK	69	ARG
11	CK	70	THR
11	CK	82	VAL
11	CK	92	TYR
11	CK	102	ASN
11	CK	121	LYS
11	CK	122	LYS
11	CK	129	ARG
11	CK	132	VAL
11	CK	133	THR
11	CK	151	VAL
11	CK	157	ASN
11	CK	161	LEU
11	CK	162	GLN
11	CK	164	ILE
11	CK	166	ARG
11	CK	172	ILE

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Mol	Chain	Res	Type
11	CK	173	ARG
11	CK	190	ASP
12	CL	3	ARG
12	CL	24	ARG
12	CL	28	ASP
12	CL	30	LYS
12	CL	32	ARG
12	CL	33	ILE
12	CL	40	LYS
12	CL	42	THR
12	CL	52	LEU
12	CL	57	LEU
12	CL	58	GLU
12	CL	63	GLU
12	CL	71	CYS
12	CL	74	LYS
12	CL	77	THR
12	CL	87	LEU
12	CL	91	VAL
12	CL	139	ARG
12	CL	153	ARG
12	CL	165	ILE
12	CL	169	LYS
12	CL	185	ARG
12	CL	197	VAL
12	CL	206	LEU
12	CL	208	ASN
12	CL	212	GLU
13	CM	9	MET
13	CM	10	ARG
13	CM	12	LEU
13	CM	29	ARG
13	CM	40	LEU
13	CM	44	THR
13	CM	56	THR
13	CM	80	LEU
13	CM	82	ARG
13	CM	106	ILE
13	CM	107	ASP
13	CM	112	LEU
13	CM	115	LYS
13	CM	130	VAL

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Mol	Chain	Res	Type
13	CM	137	ARG
13	CM	140	ARG
13	CM	142	LYS
13	CM	145	LYS
13	CM	147	THR
13	CM	168	ASP
13	CM	171	VAL
13	CM	172	LEU
14	CN	4	SER
14	CN	5	LYS
14	CN	23	LYS
14	CN	42	ARG
14	CN	52	ASP
14	CN	53	LEU
14	CN	54	LEU
14	CN	55	ARG
14	CN	57	VAL
14	CN	58	VAL
14	CN	59	ARG
14	CN	63	VAL
14	CN	67	ARG
14	CN	69	VAL
14	CN	85	LEU
14	CN	107	GLU
14	CN	118	GLU
14	CN	124	ILE
14	CN	128	ARG
14	CN	131	LYS
14	CN	153	ASP
14	CN	154	VAL
14	CN	164	GLU
14	CN	165	SER
14	CN	168	ARG
14	CN	171	ARG
15	CO	4	ASP
15	CO	5	SER
15	CO	8	LYS
15	CO	15	VAL
15	CO	38	ILE
15	CO	45	LEU
15	CO	53	VAL
15	CO	63	VAL

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Mol	Chain	Res	Type
15	CO	66	THR
15	CO	90	VAL
15	CO	121	MET
15	CO	123	LEU
15	CO	124	ARG
15	CO	130	THR
16	CP	10	LEU
16	CP	17	ASP
16	CP	20	ARG
16	CP	22	LEU
16	CP	68	ARG
16	CP	80	THR
16	CP	85	THR
16	CP	133	ILE
16	CP	138	GLN
16	CP	151	ILE
16	CP	153	ASP
16	CP	182	ASN
16	CP	183	THR
16	CP	190	THR
16	CP	198	SER
17	CQ	41	LEU
17	CQ	58	LEU
17	CQ	67	THR
17	CQ	74	ARG
17	CQ	78	ARG
17	CQ	85	ARG
17	CQ	106	GLU
17	CQ	110	PRO
17	CQ	115	LYS
17	CQ	117	ARG
17	CQ	124	LEU
17	CQ	126	VAL
17	CQ	128	ARG
17	CQ	129	LEU
17	CQ	134	LYS
17	CQ	180	SER
18	CR	7	THR
18	CR	9	THR
18	CR	24	VAL
18	CR	32	THR
18	CR	42	THR

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Mol	Chain	Res	Type
18	CR	49	GLU
18	CR	52	LEU
18	CR	56	ARG
18	CR	70	THR
18	CR	78	VAL
18	CR	111	LYS
18	CR	112	LEU
18	CR	114	VAL
18	CR	119	VAL
18	CR	128	ARG
18	CR	144	SER
18	CR	166	VAL
18	CR	168	LEU
18	CR	171	ARG
18	CR	175	ARG
19	CS	3	ILE
19	CS	7	SER
19	CS	11	LYS
19	CS	17	THR
19	CS	24	VAL
19	CS	26	LEU
19	CS	32	LEU
19	CS	41	ASP
19	CS	49	LEU
19	CS	69	ARG
19	CS	80	THR
19	CS	81	VAL
19	CS	82	VAL
19	CS	86	THR
19	CS	93	ILE
19	CS	113	LYS
19	CS	135	GLN
19	CS	138	LEU
19	CS	150	VAL
19	CS	170	ARG
19	CS	180	ARG
19	CS	181	SER
20	CT	5	ARG
20	CT	10	LEU
20	CT	17	VAL
20	CT	22	VAL
20	CT	30	SER

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Mol	Chain	Res	Type
20	CT	43	LYS
20	CT	57	VAL
20	CT	74	ARG
20	CT	81	ARG
20	CT	98	ARG
20	CT	99	LEU
20	CT	103	ARG
20	CT	104	ARG
20	CT	126	GLU
20	CT	130	ASN
20	CT	134	HIS
20	CT	144	GLN
20	CT	148	ASP
20	CT	165	LYS
20	CT	166	ASN
20	CT	180	LYS
21	CU	1	MET
21	CU	24	LEU
21	CU	45	LEU
21	CU	58	ILE
21	CU	61	ILE
21	CU	71	LYS
21	CU	80	ARG
21	CU	81	TYR
21	CU	82	ASP
21	CU	97	VAL
21	CU	100	VAL
21	CU	104	GLU
21	CU	117	ARG
21	CU	132	THR
21	CU	137	ARG
21	CU	145	THR
21	CU	149	LYS
21	CU	155	ARG
21	CU	156	VAL
21	CU	160	THR
21	CU	162	THR
21	CU	167	ARG
21	CU	172	TYR
22	CV	9	SER
22	CV	16	GLN
22	CV	25	VAL

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Mol	Chain	Res	Type
22	CV	26	HIS
22	CV	27	LEU
22	CV	32	LYS
22	CV	75	ILE
22	CV	78	LYS
22	CV	79	MET
22	CV	80	VAL
22	CV	88	ARG
22	CV	92	ARG
22	CV	96	ILE
22	CV	97	LYS
22	CV	100	LYS
22	CV	101	CYS
22	CV	102	ARG
22	CV	103	GLN
22	CV	106	LEU
22	CV	126	VAL
22	CV	127	GLN
22	CV	128	LEU
22	CV	139	ARG
22	CV	143	THR
23	CW	10	LYS
23	CW	38	ILE
23	CW	43	VAL
23	CW	49	ASN
23	CW	55	THR
23	CW	58	GLU
23	CW	59	ASP
23	CW	100	THR
23	CW	104	ARG
23	CW	105	LEU
24	CX	13	ILE
24	CX	32	ARG
24	CX	45	ARG
24	CX	69	LEU
24	CX	73	VAL
24	CX	83	LYS
24	CX	88	ARG
24	CX	93	LEU
24	CX	102	ILE
24	CX	120	LYS
24	CX	128	ARG

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Mol	Chain	Res	Type
26	CY	1	MET
26	CY	4	GLU
26	CY	5	ILE
26	CY	19	THR
26	CY	25	ASP
26	CY	34	SER
26	CY	39	LEU
26	CY	43	ARG
26	CY	54	LEU
26	CY	63	ILE
27	CZ	26	VAL
27	CZ	27	ARG
27	CZ	37	THR
27	CZ	38	LEU
27	CZ	39	LYS
27	CZ	63	ILE
27	CZ	71	THR
27	CZ	92	LYS
27	CZ	108	LEU
27	CZ	115	ARG
27	CZ	117	ASN
27	CZ	125	ARG
27	CZ	133	LEU
27	CZ	135	ILE
28	DA	8	VAL
28	DA	9	SER
28	DA	13	ARG
28	DA	17	LYS
28	DA	37	LYS
28	DA	45	ILE
28	DA	50	ILE
28	DA	56	VAL
28	DA	57	LEU
28	DA	59	VAL
28	DA	67	GLU
28	DA	74	TYR
28	DA	76	LEU
28	DA	105	VAL
29	DB	14	VAL
29	DB	17	ARG
29	DB	24	VAL
29	DB	26	VAL

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Mol	Chain	Res	Type
29	DB	30	ASP
29	DB	46	ILE
29	DB	66	THR
29	DB	81	LEU
29	DB	86	THR
29	DB	92	PHE
29	DB	103	GLN
30	DC	4	ARG
30	DC	8	THR
30	DC	10	LYS
30	DC	14	HIS
30	DC	42	ARG
30	DC	46	ASP
30	DC	56	VAL
30	DC	60	TYR
30	DC	76	ASP
30	DC	77	LYS
30	DC	85	ASP
30	DC	88	ASP
30	DC	91	LEU
30	DC	115	LYS
30	DC	139	ARG
31	DD	13	THR
31	DD	14	ARG
31	DD	21	ILE
31	DD	22	LYS
31	DD	23	LYS
31	DD	26	THR
31	DD	59	LYS
32	DE	40	LYS
32	DE	61	MET
32	DE	83	LYS
32	DE	102	THR
32	DE	103	THR
33	DF	8	VAL
33	DF	13	THR
33	DF	16	LEU
33	DF	26	LYS
33	DF	31	ARG
33	DF	46	THR
33	DF	64	VAL
33	DF	68	GLU

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Mol	Chain	Res	Type
33	DF	76	SER
33	DF	79	ARG
33	DF	86	LYS
33	DF	93	VAL
33	DF	96	VAL
33	DF	100	SER
33	DF	104	LEU
33	DF	106	THR
33	DF	110	GLU
34	DG	4	LEU
34	DG	19	ARG
34	DG	31	ASN
34	DG	33	ARG
34	DG	34	LYS
34	DG	40	SER
34	DG	73	THR
34	DG	75	LEU
34	DG	82	LEU
34	DG	91	THR
34	DG	109	LEU
34	DG	125	ARG
34	DG	128	LEU
35	DH	20	LYS
35	DH	31	LYS
35	DH	60	ARG
35	DH	70	LYS
35	DH	81	VAL
35	DH	92	LYS
35	DH	98	VAL
36	DI	5	VAL
36	DI	20	ILE
36	DI	23	VAL
36	DI	29	ILE
36	DI	31	ARG
36	DI	36	LYS
36	DI	58	ARG
36	DI	64	THR
36	DI	65	VAL
36	DI	71	THR
37	DJ	11	THR
37	DJ	20	GLN
37	DJ	21	LEU

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Mol	Chain	Res	Type
37	DJ	27	GLU
37	DJ	28	LEU
37	DJ	36	LEU
37	DJ	46	THR
37	DJ	48	ARG
37	DJ	49	LYS
37	DJ	59	ASN
37	DJ	64	GLU
37	DJ	68	GLN
37	DJ	69	LEU
37	DJ	71	LYS
37	DJ	89	ARG
37	DJ	101	THR
37	DJ	107	LYS
37	DJ	119	LYS
38	DK	2	THR
38	DK	17	VAL
38	DK	21	THR
38	DK	26	ILE
38	DK	43	LEU
38	DK	45	ARG
38	DK	68	ARG
38	DK	76	ARG
38	DK	81	THR
38	DK	99	ARG
39	DL	17	THR
39	DL	24	ARG
39	DL	25	ARG
39	DL	33	THR
39	DL	36	SER
39	DL	44	THR
39	DL	45	ARG
39	DL	55	ARG
39	DL	59	THR
39	DL	67	LEU
39	DL	80	THR
40	DM	24	THR
40	DM	41	THR
40	DM	53	THR
40	DM	65	LEU
40	DM	69	LEU
40	DM	72	THR

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Mol	Chain	Res	Type
40	DM	77	ARG
41	DN	4	GLN
41	DN	21	ARG
41	DN	45	ARG
41	DN	48	LYS
42	DO	85	LEU
42	DO	112	LYS
42	DO	113	ARG
42	DO	114	LYS
42	DO	127	LEU
43	DP	6	ARG
43	DP	9	ARG
43	DP	11	ARG
43	DP	13	LEU
44	DQ	7	THR
44	DQ	35	LEU
44	DQ	78	LYS
44	DQ	79	THR
44	DQ	83	LEU
44	DQ	84	THR
44	DQ	85	LEU
44	DQ	100	LYS
44	DQ	105	GLN
45	DR	7	LYS
45	DR	10	ILE
45	DR	11	THR
45	DR	25	GLN
45	DR	49	ARG
45	DR	56	THR
45	DR	60	CYS
45	DR	70	THR
48	sM	33	LYS
48	sM	43	ASP
48	sM	50	ASN
48	sM	68	ARG
48	sM	71	ASN
48	sM	74	LYS
48	sM	77	THR
49	p0	4	ILE
49	p0	5	ARG
49	p0	30	VAL
49	p0	42	ARG

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Mol	Chain	Res	Type
49	p0	44	GLU
49	p0	48	ARG
49	p0	51	VAL
49	p0	70	LEU
49	p0	72	ASP
49	p0	76	LEU
49	p0	93	LEU
49	p0	97	LYS
49	p0	104	ARG
49	p0	192	ASP
50	B	6	THR
50	B	10	THR
50	B	37	VAL
50	B	59	LEU
50	B	62	ARG
50	B	84	ARG
50	B	87	LEU
50	B	88	LYS
50	B	96	THR
50	B	111	ILE
50	B	155	PHE
50	B	168	HIS
50	B	172	LEU
50	B	188	LEU
50	B	197	ILE
50	B	198	MET
50	B	200	ASP
50	B	203	PHE
51	C	21	VAL
51	C	25	THR
51	C	29	TRP
51	C	46	THR
51	C	61	LEU
51	C	70	LEU
51	C	74	GLN
51	C	77	GLU
51	C	78	ASP
51	C	89	ASP
51	C	95	ASN
51	C	97	LEU
51	C	105	PHE
51	C	111	ARG

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Mol	Chain	Res	Type
51	C	117	TRP
51	C	129	THR
51	C	177	GLN
51	C	181	LEU
51	C	198	GLU
51	C	202	LYS
51	C	218	LEU
51	C	220	GLN
51	C	222	LYS
51	C	223	PHE
52	D	53	ILE
52	D	69	ILE
52	D	72	LEU
52	D	73	LEU
52	D	76	LEU
52	D	91	ARG
52	D	95	ARG
52	D	96	THR
52	D	97	ARG
52	D	99	LYS
52	D	111	VAL
52	D	113	LEU
52	D	117	THR
52	D	134	LEU
52	D	137	ILE
52	D	141	ARG
52	D	147	ASN
52	D	148	LEU
52	D	207	LEU
52	D	221	THR
52	D	225	LEU
52	D	226	THR
52	D	235	LEU
52	D	244	SER
52	D	245	ASP
53	E	4	LEU
53	E	21	LEU
53	E	23	GLU
53	E	76	ARG
53	E	84	ILE
53	E	92	GLN
53	E	105	MET

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Mol	Chain	Res	Type
53	E	117	ARG
53	E	151	LYS
53	E	158	ILE
53	E	172	THR
53	E	174	HIS
53	E	175	VAL
53	E	176	LEU
53	E	178	ARG
53	E	181	VAL
53	E	182	LEU
53	E	195	SER
53	E	196	ARG
53	E	215	GLU
53	E	217	ILE
53	E	222	VAL
53	E	224	ASP
54	F	6	LYS
54	F	7	LYS
54	F	9	LEU
54	F	38	LEU
54	F	39	ARG
54	F	48	LEU
54	F	68	ARG
54	F	70	VAL
54	F	71	LYS
54	F	77	ARG
54	F	102	VAL
54	F	105	VAL
54	F	115	THR
54	F	116	ASP
54	F	126	VAL
54	F	131	LEU
54	F	142	HIS
54	F	180	LEU
54	F	182	TYR
54	F	187	ARG
54	F	192	ILE
54	F	227	VAL
54	F	240	LYS
54	F	242	LYS
54	F	258	GLN
55	G	25	LEU

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Mol	Chain	Res	Type
55	G	32	GLU
55	G	38	THR
55	G	40	ILE
55	G	41	LYS
55	G	43	PHE
55	G	45	LYS
55	G	48	PHE
55	G	58	LEU
55	G	65	ARG
55	G	76	ARG
55	G	79	ASN
55	G	93	LEU
55	G	146	THR
55	G	149	VAL
55	G	156	ARG
55	G	162	VAL
55	G	186	ASN
55	G	194	LEU
55	G	216	GLU
56	H	7	TYR
56	H	10	ASN
56	H	15	THR
56	H	25	ARG
56	H	39	GLU
56	H	45	PHE
56	H	71	THR
56	H	81	VAL
56	H	82	SER
56	H	109	LEU
56	H	120	GLU
56	H	126	ASP
56	H	127	THR
56	H	128	THR
56	H	129	VAL
56	H	133	LEU
56	H	137	ARG
56	H	154	ARG
56	H	155	ASP
56	H	158	ILE
56	H	169	TYR
56	H	170	THR
56	H	174	LYS

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Mol	Chain	Res	Type
56	H	193	LEU
56	H	211	LEU
57	I	15	GLU
57	I	16	LEU
57	I	31	SER
57	I	50	ASP
57	I	67	LEU
57	I	80	GLU
57	I	85	PHE
57	I	87	ASP
57	I	97	ARG
57	I	99	LEU
57	I	104	ARG
57	I	110	GLN
57	I	114	ARG
57	I	116	ARG
57	I	126	LEU
57	I	133	THR
57	I	147	ASN
57	I	166	LEU
57	I	185	ILE
58	J	21	PHE
58	J	22	ARG
58	J	29	LEU
58	J	36	THR
58	J	58	LEU
58	J	107	THR
58	J	138	ASN
58	J	151	LYS
58	J	152	ILE
58	J	184	LEU
58	J	196	LEU
59	K	3	ARG
59	K	6	ARG
59	K	7	THR
59	K	14	THR
59	K	28	LEU
59	K	39	LYS
59	K	40	LYS
59	K	78	ARG
59	K	89	ASP
59	K	92	LYS

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Mol	Chain	Res	Type
59	K	93	LEU
59	K	97	LEU
59	K	99	LEU
59	K	101	VAL
59	K	109	LEU
59	K	110	GLN
59	K	134	ILE
59	K	138	LYS
59	K	149	ARG
59	K	161	THR
59	K	171	ARG
59	K	172	VAL
59	K	174	ARG
59	K	182	GLU
60	L	5	LYS
60	L	8	ARG
60	L	20	VAL
60	L	27	PHE
60	L	28	ASN
60	L	55	VAL
60	L	62	GLN
60	L	76	LEU
60	L	82	LEU
61	M	21	ASN
61	M	29	LYS
61	M	44	THR
61	M	67	ARG
61	M	69	LYS
61	M	74	THR
61	M	80	MET
61	M	99	ARG
61	M	123	VAL
62	N	28	LEU
62	N	36	LEU
62	N	37	VAL
62	N	43	ARG
62	N	45	LEU
62	N	50	LYS
62	N	61	VAL
62	N	74	LEU
62	N	89	ILE
62	N	103	LEU

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Mol	Chain	Res	Type
62	N	125	ASN
62	N	126	TRP
62	N	129	GLU
62	N	132	GLU
62	N	140	PHE
63	O	3	ARG
63	O	6	SER
63	O	9	LYS
63	O	27	LYS
63	O	28	LEU
63	O	32	SER
63	O	39	LYS
63	O	64	ARG
63	O	66	ILE
63	O	76	LYS
63	O	83	GLU
63	O	88	LEU
63	O	102	LEU
63	O	115	LEU
63	O	125	LEU
63	O	134	VAL
63	O	149	LEU
64	P	29	HIS
64	P	31	THR
64	P	42	VAL
64	P	81	VAL
64	P	83	ILE
64	P	92	LYS
64	P	103	ARG
64	P	115	ILE
64	P	123	SER
64	P	132	ARG
64	P	137	LEU
65	Q	22	LEU
65	Q	26	LEU
65	Q	34	VAL
65	Q	36	LEU
65	Q	44	ARG
65	Q	52	LYS
65	Q	110	GLU
65	Q	121	ILE
65	Q	124	THR

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Mol	Chain	Res	Type
66	R	29	ILE
66	R	31	VAL
66	R	40	GLU
66	R	42	GLU
66	R	43	ILE
66	R	58	ASP
66	R	65	ILE
66	R	66	ARG
66	R	69	VAL
66	R	98	ASP
66	R	106	LYS
66	R	109	PHE
66	R	114	ARG
66	R	123	ARG
66	R	128	LYS
66	R	137	ARG
67	S	18	GLU
67	S	29	GLN
67	S	34	LEU
67	S	38	ILE
67	S	40	THR
67	S	43	SER
67	S	46	LEU
67	S	62	GLN
67	S	69	ILE
67	S	72	LYS
67	S	84	TYR
67	S	105	GLN
67	S	113	LEU
67	S	115	LEU
68	T	3	LEU
68	T	5	VAL
68	T	6	GLN
68	T	7	GLU
68	T	8	GLN
68	T	11	PHE
68	T	12	GLN
68	T	13	HIS
68	T	15	LEU
68	T	26	ILE
68	T	28	ILE
68	T	40	ARG

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Mol	Chain	Res	Type
68	T	71	GLN
68	T	77	THR
68	T	80	LYS
68	T	136	GLN
68	T	138	THR
68	T	140	THR
68	T	143	ARG
68	T	145	ARG
69	U	4	VAL
69	U	6	VAL
69	U	18	TYR
69	U	22	LEU
69	U	28	LEU
69	U	33	TYR
69	U	35	ASP
69	U	36	ILE
69	U	57	ARG
69	U	67	MET
69	U	70	GLN
69	U	71	VAL
69	U	94	ILE
69	U	126	GLU
69	U	127	ASN
69	U	130	ARG
69	U	131	ASP
69	U	139	THR
69	U	143	ASP
69	U	144	GLU
70	V	15	GLN
70	V	23	ARG
70	V	27	THR
70	V	30	LYS
70	V	31	VAL
70	V	57	ARG
70	V	60	THR
70	V	61	LYS
70	V	62	VAL
70	V	74	GLU
70	V	76	SER
70	V	89	ARG
70	V	103	ILE
70	V	117	VAL

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Mol	Chain	Res	Type
71	W	5	LYS
71	W	9	VAL
71	W	10	GLU
71	W	11	LEU
71	W	25	LYS
71	W	32	VAL
71	W	41	GLU
71	W	68	SER
71	W	69	LEU
71	W	76	ASP
71	W	78	LEU
71	W	80	LYS
72	X	4	SER
72	X	7	LEU
72	X	24	GLN
72	X	25	VAL
72	X	26	LEU
72	X	53	ILE
72	X	65	LEU
72	X	76	SER
72	X	81	VAL
72	X	87	GLU
72	X	98	GLN
72	X	103	ILE
72	X	119	LYS
72	X	121	VAL
72	X	126	LEU
73	Y	7	ARG
73	Y	9	LEU
73	Y	18	HIS
73	Y	19	ARG
73	Y	32	ARG
73	Y	69	ARG
73	Y	73	ARG
73	Y	75	GLN
73	Y	84	THR
73	Y	96	VAL
73	Y	107	PHE
73	Y	110	LYS
73	Y	114	LYS
73	Y	117	ILE
73	Y	132	LEU

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Mol	Chain	Res	Type
73	Y	140	LYS
73	Y	144	ARG
74	Z	21	LYS
74	Z	32	ARG
74	Z	57	VAL
74	Z	81	GLU
74	Z	84	LYS
74	Z	99	LYS
74	Z	102	LYS
74	Z	104	SER
74	Z	124	ARG
74	Z	127	LYS
74	Z	133	ASN
75	a	40	VAL
75	a	42	LEU
75	a	43	ASP
75	a	58	ARG
75	a	60	VAL
75	a	69	LEU
75	a	71	ILE
75	a	75	LEU
75	a	78	ILE
75	a	85	LYS
75	a	92	ILE
75	a	96	SER
76	b	41	ILE
76	b	44	ILE
76	b	62	TYR
76	b	64	LEU
76	b	76	SER
76	b	85	ARG
76	b	90	GLU
77	c	33	LEU
77	c	65	THR
77	c	77	THR
78	d	15	VAL
78	d	19	THR
78	d	31	GLU
78	d	32	PHE
78	d	35	ASP
78	d	48	VAL
78	d	49	ARG

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Mol	Chain	Res	Type
78	d	58	GLU
79	e	9	SER
79	e	12	ARG
79	e	30	LEU
79	e	32	ARG
79	e	49	ASP
80	f	3	LYS
80	f	21	VAL
80	f	22	GLU
80	f	28	LYS
81	g	83	LYS
81	g	97	LYS
81	g	102	VAL
81	g	106	TYR
81	g	114	VAL
81	g	120	GLU
81	g	130	VAL
81	g	135	HIS
81	g	137	ASP
81	g	138	ARG
81	g	147	VAL
81	g	151	ASN
82	h	16	HIS
82	h	29	GLN
82	h	52	GLN
82	h	66	HIS
82	h	74	THR
82	h	76	ASP
82	h	117	LYS
82	h	136	ILE
82	h	141	LEU
82	h	149	ASP
82	h	184	ASN
82	h	191	ASP
82	h	281	TYR
82	h	292	LEU
82	h	300	THR
82	h	308	ASN
82	h	317	THR
50	s0	12	GLU
50	s0	29	VAL
50	s0	30	GLN

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Mol	Chain	Res	Type
50	s0	41	ARG
50	s0	45	VAL
50	s0	50	VAL
50	s0	55	GLU
50	s0	59	LEU
50	s0	87	LEU
50	s0	96	THR
50	s0	101	ARG
50	s0	119	ARG
50	s0	146	LEU
50	s0	154	GLU
50	s0	156	VAL
50	s0	158	VAL
50	s0	164	ASN
50	s0	165	ARG
50	s0	172	LEU
50	s0	179	ARG
50	s0	185	ARG
50	s0	188	LEU
50	s0	189	VAL
50	s0	191	ARG
50	s0	198	MET
51	s1	21	VAL
51	s1	25	THR
51	s1	37	THR
51	s1	47	LEU
51	s1	48	VAL
51	s1	68	VAL
51	s1	70	LEU
51	s1	73	LEU
51	s1	81	PHE
51	s1	91	VAL
51	s1	105	PHE
51	s1	110	LEU
51	s1	126	THR
51	s1	127	VAL
51	s1	135	LEU
51	s1	153	HIS
51	s1	159	SER
51	s1	173	THR
51	s1	175	GLU
51	s1	181	LEU

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Mol	Chain	Res	Type
51	s1	183	GLN
51	s1	185	THR
51	s1	194	ASN
51	s1	205	PHE
51	s1	222	LYS
51	s1	223	PHE
51	s1	231	LEU
51	s1	234	GLU
52	s2	41	LEU
52	s2	51	THR
52	s2	53	ILE
52	s2	55	GLU
52	s2	69	ILE
52	s2	72	LEU
52	s2	73	LEU
52	s2	84	LYS
52	s2	90	THR
52	s2	91	ARG
52	s2	95	ARG
52	s2	97	ARG
52	s2	111	VAL
52	s2	113	LEU
52	s2	117	THR
52	s2	134	LEU
52	s2	137	ILE
52	s2	139	ILE
52	s2	140	ARG
52	s2	141	ARG
52	s2	148	LEU
52	s2	150	GLN
52	s2	153	SER
52	s2	166	THR
52	s2	206	THR
52	s2	225	LEU
52	s2	228	ASN
52	s2	237	VAL
52	s2	238	SER
52	s2	245	ASP
52	s2	246	GLU
52	s2	250	GLN
53	s3	4	LEU
53	s3	21	LEU

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Mol	Chain	Res	Type
53	s3	45	LYS
53	s3	66	ILE
53	s3	69	LEU
53	s3	84	ILE
53	s3	90	ARG
53	s3	115	ILE
53	s3	142	LEU
53	s3	158	ILE
53	s3	164	VAL
53	s3	168	ILE
53	s3	178	ARG
53	s3	196	ARG
53	s3	215	GLU
53	s3	217	ILE
53	s3	223	LYS
53	s3	224	ASP
54	s4	9	LEU
54	s4	38	LEU
54	s4	42	LEU
54	s4	49	ARG
54	s4	51	ARG
54	s4	67	GLN
54	s4	70	VAL
54	s4	78	THR
54	s4	89	VAL
54	s4	95	THR
54	s4	104	ASP
54	s4	131	LEU
54	s4	156	VAL
54	s4	176	ASP
54	s4	180	LEU
54	s4	181	VAL
54	s4	182	TYR
54	s4	221	ARG
54	s4	222	LEU
54	s4	227	VAL
54	s4	245	LYS
55	s5	24	VAL
55	s5	25	LEU
55	s5	27	THR
55	s5	43	PHE
55	s5	45	LYS

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Mol	Chain	Res	Type
55	s5	59	VAL
55	s5	66	GLN
55	s5	68	ILE
55	s5	76	ARG
55	s5	100	ASN
55	s5	104	ASN
55	s5	125	THR
55	s5	146	THR
55	s5	149	VAL
55	s5	157	ARG
55	s5	194	LEU
55	s5	208	SER
55	s5	216	GLU
56	s6	9	VAL
56	s6	65	GLN
56	s6	67	VAL
56	s6	68	LEU
56	s6	71	THR
56	s6	76	LEU
56	s6	78	THR
56	s6	97	VAL
56	s6	98	ARG
56	s6	108	VAL
56	s6	120	GLU
56	s6	121	LEU
56	s6	126	ASP
56	s6	128	THR
56	s6	129	VAL
56	s6	133	LEU
56	s6	143	LYS
56	s6	151	ASP
56	s6	177	ARG
56	s6	179	VAL
56	s6	182	GLN
56	s6	193	LEU
56	s6	215	ARG
56	s6	216	LEU
57	s7	10	SER
57	s7	17	GLU
57	s7	30	SER
57	s7	33	GLU
57	s7	49	ILE

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Mol	Chain	Res	Type
57	s7	50	ASP
57	s7	67	LEU
57	s7	79	ARG
57	s7	80	GLU
57	s7	101	LYS
57	s7	105	THR
57	s7	110	GLN
57	s7	111	LYS
57	s7	114	ARG
57	s7	116	ARG
57	s7	117	THR
57	s7	129	LEU
57	s7	143	LEU
57	s7	144	VAL
57	s7	185	ILE
58	s8	20	GLN
58	s8	22	ARG
58	s8	29	LEU
58	s8	36	THR
58	s8	46	VAL
58	s8	89	GLU
58	s8	138	ASN
58	s8	151	LYS
58	s8	183	ILE
58	s8	184	LEU
59	s9	3	ARG
59	s9	6	ARG
59	s9	7	THR
59	s9	16	LYS
59	s9	20	GLU
59	s9	21	SER
59	s9	28	LEU
59	s9	37	LYS
59	s9	39	LYS
59	s9	49	LEU
59	s9	54	ARG
59	s9	78	ARG
59	s9	89	ASP
59	s9	93	LEU
59	s9	96	VAL
59	s9	99	LEU
59	s9	103	ASP

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Mol	Chain	Res	Type
59	s9	109	LEU
59	s9	111	THR
59	s9	116	LEU
59	s9	118	LEU
59	s9	130	THR
59	s9	132	ARG
59	s9	134	ILE
59	s9	145	SER
59	s9	151	ASP
59	s9	172	VAL
59	s9	180	LYS
59	s9	182	GLU
60	c0	3	MET
60	c0	15	LEU
60	c0	20	VAL
60	c0	28	ASN
60	c0	33	GLU
60	c0	35	ILE
60	c0	55	VAL
60	c0	71	GLU
61	c1	5	LEU
61	c1	10	GLU
61	c1	26	LYS
61	c1	27	THR
61	c1	31	THR
61	c1	32	LYS
61	c1	40	LEU
61	c1	44	THR
61	c1	47	THR
61	c1	60	PHE
61	c1	67	ARG
61	c1	74	THR
61	c1	76	VAL
61	c1	83	THR
61	c1	109	VAL
61	c1	129	ARG
62	c2	28	LEU
62	c2	43	ARG
62	c2	52	LEU
62	c2	58	LEU
62	c2	61	VAL
62	c2	62	LEU

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Mol	Chain	Res	Type
62	c2	71	ILE
62	c2	86	VAL
62	c2	89	ILE
62	c2	90	LYS
62	c2	103	LEU
62	c2	129	GLU
62	c2	132	GLU
62	c2	137	MET
62	c2	140	PHE
63	c3	6	SER
63	c3	12	SER
63	c3	14	SER
63	c3	16	ILE
63	c3	19	SER
63	c3	28	LEU
63	c3	39	LYS
63	c3	60	VAL
63	c3	66	ILE
63	c3	76	LYS
63	c3	97	SER
63	c3	102	LEU
63	c3	115	LEU
63	c3	125	LEU
63	c3	127	ARG
63	c3	138	ASN
64	c4	18	ARG
64	c4	49	LYS
64	c4	51	ASP
64	c4	52	ARG
64	c4	81	VAL
64	c4	91	THR
64	c4	107	ARG
64	c4	114	ARG
64	c4	119	THR
64	c4	124	ASP
64	c4	133	ARG
64	c4	136	ARG
65	c5	12	PHE
65	c5	28	MET
65	c5	36	LEU
65	c5	60	LEU
65	c5	65	LEU

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Mol	Chain	Res	Type
65	c5	69	GLU
65	c5	72	LYS
65	c5	84	ILE
65	c5	110	GLU
65	c5	122	THR
65	c5	127	ARG
65	c5	128	HIS
66	c6	15	SER
66	c6	17	THR
66	c6	23	LYS
66	c6	26	LYS
66	c6	28	LEU
66	c6	37	THR
66	c6	42	GLU
66	c6	43	ILE
66	c6	48	VAL
66	c6	53	LEU
66	c6	57	LEU
66	c6	63	ILE
66	c6	68	ARG
66	c6	69	VAL
66	c6	82	ARG
66	c6	94	GLN
66	c6	127	LYS
66	c6	128	LYS
66	c6	137	ARG
66	c6	143	ARG
67	c7	3	ARG
67	c7	8	THR
67	c7	29	GLN
67	c7	34	LEU
67	c7	46	LEU
67	c7	69	ILE
67	c7	72	LYS
67	c7	82	ASP
67	c7	85	VAL
67	c7	106	THR
67	c7	110	VAL
68	c8	3	LEU
68	c8	4	VAL
68	c8	5	VAL
68	c8	6	GLN

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Mol	Chain	Res	Type
68	c8	12	GLN
68	c8	14	ILE
68	c8	25	ASN
68	c8	40	ARG
68	c8	61	LEU
68	c8	77	THR
68	c8	85	PHE
68	c8	92	ILE
68	c8	111	ASP
68	c8	112	ASP
68	c8	116	LEU
68	c8	133	VAL
68	c8	136	GLN
68	c8	138	THR
68	c8	143	ARG
69	c9	6	VAL
69	c9	13	ASP
69	c9	28	LEU
69	c9	29	GLU
69	c9	34	VAL
69	c9	37	VAL
69	c9	68	ARG
69	c9	70	GLN
69	c9	115	GLU
69	c9	122	ARG
69	c9	126	GLU
69	c9	131	ASP
69	c9	135	ILE
69	c9	140	LEU
69	c9	142	GLU
69	c9	143	ASP
70	d0	21	LYS
70	d0	23	ARG
70	d0	27	THR
70	d0	30	LYS
70	d0	51	VAL
70	d0	57	ARG
70	d0	60	THR
70	d0	70	THR
70	d0	72	ASN
70	d0	74	GLU
70	d0	103	ILE

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Mol	Chain	Res	Type
70	d0	107	THR
70	d0	108	ILE
71	d1	2	GLU
71	d1	4	ASP
71	d1	5	LYS
71	d1	12	TYR
71	d1	17	CYS
71	d1	32	VAL
71	d1	44	ARG
71	d1	50	TYR
71	d1	52	THR
71	d1	78	LEU
71	d1	80	LYS
72	d2	7	LEU
72	d2	15	ASN
72	d2	23	ARG
72	d2	25	VAL
72	d2	26	LEU
72	d2	31	SER
72	d2	103	ILE
73	d3	9	LEU
73	d3	16	ARG
73	d3	19	ARG
73	d3	27	ASN
73	d3	28	ASN
73	d3	33	LEU
73	d3	52	ILE
73	d3	55	GLU
73	d3	73	ARG
73	d3	84	THR
73	d3	96	VAL
73	d3	100	ASP
73	d3	103	LEU
73	d3	107	PHE
73	d3	132	LEU
74	d4	5	VAL
74	d4	34	ASN
74	d4	43	LYS
74	d4	47	VAL
74	d4	49	LYS
74	d4	62	THR
74	d4	105	ARG

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Mol	Chain	Res	Type
75	d5	46	LYS
75	d5	51	LEU
75	d5	57	TYR
76	d6	8	ASN
76	d6	10	ARG
76	d6	11	ASN
76	d6	12	LYS
76	d6	18	VAL
76	d6	45	VAL
76	d6	46	GLU
76	d6	51	ARG
76	d6	55	GLU
76	d6	82	ARG
76	d6	85	ARG
76	d6	90	GLU
77	d7	3	LEU
77	d7	4	VAL
77	d7	43	ILE
77	d7	59	CYS
77	d7	77	THR
78	d8	8	THR
78	d8	16	LEU
78	d8	22	ARG
78	d8	39	THR
78	d8	52	ASP
78	d8	58	GLU
78	d8	64	ARG
78	d8	65	ARG
78	d8	66	LEU
79	d9	12	ARG
79	d9	21	CYS
79	d9	30	LEU
79	d9	54	LYS
80	e0	22	GLU
80	e0	25	GLU
80	e0	26	LYS
80	e0	29	LYS
80	e0	46	ASN
80	e0	48	THR
80	e0	55	ARG
80	e0	61	SER
83	e1	106	TYR

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Mol	Chain	Res	Type
83	e1	113	LYS
83	e1	119	ARG
83	e1	126	CYS
83	e1	137	ASP
83	e1	147	VAL
83	e1	148	TYR
83	e1	150	VAL
82	sR	16	HIS
82	sR	48	THR
82	sR	52	GLN
82	sR	66	HIS
82	sR	70	ASP
82	sR	76	ASP
82	sR	96	THR
82	sR	145	LEU
82	sR	149	ASP
82	sR	159	ASN
82	sR	166	SER
82	sR	167	VAL
82	sR	201	THR
82	sR	232	TYR
82	sR	275	ARG
82	sR	281	TYR
82	sR	297	ASP
82	sR	317	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
4	j	132	ASN
6	l	307	GLN
7	m	40	HIS
12	r	144	ASN
12	r	163	GLN
29	AA	29	HIS
29	AA	57	HIS
6	CF	110	ASN
7	CG	40	HIS
11	CK	49	ASN
11	CK	51	GLN
18	CR	137	ASN
40	DM	32	ASN

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Mol	Chain	Res	Type
51	C	177	GLN
55	G	103	ASN
57	I	74	GLN
59	K	110	GLN
62	N	125	ASN
67	S	105	GLN
68	T	136	GLN
69	U	16	ASN
74	Z	107	GLN
82	h	159	ASN
56	s6	34	GLN
57	s7	71	HIS
64	c4	10	ASN
65	c5	103	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3145/3396 (92%)	559 (17%)	46 (1%)
1	AR	3145/3396 (92%)	562 (17%)	58 (1%)
2	3	120/121 (99%)	13 (10%)	0
2	AS	120/121 (99%)	14 (11%)	1 (0%)
25	6	1780/1800 (98%)	376 (21%)	32 (1%)
25	A	1778/1800 (98%)	419 (23%)	45 (2%)
3	4	157/158 (99%)	34 (21%)	2 (1%)
3	AT	157/158 (99%)	29 (18%)	2 (1%)
All	All	10402/10950 (94%)	2006 (19%)	186 (1%)

All (2006) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	26	A
1	1	40	A
1	1	43	A
1	1	45	A
1	1	49	A
1	1	57	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A

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Mol	Chain	Res	Type
1	1	72	C
1	1	73	C
1	1	76	G
1	1	83	U
1	1	92	G
1	1	93	C
1	1	99	A
1	1	109	A
1	1	110	G
1	1	113	C
1	1	117	U
1	1	121	A
1	1	122	A
1	1	133	U
1	1	135	C
1	1	136	G
1	1	156	G
1	1	157	A
1	1	166	C
1	1	170	G
1	1	187	A
1	1	190	U
1	1	191	U
1	1	192	C
1	1	210	U
1	1	213	A
1	1	218	G
1	1	219	A
1	1	240	U
1	1	243	G
1	1	247	C
1	1	249	U
1	1	250	U
1	1	251	G
1	1	252	U
1	1	269	G
1	1	282	G
1	1	283	G
1	1	284	A
1	1	286	U
1	1	295	A
1	1	298	U

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Mol	Chain	Res	Type
1	1	315	C
1	1	323	A
1	1	329	U
1	1	337	G
1	1	338	A
1	1	339	C
1	1	349	A
1	1	350	C
1	1	351	A
1	1	352	A
1	1	376	G
1	1	398	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	414	U
1	1	421	G
1	1	422	A
1	1	438	A
1	1	439	C
1	1	440	A
1	1	495	G
1	1	498	A
1	1	507	U
1	1	520	U
1	1	521	A
1	1	535	G
1	1	544	C
1	1	546	C
1	1	547	G
1	1	548	G
1	1	552	G
1	1	555	U
1	1	557	A
1	1	559	A
1	1	578	A
1	1	579	G
1	1	592	A
1	1	604	G
1	1	609	G
1	1	611	A
1	1	619	A

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Mol	Chain	Res	Type
1	1	620	U
1	1	621	A
1	1	636	C
1	1	649	A
1	1	651	G
1	1	658	G
1	1	660	A
1	1	677	A
1	1	681	U
1	1	691	A
1	1	705	A
1	1	712	G
1	1	715	A
1	1	716	A
1	1	727	G
1	1	764	U
1	1	766	U
1	1	767	U
1	1	776	U
1	1	777	U
1	1	780	A
1	1	781	G
1	1	785	G
1	1	806	A
1	1	817	A
1	1	830	A
1	1	849	C
1	1	861	C
1	1	869	G
1	1	874	U
1	1	879	U
1	1	890	C
1	1	896	A
1	1	907	G
1	1	908	G
1	1	914	A
1	1	916	G
1	1	917	A
1	1	921	A
1	1	923	C
1	1	924	G
1	1	925	A

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Mol	Chain	Res	Type
1	1	937	G
1	1	938	C
1	1	943	U
1	1	944	C
1	1	959	C
1	1	960	U
1	1	979	U
1	1	980	A
1	1	981	U
1	1	982	C
1	1	994	G
1	1	1001	G
1	1	1002	A
1	1	1010	G
1	1	1017	C
1	1	1018	G
1	1	1020	G
1	1	1024	G
1	1	1025	A
1	1	1029	G
1	1	1036	A
1	1	1037	C
1	1	1047	A
1	1	1049	C
1	1	1052	U
1	1	1064	A
1	1	1065	A
1	1	1072	G
1	1	1081	U
1	1	1082	U
1	1	1083	G
1	1	1087	G
1	1	1093	A
1	1	1094	U
1	1	1095	U
1	1	1097	G
1	1	1098	A
1	1	1102	A
1	1	1103	A
1	1	1104	G
1	1	1116	G
1	1	1117	G

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Mol	Chain	Res	Type
1	1	1131	G
1	1	1153	A
1	1	1159	A
1	1	1160	C
1	1	1168	U
1	1	1180	A
1	1	1181	U
1	1	1185	C
1	1	1190	A
1	1	1191	U
1	1	1192	C
1	1	1201	C
1	1	1209	G
1	1	1217	A
1	1	1222	G
1	1	1227	C
1	1	1232	C
1	1	1235	U
1	1	1236	G
1	1	1237	G
1	1	1243	G
1	1	1245	A
1	1	1246	G
1	1	1248	C
1	1	1249	G
1	1	1258	U
1	1	1262	G
1	1	1263	A
1	1	1264	G
1	1	1265	U
1	1	1267	U
1	1	1269	U
1	1	1270	A
1	1	1271	A
1	1	1274	A
1	1	1278	A
1	1	1279	C
1	1	1285	G
1	1	1286	A
1	1	1287	A
1	1	1292	C
1	1	1308	A

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Mol	Chain	Res	Type
1	1	1309	U
1	1	1313	G
1	1	1330	A
1	1	1348	U
1	1	1349	G
1	1	1351	U
1	1	1352	A
1	1	1353	U
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1386	A
1	1	1399	A
1	1	1400	G
1	1	1418	A
1	1	1419	A
1	1	1421	G
1	1	1429	G
1	1	1433	A
1	1	1434	G
1	1	1437	C
1	1	1443	G
1	1	1446	A
1	1	1450	G
1	1	1481	A
1	1	1482	A
1	1	1485	G
1	1	1491	A
1	1	1508	C
1	1	1527	C
1	1	1533	U
1	1	1536	G
1	1	1556	C
1	1	1560	G
1	1	1561	G
1	1	1562	C
1	1	1563	C
1	1	1564	U
1	1	1567	U
1	1	1568	U
1	1	1569	U
1	1	1570	U

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Mol	Chain	Res	Type
1	1	1576	G
1	1	1580	A
1	1	1582	C
1	1	1583	A
1	1	1587	A
1	1	1589	A
1	1	1605	A
1	1	1620	U
1	1	1629	U
1	1	1639	C
1	1	1643	A
1	1	1655	G
1	1	1656	A
1	1	1657	C
1	1	1658	G
1	1	1683	A
1	1	1716	U
1	1	1717	U
1	1	1724	U
1	1	1729	A
1	1	1736	G
1	1	1741	A
1	1	1750	A
1	1	1751	G
1	1	1765	U
1	1	1766	G
1	1	1769	G
1	1	1770	G
1	1	1780	G
1	1	1797	A
1	1	1810	A
1	1	1812	G
1	1	1814	A
1	1	1815	U
1	1	1816	A
1	1	1817	G
1	1	1819	U
1	1	1820	U
1	1	1821	U
1	1	1835	A
1	1	1839	A
1	1	1842	A

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Mol	Chain	Res	Type
1	1	1846	C
1	1	1849	C
1	1	1850	A
1	1	1858	A
1	1	1866	C
1	1	1879	A
1	1	1880	U
1	1	1895	A
1	1	1901	A
1	1	1906	G
1	1	1951	C
1	1	1952	G
1	1	1953	G
1	1	1954	G
1	1	2094	C
1	1	2101	C
1	1	2102	U
1	1	2111	G
1	1	2112	U
1	1	2113	A
1	1	2121	G
1	1	2122	G
1	1	2131	A
1	1	2134	G
1	1	2140	U
1	1	2145	A
1	1	2158	A
1	1	2169	G
1	1	2170	U
1	1	2177	G
1	1	2205	U
1	1	2210	G
1	1	2228	A
1	1	2244	A
1	1	2246	G
1	1	2249	G
1	1	2250	G
1	1	2255	A
1	1	2256	A
1	1	2262	A
1	1	2272	G
1	1	2273	G

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Mol	Chain	Res	Type
1	1	2281	A
1	1	2282	U
1	1	2288	G
1	1	2298	U
1	1	2301	U
1	1	2303	A
1	1	2307	G
1	1	2310	U
1	1	2313	A
1	1	2314	U
1	1	2315	G
1	1	2334	U
1	1	2336	U
1	1	2361	A
1	1	2362	C
1	1	2372	A
1	1	2373	A
1	1	2374	C
1	1	2375	G
1	1	2382	G
1	1	2385	G
1	1	2393	G
1	1	2397	A
1	1	2398	A
1	1	2402	A
1	1	2403	G
1	1	2404	A
1	1	2405	C
1	1	2411	U
1	1	2418	G
1	1	2419	A
1	1	2444	C
1	1	2445	A
1	1	2502	A
1	1	2503	G
1	1	2514	U
1	1	2515	A
1	1	2522	G
1	1	2523	A
1	1	2532	U
1	1	2533	G
1	1	2537	U

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Mol	Chain	Res	Type
1	1	2538	U
1	1	2539	C
1	1	2540	A
1	1	2541	U
1	1	2542	U
1	1	2543	U
1	1	2547	A
1	1	2548	C
1	1	2549	G
1	1	2552	C
1	1	2555	G
1	1	2561	A
1	1	2568	C
1	1	2569	A
1	1	2570	U
1	1	2571	U
1	1	2572	C
1	1	2573	G
1	1	2581	U
1	1	2582	C
1	1	2585	G
1	1	2593	A
1	1	2594	C
1	1	2606	G
1	1	2607	G
1	1	2614	G
1	1	2626	A
1	1	2637	A
1	1	2652	U
1	1	2656	A
1	1	2674	A
1	1	2677	G
1	1	2689	A
1	1	2690	G
1	1	2691	A
1	1	2694	A
1	1	2696	A
1	1	2714	G
1	1	2728	G
1	1	2729	U
1	1	2737	C
1	1	2752	U

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Mol	Chain	Res	Type
1	1	2753	G
1	1	2755	C
1	1	2771	U
1	1	2772	C
1	1	2773	C
1	1	2777	G
1	1	2778	G
1	1	2780	A
1	1	2796	G
1	1	2797	C
1	1	2799	A
1	1	2800	G
1	1	2801	A
1	1	2810	C
1	1	2814	G
1	1	2816	G
1	1	2817	A
1	1	2818	U
1	1	2842	U
1	1	2843	U
1	1	2845	A
1	1	2849	C
1	1	2860	U
1	1	2867	C
1	1	2871	G
1	1	2872	A
1	1	2875	U
1	1	2876	C
1	1	2887	A
1	1	2899	C
1	1	2910	A
1	1	2914	G
1	1	2923	U
1	1	2927	C
1	1	2935	U
1	1	2936	A
1	1	2942	C
1	1	2945	G
1	1	2947	G
1	1	2954	U
1	1	2955	U
1	1	2971	A

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Mol	Chain	Res	Type
1	1	2980	U
1	1	2983	C
1	1	2990	G
1	1	2992	U
1	1	2997	G
1	1	3012	A
1	1	3056	U
1	1	3059	G
1	1	3078	U
1	1	3079	U
1	1	3080	G
1	1	3086	A
1	1	3092	C
1	1	3113	A
1	1	3119	U
1	1	3122	A
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3143	C
1	1	3150	A
1	1	3151	U
1	1	3153	U
1	1	3154	C
1	1	3155	U
1	1	3156	U
1	1	3157	U
1	1	3164	C
1	1	3165	A
1	1	3168	A
1	1	3171	U
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3181	C
1	1	3187	A
1	1	3196	U
1	1	3199	G
1	1	3207	U
1	1	3210	A
1	1	3217	C

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Mol	Chain	Res	Type
1	1	3218	A
1	1	3219	G
1	1	3228	C
1	1	3229	G
1	1	3243	A
1	1	3245	A
1	1	3246	G
1	1	3247	G
1	1	3259	U
1	1	3270	U
1	1	3271	G
1	1	3272	C
1	1	3273	A
1	1	3276	G
1	1	3281	U
1	1	3286	G
1	1	3287	U
1	1	3288	G
1	1	3289	G
1	1	3294	A
1	1	3295	A
1	1	3304	U
1	1	3309	G
1	1	3313	U
1	1	3316	A
1	1	3318	G
1	1	3319	U
1	1	3341	U
1	1	3342	A
1	1	3345	G
1	1	3347	A
1	1	3351	U
1	1	3352	U
1	1	3353	G
1	1	3354	U
1	1	3355	U
1	1	3369	G
1	1	3375	A
1	1	3376	A
1	1	3378	C
1	1	3381	U
1	1	3382	U

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Mol	Chain	Res	Type
1	1	3389	U
1	1	3390	G
1	1	3396	U
2	3	7	G
2	3	11	A
2	3	13	A
2	3	22	A
2	3	54	U
2	3	65	G
2	3	73	C
2	3	74	C
2	3	76	A
2	3	95	A
2	3	102	A
2	3	112	G
2	3	121	U
3	4	2	A
3	4	23	U
3	4	34	U
3	4	35	C
3	4	48	A
3	4	53	A
3	4	57	C
3	4	58	G
3	4	59	A
3	4	62	C
3	4	63	G
3	4	79	A
3	4	80	A
3	4	81	U
3	4	82	U
3	4	85	G
3	4	86	U
3	4	87	G
3	4	90	U
3	4	95	G
3	4	96	A
3	4	104	A
3	4	105	A
3	4	106	C
3	4	111	A
3	4	113	U

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Mol	Chain	Res	Type
3	4	125	U
3	4	126	A
3	4	128	U
3	4	138	A
3	4	152	G
3	4	155	A
3	4	157	U
3	4	158	U
25	6	2	A
25	6	4	C
25	6	17	C
25	6	25	C
25	6	26	A
25	6	27	U
25	6	34	G
25	6	47	A
25	6	57	G
25	6	60	U
25	6	61	A
25	6	67	A
25	6	68	A
25	6	69	G
25	6	72	A
25	6	73	U
25	6	75	U
25	6	76	A
25	6	77	U
25	6	104	A
25	6	114	C
25	6	126	A
25	6	132	U
25	6	137	U
25	6	138	A
25	6	140	A
25	6	141	U
25	6	144	U
25	6	145	A
25	6	146	U
25	6	153	G
25	6	159	U
25	6	166	C
25	6	178	U

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Mol	Chain	Res	Type
25	6	181	A
25	6	185	U
25	6	188	A
25	6	191	C
25	6	192	U
25	6	193	U
25	6	194	U
25	6	195	G
25	6	200	A
25	6	215	A
25	6	216	U
25	6	217	A
25	6	218	A
25	6	219	A
25	6	220	A
25	6	227	U
25	6	228	G
25	6	232	U
25	6	233	C
25	6	240	U
25	6	241	U
25	6	249	U
25	6	250	C
25	6	261	U
25	6	265	A
25	6	271	A
25	6	272	U
25	6	273	G
25	6	275	C
25	6	278	U
25	6	280	U
25	6	285	G
25	6	299	A
25	6	302	U
25	6	308	C
25	6	314	C
25	6	316	A
25	6	319	U
25	6	320	U
25	6	321	C
25	6	322	G
25	6	337	G

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Mol	Chain	Res	Type
25	6	338	C
25	6	352	A
25	6	359	A
25	6	360	A
25	6	361	C
25	6	400	A
25	6	401	A
25	6	402	C
25	6	404	G
25	6	416	A
25	6	418	G
25	6	424	C
25	6	425	A
25	6	426	G
25	6	434	G
25	6	439	U
25	6	444	C
25	6	445	A
25	6	448	C
25	6	454	U
25	6	468	A
25	6	477	A
25	6	480	G
25	6	486	G
25	6	488	G
25	6	489	C
25	6	490	C
25	6	492	A
25	6	493	U
25	6	494	U
25	6	496	G
25	6	497	G
25	6	500	C
25	6	501	U
25	6	504	U
25	6	505	A
25	6	506	A
25	6	507	U
25	6	510	G
25	6	511	A
25	6	512	A
25	6	513	U

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Mol	Chain	Res	Type
25	6	514	G
25	6	515	A
25	6	516	G
25	6	519	C
25	6	527	A
25	6	538	A
25	6	539	G
25	6	540	G
25	6	541	A
25	6	542	A
25	6	543	C
25	6	544	A
25	6	548	G
25	6	557	G
25	6	558	U
25	6	559	C
25	6	565	C
25	6	568	G
25	6	570	A
25	6	574	G
25	6	579	A
25	6	580	A
25	6	582	U
25	6	594	A
25	6	595	G
25	6	611	U
25	6	619	A
25	6	620	A
25	6	621	A
25	6	622	A
25	6	623	A
25	6	624	G
25	6	639	U
25	6	640	U
25	6	650	U
25	6	652	G
25	6	653	C
25	6	658	C
25	6	676	G
25	6	679	U
25	6	680	U
25	6	681	U

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Mol	Chain	Res	Type
25	6	682	C
25	6	683	C
25	6	684	A
25	6	685	A
25	6	691	C
25	6	696	C
25	6	709	C
25	6	711	U
25	6	714	G
25	6	715	U
25	6	718	U
25	6	719	U
25	6	720	G
25	6	721	U
25	6	722	G
25	6	723	G
25	6	730	G
25	6	742	U
25	6	745	U
25	6	753	A
25	6	754	A
25	6	755	A
25	6	756	A
25	6	765	G
25	6	766	U
25	6	774	A
25	6	775	G
25	6	780	A
25	6	781	U
25	6	782	U
25	6	783	G
25	6	789	A
25	6	793	A
25	6	794	U
25	6	803	A
25	6	811	A
25	6	812	A
25	6	815	G
25	6	821	U
25	6	823	G
25	6	825	U
25	6	826	U

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Mol	Chain	Res	Type
25	6	829	A
25	6	830	U
25	6	831	U
25	6	832	U
25	6	834	G
25	6	835	U
25	6	863	A
25	6	876	G
25	6	898	A
25	6	906	A
25	6	912	U
25	6	913	G
25	6	914	G
25	6	916	U
25	6	933	A
25	6	935	U
25	6	942	G
25	6	959	U
25	6	960	U
25	6	966	A
25	6	970	A
25	6	971	A
25	6	983	A
25	6	992	A
25	6	1003	A
25	6	1004	U
25	6	1005	A
25	6	1021	C
25	6	1026	A
25	6	1028	C
25	6	1039	A
25	6	1040	G
25	6	1052	U
25	6	1053	G
25	6	1057	U
25	6	1058	U
25	6	1059	U
25	6	1060	U
25	6	1072	C
25	6	1073	G
25	6	1076	A
25	6	1082	C

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Mol	Chain	Res	Type
25	6	1092	A
25	6	1096	C
25	6	1097	U
25	6	1098	U
25	6	1099	U
25	6	1100	G
25	6	1109	G
25	6	1137	A
25	6	1138	A
25	6	1151	A
25	6	1155	G
25	6	1158	C
25	6	1159	C
25	6	1160	A
25	6	1167	G
25	6	1185	U
25	6	1194	A
25	6	1196	A
25	6	1199	G
25	6	1200	G
25	6	1202	A
25	6	1208	A
25	6	1217	A
25	6	1218	G
25	6	1225	U
25	6	1228	G
25	6	1229	G
25	6	1230	A
25	6	1231	U
25	6	1241	G
25	6	1243	G
25	6	1244	A
25	6	1245	G
25	6	1246	C
25	6	1255	G
25	6	1256	A
25	6	1257	U
25	6	1258	U
25	6	1286	U
25	6	1291	G
25	6	1314	U
25	6	1315	U

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Mol	Chain	Res	Type
25	6	1316	G
25	6	1321	A
25	6	1344	A
25	6	1345	A
25	6	1346	A
25	6	1354	G
25	6	1361	U
25	6	1363	U
25	6	1364	G
25	6	1371	A
25	6	1372	U
25	6	1388	A
25	6	1390	U
25	6	1398	U
25	6	1399	C
25	6	1400	A
25	6	1402	G
25	6	1413	U
25	6	1414	U
25	6	1415	U
25	6	1427	A
25	6	1428	G
25	6	1433	G
25	6	1445	G
25	6	1446	A
25	6	1448	G
25	6	1458	G
25	6	1459	C
25	6	1461	C
25	6	1471	A
25	6	1481	C
25	6	1482	C
25	6	1490	C
25	6	1491	U
25	6	1492	A
25	6	1493	A
25	6	1506	G
25	6	1514	U
25	6	1515	A
25	6	1516	A
25	6	1521	G
25	6	1523	G

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Mol	Chain	Res	Type
25	6	1524	A
25	6	1535	U
25	6	1536	G
25	6	1537	C
25	6	1538	U
25	6	1540	G
25	6	1554	U
25	6	1557	U
25	6	1559	A
25	6	1569	A
25	6	1573	A
25	6	1574	G
25	6	1584	G
25	6	1590	G
25	6	1601	G
25	6	1616	G
25	6	1621	U
25	6	1657	U
25	6	1658	G
25	6	1682	U
25	6	1683	C
25	6	1696	G
25	6	1697	G
25	6	1698	G
25	6	1699	G
25	6	1700	C
25	6	1701	A
25	6	1702	A
25	6	1703	C
25	6	1712	A
25	6	1716	C
25	6	1717	G
25	6	1731	A
25	6	1760	G
25	6	1762	A
25	6	1766	A
25	6	1767	G
25	6	1769	U
25	6	1780	G
25	6	1782	A
25	6	1783	C
25	6	1792	G

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Mol	Chain	Res	Type
25	6	1793	G
25	6	1794	A
25	6	1795	U
25	6	1796	C
25	6	1799	U
25	6	1800	A
1	AR	16	A
1	AR	24	G
1	AR	26	A
1	AR	40	A
1	AR	43	A
1	AR	49	A
1	AR	57	A
1	AR	59	G
1	AR	60	A
1	AR	65	A
1	AR	66	A
1	AR	76	G
1	AR	92	G
1	AR	93	C
1	AR	99	A
1	AR	109	A
1	AR	110	G
1	AR	111	C
1	AR	113	C
1	AR	116	A
1	AR	120	G
1	AR	121	A
1	AR	122	A
1	AR	133	U
1	AR	135	C
1	AR	136	G
1	AR	156	G
1	AR	157	A
1	AR	165	A
1	AR	166	C
1	AR	172	G
1	AR	173	G
1	AR	174	C
1	AR	187	A
1	AR	190	U
1	AR	191	U

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Mol	Chain	Res	Type
1	AR	192	C
1	AR	200	C
1	AR	210	U
1	AR	211	A
1	AR	213	A
1	AR	218	G
1	AR	219	A
1	AR	231	G
1	AR	240	U
1	AR	241	G
1	AR	243	G
1	AR	245	U
1	AR	249	U
1	AR	250	U
1	AR	251	G
1	AR	252	U
1	AR	269	G
1	AR	270	U
1	AR	286	U
1	AR	295	A
1	AR	298	U
1	AR	323	A
1	AR	329	U
1	AR	334	A
1	AR	338	A
1	AR	339	C
1	AR	350	C
1	AR	351	A
1	AR	370	U
1	AR	376	G
1	AR	399	A
1	AR	401	U
1	AR	402	A
1	AR	403	C
1	AR	404	G
1	AR	409	A
1	AR	421	G
1	AR	422	A
1	AR	439	C
1	AR	440	A
1	AR	495	G
1	AR	516	A

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Mol	Chain	Res	Type
1	AR	521	A
1	AR	535	G
1	AR	544	C
1	AR	546	C
1	AR	548	G
1	AR	551	A
1	AR	552	G
1	AR	555	U
1	AR	557	A
1	AR	558	U
1	AR	559	A
1	AR	578	A
1	AR	579	G
1	AR	592	A
1	AR	600	G
1	AR	604	G
1	AR	607	A
1	AR	609	G
1	AR	611	A
1	AR	621	A
1	AR	622	A
1	AR	636	C
1	AR	638	C
1	AR	649	A
1	AR	651	G
1	AR	660	A
1	AR	677	A
1	AR	681	U
1	AR	691	A
1	AR	705	A
1	AR	712	G
1	AR	715	A
1	AR	716	A
1	AR	726	G
1	AR	727	G
1	AR	758	C
1	AR	764	U
1	AR	765	C
1	AR	766	U
1	AR	767	U
1	AR	776	U
1	AR	777	U

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Mol	Chain	Res	Type
1	AR	780	A
1	AR	781	G
1	AR	785	G
1	AR	806	A
1	AR	817	A
1	AR	830	A
1	AR	849	C
1	AR	861	C
1	AR	874	U
1	AR	879	U
1	AR	896	A
1	AR	907	G
1	AR	908	G
1	AR	914	A
1	AR	916	G
1	AR	917	A
1	AR	921	A
1	AR	923	C
1	AR	924	G
1	AR	937	G
1	AR	944	C
1	AR	959	C
1	AR	960	U
1	AR	964	G
1	AR	979	U
1	AR	980	A
1	AR	981	U
1	AR	982	C
1	AR	984	G
1	AR	994	G
1	AR	1001	G
1	AR	1002	A
1	AR	1006	A
1	AR	1010	G
1	AR	1015	U
1	AR	1016	C
1	AR	1017	C
1	AR	1018	G
1	AR	1020	G
1	AR	1021	G
1	AR	1024	G
1	AR	1029	G

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Mol	Chain	Res	Type
1	AR	1036	A
1	AR	1037	C
1	AR	1047	A
1	AR	1049	C
1	AR	1064	A
1	AR	1065	A
1	AR	1072	G
1	AR	1081	U
1	AR	1082	U
1	AR	1093	A
1	AR	1094	U
1	AR	1095	U
1	AR	1096	U
1	AR	1097	G
1	AR	1098	A
1	AR	1103	A
1	AR	1104	G
1	AR	1117	G
1	AR	1131	G
1	AR	1143	A
1	AR	1153	A
1	AR	1159	A
1	AR	1180	A
1	AR	1181	U
1	AR	1190	A
1	AR	1192	C
1	AR	1196	C
1	AR	1201	C
1	AR	1202	A
1	AR	1209	G
1	AR	1214	U
1	AR	1216	C
1	AR	1217	A
1	AR	1222	G
1	AR	1235	U
1	AR	1236	G
1	AR	1237	G
1	AR	1239	C
1	AR	1241	U
1	AR	1242	G
1	AR	1244	A
1	AR	1245	A

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Mol	Chain	Res	Type
1	AR	1246	G
1	AR	1252	A
1	AR	1258	U
1	AR	1262	G
1	AR	1263	A
1	AR	1285	G
1	AR	1292	C
1	AR	1295	G
1	AR	1307	G
1	AR	1308	A
1	AR	1309	U
1	AR	1313	G
1	AR	1330	A
1	AR	1348	U
1	AR	1349	G
1	AR	1351	U
1	AR	1352	A
1	AR	1353	U
1	AR	1355	A
1	AR	1356	U
1	AR	1357	G
1	AR	1385	C
1	AR	1386	A
1	AR	1399	A
1	AR	1400	G
1	AR	1418	A
1	AR	1419	A
1	AR	1421	G
1	AR	1431	G
1	AR	1434	G
1	AR	1437	C
1	AR	1446	A
1	AR	1450	G
1	AR	1453	A
1	AR	1481	A
1	AR	1482	A
1	AR	1488	G
1	AR	1508	C
1	AR	1536	G
1	AR	1555	U
1	AR	1556	C
1	AR	1560	G

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Mol	Chain	Res	Type
1	AR	1562	C
1	AR	1563	C
1	AR	1566	A
1	AR	1567	U
1	AR	1568	U
1	AR	1569	U
1	AR	1570	U
1	AR	1572	U
1	AR	1576	G
1	AR	1578	C
1	AR	1579	C
1	AR	1580	A
1	AR	1581	C
1	AR	1582	C
1	AR	1583	A
1	AR	1589	A
1	AR	1593	A
1	AR	1605	A
1	AR	1607	U
1	AR	1620	U
1	AR	1629	U
1	AR	1639	C
1	AR	1643	A
1	AR	1645	U
1	AR	1657	C
1	AR	1658	G
1	AR	1683	A
1	AR	1716	U
1	AR	1717	U
1	AR	1724	U
1	AR	1725	C
1	AR	1736	G
1	AR	1741	A
1	AR	1742	U
1	AR	1750	A
1	AR	1751	G
1	AR	1762	C
1	AR	1765	U
1	AR	1766	G
1	AR	1769	G
1	AR	1770	G
1	AR	1780	G

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Mol	Chain	Res	Type
1	AR	1797	A
1	AR	1809	A
1	AR	1810	A
1	AR	1814	A
1	AR	1815	U
1	AR	1816	A
1	AR	1817	G
1	AR	1820	U
1	AR	1821	U
1	AR	1835	A
1	AR	1839	A
1	AR	1841	A
1	AR	1842	A
1	AR	1846	C
1	AR	1849	C
1	AR	1878	G
1	AR	1879	A
1	AR	1893	A
1	AR	1906	G
1	AR	1952	G
1	AR	1953	G
1	AR	1954	G
1	AR	2094	C
1	AR	2101	C
1	AR	2102	U
1	AR	2111	G
1	AR	2112	U
1	AR	2113	A
1	AR	2114	C
1	AR	2121	G
1	AR	2122	G
1	AR	2131	A
1	AR	2134	G
1	AR	2140	U
1	AR	2144	A
1	AR	2158	A
1	AR	2169	G
1	AR	2187	G
1	AR	2198	A
1	AR	2201	G
1	AR	2205	U
1	AR	2209	U

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Mol	Chain	Res	Type
1	AR	2210	G
1	AR	2223	A
1	AR	2225	U
1	AR	2228	A
1	AR	2244	A
1	AR	2252	A
1	AR	2253	G
1	AR	2254	U
1	AR	2255	A
1	AR	2256	A
1	AR	2261	G
1	AR	2264	U
1	AR	2269	U
1	AR	2270	A
1	AR	2271	A
1	AR	2272	G
1	AR	2273	G
1	AR	2279	A
1	AR	2280	A
1	AR	2281	A
1	AR	2282	U
1	AR	2288	G
1	AR	2307	G
1	AR	2310	U
1	AR	2313	A
1	AR	2314	U
1	AR	2315	G
1	AR	2334	U
1	AR	2336	U
1	AR	2372	A
1	AR	2373	A
1	AR	2374	C
1	AR	2375	G
1	AR	2385	G
1	AR	2393	G
1	AR	2397	A
1	AR	2401	A
1	AR	2402	A
1	AR	2403	G
1	AR	2404	A
1	AR	2411	U
1	AR	2418	G

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Mol	Chain	Res	Type
1	AR	2419	A
1	AR	2435	G
1	AR	2443	A
1	AR	2444	C
1	AR	2445	A
1	AR	2502	A
1	AR	2503	G
1	AR	2504	U
1	AR	2507	C
1	AR	2508	U
1	AR	2514	U
1	AR	2515	A
1	AR	2522	G
1	AR	2523	A
1	AR	2524	A
1	AR	2530	G
1	AR	2533	G
1	AR	2536	A
1	AR	2538	U
1	AR	2539	C
1	AR	2540	A
1	AR	2541	U
1	AR	2542	U
1	AR	2543	U
1	AR	2547	A
1	AR	2549	G
1	AR	2552	C
1	AR	2555	G
1	AR	2561	A
1	AR	2569	A
1	AR	2570	U
1	AR	2571	U
1	AR	2572	C
1	AR	2573	G
1	AR	2581	U
1	AR	2585	G
1	AR	2586	G
1	AR	2589	G
1	AR	2593	A
1	AR	2594	C
1	AR	2595	A
1	AR	2606	G

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Mol	Chain	Res	Type
1	AR	2607	G
1	AR	2614	G
1	AR	2634	U
1	AR	2638	C
1	AR	2652	U
1	AR	2656	A
1	AR	2674	A
1	AR	2677	G
1	AR	2681	U
1	AR	2689	A
1	AR	2691	A
1	AR	2694	A
1	AR	2696	A
1	AR	2705	A
1	AR	2714	G
1	AR	2719	U
1	AR	2727	A
1	AR	2728	G
1	AR	2729	U
1	AR	2752	U
1	AR	2753	G
1	AR	2755	C
1	AR	2762	A
1	AR	2771	U
1	AR	2772	C
1	AR	2777	G
1	AR	2778	G
1	AR	2796	G
1	AR	2799	A
1	AR	2800	G
1	AR	2801	A
1	AR	2802	A
1	AR	2810	C
1	AR	2817	A
1	AR	2818	U
1	AR	2819	A
1	AR	2842	U
1	AR	2843	U
1	AR	2845	A
1	AR	2847	A
1	AR	2860	U
1	AR	2867	C

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Mol	Chain	Res	Type
1	AR	2871	G
1	AR	2872	A
1	AR	2873	U
1	AR	2875	U
1	AR	2887	A
1	AR	2896	A
1	AR	2899	C
1	AR	2923	U
1	AR	2928	C
1	AR	2935	U
1	AR	2936	A
1	AR	2942	C
1	AR	2945	G
1	AR	2947	G
1	AR	2951	G
1	AR	2952	G
1	AR	2971	A
1	AR	2983	C
1	AR	2990	G
1	AR	2996	U
1	AR	2997	G
1	AR	3012	A
1	AR	3049	A
1	AR	3056	U
1	AR	3057	U
1	AR	3059	G
1	AR	3078	U
1	AR	3079	U
1	AR	3086	A
1	AR	3092	C
1	AR	3104	U
1	AR	3119	U
1	AR	3122	A
1	AR	3130	A
1	AR	3131	U
1	AR	3142	A
1	AR	3143	C
1	AR	3151	U
1	AR	3153	U
1	AR	3155	U
1	AR	3156	U
1	AR	3157	U

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Mol	Chain	Res	Type
1	AR	3164	C
1	AR	3165	A
1	AR	3167	A
1	AR	3168	A
1	AR	3170	A
1	AR	3171	U
1	AR	3173	G
1	AR	3174	A
1	AR	3176	G
1	AR	3179	U
1	AR	3181	C
1	AR	3187	A
1	AR	3197	G
1	AR	3207	U
1	AR	3217	C
1	AR	3218	A
1	AR	3219	G
1	AR	3222	U
1	AR	3224	G
1	AR	3229	G
1	AR	3243	A
1	AR	3244	A
1	AR	3245	A
1	AR	3246	G
1	AR	3247	G
1	AR	3253	G
1	AR	3259	U
1	AR	3266	G
1	AR	3269	U
1	AR	3270	U
1	AR	3273	A
1	AR	3276	G
1	AR	3277	U
1	AR	3281	U
1	AR	3287	U
1	AR	3289	G
1	AR	3294	A
1	AR	3295	A
1	AR	3303	G
1	AR	3304	U
1	AR	3307	A
1	AR	3313	U

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Mol	Chain	Res	Type
1	AR	3316	A
1	AR	3317	U
1	AR	3318	G
1	AR	3319	U
1	AR	3320	A
1	AR	3330	A
1	AR	3341	U
1	AR	3342	A
1	AR	3345	G
1	AR	3347	A
1	AR	3350	C
1	AR	3351	U
1	AR	3352	U
1	AR	3353	G
1	AR	3355	U
1	AR	3356	G
1	AR	3359	A
1	AR	3369	G
1	AR	3375	A
1	AR	3378	C
1	AR	3383	G
1	AR	3389	U
2	AS	7	G
2	AS	22	A
2	AS	52	G
2	AS	53	U
2	AS	54	U
2	AS	60	G
2	AS	65	G
2	AS	73	C
2	AS	74	C
2	AS	99	G
2	AS	101	G
2	AS	102	A
2	AS	112	G
2	AS	121	U
3	AT	34	U
3	AT	35	C
3	AT	48	A
3	AT	51	G
3	AT	59	A
3	AT	62	C

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Mol	Chain	Res	Type
3	AT	63	G
3	AT	79	A
3	AT	80	A
3	AT	81	U
3	AT	82	U
3	AT	83	C
3	AT	85	G
3	AT	86	U
3	AT	87	G
3	AT	90	U
3	AT	95	G
3	AT	97	A
3	AT	104	A
3	AT	106	C
3	AT	111	A
3	AT	113	U
3	AT	125	U
3	AT	126	A
3	AT	148	G
3	AT	151	C
3	AT	152	G
3	AT	155	A
3	AT	158	U
25	A	2	A
25	A	4	C
25	A	17	C
25	A	25	C
25	A	26	A
25	A	27	U
25	A	34	G
25	A	42	G
25	A	45	U
25	A	46	A
25	A	47	A
25	A	50	C
25	A	57	G
25	A	60	U
25	A	67	A
25	A	68	A
25	A	69	G
25	A	72	A
25	A	73	U

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Mol	Chain	Res	Type
25	A	74	U
25	A	104	A
25	A	114	C
25	A	116	U
25	A	128	U
25	A	130	C
25	A	131	C
25	A	132	U
25	A	133	U
25	A	134	U
25	A	135	A
25	A	136	C
25	A	137	U
25	A	140	A
25	A	141	U
25	A	144	U
25	A	145	A
25	A	146	U
25	A	153	G
25	A	158	U
25	A	159	U
25	A	161	U
25	A	176	C
25	A	178	U
25	A	179	A
25	A	185	U
25	A	186	C
25	A	187	G
25	A	188	A
25	A	190	C
25	A	191	C
25	A	192	U
25	A	193	U
25	A	194	U
25	A	195	G
25	A	196	G
25	A	197	A
25	A	200	A
25	A	215	A
25	A	217	A
25	A	218	A
25	A	219	A

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Mol	Chain	Res	Type
25	A	226	A
25	A	227	U
25	A	228	G
25	A	229	U
25	A	233	C
25	A	234	G
25	A	235	G
25	A	238	U
25	A	240	U
25	A	241	U
25	A	250	C
25	A	260	U
25	A	261	U
25	A	265	A
25	A	271	A
25	A	272	U
25	A	274	G
25	A	275	C
25	A	276	C
25	A	277	U
25	A	278	U
25	A	279	G
25	A	280	U
25	A	281	G
25	A	284	G
25	A	288	A
25	A	290	G
25	A	299	A
25	A	308	C
25	A	309	C
25	A	314	C
25	A	316	A
25	A	319	U
25	A	321	C
25	A	322	G
25	A	337	G
25	A	338	C
25	A	352	A
25	A	359	A
25	A	360	A
25	A	361	C
25	A	387	A

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Mol	Chain	Res	Type
25	A	390	G
25	A	400	A
25	A	402	C
25	A	403	G
25	A	404	G
25	A	416	A
25	A	418	G
25	A	424	C
25	A	425	A
25	A	426	G
25	A	428	A
25	A	434	G
25	A	439	U
25	A	444	C
25	A	445	A
25	A	448	C
25	A	454	U
25	A	468	A
25	A	480	G
25	A	484	C
25	A	485	A
25	A	488	G
25	A	493	U
25	A	494	U
25	A	495	C
25	A	496	G
25	A	497	G
25	A	498	G
25	A	499	U
25	A	500	C
25	A	502	U
25	A	503	G
25	A	504	U
25	A	505	A
25	A	506	A
25	A	507	U
25	A	510	G
25	A	511	A
25	A	512	A
25	A	513	U
25	A	515	A
25	A	516	G

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Mol	Chain	Res	Type
25	A	527	A
25	A	532	U
25	A	538	A
25	A	539	G
25	A	540	G
25	A	541	A
25	A	542	A
25	A	543	C
25	A	544	A
25	A	555	A
25	A	556	A
25	A	557	G
25	A	558	U
25	A	559	C
25	A	565	C
25	A	579	A
25	A	580	A
25	A	583	C
25	A	594	A
25	A	595	G
25	A	606	A
25	A	611	U
25	A	619	A
25	A	620	A
25	A	621	A
25	A	622	A
25	A	623	A
25	A	624	G
25	A	639	U
25	A	640	U
25	A	650	U
25	A	653	C
25	A	654	C
25	A	655	G
25	A	656	G
25	A	658	C
25	A	677	G
25	A	679	U
25	A	684	A
25	A	685	A
25	A	686	C
25	A	692	C

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Mol	Chain	Res	Type
25	A	694	U
25	A	696	C
25	A	697	C
25	A	700	C
25	A	702	G
25	A	703	G
25	A	704	C
25	A	705	U
25	A	707	A
25	A	708	C
25	A	709	C
25	A	710	U
25	A	711	U
25	A	712	G
25	A	714	G
25	A	717	C
25	A	718	U
25	A	719	U
25	A	721	U
25	A	722	G
25	A	723	G
25	A	725	U
25	A	727	U
25	A	728	U
25	A	731	C
25	A	732	G
25	A	733	A
25	A	734	A
25	A	735	C
25	A	736	C
25	A	737	A
25	A	738	G
25	A	742	U
25	A	743	U
25	A	745	U
25	A	754	A
25	A	755	A
25	A	756	A
25	A	765	G
25	A	766	U
25	A	774	A
25	A	775	G

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Mol	Chain	Res	Type
25	A	778	G
25	A	780	A
25	A	781	U
25	A	783	G
25	A	784	C
25	A	789	A
25	A	794	U
25	A	812	A
25	A	814	A
25	A	815	G
25	A	816	G
25	A	818	C
25	A	819	G
25	A	820	U
25	A	821	U
25	A	822	U
25	A	824	G
25	A	830	U
25	A	831	U
25	A	833	U
25	A	862	A
25	A	863	A
25	A	864	U
25	A	886	U
25	A	898	A
25	A	912	U
25	A	913	G
25	A	914	G
25	A	915	A
25	A	916	U
25	A	928	U
25	A	933	A
25	A	935	U
25	A	942	G
25	A	951	A
25	A	960	U
25	A	966	A
25	A	988	A
25	A	991	G
25	A	992	A
25	A	993	A
25	A	1003	A

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Mol	Chain	Res	Type
25	A	1004	U
25	A	1005	A
25	A	1020	A
25	A	1026	A
25	A	1028	C
25	A	1039	A
25	A	1040	G
25	A	1052	U
25	A	1053	G
25	A	1058	U
25	A	1061	A
25	A	1074	G
25	A	1076	A
25	A	1080	U
25	A	1082	C
25	A	1091	A
25	A	1092	A
25	A	1093	A
25	A	1096	C
25	A	1097	U
25	A	1100	G
25	A	1109	G
25	A	1111	G
25	A	1138	A
25	A	1146	G
25	A	1150	G
25	A	1151	A
25	A	1157	A
25	A	1158	C
25	A	1160	A
25	A	1164	G
25	A	1167	G
25	A	1185	U
25	A	1194	A
25	A	1196	A
25	A	1197	C
25	A	1199	G
25	A	1200	G
25	A	1202	A
25	A	1207	C
25	A	1208	A
25	A	1217	A

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Mol	Chain	Res	Type
25	A	1218	G
25	A	1227	A
25	A	1229	G
25	A	1243	G
25	A	1244	A
25	A	1245	G
25	A	1251	U
25	A	1256	A
25	A	1257	U
25	A	1258	U
25	A	1286	U
25	A	1314	U
25	A	1315	U
25	A	1321	A
25	A	1339	C
25	A	1340	U
25	A	1341	A
25	A	1344	A
25	A	1345	A
25	A	1349	G
25	A	1354	G
25	A	1361	U
25	A	1362	U
25	A	1363	U
25	A	1364	G
25	A	1370	U
25	A	1371	A
25	A	1372	U
25	A	1390	U
25	A	1398	U
25	A	1399	C
25	A	1400	A
25	A	1412	G
25	A	1413	U
25	A	1415	U
25	A	1427	A
25	A	1428	G
25	A	1446	A
25	A	1458	G
25	A	1459	C
25	A	1461	C
25	A	1471	A

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Mol	Chain	Res	Type
25	A	1473	U
25	A	1474	G
25	A	1475	A
25	A	1482	C
25	A	1486	G
25	A	1490	C
25	A	1491	U
25	A	1492	A
25	A	1493	A
25	A	1506	G
25	A	1515	A
25	A	1516	A
25	A	1517	U
25	A	1521	G
25	A	1523	G
25	A	1524	A
25	A	1526	A
25	A	1535	U
25	A	1536	G
25	A	1537	C
25	A	1538	U
25	A	1542	G
25	A	1557	U
25	A	1559	A
25	A	1569	A
25	A	1574	G
25	A	1584	G
25	A	1590	G
25	A	1601	G
25	A	1614	A
25	A	1616	G
25	A	1619	C
25	A	1624	C
25	A	1626	U
25	A	1631	A
25	A	1657	U
25	A	1658	G
25	A	1680	G
25	A	1683	C
25	A	1684	U
25	A	1686	C
25	A	1698	G

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Mol	Chain	Res	Type
25	A	1699	G
25	A	1700	C
25	A	1701	A
25	A	1702	A
25	A	1703	C
25	A	1711	C
25	A	1712	A
25	A	1713	G
25	A	1731	A
25	A	1750	A
25	A	1760	G
25	A	1762	A
25	A	1766	A
25	A	1769	U
25	A	1780	G
25	A	1782	A
25	A	1783	C
25	A	1792	G
25	A	1793	G
25	A	1794	A
25	A	1795	U
25	A	1796	C

All (186) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	65	A
1	1	210	U
1	1	239	G
1	1	282	G
1	1	547	G
1	1	647	A
1	1	763	G
1	1	873	C
1	1	916	G
1	1	979	U
1	1	981	U
1	1	993	G
1	1	1064	A
1	1	1094	U
1	1	1097	G
1	1	1273	A

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Mol	Chain	Res	Type
1	1	1307	G
1	1	1329	U
1	1	1352	A
1	1	1355	A
1	1	1562	C
1	1	1568	U
1	1	1716	U
1	1	1820	U
1	1	2101	C
1	1	2112	U
1	1	2209	U
1	1	2249	G
1	1	2372	A
1	1	2418	G
1	1	2537	U
1	1	2541	U
1	1	2593	A
1	1	2772	C
1	1	2801	A
1	1	2818	U
1	1	3056	U
1	1	3078	U
1	1	3121	U
1	1	3218	A
1	1	3228	C
1	1	3269	U
1	1	3350	C
1	1	3351	U
1	1	3353	G
1	1	3375	A
3	4	85	G
3	4	125	U
25	6	25	C
25	6	139	C
25	6	145	A
25	6	158	U
25	6	187	G
25	6	192	U
25	6	217	A
25	6	272	U
25	6	417	A
25	6	512	A

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Mol	Chain	Res	Type
25	6	542	A
25	6	558	U
25	6	678	A
25	6	755	A
25	6	829	A
25	6	834	G
25	6	1051	G
25	6	1058	U
25	6	1081	A
25	6	1097	U
25	6	1207	C
25	6	1244	A
25	6	1255	G
25	6	1344	A
25	6	1481	C
25	6	1489	U
25	6	1491	U
25	6	1535	U
25	6	1568	C
25	6	1573	A
25	6	1620	C
25	6	1657	U
1	AR	40	A
1	AR	65	A
1	AR	588	G
1	AR	637	C
1	AR	715	A
1	AR	763	G
1	AR	873	C
1	AR	916	G
1	AR	979	U
1	AR	981	U
1	AR	993	G
1	AR	1064	A
1	AR	1097	G
1	AR	1103	A
1	AR	1238	C
1	AR	1241	U
1	AR	1284	C
1	AR	1307	G
1	AR	1329	U
1	AR	1331	U

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Mol	Chain	Res	Type
1	AR	1352	A
1	AR	1355	A
1	AR	1554	U
1	AR	1562	C
1	AR	1589	A
1	AR	1716	U
1	AR	1815	U
1	AR	1816	A
1	AR	1820	U
1	AR	1846	C
1	AR	2101	C
1	AR	2112	U
1	AR	2209	U
1	AR	2252	A
1	AR	2255	A
1	AR	2260	U
1	AR	2269	U
1	AR	2373	A
1	AR	2374	C
1	AR	2404	A
1	AR	2418	G
1	AR	2537	U
1	AR	2541	U
1	AR	2593	A
1	AR	2728	G
1	AR	2801	A
1	AR	2818	U
1	AR	2872	A
1	AR	3078	U
1	AR	3121	U
1	AR	3218	A
1	AR	3228	C
1	AR	3269	U
1	AR	3276	G
1	AR	3316	A
1	AR	3317	U
1	AR	3350	C
1	AR	3375	A
2	AS	52	G
3	AT	82	U
3	AT	85	G
25	A	25	C

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Mol	Chain	Res	Type
25	A	45	U
25	A	73	U
25	A	130	C
25	A	131	C
25	A	139	C
25	A	158	U
25	A	187	G
25	A	218	A
25	A	240	U
25	A	278	U
25	A	280	U
25	A	417	A
25	A	497	G
25	A	499	U
25	A	501	U
25	A	503	G
25	A	512	A
25	A	555	A
25	A	685	A
25	A	704	C
25	A	720	G
25	A	721	U
25	A	755	A
25	A	829	A
25	A	1051	G
25	A	1081	A
25	A	1150	G
25	A	1157	A
25	A	1196	A
25	A	1207	C
25	A	1226	A
25	A	1244	A
25	A	1250	U
25	A	1344	A
25	A	1370	U
25	A	1481	C
25	A	1489	U
25	A	1568	C
25	A	1573	A
25	A	1600	A
25	A	1615	C
25	A	1657	U

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Mol	Chain	Res	Type
25	A	1698	G
25	A	1761	U

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2548 ligands modelled in this entry, 1 is modelled with single atom and 1477 are monoatomic - leaving 1070 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
84	OHX	AR	3514	-	0,6,6	-	-	-		
84	OHX	1	3655	-	0,6,6	-	-	-		
84	OHX	AR	3520	-	0,6,6	-	-	-		
84	OHX	AR	3676	-	0,6,6	-	-	-		
84	OHX	1	3587	-	0,6,6	-	-	-		
84	OHX	6	1947	-	0,6,6	-	-	-		
84	OHX	AR	3415	-	0,6,6	-	-	-		
84	OHX	AR	3618	-	0,6,6	-	-	-		
84	OHX	AR	3518	-	0,6,6	-	-	-		
84	OHX	A	1997	-	0,6,6	-	-	-		
84	OHX	1	3677	-	0,6,6	-	-	-		
84	OHX	AR	3461	-	0,6,6	-	-	-		
84	OHX	AR	3496	-	0,6,6	-	-	-		
84	OHX	AR	3716	-	0,6,6	-	-	-		
84	OHX	AR	3705	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3457	-	0,6,6	-	-	-		
84	OHX	AT	216	-	0,6,6	-	-	-		
84	OHX	AR	3506	-	0,6,6	-	-	-		
84	OHX	1	3571	-	0,6,6	-	-	-		
84	OHX	AR	3574	-	0,6,6	-	-	-		
84	OHX	A	1929	-	0,6,6	-	-	-		
84	OHX	A	1965	-	0,6,6	-	-	-		
84	OHX	1	3488	-	0,6,6	-	-	-		
84	OHX	1	401	-	0,6,6	-	-	-		
84	OHX	6	1919	-	0,6,6	-	-	-		
84	OHX	1	3539	84	0,6,6	-	-	-		
84	OHX	1	3654	-	0,6,6	-	-	-		
84	OHX	4	214	-	0,6,6	-	-	-		
84	OHX	1	3683	-	0,6,6	-	-	-		
84	OHX	6	1942	-	0,6,6	-	-	-		
84	OHX	6	1985	-	0,6,6	-	-	-		
84	OHX	AR	3549	-	0,6,6	-	-	-		
84	OHX	AR	3635	-	0,6,6	-	-	-		
84	OHX	AR	3666	-	0,6,6	-	-	-		
84	OHX	AR	3668	-	0,6,6	-	-	-		
84	OHX	AR	3689	-	0,6,6	-	-	-		
84	OHX	AR	3715	-	0,6,6	-	-	-		
84	OHX	6	1977	-	0,6,6	-	-	-		
84	OHX	AR	3631	-	0,6,6	-	-	-		
84	OHX	1	3438	-	0,6,6	-	-	-		
84	OHX	1	3673	-	0,6,6	-	-	-		
84	OHX	1	3501	-	0,6,6	-	-	-		
84	OHX	AR	3439	-	0,6,6	-	-	-		
84	OHX	1	3724	-	0,6,6	-	-	-		
84	OHX	1	3441	-	0,6,6	-	-	-		
84	OHX	AR	3723	-	0,6,6	-	-	-		
84	OHX	A	1998	-	0,6,6	-	-	-		
84	OHX	AR	3691	-	0,6,6	-	-	-		
84	OHX	AR	3599	-	0,6,6	-	-	-		
84	OHX	AR	3617	-	0,6,6	-	-	-		
84	OHX	1	3482	-	0,6,6	-	-	-		
84	OHX	1	3546	-	0,6,6	-	-	-		
84	OHX	1	3665	-	0,6,6	-	-	-		
84	OHX	AR	3582	-	0,6,6	-	-	-		
84	OHX	CM	201	-	0,6,6	-	-	-		
84	OHX	6	2026	-	0,6,6	-	-	-		
84	OHX	A	2036	-	0,6,6	-	-	-		
84	OHX	1	3451	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3607	-	0,6,6	-	-	-		
84	OHX	AR	3641	-	0,6,6	-	-	-		
84	OHX	AR	3678	-	0,6,6	-	-	-		
84	OHX	AR	3679	-	0,6,6	-	-	-		
84	OHX	6	2038	-	0,6,6	-	-	-		
84	OHX	AT	202	-	0,6,6	-	-	-		
84	OHX	1	3444	-	0,6,6	-	-	-		
84	OHX	1	3522	-	0,6,6	-	-	-		
84	OHX	AR	3494	-	0,6,6	-	-	-		
84	OHX	AS	201	-	0,6,6	-	-	-		
84	OHX	1	3580	-	0,6,6	-	-	-		
84	OHX	AR	3687	-	0,6,6	-	-	-		
84	OHX	1	3711	-	0,6,6	-	-	-		
84	OHX	AS	203	-	0,6,6	-	-	-		
84	OHX	A	1943	-	0,6,6	-	-	-		
84	OHX	1	3584	-	0,6,6	-	-	-		
84	OHX	1	3478	-	0,6,6	-	-	-		
84	OHX	CE	402	-	0,6,6	-	-	-		
84	OHX	1	3547	-	0,6,6	-	-	-		
84	OHX	6	1936	-	0,6,6	-	-	-		
84	OHX	1	3615	-	0,6,6	-	-	-		
84	OHX	6	1955	-	0,6,6	-	-	-		
84	OHX	AR	3438	-	0,6,6	-	-	-		
84	OHX	AR	3728	-	0,6,6	-	-	-		
84	OHX	6	1935	-	0,6,6	-	-	-		
84	OHX	1	3633	-	0,6,6	-	-	-		
84	OHX	A	1921	-	0,6,6	-	-	-		
84	OHX	A	1933	-	0,6,6	-	-	-		
84	OHX	A	1918	-	0,6,6	-	-	-		
84	OHX	AR	3486	-	0,6,6	-	-	-		
84	OHX	1	3691	-	0,6,6	-	-	-		
84	OHX	1	3567	-	0,6,6	-	-	-		
84	OHX	1	3436	-	0,6,6	-	-	-		
84	OHX	AR	3483	-	0,6,6	-	-	-		
84	OHX	AR	3658	-	0,6,6	-	-	-		
84	OHX	1	3423	-	0,6,6	-	-	-		
84	OHX	A	1932	-	0,6,6	-	-	-		
84	OHX	6	2036	-	0,6,6	-	-	-		
84	OHX	AR	3725	-	0,6,6	-	-	-		
84	OHX	A	1945	-	0,6,6	-	-	-		
84	OHX	A	1908	-	0,6,6	-	-	-		
84	OHX	6	2027	-	0,6,6	-	-	-		
84	OHX	1	3432	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	2	201	-	0,6,6	-	-	-		
84	OHX	AR	3498	-	0,6,6	-	-	-		
84	OHX	1	3641	-	0,6,6	-	-	-		
84	OHX	A	1955	-	0,6,6	-	-	-		
84	OHX	AR	3703	-	0,6,6	-	-	-		
84	OHX	T	201	-	0,6,6	-	-	-		
84	OHX	AR	3737	-	0,6,6	-	-	-		
84	OHX	A	2019	-	0,6,6	-	-	-		
84	OHX	1	3569	-	0,6,6	-	-	-		
84	OHX	c5	201	-	0,6,6	-	-	-		
84	OHX	6	2004	-	0,6,6	-	-	-		
84	OHX	CX	202	-	0,6,6	-	-	-		
84	OHX	AM	101	-	0,6,6	-	-	-		
84	OHX	AR	3669	-	0,6,6	-	-	-		
84	OHX	z	201	-	0,6,6	-	-	-		
84	OHX	A	1968	-	0,6,6	-	-	-		
84	OHX	6	1933	-	0,6,6	-	-	-		
84	OHX	AR	3736	-	0,6,6	-	-	-		
84	OHX	A	2001	-	0,6,6	-	-	-		
84	OHX	6	1912	-	0,6,6	-	-	-		
84	OHX	6	1904	-	0,6,6	-	-	-		
84	OHX	AR	3481	-	0,6,6	-	-	-		
84	OHX	AR	3526	-	0,6,6	-	-	-		
84	OHX	1	3577	-	0,6,6	-	-	-		
84	OHX	AR	3487	-	0,6,6	-	-	-		
84	OHX	6	1910	-	0,6,6	-	-	-		
84	OHX	6	1950	-	0,6,6	-	-	-		
84	OHX	1	3671	-	0,6,6	-	-	-		
84	OHX	AR	3719	-	0,6,6	-	-	-		
84	OHX	A	2018	-	0,6,6	-	-	-		
84	OHX	1	3585	-	0,6,6	-	-	-		
84	OHX	AR	3653	-	0,6,6	-	-	-		
84	OHX	1	3469	-	0,6,6	-	-	-		
84	OHX	6	1993	-	0,6,6	-	-	-		
84	OHX	A	2008	-	0,6,6	-	-	-		
84	OHX	AR	3401	-	0,6,6	-	-	-		
84	OHX	1	3428	-	0,6,6	-	-	-		
84	OHX	AR	3411	-	0,6,6	-	-	-		
84	OHX	A	1996	-	0,6,6	-	-	-		
84	OHX	A	2014	-	0,6,6	-	-	-		
84	OHX	1	3570	-	0,6,6	-	-	-		
84	OHX	1	3592	-	0,6,6	-	-	-		
84	OHX	AT	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3742	-	0,6,6	-	-	-		
84	OHX	AR	3722	-	0,6,6	-	-	-		
84	OHX	6	1971	-	0,6,6	-	-	-		
84	OHX	6	2013	-	0,6,6	-	-	-		
84	OHX	1	3714	-	0,6,6	-	-	-		
84	OHX	AR	3402	-	0,6,6	-	-	-		
84	OHX	1	3640	-	0,6,6	-	-	-		
84	OHX	6	2017	-	0,6,6	-	-	-		
84	OHX	1	3510	-	0,6,6	-	-	-		
84	OHX	A	2024	-	0,6,6	-	-	-		
84	OHX	A	1917	-	0,6,6	-	-	-		
84	OHX	1	3427	-	0,6,6	-	-	-		
84	OHX	A	1950	-	0,6,6	-	-	-		
84	OHX	1	3551	-	0,6,6	-	-	-		
84	OHX	6	1991	-	0,6,6	-	-	-		
84	OHX	1	3598	-	0,6,6	-	-	-		
84	OHX	1	3549	-	0,6,6	-	-	-		
84	OHX	1	3606	-	0,6,6	-	-	-		
84	OHX	1	3678	-	0,6,6	-	-	-		
84	OHX	x	201	-	0,6,6	-	-	-		
84	OHX	1	3564	-	0,6,6	-	-	-		
84	OHX	AR	3667	-	0,6,6	-	-	-		
84	OHX	AR	3626	-	0,6,6	-	-	-		
84	OHX	AR	3474	-	0,6,6	-	-	-		
84	OHX	AR	3596	-	0,6,6	-	-	-		
84	OHX	1	3705	-	0,6,6	-	-	-		
84	OHX	AR	3462	-	0,6,6	-	-	-		
84	OHX	A	1913	-	0,6,6	-	-	-		
84	OHX	1	3707	-	0,6,6	-	-	-		
84	OHX	6	1902	-	0,6,6	-	-	-		
84	OHX	AR	3660	-	0,6,6	-	-	-		
84	OHX	AR	3629	-	0,6,6	-	-	-		
84	OHX	AR	3627	-	0,6,6	-	-	-		
84	OHX	AR	3663	-	0,6,6	-	-	-		
84	OHX	AR	3657	-	0,6,6	-	-	-		
84	OHX	1	3662	-	0,6,6	-	-	-		
84	OHX	1	3532	-	0,6,6	-	-	-		
84	OHX	A	1949	-	0,6,6	-	-	-		
84	OHX	1	3676	-	0,6,6	-	-	-		
84	OHX	AR	3581	-	0,6,6	-	-	-		
84	OHX	6	2011	-	0,6,6	-	-	-		
84	OHX	6	2051	-	0,6,6	-	-	-		
84	OHX	CF	401	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3697	84	0,6,6	-	-	-		
84	OHX	A	2004	-	0,6,6	-	-	-		
84	OHX	AR	3673	-	0,6,6	-	-	-		
84	OHX	1	3404	-	0,6,6	-	-	-		
84	OHX	AR	3682	-	0,6,6	-	-	-		
84	OHX	1	3477	-	0,6,6	-	-	-		
84	OHX	AR	3463	-	0,6,6	-	-	-		
84	OHX	AR	3579	-	0,6,6	-	-	-		
84	OHX	1	3408	-	0,6,6	-	-	-		
84	OHX	1	3646	-	0,6,6	-	-	-		
84	OHX	1	3555	-	0,6,6	-	-	-		
84	OHX	AR	3572	-	0,6,6	-	-	-		
84	OHX	AT	204	-	0,6,6	-	-	-		
84	OHX	6	1957	-	0,6,6	-	-	-		
84	OHX	AR	3638	-	0,6,6	-	-	-		
84	OHX	1	3520	-	0,6,6	-	-	-		
84	OHX	4	203	-	0,6,6	-	-	-		
84	OHX	1	3723	1	0,6,6	-	-	-		
84	OHX	1	3631	-	0,6,6	-	-	-		
84	OHX	AT	207	-	0,6,6	-	-	-		
84	OHX	A	2021	-	0,6,6	-	-	-		
84	OHX	1	3417	-	0,6,6	-	-	-		
84	OHX	A	1962	-	0,6,6	-	-	-		
84	OHX	1	3660	-	0,6,6	-	-	-		
84	OHX	1	3704	-	0,6,6	-	-	-		
86	HN8	1	4223	-	24,26,26	0.28	0	36,41,41	1.03	2 (5%)
84	OHX	AR	3683	-	0,6,6	-	-	-		
84	OHX	1	3548	-	0,6,6	-	-	-		
84	OHX	AR	3435	-	0,6,6	-	-	-		
84	OHX	AR	3733	-	0,6,6	-	-	-		
84	OHX	1	3599	-	0,6,6	-	-	-		
84	OHX	AR	3686	-	0,6,6	-	-	-		
84	OHX	1	3466	-	0,6,6	-	-	-		
84	OHX	1	3573	-	0,6,6	-	-	-		
84	OHX	1	3559	-	0,6,6	-	-	-		
84	OHX	1	3562	-	0,6,6	-	-	-		
84	OHX	1	3651	-	0,6,6	-	-	-		
84	OHX	6	1995	-	0,6,6	-	-	-		
84	OHX	1	3602	-	0,6,6	-	-	-		
84	OHX	6	1980	-	0,6,6	-	-	-		
84	OHX	AR	3451	-	0,6,6	-	-	-		
84	OHX	1	3462	-	0,6,6	-	-	-		
84	OHX	AR	3407	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3416	-	0,6,6	-	-	-		
84	OHX	AR	3591	-	0,6,6	-	-	-		
84	OHX	4	215	-	0,6,6	-	-	-		
84	OHX	A	2042	-	0,6,6	-	-	-		
84	OHX	1	3625	-	0,6,6	-	-	-		
84	OHX	h	401	-	0,6,6	-	-	-		
84	OHX	1	3443	-	0,6,6	-	-	-		
84	OHX	1	3680	-	0,6,6	-	-	-		
84	OHX	AR	3433	-	0,6,6	-	-	-		
84	OHX	AR	3484	-	0,6,6	-	-	-		
84	OHX	AR	3616	-	0,6,6	-	-	-		
84	OHX	AR	3632	-	0,6,6	-	-	-		
84	OHX	AR	3702	-	0,6,6	-	-	-		
84	OHX	6	2044	-	0,6,6	-	-	-		
84	OHX	AR	3623	-	0,6,6	-	-	-		
84	OHX	AS	210	-	0,6,6	-	-	-		
84	OHX	1	3706	-	0,6,6	-	-	-		
84	OHX	A	1960	-	0,6,6	-	-	-		
84	OHX	1	3581	-	0,6,6	-	-	-		
84	OHX	1	3653	-	0,6,6	-	-	-		
84	OHX	1	3715	-	0,6,6	-	-	-		
84	OHX	6	1982	-	0,6,6	-	-	-		
84	OHX	1	3622	-	0,6,6	-	-	-		
84	OHX	6	2032	-	0,6,6	-	-	-		
84	OHX	1	3540	-	0,6,6	-	-	-		
84	OHX	6	2021	-	0,6,6	-	-	-		
84	OHX	1	3410	-	0,6,6	-	-	-		
84	OHX	AR	3442	-	0,6,6	-	-	-		
84	OHX	1	3494	-	0,6,6	-	-	-		
84	OHX	AR	3588	-	0,6,6	-	-	-		
84	OHX	AR	3418	-	0,6,6	-	-	-		
84	OHX	AS	202	-	0,6,6	-	-	-		
84	OHX	A	1935	-	0,6,6	-	-	-		
84	OHX	AR	3539	-	0,6,6	-	-	-		
84	OHX	1	3716	-	0,6,6	-	-	-		
84	OHX	A	1990	-	0,6,6	-	-	-		
84	OHX	6	1965	-	0,6,6	-	-	-		
84	OHX	1	3670	-	0,6,6	-	-	-		
84	OHX	AR	3469	-	0,6,6	-	-	-		
84	OHX	CG	302	-	0,6,6	-	-	-		
84	OHX	1	3700	-	0,6,6	-	-	-		
84	OHX	6	1906	-	0,6,6	-	-	-		
84	OHX	AR	3489	87	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3542	-	0,6,6	-	-	-		
84	OHX	A	1947	-	0,6,6	-	-	-		
84	OHX	A	1978	-	0,6,6	-	-	-		
84	OHX	c8	201	-	0,6,6	-	-	-		
84	OHX	6	1939	-	0,6,6	-	-	-		
84	OHX	A	1982	-	0,6,6	-	-	-		
84	OHX	6	2050	-	0,6,6	-	-	-		
84	OHX	AR	3529	-	0,6,6	-	-	-		
84	OHX	AR	3562	-	0,6,6	-	-	-		
84	OHX	A	2025	-	0,6,6	-	-	-		
84	OHX	AR	3422	-	0,6,6	-	-	-		
84	OHX	AR	3624	-	0,6,6	-	-	-		
84	OHX	AR	3650	-	0,6,6	-	-	-		
84	OHX	AS	206	-	0,6,6	-	-	-		
84	OHX	1	3583	-	0,6,6	-	-	-		
84	OHX	AR	3665	-	0,6,6	-	-	-		
84	OHX	y	201	-	0,6,6	-	-	-		
84	OHX	AR	3744	-	0,6,6	-	-	-		
84	OHX	AR	3611	-	0,6,6	-	-	-		
84	OHX	AR	3534	-	0,6,6	-	-	-		
84	OHX	3	208	-	0,6,6	-	-	-		
84	OHX	AR	3590	-	0,6,6	-	-	-		
84	OHX	A	2022	-	0,6,6	-	-	-		
84	OHX	1	3456	-	0,6,6	-	-	-		
84	OHX	AR	3730	-	0,6,6	-	-	-		
84	OHX	1	3554	-	0,6,6	-	-	-		
84	OHX	A	2006	-	0,6,6	-	-	-		
84	OHX	AR	3540	-	0,6,6	-	-	-		
84	OHX	1	3667	-	0,6,6	-	-	-		
84	OHX	1	3527	-	0,6,6	-	-	-		
84	OHX	6	1998	-	0,6,6	-	-	-		
84	OHX	AR	3429	-	0,6,6	-	-	-		
84	OHX	6	1981	-	0,6,6	-	-	-		
84	OHX	AR	3585	-	0,6,6	-	-	-		
84	OHX	AR	3681	-	0,6,6	-	-	-		
84	OHX	AR	3675	-	0,6,6	-	-	-		
84	OHX	AR	3426	-	0,6,6	-	-	-		
84	OHX	AR	3659	-	0,6,6	-	-	-		
84	OHX	A	1942	-	0,6,6	-	-	-		
84	OHX	6	2023	-	0,6,6	-	-	-		
84	OHX	AR	3656	-	0,6,6	-	-	-		
84	OHX	1	3550	-	0,6,6	-	-	-		
84	OHX	AR	3525	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3538	-	0,6,6	-	-	-		
84	OHX	A	1906	-	0,6,6	-	-	-		
84	OHX	AR	3499	-	0,6,6	-	-	-		
84	OHX	1	3531	-	0,6,6	-	-	-		
84	OHX	1	3718	-	0,6,6	-	-	-		
84	OHX	AR	3727	-	0,6,6	-	-	-		
84	OHX	1	3515	-	0,6,6	-	-	-		
84	OHX	1	3605	-	0,6,6	-	-	-		
84	OHX	1	3664	-	0,6,6	-	-	-		
84	OHX	1	3600	-	0,6,6	-	-	-		
84	OHX	A	1903	-	0,6,6	-	-	-		
84	OHX	6	1967	-	0,6,6	-	-	-		
84	OHX	AR	3557	-	0,6,6	-	-	-		
84	OHX	AS	211	-	0,6,6	-	-	-		
84	OHX	A	1963	-	0,6,6	-	-	-		
84	OHX	6	1964	-	0,6,6	-	-	-		
84	OHX	A	1988	-	0,6,6	-	-	-		
84	OHX	6	1984	-	0,6,6	-	-	-		
84	OHX	3	204	-	0,6,6	-	-	-		
84	OHX	6	2034	-	0,6,6	-	-	-		
84	OHX	1	3720	-	0,6,6	-	-	-		
84	OHX	6	1988	-	0,6,6	-	-	-		
84	OHX	1	3578	-	0,6,6	-	-	-		
84	OHX	1	3702	-	0,6,6	-	-	-		
84	OHX	1	3458	-	0,6,6	-	-	-		
84	OHX	1	3675	-	0,6,6	-	-	-		
84	OHX	1	3447	-	0,6,6	-	-	-		
84	OHX	AR	3428	-	0,6,6	-	-	-		
84	OHX	AR	3565	-	0,6,6	-	-	-		
84	OHX	AR	3739	-	0,6,6	-	-	-		
84	OHX	1	3626	-	0,6,6	-	-	-		
84	OHX	A	1938	-	0,6,6	-	-	-		
84	OHX	1	3541	-	0,6,6	-	-	-		
84	OHX	6	1926	-	0,6,6	-	-	-		
84	OHX	1	3657	-	0,6,6	-	-	-		
84	OHX	1	3476	-	0,6,6	-	-	-		
84	OHX	1	3635	-	0,6,6	-	-	-		
84	OHX	1	3514	-	0,6,6	-	-	-		
84	OHX	AR	3674	-	0,6,6	-	-	-		
84	OHX	A	1902	-	0,6,6	-	-	-		
84	OHX	AR	3712	-	0,6,6	-	-	-		
84	OHX	1	3411	-	0,6,6	-	-	-		
84	OHX	6	1940	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3439	-	0,6,6	-	-	-		
84	OHX	6	2016	-	0,6,6	-	-	-		
84	OHX	A	1966	-	0,6,6	-	-	-		
84	OHX	1	3699	-	0,6,6	-	-	-		
84	OHX	1	3496	-	0,6,6	-	-	-		
84	OHX	AR	3477	84	0,6,6	-	-	-		
84	OHX	AR	3471	-	0,6,6	-	-	-		
84	OHX	1	3473	-	0,6,6	-	-	-		
84	OHX	1	3457	-	0,6,6	-	-	-		
84	OHX	AR	3510	-	0,6,6	-	-	-		
84	OHX	AR	3555	-	0,6,6	-	-	-		
84	OHX	AR	3551	-	0,6,6	-	-	-		
84	OHX	AT	212	-	0,6,6	-	-	-		
84	OHX	1	3519	-	0,6,6	-	-	-		
84	OHX	1	3545	-	0,6,6	-	-	-		
84	OHX	6	1945	-	0,6,6	-	-	-		
84	OHX	AR	3558	-	0,6,6	-	-	-		
84	OHX	AR	3701	-	0,6,6	-	-	-		
84	OHX	A	1951	-	0,6,6	-	-	-		
84	OHX	AR	3694	-	0,6,6	-	-	-		
84	OHX	6	1911	-	0,6,6	-	-	-		
84	OHX	AR	3493	-	0,6,6	-	-	-		
84	OHX	1	3689	-	0,6,6	-	-	-		
84	OHX	4	216	-	0,6,6	-	-	-		
84	OHX	6	2009	-	0,6,6	-	-	-		
84	OHX	6	2018	-	0,6,6	-	-	-		
84	OHX	1	3472	-	0,6,6	-	-	-		
84	OHX	6	2037	-	0,6,6	-	-	-		
84	OHX	1	3572	-	0,6,6	-	-	-		
84	OHX	1	3623	-	0,6,6	-	-	-		
84	OHX	1	3629	-	0,6,6	-	-	-		
84	OHX	6	2046	-	0,6,6	-	-	-		
84	OHX	1	3674	-	0,6,6	-	-	-		
84	OHX	AR	3408	-	0,6,6	-	-	-		
84	OHX	AR	3414	-	0,6,6	-	-	-		
84	OHX	6	2048	-	0,6,6	-	-	-		
84	OHX	AR	3504	-	0,6,6	-	-	-		
84	OHX	A	1940	-	0,6,6	-	-	-		
84	OHX	1	3468	-	0,6,6	-	-	-		
84	OHX	6	1973	-	0,6,6	-	-	-		
84	OHX	AR	3453	-	0,6,6	-	-	-		
84	OHX	A	2017	-	0,6,6	-	-	-		
84	OHX	6	2005	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3491	-	0,6,6	-	-	-		
84	OHX	1	3644	-	0,6,6	-	-	-		
84	OHX	AR	3450	-	0,6,6	-	-	-		
84	OHX	AR	3521	-	0,6,6	-	-	-		
84	OHX	4	209	-	0,6,6	-	-	-		
84	OHX	6	1966	-	0,6,6	-	-	-		
84	OHX	1	3448	-	0,6,6	-	-	-		
84	OHX	AR	3619	-	0,6,6	-	-	-		
84	OHX	A	1989	-	0,6,6	-	-	-		
84	OHX	AR	3430	-	0,6,6	-	-	-		
84	OHX	6	1953	-	0,6,6	-	-	-		
84	OHX	A	2020	-	0,6,6	-	-	-		
84	OHX	1	3431	-	0,6,6	-	-	-		
84	OHX	CG	301	-	0,6,6	-	-	-		
84	OHX	A	2003	-	0,6,6	-	-	-		
84	OHX	A	1977	-	0,6,6	-	-	-		
84	OHX	1	3709	-	0,6,6	-	-	-		
84	OHX	A	2009	-	0,6,6	-	-	-		
84	OHX	A	1954	-	0,6,6	-	-	-		
84	OHX	1	3608	-	0,6,6	-	-	-		
84	OHX	AR	3655	-	0,6,6	-	-	-		
87	GOL	A	2160	-	5,5,5	0.10	0	5,5,5	0.29	0
84	OHX	r	301	-	0,6,6	-	-	-		
84	OHX	AR	3643	-	0,6,6	-	-	-		
84	OHX	1	3582	-	0,6,6	-	-	-		
84	OHX	AT	214	-	0,6,6	-	-	-		
84	OHX	A	1964	-	0,6,6	-	-	-		
84	OHX	6	1923	-	0,6,6	-	-	-		
84	OHX	1	3511	-	0,6,6	-	-	-		
84	OHX	AR	3649	-	0,6,6	-	-	-		
84	OHX	AT	211	-	0,6,6	-	-	-		
84	OHX	6	1951	-	0,6,6	-	-	-		
84	OHX	1	3690	-	0,6,6	-	-	-		
84	OHX	1	3497	-	0,6,6	-	-	-		
84	OHX	1	3628	-	0,6,6	-	-	-		
84	OHX	6	1986	-	0,6,6	-	-	-		
84	OHX	1	3425	-	0,6,6	-	-	-		
84	OHX	AR	3488	-	0,6,6	-	-	-		
84	OHX	1	3530	-	0,6,6	-	-	-		
84	OHX	A	1972	-	0,6,6	-	-	-		
84	OHX	A	2011	-	0,6,6	-	-	-		
84	OHX	6	1994	-	0,6,6	-	-	-		
84	OHX	1	3516	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3709	-	0,6,6	-	-	-		
84	OHX	AR	3405	-	0,6,6	-	-	-		
84	OHX	1	3642	-	0,6,6	-	-	-		
84	OHX	AR	3680	-	0,6,6	-	-	-		
84	OHX	AR	3651	-	0,6,6	-	-	-		
84	OHX	1	3498	-	0,6,6	-	-	-		
84	OHX	1	3566	-	0,6,6	-	-	-		
84	OHX	1	3703	-	0,6,6	-	-	-		
84	OHX	1	3588	-	0,6,6	-	-	-		
84	OHX	A	2027	-	0,6,6	-	-	-		
84	OHX	AR	3403	-	0,6,6	-	-	-		
84	OHX	6	2030	-	0,6,6	-	-	-		
84	OHX	AR	3625	-	0,6,6	-	-	-		
84	OHX	6	1974	-	0,6,6	-	-	-		
84	OHX	1	3669	-	0,6,6	-	-	-		
84	OHX	A	1952	-	0,6,6	-	-	-		
84	OHX	A	1986	-	0,6,6	-	-	-		
84	OHX	AR	3561	-	0,6,6	-	-	-		
84	OHX	A	1971	-	0,6,6	-	-	-		
84	OHX	6	2020	-	0,6,6	-	-	-		
84	OHX	A	1993	-	0,6,6	-	-	-		
84	OHX	A	1936	-	0,6,6	-	-	-		
84	OHX	1	3464	-	0,6,6	-	-	-		
84	OHX	AR	3607	-	0,6,6	-	-	-		
84	OHX	6	2035	-	0,6,6	-	-	-		
84	OHX	AR	3406	-	0,6,6	-	-	-		
84	OHX	6	1990	-	0,6,6	-	-	-		
84	OHX	AR	3434	-	0,6,6	-	-	-		
84	OHX	1	3405	-	0,6,6	-	-	-		
84	OHX	6	1938	-	0,6,6	-	-	-		
84	OHX	AR	3444	-	0,6,6	-	-	-		
84	OHX	AR	3465	-	0,6,6	-	-	-		
84	OHX	A	1957	-	0,6,6	-	-	-		
84	OHX	3	207	-	0,6,6	-	-	-		
84	OHX	AR	3536	-	0,6,6	-	-	-		
84	OHX	1	3713	-	0,6,6	-	-	-		
84	OHX	1	3401	-	0,6,6	-	-	-		
84	OHX	1	3446	-	0,6,6	-	-	-		
84	OHX	AR	3413	-	0,6,6	-	-	-		
84	OHX	AR	3554	-	0,6,6	-	-	-		
84	OHX	AR	3699	-	0,6,6	-	-	-		
84	OHX	1	3502	-	0,6,6	-	-	-		
84	OHX	AR	3580	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AS	207	-	0,6,6	-	-	-		
84	OHX	1	3686	-	0,6,6	-	-	-		
84	OHX	1	3534	-	0,6,6	-	-	-		
84	OHX	AR	3485	-	0,6,6	-	-	-		
84	OHX	A	1924	-	0,6,6	-	-	-		
84	OHX	AR	3700	-	0,6,6	-	-	-		
84	OHX	6	1972	-	0,6,6	-	-	-		
84	OHX	1	3656	-	0,6,6	-	-	-		
84	OHX	1	3529	-	0,6,6	-	-	-		
84	OHX	AR	3427	-	0,6,6	-	-	-		
84	OHX	6	2029	-	0,6,6	-	-	-		
84	OHX	6	2045	-	0,6,6	-	-	-		
84	OHX	1	3409	-	0,6,6	-	-	-		
84	OHX	A	2041	-	0,6,6	-	-	-		
84	OHX	6	1918	-	0,6,6	-	-	-		
84	OHX	A	1927	-	0,6,6	-	-	-		
84	OHX	6	1909	-	0,6,6	-	-	-		
84	OHX	AR	3513	-	0,6,6	-	-	-		
84	OHX	A	1958	-	0,6,6	-	-	-		
84	OHX	A	1923	-	0,6,6	-	-	-		
84	OHX	1	3538	-	0,6,6	-	-	-		
84	OHX	AR	3470	-	0,6,6	-	-	-		
84	OHX	AR	3556	-	0,6,6	-	-	-		
84	OHX	1	3424	-	0,6,6	-	-	-		
84	OHX	AR	3547	-	0,6,6	-	-	-		
84	OHX	AR	3519	-	0,6,6	-	-	-		
84	OHX	6	1992	-	0,6,6	-	-	-		
84	OHX	AR	3410	-	0,6,6	-	-	-		
84	OHX	6	2002	-	0,6,6	-	-	-		
84	OHX	1	3630	-	0,6,6	-	-	-		
84	OHX	AT	208	-	0,6,6	-	-	-		
84	OHX	A	1919	-	0,6,6	-	-	-		
84	OHX	AR	3597	-	0,6,6	-	-	-		
84	OHX	1	3442	-	0,6,6	-	-	-		
84	OHX	AR	3685	-	0,6,6	-	-	-		
84	OHX	AR	3695	-	0,6,6	-	-	-		
84	OHX	6	1915	-	0,6,6	-	-	-		
84	OHX	AR	3515	-	0,6,6	-	-	-		
84	OHX	AS	205	-	0,6,6	-	-	-		
84	OHX	1	3661	-	0,6,6	-	-	-		
84	OHX	CV	201	-	0,6,6	-	-	-		
84	OHX	A	1937	-	0,6,6	-	-	-		
84	OHX	1	3524	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3481	-	0,6,6	-	-	-		
84	OHX	1	3557	-	0,6,6	-	-	-		
84	OHX	AR	3569	-	0,6,6	-	-	-		
84	OHX	AT	203	-	0,6,6	-	-	-		
84	OHX	1	3415	-	0,6,6	-	-	-		
84	OHX	1	3603	-	0,6,6	-	-	-		
84	OHX	1	3556	-	0,6,6	-	-	-		
84	OHX	AR	3589	-	0,6,6	-	-	-		
84	OHX	AT	217	-	0,6,6	-	-	-		
84	OHX	AR	3664	-	0,6,6	-	-	-		
84	OHX	AT	213	-	0,6,6	-	-	-		
84	OHX	1	3509	-	0,6,6	-	-	-		
84	OHX	6	2019	-	0,6,6	-	-	-		
84	OHX	6	1931	-	0,6,6	-	-	-		
84	OHX	1	3505	-	0,6,6	-	-	-		
84	OHX	AR	3577	-	0,6,6	-	-	-		
84	OHX	AR	3460	-	0,6,6	-	-	-		
84	OHX	AR	3692	-	0,6,6	-	-	-		
84	OHX	AR	3417	-	0,6,6	-	-	-		
84	OHX	AR	3601	-	0,6,6	-	-	-		
84	OHX	A	2031	-	0,6,6	-	-	-		
84	OHX	6	1916	-	0,6,6	-	-	-		
84	OHX	6	2000	-	0,6,6	-	-	-		
84	OHX	AR	3621	-	0,6,6	-	-	-		
84	OHX	1	3579	-	0,6,6	-	-	-		
84	OHX	AR	3452	-	0,6,6	-	-	-		
84	OHX	1	3701	-	0,6,6	-	-	-		
84	OHX	AC	101	-	0,6,6	-	-	-		
84	OHX	A	1930	-	0,6,6	-	-	-		
84	OHX	6	2014	-	0,6,6	-	-	-		
84	OHX	A	1973	-	0,6,6	-	-	-		
84	OHX	AR	3454	-	0,6,6	-	-	-		
84	OHX	AR	3509	-	0,6,6	-	-	-		
84	OHX	AR	3741	-	0,6,6	-	-	-		
84	OHX	1	3561	-	0,6,6	-	-	-		
84	OHX	A	1931	-	0,6,6	-	-	-		
84	OHX	AR	3473	-	0,6,6	-	-	-		
84	OHX	AR	3706	-	0,6,6	-	-	-		
84	OHX	A	1987	-	0,6,6	-	-	-		
84	OHX	d9	101	-	0,6,6	-	-	-		
84	OHX	1	3461	-	0,6,6	-	-	-		
84	OHX	AR	3710	-	0,6,6	-	-	-		
84	OHX	6	2007	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3566	-	0,6,6	-	-	-		
84	OHX	AS	208	-	0,6,6	-	-	-		
84	OHX	1	3453	-	0,6,6	-	-	-		
84	OHX	A	1983	-	0,6,6	-	-	-		
84	OHX	AR	3608	-	0,6,6	-	-	-		
84	OHX	6	1917	-	0,6,6	-	-	-		
84	OHX	A	1992	-	0,6,6	-	-	-		
84	OHX	A	2029	-	0,6,6	-	-	-		
84	OHX	AR	3647	-	0,6,6	-	-	-		
84	OHX	AR	3423	-	0,6,6	-	-	-		
84	OHX	A	1961	-	0,6,6	-	-	-		
84	OHX	e	101	-	0,6,6	-	-	-		
84	OHX	1	3512	-	0,6,6	-	-	-		
84	OHX	1	3543	-	0,6,6	-	-	-		
84	OHX	1	3591	-	0,6,6	-	-	-		
84	OHX	AR	3482	-	0,6,6	-	-	-		
84	OHX	AR	3696	84	0,6,6	-	-	-		
84	OHX	6	2040	-	0,6,6	-	-	-		
84	OHX	AR	3495	-	0,6,6	-	-	-		
84	OHX	AR	3543	-	0,6,6	-	-	-		
84	OHX	AR	3503	-	0,6,6	-	-	-		
84	OHX	1	3617	-	0,6,6	-	-	-		
84	OHX	AR	3568	-	0,6,6	-	-	-		
84	OHX	A	1926	-	0,6,6	-	-	-		
84	OHX	6	2012	-	0,6,6	-	-	-		
84	OHX	1	3492	-	0,6,6	-	-	-		
84	OHX	1	3688	-	0,6,6	-	-	-		
84	OHX	CK	201	-	0,6,6	-	-	-		
84	OHX	1	3649	-	0,6,6	-	-	-		
84	OHX	1	3521	-	0,6,6	-	-	-		
84	OHX	AR	3693	-	0,6,6	-	-	-		
84	OHX	AR	3508	-	0,6,6	-	-	-		
84	OHX	A	2034	-	0,6,6	-	-	-		
84	OHX	AR	3404	-	0,6,6	-	-	-		
84	OHX	AR	3734	-	0,6,6	-	-	-		
84	OHX	A	2038	-	0,6,6	-	-	-		
84	OHX	6	1949	-	0,6,6	-	-	-		
84	OHX	6	1914	-	0,6,6	-	-	-		
84	OHX	6	1954	-	0,6,6	-	-	-		
84	OHX	1	3574	-	0,6,6	-	-	-		
84	OHX	AR	3517	-	0,6,6	-	-	-		
84	OHX	AR	3732	-	0,6,6	-	-	-		
84	OHX	1	3418	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3479	-	0,6,6	-	-	-		
84	OHX	1	3593	-	0,6,6	-	-	-		
84	OHX	1	3624	-	0,6,6	-	-	-		
84	OHX	1	3643	-	0,6,6	-	-	-		
84	OHX	6	1944	-	0,6,6	-	-	-		
84	OHX	AR	3628	-	0,6,6	-	-	-		
84	OHX	AS	204	-	0,6,6	-	-	-		
84	OHX	AR	3738	-	0,6,6	-	-	-		
84	OHX	A	2037	-	0,6,6	-	-	-		
84	OHX	1	3459	-	0,6,6	-	-	-		
84	OHX	1	3542	-	0,6,6	-	-	-		
84	OHX	6	2015	-	0,6,6	-	-	-		
84	OHX	6	1901	-	0,6,6	-	-	-		
84	OHX	A	1995	-	0,6,6	-	-	-		
84	OHX	6	1934	-	0,6,6	-	-	-		
84	OHX	A	1907	-	0,6,6	-	-	-		
84	OHX	AR	3613	-	0,6,6	-	-	-		
84	OHX	1	3616	-	0,6,6	-	-	-		
84	OHX	1	3596	-	0,6,6	-	-	-		
84	OHX	6	1943	-	0,6,6	-	-	-		
84	OHX	AR	3573	-	0,6,6	-	-	-		
84	OHX	1	3687	-	0,6,6	-	-	-		
84	OHX	1	3518	-	0,6,6	-	-	-		
84	OHX	A	1967	-	0,6,6	-	-	-		
84	OHX	1	3470	-	0,6,6	-	-	-		
87	GOL	AR	4261	1	5,5,5	0.14	0	5,5,5	0.33	0
84	OHX	1	3460	-	0,6,6	-	-	-		
84	OHX	AR	3502	-	0,6,6	-	-	-		
84	OHX	4	202	-	0,6,6	-	-	-		
84	OHX	6	1948	-	0,6,6	-	-	-		
84	OHX	6	1996	-	0,6,6	-	-	-		
84	OHX	AR	3633	-	0,6,6	-	-	-		
84	OHX	A	1953	-	0,6,6	-	-	-		
84	OHX	3	202	-	0,6,6	-	-	-		
84	OHX	AR	3552	-	0,6,6	-	-	-		
84	OHX	AR	3743	-	0,6,6	-	-	-		
84	OHX	6	2003	-	0,6,6	-	-	-		
84	OHX	AH	201	-	0,6,6	-	-	-		
84	OHX	AR	3731	-	0,6,6	-	-	-		
84	OHX	AR	3546	-	0,6,6	-	-	-		
84	OHX	J	301	-	0,6,6	-	-	-		
87	GOL	AR	4262	84	5,5,5	0.26	0	5,5,5	0.53	0
84	OHX	AR	3610	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3432	-	0,6,6	-	-	-		
84	OHX	6	1908	-	0,6,6	-	-	-		
84	OHX	6	1956	-	0,6,6	-	-	-		
84	OHX	4	206	-	0,6,6	-	-	-		
84	OHX	AR	3511	-	0,6,6	-	-	-		
84	OHX	AR	3505	-	0,6,6	-	-	-		
84	OHX	1	3467	-	0,6,6	-	-	-		
84	OHX	1	3475	-	0,6,6	-	-	-		
84	OHX	1	3696	-	0,6,6	-	-	-		
84	OHX	1	3681	-	0,6,6	-	-	-		
84	OHX	4	210	-	0,6,6	-	-	-		
84	OHX	6	1989	-	0,6,6	-	-	-		
84	OHX	AR	3448	-	0,6,6	-	-	-		
84	OHX	AR	3412	-	0,6,6	-	-	-		
84	OHX	AR	3537	-	0,6,6	-	-	-		
84	OHX	AR	3445	-	0,6,6	-	-	-		
84	OHX	AR	3522	-	0,6,6	-	-	-		
84	OHX	CP	501	-	0,6,6	-	-	-		
84	OHX	AR	3652	-	0,6,6	-	-	-		
84	OHX	A	2012	-	0,6,6	-	-	-		
87	GOL	6	2199	-	5,5,5	0.10	0	5,5,5	0.33	0
84	OHX	AR	3449	-	0,6,6	-	-	-		
84	OHX	AR	3576	-	0,6,6	-	-	-		
84	OHX	A	1916	-	0,6,6	-	-	-		
84	OHX	AR	3409	-	0,6,6	-	-	-		
84	OHX	AR	3604	-	0,6,6	-	-	-		
84	OHX	1	3692	-	0,6,6	-	-	-		
84	OHX	1	3499	-	0,6,6	-	-	-		
84	OHX	1	3487	-	0,6,6	-	-	-		
84	OHX	6	1959	-	0,6,6	-	-	-		
84	OHX	1	3420	-	0,6,6	-	-	-		
84	OHX	6	2031	-	0,6,6	-	-	-		
84	OHX	AR	3672	-	0,6,6	-	-	-		
84	OHX	1	3636	-	0,6,6	-	-	-		
84	OHX	1	3685	-	0,6,6	-	-	-		
84	OHX	K	201	-	0,6,6	-	-	-		
84	OHX	CL	301	-	0,6,6	-	-	-		
84	OHX	AR	3535	-	0,6,6	-	-	-		
84	OHX	A	2016	-	0,6,6	-	-	-		
84	OHX	1	3563	-	0,6,6	-	-	-		
84	OHX	A	2043	-	0,6,6	-	-	-		
84	OHX	1	3434	-	0,6,6	-	-	-		
84	OHX	M	201	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3466	-	0,6,6	-	-	-		
84	OHX	1	3679	-	0,6,6	-	-	-		
84	OHX	1	3449	-	0,6,6	-	-	-		
84	OHX	1	3544	-	0,6,6	-	-	-		
84	OHX	AT	210	-	0,6,6	-	-	-		
84	OHX	AG	201	-	0,6,6	-	-	-		
84	OHX	1	3609	-	0,6,6	-	-	-		
84	OHX	c4	201	-	0,6,6	-	-	-		
84	OHX	A	1911	-	0,6,6	-	-	-		
84	OHX	1	3612	-	0,6,6	-	-	-		
84	OHX	1	3586	-	0,6,6	-	-	-		
84	OHX	A	1984	-	0,6,6	-	-	-		
84	OHX	1	3480	-	0,6,6	-	-	-		
84	OHX	6	1903	-	0,6,6	-	-	-		
84	OHX	AR	3606	-	0,6,6	-	-	-		
84	OHX	1	3645	-	0,6,6	-	-	-		
84	OHX	AR	3500	-	0,6,6	-	-	-		
84	OHX	AR	3564	-	0,6,6	-	-	-		
84	OHX	1	3483	-	0,6,6	-	-	-		
84	OHX	1	3589	-	0,6,6	-	-	-		
84	OHX	1	3694	-	0,6,6	-	-	-		
84	OHX	A	1994	-	0,6,6	-	-	-		
84	OHX	6	1920	-	0,6,6	-	-	-		
84	OHX	AR	3662	-	0,6,6	-	-	-		
84	OHX	1	3440	-	0,6,6	-	-	-		
84	OHX	AR	3595	-	0,6,6	-	-	-		
84	OHX	6	2043	-	0,6,6	-	-	-		
84	OHX	1	3429	-	0,6,6	-	-	-		
84	OHX	6	2049	-	0,6,6	-	-	-		
84	OHX	AR	3594	-	0,6,6	-	-	-		
84	OHX	AR	3603	-	0,6,6	-	-	-		
84	OHX	AR	3637	-	0,6,6	-	-	-		
84	OHX	A	1948	-	0,6,6	-	-	-		
84	OHX	AR	3553	-	0,6,6	-	-	-		
84	OHX	3	203	-	0,6,6	-	-	-		
84	OHX	1	3601	-	0,6,6	-	-	-		
84	OHX	1	3455	-	0,6,6	-	-	-		
84	OHX	1	3658	-	0,6,6	-	-	-		
84	OHX	A	1970	-	0,6,6	-	-	-		
84	OHX	6	1921	-	0,6,6	-	-	-		
84	OHX	1	3450	-	0,6,6	-	-	-		
84	OHX	1	3619	-	0,6,6	-	-	-		
84	OHX	6	2047	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3584	-	0,6,6	-	-	-		
84	OHX	AR	3497	-	0,6,6	-	-	-		
84	OHX	AR	3645	-	0,6,6	-	-	-		
84	OHX	O	201	-	0,6,6	-	-	-		
84	OHX	AR	3458	-	0,6,6	-	-	-		
84	OHX	6	1924	-	0,6,6	-	-	-		
84	OHX	4	204	-	0,6,6	-	-	-		
84	OHX	AR	3586	-	0,6,6	-	-	-		
84	OHX	1	3523	-	0,6,6	-	-	-		
84	OHX	AR	3447	-	0,6,6	-	-	-		
84	OHX	A	1920	-	0,6,6	-	-	-		
84	OHX	1	3638	-	0,6,6	-	-	-		
84	OHX	AR	3490	-	0,6,6	-	-	-		
84	OHX	AR	3648	-	0,6,6	-	-	-		
84	OHX	A	1975	-	0,6,6	-	-	-		
84	OHX	A	1980	-	0,6,6	-	-	-		
84	OHX	6	2041	-	0,6,6	-	-	-		
84	OHX	AR	3440	-	0,6,6	-	-	-		
84	OHX	A	2013	-	0,6,6	-	-	-		
84	OHX	AR	3602	-	0,6,6	-	-	-		
84	OHX	1	3416	-	0,6,6	-	-	-		
84	OHX	AR	3587	-	0,6,6	-	-	-		
84	OHX	AR	3456	-	0,6,6	-	-	-		
84	OHX	AR	3717	-	0,6,6	-	-	-		
84	OHX	1	3495	-	0,6,6	-	-	-		
84	OHX	AR	3419	-	0,6,6	-	-	-		
84	OHX	1	3508	-	0,6,6	-	-	-		
84	OHX	1	3484	-	0,6,6	-	-	-		
84	OHX	AR	3421	-	0,6,6	-	-	-		
84	OHX	1	3568	-	0,6,6	-	-	-		
84	OHX	AR	3640	-	0,6,6	-	-	-		
84	OHX	sR	401	-	0,6,6	-	-	-		
84	OHX	AR	3436	-	0,6,6	-	-	-		
84	OHX	4	212	-	0,6,6	-	-	-		
84	OHX	AR	3464	-	0,6,6	-	-	-		
84	OHX	CE	401	-	0,6,6	-	-	-		
84	OHX	A	1974	-	0,6,6	-	-	-		
87	GOL	v	305	-	5,5,5	0.18	0	5,5,5	0.54	0
84	OHX	AK	102	-	0,6,6	-	-	-		
84	OHX	AR	3531	-	0,6,6	-	-	-		
84	OHX	1	3560	-	0,6,6	-	-	-		
84	OHX	1	3719	-	0,6,6	-	-	-		
84	OHX	1	3611	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3698	-	0,6,6	-	-	-		
84	OHX	AR	3524	-	0,6,6	-	-	-		
84	OHX	1	3490	-	0,6,6	-	-	-		
84	OHX	AR	3677	-	0,6,6	-	-	-		
84	OHX	DQ	201	-	0,6,6	-	-	-		
84	OHX	6	2028	-	0,6,6	-	-	-		
84	OHX	AR	3507	-	0,6,6	-	-	-		
84	OHX	DD	101	-	0,6,6	-	-	-		
84	OHX	AR	3443	-	0,6,6	-	-	-		
84	OHX	6	2042	-	0,6,6	-	-	-		
84	OHX	AR	3684	-	0,6,6	-	-	-		
84	OHX	1	3672	-	0,6,6	-	-	-		
84	OHX	6	1925	-	0,6,6	-	-	-		
84	OHX	AR	3646	-	0,6,6	-	-	-		
84	OHX	1	3536	-	0,6,6	-	-	-		
84	OHX	AR	3622	-	0,6,6	-	-	-		
84	OHX	AR	3654	-	0,6,6	-	-	-		
84	OHX	CF	402	-	0,6,6	-	-	-		
84	OHX	AR	3578	-	0,6,6	-	-	-		
84	OHX	AR	3492	-	0,6,6	-	-	-		
84	OHX	AR	3634	-	0,6,6	-	-	-		
84	OHX	1	3668	-	0,6,6	-	-	-		
84	OHX	A	2010	-	0,6,6	-	-	-		
84	OHX	A	1909	-	0,6,6	-	-	-		
84	OHX	AR	3431	-	0,6,6	-	-	-		
84	OHX	6	1987	-	0,6,6	-	-	-		
84	OHX	1	3620	-	0,6,6	-	-	-		
84	OHX	6	1927	-	0,6,6	-	-	-		
84	OHX	AR	3528	-	0,6,6	-	-	-		
84	OHX	1	3553	-	0,6,6	-	-	-		
84	OHX	6	1960	-	0,6,6	-	-	-		
84	OHX	A	1925	-	0,6,6	-	-	-		
84	OHX	6	1907	-	0,6,6	-	-	-		
84	OHX	AR	3527	-	0,6,6	-	-	-		
84	OHX	A	2026	-	0,6,6	-	-	-		
84	OHX	1	3526	-	0,6,6	-	-	-		
84	OHX	1	3485	-	0,6,6	-	-	-		
84	OHX	1	3552	-	0,6,6	-	-	-		
84	OHX	AR	3512	-	0,6,6	-	-	-		
84	OHX	6	1961	-	0,6,6	-	-	-		
84	OHX	1	3426	-	0,6,6	-	-	-		
84	OHX	x	202	-	0,6,6	-	-	-		
84	OHX	AR	3425	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	6	1976	-	0,6,6	-	-	-		
84	OHX	A	1939	-	0,6,6	-	-	-		
84	OHX	A	1904	-	0,6,6	-	-	-		
84	OHX	AR	3476	-	0,6,6	-	-	-		
84	OHX	A	2039	-	0,6,6	-	-	-		
84	OHX	1	3610	-	0,6,6	-	-	-		
84	OHX	AR	3559	-	0,6,6	-	-	-		
84	OHX	A	2005	-	0,6,6	-	-	-		
84	OHX	AR	3718	-	0,6,6	-	-	-		
84	OHX	1	3507	-	0,6,6	-	-	-		
84	OHX	6	1922	-	0,6,6	-	-	-		
84	OHX	6	1999	-	0,6,6	-	-	-		
84	OHX	AR	3478	-	0,6,6	-	-	-		
84	OHX	1	3537	-	0,6,6	-	-	-		
84	OHX	1	3712	-	0,6,6	-	-	-		
84	OHX	Q	201	-	0,6,6	-	-	-		
84	OHX	AR	3639	-	0,6,6	-	-	-		
84	OHX	AR	3721	-	0,6,6	-	-	-		
84	OHX	AR	3745	-	0,6,6	-	-	-		
84	OHX	1	3576	-	0,6,6	-	-	-		
84	OHX	1	3604	-	0,6,6	-	-	-		
84	OHX	A	1976	-	0,6,6	-	-	-		
84	OHX	A	2015	-	0,6,6	-	-	-		
84	OHX	AR	3670	-	0,6,6	-	-	-		
84	OHX	DH	201	-	0,6,6	-	-	-		
84	OHX	4	211	-	0,6,6	-	-	-		
84	OHX	A	1905	-	0,6,6	-	-	-		
84	OHX	AR	3605	-	0,6,6	-	-	-		
84	OHX	6	1952	-	0,6,6	-	-	-		
84	OHX	6	1946	-	0,6,6	-	-	-		
84	OHX	4	208	-	0,6,6	-	-	-		
84	OHX	1	3474	-	0,6,6	-	-	-		
84	OHX	AP	502	-	0,6,6	-	-	-		
84	OHX	AR	3713	-	0,6,6	-	-	-		
84	OHX	6	1997	-	0,6,6	-	-	-		
84	OHX	1	3421	-	0,6,6	-	-	-		
84	OHX	k	401	-	0,6,6	-	-	-		
84	OHX	A	2000	-	0,6,6	-	-	-		
84	OHX	AR	3593	-	0,6,6	-	-	-		
84	OHX	AR	3698	-	0,6,6	-	-	-		
84	OHX	1	3663	-	0,6,6	-	-	-		
84	OHX	3	206	-	0,6,6	-	-	-		
86	HN8	AR	4263	-	24,26,26	0.29	0	36,41,41	1.60	4 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	2033	-	0,6,6	-	-	-		
84	OHX	AR	3720	-	0,6,6	-	-	-		
84	OHX	1	3433	-	0,6,6	-	-	-		
84	OHX	6	2039	-	0,6,6	-	-	-		
84	OHX	s8	301	-	0,6,6	-	-	-		
84	OHX	6	1978	-	0,6,6	-	-	-		
84	OHX	4	213	-	0,6,6	-	-	-		
84	OHX	6	2001	-	0,6,6	-	-	-		
84	OHX	AR	3740	-	0,6,6	-	-	-		
84	OHX	AR	3575	-	0,6,6	-	-	-		
84	OHX	A	1946	-	0,6,6	-	-	-		
84	OHX	1	3414	-	0,6,6	-	-	-		
84	OHX	1	3621	-	0,6,6	-	-	-		
84	OHX	1	3528	-	0,6,6	-	-	-		
84	OHX	1	3504	-	0,6,6	-	-	-		
84	OHX	1	3463	-	0,6,6	-	-	-		
84	OHX	1	3613	-	0,6,6	-	-	-		
84	OHX	1	3565	-	0,6,6	-	-	-		
84	OHX	1	3648	-	0,6,6	-	-	-		
84	OHX	1	3682	-	0,6,6	-	-	-		
84	OHX	AR	3424	-	0,6,6	-	-	-		
84	OHX	AR	3583	-	0,6,6	-	-	-		
84	OHX	6	2008	-	0,6,6	-	-	-		
84	OHX	A	2035	-	0,6,6	-	-	-		
84	OHX	AR	3467	-	0,6,6	-	-	-		
84	OHX	A	2040	-	0,6,6	-	-	-		
84	OHX	6	1932	-	0,6,6	-	-	-		
84	OHX	AR	3563	-	0,6,6	-	-	-		
84	OHX	AR	3671	-	0,6,6	-	-	-		
84	OHX	1	3595	-	0,6,6	-	-	-		
84	OHX	AR	3630	-	0,6,6	-	-	-		
84	OHX	1	3430	-	0,6,6	-	-	-		
84	OHX	AT	215	-	0,6,6	-	-	-		
84	OHX	AR	3614	-	0,6,6	-	-	-		
84	OHX	1	3435	-	0,6,6	-	-	-		
84	OHX	AR	3598	-	0,6,6	-	-	-		
84	OHX	AR	3724	-	0,6,6	-	-	-		
84	OHX	6	1979	-	0,6,6	-	-	-		
84	OHX	AR	3661	-	0,6,6	-	-	-		
84	OHX	AR	3612	-	0,6,6	-	-	-		
84	OHX	A	1922	-	0,6,6	-	-	-		
84	OHX	1	3419	-	0,6,6	-	-	-		
84	OHX	A	1985	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3541	-	0,6,6	-	-	-		
84	OHX	1	3590	-	0,6,6	-	-	-		
84	OHX	1	3647	-	0,6,6	-	-	-		
84	OHX	AR	3548	-	0,6,6	-	-	-		
84	OHX	1	3407	-	0,6,6	-	-	-		
84	OHX	1	3422	-	0,6,6	-	-	-		
84	OHX	1	3639	-	0,6,6	-	-	-		
84	OHX	AR	3441	-	0,6,6	-	-	-		
84	OHX	AR	3455	-	0,6,6	-	-	-		
84	OHX	6	2022	-	0,6,6	-	-	-		
84	OHX	1	3632	-	0,6,6	-	-	-		
84	OHX	AR	3550	-	0,6,6	-	-	-		
84	OHX	AR	3690	-	0,6,6	-	-	-		
84	OHX	CX	201	-	0,6,6	-	-	-		
84	OHX	1	3493	-	0,6,6	-	-	-		
84	OHX	1	3503	-	0,6,6	-	-	-		
84	OHX	4	201	-	0,6,6	-	-	-		
84	OHX	A	2032	-	0,6,6	-	-	-		
84	OHX	1	3479	-	0,6,6	-	-	-		
84	OHX	A	1914	-	0,6,6	-	-	-		
84	OHX	6	1913	-	0,6,6	-	-	-		
84	OHX	c3	201	-	0,6,6	-	-	-		
84	OHX	AR	3459	-	0,6,6	-	-	-		
84	OHX	AR	3437	-	0,6,6	-	-	-		
84	OHX	1	3717	-	0,6,6	-	-	-		
84	OHX	AR	3544	-	0,6,6	-	-	-		
84	OHX	AR	3600	-	0,6,6	-	-	-		
84	OHX	1	3618	-	0,6,6	-	-	-		
84	OHX	AR	3560	-	0,6,6	-	-	-		
84	OHX	AT	209	-	0,6,6	-	-	-		
84	OHX	A	1912	-	0,6,6	-	-	-		
84	OHX	1	3471	-	0,6,6	-	-	-		
84	OHX	6	1983	-	0,6,6	-	-	-		
84	OHX	1	3627	-	0,6,6	-	-	-		
84	OHX	AR	3545	-	0,6,6	-	-	-		
84	OHX	AR	3704	-	0,6,6	-	-	-		
84	OHX	A	2030	-	0,6,6	-	-	-		
84	OHX	6	1975	-	0,6,6	-	-	-		
84	OHX	1	3525	-	0,6,6	-	-	-		
84	OHX	6	1905	-	0,6,6	-	-	-		
84	OHX	A	1928	-	0,6,6	-	-	-		
84	OHX	1	3437	-	0,6,6	-	-	-		
84	OHX	6	2025	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3708	-	0,6,6	-	-	-		
84	OHX	6	1962	-	0,6,6	-	-	-		
84	OHX	AR	3530	-	0,6,6	-	-	-		
84	OHX	AR	3532	-	0,6,6	-	-	-		
84	OHX	AR	3729	-	0,6,6	-	-	-		
84	OHX	1	3634	-	0,6,6	-	-	-		
84	OHX	AR	3615	-	0,6,6	-	-	-		
84	OHX	1	3650	-	0,6,6	-	-	-		
84	OHX	1	3454	-	0,6,6	-	-	-		
84	OHX	AR	3697	-	0,6,6	-	-	-		
84	OHX	AR	3480	-	0,6,6	-	-	-		
84	OHX	1	3486	-	0,6,6	-	-	-		
84	OHX	6	1930	-	0,6,6	-	-	-		
84	OHX	6	1941	-	0,6,6	-	-	-		
84	OHX	AR	3644	-	0,6,6	-	-	-		
84	OHX	A	1944	-	0,6,6	-	-	-		
84	OHX	AR	3475	-	0,6,6	-	-	-		
84	OHX	A	2002	-	0,6,6	-	-	-		
84	OHX	1	3403	-	0,6,6	-	-	-		
84	OHX	6	1970	-	0,6,6	-	-	-		
84	OHX	AR	3711	-	0,6,6	-	-	-		
84	OHX	1	3684	-	0,6,6	-	-	-		
84	OHX	AR	3472	-	0,6,6	-	-	-		
84	OHX	3	209	-	0,6,6	-	-	-		
84	OHX	4	205	-	0,6,6	-	-	-		
84	OHX	AR	3523	-	0,6,6	-	-	-		
84	OHX	AR	3726	-	0,6,6	-	-	-		
84	OHX	AR	3688	-	0,6,6	-	-	-		
84	OHX	AR	3735	-	0,6,6	-	-	-		
84	OHX	A	1981	-	0,6,6	-	-	-		
84	OHX	AR	3570	-	0,6,6	-	-	-		
84	OHX	AR	3446	-	0,6,6	-	-	-		
84	OHX	AR	3468	-	0,6,6	-	-	-		
84	OHX	AR	3533	-	0,6,6	-	-	-		
84	OHX	1	3465	-	0,6,6	-	-	-		
84	OHX	A	1979	-	0,6,6	-	-	-		
84	OHX	AR	3636	-	0,6,6	-	-	-		
84	OHX	AS	209	-	0,6,6	-	-	-		
84	OHX	A	1991	-	0,6,6	-	-	-		
84	OHX	1	3412	-	0,6,6	-	-	-		
84	OHX	6	2052	-	0,6,6	-	-	-		
84	OHX	1	3445	-	0,6,6	-	-	-		
84	OHX	AR	3571	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3652	-	0,6,6	-	-	-		
84	OHX	6	2024	-	0,6,6	-	-	-		
84	OHX	3	205	-	0,6,6	-	-	-		
84	OHX	AR	3609	-	0,6,6	-	-	-		
84	OHX	6	1928	-	0,6,6	-	-	-		
84	OHX	A	1915	-	0,6,6	-	-	-		
84	OHX	A	1969	-	0,6,6	-	-	-		
84	OHX	A	1910	-	0,6,6	-	-	-		
84	OHX	1	3513	-	0,6,6	-	-	-		
84	OHX	1	3413	-	0,6,6	-	-	-		
84	OHX	1	3637	-	0,6,6	-	-	-		
84	OHX	AR	3516	-	0,6,6	-	-	-		
84	OHX	AR	3642	-	0,6,6	-	-	-		
84	OHX	6	1929	-	0,6,6	-	-	-		
84	OHX	1	3535	-	0,6,6	-	-	-		
84	OHX	1	3406	-	0,6,6	-	-	-		
84	OHX	AR	3620	-	0,6,6	-	-	-		
84	OHX	AT	206	-	0,6,6	-	-	-		
84	OHX	AR	3567	-	0,6,6	-	-	-		
84	OHX	AT	205	-	0,6,6	-	-	-		
84	OHX	A	1959	-	0,6,6	-	-	-		
84	OHX	AR	3714	-	0,6,6	-	-	-		
84	OHX	4	207	-	0,6,6	-	-	-		
84	OHX	1	3452	-	0,6,6	-	-	-		
84	OHX	A	1941	-	0,6,6	-	-	-		
84	OHX	6	1963	-	0,6,6	-	-	-		
84	OHX	A	1901	-	0,6,6	-	-	-		
84	OHX	6	1958	-	0,6,6	-	-	-		
84	OHX	1	3489	-	0,6,6	-	-	-		
84	OHX	1	3500	-	0,6,6	-	-	-		
84	OHX	1	3558	-	0,6,6	-	-	-		
84	OHX	1	3597	-	0,6,6	-	-	-		
84	OHX	1	3721	-	0,6,6	-	-	-		
84	OHX	1	3575	-	0,6,6	-	-	-		
84	OHX	1	3594	-	0,6,6	-	-	-		
84	OHX	v	301	-	0,6,6	-	-	-		
84	OHX	6	2006	-	0,6,6	-	-	-		
84	OHX	6	2010	-	0,6,6	-	-	-		
84	OHX	6	2033	-	0,6,6	-	-	-		
84	OHX	AR	3592	-	0,6,6	-	-	-		
84	OHX	1	3710	-	0,6,6	-	-	-		
84	OHX	AR	3491	-	0,6,6	-	-	-		
84	OHX	1	3695	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	3	201	-	0,6,6	-	-	-		
84	OHX	1	3533	-	0,6,6	-	-	-		
84	OHX	AR	3420	-	0,6,6	-	-	-		
84	OHX	1	3708	-	0,6,6	-	-	-		
84	OHX	A	2028	-	0,6,6	-	-	-		
84	OHX	c1	201	-	0,6,6	-	-	-		
84	OHX	6	1969	-	0,6,6	-	-	-		
84	OHX	1	3693	-	0,6,6	-	-	-		
84	OHX	1	3666	-	0,6,6	-	-	-		
84	OHX	6	1968	-	0,6,6	-	-	-		
84	OHX	A	1934	-	0,6,6	-	-	-		
84	OHX	1	3506	-	0,6,6	-	-	-		
84	OHX	1	3402	-	0,6,6	-	-	-		
84	OHX	6	1937	-	0,6,6	-	-	-		
84	OHX	A	2007	-	0,6,6	-	-	-		
84	OHX	1	3614	-	0,6,6	-	-	-		
84	OHX	1	3659	-	0,6,6	-	-	-		
84	OHX	A	2023	-	0,6,6	-	-	-		
84	OHX	1	3517	-	0,6,6	-	-	-		
84	OHX	AR	3707	-	0,6,6	-	-	-		
84	OHX	AR	3501	-	0,6,6	-	-	-		
84	OHX	A	1999	-	0,6,6	-	-	-		
84	OHX	A	1956	-	0,6,6	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	GOL	v	305	-	-	2/4/4/4	-
86	HN8	AR	4263	-	-	0/2/48/48	0/6/5/5
87	GOL	AR	4261	1	-	2/4/4/4	-
87	GOL	6	2199	-	-	0/4/4/4	-
87	GOL	A	2160	-	-	0/4/4/4	-
87	GOL	AR	4262	84	-	1/4/4/4	-
86	HN8	1	4223	-	-	0/2/48/48	0/6/5/5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	AR	4263	HN8	C5-C1-C3	-5.16	100.15	106.09
86	AR	4263	HN8	C5-C1-C2	-5.00	102.67	106.70
86	AR	4263	HN8	C5-C1-C7	4.00	116.29	114.53
86	1	4223	HN8	C5-C1-C7	3.71	116.17	114.53
86	AR	4263	HN8	C3-C1-C2	2.87	107.05	102.28
86	1	4223	HN8	O1-C9-C17	-2.42	102.25	109.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

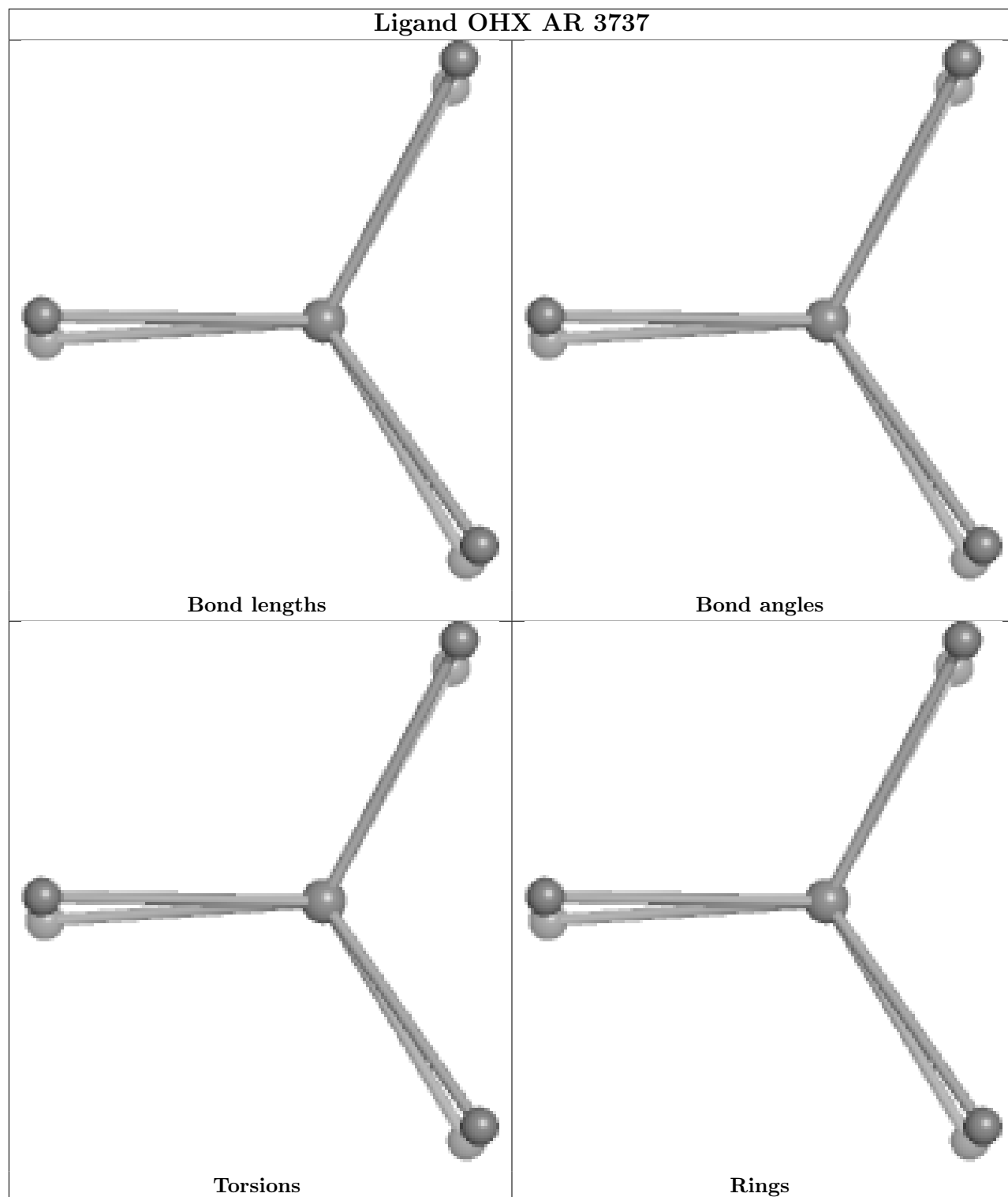
Mol	Chain	Res	Type	Atoms
87	v	305	GOL	O1-C1-C2-C3
87	AR	4261	GOL	C1-C2-C3-O3
87	v	305	GOL	O1-C1-C2-O2
87	AR	4261	GOL	O2-C2-C3-O3
87	AR	4262	GOL	C1-C2-C3-O3

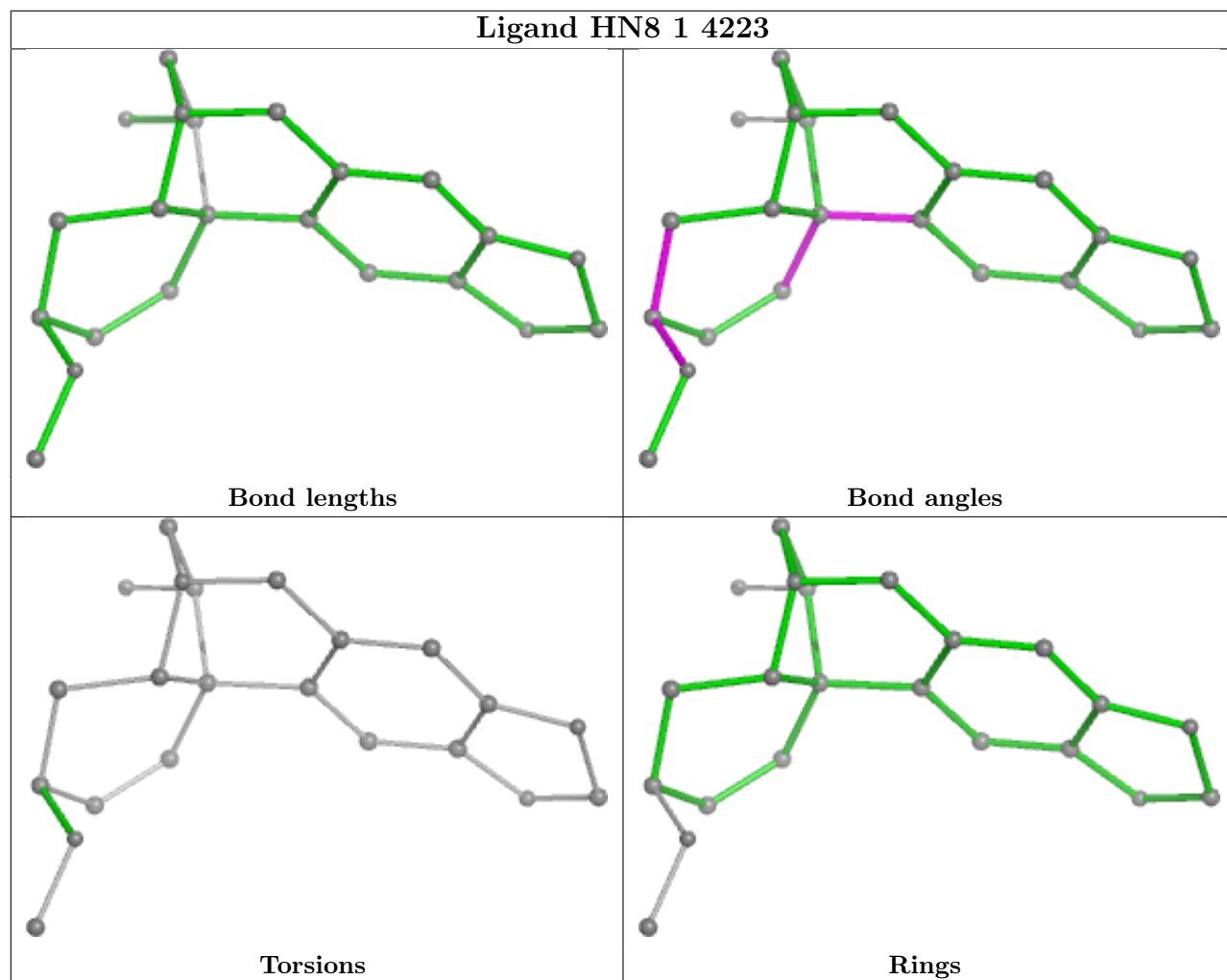
There are no ring outliers.

No monomer is involved in short contacts.

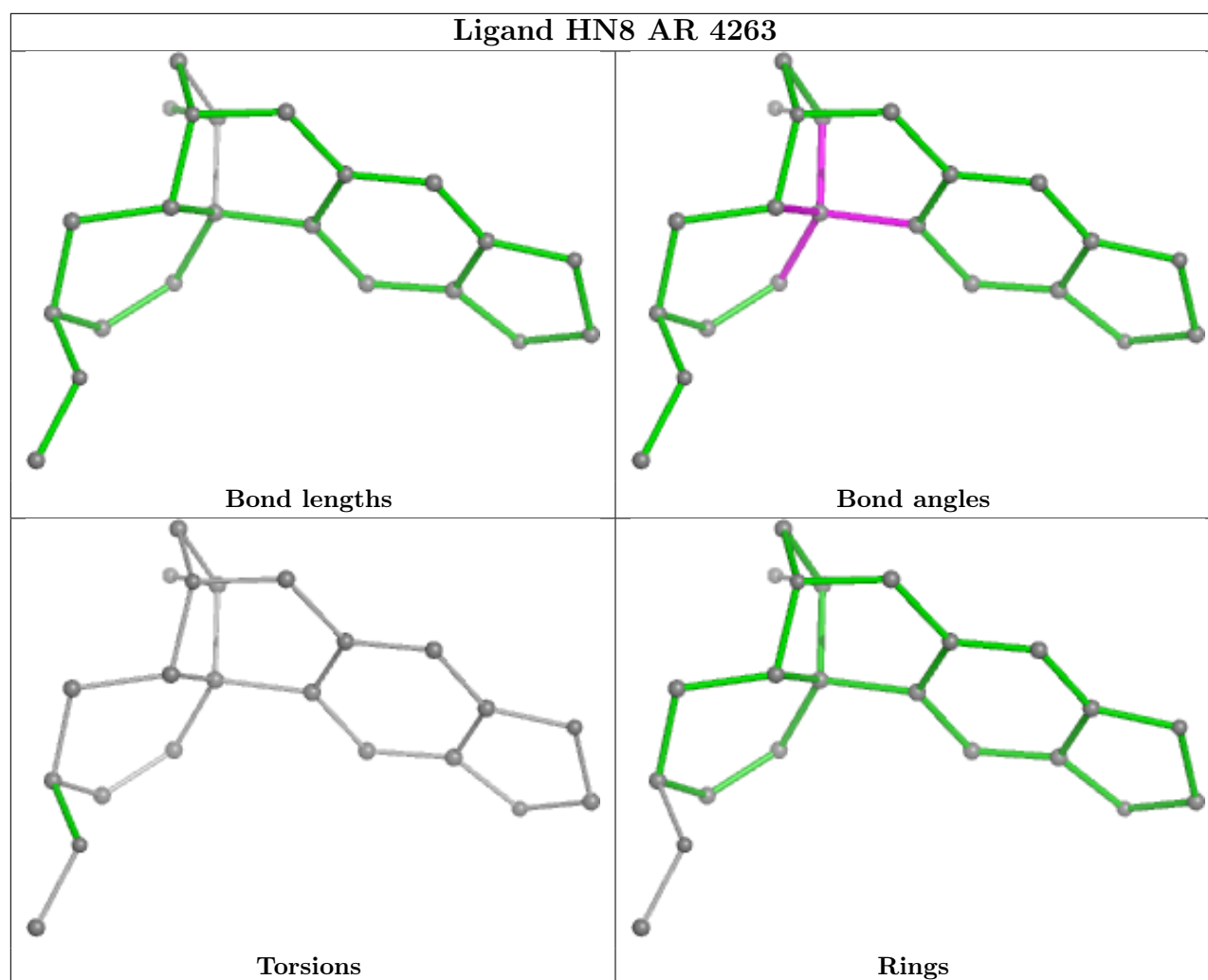
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand OHX AR 3737









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	sM	2
25	A	1
47	m2	1
5	CE	1
50	s0	1
54	s4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	85:SER	C	119:UNK	N	44.14
1	sM	139:UNK	C	155:UNK	N	37.59
1	A	1716:C	O3'	1717:G	P	4.52
1	m2	23:UNK	C	28:UNK	N	3.62
1	CE	168:LYS	C	169:THR	N	1.19
1	s0	160:ILE	C	161:PRO	N	1.19
1	s4	82:TYR	C	83:PRO	N	1.18

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	3149/3396 (92%)	0.22	98 (3%) 49 26	26, 47, 129, 223	0
1	AR	3149/3396 (92%)	0.30	104 (3%) 46 24	27, 49, 123, 225	0
2	3	121/121 (100%)	-0.11	0 100 100	35, 63, 75, 82	0
2	AS	121/121 (100%)	-0.04	1 (0%) 86 72	34, 52, 66, 73	0
3	4	158/158 (100%)	0.21	5 (3%) 47 25	34, 51, 91, 138	0
3	AT	158/158 (100%)	0.25	6 (3%) 40 20	34, 60, 99, 128	0
4	CD	252/252 (100%)	0.04	3 (1%) 79 61	33, 52, 74, 82	0
4	j	252/252 (100%)	0.04	1 (0%) 92 84	31, 46, 64, 77	0
5	CE	386/386 (100%)	-0.18	1 (0%) 94 88	25, 41, 55, 95	0
5	k	386/386 (100%)	-0.02	3 (0%) 86 72	25, 48, 62, 80	0
6	CF	361/361 (100%)	-0.11	1 (0%) 94 88	31, 47, 65, 88	0
6	l	361/361 (100%)	-0.12	1 (0%) 94 88	27, 44, 62, 71	0
7	CG	296/296 (100%)	0.15	13 (4%) 34 17	39, 57, 83, 104	0
7	m	296/296 (100%)	0.48	17 (5%) 23 11	46, 69, 89, 115	0
8	CH	156/175 (89%)	0.07	3 (1%) 66 46	37, 46, 68, 84	0
8	n	156/175 (89%)	0.04	1 (0%) 89 78	36, 43, 66, 86	0
9	CI	222/222 (100%)	-0.13	3 (1%) 75 56	27, 35, 78, 133	0
9	o	222/222 (100%)	-0.16	4 (1%) 68 47	29, 38, 73, 123	0
10	CJ	233/233 (100%)	0.79	32 (13%) 3 1	70, 82, 123, 144	0
10	p	233/233 (100%)	0.49	13 (5%) 24 11	56, 70, 105, 116	0
11	CK	191/191 (100%)	-0.16	3 (1%) 72 51	35, 45, 66, 82	0
11	q	191/191 (100%)	-0.25	0 100 100	42, 53, 66, 86	0
12	CL	211/220 (95%)	0.45	13 (6%) 20 9	39, 59, 80, 93	0
12	r	211/220 (95%)	-0.04	2 (0%) 84 69	33, 46, 81, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	CM	169/169 (100%)	-0.19	1 (0%) 89 78	40, 61, 75, 83	0
13	s	169/169 (100%)	0.09	4 (2%) 59 37	55, 77, 90, 96	0
14	CN	193/193 (100%)	0.54	15 (7%) 13 5	41, 62, 101, 119	0
14	t	193/193 (100%)	-0.05	0 100 100	33, 53, 95, 125	0
15	CO	136/136 (100%)	-0.34	1 (0%) 87 75	34, 40, 63, 71	0
15	u	136/136 (100%)	-0.29	3 (2%) 62 41	37, 43, 60, 68	0
16	CP	203/203 (100%)	-0.11	0 100 100	38, 55, 67, 71	0
16	v	203/203 (100%)	-0.17	0 100 100	33, 44, 57, 64	0
17	CQ	197/197 (100%)	-0.20	3 (1%) 73 54	25, 30, 60, 66	0
17	w	197/197 (100%)	-0.27	0 100 100	28, 34, 55, 60	0
18	CR	183/183 (100%)	1.33	29 (15%) 2 1	31, 39, 137, 167	0
18	x	183/183 (100%)	0.53	21 (11%) 4 2	32, 40, 105, 140	0
19	CS	185/185 (100%)	-0.16	0 100 100	32, 45, 56, 60	0
19	y	185/185 (100%)	-0.14	0 100 100	33, 43, 63, 87	0
20	CT	188/188 (100%)	0.12	9 (4%) 30 14	48, 63, 158, 169	0
20	z	188/188 (100%)	0.16	7 (3%) 41 21	48, 64, 150, 167	0
21	0	172/172 (100%)	-0.19	1 (0%) 89 78	35, 41, 55, 65	0
21	CU	172/172 (100%)	-0.35	0 100 100	30, 37, 50, 57	0
22	2	159/159 (100%)	-0.07	2 (1%) 77 59	34, 45, 87, 97	0
22	CV	159/159 (100%)	-0.21	0 100 100	31, 41, 74, 84	0
23	5	100/100 (100%)	0.81	12 (12%) 4 2	79, 93, 105, 123	0
23	CW	100/100 (100%)	1.11	21 (21%) 1 0	77, 87, 98, 119	0
24	CX	136/136 (100%)	0.14	1 (0%) 87 75	29, 38, 57, 59	0
24	IR	136/136 (100%)	0.04	4 (2%) 51 28	31, 43, 56, 62	0
25	6	1783/1800 (99%)	0.43	115 (6%) 19 8	41, 78, 169, 233	0
25	A	1781/1800 (98%)	0.51	128 (7%) 15 6	49, 87, 186, 250	0
26	7	98/98 (100%)	1.75	29 (29%) 0 0	43, 59, 150, 157	0
26	CY	98/98 (100%)	0.41	11 (11%) 5 2	38, 53, 145, 177	0
27	8	121/121 (100%)	-0.03	1 (0%) 86 72	44, 57, 77, 117	0
27	CZ	121/121 (100%)	0.05	4 (3%) 46 24	48, 64, 85, 100	0
28	9	126/126 (100%)	0.67	6 (4%) 30 14	40, 55, 64, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
28	DA	126/126 (100%)	0.69	7 (5%)	24 11	40, 57, 73, 82	0
29	AA	135/135 (100%)	1.73	47 (34%)	0 0	69, 83, 94, 104	0
29	DB	135/135 (100%)	0.90	16 (11%)	4 2	81, 95, 110, 120	0
30	AB	148/148 (100%)	-0.08	0	100 100	27, 46, 73, 86	0
30	DC	148/148 (100%)	0.02	1 (0%)	87 75	30, 51, 71, 77	0
31	AC	58/58 (100%)	-0.07	0	100 100	32, 52, 102, 122	0
31	DD	58/58 (100%)	-0.06	0	100 100	38, 51, 80, 88	0
32	AD	97/97 (100%)	0.38	6 (6%)	20 9	67, 77, 99, 110	0
32	DE	97/97 (100%)	-0.29	0	100 100	71, 83, 105, 109	0
33	AE	109/109 (100%)	0.20	2 (1%)	68 47	42, 56, 95, 106	0
33	DF	109/109 (100%)	0.18	3 (2%)	53 30	41, 52, 92, 111	0
34	AF	127/127 (100%)	0.01	3 (2%)	59 37	25, 40, 52, 69	0
34	DG	127/127 (100%)	0.06	2 (1%)	72 51	24, 43, 55, 77	0
35	AG	106/106 (100%)	-0.15	1 (0%)	84 69	31, 36, 61, 72	0
35	DH	106/106 (100%)	-0.13	1 (0%)	84 69	28, 35, 64, 87	0
36	AH	112/112 (100%)	0.26	6 (5%)	25 12	43, 63, 104, 114	0
36	DI	112/112 (100%)	0.29	1 (0%)	84 69	46, 68, 113, 125	0
37	AI	119/119 (100%)	0.27	6 (5%)	28 13	46, 61, 70, 77	0
37	DJ	119/119 (100%)	0.27	6 (5%)	28 13	51, 67, 81, 88	0
38	AJ	99/99 (100%)	0.24	3 (3%)	50 27	52, 61, 93, 113	0
38	DK	99/99 (100%)	0.26	4 (4%)	38 19	59, 70, 92, 110	0
39	AK	87/87 (100%)	0.10	3 (3%)	45 24	32, 36, 63, 86	0
39	DL	87/87 (100%)	0.24	3 (3%)	45 24	36, 42, 77, 113	0
40	AL	77/77 (100%)	0.19	2 (2%)	56 33	67, 79, 101, 108	0
40	DM	77/77 (100%)	1.93	30 (38%)	0 0	76, 88, 107, 115	0
41	AM	50/50 (100%)	-0.07	0	100 100	42, 45, 52, 62	0
41	DN	50/50 (100%)	-0.04	0	100 100	45, 49, 59, 70	0
42	AN	52/52 (100%)	0.61	5 (9%)	8 2	37, 43, 61, 69	0
42	DO	52/52 (100%)	0.02	1 (1%)	66 46	32, 35, 48, 62	0
43	AO	25/25 (100%)	-0.14	0	100 100	52, 54, 59, 59	0
43	DP	25/25 (100%)	-0.20	0	100 100	43, 46, 59, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	AP	105/105 (100%)	0.66	9 (8%) 10 4	34, 50, 74, 103	0
44	DQ	105/105 (100%)	0.25	0 100 100	37, 50, 65, 97	0
45	AQ	91/91 (100%)	-0.22	0 100 100	40, 50, 67, 80	0
45	DR	91/91 (100%)	-0.24	0 100 100	39, 53, 69, 79	0
46	i	159/272 (58%)	0.57	19 (11%) 4 2	70, 90, 143, 148	0
47	m2	0/150	-	-	-	-
48	sM	63/104 (60%)	0.77	6 (9%) 8 2	62, 91, 108, 114	0
49	p0	143/311 (45%)	1.60	53 (37%) 0 0	89, 108, 172, 179	0
50	B	206/206 (100%)	0.86	27 (13%) 3 1	93, 110, 125, 146	0
50	s0	206/206 (100%)	0.32	8 (3%) 39 20	77, 97, 115, 120	0
51	C	214/216 (99%)	1.64	78 (36%) 0 0	93, 121, 142, 150	0
51	s1	216/216 (100%)	0.53	13 (6%) 21 10	68, 83, 110, 129	0
52	D	217/217 (100%)	0.03	2 (0%) 84 69	68, 87, 108, 125	0
52	s2	217/217 (100%)	0.07	2 (0%) 84 69	57, 76, 92, 106	0
53	E	223/223 (100%)	0.65	19 (8%) 10 4	74, 91, 118, 137	0
53	s3	223/223 (100%)	0.70	27 (12%) 4 1	75, 103, 134, 148	0
54	F	260/260 (100%)	0.62	22 (8%) 10 4	63, 87, 97, 121	0
54	s4	260/260 (100%)	0.16	7 (2%) 54 31	53, 84, 98, 128	0
55	G	206/206 (100%)	0.77	22 (10%) 6 2	92, 112, 131, 141	0
55	s5	206/206 (100%)	0.95	34 (16%) 1 1	74, 95, 114, 122	0
56	H	226/226 (100%)	0.87	39 (17%) 1 0	61, 94, 116, 143	0
56	s6	218/226 (96%)	0.63	26 (11%) 4 2	52, 83, 111, 124	0
57	I	184/186 (98%)	1.03	29 (15%) 2 1	87, 119, 148, 156	0
57	s7	186/186 (100%)	1.00	32 (17%) 1 0	77, 112, 147, 152	0
58	J	188/199 (94%)	0.29	9 (4%) 30 14	53, 70, 111, 126	0
58	s8	188/199 (94%)	0.57	14 (7%) 14 5	49, 73, 124, 140	0
59	K	185/185 (100%)	1.06	34 (18%) 1 0	77, 95, 129, 158	0
59	s9	185/185 (100%)	0.68	15 (8%) 12 5	67, 85, 116, 151	0
60	L	96/105 (91%)	1.12	16 (16%) 1 1	81, 102, 129, 139	0
60	c0	96/105 (91%)	2.34	55 (57%) 0 0	96, 126, 139, 147	0
61	M	155/155 (100%)	0.82	16 (10%) 6 2	56, 70, 126, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
61	c1	146/155 (94%)	0.46	8 (5%) 25 11	55, 70, 104, 131	0
62	N	124/124 (100%)	1.99	64 (51%) 0 0	133, 140, 152, 160	0
62	c2	124/124 (100%)	3.01	87 (70%) 0 0	161, 169, 184, 190	0
63	O	150/150 (100%)	0.41	9 (6%) 21 10	64, 85, 100, 104	0
63	c3	150/150 (100%)	0.16	4 (2%) 54 31	59, 78, 96, 111	0
64	P	127/128 (99%)	1.40	36 (28%) 0 0	66, 119, 135, 138	0
64	c4	128/128 (100%)	0.63	11 (8%) 10 4	57, 81, 91, 94	0
65	Q	124/141 (87%)	0.49	7 (5%) 24 11	75, 89, 126, 146	0
65	c5	135/141 (95%)	0.80	16 (11%) 4 2	82, 97, 118, 131	0
66	R	141/142 (99%)	1.05	25 (17%) 1 0	81, 107, 115, 120	0
66	c6	142/142 (100%)	0.69	15 (10%) 6 2	67, 91, 106, 127	0
67	S	120/125 (96%)	0.56	14 (11%) 4 2	90, 109, 134, 138	0
67	c7	117/125 (93%)	0.13	6 (5%) 28 13	78, 97, 122, 130	0
68	T	145/145 (100%)	0.79	17 (11%) 4 2	71, 99, 129, 140	0
68	c8	145/145 (100%)	0.71	16 (11%) 5 2	79, 91, 116, 127	0
69	U	143/143 (100%)	1.00	22 (15%) 2 1	84, 102, 119, 133	0
69	c9	143/143 (100%)	1.11	30 (20%) 1 0	71, 86, 106, 119	0
70	V	107/110 (97%)	0.14	2 (1%) 66 46	73, 109, 141, 145	0
70	d0	110/110 (100%)	0.46	12 (10%) 5 2	70, 111, 154, 172	0
71	W	87/87 (100%)	0.61	8 (9%) 9 3	90, 96, 115, 124	0
71	d1	87/87 (100%)	0.14	4 (4%) 32 16	75, 83, 110, 121	0
72	X	129/129 (100%)	0.15	2 (1%) 72 51	68, 81, 88, 101	0
72	d2	129/129 (100%)	0.05	1 (0%) 86 72	57, 70, 81, 97	0
73	Y	144/144 (100%)	0.22	3 (2%) 63 43	57, 62, 73, 88	0
73	d3	144/144 (100%)	-0.08	0 100 100	46, 52, 66, 78	0
74	Z	134/134 (100%)	0.47	15 (11%) 5 2	69, 97, 114, 125	0
74	d4	134/134 (100%)	0.23	11 (8%) 11 4	62, 88, 103, 122	0
75	a	70/70 (100%)	2.04	28 (40%) 0 0	111, 123, 138, 139	0
75	d5	69/70 (98%)	1.43	22 (31%) 0 0	93, 113, 124, 127	0
76	b	97/97 (100%)	0.42	5 (5%) 27 12	67, 83, 135, 138	0
76	d6	97/97 (100%)	0.14	1 (1%) 82 67	51, 63, 95, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
77	c	81/81 (100%)	1.03	15 (18%) 1 0	82, 95, 127, 134	0
77	d7	81/81 (100%)	1.14	15 (18%) 1 0	72, 87, 126, 132	0
78	d	63/63 (100%)	0.96	7 (11%) 5 2	104, 121, 132, 134	0
78	d8	63/63 (100%)	1.97	34 (53%) 0 0	91, 107, 121, 125	0
79	d9	53/53 (100%)	1.20	10 (18%) 1 0	71, 82, 120, 128	0
79	e	53/53 (100%)	0.69	4 (7%) 14 5	75, 80, 96, 104	0
80	e0	62/62 (100%)	0.97	9 (14%) 2 1	59, 83, 113, 125	0
80	f	60/62 (96%)	1.14	11 (18%) 1 0	63, 92, 131, 134	0
81	g	71/71 (100%)	1.75	29 (40%) 0 0	105, 124, 144, 150	0
82	h	318/318 (100%)	1.11	70 (22%) 0 0	97, 115, 135, 147	0
82	sR	318/318 (100%)	0.61	32 (10%) 7 2	99, 121, 140, 157	0
83	e1	51/51 (100%)	2.31	23 (45%) 0 0	145, 157, 165, 167	0
All	All	33004/34167 (96%)	0.39	2308 (6%) 16 7	24, 66, 132, 250	0

All (2308) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	CR	161	ALA	24.1
18	CR	162	GLU	20.5
26	7	76	VAL	18.1
18	CR	160	ALA	16.2
26	7	75	THR	15.8
18	CR	159	LYS	15.5
18	CR	179	GLN	14.3
18	x	162	GLU	13.0
18	CR	178	ALA	12.4
18	CR	158	ALA	12.1
55	G	152	GLY	11.8
75	a	36	ALA	11.2
28	DA	127	GLU	10.9
25	A	1702	A	10.6
26	7	84	GLY	10.4
1	AR	1569	U	10.1
18	x	161	ALA	10.0
61	M	147	GLY	9.9
25	A	1709	C	9.7
25	A	1708	U	9.6
61	c1	3	THR	9.6

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Mol	Chain	Res	Type	RSRZ
62	c2	105	LYS	9.2
18	CR	165	VAL	9.1
26	7	88	ASP	8.8
51	C	100	PHE	8.7
25	A	913	G	8.7
61	M	145	ALA	8.6
61	M	146	ALA	8.5
25	A	1694	A	8.4
18	x	163	LYS	8.4
1	AR	2445	A	8.4
18	CR	168	LEU	8.3
18	x	184	ALA	8.2
26	7	81	PRO	8.2
18	CR	167	ARG	8.0
18	CR	176	ILE	8.0
80	e0	62	VAL	7.9
62	c2	63	VAL	7.8
49	p0	192	ASP	7.7
18	CR	174	GLY	7.7
77	c	38	PRO	7.7
26	7	86	SER	7.7
55	G	151	GLY	7.6
18	CR	163	LYS	7.6
25	A	1703	C	7.6
10	CJ	254	ASP	7.5
23	CW	9	GLN	7.5
44	AP	106	PHE	7.5
61	M	2	SER	7.5
18	CR	175	ARG	7.5
25	A	1698	G	7.5
1	1	1569	U	7.4
25	A	1699	G	7.4
74	d4	134	ALA	7.4
25	A	194	U	7.3
25	A	1704	U	7.3
20	CT	182	ASP	7.3
61	M	152	GLN	7.3
59	K	181	ALA	7.3
25	A	1711	C	7.2
60	c0	79	TYR	7.2
25	A	1696	G	7.2
18	CR	180	LYS	7.2

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Mol	Chain	Res	Type	RSRZ
61	M	150	ASN	7.2
18	x	160	ALA	7.1
26	CY	81	PRO	7.1
18	CR	170	SER	7.1
1	1	1568	U	7.1
65	c5	4	ALA	7.0
74	d4	135	ASP	7.0
25	A	1693	A	7.0
1	AR	2502	A	7.0
1	1	1570	U	7.0
18	CR	164	LYS	6.9
1	AR	252	U	6.9
82	h	4	ASN	6.8
83	e1	102	VAL	6.8
25	A	134	U	6.8
1	AR	2535	A	6.8
61	M	153	PHE	6.7
26	CY	95	SER	6.7
1	1	2539	C	6.7
62	c2	64	SER	6.6
64	P	16	VAL	6.6
26	7	85	ALA	6.6
25	A	1059	U	6.6
25	A	1697	G	6.6
55	G	153	GLY	6.6
66	R	92	TYR	6.5
62	N	62	LEU	6.5
18	x	159	LYS	6.5
18	x	164	LYS	6.5
25	A	1700	C	6.5
25	A	135	A	6.5
46	i	16	ASP	6.5
46	i	85	SER	6.5
82	h	52	GLN	6.5
82	h	3	SER	6.4
18	CR	184	ALA	6.4
25	A	1705	C	6.4
18	CR	157	VAL	6.4
26	7	82	ILE	6.4
64	P	15	GLY	6.4
79	d9	4	GLU	6.3
25	6	718	U	6.2

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Mol	Chain	Res	Type	RSRZ
46	i	88	ARG	6.2
77	d7	59	CYS	6.2
25	6	1694	A	6.2
26	7	77	LYS	6.2
62	c2	47	GLU	6.2
26	7	74	LYS	6.2
82	h	212	ALA	6.2
66	R	66	ARG	6.1
1	1	1955	U	6.1
1	AR	2504	U	6.1
1	AR	1567	U	6.1
10	CJ	253	SER	6.0
25	A	238	U	6.0
83	e1	113	LYS	6.0
51	C	98	THR	6.0
62	c2	43	ARG	6.0
79	d9	5	ASN	6.0
51	C	230	ALA	6.0
1	AR	2539	C	6.0
62	c2	121	VAL	5.9
60	c0	67	THR	5.9
62	c2	123	VAL	5.9
3	AT	81	U	5.9
1	1	1952	G	5.9
18	CR	183	ALA	5.9
25	6	658	C	5.9
25	A	1692	G	5.8
82	h	2	ALA	5.8
26	7	87	LEU	5.8
40	DM	34	ALA	5.8
61	M	155	LYS	5.8
28	9	127	GLU	5.8
66	R	21	HIS	5.8
26	7	90	ILE	5.8
61	c1	2	SER	5.8
66	R	20	ALA	5.7
80	f	60	PRO	5.7
51	C	20	VAL	5.7
25	6	225	A	5.7
55	s5	152	GLY	5.7
25	6	194	U	5.7
62	c2	28	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	AR	1570	U	5.6
26	CY	96	LEU	5.6
25	A	656	G	5.6
39	DL	88	ALA	5.6
1	AR	2503	G	5.6
62	c2	65	SER	5.6
25	6	1228	G	5.5
7	CG	295	GLY	5.5
83	e1	112	GLY	5.5
51	C	96	LEU	5.5
55	s5	37	GLN	5.5
55	G	154	ALA	5.5
25	6	1256	A	5.4
25	A	1707	A	5.4
62	c2	75	VAL	5.4
1	AR	1571	A	5.4
61	M	3	THR	5.4
25	6	239	C	5.4
80	e0	63	GLN	5.4
66	R	5	PRO	5.4
64	P	75	GLY	5.4
1	1	1349	G	5.4
82	h	79	TYR	5.4
1	1	2205	U	5.4
1	AR	2506	U	5.3
60	c0	48	SER	5.3
25	6	656	G	5.3
53	s3	145	ALA	5.3
82	h	7	LEU	5.3
1	AR	3154	C	5.3
25	A	719	U	5.3
62	c2	92	ALA	5.3
1	AR	1581	C	5.3
25	6	1695	G	5.3
10	CJ	121	SER	5.3
62	c2	74	LEU	5.3
75	a	67	ASP	5.2
10	CJ	118	GLU	5.2
60	c0	64	TYR	5.2
1	AR	2537	U	5.2
39	DL	87	SER	5.2
1	AR	3275	U	5.2

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Mol	Chain	Res	Type	RSRZ
1	AR	1572	U	5.2
56	s6	169	TYR	5.2
26	7	69	LYS	5.2
65	c5	50	THR	5.2
1	AR	1351	U	5.1
44	AP	104	LEU	5.1
60	c0	76	LEU	5.1
80	f	53	LYS	5.1
1	AR	2505	U	5.1
61	M	149	ALA	5.1
25	6	506	A	5.1
23	CW	11	ILE	5.1
51	C	95	ASN	5.1
75	a	97	LYS	5.0
53	s3	176	LEU	5.0
74	Z	2	SER	5.0
83	e1	146	SER	5.0
50	B	28	ASN	5.0
25	A	132	U	5.0
55	G	222	LYS	5.0
18	CR	169	THR	5.0
62	c2	103	LEU	5.0
1	AR	1566	A	5.0
25	6	229	U	5.0
25	A	1695	G	5.0
25	A	261	U	5.0
57	I	74	GLN	5.0
51	C	231	LEU	5.0
18	x	158	ALA	5.0
65	Q	51	SER	5.0
10	CJ	107	GLU	4.9
62	c2	30	VAL	4.9
25	6	676	G	4.9
82	sR	319	ASN	4.9
81	g	146	SER	4.9
1	1	1571	A	4.9
25	A	914	G	4.9
25	A	1686	C	4.9
75	d5	37	GLN	4.9
1	AR	1025	A	4.9
25	6	1227	A	4.9
34	AF	128	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
65	c5	5	VAL	4.9
82	h	6	VAL	4.9
26	CY	97	LYS	4.9
51	C	86	LEU	4.8
18	CR	177	ALA	4.8
55	G	155	ALA	4.8
1	AR	1574	C	4.8
26	7	68	ALA	4.8
62	c2	45	LEU	4.8
26	7	80	ARG	4.8
1	AR	3156	U	4.8
7	CG	290	ILE	4.8
7	CG	296	GLN	4.8
55	s5	151	GLY	4.8
26	7	95	SER	4.8
40	DM	32	ASN	4.8
1	1	1243	G	4.8
62	c2	59	LEU	4.8
60	c0	98	THR	4.8
1	AR	2507	C	4.7
25	6	1707	A	4.7
51	C	101	HIS	4.7
25	6	678	A	4.7
62	c2	104	GLY	4.7
40	DM	31	LEU	4.7
26	CY	67	VAL	4.7
75	a	69	LEU	4.7
77	c	33	LEU	4.7
62	c2	34	THR	4.7
1	AR	2444	C	4.7
57	I	87	ASP	4.7
75	a	48	ASP	4.7
25	6	1229	G	4.7
62	c2	60	VAL	4.7
69	c9	4	VAL	4.7
62	N	67	THR	4.6
46	i	89	ARG	4.6
65	c5	10	ARG	4.6
69	c9	2	PRO	4.6
62	c2	107	ASP	4.6
80	e0	49	LEU	4.6
57	I	32	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
82	sR	121	MET	4.6
62	c2	80	ASN	4.6
78	d8	65	ARG	4.6
65	Q	50	THR	4.6
1	1	1236	G	4.6
1	1	1268	G	4.6
25	A	133	U	4.6
62	c2	112	ALA	4.6
1	1	1350	A	4.6
25	A	1701	A	4.6
61	M	4	GLU	4.6
64	P	40	ALA	4.6
18	x	174	GLY	4.6
25	6	721	U	4.6
39	AK	87	SER	4.6
60	c0	50	THR	4.6
83	e1	115	THR	4.6
83	e1	104	SER	4.6
3	AT	80	A	4.6
25	A	718	U	4.5
25	A	1687	U	4.5
1	1	1266	G	4.5
18	x	179	GLN	4.5
55	s5	155	ALA	4.5
59	K	138	LYS	4.5
61	M	154	ALA	4.5
56	s6	217	SER	4.5
1	1	1242	G	4.5
60	c0	57	THR	4.5
40	DM	11	PHE	4.5
55	s5	156	ARG	4.5
26	7	83	THR	4.5
69	U	71	VAL	4.5
62	N	49	THR	4.5
25	A	658	C	4.5
68	T	2	SER	4.5
25	A	241	U	4.5
29	AA	95	VAL	4.5
1	1	1352	A	4.5
26	7	96	LEU	4.4
60	c0	65	TYR	4.4
1	AR	2536	A	4.4

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Mol	Chain	Res	Type	RSRZ
29	AA	5	LEU	4.4
1	1	1762	C	4.4
64	P	29	HIS	4.4
26	7	70	LYS	4.4
10	CJ	115	ALA	4.4
25	A	715	U	4.4
40	DM	71	PRO	4.4
1	AR	1579	C	4.4
7	CG	297	GLN	4.4
18	CR	172	GLN	4.4
37	DJ	120	ALA	4.4
25	A	239	C	4.4
62	N	50	LYS	4.4
62	N	64	SER	4.4
51	C	47	LEU	4.4
75	a	65	LEU	4.4
25	A	1710	U	4.4
23	5	89	LEU	4.4
60	c0	69	THR	4.4
65	c5	52	LYS	4.4
26	CY	68	ALA	4.3
57	I	38	LEU	4.3
62	c2	71	ILE	4.3
51	C	226	GLY	4.3
25	A	1706	C	4.3
10	CJ	106	LYS	4.3
29	AA	99	GLU	4.3
58	s8	67	TRP	4.3
46	i	87	THR	4.3
62	c2	115	VAL	4.3
68	T	13	HIS	4.3
62	N	111	ASN	4.3
79	e	4	GLU	4.3
29	AA	72	ILE	4.3
51	C	84	ILE	4.3
1	AR	2501	U	4.3
51	C	99	ASN	4.3
62	c2	116	VAL	4.3
18	CR	166	VAL	4.3
22	2	121	ALA	4.3
33	DF	82	GLU	4.3
40	DM	30	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
53	E	217	ILE	4.3
54	F	167	GLY	4.3
62	c2	114	LYS	4.3
83	e1	145	HIS	4.3
53	s3	174	HIS	4.3
1	1	1567	U	4.2
62	c2	56	GLU	4.2
51	C	55	LYS	4.2
62	c2	76	GLU	4.2
25	6	226	A	4.2
56	s6	166	GLU	4.2
25	6	240	U	4.2
61	M	148	LYS	4.2
61	M	151	LYS	4.2
25	A	136	C	4.2
60	c0	68	LEU	4.2
1	1	1265	U	4.2
51	C	41	ARG	4.2
55	G	41	LYS	4.2
62	c2	119	SER	4.2
61	M	156	PHE	4.2
1	AR	3276	G	4.2
59	K	186	GLU	4.2
63	O	151	ASN	4.2
78	d8	13	ILE	4.2
78	d8	43	ASN	4.2
25	A	183	U	4.2
62	c2	91	VAL	4.2
28	9	120	GLN	4.2
81	g	104	SER	4.2
33	AE	82	GLU	4.2
82	sR	51	ASP	4.2
62	c2	113	ARG	4.2
70	d0	121	ASN	4.2
82	h	253	ALA	4.2
75	a	73	GLY	4.2
1	1	1351	U	4.1
10	CJ	252	ASN	4.1
26	7	89	LEU	4.1
60	c0	70	GLU	4.1
77	d7	33	LEU	4.1
83	e1	107	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
9	CI	26	VAL	4.1
62	N	41	LEU	4.1
29	AA	107	ARG	4.1
82	sR	46	LYS	4.1
1	AR	1815	U	4.1
25	A	820	U	4.1
62	c2	61	VAL	4.1
7	CG	287	ALA	4.1
25	6	679	U	4.1
49	p0	197	PHE	4.1
46	i	18	VAL	4.1
60	c0	9	ASN	4.1
83	e1	114	VAL	4.1
49	p0	25	LEU	4.1
10	CJ	117	ALA	4.1
60	c0	3	MET	4.1
10	CJ	111	LYS	4.1
38	AJ	99	ARG	4.1
77	c	41	LEU	4.1
60	c0	37	THR	4.0
1	1	2207	A	4.0
25	A	1690	G	4.0
26	7	72	SER	4.0
65	c5	6	ASN	4.0
12	CL	112	GLN	4.0
51	C	91	VAL	4.0
62	c2	125	ASN	4.0
68	T	8	GLN	4.0
75	a	71	ILE	4.0
1	1	1267	U	4.0
48	sM	84	LYS	4.0
62	c2	29	LYS	4.0
1	1	1278	A	4.0
25	6	214	G	4.0
23	CW	10	LYS	4.0
62	c2	93	ASP	4.0
55	s5	153	GLY	4.0
57	s7	93	LEU	4.0
25	A	131	C	4.0
64	P	27	PHE	4.0
62	c2	46	ARG	4.0
25	A	506	A	4.0

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Mol	Chain	Res	Type	RSRZ
60	c0	55	VAL	4.0
40	DM	33	LYS	4.0
82	h	115	ILE	4.0
67	S	126	ALA	4.0
60	c0	95	ARG	3.9
39	AK	84	SER	3.9
55	G	150	GLY	3.9
62	c2	111	ASN	3.9
75	a	60	VAL	3.9
26	7	79	GLN	3.9
62	N	110	GLY	3.9
82	h	262	VAL	3.9
51	C	38	PHE	3.9
77	d7	62	ILE	3.9
1	AR	2441	A	3.9
40	DM	72	THR	3.9
51	C	25	THR	3.9
69	c9	19	ALA	3.9
46	i	17	VAL	3.9
25	6	487	G	3.9
70	d0	17	GLN	3.9
60	c0	49	LEU	3.9
21	0	1	MET	3.9
1	AR	1580	A	3.9
25	6	1255	G	3.9
25	6	712	G	3.9
25	6	1700	C	3.9
54	s4	261	LEU	3.9
82	h	315	VAL	3.9
71	d1	43	GLY	3.9
55	G	181	GLU	3.9
60	c0	42	VAL	3.8
67	S	86	PRO	3.8
62	N	78	LEU	3.8
25	A	195	G	3.8
18	x	181	ARG	3.8
70	d0	18	GLN	3.8
10	CJ	250	ALA	3.8
55	s5	154	ALA	3.8
1	1	1271	A	3.8
82	h	263	PHE	3.8
49	p0	292	GLU	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
65	c5	134	THR	3.8
62	N	28	LEU	3.8
64	P	41	ARG	3.8
20	CT	175	GLN	3.8
29	AA	106	GLN	3.8
62	N	20	ALA	3.8
66	c6	4	VAL	3.8
83	e1	106	TYR	3.8
54	F	143	ASP	3.8
62	N	63	VAL	3.8
56	s6	164	LYS	3.8
68	c8	18	LEU	3.8
25	A	228	G	3.8
46	i	273	THR	3.8
59	K	182	GLU	3.8
69	U	5	SER	3.8
10	CJ	122	LYS	3.8
25	6	75	U	3.8
25	6	1710	U	3.8
51	C	59	ASP	3.8
55	G	210	ALA	3.8
1	1	3154	C	3.8
20	CT	183	ALA	3.8
25	A	899	G	3.8
62	c2	72	ILE	3.8
7	m	124	GLU	3.7
49	p0	284	ALA	3.7
62	c2	102	GLY	3.7
23	5	108	TYR	3.7
62	c2	62	LEU	3.7
10	CJ	249	ARG	3.7
55	s5	61	TYR	3.7
60	L	12	HIS	3.7
1	AR	546	C	3.7
62	N	32	LEU	3.7
48	sM	85	SER	3.7
1	AR	2538	U	3.7
26	7	67	VAL	3.7
10	p	121	SER	3.7
51	C	130	SER	3.7
53	s3	44	THR	3.7
68	c8	17	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
57	s7	90	VAL	3.7
60	c0	73	VAL	3.7
1	AR	1568	U	3.7
25	6	1692	G	3.7
62	c2	124	LYS	3.7
68	T	44	ASN	3.7
23	CW	97	SER	3.7
62	c2	23	THR	3.7
81	g	87	THR	3.7
51	C	29	TRP	3.7
1	AR	1352	A	3.7
1	1	1576	G	3.7
68	T	6	GLN	3.7
81	g	105	TYR	3.7
1	1	1259	A	3.7
25	6	1693	A	3.7
53	E	179	GLN	3.7
55	G	37	GLN	3.7
62	c2	122	VAL	3.7
46	i	15	ALA	3.7
57	s7	3	ALA	3.7
61	c1	145	ALA	3.7
62	N	85	LYS	3.7
25	6	675	U	3.7
20	z	187	GLU	3.7
7	m	131	LEU	3.7
82	sR	191	ASP	3.7
14	CN	131	LYS	3.7
51	C	94	LYS	3.7
25	6	1699	G	3.7
60	c0	54	TYR	3.7
62	N	91	VAL	3.7
75	a	38	HIS	3.7
7	m	297	GLN	3.7
56	H	217	SER	3.7
63	O	61	THR	3.7
62	c2	120	VAL	3.7
68	T	22	VAL	3.7
25	6	727	U	3.6
10	p	115	ALA	3.6
59	K	184	SER	3.6
77	c	32	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	AR	1016	C	3.6
7	m	295	GLY	3.6
25	6	1059	U	3.6
78	d8	31	GLU	3.6
1	AR	1562	C	3.6
1	AR	2546	C	3.6
51	C	207	LEU	3.6
56	H	147	LEU	3.6
39	AK	86	ALA	3.6
25	6	1257	U	3.6
1	AR	2442	G	3.6
18	x	180	LYS	3.6
29	AA	109	GLU	3.6
25	A	1060	U	3.6
53	E	88	ALA	3.6
29	AA	94	SER	3.6
62	N	66	VAL	3.6
14	CN	129	ASN	3.6
1	1	1566	A	3.6
62	N	52	LEU	3.6
26	7	78	ALA	3.6
29	AA	2	ALA	3.6
25	A	182	A	3.6
25	A	488	G	3.6
53	s3	175	VAL	3.6
62	N	112	ALA	3.6
49	p0	50	VAL	3.6
49	p0	293	GLU	3.6
50	B	198	MET	3.6
57	s7	2	SER	3.6
81	g	93	HIS	3.6
25	A	232	U	3.6
25	A	196	G	3.6
75	a	42	LEU	3.6
11	CK	189	GLU	3.6
18	x	176	ILE	3.6
62	c2	94	ALA	3.6
67	S	125	SER	3.6
56	s6	165	GLY	3.6
80	f	49	LEU	3.6
1	AR	2545	C	3.6
25	6	710	U	3.6

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Mol	Chain	Res	Type	RSRZ
1	1	1577	G	3.6
1	AR	1349	G	3.6
1	AR	2440	G	3.6
14	CN	93	ILE	3.6
25	A	201	G	3.6
50	B	39	ASN	3.6
67	c7	104	ASN	3.6
77	d7	57	GLU	3.6
80	e0	50	VAL	3.6
50	B	196	SER	3.6
83	e1	111	GLU	3.5
53	E	218	LEU	3.5
82	h	296	ALA	3.5
25	6	493	U	3.5
62	c2	117	GLY	3.5
62	N	109	GLU	3.5
56	s6	215	ARG	3.5
14	CN	95	ILE	3.5
53	s3	71	LEU	3.5
81	g	129	GLY	3.5
7	m	117	GLU	3.5
51	C	31	ASP	3.5
10	p	116	VAL	3.5
58	s8	123	LYS	3.5
82	h	314	GLN	3.5
66	R	3	ALA	3.5
76	d6	45	VAL	3.5
59	K	178	ALA	3.5
69	U	50	ALA	3.5
18	x	166	VAL	3.5
51	s1	89	ASP	3.5
23	CW	14	THR	3.5
29	AA	100	THR	3.5
75	a	44	GLN	3.5
49	p0	191	TYR	3.5
79	d9	23	VAL	3.5
64	P	80	HIS	3.5
29	AA	92	PHE	3.5
50	B	97	PRO	3.5
82	h	261	LYS	3.5
1	AR	544	C	3.5
23	5	27	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
68	T	5	VAL	3.5
1	1	1572	U	3.5
60	c0	78	GLU	3.5
64	P	79	VAL	3.5
46	i	274	LYS	3.5
1	1	1764	U	3.5
1	1	2570	U	3.5
1	AR	2443	A	3.5
61	M	144	ALA	3.5
56	H	12	SER	3.5
62	N	68	GLU	3.5
51	C	32	ILE	3.5
54	F	261	LEU	3.5
68	c8	14	ILE	3.5
10	CJ	255	SER	3.4
57	I	78	THR	3.4
64	P	14	PHE	3.4
56	H	41	VAL	3.4
81	g	109	ASP	3.4
40	DM	74	LYS	3.4
62	c2	85	LYS	3.4
64	P	33	LEU	3.4
77	d7	82	LYS	3.4
77	d7	58	SER	3.4
20	z	188	ASP	3.4
50	B	199	PRO	3.4
53	s3	42	THR	3.4
77	c	45	THR	3.4
58	s8	200	LYS	3.4
59	s9	93	LEU	3.4
65	c5	136	SER	3.4
51	C	97	LEU	3.4
60	c0	46	LEU	3.4
50	B	166	GLY	3.4
55	s5	92	ARG	3.4
51	C	217	LEU	3.4
60	L	66	TYR	3.4
18	CR	181	ARG	3.4
56	H	50	PHE	3.4
25	A	1691	A	3.4
62	c2	79	ALA	3.4
74	Z	34	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
29	AA	105	SER	3.4
32	AD	35	ARG	3.4
25	A	192	U	3.4
25	6	228	G	3.4
1	1	1248	C	3.4
60	c0	1	MET	3.4
83	e1	109	ASP	3.4
78	d	44	VAL	3.4
65	c5	51	SER	3.4
74	d4	2	SER	3.4
25	A	1058	U	3.4
58	s8	199	LYS	3.4
83	e1	143	LYS	3.4
23	CW	44	GLU	3.4
23	5	10	LYS	3.4
3	4	82	U	3.4
25	A	240	U	3.4
29	AA	70	PRO	3.4
51	s1	54	LEU	3.4
52	s2	92	ALA	3.4
62	c2	27	ALA	3.4
66	c6	142	TYR	3.4
81	g	85	TYR	3.4
75	d5	86	GLU	3.4
62	c2	86	VAL	3.3
69	U	108	LEU	3.3
82	h	221	MET	3.4
82	h	252	LEU	3.3
18	x	177	ALA	3.3
37	DJ	2	ALA	3.3
55	s5	35	GLN	3.3
51	s1	97	LEU	3.3
62	N	71	ILE	3.3
62	c2	89	ILE	3.3
82	h	313	TRP	3.3
1	1	1269	U	3.3
74	Z	133	ASN	3.3
18	x	165	VAL	3.3
71	d1	39	VAL	3.3
53	E	183	GLY	3.3
28	DA	126	LEU	3.3
64	P	11	SER	3.3

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Mol	Chain	Res	Type	RSRZ
26	7	71	ARG	3.3
12	CL	186	GLU	3.3
77	d7	38	PRO	3.3
82	sR	314	GLN	3.3
51	C	42	ASN	3.3
1	AR	1350	A	3.3
25	6	719	U	3.3
25	A	912	U	3.3
82	h	248	ASN	3.3
25	6	1221	A	3.3
25	A	713	A	3.3
59	K	180	LYS	3.3
25	6	484	C	3.3
25	6	495	C	3.3
25	A	231	U	3.3
29	AA	108	GLU	3.3
51	C	40	ASN	3.3
82	h	254	ALA	3.3
74	Z	67	GLY	3.3
78	d8	66	LEU	3.3
20	z	177	VAL	3.3
62	N	94	ALA	3.3
1	AR	250	U	3.3
81	g	143	LYS	3.3
62	c2	126	TRP	3.3
83	e1	108	VAL	3.3
25	6	483	A	3.3
25	A	1712	A	3.3
25	6	655	G	3.3
68	c8	15	LEU	3.3
66	c6	19	VAL	3.3
81	g	124	PRO	3.3
49	p0	280	ALA	3.3
69	c9	55	TYR	3.3
57	I	89	HIS	3.3
1	AR	3157	U	3.3
37	AI	13	SER	3.3
66	R	26	LYS	3.3
51	C	26	ARG	3.3
9	o	27	ALA	3.3
57	I	52	ALA	3.3
62	N	40	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
51	C	45	LYS	3.3
1	1	1270	A	3.2
7	m	126	GLU	3.2
60	c0	74	GLU	3.2
75	d5	89	ILE	3.2
25	A	730	G	3.2
65	c5	133	ALA	3.2
62	N	74	LEU	3.2
82	h	71	CYS	3.2
32	AD	83	LYS	3.2
81	g	107	LYS	3.2
25	6	241	U	3.2
25	6	1226	A	3.2
26	7	91	LYS	3.2
27	CZ	22	LYS	3.2
60	c0	41	TYR	3.2
62	N	73	LYS	3.2
25	6	224	C	3.2
55	s5	30	PRO	3.2
58	J	136	SER	3.2
58	s8	148	ALA	3.2
64	P	78	ALA	3.2
29	AA	18	TYR	3.2
25	A	1681	A	3.2
55	G	161	ASP	3.2
55	s5	145	ASP	3.2
67	c7	87	GLU	3.2
60	c0	44	LYS	3.2
62	c2	96	GLN	3.2
71	W	34	ILE	3.2
49	p0	296	ALA	3.2
67	S	123	ASN	3.2
18	x	157	VAL	3.2
77	d7	77	THR	3.2
25	6	1231	U	3.2
25	6	1708	U	3.2
68	T	17	LEU	3.2
82	h	81	LEU	3.2
59	K	141	VAL	3.2
78	d	7	VAL	3.2
29	DB	56	LYS	3.2
57	I	108	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
65	Q	12	PHE	3.2
82	sR	303	ALA	3.2
25	6	490	C	3.2
56	s6	218	GLU	3.2
1	AR	245	U	3.2
1	AR	2571	U	3.2
25	A	193	U	3.2
51	C	233	GLY	3.2
61	c1	147	GLY	3.2
10	CJ	114	ALA	3.2
64	P	13	VAL	3.2
64	P	20	TYR	3.2
81	g	102	VAL	3.2
80	e0	61	SER	3.2
8	CH	130	ILE	3.2
51	C	37	THR	3.2
66	R	57	LEU	3.2
71	W	69	LEU	3.2
11	CK	190	ASP	3.2
50	B	175	TYR	3.2
1	1	1237	G	3.2
18	CR	173	ARG	3.2
25	6	1712	A	3.2
50	s0	24	LEU	3.2
59	s9	128	LEU	3.2
62	c2	38	HIS	3.2
68	T	23	ASP	3.2
7	m	123	GLU	3.2
17	CQ	182	ASN	3.2
25	6	1696	G	3.2
4	CD	252	THR	3.2
10	CJ	116	VAL	3.2
53	s3	177	MET	3.2
56	H	156	PHE	3.2
66	c6	46	PHE	3.2
9	CI	25	GLN	3.2
49	p0	285	SER	3.2
62	c2	143	GLN	3.2
69	c9	5	SER	3.2
51	C	85	LYS	3.1
53	s3	217	ILE	3.1
65	Q	10	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
50	B	50	VAL	3.1
64	P	42	VAL	3.1
67	c7	88	VAL	3.1
51	C	56	SER	3.1
75	a	98	GLN	3.1
57	s7	58	LEU	3.1
25	6	238	U	3.1
25	A	1370	U	3.1
60	c0	20	VAL	3.1
60	c0	94	GLU	3.1
23	CW	52	ASN	3.1
62	c2	44	GLY	3.1
8	CH	129	GLU	3.1
1	AR	251	G	3.1
69	c9	66	TYR	3.1
10	CJ	256	ALA	3.1
49	p0	288	ALA	3.1
1	AR	246	U	3.1
5	k	387	LEU	3.1
25	A	230	C	3.1
56	s6	212	LEU	3.1
39	DL	86	ALA	3.1
66	R	29	ILE	3.1
66	c6	36	ILE	3.1
59	s9	184	SER	3.1
74	d4	133	ASN	3.1
1	1	439	C	3.1
1	1	1574	C	3.1
1	AR	1563	C	3.1
1	AR	2572	C	3.1
81	g	145	HIS	3.1
51	C	221	PRO	3.1
62	c2	132	GLU	3.1
82	h	74	THR	3.1
25	A	729	G	3.1
55	s5	36	ALA	3.1
7	CG	5	LYS	3.1
82	sR	52	GLN	3.1
57	s7	60	ILE	3.1
26	CY	98	PRO	3.1
62	N	48	SER	3.1
54	F	168	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
56	H	221	ALA	3.1
57	s7	72	LYS	3.1
62	c2	73	LYS	3.1
9	o	25	GLN	3.1
54	F	252	ARG	3.1
7	CG	291	ALA	3.1
40	DM	29	LYS	3.1
51	C	227	ALA	3.1
1	1	1761	C	3.1
25	A	188	A	3.1
54	F	255	ARG	3.1
64	P	83	ILE	3.1
75	a	41	ILE	3.1
51	C	28	GLU	3.1
53	s3	148	LYS	3.1
62	c2	90	LYS	3.1
81	g	151	ASN	3.1
20	CT	176	ARG	3.1
82	h	294	TRP	3.1
60	c0	47	GLN	3.1
62	N	89	ILE	3.1
74	d4	67	GLY	3.1
29	AA	96	VAL	3.1
10	p	152	LEU	3.1
29	AA	91	ALA	3.1
82	h	33	LEU	3.1
83	e1	110	ALA	3.1
50	B	54	TRP	3.1
64	P	43	THR	3.1
69	c9	112	GLY	3.1
77	c	44	THR	3.1
29	AA	114	VAL	3.1
59	K	87	SER	3.0
83	e1	134	ASN	3.0
10	p	202	GLU	3.0
56	s6	162	VAL	3.0
64	P	102	LEU	3.0
59	K	164	PHE	3.0
62	c2	128	ALA	3.0
63	O	15	ALA	3.0
82	h	36	ALA	3.0
1	1	1272	C	3.0

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Mol	Chain	Res	Type	RSRZ
25	6	489	C	3.0
62	N	119	SER	3.0
25	6	1491	U	3.0
29	DB	75	VAL	3.0
58	s8	141	ARG	3.0
68	c8	32	LEU	3.0
51	C	223	PHE	3.0
54	F	133	LYS	3.0
69	U	21	PHE	3.0
68	c8	53	ASP	3.0
23	CW	68	THR	3.0
42	AN	108	THR	3.0
50	B	24	LEU	3.0
56	s6	168	THR	3.0
71	W	53	TYR	3.0
25	A	845	G	3.0
40	DM	73	LEU	3.0
1	1	1580	A	3.0
69	U	6	VAL	3.0
64	P	99	GLN	3.0
82	h	283	LYS	3.0
62	c2	39	ASP	3.0
1	1	1277	C	3.0
1	AR	1354	G	3.0
25	6	227	U	3.0
29	DB	74	VAL	3.0
69	c9	131	ASP	3.0
9	CI	27	ALA	3.0
55	s5	68	ILE	3.0
1	1	2538	U	3.0
1	AR	545	U	3.0
25	A	191	C	3.0
28	DA	120	GLN	3.0
56	s6	216	LEU	3.0
82	sR	252	LEU	3.0
56	H	27	PHE	3.0
29	AA	93	LYS	3.0
55	G	36	ALA	3.0
82	h	295	SER	3.0
66	R	96	TYR	3.0
64	P	93	THR	3.0
4	CD	253	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	AR	1816	A	3.0
25	6	1223	A	3.0
1	1	547	G	3.0
23	CW	53	ALA	3.0
25	A	1229	G	3.0
27	CZ	23	ALA	3.0
64	c4	45	GLY	3.0
54	F	138	TYR	3.0
55	s5	78	ALA	3.0
66	c6	64	ASP	3.0
68	c8	5	VAL	3.0
23	5	80	THR	3.0
1	1	1815	U	3.0
3	4	158	U	3.0
7	m	119	TYR	3.0
57	s7	162	ILE	3.0
40	DM	45	VAL	3.0
49	p0	190	VAL	3.0
68	c8	22	VAL	3.0
25	A	1713	G	3.0
51	C	39	GLU	3.0
66	R	56	GLY	3.0
55	s5	148	ARG	3.0
1	1	1260	A	3.0
51	C	36	SER	3.0
51	C	74	GLN	3.0
75	d5	44	GLN	3.0
1	1	1261	G	2.9
51	C	44	GLY	2.9
29	AA	26	VAL	2.9
46	i	19	VAL	2.9
10	CJ	245	LYS	2.9
61	c1	5	LEU	2.9
62	c2	133	LEU	2.9
12	r	209	ASN	2.9
12	CL	209	ASN	2.9
25	A	189	C	2.9
57	s7	52	ALA	2.9
81	g	100	LEU	2.9
82	h	32	LEU	2.9
12	CL	213	PHE	2.9
36	AH	73	SER	2.9

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Mol	Chain	Res	Type	RSRZ
56	H	80	ASN	2.9
3	AT	83	C	2.9
25	A	696	C	2.9
83	e1	135	HIS	2.9
1	1	1240	A	2.9
58	s8	139	ALA	2.9
82	h	78	ALA	2.9
78	d8	64	ARG	2.9
1	AR	547	G	2.9
25	6	677	G	2.9
75	d5	52	LYS	2.9
25	6	726	C	2.9
34	AF	2	ALA	2.9
65	c5	128	HIS	2.9
71	W	54	ALA	2.9
74	Z	129	VAL	2.9
75	a	82	HIS	2.9
25	6	1285	U	2.9
78	d	26	THR	2.9
80	f	54	ARG	2.9
1	AR	543	C	2.9
25	6	1220	C	2.9
69	U	72	GLY	2.9
1	AR	249	U	2.9
29	AA	42	LEU	2.9
50	B	9	LEU	2.9
38	DK	27	SER	2.9
60	c0	51	SER	2.9
66	R	143	ARG	2.9
69	c9	18	TYR	2.9
60	c0	56	LYS	2.9
62	N	47	GLU	2.9
1	1	1759	C	2.9
51	s1	53	GLY	2.9
29	AA	80	LEU	2.9
32	AD	24	THR	2.9
14	CN	182	ILE	2.9
23	CW	105	LEU	2.9
62	N	88	LEU	2.9
67	S	85	VAL	2.9
53	s3	151	LYS	2.9
54	F	134	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
54	s4	134	LYS	2.9
1	1	1256	G	2.9
25	6	1217	A	2.9
78	d	43	ASN	2.9
81	g	134	ASN	2.9
49	p0	64	ARG	2.9
50	B	41	ARG	2.9
62	c2	77	GLY	2.9
66	c6	114	ARG	2.9
78	d8	8	THR	2.9
56	H	212	LEU	2.9
75	d5	50	ILE	2.9
53	s3	107	PHE	2.9
58	J	148	ALA	2.9
1	AR	1028	U	2.9
59	s9	185	GLY	2.9
53	s3	184	ILE	2.9
56	H	153	VAL	2.9
66	R	63	ILE	2.9
78	d8	9	LEU	2.9
62	c2	101	ALA	2.9
70	d0	14	GLN	2.9
51	C	89	ASP	2.9
25	A	184	C	2.9
64	P	34	SER	2.9
25	6	192	U	2.9
25	A	137	U	2.9
42	DO	77	ILE	2.9
62	N	86	VAL	2.9
77	d7	37	CYS	2.9
49	p0	290	PRO	2.9
82	sR	301	LEU	2.9
24	lR	4	ASN	2.8
1	1	1763	U	2.8
18	CR	156	ALA	2.8
53	E	148	LYS	2.8
83	e1	105	TYR	2.8
49	p0	287	ASP	2.8
20	CT	185	LEU	2.8
25	6	722	G	2.8
25	6	829	A	2.8
54	s4	131	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
57	I	77	LEU	2.8
59	K	116	LEU	2.8
82	sR	49	GLY	2.8
51	C	35	PRO	2.8
68	T	58	ALA	2.8
1	AR	3153	U	2.8
25	A	921	U	2.8
40	DM	69	LEU	2.8
75	d5	87	GLY	2.8
51	C	66	VAL	2.8
12	r	217	PHE	2.8
29	AA	69	LYS	2.8
55	s5	20	PHE	2.8
60	c0	45	ALA	2.8
1	AR	3155	U	2.8
50	B	18	LEU	2.8
53	s3	150	MET	2.8
68	T	11	PHE	2.8
7	CG	294	ALA	2.8
23	CW	106	ALA	2.8
29	AA	35	SER	2.8
65	Q	101	ALA	2.8
82	h	319	ASN	2.8
7	m	236	LEU	2.8
57	I	165	LYS	2.8
67	S	110	VAL	2.8
24	CX	4	ASN	2.8
69	c9	127	ASN	2.8
82	h	34	LEU	2.8
49	p0	196	VAL	2.8
53	s3	152	PHE	2.8
82	h	211	ILE	2.8
1	1	2095	G	2.8
3	AT	158	U	2.8
38	DK	100	HIS	2.8
57	I	80	GLU	2.8
34	DG	2	ALA	2.8
77	c	37	CYS	2.8
78	d8	24	GLY	2.8
75	d5	60	VAL	2.8
1	AR	1814	A	2.8
25	6	1058	U	2.8

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Mol	Chain	Res	Type	RSRZ
25	A	657	U	2.8
62	c2	57	ALA	2.8
69	c9	130	ARG	2.8
34	DG	128	LEU	2.8
53	s3	182	LEU	2.8
54	F	123	LEU	2.8
82	h	305	TYR	2.8
1	1	1234	G	2.8
57	I	86	GLN	2.8
18	x	182	ILE	2.8
23	5	11	ILE	2.8
25	A	491	C	2.8
40	AL	5	ILE	2.8
59	s9	148	VAL	2.8
60	c0	22	VAL	2.8
75	d5	51	LEU	2.8
51	C	220	GLN	2.8
66	R	22	VAL	2.8
81	g	130	VAL	2.8
69	c9	113	ILE	2.8
26	CY	66	GLU	2.8
37	DJ	24	LEU	2.8
62	N	36	LEU	2.8
82	sR	244	ALA	2.8
1	1	2569	A	2.8
1	AR	2540	A	2.8
25	6	1701	A	2.8
25	A	197	A	2.8
54	F	129	VAL	2.8
54	F	256	ARG	2.8
60	c0	35	ILE	2.8
83	e1	131	PHE	2.8
62	N	43	ARG	2.8
64	P	18	ARG	2.8
32	AD	95	ALA	2.8
33	DF	112	ASP	2.8
59	K	185	GLY	2.8
49	p0	26	PHE	2.8
62	N	113	ARG	2.8
69	U	25	GLN	2.8
75	a	40	VAL	2.8
51	C	67	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
80	f	56	MET	2.8
79	d9	17	GLY	2.8
46	i	84	LYS	2.8
81	g	83	LYS	2.8
44	AP	105	GLN	2.7
81	g	137	ASP	2.8
1	1	1765	U	2.7
1	AR	1564	U	2.7
3	4	81	U	2.7
56	H	1	MET	2.7
60	L	49	LEU	2.7
57	s7	92	PHE	2.7
58	J	8	ARG	2.7
79	d9	6	VAL	2.7
29	AA	102	GLU	2.7
54	F	163	ASP	2.7
23	CW	13	LYS	2.7
66	c6	38	LEU	2.7
1	AR	1954	G	2.7
25	6	837	G	2.7
28	9	71	SER	2.7
63	O	59	GLY	2.7
68	T	10	SER	2.7
3	AT	79	A	2.7
33	AE	79	ARG	2.7
73	Y	57	LEU	2.7
1	AR	3277	U	2.7
25	6	657	U	2.7
25	6	1052	U	2.7
29	AA	11	ALA	2.7
32	AD	23	TYR	2.7
60	c0	23	ALA	2.7
82	sR	24	ALA	2.7
10	p	89	GLU	2.7
53	E	139	SER	2.7
57	s7	31	SER	2.7
1	AR	2573	G	2.7
50	s0	46	HIS	2.7
1	1	1244	A	2.7
28	9	85	VAL	2.7
50	B	189	VAL	2.7
59	K	104	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
62	c2	37	VAL	2.7
3	AT	84	C	2.7
25	A	716	C	2.7
25	A	911	U	2.7
75	d5	88	ILE	2.7
42	AN	106	ARG	2.7
53	E	143	ARG	2.7
7	m	293	LEU	2.7
59	K	118	LEU	2.7
56	H	152	ASP	2.7
29	AA	71	PHE	2.7
62	N	117	GLY	2.7
78	d8	32	PHE	2.7
37	AI	2	ALA	2.7
49	p0	28	VAL	2.7
48	sM	83	LYS	2.7
62	N	108	ARG	2.7
52	s2	105	GLY	2.7
59	K	183	ALA	2.7
40	DM	5	ILE	2.7
82	h	310	ILE	2.7
1	AR	1573	G	2.7
1	AR	1576	G	2.7
25	6	496	G	2.7
25	A	714	G	2.7
67	S	74	GLN	2.7
68	c8	10	SER	2.7
78	d8	6	PRO	2.7
82	sR	235	SER	2.7
25	6	320	U	2.7
25	A	794	U	2.7
10	CJ	119	GLY	2.7
10	CJ	251	LYS	2.7
49	p0	88	PHE	2.7
77	d7	46	VAL	2.7
23	CW	108	TYR	2.7
58	J	72	ILE	2.7
25	A	200	A	2.7
59	K	54	ARG	2.7
64	c4	47	LYS	2.7
82	sR	309	VAL	2.7
51	C	60	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
62	c2	52	LEU	2.7
78	d8	54	LEU	2.7
37	DJ	119	LYS	2.7
57	s7	24	PHE	2.7
75	a	37	GLN	2.7
53	s3	221	SER	2.7
55	G	24	VAL	2.7
14	CN	132	ALA	2.7
49	p0	295	ALA	2.7
59	s9	183	ALA	2.7
60	L	41	TYR	2.7
60	c0	66	TYR	2.7
74	d4	26	ASP	2.7
1	AR	1577	G	2.7
25	A	1255	G	2.7
53	E	54	ARG	2.7
50	B	32	HIS	2.7
12	CL	218	ALA	2.7
51	s1	56	SER	2.7
54	F	24	SER	2.7
69	c9	125	SER	2.7
1	AR	601	U	2.7
40	DM	54	LEU	2.7
25	6	1703	C	2.7
37	AI	8	GLU	2.7
29	DB	116	LYS	2.6
51	C	133	TYR	2.6
56	H	175	ILE	2.7
57	I	55	LYS	2.6
60	c0	14	TYR	2.6
63	c3	22	ALA	2.7
66	c6	29	ILE	2.7
78	d8	56	LEU	2.6
25	6	1232	U	2.6
7	m	127	GLY	2.6
68	c8	6	GLN	2.6
77	d7	35	VAL	2.6
1	1	1228	C	2.6
1	1	1238	C	2.6
1	1	1581	C	2.6
29	AA	46	ILE	2.6
35	AG	2	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
25	6	488	G	2.6
49	p0	24	SER	2.6
58	J	143	TRP	2.6
40	DM	43	PHE	2.6
79	e	5	ASN	2.6
25	A	917	U	2.6
49	p0	47	GLY	2.6
49	p0	80	VAL	2.6
62	N	127	GLY	2.6
60	c0	71	GLU	2.6
60	c0	93	GLN	2.6
38	DK	98	ARG	2.6
51	C	182	ALA	2.6
60	L	23	ALA	2.6
64	P	110	LEU	2.6
64	c4	60	ALA	2.6
68	T	102	ALA	2.6
75	a	80	LEU	2.6
82	sR	172	ALA	2.6
82	sR	226	ALA	2.6
1	1	2772	C	2.6
1	AR	247	C	2.6
1	AR	439	C	2.6
50	B	203	PHE	2.6
52	D	144	TRP	2.6
1	AR	1565	G	2.6
25	6	1698	G	2.6
59	K	142	ASN	2.6
62	c2	40	GLY	2.6
40	DM	16	ARG	2.6
49	p0	60	ARG	2.6
75	a	53	GLU	2.6
1	AR	2543	U	2.6
38	DK	58	ILE	2.6
48	sM	66	ALA	2.6
63	O	16	ILE	2.6
82	h	23	LEU	2.6
1	AR	621	A	2.6
82	h	251	TRP	2.6
75	a	68	ARG	2.6
70	d0	15	GLN	2.6
26	CY	82	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
59	K	76	LEU	2.6
1	1	2522	G	2.6
1	1	3319	U	2.6
25	A	178	U	2.6
49	p0	86	PHE	2.6
17	CQ	187	GLU	2.6
29	AA	47	GLU	2.6
66	c6	141	SER	2.6
78	d8	44	VAL	2.6
1	AR	1582	C	2.6
51	C	92	GLN	2.6
10	CJ	109	LEU	2.6
60	c0	11	ILE	2.6
63	c3	66	ILE	2.6
75	a	51	LEU	2.6
78	d	54	LEU	2.6
53	s3	223	LYS	2.6
25	6	725	U	2.6
25	6	1254	U	2.6
25	A	918	U	2.6
57	I	63	PRO	2.6
1	1	1954	G	2.6
1	1	2206	G	2.6
10	CJ	161	GLU	2.6
29	AA	45	GLY	2.6
62	c2	127	GLY	2.6
83	e1	127	GLY	2.6
57	I	31	SER	2.6
10	CJ	26	LEU	2.6
18	x	168	LEU	2.6
25	6	1230	A	2.6
40	DM	36	LYS	2.6
62	c2	97	LEU	2.6
72	X	55	ASP	2.6
1	1	1275	C	2.6
51	C	46	THR	2.6
1	AR	1765	U	2.6
25	6	1704	U	2.6
26	7	92	GLU	2.6
29	DB	102	GLU	2.6
29	AA	111	LYS	2.6
60	L	68	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
75	a	88	ILE	2.6
79	d9	20	GLN	2.6
10	p	97	TYR	2.6
25	6	729	G	2.6
25	A	142	G	2.6
26	7	73	ARG	2.6
37	AI	120	ALA	2.6
77	c	79	PHE	2.6
25	A	541	A	2.6
49	p0	29	GLY	2.6
49	p0	188	VAL	2.6
51	C	229	MET	2.6
64	c4	125	SER	2.6
14	CN	112	ASN	2.6
23	CW	56	VAL	2.6
25	A	235	G	2.6
55	G	70	VAL	2.6
57	s7	7	LYS	2.6
60	L	67	THR	2.6
76	b	60	PRO	2.6
81	g	115	THR	2.6
1	AR	3319	U	2.6
25	6	1687	U	2.6
57	s7	49	ILE	2.6
15	CO	138	ALA	2.6
23	CW	15	PHE	2.6
49	p0	286	GLY	2.6
58	J	181	GLY	2.6
62	N	75	VAL	2.6
62	N	121	VAL	2.6
62	N	53	THR	2.6
66	c6	115	THR	2.6
75	d5	105	THR	2.6
29	DB	36	HIS	2.6
18	x	183	ALA	2.6
59	s9	139	GLN	2.6
29	AA	113	VAL	2.6
51	C	43	VAL	2.6
53	s3	142	LEU	2.6
29	DB	72	ILE	2.6
51	C	232	HIS	2.6
70	d0	78	THR	2.6

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Mol	Chain	Res	Type	RSRZ
10	CJ	120	LYS	2.5
34	AF	127	ALA	2.5
57	I	76	LYS	2.5
58	s8	162	ALA	2.5
65	c5	7	ALA	2.5
65	c5	9	LYS	2.5
1	1	252	U	2.5
1	1	2208	A	2.5
25	A	181	A	2.5
25	6	1690	G	2.5
27	CZ	33	ARG	2.5
82	h	213	SER	2.5
28	9	126	LEU	2.5
56	s6	173	PRO	2.5
60	c0	97	PRO	2.5
29	AA	101	PHE	2.5
80	f	48	THR	2.5
35	DH	60	ARG	2.5
57	s7	57	ALA	2.5
70	d0	98	GLN	2.5
62	N	120	VAL	2.5
25	A	910	C	2.5
50	B	194	PRO	2.5
51	C	23	PRO	2.5
56	H	173	PRO	2.5
57	s7	157	LYS	2.5
62	c2	136	ILE	2.5
74	d4	34	ASN	2.5
10	CJ	110	THR	2.5
82	h	318	ALA	2.5
69	c9	114	VAL	2.5
58	s8	137	LYS	2.5
55	s5	55	ASP	2.5
75	a	93	SER	2.5
82	h	264	SER	2.5
55	s5	129	PRO	2.5
64	P	94	PRO	2.5
36	AH	71	THR	2.5
50	s0	20	ALA	2.5
55	s5	79	ASN	2.5
64	P	101	ALA	2.5
25	6	1265	G	2.5

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Mol	Chain	Res	Type	RSRZ
25	6	1697	G	2.5
58	J	71	GLY	2.5
64	P	28	VAL	2.5
57	I	81	LEU	2.5
77	d7	36	LYS	2.5
61	c1	20	PHE	2.5
82	sR	316	MET	2.5
55	G	96	SER	2.5
55	G	223	SER	2.5
46	i	137	GLU	2.5
44	AP	11	TYR	2.5
1	1	1239	C	2.5
13	CM	174	LYS	2.5
25	6	1219	A	2.5
40	DM	6	THR	2.5
49	p0	89	THR	2.5
50	B	139	VAL	2.5
59	K	95	TYR	2.5
62	N	116	VAL	2.5
62	N	124	LYS	2.5
64	c4	97	GLY	2.5
74	Z	29	HIS	2.5
59	K	3	ARG	2.5
51	s1	90	GLU	2.5
77	c	28	PRO	2.5
7	m	122	VAL	2.5
25	6	494	U	2.5
44	AP	102	GLN	2.5
53	s3	222	VAL	2.5
60	c0	13	GLN	2.5
66	R	90	VAL	2.5
71	W	32	VAL	2.5
82	h	309	VAL	2.5
57	I	29	ASN	2.5
38	AJ	98	ARG	2.5
1	1	1103	A	2.5
1	AR	2569	A	2.5
27	CZ	142	ILE	2.5
69	U	35	ASP	2.5
69	U	103	LYS	2.5
12	CL	188	GLY	2.5
57	I	90	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
61	c1	146	ALA	2.5
81	g	88	PRO	2.5
25	A	499	U	2.5
50	B	201	LEU	2.5
66	R	114	ARG	2.5
42	AN	119	ASN	2.5
49	p0	81	LYS	2.5
9	o	23	ALA	2.5
18	x	178	ALA	2.5
26	CY	85	ALA	2.5
51	C	131	ASP	2.5
51	C	190	PRO	2.5
55	G	182	ALA	2.5
57	s7	123	ASP	2.5
62	c2	42	ALA	2.5
75	a	61	SER	2.5
78	d8	59	SER	2.5
55	s5	130	ILE	2.5
62	N	100	TRP	2.5
62	c2	100	TRP	2.5
25	6	142	G	2.5
70	d0	72	ASN	2.5
82	sR	168	THR	2.5
82	sR	177	MET	2.5
62	N	122	VAL	2.5
66	R	55	VAL	2.5
74	Z	61	ARG	2.5
20	z	185	LEU	2.5
69	U	132	LEU	2.5
56	H	45	PHE	2.5
25	A	507	U	2.5
55	s5	224	ASN	2.5
65	c5	89	MET	2.5
10	CJ	113	ALA	2.5
25	6	720	G	2.5
49	p0	87	VAL	2.5
53	E	142	LEU	2.5
23	5	9	GLN	2.5
63	O	17	PRO	2.5
1	1	1025	A	2.5
3	4	79	A	2.5
60	c0	34	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
62	c2	106	ILE	2.5
75	a	89	ILE	2.5
25	6	711	U	2.5
56	H	66	GLY	2.5
63	O	60	VAL	2.5
74	Z	6	THR	2.5
78	d8	41	VAL	2.5
46	i	105	LYS	2.5
66	R	60	PHE	2.5
26	CY	94	ARG	2.5
68	c8	144	ARG	2.5
82	h	5	GLU	2.5
2	AS	73	C	2.4
82	sR	313	TRP	2.4
82	h	271	VAL	2.4
25	6	1361	U	2.4
25	A	920	U	2.4
80	f	55	ARG	2.4
56	H	218	GLU	2.4
59	K	162	SER	2.4
51	C	225	VAL	2.4
1	1	1232	C	2.4
49	p0	79	PHE	2.4
82	sR	227	ALA	2.4
55	s5	157	ARG	2.4
64	P	114	ARG	2.4
78	d8	27	GLN	2.4
5	CE	386	ASP	2.4
51	C	215	VAL	2.4
67	S	124	VAL	2.4
69	c9	128	GLY	2.4
74	Z	35	VAL	2.4
49	p0	283	ALA	2.4
1	AR	1353	U	2.4
1	AR	2544	U	2.4
10	p	122	LYS	2.4
25	A	227	U	2.4
56	H	226	ILE	2.4
14	CN	94	GLY	2.4
49	p0	76	LEU	2.4
50	B	23	HIS	2.4
54	F	76	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
60	L	48	SER	2.4
56	s6	213	ALA	2.4
62	c2	69	ALA	2.4
69	U	107	ALA	2.4
78	d8	63	ALA	2.4
53	E	213	GLU	2.4
40	DM	10	GLN	2.4
68	T	14	ILE	2.4
80	e0	48	THR	2.4
25	A	894	U	2.4
56	H	177	ARG	2.4
69	c9	9	VAL	2.4
75	d5	42	LEU	2.4
78	d8	48	VAL	2.4
78	d8	57	MET	2.4
25	6	714	G	2.4
51	C	132	ASP	2.4
59	s9	146	PHE	2.4
56	H	148	SER	2.4
67	S	107	SER	2.4
37	AI	64	GLU	2.4
50	s0	173	ILE	2.4
49	p0	104	ARG	2.4
51	C	183	GLN	2.4
64	P	12	GLN	2.4
81	g	117	LEU	2.4
7	m	201	GLY	2.4
37	AI	3	GLY	2.4
57	s7	69	GLY	2.4
12	CL	217	PHE	2.4
57	s7	158	ASP	2.4
60	c0	75	TYR	2.4
11	CK	191	LEU	2.4
29	AA	103	GLN	2.4
55	s5	165	LEU	2.4
58	s8	111	GLN	2.4
67	c7	105	GLN	2.4
75	d5	68	ARG	2.4
10	CJ	35	GLY	2.4
36	AH	72	VAL	2.4
60	L	3	MET	2.4
66	R	11	GLY	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
70	d0	36	ASN	2.4
77	c	39	GLY	2.4
78	d8	5	THR	2.4
78	d8	45	LYS	2.4
78	d	35	ASP	2.4
80	f	2	ALA	2.4
1	AR	1628	C	2.4
18	CR	182	ILE	2.4
25	6	1706	C	2.4
50	s0	185	ARG	2.4
28	DA	90	VAL	2.4
44	AP	99	GLN	2.4
51	C	73	LEU	2.4
55	s5	150	GLY	2.4
40	DM	37	PRO	2.4
53	s3	65	ARG	2.4
63	c3	15	ALA	2.4
69	U	51	GLU	2.4
1	1	3155	U	2.4
57	s7	73	VAL	2.4
59	K	148	VAL	2.4
62	N	105	LYS	2.4
68	T	43	SER	2.4
10	CJ	182	GLY	2.4
25	A	793	A	2.4
29	AA	38	PHE	2.4
55	s5	43	PHE	2.4
23	CW	98	THR	2.4
62	N	51	ALA	2.4
1	1	1229	G	2.4
40	DM	27	ILE	2.4
60	c0	26	ASP	2.4
24	lR	5	GLY	2.4
51	C	93	GLY	2.4
1	AR	1762	C	2.4
25	6	1709	C	2.4
25	A	233	C	2.4
26	7	93	ARG	2.4
55	s5	225	ARG	2.4
78	d8	67	ARG	2.4
1	1	440	A	2.4
68	c8	19	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
77	d7	53	ALA	2.4
78	d8	39	THR	2.4
25	6	794	U	2.4
29	DB	58	GLY	2.4
50	B	29	VAL	2.4
57	I	56	LYS	2.4
53	E	184	ILE	2.4
54	F	162	ILE	2.4
62	N	128	ALA	2.4
62	c2	84	ASN	2.4
69	c9	136	ALA	2.4
82	sR	317	THR	2.4
29	DB	95	VAL	2.3
36	AH	77	GLY	2.3
56	H	36	VAL	2.3
53	s3	25	PHE	2.3
56	H	190	GLN	2.3
57	I	101	LYS	2.3
10	p	129	PRO	2.3
69	c9	111	ILE	2.3
76	b	65	PRO	2.3
62	c2	32	LEU	2.3
74	Z	125	LEU	2.3
29	AA	74	VAL	2.3
82	h	25	THR	2.3
72	X	73	GLY	2.3
28	DA	113	LYS	2.3
25	6	705	U	2.3
49	p0	18	TYR	2.3
56	H	169	TYR	2.3
60	c0	43	ILE	2.3
12	CL	185	ARG	2.3
29	DB	10	VAL	2.3
1	AR	1024	G	2.3
51	C	50	LYS	2.3
56	H	16	PHE	2.3
62	N	80	ASN	2.3
65	c5	135	THR	2.3
82	h	99	THR	2.3
55	s5	31	GLU	2.3
57	I	150	GLN	2.3
7	m	192	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
10	p	109	LEU	2.3
25	A	919	A	2.3
53	E	178	ARG	2.3
54	s4	149	TYR	2.3
55	s5	77	TYR	2.3
62	c2	48	SER	2.3
82	h	301	LEU	2.3
68	T	56	LYS	2.3
29	AA	90	GLU	2.3
79	d9	45	GLU	2.3
50	B	43	ASP	2.3
51	C	224	ASP	2.3
1	AR	1031	C	2.3
78	d8	42	ARG	2.3
15	u	9	ALA	2.3
51	C	54	LEU	2.3
58	s8	115	ALA	2.3
59	K	156	ILE	2.3
7	m	125	VAL	2.3
29	AA	61	LYS	2.3
59	s9	177	ALA	2.3
51	C	21	VAL	2.3
55	s5	168	VAL	2.3
75	d5	70	LYS	2.3
1	AR	1103	A	2.3
25	A	728	U	2.3
54	F	25	GLY	2.3
59	K	111	THR	2.3
75	d5	102	THR	2.3
40	DM	7	ASP	2.3
17	CQ	183	ALA	2.3
29	AA	25	ILE	2.3
62	N	42	ALA	2.3
62	N	59	LEU	2.3
69	U	28	LEU	2.3
69	c9	17	ALA	2.3
75	d5	46	LYS	2.3
1	AR	3278	C	2.3
49	p0	27	VAL	2.3
12	CL	194	GLY	2.3
25	6	234	G	2.3
46	i	98	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
49	p0	282	SER	2.3
51	C	24	PHE	2.3
62	N	55	GLY	2.3
67	c7	86	PRO	2.3
14	CN	136	GLU	2.3
25	6	242	U	2.3
78	d8	29	ARG	2.3
15	u	137	LYS	2.3
29	DB	21	LYS	2.3
38	AJ	29	LYS	2.3
42	AN	121	LEU	2.3
60	L	5	LYS	2.3
62	c2	41	LEU	2.3
65	Q	78	THR	2.3
49	p0	73	PHE	2.3
64	P	74	VAL	2.3
82	h	54	PHE	2.3
20	CT	170	ARG	2.3
57	s7	32	PRO	2.3
59	s9	186	GLU	2.3
62	c2	25	GLU	2.3
71	W	18	SER	2.3
82	h	246	SER	2.3
56	s6	171	LYS	2.3
1	1	1353	U	2.3
25	A	486	G	2.3
57	s7	89	HIS	2.3
59	K	105	LEU	2.3
76	b	44	ILE	2.3
82	h	182	ASN	2.3
13	s	11	ASP	2.3
56	s6	156	PHE	2.3
82	h	77	GLY	2.3
29	DB	73	LYS	2.3
60	L	4	PRO	2.3
82	h	206	PRO	2.3
56	s6	148	SER	2.3
25	6	189	C	2.3
69	c9	22	LEU	2.3
74	Z	63	GLN	2.3
10	p	130	TYR	2.3
53	E	25	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
53	E	27	ARG	2.3
53	s3	40	ARG	2.3
66	R	7	VAL	2.3
1	1	1635	G	2.3
62	c2	98	GLY	2.3
62	c2	68	GLU	2.3
69	U	38	LYS	2.3
10	p	99	PRO	2.3
70	d0	105	GLN	2.3
56	H	186	ARG	2.3
79	e	23	VAL	2.3
81	g	106	TYR	2.3
82	h	8	VAL	2.3
23	5	52	ASN	2.3
55	G	186	ASN	2.3
64	P	31	THR	2.3
64	P	38	THR	2.3
66	R	62	ASN	2.3
82	h	146	GLY	2.3
37	DJ	8	GLU	2.3
66	R	105	LEU	2.3
60	L	11	ILE	2.3
56	s6	167	LYS	2.3
71	W	37	ALA	2.3
75	d5	104	ALA	2.3
51	C	102	GLY	2.3
56	H	165	GLY	2.3
74	Z	46	GLU	2.3
80	f	52	GLY	2.3
25	A	490	C	2.3
25	A	558	U	2.3
53	E	111	ASN	2.3
82	sR	224	ASN	2.3
53	s3	178	ARG	2.3
65	c5	109	PRO	2.3
82	h	247	PRO	2.3
14	CN	145	PHE	2.3
59	s9	141	VAL	2.3
64	P	17	ALA	2.3
78	d8	55	VAL	2.3
1	1	3351	U	2.2
49	p0	31	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
51	s1	98	THR	2.2
62	c2	58	LEU	2.2
78	d8	61	ARG	2.2
82	h	202	LEU	2.2
1	1	1582	C	2.2
54	F	127	LYS	2.2
69	U	124	ILE	2.2
51	s1	91	VAL	2.2
56	H	210	GLN	2.2
60	L	22	VAL	2.2
20	z	178	ALA	2.2
44	AP	90	HIS	2.2
59	s9	182	GLU	2.2
75	d5	38	HIS	2.2
81	g	110	ALA	2.2
25	6	188	A	2.2
57	I	79	ARG	2.2
74	d4	32	ARG	2.2
62	N	84	ASN	2.2
56	H	5	ILE	2.2
57	s7	177	THR	2.2
69	U	101	ASN	2.2
82	sR	165	ASP	2.2
1	1	3352	U	2.2
24	lR	137	VAL	2.2
29	DB	96	VAL	2.2
14	CN	114	GLN	2.2
40	DM	60	GLY	2.2
57	s7	11	GLN	2.2
23	5	94	ARG	2.2
25	A	898	A	2.2
54	F	171	ASP	2.2
62	c2	70	ASN	2.2
74	d4	3	ASP	2.2
82	h	317	THR	2.2
1	1	1262	G	2.2
1	1	2209	U	2.2
1	1	2501	U	2.2
20	CT	178	ALA	2.2
49	p0	62	ALA	2.2
54	s4	258	GLN	2.2
71	d1	44	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
76	b	62	TYR	2.2
82	h	27	ALA	2.2
1	AR	1759	C	2.2
25	6	1711	C	2.2
29	AA	33	SER	2.2
66	c6	89	LEU	2.2
29	DB	118	PHE	2.2
82	h	312	VAL	2.2
1	1	1245	A	2.2
18	CR	171	ARG	2.2
7	m	100	ALA	2.2
9	o	28	ALA	2.2
55	s5	28	PRO	2.2
13	s	90	GLN	2.2
62	c2	20	ALA	2.2
71	d1	42	GLU	2.2
25	6	1258	U	2.2
14	CN	116	LEU	2.2
56	H	178	LEU	2.2
69	U	40	SER	2.2
50	s0	41	ARG	2.2
62	N	33	ARG	2.2
23	5	22	PRO	2.2
53	E	93	ASP	2.2
53	s3	34	TYR	2.2
64	c4	70	LYS	2.2
81	g	94	LYS	2.2
59	s9	112	GLN	2.2
62	N	69	ALA	2.2
67	c7	25	THR	2.2
76	b	48	ALA	2.2
82	h	180	ALA	2.2
1	AR	2508	U	2.2
25	6	232	U	2.2
25	6	501	U	2.2
25	6	1702	A	2.2
25	A	280	U	2.2
25	A	1688	U	2.2
63	c3	25	TRP	2.2
23	5	38	ILE	2.2
49	p0	187	VAL	2.2
51	C	65	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
56	s6	175	ILE	2.2
67	S	88	VAL	2.2
25	6	1233	G	2.2
25	A	682	C	2.2
51	C	90	GLU	2.2
51	s1	228	LEU	2.2
55	G	198	LEU	2.2
23	5	28	PHE	2.2
25	6	754	A	2.2
25	6	1224	A	2.2
51	s1	20	VAL	2.2
64	c4	83	ILE	2.2
70	V	120	SER	2.2
77	c	30	SER	2.2
78	d8	28	VAL	2.2
75	d5	72	GLY	2.2
62	N	79	ALA	2.2
62	N	101	ALA	2.2
60	L	46	LEU	2.2
82	h	267	PRO	2.2
1	1	1246	G	2.2
1	1	1573	G	2.2
5	k	287	LYS	2.2
46	i	86	ASN	2.2
48	sM	82	THR	2.2
60	c0	10	LYS	2.2
75	a	56	THR	2.2
74	d4	27	VAL	2.2
25	A	493	U	2.2
53	E	87	TYR	2.2
58	s8	117	TYR	2.2
74	Z	69	SER	2.2
56	H	124	LEU	2.2
59	K	119	ALA	2.2
83	e1	140	TYR	2.2
28	DA	83	ASP	2.2
68	c8	12	GLN	2.2
69	c9	35	ASP	2.2
60	c0	96	ASN	2.2
69	c9	14	PHE	2.2
25	6	1235	C	2.2
50	B	48	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
81	g	86	THR	2.2
14	CN	130	GLY	2.2
25	A	720	G	2.2
7	CG	293	LEU	2.2
20	CT	181	ARG	2.2
40	DM	26	LYS	2.2
74	Z	132	ARG	2.2
25	6	579	A	2.2
55	s5	158	GLN	2.2
57	s7	22	GLN	2.2
71	W	40	ASP	2.2
49	p0	59	VAL	2.2
56	s6	36	VAL	2.2
57	I	51	VAL	2.2
59	K	113	VAL	2.2
82	h	43	ILE	2.2
1	1	2572	C	2.2
60	L	44	LYS	2.2
68	T	3	LEU	2.2
1	1	2571	U	2.2
1	1	1953	G	2.2
25	6	1050	G	2.2
60	c0	36	ASP	2.2
82	sR	30	PRO	2.2
62	N	106	ILE	2.2
12	CL	204	GLY	2.2
29	AA	79	HIS	2.2
57	s7	126	LEU	2.1
59	K	60	LEU	2.1
59	K	86	LEU	2.1
1	1	1255	C	2.1
1	1	2507	C	2.1
6	CF	218	ALA	2.1
15	u	138	ALA	2.1
40	AL	34	ALA	2.1
75	a	47	TYR	2.1
12	CL	205	SER	2.1
1	AR	1630	U	2.1
1	AR	1763	U	2.1
33	DF	110	GLU	2.1
36	AH	110	GLU	2.1
40	DM	70	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
80	e0	45	VAL	2.1
82	sR	315	VAL	2.1
1	1	1230	G	2.1
1	AR	1561	G	2.1
49	p0	82	GLY	2.1
54	F	144	GLY	2.1
55	G	75	GLY	2.1
60	c0	19	GLY	2.1
69	c9	32	GLY	2.1
23	CW	57	THR	2.1
51	s1	61	LEU	2.1
51	s1	217	LEU	2.1
55	G	175	LEU	2.1
60	c0	28	ASN	2.1
63	O	138	ASN	2.1
83	e1	123	ASN	2.1
49	p0	289	ALA	2.1
73	Y	85	ALA	2.1
6	l	2	SER	2.1
49	p0	48	ARG	2.1
62	c2	82	PRO	2.1
69	U	126	GLU	2.1
70	d0	102	ARG	2.1
77	c	36	LYS	2.1
63	O	53	LEU	2.1
66	R	52	LEU	2.1
69	U	80	TYR	2.1
69	c9	16	ASN	2.1
69	c9	43	ASN	2.1
75	a	101	TYR	2.1
79	d9	27	HIS	2.1
82	h	306	THR	2.1
12	CL	183	LYS	2.1
40	DM	56	ILE	2.1
51	C	68	VAL	2.1
58	s8	152	ILE	2.1
62	N	21	GLU	2.1
77	d7	54	VAL	2.1
51	C	103	MET	2.1
1	AR	2542	U	2.1
25	A	237	C	2.1
25	A	717	C	2.1

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Mol	Chain	Res	Type	RSRZ
49	p0	46	ARG	2.1
50	B	147	THR	2.1
66	R	23	LYS	2.1
66	c6	143	ARG	2.1
64	P	39	ILE	2.1
64	c4	48	VAL	2.1
78	d8	58	GLU	2.1
7	CG	9	SER	2.1
25	A	505	A	2.1
80	f	6	GLY	2.1
83	e1	122	SER	2.1
4	CD	34	TYR	2.1
57	I	43	PHE	2.1
59	K	120	LYS	2.1
69	c9	119	LYS	2.1
80	e0	55	ARG	2.1
82	sR	214	ALA	2.1
7	m	221	GLU	2.1
10	CJ	123	GLN	2.1
14	CN	57	VAL	2.1
56	H	162	VAL	2.1
57	s7	29	ASN	2.1
68	c8	20	THR	2.1
75	d5	41	ILE	2.1
77	d7	40	CYS	2.1
57	s7	154	LEU	2.1
69	U	105	LEU	2.1
32	AD	22	LYS	2.1
56	H	149	LYS	2.1
77	c	80	ARG	2.1
23	CW	33	TYR	2.1
79	d9	43	PHE	2.1
23	CW	34	ALA	2.1
56	s6	205	ALA	2.1
29	AA	40	HIS	2.1
44	AP	92	GLU	2.1
46	i	116	GLU	2.1
23	CW	100	THR	2.1
64	P	97	GLY	2.1
64	c4	44	GLY	2.1
64	c4	65	GLN	2.1
79	d9	31	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
60	L	59	PHE	2.1
60	c0	16	PHE	2.1
80	e0	27	PRO	2.1
82	sR	26	SER	2.1
5	k	386	ASP	2.1
20	z	189	ALA	2.1
50	s0	40	ALA	2.1
65	Q	54	ALA	2.1
67	S	87	GLU	2.1
69	c9	29	GLU	2.1
25	A	1227	A	2.1
72	d2	56	HIS	2.1
82	h	113	VAL	2.1
10	p	201	THR	2.1
20	z	181	ARG	2.1
25	A	1237	G	2.1
56	H	180	THR	2.1
70	V	67	THR	2.1
79	e	30	LEU	2.1
82	h	137	LYS	2.1
51	s1	23	PRO	2.1
27	8	23	ALA	2.1
53	s3	144	ALA	2.1
69	c9	51	GLU	2.1
51	C	72	ASP	2.1
54	F	254	ARG	2.1
69	U	24	ARG	2.1
25	6	138	A	2.1
25	A	830	U	2.1
25	A	1240	U	2.1
29	AA	118	PHE	2.1
57	s7	131	PHE	2.1
78	d8	19	THR	2.1
1	1	1233	G	2.1
25	A	1716	C	2.1
29	AA	117	ALA	2.1
30	DC	97	GLU	2.1
49	p0	44	GLU	2.1
8	CH	15	VAL	2.1
24	lR	2	SER	2.1
29	DB	69	LYS	2.1
60	c0	52	LYS	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	s4	253	ASP	2.1
56	H	18	ILE	2.1
62	N	46	ARG	2.1
77	c	35	VAL	2.1
81	g	149	LYS	2.1
54	F	259	GLN	2.1
57	I	11	GLN	2.1
62	N	126	TRP	2.1
1	AR	1356	U	2.1
1	AR	1764	U	2.1
1	AR	2565	U	2.1
4	j	252	THR	2.1
25	6	231	U	2.1
25	A	725	U	2.1
1	1	1231	A	2.1
3	4	80	A	2.1
7	CG	263	GLU	2.1
13	s	167	TYR	2.1
56	s6	177	ARG	2.1
56	s6	209	ALA	2.1
57	I	17	GLU	2.1
68	c8	146	ALA	2.1
69	c9	137	ALA	2.1
74	d4	4	ALA	2.1
78	d8	10	ALA	2.1
82	sR	318	ALA	2.1
55	s5	96	SER	2.1
59	K	63	ASP	2.1
62	c2	78	LEU	2.1
82	sR	205	SER	2.1
1	AR	1268	G	2.1
29	DB	57	HIS	2.1
10	CJ	137	ASN	2.1
28	9	98	ASN	2.1
29	AA	3	LYS	2.1
37	DJ	102	GLU	2.1
50	B	21	ASN	2.1
59	K	6	ARG	2.1
75	d5	103	ARG	2.1
7	CG	288	ALA	2.1
49	p0	51	VAL	2.1
49	p0	277	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
56	s6	206	ALA	2.1
1	1	1263	A	2.1
1	AR	1575	A	2.1
82	h	73	LEU	2.1
57	s7	66	SER	2.1
58	s8	149	SER	2.1
29	AA	130	PHE	2.0
44	AP	22	GLN	2.0
54	s4	133	LYS	2.0
68	c8	11	PHE	2.0
56	H	225	GLU	2.0
56	s6	160	ARG	2.0
81	g	116	LYS	2.0
1	AR	243	G	2.0
20	CT	179	GLU	2.0
10	CJ	45	ASN	2.0
36	AH	112	ALA	2.0
36	DI	59	PRO	2.0
56	H	49	VAL	2.0
56	s6	163	THR	2.0
59	K	4	ALA	2.0
66	c6	39	VAL	2.0
70	d0	107	THR	2.0
82	h	83	ALA	2.0
40	DM	35	GLY	2.0
50	B	188	LEU	2.0
56	s6	147	LEU	2.0
66	R	65	ILE	2.0
78	d	56	LEU	2.0
1	AR	253	A	2.0
49	p0	195	GLN	2.0
57	I	85	PHE	2.0
57	s7	161	GLN	2.0
58	J	141	ARG	2.0
82	h	59	ARG	2.0
40	DM	2	ALA	2.0
51	C	34	ALA	2.0
59	s9	181	ALA	2.0
80	f	45	VAL	2.0
8	n	97	ASN	2.0
28	DA	91	ASN	2.0
1	1	250	U	2.0

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Mol	Chain	Res	Type	RSRZ
50	s0	166	GLY	2.0
60	c0	53	GLY	2.0
62	N	125	ASN	2.0
51	C	30	PHE	2.0
53	s3	51	ARG	2.0
69	c9	122	ARG	2.0
75	d5	58	ARG	2.0
82	h	231	MET	2.0
25	A	733	A	2.0
10	CJ	67	ILE	2.0
29	AA	6	LYS	2.0
49	p0	43	LYS	2.0
59	s9	180	LYS	2.0
82	sR	47	LEU	2.0
13	s	60	ARG	2.0
14	CN	133	PRO	2.0
62	N	102	GLY	2.0
73	Y	2	GLY	2.0
1	1	545	U	2.0
25	6	74	U	2.0
25	A	187	G	2.0
53	E	214	GLU	2.0
55	s5	39	GLU	2.0
67	S	70	SER	2.0
66	c6	28	LEU	2.0
81	g	152	ALA	2.0
25	6	491	C	2.0
48	sM	50	ASN	2.0
77	c	42	ASN	2.0
40	DM	4	GLU	2.0
1	1	1241	U	2.0
1	1	1348	U	2.0
1	AR	2541	U	2.0
22	2	120	LYS	2.0
23	CW	70	LYS	2.0
25	A	1682	U	2.0
42	AN	120	GLN	2.0
59	K	112	GLN	2.0
57	s7	175	LYS	2.0
61	c1	117	VAL	2.0
67	S	53	TYR	2.0
78	d8	30	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
46	i	255	ALA	2.0
58	J	147	ALA	2.0
64	c4	62	LEU	2.0
7	CG	3	PHE	2.0
25	A	895	G	2.0
52	D	145	GLY	2.0
56	H	33	GLY	2.0
74	Z	66	GLY	2.0
78	d8	53	ILE	2.0
25	A	217	A	2.0
64	P	37	GLU	2.0
67	S	101	ASN	2.0
82	h	316	MET	2.0
25	A	500	C	2.0
46	i	83	LYS	2.0
12	CL	181	TYR	2.0
56	H	216	LEU	2.0
57	I	34	LEU	2.0
62	N	60	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	6	2176	1/1	0.31	0.68	93,93,93,93	0
85	MG	1	3951	1/1	0.45	0.33	69,69,69,69	0
85	MG	6	2158	1/1	0.46	0.75	74,74,74,74	0
85	MG	1	4140	1/1	0.46	0.29	187,187,187,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	A	2130	1/1	0.46	0.62	74,74,74,74	0
85	MG	1	3813	1/1	0.48	0.37	61,61,61,61	0
85	MG	1	3958	1/1	0.49	0.38	44,44,44,44	0
85	MG	1	4053	1/1	0.49	0.41	74,74,74,74	0
85	MG	1	3965	1/1	0.51	0.57	94,94,94,94	0
85	MG	A	2121	1/1	0.52	0.31	62,62,62,62	0
85	MG	1	3948	1/1	0.55	0.23	73,73,73,73	0
85	MG	AR	4196	1/1	0.55	0.43	43,43,43,43	0
85	MG	4	229	1/1	0.56	0.41	54,54,54,54	0
85	MG	AS	228	1/1	0.56	0.42	84,84,84,84	0
85	MG	AR	4102	1/1	0.57	0.98	30,30,30,30	0
85	MG	AR	4104	1/1	0.57	0.39	66,66,66,66	0
85	MG	1	4150	1/1	0.57	0.26	49,49,49,49	0
85	MG	A	2150	1/1	0.57	0.16	86,86,86,86	0
85	MG	1	4152	1/1	0.59	0.80	111,111,111,111	0
85	MG	AR	4122	1/1	0.60	0.25	68,68,68,68	0
85	MG	1	4104	1/1	0.60	0.45	53,53,53,53	0
85	MG	AR	3890	1/1	0.60	0.42	29,29,29,29	0
85	MG	AR	4013	1/1	0.60	0.29	65,65,65,65	0
85	MG	1	3989	1/1	0.60	0.26	55,55,55,55	0
85	MG	6	2168	1/1	0.60	0.31	132,132,132,132	0
85	MG	1	3772	1/1	0.61	0.20	35,35,35,35	0
85	MG	6	2180	1/1	0.61	0.60	64,64,64,64	0
85	MG	A	2124	1/1	0.61	0.30	68,68,68,68	0
85	MG	6	2185	1/1	0.61	0.46	89,89,89,89	0
85	MG	AR	4254	1/1	0.61	0.38	56,56,56,56	0
85	MG	A	2155	1/1	0.61	0.46	75,75,75,75	0
85	MG	6	2194	1/1	0.62	0.15	108,108,108,108	0
85	MG	6	2160	1/1	0.62	0.38	85,85,85,85	0
85	MG	4	221	1/1	0.63	0.54	51,51,51,51	0
85	MG	1	4004	1/1	0.64	0.26	44,44,44,44	0
85	MG	AR	4125	1/1	0.64	0.29	82,82,82,82	0
85	MG	AS	220	1/1	0.64	0.36	68,68,68,68	0
85	MG	AR	3950	1/1	0.65	0.27	47,47,47,47	0
85	MG	1	3823	1/1	0.65	0.27	41,41,41,41	0
85	MG	6	2191	1/1	0.65	0.44	87,87,87,87	0
85	MG	AR	3955	1/1	0.66	0.17	34,34,34,34	0
85	MG	AR	4255	1/1	0.67	0.64	57,57,57,57	0
85	MG	1	4124	1/1	0.68	0.22	48,48,48,48	0
85	MG	t	202	1/1	0.68	0.26	101,101,101,101	0
85	MG	AR	4219	1/1	0.68	0.17	67,67,67,67	0
85	MG	AR	4074	1/1	0.68	0.23	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4174	1/1	0.69	0.42	39,39,39,39	0
85	MG	AT	218	1/1	0.69	0.34	30,30,30,30	0
85	MG	A	2099	1/1	0.69	0.69	71,71,71,71	0
85	MG	A	2103	1/1	0.69	0.55	73,73,73,73	0
85	MG	AR	3833	1/1	0.69	0.30	49,49,49,49	0
85	MG	1	3930	1/1	0.69	0.57	40,40,40,40	0
85	MG	1	3952	1/1	0.69	0.24	77,77,77,77	0
85	MG	1	3820	1/1	0.69	0.60	65,65,65,65	0
85	MG	6	2086	1/1	0.69	0.25	82,82,82,82	0
85	MG	A	2117	1/1	0.70	0.19	71,71,71,71	0
85	MG	6	2133	1/1	0.70	0.66	61,61,61,61	0
85	MG	A	2085	1/1	0.70	0.40	63,63,63,63	0
85	MG	AR	4170	1/1	0.70	0.27	32,32,32,32	0
85	MG	A	2139	1/1	0.70	0.36	64,64,64,64	0
85	MG	6	2174	1/1	0.70	0.44	58,58,58,58	0
85	MG	A	2151	1/1	0.70	0.69	52,52,52,52	0
85	MG	A	2112	1/1	0.70	0.37	86,86,86,86	0
85	MG	Y	201	1/1	0.70	0.20	61,61,61,61	0
85	MG	6	2154	1/1	0.71	0.41	54,54,54,54	0
85	MG	l	403	1/1	0.71	0.47	37,37,37,37	0
85	MG	1	4061	1/1	0.71	0.31	54,54,54,54	0
85	MG	AR	4119	1/1	0.71	0.39	91,91,91,91	0
84	OHX	AR	3737	7/7	0.71	0.46	158,158,158,159	0
85	MG	4	233	1/1	0.71	0.20	48,48,48,48	0
85	MG	AR	4037	1/1	0.71	0.34	70,70,70,70	0
85	MG	AR	4003	1/1	0.72	0.43	45,45,45,45	0
85	MG	AR	4222	1/1	0.72	0.39	58,58,58,58	0
85	MG	1	3814	1/1	0.72	0.22	77,77,77,77	0
85	MG	AR	4030	1/1	0.72	0.57	59,59,59,59	0
85	MG	s	300	1/1	0.72	0.27	70,70,70,70	0
85	MG	AR	4049	1/1	0.72	0.19	50,50,50,50	0
85	MG	1	4101	1/1	0.72	0.51	38,38,38,38	0
85	MG	A	2046	1/1	0.72	0.29	67,67,67,67	0
85	MG	A	2062	1/1	0.72	0.71	65,65,65,65	0
85	MG	AR	4181	1/1	0.72	0.24	50,50,50,50	0
85	MG	AR	3817	1/1	0.72	0.24	112,112,112,112	0
85	MG	AR	4034	1/1	0.73	0.45	60,60,60,60	0
85	MG	AR	4214	1/1	0.73	0.24	55,55,55,55	0
85	MG	AT	224	1/1	0.73	0.23	68,68,68,68	0
85	MG	CD	302	1/1	0.73	0.49	36,36,36,36	0
85	MG	A	2128	1/1	0.73	0.50	78,78,78,78	0
85	MG	DC	203	1/1	0.73	0.31	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2124	1/1	0.73	0.28	66,66,66,66	0
85	MG	A	2146	1/1	0.73	0.16	120,120,120,120	0
85	MG	1	4161	1/1	0.73	0.25	69,69,69,69	0
85	MG	AR	4011	1/1	0.73	0.39	58,58,58,58	0
85	MG	1	4190	1/1	0.73	0.56	25,25,25,25	0
85	MG	1	3988	1/1	0.73	0.37	34,34,34,34	0
85	MG	AR	4024	1/1	0.74	0.78	53,53,53,53	0
85	MG	AS	225	1/1	0.74	0.35	58,58,58,58	0
85	MG	AR	4161	1/1	0.74	0.27	39,39,39,39	0
85	MG	AR	3783	1/1	0.74	0.32	44,44,44,44	0
85	MG	1	3983	1/1	0.74	0.52	55,55,55,55	0
85	MG	1	4151	1/1	0.74	0.28	41,41,41,41	0
85	MG	A	2131	1/1	0.74	0.43	64,64,64,64	0
85	MG	A	2135	1/1	0.74	0.56	55,55,55,55	0
85	MG	1	4081	1/1	0.74	0.39	29,29,29,29	0
85	MG	1	4129	1/1	0.74	0.43	33,33,33,33	0
85	MG	1	4131	1/1	0.74	0.32	48,48,48,48	0
85	MG	6	2192	1/1	0.74	0.67	74,74,74,74	0
85	MG	1	4056	1/1	0.74	0.30	51,51,51,51	0
85	MG	AR	3782	1/1	0.74	0.35	36,36,36,36	0
85	MG	A	2118	1/1	0.75	0.92	80,80,80,80	0
85	MG	AR	4215	1/1	0.75	0.28	70,70,70,70	0
85	MG	AR	3995	1/1	0.75	0.34	65,65,65,65	0
85	MG	AR	3827	1/1	0.75	0.35	58,58,58,58	0
85	MG	A	2045	1/1	0.75	0.79	58,58,58,58	0
85	MG	1	4158	1/1	0.75	0.46	47,47,47,47	0
85	MG	A	2054	1/1	0.75	0.23	66,66,66,66	0
85	MG	A	2136	1/1	0.75	0.71	74,74,74,74	0
85	MG	6	2083	1/1	0.75	0.46	63,63,63,63	0
85	MG	AR	4022	1/1	0.75	0.44	30,30,30,30	0
85	MG	1	3816	1/1	0.75	0.34	44,44,44,44	0
85	MG	AR	4117	1/1	0.75	0.31	64,64,64,64	0
85	MG	6	2117	1/1	0.75	0.28	65,65,65,65	0
85	MG	AT	222	1/1	0.75	0.34	43,43,43,43	0
85	MG	4	235	1/1	0.76	0.50	70,70,70,70	0
85	MG	CM	202	1/1	0.76	0.15	62,62,62,62	0
85	MG	1	3790	1/1	0.76	0.12	43,43,43,43	0
85	MG	1	3857	1/1	0.76	0.25	56,56,56,56	0
85	MG	1	4093	1/1	0.76	0.37	57,57,57,57	0
85	MG	6	2188	1/1	0.76	0.54	66,66,66,66	0
85	MG	AR	4257	1/1	0.76	0.32	51,51,51,51	0
85	MG	6	2189	1/1	0.76	0.34	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4155	1/1	0.76	0.23	53,53,53,53	0
85	MG	1	4148	1/1	0.76	0.18	53,53,53,53	0
85	MG	6	2088	1/1	0.76	0.35	82,82,82,82	0
85	MG	AR	4087	1/1	0.76	0.36	63,63,63,63	0
85	MG	AR	3776	1/1	0.76	0.33	76,76,76,76	0
85	MG	AS	219	1/1	0.77	0.24	58,58,58,58	0
85	MG	6	2162	1/1	0.77	0.26	60,60,60,60	0
85	MG	6	2163	1/1	0.77	0.42	48,48,48,48	0
85	MG	AR	4171	1/1	0.77	0.17	88,88,88,88	0
85	MG	AR	4085	1/1	0.77	0.46	35,35,35,35	0
85	MG	6	2081	1/1	0.77	0.25	55,55,55,55	0
84	OHX	1	3691	7/7	0.77	0.31	201,201,201,201	0
85	MG	1	3744	1/1	0.77	0.42	83,83,83,83	0
85	MG	AR	3921	1/1	0.77	0.31	38,38,38,38	0
85	MG	1	3801	1/1	0.77	0.54	37,37,37,37	0
85	MG	6	2074	1/1	0.77	0.37	62,62,62,62	0
85	MG	AR	4225	1/1	0.77	0.35	34,34,34,34	0
85	MG	AR	4244	1/1	0.77	0.40	45,45,45,45	0
85	MG	AR	3976	1/1	0.77	0.44	81,81,81,81	0
85	MG	A	2084	1/1	0.77	0.22	72,72,72,72	0
85	MG	AR	4156	1/1	0.77	1.08	72,72,72,72	0
85	MG	V	201	1/1	0.77	0.50	70,70,70,70	0
85	MG	AR	4160	1/1	0.77	0.26	78,78,78,78	0
85	MG	b	101	1/1	0.77	0.45	65,65,65,65	0
85	MG	1	3811	1/1	0.78	0.30	44,44,44,44	0
85	MG	6	2197	1/1	0.78	0.57	56,56,56,56	0
85	MG	AF	202	1/1	0.78	0.27	28,28,28,28	0
85	MG	AR	4123	1/1	0.78	0.36	57,57,57,57	0
85	MG	AR	4005	1/1	0.78	0.62	40,40,40,40	0
85	MG	AR	4141	1/1	0.78	0.36	37,37,37,37	0
85	MG	1	3976	1/1	0.78	0.14	61,61,61,61	0
85	MG	1	3941	1/1	0.78	0.41	78,78,78,78	0
85	MG	1	4012	1/1	0.78	0.44	50,50,50,50	0
85	MG	AR	3803	1/1	0.78	0.51	35,35,35,35	0
85	MG	1	4087	1/1	0.78	0.23	59,59,59,59	0
85	MG	1	4092	1/1	0.78	0.64	54,54,54,54	0
85	MG	1	4187	1/1	0.78	0.35	43,43,43,43	0
85	MG	x	206	1/1	0.78	0.58	35,35,35,35	0
85	MG	6	2157	1/1	0.78	0.28	56,56,56,56	0
85	MG	1	4046	1/1	0.78	0.34	37,37,37,37	0
85	MG	6	2076	1/1	0.78	0.58	105,105,105,105	0
85	MG	AR	4220	1/1	0.78	0.39	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3968	1/1	0.78	0.32	30,30,30,30	0
85	MG	AR	3971	1/1	0.78	0.42	57,57,57,57	0
87	GOL	AR	4261	6/6	0.78	0.34	48,48,48,48	0
85	MG	6	2183	1/1	0.79	0.58	71,71,71,71	0
85	MG	AR	4097	1/1	0.79	0.58	40,40,40,40	0
85	MG	4	236	1/1	0.79	0.19	50,50,50,50	0
85	MG	4	238	1/1	0.79	0.26	35,35,35,35	0
85	MG	AR	4110	1/1	0.79	0.50	46,46,46,46	0
85	MG	1	3751	1/1	0.79	0.35	40,40,40,40	0
85	MG	1	3800	1/1	0.79	0.61	45,45,45,45	0
85	MG	DI	202	1/1	0.79	0.36	56,56,56,56	0
85	MG	6	2092	1/1	0.79	0.58	93,93,93,93	0
85	MG	6	2193	1/1	0.79	0.45	55,55,55,55	0
85	MG	6	2167	1/1	0.79	0.50	53,53,53,53	0
85	MG	1	4023	1/1	0.79	0.48	57,57,57,57	0
85	MG	AR	3964	1/1	0.79	0.29	35,35,35,35	0
85	MG	1	3750	1/1	0.79	0.18	55,55,55,55	0
85	MG	AR	4063	1/1	0.79	0.12	54,54,54,54	0
85	MG	1	3994	1/1	0.79	0.27	47,47,47,47	0
85	MG	1	4001	1/1	0.79	0.45	47,47,47,47	0
87	GOL	6	2199	6/6	0.79	0.44	49,49,49,49	0
85	MG	A	2116	1/1	0.79	0.61	67,67,67,67	0
88	ZN	d7	101	1/1	0.79	0.47	143,143,143,143	0
85	MG	AT	231	1/1	0.80	0.83	52,52,52,52	0
85	MG	1	3807	1/1	0.80	0.18	41,41,41,41	0
85	MG	1	4040	1/1	0.80	0.30	74,74,74,74	0
85	MG	AR	3986	1/1	0.80	0.21	56,56,56,56	0
85	MG	AR	4223	1/1	0.80	0.30	61,61,61,61	0
85	MG	1	4074	1/1	0.80	0.24	37,37,37,37	0
85	MG	AR	3998	1/1	0.80	0.45	40,40,40,40	0
85	MG	1	4044	1/1	0.80	0.32	47,47,47,47	0
85	MG	1	4127	1/1	0.80	0.26	45,45,45,45	0
85	MG	6	2130	1/1	0.80	0.31	66,66,66,66	0
85	MG	4	232	1/1	0.80	0.28	37,37,37,37	0
85	MG	A	2091	1/1	0.80	0.43	71,71,71,71	0
85	MG	1	3852	1/1	0.80	0.33	38,38,38,38	0
85	MG	AR	4194	1/1	0.80	0.27	53,53,53,53	0
85	MG	1	4014	1/1	0.80	0.37	57,57,57,57	0
85	MG	AR	4198	1/1	0.80	0.59	51,51,51,51	0
85	MG	AR	3779	1/1	0.80	0.38	73,73,73,73	0
87	GOL	AR	4262	6/6	0.80	0.34	48,48,48,48	0
85	MG	1	4159	1/1	0.80	0.39	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	A	2083	1/1	0.81	0.18	68,68,68,68	0
85	MG	6	2146	1/1	0.81	1.00	80,80,80,80	0
84	OHX	1	3668	7/7	0.81	0.45	124,124,124,124	0
85	MG	AR	4128	1/1	0.81	0.21	55,55,55,55	0
85	MG	1	4027	1/1	0.81	0.39	35,35,35,35	0
85	MG	AR	4155	1/1	0.81	0.45	34,34,34,34	0
85	MG	1	4203	1/1	0.81	0.24	31,31,31,31	0
85	MG	A	2114	1/1	0.81	0.39	76,76,76,76	0
85	MG	1	4088	1/1	0.81	0.25	44,44,44,44	0
85	MG	AS	217	1/1	0.81	0.47	44,44,44,44	0
85	MG	1	3963	1/1	0.81	0.25	45,45,45,45	0
85	MG	AR	4169	1/1	0.81	0.29	46,46,46,46	0
85	MG	1	3840	1/1	0.81	0.31	78,78,78,78	0
85	MG	1	3998	1/1	0.81	0.34	36,36,36,36	0
85	MG	AR	3760	1/1	0.81	0.14	53,53,53,53	0
85	MG	AR	3761	1/1	0.81	0.33	31,31,31,31	0
85	MG	AR	4182	1/1	0.81	0.37	79,79,79,79	0
85	MG	1	3966	1/1	0.81	0.18	69,69,69,69	0
84	OHX	1	3717	7/7	0.81	0.54	144,144,144,145	0
85	MG	CE	407	1/1	0.81	0.59	41,41,41,41	0
85	MG	CG	304	1/1	0.81	0.25	56,56,56,56	0
85	MG	CJ	301	1/1	0.81	0.22	78,78,78,78	0
85	MG	A	2152	1/1	0.81	0.70	43,43,43,43	0
85	MG	AR	3780	1/1	0.81	0.17	88,88,88,88	0
85	MG	AR	4200	1/1	0.81	0.25	48,48,48,48	0
85	MG	DE	201	1/1	0.81	0.28	72,72,72,72	0
85	MG	AR	4206	1/1	0.81	0.28	33,33,33,33	0
85	MG	1	3954	1/1	0.81	0.15	46,46,46,46	0
85	MG	j	302	1/1	0.81	0.25	35,35,35,35	0
85	MG	1	3987	1/1	0.81	0.68	65,65,65,65	0
85	MG	1	4170	1/1	0.81	0.49	41,41,41,41	0
85	MG	AR	4039	1/1	0.82	0.38	56,56,56,56	0
85	MG	6	2152	1/1	0.82	0.43	62,62,62,62	0
85	MG	AR	4056	1/1	0.82	0.38	44,44,44,44	0
85	MG	AR	4060	1/1	0.82	0.27	70,70,70,70	0
85	MG	AR	3836	1/1	0.82	0.45	48,48,48,48	0
85	MG	1	3985	1/1	0.82	0.60	50,50,50,50	0
85	MG	AR	3903	1/1	0.82	0.69	39,39,39,39	0
85	MG	6	2072	1/1	0.82	0.70	40,40,40,40	0
85	MG	AR	3944	1/1	0.82	0.17	38,38,38,38	0
85	MG	A	2098	1/1	0.82	0.48	65,65,65,65	0
85	MG	AR	4101	1/1	0.82	0.25	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4224	1/1	0.82	0.49	47,47,47,47	0
85	MG	A	2107	1/1	0.82	0.31	80,80,80,80	0
85	MG	AR	3945	1/1	0.82	0.15	40,40,40,40	0
85	MG	AR	4239	1/1	0.82	0.42	39,39,39,39	0
85	MG	1	4045	1/1	0.82	0.34	39,39,39,39	0
85	MG	1	3925	1/1	0.82	0.13	46,46,46,46	0
85	MG	1	3855	1/1	0.82	0.32	44,44,44,44	0
85	MG	AR	3749	1/1	0.82	0.19	42,42,42,42	0
85	MG	AR	3751	1/1	0.82	0.36	36,36,36,36	0
85	MG	AR	3756	1/1	0.82	0.36	36,36,36,36	0
85	MG	AR	3984	1/1	0.82	0.65	50,50,50,50	0
85	MG	1	4013	1/1	0.82	0.33	52,52,52,52	0
85	MG	1	4119	1/1	0.82	0.28	35,35,35,35	0
85	MG	1	4060	1/1	0.82	0.36	44,44,44,44	0
85	MG	AT	221	1/1	0.82	0.76	52,52,52,52	0
85	MG	A	2140	1/1	0.82	0.82	82,82,82,82	0
85	MG	1	3863	1/1	0.82	0.20	55,55,55,55	0
85	MG	6	2099	1/1	0.82	0.39	51,51,51,51	0
85	MG	AT	228	1/1	0.82	0.37	47,47,47,47	0
85	MG	1	4165	1/1	0.82	0.40	24,24,24,24	0
85	MG	1	3955	1/1	0.82	0.43	51,51,51,51	0
85	MG	CE	403	1/1	0.82	0.32	22,22,22,22	0
85	MG	AR	4014	1/1	0.82	0.39	57,57,57,57	0
85	MG	AR	3794	1/1	0.82	0.24	34,34,34,34	0
85	MG	c6	201	1/1	0.82	0.22	89,89,89,89	0
85	MG	c9	201	1/1	0.82	0.10	79,79,79,79	0
85	MG	1	3997	1/1	0.82	0.17	54,54,54,54	0
85	MG	AR	3811	1/1	0.82	0.20	50,50,50,50	0
85	MG	1	3866	1/1	0.82	0.39	34,34,34,34	0
87	GOL	A	2160	6/6	0.82	0.35	60,60,60,60	0
85	MG	x	203	1/1	0.82	0.39	63,63,63,63	0
85	MG	1	3761	1/1	0.83	0.30	41,41,41,41	0
85	MG	6	2178	1/1	0.83	0.36	57,57,57,57	0
85	MG	AR	3812	1/1	0.83	0.42	32,32,32,32	0
85	MG	AR	3816	1/1	0.83	0.24	39,39,39,39	0
85	MG	A	2048	1/1	0.83	0.33	52,52,52,52	0
84	OHX	A	2034	7/7	0.83	0.20	231,232,232,232	0
85	MG	4	234	1/1	0.83	0.43	44,44,44,44	0
85	MG	A	2081	1/1	0.83	0.31	66,66,66,66	0
85	MG	1	3779	1/1	0.83	0.48	55,55,55,55	0
85	MG	6	2186	1/1	0.83	0.31	107,107,107,107	0
85	MG	1	3739	1/1	0.83	0.32	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2111	1/1	0.83	0.42	61,61,61,61	0
85	MG	A	2094	1/1	0.83	0.38	110,110,110,110	0
85	MG	AR	3911	1/1	0.83	0.42	40,40,40,40	0
85	MG	AR	4075	1/1	0.83	0.31	36,36,36,36	0
85	MG	AR	4221	1/1	0.83	0.28	35,35,35,35	0
85	MG	AR	4076	1/1	0.83	0.32	48,48,48,48	0
85	MG	1	3993	1/1	0.83	0.62	42,42,42,42	0
85	MG	1	4098	1/1	0.83	0.27	47,47,47,47	0
85	MG	AR	4089	1/1	0.83	0.10	62,62,62,62	0
85	MG	AR	4232	1/1	0.83	0.43	28,28,28,28	0
85	MG	AR	4090	1/1	0.83	0.49	57,57,57,57	0
85	MG	AR	4240	1/1	0.83	0.55	70,70,70,70	0
85	MG	AR	4094	1/1	0.83	0.31	43,43,43,43	0
85	MG	A	2127	1/1	0.83	0.29	83,83,83,83	0
85	MG	AR	4245	1/1	0.83	0.22	26,26,26,26	0
85	MG	1	3819	1/1	0.83	0.40	27,27,27,27	0
85	MG	1	3870	1/1	0.83	0.28	47,47,47,47	0
85	MG	6	2138	1/1	0.83	0.30	73,73,73,73	0
85	MG	6	2140	1/1	0.83	0.40	69,69,69,69	0
85	MG	1	4118	1/1	0.83	0.34	43,43,43,43	0
85	MG	AR	4116	1/1	0.83	0.30	99,99,99,99	0
85	MG	v	303	1/1	0.83	0.24	44,44,44,44	0
85	MG	AR	3973	1/1	0.83	0.23	40,40,40,40	0
85	MG	AR	3975	1/1	0.83	0.27	31,31,31,31	0
85	MG	AR	3752	1/1	0.83	0.21	37,37,37,37	0
85	MG	1	4050	1/1	0.83	0.36	31,31,31,31	0
84	OHX	AR	3664	7/7	0.83	0.43	180,180,181,181	0
85	MG	AR	3994	1/1	0.83	0.32	25,25,25,25	0
85	MG	6	2064	1/1	0.83	0.68	53,53,53,53	0
85	MG	6	2068	1/1	0.83	0.46	61,61,61,61	0
85	MG	6	2070	1/1	0.83	0.39	73,73,73,73	0
84	OHX	AR	3686	7/7	0.83	0.38	156,156,156,157	0
85	MG	1	3972	1/1	0.83	0.85	45,45,45,45	0
84	OHX	6	2045	7/7	0.83	0.34	141,141,142,142	0
85	MG	1	3843	1/1	0.83	0.41	24,24,24,24	0
85	MG	AR	4173	1/1	0.83	0.31	53,53,53,53	0
85	MG	AR	3841	1/1	0.84	0.29	54,54,54,54	0
85	MG	1	4145	1/1	0.84	0.33	42,42,42,42	0
85	MG	1	4070	1/1	0.84	0.20	68,68,68,68	0
85	MG	1	3853	1/1	0.84	0.55	48,48,48,48	0
85	MG	AR	4086	1/1	0.84	0.40	42,42,42,42	0
85	MG	1	4202	1/1	0.84	0.56	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4003	1/1	0.84	0.35	79,79,79,79	0
85	MG	AR	4188	1/1	0.84	1.10	31,31,31,31	0
84	OHX	AR	3719	7/7	0.84	0.42	133,133,133,133	0
85	MG	1	4006	1/1	0.84	0.57	47,47,47,47	0
85	MG	AR	4019	1/1	0.84	0.27	45,45,45,45	0
85	MG	AT	226	1/1	0.84	0.30	63,63,63,63	0
85	MG	AR	4021	1/1	0.84	0.17	82,82,82,82	0
85	MG	1	4091	1/1	0.84	0.32	47,47,47,47	0
85	MG	AR	3960	1/1	0.84	0.21	41,41,41,41	0
85	MG	6	2118	1/1	0.84	0.14	93,93,93,93	0
85	MG	AR	4113	1/1	0.84	0.58	37,37,37,37	0
85	MG	AR	4032	1/1	0.84	0.37	48,48,48,48	0
85	MG	1	3931	1/1	0.84	0.53	32,32,32,32	0
85	MG	AR	4035	1/1	0.84	0.38	43,43,43,43	0
85	MG	CP	502	1/1	0.84	0.42	45,45,45,45	0
85	MG	CQ	204	1/1	0.84	0.41	30,30,30,30	0
85	MG	CR	202	1/1	0.84	0.28	29,29,29,29	0
85	MG	AB	207	1/1	0.84	0.24	34,34,34,34	0
85	MG	6	2173	1/1	0.84	0.73	48,48,48,48	0
85	MG	AR	4044	1/1	0.84	0.56	60,60,60,60	0
85	MG	AR	4045	1/1	0.84	0.30	55,55,55,55	0
85	MG	A	2159	1/1	0.84	0.93	64,64,64,64	0
85	MG	AR	4234	1/1	0.84	0.45	32,32,32,32	0
85	MG	A	2047	1/1	0.84	0.65	55,55,55,55	0
85	MG	AR	4046	1/1	0.84	0.26	46,46,46,46	0
85	MG	1	4160	1/1	0.84	0.32	34,34,34,34	0
84	OHX	AR	3717	7/7	0.84	0.42	144,144,144,144	0
85	MG	A	2068	1/1	0.84	0.56	84,84,84,84	0
85	MG	A	2069	1/1	0.84	0.49	58,58,58,58	0
85	MG	1	4163	1/1	0.84	0.24	44,44,44,44	0
85	MG	AR	4253	1/1	0.84	0.17	41,41,41,41	0
85	MG	1	4065	1/1	0.84	0.31	48,48,48,48	0
85	MG	1	3940	1/1	0.85	0.37	43,43,43,43	0
85	MG	A	2089	1/1	0.85	0.19	90,90,90,90	0
85	MG	1	3967	1/1	0.85	0.20	38,38,38,38	0
85	MG	1	3799	1/1	0.85	0.41	37,37,37,37	0
85	MG	A	2095	1/1	0.85	0.25	96,96,96,96	0
85	MG	1	3754	1/1	0.85	0.52	37,37,37,37	0
85	MG	1	4111	1/1	0.85	0.55	44,44,44,44	0
85	MG	A	2101	1/1	0.85	0.38	64,64,64,64	0
85	MG	AS	226	1/1	0.85	0.21	67,67,67,67	0
84	OHX	AR	3705	7/7	0.85	0.36	141,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3988	1/1	0.85	0.81	50,50,50,50	0
85	MG	1	3984	1/1	0.85	0.27	70,70,70,70	0
85	MG	6	2145	1/1	0.85	0.20	59,59,59,59	0
85	MG	1	4064	1/1	0.85	0.30	58,58,58,58	0
85	MG	AR	4183	1/1	0.85	0.23	55,55,55,55	0
85	MG	1	3805	1/1	0.85	0.20	29,29,29,29	0
84	OHX	A	1971	7/7	0.85	0.23	149,150,151,151	0
85	MG	1	3874	1/1	0.85	0.55	49,49,49,49	0
85	MG	AR	4093	1/1	0.85	0.37	46,46,46,46	0
85	MG	AR	3862	1/1	0.85	0.21	56,56,56,56	0
85	MG	AR	4096	1/1	0.85	0.32	54,54,54,54	0
85	MG	AR	3873	1/1	0.85	0.46	31,31,31,31	0
85	MG	AR	4017	1/1	0.85	0.31	95,95,95,95	0
85	MG	4	220	1/1	0.85	0.34	64,64,64,64	0
85	MG	AR	4103	1/1	0.85	0.19	47,47,47,47	0
85	MG	A	2142	1/1	0.85	0.13	80,80,80,80	0
85	MG	1	4135	1/1	0.85	0.48	51,51,51,51	0
85	MG	1	4077	1/1	0.85	0.27	33,33,33,33	0
84	OHX	AR	3728	7/7	0.85	0.42	151,152,152,152	0
85	MG	AR	4025	1/1	0.85	0.25	31,31,31,31	0
85	MG	1	4082	1/1	0.85	0.30	35,35,35,35	0
85	MG	AR	3759	1/1	0.85	0.62	34,34,34,34	0
85	MG	1	3959	1/1	0.85	0.27	66,66,66,66	0
85	MG	AR	4238	1/1	0.85	0.38	36,36,36,36	0
85	MG	A	2050	1/1	0.85	0.39	67,67,67,67	0
85	MG	1	4042	1/1	0.85	0.41	48,48,48,48	0
85	MG	AR	3958	1/1	0.85	0.56	38,38,38,38	0
85	MG	1	3731	1/1	0.85	0.49	36,36,36,36	0
85	MG	AR	4140	1/1	0.85	0.49	44,44,44,44	0
85	MG	6	2110	1/1	0.85	0.54	54,54,54,54	0
85	MG	AR	4142	1/1	0.85	0.31	46,46,46,46	0
85	MG	1	3797	1/1	0.85	0.18	79,79,79,79	0
85	MG	DC	202	1/1	0.86	0.30	48,48,48,48	0
85	MG	6	2066	1/1	0.86	0.35	74,74,74,74	0
85	MG	AR	3954	1/1	0.86	0.30	44,44,44,44	0
85	MG	1	4038	1/1	0.86	0.72	41,41,41,41	0
85	MG	DQ	203	1/1	0.86	0.22	45,45,45,45	0
85	MG	AR	4187	1/1	0.86	0.43	36,36,36,36	0
85	MG	AR	3957	1/1	0.86	0.13	55,55,55,55	0
85	MG	AR	4071	1/1	0.86	0.27	39,39,39,39	0
85	MG	3	216	1/1	0.86	0.40	58,58,58,58	0
85	MG	1	3759	1/1	0.86	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3926	1/1	0.86	0.16	37,37,37,37	0
84	OHX	1	3709	7/7	0.86	0.35	157,158,158,158	0
85	MG	6	2161	1/1	0.86	0.49	58,58,58,58	0
84	OHX	6	2046	7/7	0.86	0.36	151,152,152,152	0
85	MG	A	2075	1/1	0.86	0.43	74,74,74,74	0
85	MG	1	3936	1/1	0.86	0.54	61,61,61,61	0
84	OHX	1	3714	7/7	0.86	0.51	146,147,147,148	0
85	MG	AR	4092	1/1	0.86	0.32	47,47,47,47	0
85	MG	AR	3982	1/1	0.86	0.24	53,53,53,53	0
85	MG	6	2087	1/1	0.86	0.30	56,56,56,56	0
84	OHX	AR	3734	7/7	0.86	0.55	148,148,148,149	0
85	MG	A	2092	1/1	0.86	0.27	91,91,91,91	0
85	MG	6	2090	1/1	0.86	0.31	49,49,49,49	0
85	MG	AR	3991	1/1	0.86	0.14	98,98,98,98	0
84	OHX	1	3702	7/7	0.86	0.22	219,219,219,219	0
85	MG	1	3981	1/1	0.86	0.50	50,50,50,50	0
85	MG	6	2105	1/1	0.86	0.48	64,64,64,64	0
85	MG	AR	3814	1/1	0.86	0.31	105,105,105,105	0
85	MG	1	4007	1/1	0.86	0.42	29,29,29,29	0
85	MG	A	2109	1/1	0.86	0.41	60,60,60,60	0
85	MG	A	2110	1/1	0.86	0.67	116,116,116,116	0
85	MG	1	4009	1/1	0.86	0.66	42,42,42,42	0
85	MG	AR	4248	1/1	0.86	0.94	45,45,45,45	0
85	MG	6	2115	1/1	0.86	0.41	85,85,85,85	0
85	MG	AR	4118	1/1	0.86	0.41	31,31,31,31	0
85	MG	AR	3829	1/1	0.86	0.66	66,66,66,66	0
85	MG	AR	4120	1/1	0.86	0.27	31,31,31,31	0
84	OHX	A	1946	7/7	0.86	0.22	165,166,166,167	0
85	MG	1	3752	1/1	0.86	0.42	57,57,57,57	0
85	MG	AR	3840	1/1	0.86	0.31	47,47,47,47	0
85	MG	AR	4127	1/1	0.86	0.17	77,77,77,77	0
85	MG	6	2122	1/1	0.86	0.48	61,61,61,61	0
85	MG	AR	3852	1/1	0.86	0.24	37,37,37,37	0
85	MG	1	4183	1/1	0.86	0.17	44,44,44,44	0
85	MG	AR	4029	1/1	0.86	0.22	42,42,42,42	0
85	MG	AR	4145	1/1	0.86	0.20	70,70,70,70	0
85	MG	AR	4146	1/1	0.86	0.19	34,34,34,34	0
85	MG	AT	225	1/1	0.86	0.91	53,53,53,53	0
85	MG	v	304	1/1	0.86	0.62	52,52,52,52	0
85	MG	AT	227	1/1	0.86	0.89	79,79,79,79	0
85	MG	1	3953	1/1	0.86	0.20	46,46,46,46	0
85	MG	AR	4157	1/1	0.86	0.28	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	A	2156	1/1	0.86	0.62	45,45,45,45	0
85	MG	AR	4159	1/1	0.86	0.38	36,36,36,36	0
85	MG	T	202	1/1	0.86	0.09	97,97,97,97	0
85	MG	U	201	1/1	0.86	0.42	76,76,76,76	0
85	MG	AR	3894	1/1	0.86	0.53	45,45,45,45	0
85	MG	6	2195	1/1	0.86	0.65	35,35,35,35	0
85	MG	AR	4164	1/1	0.86	0.23	41,41,41,41	0
84	OHX	1	3724	7/7	0.86	0.22	113,113,113,113	0
85	MG	AB	202	1/1	0.86	0.31	29,29,29,29	0
87	GOL	v	305	6/6	0.86	0.26	38,38,38,38	0
85	MG	AR	3935	1/1	0.86	0.62	49,49,49,49	0
85	MG	6	2059	1/1	0.86	0.43	70,70,70,70	0
85	MG	1	3832	1/1	0.86	0.41	26,26,26,26	0
85	MG	CR	203	1/1	0.86	0.15	95,95,95,95	0
85	MG	CR	204	1/1	0.86	0.21	46,46,46,46	0
85	MG	1	3908	1/1	0.87	0.50	62,62,62,62	0
85	MG	1	3961	1/1	0.87	0.19	40,40,40,40	0
85	MG	A	2088	1/1	0.87	0.53	59,59,59,59	0
85	MG	1	4000	1/1	0.87	0.23	43,43,43,43	0
84	OHX	AR	3741	7/7	0.87	0.38	207,208,208,208	0
85	MG	1	4193	1/1	0.87	0.37	23,23,23,23	0
84	OHX	1	3708	7/7	0.87	0.39	134,134,134,134	0
85	MG	1	4128	1/1	0.87	0.45	51,51,51,51	0
85	MG	1	4210	1/1	0.87	0.30	24,24,24,24	0
85	MG	6	2079	1/1	0.87	0.24	45,45,45,45	0
85	MG	6	2164	1/1	0.87	0.35	53,53,53,53	0
85	MG	AR	4080	1/1	0.87	0.51	32,32,32,32	0
85	MG	1	4211	1/1	0.87	0.63	42,42,42,42	0
84	OHX	z	201	7/7	0.87	0.39	155,156,157,157	0
85	MG	6	2169	1/1	0.87	0.63	49,49,49,49	0
84	OHX	A	2007	7/7	0.87	0.26	200,200,201,201	0
85	MG	1	3971	1/1	0.87	0.46	35,35,35,35	0
85	MG	1	4138	1/1	0.87	0.28	33,33,33,33	0
85	MG	1	3845	1/1	0.87	0.40	18,18,18,18	0
84	OHX	A	2025	7/7	0.87	0.48	173,173,173,173	0
84	OHX	AR	3640	7/7	0.87	0.32	126,126,126,126	0
85	MG	CF	403	1/1	0.87	0.40	34,34,34,34	0
85	MG	1	3944	1/1	0.87	0.48	32,32,32,32	0
85	MG	1	3767	1/1	0.87	0.12	60,60,60,60	0
85	MG	A	2129	1/1	0.87	0.30	57,57,57,57	0
85	MG	CL	302	1/1	0.87	0.36	68,68,68,68	0
84	OHX	AR	3652	7/7	0.87	0.44	112,112,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	A	2134	1/1	0.87	0.35	70,70,70,70	0
85	MG	AR	4207	1/1	0.87	0.50	48,48,48,48	0
85	MG	1	4154	1/1	0.87	0.21	46,46,46,46	0
85	MG	AR	3842	1/1	0.87	0.16	47,47,47,47	0
85	MG	AR	3845	1/1	0.87	0.41	23,23,23,23	0
85	MG	AR	3851	1/1	0.87	0.29	38,38,38,38	0
85	MG	CU	201	1/1	0.87	0.40	38,38,38,38	0
85	MG	DA	201	1/1	0.87	0.28	48,48,48,48	0
85	MG	1	3778	1/1	0.87	0.46	49,49,49,49	0
85	MG	AR	4020	1/1	0.87	0.23	41,41,41,41	0
85	MG	n	201	1/1	0.87	0.26	43,43,43,43	0
85	MG	6	2120	1/1	0.87	0.42	69,69,69,69	0
84	OHX	6	1960	7/7	0.87	0.22	118,118,118,118	0
85	MG	1	3786	1/1	0.87	0.20	40,40,40,40	0
84	OHX	6	2040	7/7	0.87	0.29	184,184,185,185	0
85	MG	AR	4124	1/1	0.87	0.18	39,39,39,39	0
85	MG	1	3892	1/1	0.87	0.41	23,23,23,23	0
85	MG	AR	3913	1/1	0.87	0.43	26,26,26,26	0
85	MG	s6	301	1/1	0.87	0.29	77,77,77,77	0
85	MG	A	2053	1/1	0.87	0.72	57,57,57,57	0
85	MG	1	3996	1/1	0.87	0.44	64,64,64,64	0
85	MG	d4	201	1/1	0.87	0.38	53,53,53,53	0
85	MG	1	4108	1/1	0.87	0.21	42,42,42,42	0
85	MG	AR	4246	1/1	0.87	0.41	22,22,22,22	0
85	MG	6	2141	1/1	0.87	0.32	52,52,52,52	0
85	MG	AR	4250	1/1	0.87	0.80	59,59,59,59	0
85	MG	x	209	1/1	0.87	0.66	39,39,39,39	0
85	MG	AR	3947	1/1	0.87	0.50	44,44,44,44	0
85	MG	AS	215	1/1	0.88	0.36	58,58,58,58	0
85	MG	3	220	1/1	0.88	0.17	68,68,68,68	0
85	MG	A	2087	1/1	0.88	0.50	78,78,78,78	0
85	MG	AR	4051	1/1	0.88	0.38	40,40,40,40	0
85	MG	1	3803	1/1	0.88	0.42	41,41,41,41	0
85	MG	AS	223	1/1	0.88	0.28	41,41,41,41	0
85	MG	AS	224	1/1	0.88	0.24	55,55,55,55	0
85	MG	A	2093	1/1	0.88	0.14	100,100,100,100	0
85	MG	1	4137	1/1	0.88	0.17	55,55,55,55	0
85	MG	6	2171	1/1	0.88	0.25	56,56,56,56	0
85	MG	4	222	1/1	0.88	0.28	33,33,33,33	0
85	MG	1	3939	1/1	0.88	0.29	39,39,39,39	0
84	OHX	A	2036	7/7	0.88	0.15	252,253,253,253	0
84	OHX	A	2041	7/7	0.88	0.46	139,139,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2103	1/1	0.88	0.33	69,69,69,69	0
85	MG	1	4084	1/1	0.88	0.27	32,32,32,32	0
84	OHX	1	3687	7/7	0.88	0.42	149,149,150,150	0
85	MG	AR	4175	1/1	0.88	0.25	35,35,35,35	0
85	MG	1	3945	1/1	0.88	0.29	57,57,57,57	0
85	MG	AR	3838	1/1	0.88	0.37	27,27,27,27	0
85	MG	1	4033	1/1	0.88	0.21	58,58,58,58	0
84	OHX	AR	3707	7/7	0.88	0.25	129,129,130,130	0
85	MG	CE	404	1/1	0.88	0.29	27,27,27,27	0
84	OHX	AR	3517	7/7	0.88	0.16	145,146,146,146	0
85	MG	AR	3999	1/1	0.88	0.30	44,44,44,44	0
85	MG	1	3785	1/1	0.88	0.45	25,25,25,25	0
84	OHX	6	2018	7/7	0.88	0.23	189,189,189,189	0
85	MG	1	3787	1/1	0.88	0.46	46,46,46,46	0
85	MG	AR	3861	1/1	0.88	0.37	30,30,30,30	0
85	MG	A	2133	1/1	0.88	0.20	72,72,72,72	0
85	MG	1	3897	1/1	0.88	0.21	46,46,46,46	0
85	MG	AR	3868	1/1	0.88	0.46	25,25,25,25	0
85	MG	1	4162	1/1	0.88	0.25	40,40,40,40	0
85	MG	1	4110	1/1	0.88	0.24	30,30,30,30	0
84	OHX	AR	3720	7/7	0.88	0.33	152,152,152,152	0
85	MG	x	208	1/1	0.88	0.33	46,46,46,46	0
85	MG	AR	4023	1/1	0.88	0.23	31,31,31,31	0
85	MG	AR	3907	1/1	0.88	0.63	25,25,25,25	0
85	MG	1	4113	1/1	0.88	0.26	57,57,57,57	0
85	MG	1	4115	1/1	0.88	0.23	36,36,36,36	0
84	OHX	AR	3722	7/7	0.88	0.31	140,141,141,141	0
85	MG	DL	102	1/1	0.88	0.50	39,39,39,39	0
84	OHX	AR	3726	7/7	0.88	0.42	118,118,118,118	0
85	MG	1	3927	1/1	0.88	0.24	42,42,42,42	0
85	MG	AR	4126	1/1	0.88	0.69	83,83,83,83	0
85	MG	1	4125	1/1	0.88	0.38	23,23,23,23	0
85	MG	1	3758	1/1	0.88	0.50	32,32,32,32	0
85	MG	AR	4130	1/1	0.88	0.15	31,31,31,31	0
84	OHX	AR	3690	7/7	0.88	0.47	117,118,118,118	0
85	MG	1	3933	1/1	0.88	0.11	49,49,49,49	0
85	MG	3	212	1/1	0.88	0.44	62,62,62,62	0
85	MG	AR	4251	1/1	0.88	0.41	59,59,59,59	0
85	MG	1	3934	1/1	0.88	0.44	54,54,54,54	0
85	MG	A	2070	1/1	0.88	0.53	79,79,79,79	0
85	MG	AR	4047	1/1	0.88	0.14	54,54,54,54	0
85	MG	A	2080	1/1	0.88	0.39	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4149	1/1	0.88	0.38	66,66,66,66	0
85	MG	AR	4150	1/1	0.88	0.18	44,44,44,44	0
85	MG	DI	201	1/1	0.89	0.22	68,68,68,68	0
85	MG	AR	4050	1/1	0.89	0.31	91,91,91,91	0
85	MG	3	211	1/1	0.89	0.35	38,38,38,38	0
85	MG	AR	4186	1/1	0.89	0.21	33,33,33,33	0
85	MG	1	3873	1/1	0.89	0.23	48,48,48,48	0
85	MG	AR	4059	1/1	0.89	0.20	47,47,47,47	0
85	MG	1	3777	1/1	0.89	0.17	30,30,30,30	0
85	MG	6	2190	1/1	0.89	0.48	66,66,66,66	0
85	MG	AR	4067	1/1	0.89	0.34	34,34,34,34	0
85	MG	AR	4069	1/1	0.89	0.23	26,26,26,26	0
85	MG	1	3881	1/1	0.89	0.55	31,31,31,31	0
85	MG	AR	4073	1/1	0.89	0.39	40,40,40,40	0
85	MG	AR	4210	1/1	0.89	0.72	54,54,54,54	0
85	MG	3	221	1/1	0.89	0.47	34,34,34,34	0
85	MG	AR	3943	1/1	0.89	0.10	41,41,41,41	0
85	MG	1	3886	1/1	0.89	0.41	21,21,21,21	0
85	MG	1	4130	1/1	0.89	0.27	45,45,45,45	0
85	MG	AR	4083	1/1	0.89	0.28	31,31,31,31	0
85	MG	1	3995	1/1	0.89	0.31	34,34,34,34	0
85	MG	4	228	1/1	0.89	0.26	54,54,54,54	0
84	OHX	AR	3733	7/7	0.89	0.33	187,188,188,188	0
84	OHX	c4	201	7/7	0.89	0.53	152,152,153,153	0
85	MG	1	3726	1/1	0.89	0.84	54,54,54,54	0
85	MG	1	3999	1/1	0.89	0.33	41,41,41,41	0
85	MG	1	4073	1/1	0.89	0.38	40,40,40,40	0
85	MG	1	3956	1/1	0.89	0.54	34,34,34,34	0
85	MG	AR	3967	1/1	0.89	0.55	42,42,42,42	0
85	MG	6	2123	1/1	0.89	0.24	69,69,69,69	0
85	MG	AR	4099	1/1	0.89	0.16	41,41,41,41	0
85	MG	4	237	1/1	0.89	0.20	38,38,38,38	0
85	MG	1	3915	1/1	0.89	0.12	36,36,36,36	0
85	MG	4	240	1/1	0.89	0.57	32,32,32,32	0
85	MG	AR	3764	1/1	0.89	0.34	33,33,33,33	0
85	MG	6	2134	1/1	0.89	0.22	80,80,80,80	0
85	MG	AR	3777	1/1	0.89	0.31	37,37,37,37	0
85	MG	1	4080	1/1	0.89	0.22	35,35,35,35	0
84	OHX	6	2051	7/7	0.89	0.29	172,172,172,173	0
85	MG	1	3960	1/1	0.89	0.21	33,33,33,33	0
85	MG	6	2144	1/1	0.89	0.38	74,74,74,74	0
85	MG	r	302	1/1	0.89	0.22	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4005	1/1	0.89	0.35	36,36,36,36	0
85	MG	6	2149	1/1	0.89	0.32	46,46,46,46	0
85	MG	6	2150	1/1	0.89	0.13	77,77,77,77	0
85	MG	A	2125	1/1	0.89	0.85	56,56,56,56	0
84	OHX	6	1975	7/7	0.89	0.43	120,120,120,120	0
84	OHX	AR	3602	7/7	0.89	0.18	143,143,144,144	0
85	MG	1	3928	1/1	0.89	0.27	34,34,34,34	0
84	OHX	CF	401	7/7	0.89	0.31	146,146,147,147	0
84	OHX	6	2006	7/7	0.89	0.29	151,151,152,152	0
85	MG	AR	4135	1/1	0.89	0.18	62,62,62,62	0
85	MG	x	207	1/1	0.89	0.31	33,33,33,33	0
85	MG	AR	3834	1/1	0.89	0.47	33,33,33,33	0
85	MG	1	3932	1/1	0.89	0.19	55,55,55,55	0
84	OHX	1	3723	7/7	0.89	0.35	113,113,113,113	0
84	OHX	A	1985	7/7	0.89	0.31	140,140,141,141	0
85	MG	AT	229	1/1	0.89	0.42	55,55,55,55	0
85	MG	AR	4148	1/1	0.89	0.28	43,43,43,43	0
85	MG	A	2149	1/1	0.89	0.25	60,60,60,60	0
85	MG	1	4029	1/1	0.89	0.11	47,47,47,47	0
85	MG	1	4184	1/1	0.89	0.26	36,36,36,36	0
85	MG	AR	4153	1/1	0.89	0.19	88,88,88,88	0
85	MG	AR	4154	1/1	0.89	0.32	39,39,39,39	0
85	MG	AR	4028	1/1	0.89	0.19	41,41,41,41	0
84	OHX	1	3620	7/7	0.89	0.35	118,118,118,118	0
85	MG	D	301	1/1	0.89	0.58	58,58,58,58	0
85	MG	1	4036	1/1	0.89	0.42	70,70,70,70	0
85	MG	1	3982	1/1	0.89	0.37	32,32,32,32	0
84	OHX	A	2015	7/7	0.89	0.41	169,170,171,172	0
84	OHX	1	3712	7/7	0.89	0.34	133,133,133,133	0
85	MG	AR	4163	1/1	0.89	0.23	62,62,62,62	0
84	OHX	1	3721	7/7	0.89	0.35	127,127,127,128	0
84	OHX	AR	3729	7/7	0.89	0.46	120,120,120,121	0
85	MG	AR	4043	1/1	0.89	0.38	37,37,37,37	0
85	MG	CR	205	1/1	0.89	0.40	31,31,31,31	0
85	MG	d5	201	1/1	0.89	0.09	71,71,71,71	0
85	MG	AR	3882	1/1	0.89	0.14	47,47,47,47	0
85	MG	1	4219	1/1	0.89	0.26	98,98,98,98	0
85	MG	DC	201	1/1	0.89	0.45	30,30,30,30	0
85	MG	AR	3891	1/1	0.89	0.27	69,69,69,69	0
85	MG	6	2085	1/1	0.89	0.47	75,75,75,75	0
85	MG	AR	3899	1/1	0.89	0.60	45,45,45,45	0
85	MG	AR	3765	1/1	0.90	0.39	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	3773	1/1	0.90	0.29	41,41,41,41	0
84	OHX	A	2042	7/7	0.90	0.21	172,173,173,174	0
84	OHX	A	2043	7/7	0.90	0.19	155,156,156,157	0
85	MG	1	4102	1/1	0.90	0.37	57,57,57,57	0
84	OHX	AR	3692	7/7	0.90	0.31	170,171,171,171	0
84	OHX	1	3656	7/7	0.90	0.50	143,143,143,144	0
85	MG	1	3818	1/1	0.90	0.43	39,39,39,39	0
84	OHX	6	2001	7/7	0.90	0.28	119,120,120,120	0
85	MG	1	3737	1/1	0.90	0.93	57,57,57,57	0
85	MG	AR	3807	1/1	0.90	0.38	25,25,25,25	0
84	OHX	1	3710	7/7	0.90	0.33	136,137,137,137	0
85	MG	AR	4166	1/1	0.90	0.16	38,38,38,38	0
85	MG	1	4116	1/1	0.90	0.52	44,44,44,44	0
85	MG	4	231	1/1	0.90	0.23	58,58,58,58	0
85	MG	6	2139	1/1	0.90	0.22	45,45,45,45	0
85	MG	AR	4033	1/1	0.90	0.26	40,40,40,40	0
85	MG	1	4117	1/1	0.90	0.31	41,41,41,41	0
85	MG	AR	3821	1/1	0.90	0.21	42,42,42,42	0
85	MG	A	2051	1/1	0.90	0.47	67,67,67,67	0
85	MG	1	3830	1/1	0.90	0.22	44,44,44,44	0
84	OHX	1	3501	7/7	0.90	0.17	126,126,127,127	0
85	MG	AR	4040	1/1	0.90	0.26	43,43,43,43	0
85	MG	A	2065	1/1	0.90	0.73	57,57,57,57	0
85	MG	AR	4042	1/1	0.90	0.12	57,57,57,57	0
85	MG	1	4015	1/1	0.90	0.37	67,67,67,67	0
85	MG	1	4020	1/1	0.90	0.39	34,34,34,34	0
84	OHX	6	2021	7/7	0.90	0.25	181,181,182,182	0
84	OHX	6	2039	7/7	0.90	0.62	132,133,133,134	0
85	MG	AR	4197	1/1	0.90	0.27	35,35,35,35	0
85	MG	1	4028	1/1	0.90	0.16	46,46,46,46	0
84	OHX	1	3626	7/7	0.90	0.35	124,124,124,124	0
85	MG	1	3851	1/1	0.90	0.36	34,34,34,34	0
84	OHX	6	2041	7/7	0.90	0.34	143,144,145,145	0
84	OHX	1	3642	7/7	0.90	0.45	135,135,136,136	0
84	OHX	1	3718	7/7	0.90	0.39	149,149,149,149	0
85	MG	t	201	1/1	0.90	0.17	51,51,51,51	0
85	MG	1	3962	1/1	0.90	0.41	39,39,39,39	0
85	MG	AR	4064	1/1	0.90	0.24	38,38,38,38	0
84	OHX	1	3719	7/7	0.90	0.52	120,120,121,121	0
85	MG	6	2166	1/1	0.90	0.49	53,53,53,53	0
85	MG	AR	4070	1/1	0.90	0.19	50,50,50,50	0
85	MG	1	4147	1/1	0.90	0.21	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3762	1/1	0.90	0.56	30,30,30,30	0
85	MG	A	2102	1/1	0.90	0.49	58,58,58,58	0
85	MG	x	205	1/1	0.90	0.66	33,33,33,33	0
85	MG	A	2106	1/1	0.90	0.50	58,58,58,58	0
85	MG	1	3766	1/1	0.90	0.16	73,73,73,73	0
85	MG	1	3869	1/1	0.90	0.49	34,34,34,34	0
84	OHX	6	2052	7/7	0.90	0.33	143,144,144,144	0
85	MG	1	4055	1/1	0.90	0.17	33,33,33,33	0
85	MG	A	2113	1/1	0.90	0.48	73,73,73,73	0
85	MG	AR	4084	1/1	0.90	0.22	34,34,34,34	0
85	MG	1	3771	1/1	0.90	0.42	33,33,33,33	0
85	MG	1	4156	1/1	0.90	0.19	44,44,44,44	0
85	MG	AR	3914	1/1	0.90	0.43	32,32,32,32	0
84	OHX	AR	3738	7/7	0.90	0.15	141,142,142,142	0
85	MG	A	2122	1/1	0.90	0.17	86,86,86,86	0
84	OHX	AM	101	7/7	0.90	0.43	121,121,121,121	0
85	MG	AR	4252	1/1	0.90	0.37	50,50,50,50	0
84	OHX	1	3696	7/7	0.90	0.39	146,146,147,147	0
84	OHX	1	3700	7/7	0.90	0.36	148,148,149,149	0
84	OHX	AR	3604	7/7	0.90	0.19	158,159,159,159	0
85	MG	AR	3946	1/1	0.90	0.30	59,59,59,59	0
85	MG	AS	213	1/1	0.90	0.45	26,26,26,26	0
85	MG	A	2132	1/1	0.90	0.26	98,98,98,98	0
85	MG	1	3898	1/1	0.90	0.46	33,33,33,33	0
85	MG	AR	4098	1/1	0.90	0.20	46,46,46,46	0
85	MG	AS	218	1/1	0.90	0.30	33,33,33,33	0
85	MG	AR	3948	1/1	0.90	0.54	40,40,40,40	0
85	MG	6	2078	1/1	0.90	0.45	42,42,42,42	0
84	OHX	AR	3631	7/7	0.90	0.18	175,176,177,177	0
85	MG	6	2080	1/1	0.90	0.64	69,69,69,69	0
85	MG	AR	3956	1/1	0.90	0.22	29,29,29,29	0
84	OHX	1	3644	7/7	0.90	0.25	166,167,167,167	0
85	MG	6	2082	1/1	0.90	0.48	54,54,54,54	0
84	OHX	AR	3646	7/7	0.90	0.37	108,108,108,108	0
85	MG	6	2198	1/1	0.90	0.56	49,49,49,49	0
85	MG	1	3793	1/1	0.90	0.30	37,37,37,37	0
85	MG	AB	204	1/1	0.90	0.29	52,52,52,52	0
84	OHX	3	209	7/7	0.90	0.28	152,152,152,152	0
84	OHX	A	2026	7/7	0.90	0.40	123,123,124,124	0
85	MG	AG	202	1/1	0.90	0.20	43,43,43,43	0
85	MG	AH	202	1/1	0.90	0.15	58,58,58,58	0
85	MG	1	4085	1/1	0.90	0.39	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3750	1/1	0.90	0.41	27,27,27,27	0
85	MG	CD	301	1/1	0.90	0.36	34,34,34,34	0
85	MG	s4	301	1/1	0.90	0.23	59,59,59,59	0
85	MG	1	4198	1/1	0.90	0.60	43,43,43,43	0
84	OHX	A	2029	7/7	0.90	0.20	184,184,184,184	0
85	MG	AR	3753	1/1	0.90	0.33	26,26,26,26	0
85	MG	AR	4134	1/1	0.90	0.27	44,44,44,44	0
85	MG	AR	3755	1/1	0.90	0.18	56,56,56,56	0
84	OHX	A	2030	7/7	0.90	0.47	142,143,143,144	0
85	MG	1	4209	1/1	0.90	0.67	48,48,48,48	0
84	OHX	x	201	7/7	0.90	0.39	110,110,110,110	0
84	OHX	1	3707	7/7	0.90	0.40	125,125,126,126	0
84	OHX	1	3653	7/7	0.90	0.29	133,133,133,133	0
85	MG	AR	4009	1/1	0.90	0.34	37,37,37,37	0
85	MG	1	4035	1/1	0.91	0.60	47,47,47,47	0
85	MG	1	3746	1/1	0.91	0.41	26,26,26,26	0
85	MG	1	4037	1/1	0.91	0.30	30,30,30,30	0
85	MG	6	2196	1/1	0.91	0.76	48,48,48,48	0
84	OHX	AR	3665	7/7	0.91	0.39	133,133,133,133	0
84	OHX	AR	3745	7/7	0.91	0.34	128,128,128,128	0
85	MG	AB	201	1/1	0.91	0.28	34,34,34,34	0
84	OHX	AS	211	7/7	0.91	0.29	141,141,142,142	0
85	MG	AB	203	1/1	0.91	0.34	32,32,32,32	0
84	OHX	AT	213	7/7	0.91	0.25	137,137,137,137	0
85	MG	AB	205	1/1	0.91	0.22	40,40,40,40	0
85	MG	AR	4136	1/1	0.91	0.27	36,36,36,36	0
85	MG	AR	4137	1/1	0.91	0.48	79,79,79,79	0
85	MG	AR	4139	1/1	0.91	0.35	46,46,46,46	0
85	MG	1	3847	1/1	0.91	0.54	28,28,28,28	0
85	MG	1	3848	1/1	0.91	0.40	60,60,60,60	0
85	MG	CX	204	1/1	0.91	0.21	46,46,46,46	0
85	MG	AR	3979	1/1	0.91	0.57	41,41,41,41	0
85	MG	1	3849	1/1	0.91	0.44	23,23,23,23	0
84	OHX	AR	3677	7/7	0.91	0.38	110,111,111,111	0
85	MG	AR	4147	1/1	0.91	0.23	31,31,31,31	0
84	OHX	4	215	7/7	0.91	0.28	137,138,138,138	0
84	OHX	A	1970	7/7	0.91	0.35	132,132,133,133	0
85	MG	1	4174	1/1	0.91	0.83	55,55,55,55	0
85	MG	1	4058	1/1	0.91	0.31	51,51,51,51	0
84	OHX	1	3596	7/7	0.91	0.49	143,144,144,144	0
85	MG	DQ	204	1/1	0.91	0.35	32,32,32,32	0
85	MG	1	3765	1/1	0.91	0.49	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3861	1/1	0.91	0.24	34,34,34,34	0
84	OHX	1	3695	7/7	0.91	0.61	154,154,155,155	0
85	MG	1	3865	1/1	0.91	0.32	45,45,45,45	0
85	MG	6	2109	1/1	0.91	0.42	56,56,56,56	0
84	OHX	A	1993	7/7	0.91	0.38	151,151,152,152	0
84	OHX	AR	3695	7/7	0.91	0.30	122,122,123,123	0
85	MG	AR	3770	1/1	0.91	0.44	32,32,32,32	0
85	MG	A	2056	1/1	0.91	0.34	65,65,65,65	0
85	MG	AR	3771	1/1	0.91	0.36	42,42,42,42	0
85	MG	1	3979	1/1	0.91	0.31	39,39,39,39	0
85	MG	A	2067	1/1	0.91	0.81	64,64,64,64	0
84	OHX	6	2048	7/7	0.91	0.35	173,174,174,174	0
84	OHX	A	2021	7/7	0.91	0.43	133,133,134,134	0
85	MG	AR	3778	1/1	0.91	0.26	42,42,42,42	0
85	MG	1	4213	1/1	0.91	0.64	50,50,50,50	0
84	OHX	A	2023	7/7	0.91	0.26	144,145,145,145	0
85	MG	AR	4176	1/1	0.91	0.23	33,33,33,33	0
85	MG	AR	4177	1/1	0.91	0.30	32,32,32,32	0
85	MG	AR	4180	1/1	0.91	0.39	48,48,48,48	0
84	OHX	1	3673	7/7	0.91	0.56	133,133,133,133	0
85	MG	A	2086	1/1	0.91	0.24	66,66,66,66	0
85	MG	AR	4026	1/1	0.91	0.33	60,60,60,60	0
85	MG	1	3884	1/1	0.91	0.34	29,29,29,29	0
85	MG	AR	4184	1/1	0.91	0.16	69,69,69,69	0
85	MG	AR	3789	1/1	0.91	0.39	36,36,36,36	0
85	MG	6	2127	1/1	0.91	0.47	54,54,54,54	0
85	MG	AR	3796	1/1	0.91	0.41	64,64,64,64	0
85	MG	6	2129	1/1	0.91	0.38	62,62,62,62	0
85	MG	1	3782	1/1	0.91	0.45	58,58,58,58	0
85	MG	3	217	1/1	0.91	0.36	40,40,40,40	0
84	OHX	1	3720	7/7	0.91	0.28	128,128,129,129	0
84	OHX	AR	3718	7/7	0.91	0.47	166,167,167,167	0
85	MG	AR	4205	1/1	0.91	0.24	59,59,59,59	0
85	MG	AR	3815	1/1	0.91	0.24	32,32,32,32	0
85	MG	1	3992	1/1	0.91	0.24	40,40,40,40	0
84	OHX	1	3676	7/7	0.91	0.30	149,150,150,150	0
85	MG	1	3899	1/1	0.91	0.35	39,39,39,39	0
85	MG	AR	3824	1/1	0.91	0.13	77,77,77,77	0
85	MG	AR	4216	1/1	0.91	0.20	44,44,44,44	0
85	MG	6	2142	1/1	0.91	0.24	83,83,83,83	0
85	MG	6	2143	1/1	0.91	0.31	75,75,75,75	0
85	MG	AR	3832	1/1	0.91	0.53	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	4	227	1/1	0.91	0.40	52,52,52,52	0
85	MG	1	4100	1/1	0.91	0.27	53,53,53,53	0
85	MG	1	3901	1/1	0.91	0.49	39,39,39,39	0
85	MG	1	3789	1/1	0.91	0.17	42,42,42,42	0
85	MG	AR	4231	1/1	0.91	0.35	32,32,32,32	0
85	MG	1	3913	1/1	0.91	0.59	28,28,28,28	0
84	OHX	6	2002	7/7	0.91	0.27	132,133,133,134	0
85	MG	AR	4236	1/1	0.91	0.42	23,23,23,23	0
85	MG	1	4109	1/1	0.91	0.14	66,66,66,66	0
85	MG	1	3917	1/1	0.91	0.26	30,30,30,30	0
85	MG	AR	4068	1/1	0.91	0.12	99,99,99,99	0
85	MG	1	3920	1/1	0.91	0.10	41,41,41,41	0
84	OHX	A	2035	7/7	0.91	0.48	130,131,131,131	0
84	OHX	6	2004	7/7	0.91	0.40	157,157,158,158	0
84	OHX	A	2038	7/7	0.91	0.34	146,147,147,147	0
84	OHX	A	2039	7/7	0.91	0.41	166,167,168,168	0
85	MG	k	402	1/1	0.91	0.37	37,37,37,37	0
85	MG	6	2165	1/1	0.91	0.35	51,51,51,51	0
85	MG	AR	3889	1/1	0.91	0.36	35,35,35,35	0
85	MG	1	3929	1/1	0.91	0.30	34,34,34,34	0
84	OHX	1	3701	7/7	0.91	0.31	139,139,140,140	0
85	MG	AR	4256	1/1	0.91	0.43	49,49,49,49	0
85	MG	AR	3892	1/1	0.91	0.48	31,31,31,31	0
84	OHX	AR	3727	7/7	0.91	0.23	187,188,188,188	0
85	MG	AR	3896	1/1	0.91	0.55	36,36,36,36	0
85	MG	AR	3897	1/1	0.91	0.44	51,51,51,51	0
85	MG	1	4011	1/1	0.91	0.37	44,44,44,44	0
84	OHX	6	2008	7/7	0.91	0.18	136,136,136,136	0
85	MG	H	301	1/1	0.91	0.10	83,83,83,83	0
84	OHX	s8	301	7/7	0.91	0.32	167,167,168,168	0
84	OHX	c3	201	7/7	0.91	0.24	155,156,156,157	0
84	OHX	AR	3639	7/7	0.91	0.22	138,139,139,139	0
85	MG	w	202	1/1	0.91	0.32	31,31,31,31	0
84	OHX	AR	3730	7/7	0.91	0.33	176,176,176,176	0
85	MG	AR	3922	1/1	0.91	0.49	31,31,31,31	0
85	MG	AR	4100	1/1	0.91	0.28	57,57,57,57	0
85	MG	AR	3929	1/1	0.91	0.37	25,25,25,25	0
85	MG	c8	202	1/1	0.91	0.33	79,79,79,79	0
85	MG	AR	3934	1/1	0.91	0.31	32,32,32,32	0
85	MG	1	4021	1/1	0.91	0.15	44,44,44,44	0
85	MG	1	4022	1/1	0.91	0.59	53,53,53,53	0
85	MG	d6	101	1/1	0.91	0.34	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3659	7/7	0.91	0.32	140,140,140,141	0
85	MG	1	3732	1/1	0.91	0.44	26,26,26,26	0
84	OHX	3	205	7/7	0.91	0.21	127,128,128,128	0
84	OHX	1	3716	7/7	0.91	0.45	138,138,139,139	0
85	MG	1	4030	1/1	0.91	0.73	72,72,72,72	0
84	OHX	4	213	7/7	0.91	0.31	117,117,117,117	0
84	OHX	CF	402	7/7	0.92	0.34	145,146,146,146	0
85	MG	AT	220	1/1	0.92	0.47	53,53,53,53	0
84	OHX	CG	302	7/7	0.92	0.38	147,147,147,148	0
85	MG	1	3755	1/1	0.92	0.42	36,36,36,36	0
85	MG	1	4079	1/1	0.92	0.21	97,97,97,97	0
85	MG	1	3969	1/1	0.92	0.21	41,41,41,41	0
85	MG	1	3970	1/1	0.92	0.30	31,31,31,31	0
85	MG	4	225	1/1	0.92	0.32	25,25,25,25	0
84	OHX	AR	3668	7/7	0.92	0.37	131,132,132,132	0
85	MG	1	3862	1/1	0.92	0.46	52,52,52,52	0
85	MG	1	3974	1/1	0.92	0.22	28,28,28,28	0
85	MG	AR	3902	1/1	0.92	0.57	42,42,42,42	0
84	OHX	6	2033	7/7	0.92	0.39	150,151,151,152	0
85	MG	1	3864	1/1	0.92	0.25	38,38,38,38	0
85	MG	1	4089	1/1	0.92	0.21	42,42,42,42	0
84	OHX	1	3627	7/7	0.92	0.28	141,142,142,143	0
84	OHX	A	1981	7/7	0.92	0.16	194,195,195,195	0
85	MG	1	3764	1/1	0.92	0.58	41,41,41,41	0
84	OHX	1	3692	7/7	0.92	0.29	113,113,113,113	0
85	MG	AR	3924	1/1	0.92	0.49	27,27,27,27	0
85	MG	AR	3927	1/1	0.92	0.45	35,35,35,35	0
85	MG	1	4099	1/1	0.92	0.23	44,44,44,44	0
85	MG	1	3871	1/1	0.92	0.47	30,30,30,30	0
84	OHX	l	401	7/7	0.92	0.41	143,143,144,144	0
84	OHX	A	2006	7/7	0.92	0.31	149,150,150,150	0
85	MG	l	402	1/1	0.92	0.33	57,57,57,57	0
85	MG	1	3877	1/1	0.92	0.71	36,36,36,36	0
85	MG	1	4107	1/1	0.92	0.16	40,40,40,40	0
85	MG	o	302	1/1	0.92	0.21	39,39,39,39	0
85	MG	1	3990	1/1	0.92	0.30	24,24,24,24	0
85	MG	DA	202	1/1	0.92	0.20	45,45,45,45	0
84	OHX	AR	3694	7/7	0.92	0.33	146,147,147,147	0
84	OHX	A	2011	7/7	0.92	0.23	149,149,150,150	0
84	OHX	A	2012	7/7	0.92	0.37	139,140,140,140	0
85	MG	t	203	1/1	0.92	0.42	29,29,29,29	0
84	OHX	1	3665	7/7	0.92	0.36	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	A	2017	7/7	0.92	0.31	158,159,160,160	0
84	OHX	A	2019	7/7	0.92	0.29	176,176,176,176	0
85	MG	AR	3961	1/1	0.92	0.53	43,43,43,43	0
84	OHX	1	3666	7/7	0.92	0.42	117,118,118,118	0
85	MG	x	204	1/1	0.92	0.35	28,28,28,28	0
84	OHX	1	3698	7/7	0.92	0.30	162,163,163,163	0
85	MG	1	3905	1/1	0.92	0.47	38,38,38,38	0
84	OHX	AR	3709	7/7	0.92	0.28	110,111,111,111	0
85	MG	1	4002	1/1	0.92	0.56	37,37,37,37	0
84	OHX	AR	3716	7/7	0.92	0.37	143,143,143,143	0
85	MG	AR	3977	1/1	0.92	0.41	41,41,41,41	0
85	MG	6	2056	1/1	0.92	0.22	77,77,77,77	0
85	MG	AR	3980	1/1	0.92	0.86	40,40,40,40	0
85	MG	A	2057	1/1	0.92	0.46	70,70,70,70	0
85	MG	A	2061	1/1	0.92	0.50	59,59,59,59	0
84	OHX	6	2050	7/7	0.92	0.47	159,159,160,160	0
85	MG	6	2060	1/1	0.92	0.34	47,47,47,47	0
84	OHX	1	3651	7/7	0.92	0.26	130,130,131,131	0
84	OHX	6	1977	7/7	0.92	0.25	150,151,151,152	0
85	MG	AR	3747	1/1	0.92	0.30	23,23,23,23	0
85	MG	AR	3992	1/1	0.92	0.64	67,67,67,67	0
85	MG	AR	4165	1/1	0.92	0.21	43,43,43,43	0
84	OHX	1	3672	7/7	0.92	0.41	147,147,147,148	0
85	MG	1	4008	1/1	0.92	0.29	37,37,37,37	0
85	MG	AR	3996	1/1	0.92	0.33	56,56,56,56	0
84	OHX	AR	3721	7/7	0.92	0.38	139,139,140,140	0
84	OHX	A	2037	7/7	0.92	0.44	153,154,154,155	0
85	MG	1	3802	1/1	0.92	0.18	86,86,86,86	0
85	MG	6	2077	1/1	0.92	0.54	39,39,39,39	0
84	OHX	AR	3506	7/7	0.92	0.21	112,112,112,112	0
85	MG	1	4146	1/1	0.92	0.17	48,48,48,48	0
85	MG	AR	4178	1/1	0.92	0.19	24,24,24,24	0
84	OHX	1	3652	7/7	0.92	0.33	110,110,110,110	0
84	OHX	AR	3599	7/7	0.92	0.24	136,136,136,136	0
84	OHX	1	3722	1/7	0.92	0.12	136,136,136,136	0
85	MG	AR	4018	1/1	0.92	0.21	36,36,36,36	0
84	OHX	6	2005	7/7	0.92	0.42	126,126,127,127	0
84	OHX	1	3488	7/7	0.92	0.17	109,109,109,110	0
85	MG	A	2100	1/1	0.92	0.44	92,92,92,92	0
84	OHX	AR	3732	7/7	0.92	0.52	146,146,147,147	0
85	MG	1	4026	1/1	0.92	0.41	65,65,65,65	0
85	MG	AR	4189	1/1	0.92	1.14	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4192	1/1	0.92	0.19	29,29,29,29	0
85	MG	1	3937	1/1	0.92	0.12	68,68,68,68	0
85	MG	1	3938	1/1	0.92	0.21	34,34,34,34	0
85	MG	6	2091	1/1	0.92	0.41	61,61,61,61	0
84	OHX	6	2007	7/7	0.92	0.28	145,146,146,146	0
85	MG	AR	4027	1/1	0.92	0.23	76,76,76,76	0
85	MG	6	2095	1/1	0.92	0.43	41,41,41,41	0
85	MG	A	2115	1/1	0.92	0.38	83,83,83,83	0
84	OHX	c5	201	7/7	0.92	0.19	161,161,161,161	0
85	MG	6	2100	1/1	0.92	0.51	36,36,36,36	0
85	MG	AR	4209	1/1	0.92	0.40	74,74,74,74	0
85	MG	AR	4031	1/1	0.92	0.20	39,39,39,39	0
85	MG	AR	3785	1/1	0.92	0.47	57,57,57,57	0
84	OHX	d9	101	7/7	0.92	0.48	153,153,154,154	0
85	MG	AR	3792	1/1	0.92	0.51	43,43,43,43	0
85	MG	A	2126	1/1	0.92	0.68	64,64,64,64	0
85	MG	1	3942	1/1	0.92	0.26	32,32,32,32	0
85	MG	6	2106	1/1	0.92	0.39	50,50,50,50	0
85	MG	AR	4038	1/1	0.92	0.23	35,35,35,35	0
85	MG	1	3943	1/1	0.92	0.54	37,37,37,37	0
85	MG	AR	3804	1/1	0.92	0.45	27,27,27,27	0
85	MG	1	3821	1/1	0.92	0.52	66,66,66,66	0
85	MG	AR	3808	1/1	0.92	0.34	28,28,28,28	0
85	MG	AR	4226	1/1	0.92	0.41	24,24,24,24	0
85	MG	AR	4230	1/1	0.92	0.55	18,18,18,18	0
84	OHX	1	3643	7/7	0.92	0.39	114,114,114,114	0
85	MG	1	4039	1/1	0.92	0.48	40,40,40,40	0
85	MG	AR	4233	1/1	0.92	0.33	31,31,31,31	0
85	MG	1	3947	1/1	0.92	0.21	26,26,26,26	0
85	MG	A	2143	1/1	0.92	0.38	106,106,106,106	0
85	MG	1	3728	1/1	0.92	0.61	52,52,52,52	0
85	MG	1	3949	1/1	0.92	0.47	44,44,44,44	0
85	MG	6	2121	1/1	0.92	0.28	41,41,41,41	0
85	MG	AR	3820	1/1	0.92	0.26	43,43,43,43	0
85	MG	AR	4055	1/1	0.92	0.17	40,40,40,40	0
84	OHX	AR	3644	7/7	0.92	0.31	126,127,127,127	0
85	MG	1	3833	1/1	0.92	0.70	24,24,24,24	0
85	MG	A	2157	1/1	0.92	0.79	75,75,75,75	0
85	MG	1	3834	1/1	0.92	0.51	22,22,22,22	0
85	MG	AR	4061	1/1	0.92	0.53	50,50,50,50	0
85	MG	F	301	1/1	0.92	0.33	64,64,64,64	0
84	OHX	1	3688	7/7	0.92	0.25	129,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4054	1/1	0.92	0.21	56,56,56,56	0
84	OHX	AR	3647	7/7	0.92	0.29	126,126,127,127	0
85	MG	6	2132	1/1	0.92	0.35	42,42,42,42	0
85	MG	AR	3835	1/1	0.92	0.41	45,45,45,45	0
84	OHX	1	3690	7/7	0.92	0.41	122,123,123,123	0
85	MG	1	3740	1/1	0.92	0.36	30,30,30,30	0
85	MG	AR	4072	1/1	0.92	0.25	70,70,70,70	0
85	MG	AS	214	1/1	0.92	0.30	52,52,52,52	0
84	OHX	AS	210	7/7	0.92	0.24	115,115,116,116	0
85	MG	1	4214	1/1	0.92	0.39	43,43,43,43	0
85	MG	1	4218	1/1	0.92	0.14	32,32,32,32	0
84	OHX	AR	3657	7/7	0.92	0.39	114,114,115,115	0
85	MG	3	210	1/1	0.92	0.39	59,59,59,59	0
85	MG	1	3850	1/1	0.92	0.48	31,31,31,31	0
84	OHX	6	2023	7/7	0.92	0.38	161,161,162,162	0
85	MG	3	214	1/1	0.92	0.52	34,34,34,34	0
85	MG	AR	3864	1/1	0.92	0.29	40,40,40,40	0
85	MG	AS	227	1/1	0.92	0.32	45,45,45,45	0
84	OHX	6	2030	7/7	0.92	0.29	118,118,118,119	0
85	MG	AR	4058	1/1	0.93	0.53	61,61,61,61	0
85	MG	1	4017	1/1	0.93	0.21	101,101,101,101	0
85	MG	1	4018	1/1	0.93	0.33	38,38,38,38	0
84	OHX	AR	3739	7/7	0.93	0.51	148,149,149,150	0
85	MG	6	2112	1/1	0.93	0.53	46,46,46,46	0
85	MG	AR	3823	1/1	0.93	0.51	39,39,39,39	0
84	OHX	AR	3740	7/7	0.93	0.25	161,161,161,162	0
85	MG	6	2116	1/1	0.93	0.21	62,62,62,62	0
84	OHX	1	3614	7/7	0.93	0.28	133,133,133,134	0
84	OHX	1	3618	7/7	0.93	0.19	190,190,190,190	0
85	MG	1	4178	1/1	0.93	0.40	28,28,28,28	0
85	MG	1	4025	1/1	0.93	0.48	32,32,32,32	0
85	MG	1	3921	1/1	0.93	0.12	57,57,57,57	0
84	OHX	AS	209	7/7	0.93	0.31	140,140,140,140	0
85	MG	1	4189	1/1	0.93	0.36	27,27,27,27	0
85	MG	AR	3839	1/1	0.93	0.43	33,33,33,33	0
85	MG	AR	4077	1/1	0.93	0.32	40,40,40,40	0
85	MG	AR	4078	1/1	0.93	0.52	60,60,60,60	0
85	MG	AT	223	1/1	0.93	0.79	45,45,45,45	0
85	MG	6	2125	1/1	0.93	0.32	75,75,75,75	0
84	OHX	AR	3606	7/7	0.93	0.31	113,113,114,114	0
84	OHX	1	3552	7/7	0.93	0.10	150,150,151,151	0
85	MG	1	3773	1/1	0.93	0.21	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3847	1/1	0.93	0.16	38,38,38,38	0
84	OHX	AR	3635	7/7	0.93	0.22	137,138,138,138	0
84	OHX	AT	217	7/7	0.93	0.37	128,128,128,128	0
84	OHX	CE	402	7/7	0.93	0.38	138,139,139,139	0
85	MG	6	2137	1/1	0.93	0.12	82,82,82,82	0
84	OHX	AR	3636	7/7	0.93	0.48	133,133,134,134	0
84	OHX	1	3556	7/7	0.93	0.27	117,117,117,117	0
84	OHX	1	3704	7/7	0.93	0.33	116,117,117,117	0
84	OHX	A	1918	7/7	0.93	0.23	128,129,129,129	0
85	MG	CG	303	1/1	0.93	0.13	62,62,62,62	0
85	MG	1	4217	1/1	0.93	0.92	58,58,58,58	0
85	MG	1	4041	1/1	0.93	0.16	45,45,45,45	0
84	OHX	AR	3641	7/7	0.93	0.48	133,133,133,133	0
84	OHX	A	1966	7/7	0.93	0.19	131,131,132,132	0
84	OHX	1	3686	7/7	0.93	0.58	156,156,157,157	0
85	MG	CQ	201	1/1	0.93	0.38	34,34,34,34	0
84	OHX	1	3655	7/7	0.93	0.37	138,138,138,139	0
84	OHX	6	2013	7/7	0.93	0.32	121,122,122,122	0
85	MG	AR	4109	1/1	0.93	0.16	39,39,39,39	0
84	OHX	AR	3649	7/7	0.93	0.50	144,144,144,144	0
84	OHX	AR	3650	7/7	0.93	0.44	118,118,118,118	0
84	OHX	A	1996	7/7	0.93	0.32	139,140,140,141	0
85	MG	AR	3905	1/1	0.93	0.48	29,29,29,29	0
84	OHX	1	3563	7/7	0.93	0.24	114,114,115,115	0
85	MG	3	222	1/1	0.93	0.38	52,52,52,52	0
85	MG	4	217	1/1	0.93	0.56	52,52,52,52	0
85	MG	1	3946	1/1	0.93	0.28	34,34,34,34	0
85	MG	AR	3920	1/1	0.93	0.50	27,27,27,27	0
85	MG	1	3804	1/1	0.93	0.50	35,35,35,35	0
84	OHX	1	3636	7/7	0.93	0.32	126,126,126,126	0
85	MG	1	4062	1/1	0.93	0.16	45,45,45,45	0
85	MG	AR	3925	1/1	0.93	0.41	34,34,34,34	0
85	MG	DO	202	1/1	0.93	0.25	42,42,42,42	0
84	OHX	AR	3663	7/7	0.93	0.29	147,148,148,148	0
85	MG	AR	3928	1/1	0.93	0.46	39,39,39,39	0
85	MG	sM	201	1/1	0.93	0.12	41,41,41,41	0
85	MG	A	2044	1/1	0.93	0.80	50,50,50,50	0
84	OHX	6	2022	7/7	0.93	0.29	153,154,154,155	0
85	MG	1	4068	1/1	0.93	0.46	42,42,42,42	0
85	MG	4	230	1/1	0.93	0.34	35,35,35,35	0
84	OHX	1	3711	7/7	0.93	0.59	119,120,120,120	0
84	OHX	6	2024	7/7	0.93	0.35	151,152,152,153	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3670	7/7	0.93	0.19	143,143,144,144	0
85	MG	A	2052	1/1	0.93	0.42	53,53,53,53	0
84	OHX	A	2020	7/7	0.93	0.23	147,148,148,148	0
84	OHX	AR	3674	7/7	0.93	0.46	130,130,130,131	0
85	MG	A	2055	1/1	0.93	0.47	71,71,71,71	0
85	MG	AR	4143	1/1	0.93	0.26	34,34,34,34	0
85	MG	AR	4144	1/1	0.93	0.33	41,41,41,41	0
85	MG	A	2060	1/1	0.93	0.62	55,55,55,55	0
84	OHX	AR	3675	7/7	0.93	0.33	138,139,139,139	0
84	OHX	4	216	7/7	0.93	0.26	126,126,126,126	0
84	OHX	AR	3678	7/7	0.93	0.42	137,137,137,138	0
85	MG	1	3826	1/1	0.93	0.25	33,33,33,33	0
85	MG	j	301	1/1	0.93	0.21	29,29,29,29	0
85	MG	1	3828	1/1	0.93	0.55	30,30,30,30	0
85	MG	AR	4152	1/1	0.93	0.23	38,38,38,38	0
85	MG	A	2072	1/1	0.93	0.39	66,66,66,66	0
85	MG	1	4086	1/1	0.93	0.29	32,32,32,32	0
85	MG	A	2076	1/1	0.93	0.35	51,51,51,51	0
85	MG	A	2078	1/1	0.93	0.68	54,54,54,54	0
84	OHX	6	2032	7/7	0.93	0.50	131,131,132,132	0
85	MG	1	3964	1/1	0.93	0.47	68,68,68,68	0
85	MG	AR	3962	1/1	0.93	0.19	93,93,93,93	0
84	OHX	1	3661	7/7	0.93	0.32	119,120,120,120	0
85	MG	AR	4158	1/1	0.93	0.20	29,29,29,29	0
85	MG	AR	3965	1/1	0.93	0.25	50,50,50,50	0
85	MG	AR	3966	1/1	0.93	0.45	38,38,38,38	0
85	MG	o	301	1/1	0.93	0.19	34,34,34,34	0
84	OHX	6	2035	7/7	0.93	0.36	142,142,143,143	0
85	MG	A	2090	1/1	0.93	0.20	57,57,57,57	0
84	OHX	6	2036	7/7	0.93	0.40	135,135,136,136	0
85	MG	1	3837	1/1	0.93	0.33	26,26,26,26	0
84	OHX	6	2037	7/7	0.93	0.40	137,137,138,138	0
85	MG	AR	4167	1/1	0.93	0.25	71,71,71,71	0
84	OHX	AR	3701	7/7	0.93	0.29	128,128,128,128	0
84	OHX	AR	3704	7/7	0.93	0.38	133,133,133,133	0
85	MG	1	3973	1/1	0.93	0.47	37,37,37,37	0
84	OHX	6	2038	7/7	0.93	0.41	148,148,148,148	0
85	MG	1	3975	1/1	0.93	0.33	42,42,42,42	0
84	OHX	A	2040	7/7	0.93	0.37	162,162,162,162	0
85	MG	AF	201	1/1	0.93	0.30	41,41,41,41	0
85	MG	A	2104	1/1	0.93	0.15	137,137,137,137	0
85	MG	A	2105	1/1	0.93	0.43	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AR	3706	7/7	0.93	0.34	155,155,155,156	0
84	OHX	1	3713	7/7	0.93	0.26	138,138,138,139	0
84	OHX	AR	3708	7/7	0.93	0.26	138,138,139,139	0
84	OHX	K	201	7/7	0.93	0.51	137,137,138,138	0
85	MG	AR	3748	1/1	0.93	0.38	44,44,44,44	0
84	OHX	x	202	7/7	0.93	0.36	144,144,145,145	0
84	OHX	AR	3711	7/7	0.93	0.37	144,144,145,145	0
85	MG	AR	4185	1/1	0.93	0.37	38,38,38,38	0
84	OHX	1	3664	7/7	0.93	0.35	124,124,124,124	0
85	MG	AR	4002	1/1	0.93	0.50	28,28,28,28	0
84	OHX	6	2043	7/7	0.93	0.31	145,145,146,146	0
84	OHX	6	1932	7/7	0.93	0.23	132,132,133,133	0
85	MG	AR	3754	1/1	0.93	0.31	40,40,40,40	0
85	MG	A	2123	1/1	0.93	0.51	55,55,55,55	0
85	MG	AR	4193	1/1	0.93	0.32	38,38,38,38	0
84	OHX	6	1950	7/7	0.93	0.21	135,135,136,136	0
85	MG	6	2065	1/1	0.93	0.58	40,40,40,40	0
85	MG	AR	3757	1/1	0.93	0.41	31,31,31,31	0
85	MG	AR	4015	1/1	0.93	0.16	45,45,45,45	0
85	MG	AR	4016	1/1	0.93	0.36	33,33,33,33	0
85	MG	AR	4201	1/1	0.93	0.27	35,35,35,35	0
85	MG	AR	4204	1/1	0.93	0.30	38,38,38,38	0
85	MG	AR	3758	1/1	0.93	0.30	37,37,37,37	0
84	OHX	1	3694	7/7	0.93	0.41	116,116,117,117	0
85	MG	6	2067	1/1	0.93	0.30	45,45,45,45	0
85	MG	1	3729	1/1	0.93	0.32	90,90,90,90	0
84	OHX	6	2049	7/7	0.93	0.33	170,171,171,171	0
85	MG	AR	4211	1/1	0.93	0.14	73,73,73,73	0
85	MG	1	3868	1/1	0.93	0.42	29,29,29,29	0
85	MG	AR	3767	1/1	0.93	0.58	35,35,35,35	0
85	MG	AR	3769	1/1	0.93	0.26	59,59,59,59	0
85	MG	AR	4218	1/1	0.93	0.27	54,54,54,54	0
85	MG	A	2147	1/1	0.93	0.26	79,79,79,79	0
84	OHX	6	1961	7/7	0.93	0.19	128,129,129,130	0
85	MG	1	3734	1/1	0.93	0.34	43,43,43,43	0
84	OHX	AR	3723	7/7	0.93	0.28	146,146,147,147	0
84	OHX	AR	3725	7/7	0.93	0.20	165,165,165,165	0
85	MG	1	4136	1/1	0.93	0.27	40,40,40,40	0
84	OHX	1	3485	7/7	0.93	0.16	120,121,121,121	0
84	OHX	1	3609	7/7	0.93	0.40	119,120,120,120	0
85	MG	A	2158	1/1	0.93	0.34	67,67,67,67	0
84	OHX	6	1986	7/7	0.93	0.32	147,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	6	1987	7/7	0.93	0.28	137,137,138,138	0
84	OHX	6	1989	7/7	0.93	0.43	143,144,144,145	0
84	OHX	AR	3527	7/7	0.93	0.20	112,112,112,112	0
85	MG	AR	3788	1/1	0.93	0.50	28,28,28,28	0
85	MG	1	3896	1/1	0.93	0.30	36,36,36,36	0
84	OHX	AR	3571	7/7	0.93	0.18	125,125,125,125	0
84	OHX	AR	3596	7/7	0.93	0.24	121,121,122,122	0
85	MG	AR	4041	1/1	0.93	0.36	34,34,34,34	0
85	MG	1	3756	1/1	0.93	0.42	32,32,32,32	0
85	MG	AR	4242	1/1	0.93	0.46	35,35,35,35	0
85	MG	c1	202	1/1	0.93	0.41	67,67,67,67	0
85	MG	AR	4243	1/1	0.93	0.59	30,30,30,30	0
85	MG	AR	3798	1/1	0.93	0.33	33,33,33,33	0
85	MG	1	4153	1/1	0.93	0.18	39,39,39,39	0
85	MG	6	2094	1/1	0.93	0.22	37,37,37,37	0
85	MG	AR	3805	1/1	0.93	0.44	36,36,36,36	0
84	OHX	AR	3736	7/7	0.93	0.28	132,132,132,133	0
84	OHX	AR	3597	7/7	0.93	0.30	150,151,151,151	0
85	MG	1	3906	1/1	0.93	0.36	42,42,42,42	0
84	OHX	6	1992	7/7	0.93	0.23	137,137,138,138	0
85	MG	1	3912	1/1	0.93	0.59	22,22,22,22	0
85	MG	1	4016	1/1	0.93	0.18	39,39,39,39	0
88	ZN	c	101	1/1	0.93	0.34	145,145,145,145	0
85	MG	AR	4057	1/1	0.93	0.39	41,41,41,41	0
85	MG	AR	4227	1/1	0.94	0.33	22,22,22,22	0
84	OHX	AR	3685	7/7	0.94	0.33	120,121,121,121	0
84	OHX	A	2032	7/7	0.94	0.20	154,154,155,155	0
84	OHX	A	2033	7/7	0.94	0.25	146,146,147,147	0
85	MG	AR	3997	1/1	0.94	0.12	44,44,44,44	0
84	OHX	6	1940	7/7	0.94	0.13	149,150,151,151	0
84	OHX	AR	3689	7/7	0.94	0.34	118,118,119,119	0
85	MG	AR	4001	1/1	0.94	0.22	38,38,38,38	0
84	OHX	1	3641	7/7	0.94	0.36	141,141,141,141	0
84	OHX	AR	3691	7/7	0.94	0.41	116,116,116,117	0
85	MG	AR	4004	1/1	0.94	0.16	32,32,32,32	0
84	OHX	6	2042	7/7	0.94	0.34	151,151,151,151	0
85	MG	AR	4006	1/1	0.94	0.55	47,47,47,47	0
85	MG	AR	4008	1/1	0.94	0.25	26,26,26,26	0
84	OHX	1	3498	7/7	0.94	0.21	115,116,116,116	0
85	MG	AR	4010	1/1	0.94	0.30	30,30,30,30	0
84	OHX	1	3675	7/7	0.94	0.30	140,141,141,141	0
84	OHX	AR	3698	7/7	0.94	0.41	123,123,123,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	6	1962	7/7	0.94	0.30	136,137,137,137	0
84	OHX	AR	3702	7/7	0.94	0.40	139,139,140,140	0
85	MG	4	223	1/1	0.94	0.59	27,27,27,27	0
85	MG	1	3880	1/1	0.94	0.59	31,31,31,31	0
85	MG	AB	206	1/1	0.94	0.27	26,26,26,26	0
84	OHX	6	2047	7/7	0.94	0.32	161,162,162,162	0
84	OHX	Q	201	7/7	0.94	0.26	165,165,165,165	0
84	OHX	6	1969	7/7	0.94	0.15	127,127,128,128	0
85	MG	1	3890	1/1	0.94	0.47	34,34,34,34	0
84	OHX	6	1971	7/7	0.94	0.24	136,136,136,137	0
84	OHX	1	3610	7/7	0.94	0.23	130,130,131,131	0
84	OHX	1	3679	7/7	0.94	0.30	131,131,132,132	0
84	OHX	6	1979	7/7	0.94	0.46	135,135,136,136	0
84	OHX	AR	3710	7/7	0.94	0.34	137,137,137,138	0
85	MG	1	3727	1/1	0.94	0.28	37,37,37,37	0
84	OHX	1	3462	7/7	0.94	0.21	119,120,120,120	0
85	MG	1	4049	1/1	0.94	0.25	32,32,32,32	0
84	OHX	AR	3712	7/7	0.94	0.27	109,109,109,109	0
85	MG	4	241	1/1	0.94	0.58	45,45,45,45	0
85	MG	AS	230	1/1	0.94	0.42	36,36,36,36	0
85	MG	1	3730	1/1	0.94	0.35	36,36,36,36	0
84	OHX	AR	3713	7/7	0.94	0.24	178,178,179,179	0
84	OHX	1	3648	7/7	0.94	0.25	119,120,120,120	0
85	MG	AR	4036	1/1	0.94	0.27	41,41,41,41	0
85	MG	k	403	1/1	0.94	0.20	30,30,30,30	0
84	OHX	1	3650	7/7	0.94	0.27	128,128,128,128	0
85	MG	1	4057	1/1	0.94	0.23	26,26,26,26	0
85	MG	1	3735	1/1	0.94	0.35	24,24,24,24	0
84	OHX	AR	3524	7/7	0.94	0.29	118,119,119,119	0
85	MG	1	3738	1/1	0.94	0.35	28,28,28,28	0
85	MG	AR	3768	1/1	0.94	0.18	39,39,39,39	0
85	MG	1	3922	1/1	0.94	0.45	45,45,45,45	0
85	MG	1	3923	1/1	0.94	0.39	51,51,51,51	0
84	OHX	1	3689	7/7	0.94	0.52	140,140,141,141	0
85	MG	1	4066	1/1	0.94	0.27	20,20,20,20	0
84	OHX	AR	3528	7/7	0.94	0.21	108,108,108,108	0
85	MG	CE	406	1/1	0.94	0.19	25,25,25,25	0
85	MG	1	3742	1/1	0.94	0.47	38,38,38,38	0
84	OHX	AR	3531	7/7	0.94	0.19	115,115,115,115	0
84	OHX	AR	3552	7/7	0.94	0.28	114,114,114,114	0
85	MG	1	3747	1/1	0.94	0.34	37,37,37,37	0
85	MG	CI	301	1/1	0.94	0.26	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3563	7/7	0.94	0.17	122,122,123,123	0
84	OHX	AR	3564	7/7	0.94	0.14	155,155,155,155	0
85	MG	AR	3784	1/1	0.94	0.24	51,51,51,51	0
84	OHX	6	1993	7/7	0.94	0.28	134,135,135,135	0
85	MG	1	3753	1/1	0.94	0.54	35,35,35,35	0
85	MG	CQ	202	1/1	0.94	0.33	32,32,32,32	0
85	MG	1	4083	1/1	0.94	0.29	41,41,41,41	0
85	MG	CR	201	1/1	0.94	0.65	29,29,29,29	0
85	MG	AR	3791	1/1	0.94	0.26	34,34,34,34	0
84	OHX	AR	3590	7/7	0.94	0.37	113,113,113,113	0
85	MG	6	2054	1/1	0.94	0.39	49,49,49,49	0
84	OHX	AR	3593	7/7	0.94	0.23	113,114,114,114	0
84	OHX	6	1999	7/7	0.94	0.26	138,139,139,140	0
85	MG	AR	3800	1/1	0.94	0.65	33,33,33,33	0
85	MG	AR	3801	1/1	0.94	0.38	32,32,32,32	0
84	OHX	1	3615	7/7	0.94	0.38	133,133,133,134	0
84	OHX	1	3514	7/7	0.94	0.18	112,112,112,112	0
84	OHX	AR	3600	7/7	0.94	0.33	119,119,119,119	0
85	MG	1	4090	1/1	0.94	0.21	42,42,42,42	0
85	MG	DC	204	1/1	0.94	0.14	35,35,35,35	0
84	OHX	1	3619	7/7	0.94	0.22	127,127,127,127	0
85	MG	AR	3809	1/1	0.94	0.65	37,37,37,37	0
85	MG	1	3763	1/1	0.94	0.65	29,29,29,29	0
85	MG	AR	4082	1/1	0.94	0.34	24,24,24,24	0
85	MG	6	2069	1/1	0.94	0.35	65,65,65,65	0
85	MG	AR	3813	1/1	0.94	0.16	55,55,55,55	0
84	OHX	AR	3735	7/7	0.94	0.30	129,129,129,129	0
84	OHX	1	3591	7/7	0.94	0.28	109,109,109,109	0
85	MG	sM	202	1/1	0.94	0.54	42,42,42,42	0
84	OHX	1	3594	7/7	0.94	0.20	131,131,132,132	0
84	OHX	AR	3607	7/7	0.94	0.30	113,113,113,113	0
85	MG	1	3768	1/1	0.94	0.41	36,36,36,36	0
85	MG	1	3770	1/1	0.94	0.25	29,29,29,29	0
85	MG	1	3950	1/1	0.94	0.14	38,38,38,38	0
85	MG	A	2049	1/1	0.94	0.50	54,54,54,54	0
84	OHX	AR	3608	7/7	0.94	0.34	131,131,132,132	0
85	MG	AR	3825	1/1	0.94	0.27	33,33,33,33	0
84	OHX	AR	3611	7/7	0.94	0.23	126,126,126,126	0
84	OHX	AR	3615	7/7	0.94	0.36	132,133,133,133	0
85	MG	AR	3831	1/1	0.94	0.23	44,44,44,44	0
84	OHX	AR	3742	7/7	0.94	0.25	128,129,129,129	0
84	OHX	AR	3622	7/7	0.94	0.24	130,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3540	7/7	0.94	0.18	111,111,111,111	0
85	MG	1	3957	1/1	0.94	0.39	37,37,37,37	0
84	OHX	AR	3634	7/7	0.94	0.26	112,112,113,113	0
85	MG	AR	4107	1/1	0.94	0.13	78,78,78,78	0
85	MG	AR	4108	1/1	0.94	0.19	36,36,36,36	0
84	OHX	3	206	7/7	0.94	0.20	127,127,128,128	0
84	OHX	AT	212	7/7	0.94	0.30	128,128,128,128	0
84	OHX	6	2010	7/7	0.94	0.33	154,155,155,155	0
85	MG	AR	4114	1/1	0.94	0.28	40,40,40,40	0
85	MG	A	2071	1/1	0.94	0.33	64,64,64,64	0
85	MG	1	4123	1/1	0.94	0.22	51,51,51,51	0
84	OHX	AT	215	7/7	0.94	0.20	137,138,138,138	0
85	MG	AR	3843	1/1	0.94	0.35	30,30,30,30	0
85	MG	6	2096	1/1	0.94	0.57	68,68,68,68	0
85	MG	6	2097	1/1	0.94	0.42	46,46,46,46	0
84	OHX	1	3660	7/7	0.94	0.28	153,153,154,154	0
85	MG	A	2082	1/1	0.94	0.23	61,61,61,61	0
85	MG	1	4126	1/1	0.94	0.98	33,33,33,33	0
85	MG	AR	3854	1/1	0.94	0.40	48,48,48,48	0
85	MG	AR	3859	1/1	0.94	0.49	29,29,29,29	0
85	MG	6	2102	1/1	0.94	0.46	45,45,45,45	0
85	MG	1	3791	1/1	0.94	0.60	54,54,54,54	0
84	OHX	6	2016	7/7	0.94	0.25	120,120,121,121	0
85	MG	1	3794	1/1	0.94	0.53	34,34,34,34	0
85	MG	AR	3872	1/1	0.94	0.34	43,43,43,43	0
85	MG	6	2108	1/1	0.94	0.56	50,50,50,50	0
85	MG	AR	3875	1/1	0.94	0.16	45,45,45,45	0
85	MG	AR	3879	1/1	0.94	0.64	22,22,22,22	0
85	MG	1	3795	1/1	0.94	0.29	26,26,26,26	0
85	MG	AR	3883	1/1	0.94	0.54	32,32,32,32	0
85	MG	A	2096	1/1	0.94	0.41	62,62,62,62	0
85	MG	A	2097	1/1	0.94	0.57	53,53,53,53	0
85	MG	AR	3888	1/1	0.94	0.67	24,24,24,24	0
84	OHX	1	3629	7/7	0.94	0.22	148,148,148,149	0
84	OHX	6	2019	7/7	0.94	0.30	140,140,141,141	0
84	OHX	CG	301	7/7	0.94	0.16	142,143,143,144	0
85	MG	6	2113	1/1	0.94	0.23	77,77,77,77	0
85	MG	AR	3893	1/1	0.94	0.95	50,50,50,50	0
84	OHX	4	214	7/7	0.94	0.46	140,140,140,140	0
84	OHX	CM	201	7/7	0.94	0.34	150,150,151,151	0
85	MG	1	4139	1/1	0.94	0.28	31,31,31,31	0
84	OHX	1	3663	7/7	0.94	0.19	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3900	1/1	0.94	0.81	37,37,37,37	0
84	OHX	1	3631	7/7	0.94	0.32	116,116,117,117	0
85	MG	A	2111	1/1	0.94	0.26	90,90,90,90	0
84	OHX	A	1953	7/7	0.94	0.41	146,147,147,147	0
85	MG	1	3978	1/1	0.94	0.35	46,46,46,46	0
84	OHX	A	1959	7/7	0.94	0.20	137,138,139,139	0
85	MG	1	3808	1/1	0.94	0.47	43,43,43,43	0
85	MG	AR	3912	1/1	0.94	0.54	23,23,23,23	0
84	OHX	A	1963	7/7	0.94	0.18	150,151,152,152	0
84	OHX	1	3632	7/7	0.94	0.34	156,156,156,156	0
85	MG	AR	3917	1/1	0.94	0.50	42,42,42,42	0
85	MG	AR	4162	1/1	0.94	0.60	56,56,56,56	0
84	OHX	AR	3651	7/7	0.94	0.31	150,151,151,151	0
84	OHX	6	2025	7/7	0.94	0.39	120,120,121,121	0
85	MG	1	3986	1/1	0.94	0.26	42,42,42,42	0
85	MG	AR	3923	1/1	0.94	0.66	38,38,38,38	0
84	OHX	A	1974	7/7	0.94	0.14	167,167,168,168	0
84	OHX	AR	3654	7/7	0.94	0.50	137,137,138,138	0
84	OHX	AR	3655	7/7	0.94	0.24	129,129,130,130	0
84	OHX	A	1991	7/7	0.94	0.24	157,157,158,158	0
84	OHX	6	2028	7/7	0.94	0.40	123,124,124,124	0
84	OHX	AR	3659	7/7	0.94	0.54	136,136,137,137	0
84	OHX	AR	3660	7/7	0.94	0.43	123,123,124,124	0
85	MG	1	3829	1/1	0.94	0.53	16,16,16,16	0
85	MG	1	4166	1/1	0.94	0.16	47,47,47,47	0
85	MG	1	4167	1/1	0.94	0.23	23,23,23,23	0
85	MG	1	4169	1/1	0.94	0.27	30,30,30,30	0
84	OHX	r	301	7/7	0.94	0.20	115,115,115,115	0
85	MG	1	3831	1/1	0.94	0.47	26,26,26,26	0
85	MG	AR	3949	1/1	0.94	0.19	32,32,32,32	0
84	OHX	6	2031	7/7	0.94	0.31	125,126,126,126	0
85	MG	1	4181	1/1	0.94	0.35	23,23,23,23	0
84	OHX	1	3705	7/7	0.94	0.38	131,131,132,132	0
85	MG	6	2155	1/1	0.94	0.86	58,58,58,58	0
84	OHX	A	2013	7/7	0.94	0.34	132,133,133,133	0
84	OHX	A	2014	7/7	0.94	0.35	127,128,128,128	0
85	MG	A	2153	1/1	0.94	0.58	51,51,51,51	0
85	MG	AR	3959	1/1	0.94	0.28	32,32,32,32	0
85	MG	6	2159	1/1	0.94	0.08	82,82,82,82	0
84	OHX	AR	3666	7/7	0.94	0.27	130,131,131,131	0
84	OHX	AR	3667	7/7	0.94	0.38	146,147,147,147	0
85	MG	AR	3963	1/1	0.94	0.20	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	A	2018	7/7	0.94	0.34	155,155,156,156	0
85	MG	1	4194	1/1	0.94	0.50	22,22,22,22	0
85	MG	1	4195	1/1	0.94	0.46	29,29,29,29	0
85	MG	AR	4203	1/1	0.94	0.24	29,29,29,29	0
84	OHX	1	3605	7/7	0.94	0.33	129,130,130,130	0
85	MG	1	4201	1/1	0.94	0.49	28,28,28,28	0
85	MG	AR	3969	1/1	0.94	0.13	60,60,60,60	0
84	OHX	y	201	7/7	0.94	0.32	128,129,129,129	0
84	OHX	1	3639	7/7	0.94	0.32	132,132,132,132	0
85	MG	1	4206	1/1	0.94	0.30	30,30,30,30	0
84	OHX	A	2022	7/7	0.94	0.36	167,167,167,167	0
85	MG	AR	4213	1/1	0.94	0.14	53,53,53,53	0
84	OHX	6	1919	7/7	0.94	0.21	121,121,122,122	0
85	MG	AR	3978	1/1	0.94	0.36	49,49,49,49	0
85	MG	d3	201	1/1	0.94	0.25	49,49,49,49	0
85	MG	1	4010	1/1	0.94	0.46	30,30,30,30	0
85	MG	1	4212	1/1	0.94	0.42	39,39,39,39	0
85	MG	AR	3981	1/1	0.94	0.14	33,33,33,33	0
84	OHX	6	1929	7/7	0.94	0.11	157,158,159,159	0
84	OHX	1	3669	7/7	0.94	0.39	131,131,131,131	0
84	OHX	A	2028	7/7	0.94	0.34	157,157,158,158	0
84	OHX	AR	3681	7/7	0.94	0.23	140,140,140,141	0
85	MG	1	3860	1/1	0.94	0.47	36,36,36,36	0
85	MG	1	4220	1/1	0.94	0.57	35,35,35,35	0
85	MG	AR	3993	1/1	0.94	0.35	28,28,28,28	0
85	MG	AR	4012	1/1	0.95	0.35	30,30,30,30	0
85	MG	1	404	1/1	0.95	0.34	35,35,35,35	0
85	MG	1	4071	1/1	0.95	0.20	40,40,40,40	0
84	OHX	AR	3605	7/7	0.95	0.16	128,128,128,129	0
84	OHX	1	3604	7/7	0.95	0.34	116,116,117,117	0
85	MG	1	4075	1/1	0.95	0.43	41,41,41,41	0
85	MG	1	3924	1/1	0.95	0.37	60,60,60,60	0
85	MG	AR	4247	1/1	0.95	0.46	22,22,22,22	0
85	MG	1	3749	1/1	0.95	0.26	24,24,24,24	0
84	OHX	6	2020	7/7	0.95	0.18	135,136,136,137	0
84	OHX	1	3539	7/7	0.95	0.28	119,119,119,119	0
84	OHX	AR	3610	7/7	0.95	0.38	137,138,138,138	0
84	OHX	1	3606	7/7	0.95	0.40	138,138,138,138	0
85	MG	w	201	1/1	0.95	0.42	37,37,37,37	0
84	OHX	1	3469	7/7	0.95	0.21	117,117,118,118	0
84	OHX	AR	3618	7/7	0.95	0.21	113,113,114,114	0
84	OHX	1	3544	7/7	0.95	0.16	116,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4259	1/1	0.95	0.49	16,16,16,16	0
85	MG	AS	212	1/1	0.95	0.33	41,41,41,41	0
84	OHX	AR	3624	7/7	0.95	0.33	150,150,151,151	0
84	OHX	1	3612	7/7	0.95	0.31	122,122,122,122	0
84	OHX	6	2026	7/7	0.95	0.25	146,146,147,147	0
84	OHX	6	2027	7/7	0.95	0.47	146,147,147,148	0
84	OHX	1	3657	7/7	0.95	0.28	123,123,124,124	0
84	OHX	AT	214	7/7	0.95	0.33	131,131,131,132	0
84	OHX	AR	3637	7/7	0.95	0.40	129,129,129,129	0
85	MG	AS	221	1/1	0.95	0.16	60,60,60,60	0
84	OHX	AT	216	7/7	0.95	0.40	132,132,132,132	0
84	OHX	AR	3638	7/7	0.95	0.42	119,119,119,119	0
85	MG	AR	3793	1/1	0.95	0.31	29,29,29,29	0
85	MG	6	2062	1/1	0.95	0.42	51,51,51,51	0
84	OHX	1	3545	7/7	0.95	0.21	120,120,120,120	0
85	MG	1	3769	1/1	0.95	0.19	45,45,45,45	0
84	OHX	1	3550	7/7	0.95	0.18	115,115,115,116	0
84	OHX	1	3706	7/7	0.95	0.30	136,137,137,138	0
85	MG	AR	3802	1/1	0.95	0.12	40,40,40,40	0
85	MG	1	4106	1/1	0.95	0.34	67,67,67,67	0
84	OHX	1	3616	7/7	0.95	0.31	146,146,147,147	0
84	OHX	6	1954	7/7	0.95	0.09	178,178,178,178	0
85	MG	1	3774	1/1	0.95	0.54	43,43,43,43	0
85	MG	6	2073	1/1	0.95	0.52	48,48,48,48	0
84	OHX	CL	301	7/7	0.95	0.21	121,122,122,122	0
84	OHX	6	1956	7/7	0.95	0.12	174,174,175,175	0
84	OHX	A	1909	7/7	0.95	0.24	151,151,152,153	0
84	OHX	A	1915	7/7	0.95	0.21	142,143,143,144	0
84	OHX	1	3662	7/7	0.95	0.31	116,116,116,116	0
84	OHX	A	1935	7/7	0.95	0.23	140,140,141,141	0
84	OHX	1	3487	7/7	0.95	0.17	115,115,116,116	0
85	MG	1	3788	1/1	0.95	0.53	45,45,45,45	0
84	OHX	1	3554	7/7	0.95	0.24	129,129,130,130	0
85	MG	CE	405	1/1	0.95	0.89	26,26,26,26	0
85	MG	AR	4062	1/1	0.95	0.17	42,42,42,42	0
84	OHX	A	1958	7/7	0.95	0.22	173,173,173,173	0
85	MG	AR	3822	1/1	0.95	0.31	46,46,46,46	0
85	MG	AR	4065	1/1	0.95	0.25	31,31,31,31	0
85	MG	AR	4066	1/1	0.95	0.14	56,56,56,56	0
84	OHX	6	1966	7/7	0.95	0.15	133,133,134,134	0
84	OHX	A	1960	7/7	0.95	0.18	151,151,151,152	0
84	OHX	1	3481	7/7	0.95	0.19	116,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3826	1/1	0.95	0.32	23,23,23,23	0
85	MG	CM	203	1/1	0.95	0.21	55,55,55,55	0
85	MG	6	2089	1/1	0.95	0.44	44,44,44,44	0
85	MG	CP	504	1/1	0.95	0.23	46,46,46,46	0
84	OHX	A	1964	7/7	0.95	0.28	122,122,123,123	0
85	MG	1	3796	1/1	0.95	0.54	18,18,18,18	0
85	MG	CQ	203	1/1	0.95	0.15	34,34,34,34	0
84	OHX	1	3621	7/7	0.95	0.23	125,126,126,126	0
84	OHX	A	1969	7/7	0.95	0.34	144,144,145,145	0
84	OHX	6	1972	7/7	0.95	0.42	142,143,143,144	0
84	OHX	AR	3658	7/7	0.95	0.35	122,123,123,123	0
84	OHX	A	1973	7/7	0.95	0.28	167,168,169,169	0
84	OHX	6	1973	7/7	0.95	0.22	137,138,138,138	0
84	OHX	A	1977	7/7	0.95	0.25	153,154,154,155	0
84	OHX	1	3667	7/7	0.95	0.30	127,127,128,128	0
85	MG	1	4141	1/1	0.95	0.38	64,64,64,64	0
85	MG	1	4144	1/1	0.95	0.16	53,53,53,53	0
84	OHX	1	3559	7/7	0.95	0.17	143,143,143,144	0
85	MG	6	2107	1/1	0.95	0.55	43,43,43,43	0
85	MG	AR	4088	1/1	0.95	0.40	25,25,25,25	0
84	OHX	A	1986	7/7	0.95	0.29	168,169,170,170	0
85	MG	1	3809	1/1	0.95	0.27	39,39,39,39	0
85	MG	DH	203	1/1	0.95	0.28	31,31,31,31	0
85	MG	1	3977	1/1	0.95	0.14	48,48,48,48	0
85	MG	AR	3853	1/1	0.95	0.26	43,43,43,43	0
84	OHX	1	3715	7/7	0.95	0.09	166,166,167,167	0
85	MG	AR	3855	1/1	0.95	0.43	33,33,33,33	0
85	MG	AR	3856	1/1	0.95	0.71	27,27,27,27	0
85	MG	AR	3857	1/1	0.95	0.53	20,20,20,20	0
84	OHX	6	1984	7/7	0.95	0.26	150,150,151,151	0
84	OHX	A	1995	7/7	0.95	0.17	151,152,152,152	0
84	OHX	1	3517	7/7	0.95	0.26	119,119,120,120	0
84	OHX	A	2000	7/7	0.95	0.24	140,141,141,141	0
85	MG	AR	3865	1/1	0.95	0.41	24,24,24,24	0
85	MG	AR	3867	1/1	0.95	0.55	18,18,18,18	0
85	MG	AR	4105	1/1	0.95	0.14	42,42,42,42	0
84	OHX	A	2002	7/7	0.95	0.31	147,148,149,149	0
84	OHX	1	3671	7/7	0.95	0.24	149,150,150,150	0
84	OHX	1	3567	7/7	0.95	0.24	128,129,129,129	0
84	OHX	AH	201	7/7	0.95	0.44	129,129,129,130	0
85	MG	AR	4111	1/1	0.95	0.35	37,37,37,37	0
85	MG	AR	3877	1/1	0.95	0.34	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3824	1/1	0.95	0.39	25,25,25,25	0
85	MG	AR	3880	1/1	0.95	0.47	42,42,42,42	0
85	MG	AR	3881	1/1	0.95	0.29	30,30,30,30	0
85	MG	A	2059	1/1	0.95	0.61	53,53,53,53	0
84	OHX	AR	3673	7/7	0.95	0.19	125,125,125,125	0
84	OHX	AK	102	7/7	0.95	0.18	105,105,105,105	0
85	MG	AR	3886	1/1	0.95	0.70	30,30,30,30	0
85	MG	A	2063	1/1	0.95	0.50	51,51,51,51	0
85	MG	A	2064	1/1	0.95	0.34	65,65,65,65	0
85	MG	AR	4121	1/1	0.95	0.30	27,27,27,27	0
84	OHX	1	3575	7/7	0.95	0.27	116,117,117,117	0
85	MG	6	2126	1/1	0.95	0.29	53,53,53,53	0
84	OHX	AR	3427	7/7	0.95	0.29	110,110,111,111	0
85	MG	6	2128	1/1	0.95	0.23	47,47,47,47	0
84	OHX	AR	3460	7/7	0.95	0.20	112,112,112,112	0
84	OHX	AR	3680	7/7	0.95	0.42	141,141,142,142	0
85	MG	A	2073	1/1	0.95	0.57	50,50,50,50	0
84	OHX	AR	3472	7/7	0.95	0.16	111,111,111,112	0
85	MG	AR	4129	1/1	0.95	0.36	26,26,26,26	0
84	OHX	AR	3474	7/7	0.95	0.19	114,114,114,115	0
85	MG	1	4171	1/1	0.95	0.24	85,85,85,85	0
85	MG	6	2135	1/1	0.95	0.24	49,49,49,49	0
85	MG	1	4173	1/1	0.95	0.54	36,36,36,36	0
85	MG	AR	3901	1/1	0.95	0.45	29,29,29,29	0
85	MG	AR	4138	1/1	0.95	0.47	28,28,28,28	0
84	OHX	AR	3495	7/7	0.95	0.17	113,113,114,114	0
85	MG	1	4175	1/1	0.95	0.44	39,39,39,39	0
85	MG	AR	3904	1/1	0.95	0.52	21,21,21,21	0
85	MG	1	3839	1/1	0.95	0.19	27,27,27,27	0
85	MG	1	4179	1/1	0.95	0.23	38,38,38,38	0
84	OHX	AR	3688	7/7	0.95	0.29	136,136,137,137	0
85	MG	1	3841	1/1	0.95	0.59	29,29,29,29	0
84	OHX	AR	3499	7/7	0.95	0.15	125,126,126,126	0
85	MG	1	4186	1/1	0.95	0.52	25,25,25,25	0
85	MG	AR	3915	1/1	0.95	0.61	28,28,28,28	0
84	OHX	A	2024	7/7	0.95	0.24	151,152,153,153	0
85	MG	AR	3918	1/1	0.95	0.48	27,27,27,27	0
85	MG	AR	4151	1/1	0.95	0.10	148,148,148,148	0
85	MG	6	2147	1/1	0.95	0.12	57,57,57,57	0
85	MG	6	2148	1/1	0.95	0.43	48,48,48,48	0
85	MG	1	3846	1/1	0.95	0.28	39,39,39,39	0
84	OHX	AR	3503	7/7	0.95	0.17	120,120,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	1	3674	7/7	0.95	0.28	136,136,137,137	0
85	MG	6	2153	1/1	0.95	0.27	97,97,97,97	0
84	OHX	A	2027	7/7	0.95	0.33	159,160,161,161	0
84	OHX	AR	3511	7/7	0.95	0.26	108,108,108,108	0
85	MG	6	2156	1/1	0.95	0.16	101,101,101,101	0
84	OHX	6	1997	7/7	0.95	0.36	132,132,133,133	0
84	OHX	1	3577	7/7	0.95	0.31	118,118,119,119	0
85	MG	AR	3937	1/1	0.95	0.67	27,27,27,27	0
85	MG	AR	3942	1/1	0.95	0.56	31,31,31,31	0
84	OHX	A	2031	7/7	0.95	0.35	159,160,161,161	0
84	OHX	1	3634	7/7	0.95	0.17	132,132,132,133	0
84	OHX	AR	3700	7/7	0.95	0.47	135,135,135,135	0
85	MG	1	4207	1/1	0.95	0.28	36,36,36,36	0
85	MG	1	4208	1/1	0.95	0.32	37,37,37,37	0
85	MG	1	3859	1/1	0.95	0.44	28,28,28,28	0
84	OHX	1	3581	7/7	0.95	0.22	112,113,113,113	0
85	MG	A	2120	1/1	0.95	0.22	85,85,85,85	0
84	OHX	1	3681	7/7	0.95	0.32	127,127,127,128	0
84	OHX	AR	3703	7/7	0.95	0.51	136,136,136,136	0
84	OHX	AR	3532	7/7	0.95	0.14	135,136,136,137	0
84	OHX	AR	3537	7/7	0.95	0.15	131,132,132,132	0
84	OHX	AR	3538	7/7	0.95	0.17	123,123,124,124	0
84	OHX	AR	3544	7/7	0.95	0.16	109,109,110,110	0
85	MG	1	3867	1/1	0.95	0.43	35,35,35,35	0
85	MG	1	4024	1/1	0.95	0.21	61,61,61,61	0
84	OHX	1	3583	7/7	0.95	0.16	131,132,132,132	0
85	MG	6	2179	1/1	0.95	0.36	43,43,43,43	0
84	OHX	1	3588	7/7	0.95	0.19	128,128,128,128	0
84	OHX	1	3525	7/7	0.95	0.21	114,114,114,115	0
84	OHX	AR	3565	7/7	0.95	0.20	113,113,113,113	0
85	MG	1	3872	1/1	0.95	0.59	32,32,32,32	0
84	OHX	AR	3568	7/7	0.95	0.25	117,117,117,117	0
84	OHX	4	210	7/7	0.95	0.27	108,108,108,108	0
84	OHX	AR	3714	7/7	0.95	0.33	132,132,133,133	0
85	MG	1	3879	1/1	0.95	0.38	45,45,45,45	0
85	MG	AR	3972	1/1	0.95	0.53	39,39,39,39	0
84	OHX	AR	3575	7/7	0.95	0.28	119,120,120,120	0
85	MG	4	218	1/1	0.95	0.60	49,49,49,49	0
85	MG	AR	4199	1/1	0.95	0.36	45,45,45,45	0
85	MG	A	2148	1/1	0.95	0.37	64,64,64,64	0
85	MG	4	219	1/1	0.95	0.68	42,42,42,42	0
84	OHX	AR	3577	7/7	0.95	0.09	156,157,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4202	1/1	0.95	0.56	29,29,29,29	0
84	OHX	AR	3579	7/7	0.95	0.35	130,130,130,130	0
84	OHX	AR	3583	7/7	0.95	0.22	113,114,114,114	0
84	OHX	AR	3587	7/7	0.95	0.24	126,126,126,126	0
85	MG	4	224	1/1	0.95	0.40	33,33,33,33	0
84	OHX	6	2009	7/7	0.95	0.18	126,127,127,128	0
85	MG	1	3894	1/1	0.95	0.48	22,22,22,22	0
84	OHX	AR	3592	7/7	0.95	0.34	114,114,114,114	0
84	OHX	1	3527	7/7	0.95	0.12	135,135,136,136	0
85	MG	AR	4212	1/1	0.95	0.27	31,31,31,31	0
85	MG	AR	3989	1/1	0.95	0.23	44,44,44,44	0
85	MG	AR	3990	1/1	0.95	0.08	39,39,39,39	0
85	MG	1	4048	1/1	0.95	0.83	33,33,33,33	0
84	OHX	AR	3724	7/7	0.95	0.27	130,130,131,131	0
84	OHX	AR	3595	7/7	0.95	0.31	131,131,131,132	0
85	MG	1	3733	1/1	0.95	0.49	26,26,26,26	0
85	MG	1	3902	1/1	0.95	0.50	35,35,35,35	0
84	OHX	6	2012	7/7	0.95	0.21	136,136,137,137	0
85	MG	AR	3746	1/1	0.95	0.26	58,58,58,58	0
84	OHX	1	3537	7/7	0.95	0.25	115,115,115,116	0
85	MG	1	3907	1/1	0.95	0.33	40,40,40,40	0
84	OHX	6	2014	7/7	0.95	0.34	129,129,129,130	0
84	OHX	6	2015	7/7	0.95	0.35	135,135,136,136	0
84	OHX	AR	3601	7/7	0.95	0.42	127,127,128,128	0
85	MG	AR	4228	1/1	0.95	0.38	27,27,27,27	0
85	MG	1	3914	1/1	0.95	0.50	19,19,19,19	0
86	HN8	1	4223	22/22	0.95	0.24	32,32,32,32	0
86	HN8	AR	4263	22/22	0.95	0.26	27,27,27,27	22
84	OHX	1	3599	7/7	0.95	0.43	115,116,116,116	0
85	MG	1	3741	1/1	0.95	0.25	37,37,37,37	0
85	MG	1	3919	1/1	0.95	0.27	33,33,33,33	0
85	MG	k	404	1/1	0.95	0.67	32,32,32,32	0
84	OHX	AR	3603	7/7	0.95	0.24	107,107,107,107	0
85	MG	AR	4237	1/1	0.95	0.21	39,39,39,39	0
88	ZN	g	501	1/1	0.95	0.06	119,119,119,119	0
84	OHX	1	3649	7/7	0.95	0.35	113,113,113,113	0
84	OHX	AR	3682	7/7	0.96	0.52	144,144,144,145	0
84	OHX	AR	3684	7/7	0.96	0.52	124,125,125,125	0
84	OHX	1	3519	7/7	0.96	0.22	116,116,116,116	0
84	OHX	O	201	7/7	0.96	0.28	158,159,159,160	0
84	OHX	6	1978	7/7	0.96	0.29	117,117,117,118	0
85	MG	AR	4217	1/1	0.96	0.60	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	T	201	7/7	0.96	0.19	145,146,146,147	0
85	MG	AR	3951	1/1	0.96	0.53	29,29,29,29	0
85	MG	AR	3952	1/1	0.96	0.36	28,28,28,28	0
84	OHX	e	101	7/7	0.96	0.41	143,144,145,145	0
84	OHX	AR	3687	7/7	0.96	0.37	121,121,122,122	0
85	MG	1	4143	1/1	0.96	0.21	29,29,29,29	0
84	OHX	c1	201	7/7	0.96	0.41	147,148,148,149	0
84	OHX	1	3703	7/7	0.96	0.46	131,131,132,132	0
84	OHX	6	1980	7/7	0.96	0.34	116,116,116,116	0
84	OHX	AR	3512	7/7	0.96	0.18	118,118,119,119	0
84	OHX	AR	3514	7/7	0.96	0.19	112,112,112,113	0
84	OHX	6	1982	7/7	0.96	0.17	147,147,148,148	0
84	OHX	AR	3693	7/7	0.96	0.41	131,131,131,131	0
84	OHX	AR	3521	7/7	0.96	0.28	117,118,118,118	0
84	OHX	AR	3522	7/7	0.96	0.13	114,114,115,115	0
85	MG	6	2151	1/1	0.96	0.15	60,60,60,60	0
84	OHX	AR	3697	7/7	0.96	0.25	114,115,115,115	0
84	OHX	1	3584	7/7	0.96	0.25	114,114,114,114	0
84	OHX	AR	3699	7/7	0.96	0.36	117,117,117,117	0
84	OHX	AR	3526	7/7	0.96	0.18	117,117,117,118	0
84	OHX	6	1985	7/7	0.96	0.33	130,130,131,131	0
84	OHX	1	3586	7/7	0.96	0.23	121,122,122,122	0
84	OHX	AR	3530	7/7	0.96	0.17	112,113,113,113	0
84	OHX	1	3520	7/7	0.96	0.18	123,123,124,124	0
84	OHX	6	1988	7/7	0.96	0.14	133,133,133,134	0
84	OHX	AR	3534	7/7	0.96	0.16	109,109,109,109	0
84	OHX	AR	3536	7/7	0.96	0.22	123,124,124,124	0
84	OHX	1	3589	7/7	0.96	0.23	113,113,113,113	0
85	MG	AR	4249	1/1	0.96	0.44	24,24,24,24	0
85	MG	1	4168	1/1	0.96	0.45	20,20,20,20	0
85	MG	1	3743	1/1	0.96	0.28	79,79,79,79	0
84	OHX	6	1990	7/7	0.96	0.29	129,130,130,130	0
84	OHX	AR	3541	7/7	0.96	0.19	125,125,125,125	0
85	MG	1	4172	1/1	0.96	0.41	67,67,67,67	0
84	OHX	AR	3543	7/7	0.96	0.24	123,123,123,123	0
84	OHX	1	3473	7/7	0.96	0.15	114,115,115,115	0
85	MG	6	2172	1/1	0.96	0.26	38,38,38,38	0
85	MG	AR	4258	1/1	0.96	0.54	34,34,34,34	0
84	OHX	AR	3545	7/7	0.96	0.24	108,108,108,108	0
85	MG	1	4176	1/1	0.96	0.62	34,34,34,34	0
85	MG	1	4177	1/1	0.96	0.44	27,27,27,27	0
85	MG	6	2177	1/1	0.96	0.19	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AR	3546	7/7	0.96	0.21	123,124,124,124	0
85	MG	AS	216	1/1	0.96	0.50	23,23,23,23	0
84	OHX	AR	3715	7/7	0.96	0.29	118,118,119,119	0
84	OHX	AR	3548	7/7	0.96	0.16	121,121,122,122	0
84	OHX	AR	3551	7/7	0.96	0.14	129,129,130,130	0
85	MG	AR	4000	1/1	0.96	0.43	25,25,25,25	0
84	OHX	1	3592	7/7	0.96	0.33	117,117,117,117	0
84	OHX	AR	3553	7/7	0.96	0.29	113,113,113,113	0
85	MG	6	2187	1/1	0.96	0.18	82,82,82,82	0
85	MG	1	3968	1/1	0.96	0.47	29,29,29,29	0
85	MG	1	4188	1/1	0.96	0.36	28,28,28,28	0
85	MG	1	3757	1/1	0.96	0.19	38,38,38,38	0
85	MG	AR	4007	1/1	0.96	0.28	29,29,29,29	0
85	MG	AS	229	1/1	0.96	0.24	46,46,46,46	0
84	OHX	AR	3555	7/7	0.96	0.21	115,115,115,115	0
84	OHX	AR	3556	7/7	0.96	0.21	109,109,109,109	0
84	OHX	AR	3557	7/7	0.96	0.17	123,123,124,124	0
84	OHX	AR	3562	7/7	0.96	0.24	124,124,124,124	0
85	MG	1	4197	1/1	0.96	0.34	32,32,32,32	0
84	OHX	6	1994	7/7	0.96	0.25	170,170,170,170	0
85	MG	1	4199	1/1	0.96	0.59	24,24,24,24	0
84	OHX	6	1995	7/7	0.96	0.24	133,134,134,135	0
84	OHX	6	1996	7/7	0.96	0.20	154,154,155,155	0
84	OHX	AR	3567	7/7	0.96	0.15	121,121,121,121	0
84	OHX	1	3593	7/7	0.96	0.15	166,167,167,167	0
84	OHX	AR	3570	7/7	0.96	0.25	120,121,121,121	0
85	MG	1	3980	1/1	0.96	0.26	73,73,73,73	0
84	OHX	6	1998	7/7	0.96	0.33	146,146,147,147	0
84	OHX	AR	3731	7/7	0.96	0.19	117,117,117,117	0
84	OHX	1	3526	7/7	0.96	0.29	114,115,115,115	0
84	OHX	6	2000	7/7	0.96	0.17	130,130,131,131	0
84	OHX	1	3654	7/7	0.96	0.14	136,136,136,137	0
84	OHX	AR	3580	7/7	0.96	0.20	117,118,118,118	0
85	MG	AK	103	1/1	0.96	0.44	36,36,36,36	0
85	MG	AP	503	1/1	0.96	0.28	27,27,27,27	0
85	MG	1	4216	1/1	0.96	0.39	23,23,23,23	0
85	MG	1	3775	1/1	0.96	0.29	32,32,32,32	0
84	OHX	AR	3581	7/7	0.96	0.18	109,109,109,109	0
84	OHX	1	3595	7/7	0.96	0.11	140,140,140,140	0
85	MG	CK	202	1/1	0.96	0.20	44,44,44,44	0
84	OHX	AR	3586	7/7	0.96	0.24	119,119,120,120	0
85	MG	1	4221	1/1	0.96	0.52	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4222	1/1	0.96	0.65	13,13,13,13	0
85	MG	CO	201	1/1	0.96	0.19	44,44,44,44	0
85	MG	1	3781	1/1	0.96	0.39	33,33,33,33	0
84	OHX	1	3445	7/7	0.96	0.26	111,112,112,112	0
85	MG	CP	505	1/1	0.96	0.27	71,71,71,71	0
84	OHX	AR	3588	7/7	0.96	0.27	112,112,112,113	0
85	MG	3	213	1/1	0.96	0.45	48,48,48,48	0
84	OHX	1	3597	7/7	0.96	0.39	117,117,118,118	0
85	MG	3	215	1/1	0.96	0.57	31,31,31,31	0
84	OHX	1	3531	7/7	0.96	0.19	114,114,114,114	0
84	OHX	AR	3743	7/7	0.96	0.33	109,109,109,109	0
85	MG	3	219	1/1	0.96	0.21	56,56,56,56	0
84	OHX	1	3601	7/7	0.96	0.30	112,112,112,112	0
84	OHX	1	3483	7/7	0.96	0.12	113,113,113,113	0
85	MG	AR	3766	1/1	0.96	0.14	96,96,96,96	0
84	OHX	1	3446	7/7	0.96	0.19	116,116,116,116	0
85	MG	1	3792	1/1	0.96	0.52	37,37,37,37	0
84	OHX	1	3451	7/7	0.96	0.22	111,111,111,111	0
84	OHX	AT	210	7/7	0.96	0.20	119,119,120,120	0
84	OHX	AT	211	7/7	0.96	0.11	137,138,138,138	0
85	MG	AR	3772	1/1	0.96	0.52	37,37,37,37	0
84	OHX	AR	3598	7/7	0.96	0.18	117,118,118,118	0
84	OHX	6	2011	7/7	0.96	0.43	146,146,147,147	0
85	MG	DH	202	1/1	0.96	0.26	40,40,40,40	0
84	OHX	1	3541	7/7	0.96	0.26	119,119,120,120	0
84	OHX	1	3543	7/7	0.96	0.22	119,119,120,120	0
84	OHX	1	3611	7/7	0.96	0.21	119,119,119,120	0
85	MG	4	226	1/1	0.96	0.59	42,42,42,42	0
84	OHX	1	3455	7/7	0.96	0.16	127,127,127,128	0
84	OHX	1	3489	7/7	0.96	0.21	113,113,114,114	0
84	OHX	6	2017	7/7	0.96	0.29	135,135,136,136	0
84	OHX	1	3547	7/7	0.96	0.11	120,121,121,121	0
85	MG	AR	3787	1/1	0.96	0.69	31,31,31,31	0
84	OHX	3	207	7/7	0.96	0.20	137,138,138,138	0
84	OHX	1	3670	7/7	0.96	0.24	111,111,111,111	0
85	MG	AR	3790	1/1	0.96	0.34	22,22,22,22	0
84	OHX	CK	201	7/7	0.96	0.21	118,118,119,119	0
84	OHX	4	206	7/7	0.96	0.16	116,116,116,116	0
85	MG	1	3812	1/1	0.96	0.64	64,64,64,64	0
84	OHX	1	3497	7/7	0.96	0.11	125,125,126,126	0
85	MG	AR	3795	1/1	0.96	0.66	49,49,49,49	0
84	OHX	CX	202	7/7	0.96	0.27	117,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AR	3612	7/7	0.96	0.34	111,111,111,111	0
85	MG	AR	4079	1/1	0.96	0.31	34,34,34,34	0
85	MG	4	239	1/1	0.96	0.69	43,43,43,43	0
84	OHX	AR	3613	7/7	0.96	0.29	112,112,112,112	0
84	OHX	AR	3614	7/7	0.96	0.20	114,114,114,114	0
84	OHX	A	1933	7/7	0.96	0.13	122,122,122,123	0
84	OHX	4	211	7/7	0.96	0.14	138,139,139,140	0
84	OHX	A	1936	7/7	0.96	0.17	126,127,127,128	0
84	OHX	A	1944	7/7	0.96	0.12	138,139,139,140	0
84	OHX	AR	3617	7/7	0.96	0.28	123,123,123,123	0
84	OHX	A	1947	7/7	0.96	0.27	129,129,130,130	0
85	MG	1	4032	1/1	0.96	0.31	42,42,42,42	0
85	MG	A	2066	1/1	0.96	0.59	79,79,79,79	0
85	MG	AR	4091	1/1	0.96	0.31	35,35,35,35	0
84	OHX	1	3617	7/7	0.96	0.23	122,122,122,122	0
84	OHX	A	1955	7/7	0.96	0.13	145,146,147,147	0
84	OHX	AR	3619	7/7	0.96	0.35	122,123,123,124	0
85	MG	AR	4095	1/1	0.96	0.22	25,25,25,25	0
84	OHX	AR	3621	7/7	0.96	0.35	135,135,136,136	0
84	OHX	1	3458	7/7	0.96	0.20	116,116,116,117	0
85	MG	A	2074	1/1	0.96	0.41	55,55,55,55	0
84	OHX	AR	3623	7/7	0.96	0.29	138,139,139,139	0
84	OHX	1	3553	7/7	0.96	0.29	121,122,122,122	0
85	MG	1	3838	1/1	0.96	0.57	33,33,33,33	0
84	OHX	AR	3626	7/7	0.96	0.30	122,123,123,123	0
84	OHX	AR	3627	7/7	0.96	0.32	127,128,128,128	0
84	OHX	AR	3628	7/7	0.96	0.32	147,148,148,148	0
85	MG	1	3842	1/1	0.96	0.55	25,25,25,25	0
84	OHX	AR	3629	7/7	0.96	0.14	141,141,141,142	0
84	OHX	1	3500	7/7	0.96	0.16	119,120,120,120	0
85	MG	AR	3828	1/1	0.96	0.61	60,60,60,60	0
84	OHX	AR	3632	7/7	0.96	0.35	117,117,118,118	0
85	MG	1	4052	1/1	0.96	0.29	21,21,21,21	0
84	OHX	A	1975	7/7	0.96	0.10	156,158,158,158	0
85	MG	AR	4112	1/1	0.96	0.15	54,54,54,54	0
84	OHX	A	1976	7/7	0.96	0.18	123,124,124,124	0
84	OHX	AR	3633	7/7	0.96	0.28	124,125,125,125	0
84	OHX	A	1978	7/7	0.96	0.26	143,144,144,145	0
85	MG	lR	201	1/1	0.96	0.36	26,26,26,26	0
84	OHX	A	1980	7/7	0.96	0.26	137,137,138,138	0
85	MG	6	2055	1/1	0.96	0.73	49,49,49,49	0
84	OHX	k	401	7/7	0.96	0.27	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	A	1983	7/7	0.96	0.24	142,142,143,143	0
85	MG	1	3854	1/1	0.96	0.62	34,34,34,34	0
85	MG	6	2061	1/1	0.96	0.32	100,100,100,100	0
85	MG	AR	3844	1/1	0.96	0.40	27,27,27,27	0
84	OHX	6	2029	7/7	0.96	0.41	152,153,153,154	0
85	MG	AR	3846	1/1	0.96	0.56	33,33,33,33	0
85	MG	1	3856	1/1	0.96	0.68	24,24,24,24	0
84	OHX	1	3431	7/7	0.96	0.30	114,114,114,114	0
84	OHX	A	1989	7/7	0.96	0.37	154,155,155,155	0
84	OHX	1	3677	7/7	0.96	0.33	116,116,117,117	0
85	MG	AR	4133	1/1	0.96	0.27	25,25,25,25	0
85	MG	1	4069	1/1	0.96	0.43	46,46,46,46	0
84	OHX	1	3622	7/7	0.96	0.27	153,154,154,154	0
84	OHX	A	1994	7/7	0.96	0.28	142,143,144,144	0
84	OHX	1	3680	7/7	0.96	0.32	122,122,122,122	0
84	OHX	6	2034	7/7	0.96	0.19	155,155,155,155	0
84	OHX	A	1997	7/7	0.96	0.28	139,140,140,140	0
85	MG	6	2075	1/1	0.96	0.14	76,76,76,76	0
84	OHX	A	1999	7/7	0.96	0.24	146,146,147,147	0
84	OHX	1	3623	7/7	0.96	0.23	114,114,115,115	0
85	MG	A	2119	1/1	0.96	0.35	57,57,57,57	0
84	OHX	A	2001	7/7	0.96	0.20	136,137,137,138	0
84	OHX	1	3683	7/7	0.96	0.33	118,118,118,118	0
85	MG	AR	3871	1/1	0.96	0.40	28,28,28,28	0
84	OHX	A	2003	7/7	0.96	0.32	129,130,130,130	0
84	OHX	A	2005	7/7	0.96	0.32	131,132,132,132	0
85	MG	AR	3874	1/1	0.96	0.60	27,27,27,27	0
84	OHX	1	3684	7/7	0.96	0.41	141,141,141,141	0
84	OHX	6	1921	7/7	0.96	0.17	141,141,142,143	0
85	MG	6	2084	1/1	0.96	0.22	48,48,48,48	0
84	OHX	A	2009	7/7	0.96	0.38	126,126,127,127	0
85	MG	1	3876	1/1	0.96	0.40	37,37,37,37	0
84	OHX	AR	3648	7/7	0.96	0.55	130,131,131,131	0
84	OHX	1	3685	7/7	0.96	0.41	121,121,121,121	0
84	OHX	1	3624	7/7	0.96	0.20	136,136,136,137	0
84	OHX	1	3507	7/7	0.96	0.23	113,113,114,114	0
84	OHX	6	1941	7/7	0.96	0.13	120,120,121,121	0
84	OHX	A	2016	7/7	0.96	0.28	142,143,143,144	0
85	MG	A	2137	1/1	0.96	0.48	58,58,58,58	0
85	MG	A	2138	1/1	0.96	0.46	66,66,66,66	0
85	MG	6	2093	1/1	0.96	0.33	47,47,47,47	0
85	MG	1	4094	1/1	0.96	0.15	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4095	1/1	0.96	0.20	61,61,61,61	0
85	MG	1	4096	1/1	0.96	0.41	27,27,27,27	0
85	MG	A	2144	1/1	0.96	0.39	69,69,69,69	0
85	MG	AR	3895	1/1	0.96	0.28	43,43,43,43	0
84	OHX	6	1946	7/7	0.96	0.17	127,128,128,129	0
84	OHX	6	2044	7/7	0.96	0.35	140,141,141,141	0
84	OHX	6	1947	7/7	0.96	0.14	121,122,122,122	0
85	MG	6	2101	1/1	0.96	0.51	53,53,53,53	0
84	OHX	6	1949	7/7	0.96	0.11	135,136,136,136	0
84	OHX	1	3509	7/7	0.96	0.14	119,120,120,120	0
85	MG	6	2104	1/1	0.96	0.20	70,70,70,70	0
85	MG	1	4103	1/1	0.96	0.27	60,60,60,60	0
84	OHX	6	1952	7/7	0.96	0.14	148,148,148,148	0
85	MG	1	4105	1/1	0.96	0.49	26,26,26,26	0
84	OHX	AR	3662	7/7	0.96	0.22	111,111,112,112	0
84	OHX	1	3628	7/7	0.96	0.26	144,145,145,145	0
84	OHX	1	3565	7/7	0.96	0.25	131,131,131,131	0
84	OHX	1	3510	7/7	0.96	0.16	111,111,111,111	0
84	OHX	1	3435	7/7	0.96	0.27	114,114,114,114	0
85	MG	AR	3916	1/1	0.96	0.58	19,19,19,19	0
84	OHX	1	3693	7/7	0.96	0.27	118,118,118,118	0
85	MG	6	2114	1/1	0.96	0.47	46,46,46,46	0
85	MG	AR	3919	1/1	0.96	0.43	34,34,34,34	0
84	OHX	1	3471	7/7	0.96	0.21	112,112,113,113	0
84	OHX	AR	3669	7/7	0.96	0.17	175,176,176,176	0
84	OHX	1	3579	7/7	0.96	0.17	119,120,120,120	0
84	OHX	AR	3671	7/7	0.96	0.28	113,113,113,113	0
84	OHX	1	3637	7/7	0.96	0.15	140,140,140,141	0
85	MG	1	3916	1/1	0.96	0.29	26,26,26,26	0
85	MG	AR	3926	1/1	0.96	0.37	33,33,33,33	0
85	MG	1	4120	1/1	0.96	0.40	27,27,27,27	0
85	MG	d3	202	1/1	0.96	0.33	47,47,47,47	0
84	OHX	AR	3441	7/7	0.96	0.18	116,117,117,117	0
84	OHX	1	3518	7/7	0.96	0.15	109,110,110,110	0
85	MG	AR	3931	1/1	0.96	0.29	17,17,17,17	0
85	MG	AR	3933	1/1	0.96	0.47	24,24,24,24	0
84	OHX	AR	3676	7/7	0.96	0.29	122,122,123,123	0
84	OHX	AR	3466	7/7	0.96	0.18	120,120,121,121	0
85	MG	AR	3936	1/1	0.96	0.52	20,20,20,20	0
84	OHX	1	3640	7/7	0.96	0.35	124,124,124,125	0
85	MG	AR	3939	1/1	0.96	0.31	31,31,31,31	0
85	MG	AR	3941	1/1	0.96	0.46	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AR	3679	7/7	0.96	0.25	153,153,153,154	0
84	OHX	1	3582	7/7	0.96	0.29	121,121,121,121	0
84	OHX	6	1976	7/7	0.96	0.13	146,147,147,148	0
88	ZN	e1	501	1/1	0.96	0.06	153,153,153,153	0
84	OHX	AR	3625	7/7	0.97	0.36	134,134,134,134	0
84	OHX	A	1968	7/7	0.97	0.34	125,125,126,126	0
84	OHX	1	3506	7/7	0.97	0.29	109,109,110,110	0
84	OHX	1	3466	7/7	0.97	0.16	114,115,115,115	0
84	OHX	6	1953	7/7	0.97	0.12	132,133,133,134	0
85	MG	AR	3930	1/1	0.97	0.62	29,29,29,29	0
84	OHX	1	3638	7/7	0.97	0.33	122,123,123,123	0
85	MG	AR	3932	1/1	0.97	0.28	63,63,63,63	0
84	OHX	AR	3630	7/7	0.97	0.13	124,125,125,125	0
84	OHX	AG	201	7/7	0.97	0.21	114,115,115,115	0
84	OHX	6	1955	7/7	0.97	0.13	179,179,179,179	0
84	OHX	1	3585	7/7	0.97	0.23	115,115,116,116	0
84	OHX	6	1957	7/7	0.97	0.14	129,130,130,131	0
85	MG	AR	3938	1/1	0.97	0.39	34,34,34,34	0
84	OHX	A	1979	7/7	0.97	0.22	142,143,144,144	0
84	OHX	AP	502	7/7	0.97	0.17	112,113,113,113	0
84	OHX	6	1959	7/7	0.97	0.17	137,138,138,139	0
85	MG	1	4112	1/1	0.97	0.43	32,32,32,32	0
84	OHX	A	1982	7/7	0.97	0.30	121,122,122,122	0
85	MG	1	4114	1/1	0.97	0.23	52,52,52,52	0
84	OHX	AR	3432	7/7	0.97	0.27	117,117,117,118	0
84	OHX	1	3542	7/7	0.97	0.17	119,119,120,120	0
84	OHX	AR	3442	7/7	0.97	0.22	112,112,112,112	0
85	MG	AR	4229	1/1	0.97	0.70	34,34,34,34	0
84	OHX	A	1987	7/7	0.97	0.15	128,128,129,129	0
84	OHX	A	1988	7/7	0.97	0.23	139,140,141,141	0
84	OHX	AR	3445	7/7	0.97	0.18	107,107,107,107	0
85	MG	6	2136	1/1	0.97	0.23	52,52,52,52	0
85	MG	AR	3953	1/1	0.97	0.19	34,34,34,34	0
85	MG	AR	4235	1/1	0.97	0.37	26,26,26,26	0
85	MG	1	4122	1/1	0.97	0.25	78,78,78,78	0
85	MG	1	3878	1/1	0.97	0.58	24,24,24,24	0
84	OHX	A	1990	7/7	0.97	0.27	135,135,136,136	0
84	OHX	AR	3447	7/7	0.97	0.25	112,112,112,112	0
84	OHX	A	1992	7/7	0.97	0.21	140,141,142,142	0
85	MG	1	3883	1/1	0.97	0.41	22,22,22,22	0
84	OHX	AR	3642	7/7	0.97	0.24	122,122,122,122	0
84	OHX	AR	3643	7/7	0.97	0.30	120,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	3887	1/1	0.97	0.83	42,42,42,42	0
84	OHX	AR	3455	7/7	0.97	0.22	111,112,112,112	0
84	OHX	AR	3456	7/7	0.97	0.19	117,117,117,117	0
84	OHX	AR	3458	7/7	0.97	0.19	114,114,114,115	0
85	MG	1	3895	1/1	0.97	0.42	28,28,28,28	0
84	OHX	A	1998	7/7	0.97	0.25	158,159,160,160	0
84	OHX	AR	3459	7/7	0.97	0.26	114,114,115,115	0
84	OHX	1	3699	7/7	0.97	0.40	130,131,131,131	0
85	MG	AR	3970	1/1	0.97	0.23	50,50,50,50	0
84	OHX	AR	3463	7/7	0.97	0.17	110,110,111,111	0
85	MG	1	3900	1/1	0.97	0.34	42,42,42,42	0
84	OHX	1	3442	7/7	0.97	0.24	120,121,121,121	0
85	MG	AR	3974	1/1	0.97	0.42	81,81,81,81	0
84	OHX	AR	3467	7/7	0.97	0.13	108,109,109,109	0
84	OHX	A	2004	7/7	0.97	0.22	139,139,140,140	0
84	OHX	AR	3653	7/7	0.97	0.30	120,120,121,121	0
84	OHX	AR	3469	7/7	0.97	0.14	121,122,122,122	0
84	OHX	6	1964	7/7	0.97	0.12	123,123,124,124	0
85	MG	1	3909	1/1	0.97	0.57	25,25,25,25	0
84	OHX	A	2008	7/7	0.97	0.16	132,132,133,133	0
84	OHX	AR	3656	7/7	0.97	0.31	134,134,134,134	0
84	OHX	AR	3473	7/7	0.97	0.11	111,111,112,112	0
85	MG	AR	3985	1/1	0.97	0.49	35,35,35,35	0
84	OHX	6	1965	7/7	0.97	0.24	116,117,117,117	0
85	MG	AR	3987	1/1	0.97	0.30	31,31,31,31	0
84	OHX	AR	3478	7/7	0.97	0.17	110,110,110,111	0
85	MG	1	4157	1/1	0.97	0.48	60,60,60,60	0
84	OHX	AR	3479	7/7	0.97	0.15	110,110,110,110	0
85	MG	1	3918	1/1	0.97	0.20	31,31,31,31	0
84	OHX	AR	3661	7/7	0.97	0.46	112,112,112,113	0
84	OHX	AR	3480	7/7	0.97	0.12	113,114,114,114	0
84	OHX	AR	3483	7/7	0.97	0.17	111,111,111,111	0
84	OHX	AR	3484	7/7	0.97	0.19	114,114,114,114	0
85	MG	AS	231	1/1	0.97	0.19	56,56,56,56	0
84	OHX	AR	3491	7/7	0.97	0.13	108,108,109,109	0
84	OHX	AR	3492	7/7	0.97	0.15	116,116,117,117	0
84	OHX	AR	3493	7/7	0.97	0.25	114,114,114,114	0
84	OHX	AR	3494	7/7	0.97	0.15	124,125,125,125	0
84	OHX	1	3425	7/7	0.97	0.25	108,109,109,109	0
84	OHX	AR	3496	7/7	0.97	0.24	112,113,113,113	0
84	OHX	6	1967	7/7	0.97	0.17	126,127,127,127	0
84	OHX	AR	3501	7/7	0.97	0.31	113,113,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	6	1968	7/7	0.97	0.26	122,122,123,123	0
84	OHX	AR	3504	7/7	0.97	0.18	110,110,110,110	0
84	OHX	1	3438	7/7	0.97	0.25	117,117,117,117	0
84	OHX	1	3546	7/7	0.97	0.17	127,127,127,127	0
84	OHX	1	3645	7/7	0.97	0.34	125,126,126,126	0
84	OHX	AR	3513	7/7	0.97	0.09	150,151,151,151	0
84	OHX	1	3646	7/7	0.97	0.25	117,118,118,118	0
84	OHX	AR	3516	7/7	0.97	0.15	112,112,112,112	0
85	MG	1	4182	1/1	0.97	0.30	25,25,25,25	0
84	OHX	6	1974	7/7	0.97	0.15	121,121,122,122	0
84	OHX	AR	3683	7/7	0.97	0.36	126,127,127,127	0
85	MG	1	4185	1/1	0.97	0.50	27,27,27,27	0
84	OHX	AR	3519	7/7	0.97	0.15	108,109,109,109	0
84	OHX	AR	3520	7/7	0.97	0.31	112,112,113,113	0
84	OHX	1	3647	7/7	0.97	0.23	118,118,118,118	0
84	OHX	1	3492	7/7	0.97	0.19	117,118,118,118	0
84	OHX	1	3548	7/7	0.97	0.11	134,134,134,134	0
85	MG	1	4191	1/1	0.97	0.44	29,29,29,29	0
85	MG	1	4192	1/1	0.97	0.66	21,21,21,21	0
84	OHX	1	3549	7/7	0.97	0.15	120,120,120,120	0
84	OHX	1	3494	7/7	0.97	0.13	119,119,120,120	0
84	OHX	J	301	7/7	0.97	0.25	157,157,158,158	0
85	MG	CP	503	1/1	0.97	0.41	38,38,38,38	0
84	OHX	1	3551	7/7	0.97	0.27	118,118,119,119	0
84	OHX	M	201	7/7	0.97	0.38	137,137,138,138	0
84	OHX	1	3598	7/7	0.97	0.27	127,127,127,127	0
85	MG	1	4200	1/1	0.97	0.49	22,22,22,22	0
84	OHX	6	1983	7/7	0.97	0.18	128,129,129,129	0
84	OHX	1	3495	7/7	0.97	0.14	114,115,115,115	0
84	OHX	AR	3533	7/7	0.97	0.18	111,111,111,111	0
85	MG	1	4204	1/1	0.97	0.51	34,34,34,34	0
85	MG	1	4205	1/1	0.97	0.24	31,31,31,31	0
84	OHX	h	401	7/7	0.97	0.15	175,176,177,177	0
84	OHX	AR	3696	7/7	0.97	0.18	112,113,113,113	0
84	OHX	1	3600	7/7	0.97	0.15	150,150,150,150	0
85	MG	CX	203	1/1	0.97	0.39	19,19,19,19	0
84	OHX	AR	3535	7/7	0.97	0.13	114,115,115,115	0
84	OHX	1	3476	7/7	0.97	0.14	111,111,111,112	0
84	OHX	1	3602	7/7	0.97	0.23	128,128,128,129	0
84	OHX	c8	201	7/7	0.97	0.20	146,147,147,148	0
84	OHX	1	3658	7/7	0.97	0.34	142,143,143,143	0
84	OHX	AR	3539	7/7	0.97	0.14	127,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3540	7/7	0.97	0.16	108,108,108,108	0
85	MG	AR	3762	1/1	0.97	0.17	24,24,24,24	0
84	OHX	1	3603	7/7	0.97	0.17	123,123,124,124	0
84	OHX	AR	3542	7/7	0.97	0.11	152,152,152,153	0
85	MG	AR	4048	1/1	0.97	0.23	34,34,34,34	0
84	OHX	1	3480	7/7	0.97	0.14	119,119,119,120	0
84	OHX	1	3449	7/7	0.97	0.23	117,117,118,118	0
84	OHX	1	3558	7/7	0.97	0.17	134,134,135,135	0
85	MG	AR	4053	1/1	0.97	0.40	30,30,30,30	0
84	OHX	1	3607	7/7	0.97	0.17	122,122,122,122	0
84	OHX	AR	3547	7/7	0.97	0.28	116,116,116,117	0
84	OHX	1	3608	7/7	0.97	0.25	118,119,119,119	0
85	MG	1	3736	1/1	0.97	0.60	31,31,31,31	0
84	OHX	AR	3549	7/7	0.97	0.20	116,117,117,117	0
85	MG	AR	3775	1/1	0.97	0.23	22,22,22,22	0
84	OHX	1	3463	7/7	0.97	0.13	121,121,122,122	0
84	OHX	3	202	7/7	0.97	0.12	115,116,116,116	0
84	OHX	3	203	7/7	0.97	0.11	118,118,118,119	0
84	OHX	AR	3554	7/7	0.97	0.15	112,112,112,112	0
85	MG	3	218	1/1	0.97	0.22	54,54,54,54	0
84	OHX	3	204	7/7	0.97	0.15	124,125,125,125	0
84	OHX	1	3561	7/7	0.97	0.26	124,124,125,125	0
84	OHX	1	3562	7/7	0.97	0.14	121,121,121,121	0
84	OHX	AR	3558	7/7	0.97	0.16	137,137,137,137	0
85	MG	AR	3786	1/1	0.97	0.48	25,25,25,25	0
84	OHX	AR	3559	7/7	0.97	0.31	121,121,121,121	0
85	MG	A	2058	1/1	0.97	0.66	46,46,46,46	0
84	OHX	AR	3560	7/7	0.97	0.19	135,135,136,136	0
84	OHX	AR	3561	7/7	0.97	0.24	110,110,110,111	0
84	OHX	1	3528	7/7	0.97	0.12	119,120,120,120	0
84	OHX	6	2003	7/7	0.97	0.13	126,126,127,127	0
84	OHX	3	208	7/7	0.97	0.30	116,116,116,116	0
84	OHX	1	3613	7/7	0.97	0.47	120,120,121,121	0
84	OHX	AR	3566	7/7	0.97	0.24	115,115,115,116	0
84	OHX	4	203	7/7	0.97	0.16	106,107,107,107	0
84	OHX	4	204	7/7	0.97	0.15	108,108,108,108	0
85	MG	AR	3797	1/1	0.97	0.27	31,31,31,31	0
84	OHX	AR	3569	7/7	0.97	0.29	137,137,137,138	0
84	OHX	4	205	7/7	0.97	0.17	106,106,106,106	0
85	MG	1	3760	1/1	0.97	0.35	27,27,27,27	0
84	OHX	1	3564	7/7	0.97	0.24	126,126,127,127	0
84	OHX	AR	3574	7/7	0.97	0.17	112,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	4	208	7/7	0.97	0.36	106,106,106,106	0
84	OHX	AR	3576	7/7	0.97	0.32	128,128,129,129	0
85	MG	AR	3806	1/1	0.97	0.29	57,57,57,57	0
85	MG	A	2077	1/1	0.97	0.59	48,48,48,48	0
84	OHX	4	209	7/7	0.97	0.23	113,113,113,113	0
85	MG	A	2079	1/1	0.97	0.64	58,58,58,58	0
84	OHX	1	3529	7/7	0.97	0.17	115,115,115,116	0
84	OHX	1	3566	7/7	0.97	0.18	113,113,114,114	0
85	MG	AR	3810	1/1	0.97	0.51	27,27,27,27	0
84	OHX	4	212	7/7	0.97	0.28	128,128,128,128	0
84	OHX	1	3502	7/7	0.97	0.18	114,114,114,114	0
84	OHX	AR	3584	7/7	0.97	0.13	131,131,131,132	0
84	OHX	AR	3585	7/7	0.97	0.20	117,117,117,117	0
84	OHX	1	3568	7/7	0.97	0.28	115,116,116,116	0
84	OHX	AS	206	7/7	0.97	0.13	124,124,125,125	0
84	OHX	AS	208	7/7	0.97	0.10	138,139,139,139	0
84	OHX	1	3569	7/7	0.97	0.28	111,111,111,111	0
85	MG	1	3776	1/1	0.97	0.50	43,43,43,43	0
84	OHX	1	3571	7/7	0.97	0.18	111,111,112,112	0
84	OHX	1	3572	7/7	0.97	0.27	118,119,119,119	0
84	OHX	AT	203	7/7	0.97	0.14	117,117,117,117	0
85	MG	1	3780	1/1	0.97	0.33	17,17,17,17	0
84	OHX	AT	205	7/7	0.97	0.15	108,108,108,108	0
85	MG	1	4019	1/1	0.97	0.24	42,42,42,42	0
84	OHX	AT	206	7/7	0.97	0.11	123,124,124,124	0
85	MG	1	3784	1/1	0.97	0.45	26,26,26,26	0
84	OHX	AT	207	7/7	0.97	0.15	117,117,117,117	0
84	OHX	AT	208	7/7	0.97	0.32	114,114,114,114	0
85	MG	AR	4115	1/1	0.97	0.33	46,46,46,46	0
84	OHX	AT	209	7/7	0.97	0.11	121,121,122,122	0
84	OHX	AR	3591	7/7	0.97	0.25	112,112,112,112	0
85	MG	v	302	1/1	0.97	0.34	36,36,36,36	0
84	OHX	1	3678	7/7	0.97	0.15	117,117,118,118	0
85	MG	AR	3837	1/1	0.97	0.59	19,19,19,19	0
85	MG	A	2108	1/1	0.97	0.62	57,57,57,57	0
84	OHX	1	3573	7/7	0.97	0.18	131,131,132,132	0
84	OHX	AR	3594	7/7	0.97	0.20	114,114,115,115	0
84	OHX	v	301	7/7	0.97	0.20	113,113,114,114	0
84	OHX	1	3574	7/7	0.97	0.28	116,116,117,117	0
84	OHX	1	3534	7/7	0.97	0.19	113,113,113,113	0
84	OHX	1	3682	7/7	0.97	0.14	110,110,111,111	0
84	OHX	1	3625	7/7	0.97	0.22	135,135,135,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	6	1905	7/7	0.97	0.34	132,133,133,134	0
84	OHX	6	1907	7/7	0.97	0.32	135,136,136,137	0
84	OHX	6	1909	7/7	0.97	0.26	137,138,138,139	0
85	MG	AR	4132	1/1	0.97	0.15	49,49,49,49	0
85	MG	AR	3848	1/1	0.97	0.28	31,31,31,31	0
85	MG	AR	3849	1/1	0.97	0.45	35,35,35,35	0
85	MG	AR	3850	1/1	0.97	0.28	24,24,24,24	0
84	OHX	6	1911	7/7	0.97	0.24	134,135,135,135	0
85	MG	6	2053	1/1	0.97	0.57	41,41,41,41	0
84	OHX	1	3576	7/7	0.97	0.14	131,131,132,132	0
84	OHX	1	3536	7/7	0.97	0.22	109,109,109,109	0
84	OHX	6	1925	7/7	0.97	0.20	122,122,122,123	0
85	MG	6	2057	1/1	0.97	0.56	51,51,51,51	0
85	MG	6	2058	1/1	0.97	0.43	45,45,45,45	0
85	MG	1	4043	1/1	0.97	0.32	27,27,27,27	0
84	OHX	6	1927	7/7	0.97	0.22	124,124,125,125	0
85	MG	1	3806	1/1	0.97	0.46	51,51,51,51	0
84	OHX	1	3578	7/7	0.97	0.19	107,107,107,107	0
85	MG	6	2063	1/1	0.97	0.20	82,82,82,82	0
84	OHX	A	1910	7/7	0.97	0.23	138,139,139,140	0
84	OHX	A	1911	7/7	0.97	0.22	139,140,141,141	0
85	MG	AR	3869	1/1	0.97	0.40	31,31,31,31	0
84	OHX	A	1913	7/7	0.97	0.20	126,126,127,127	0
85	MG	1	4051	1/1	0.97	0.22	44,44,44,44	0
84	OHX	1	3503	7/7	0.97	0.10	127,128,128,129	0
84	OHX	A	1917	7/7	0.97	0.17	130,131,131,131	0
84	OHX	6	1933	7/7	0.97	0.13	116,116,117,117	0
85	MG	6	2071	1/1	0.97	0.49	45,45,45,45	0
85	MG	1	3815	1/1	0.97	0.14	40,40,40,40	0
84	OHX	A	1921	7/7	0.97	0.22	142,143,144,144	0
84	OHX	A	1926	7/7	0.97	0.08	127,127,127,128	0
84	OHX	A	1927	7/7	0.97	0.14	138,138,139,139	0
85	MG	1	4059	1/1	0.97	0.42	51,51,51,51	0
85	MG	AR	3885	1/1	0.97	0.37	33,33,33,33	0
84	OHX	A	1928	7/7	0.97	0.13	125,126,126,126	0
84	OHX	A	1930	7/7	0.97	0.10	122,122,123,123	0
85	MG	A	2154	1/1	0.97	0.93	45,45,45,45	0
85	MG	1	3822	1/1	0.97	0.49	18,18,18,18	0
84	OHX	A	1931	7/7	0.97	0.10	139,140,140,140	0
84	OHX	A	1932	7/7	0.97	0.18	141,142,142,143	0
84	OHX	6	1934	7/7	0.97	0.13	139,139,140,140	0
84	OHX	A	1934	7/7	0.97	0.12	132,132,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	6	1935	7/7	0.97	0.14	121,121,121,122	0
84	OHX	6	1936	7/7	0.97	0.15	116,116,117,117	0
84	OHX	A	1937	7/7	0.97	0.16	153,154,155,155	0
85	MG	1	4072	1/1	0.97	0.18	46,46,46,46	0
85	MG	AR	3898	1/1	0.97	0.63	28,28,28,28	0
84	OHX	A	1939	7/7	0.97	0.11	140,141,141,142	0
84	OHX	A	1940	7/7	0.97	0.28	137,138,138,139	0
85	MG	AR	4179	1/1	0.97	0.27	43,43,43,43	0
84	OHX	A	1941	7/7	0.97	0.12	136,137,137,137	0
85	MG	1	3835	1/1	0.97	0.47	30,30,30,30	0
85	MG	s8	302	1/1	0.97	0.33	51,51,51,51	0
85	MG	1	3836	1/1	0.97	0.39	36,36,36,36	0
84	OHX	A	1943	7/7	0.97	0.21	133,133,134,134	0
84	OHX	6	1938	7/7	0.97	0.13	130,131,131,131	0
85	MG	AR	3906	1/1	0.97	0.36	33,33,33,33	0
84	OHX	A	1945	7/7	0.97	0.18	143,144,144,145	0
85	MG	AR	3908	1/1	0.97	0.53	25,25,25,25	0
84	OHX	AR	3616	7/7	0.97	0.34	109,110,110,110	0
84	OHX	6	1939	7/7	0.97	0.10	131,132,132,133	0
84	OHX	A	1948	7/7	0.97	0.13	139,140,140,140	0
85	MG	d6	102	1/1	0.97	0.50	38,38,38,38	0
84	OHX	A	1951	7/7	0.97	0.24	145,145,146,146	0
84	OHX	1	3580	7/7	0.97	0.35	115,116,116,116	0
84	OHX	A	1954	7/7	0.97	0.17	135,136,136,136	0
84	OHX	1	3538	7/7	0.97	0.09	125,125,125,126	0
84	OHX	A	1956	7/7	0.97	0.14	133,133,134,134	0
84	OHX	AR	3620	7/7	0.97	0.33	143,144,144,144	0
84	OHX	6	1943	7/7	0.97	0.09	124,124,125,125	0
84	OHX	1	3633	7/7	0.97	0.30	134,134,135,135	0
84	OHX	1	3504	7/7	0.97	0.19	127,127,127,128	0
84	OHX	1	3635	7/7	0.97	0.28	122,122,123,123	0
88	ZN	d9	102	1/1	0.97	0.13	83,83,83,83	0
84	OHX	A	1965	7/7	0.97	0.16	134,135,135,136	0
84	OHX	1	3496	7/7	0.98	0.16	115,115,115,115	0
84	OHX	1	3454	7/7	0.98	0.18	111,111,111,111	0
84	OHX	AR	3481	7/7	0.98	0.20	106,106,107,107	0
84	OHX	AR	3482	7/7	0.98	0.19	111,112,112,112	0
84	OHX	1	3404	7/7	0.98	0.35	120,120,121,121	0
84	OHX	1	3555	7/7	0.98	0.17	111,111,112,112	0
84	OHX	AR	3485	7/7	0.98	0.15	114,114,115,115	0
84	OHX	AR	3486	7/7	0.98	0.19	111,111,111,111	0
84	OHX	A	1938	7/7	0.98	0.15	126,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3798	1/1	0.98	0.23	32,32,32,32	0
84	OHX	AR	3487	7/7	0.98	0.13	107,107,107,107	0
84	OHX	AR	3488	7/7	0.98	0.09	118,118,119,119	0
84	OHX	AR	3489	7/7	0.98	0.15	114,114,114,114	0
84	OHX	A	1942	7/7	0.98	0.19	133,133,134,134	0
84	OHX	AR	3490	7/7	0.98	0.12	112,112,112,113	0
85	MG	AR	3763	1/1	0.98	0.59	17,17,17,17	0
85	MG	AR	4260	1/1	0.98	0.52	6,6,6,6	0
84	OHX	6	1991	7/7	0.98	0.29	133,134,134,135	0
84	OHX	AR	3645	7/7	0.98	0.35	118,118,118,118	0
84	OHX	1	3499	7/7	0.98	0.23	111,111,111,111	0
84	OHX	1	3557	7/7	0.98	0.16	117,118,118,118	0
84	OHX	1	3456	7/7	0.98	0.16	111,111,111,111	0
84	OHX	A	1949	7/7	0.98	0.08	148,149,149,149	0
85	MG	1	3810	1/1	0.98	0.12	32,32,32,32	0
84	OHX	A	1950	7/7	0.98	0.13	127,128,128,128	0
84	OHX	1	3457	7/7	0.98	0.18	126,127,127,128	0
84	OHX	A	1952	7/7	0.98	0.20	128,129,129,129	0
85	MG	AS	222	1/1	0.98	0.21	44,44,44,44	0
85	MG	AR	3774	1/1	0.98	0.15	30,30,30,30	0
84	OHX	1	3560	7/7	0.98	0.12	111,112,112,112	0
84	OHX	AR	3497	7/7	0.98	0.09	124,125,125,126	0
84	OHX	AR	3498	7/7	0.98	0.15	123,123,123,124	0
85	MG	1	3817	1/1	0.98	0.26	23,23,23,23	0
84	OHX	1	3432	7/7	0.98	0.27	117,117,117,117	0
84	OHX	A	1957	7/7	0.98	0.23	133,134,134,134	0
85	MG	AR	3781	1/1	0.98	0.25	23,23,23,23	0
84	OHX	AR	3500	7/7	0.98	0.12	115,115,115,115	0
84	OHX	1	3459	7/7	0.98	0.19	108,108,108,108	0
85	MG	AT	219	1/1	0.98	0.35	36,36,36,36	0
85	MG	1	4034	1/1	0.98	0.25	42,42,42,42	0
84	OHX	AR	3502	7/7	0.98	0.17	113,114,114,114	0
84	OHX	A	1961	7/7	0.98	0.11	149,150,151,151	0
84	OHX	A	1962	7/7	0.98	0.21	132,133,133,134	0
84	OHX	1	3460	7/7	0.98	0.16	118,118,118,119	0
85	MG	1	3827	1/1	0.98	0.73	32,32,32,32	0
84	OHX	1	3505	7/7	0.98	0.18	116,116,117,117	0
84	OHX	AR	3505	7/7	0.98	0.20	114,114,115,115	0
84	OHX	1	3461	7/7	0.98	0.18	110,110,111,111	0
84	OHX	A	1967	7/7	0.98	0.12	119,119,120,120	0
85	MG	AT	230	1/1	0.98	0.42	39,39,39,39	0
84	OHX	AR	3507	7/7	0.98	0.08	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3508	7/7	0.98	0.21	109,109,109,109	0
84	OHX	AR	3510	7/7	0.98	0.13	117,118,118,118	0
85	MG	1	4047	1/1	0.98	0.12	57,57,57,57	0
84	OHX	1	3434	7/7	0.98	0.25	126,127,127,127	0
84	OHX	A	1972	7/7	0.98	0.22	148,148,148,148	0
84	OHX	1	3508	7/7	0.98	0.10	113,114,114,114	0
84	OHX	6	1910	7/7	0.98	0.26	119,120,120,120	0
84	OHX	1	3630	7/7	0.98	0.33	113,113,114,114	0
84	OHX	AR	3515	7/7	0.98	0.22	113,113,114,114	0
84	OHX	6	1913	7/7	0.98	0.26	133,134,135,135	0
84	OHX	6	1916	7/7	0.98	0.21	119,120,120,120	0
84	OHX	AR	3518	7/7	0.98	0.10	118,119,119,119	0
85	MG	AR	4054	1/1	0.98	0.14	55,55,55,55	0
85	MG	1	3844	1/1	0.98	0.41	28,28,28,28	0
84	OHX	AR	3672	7/7	0.98	0.29	109,110,110,110	0
84	OHX	6	1918	7/7	0.98	0.17	116,117,117,117	0
84	OHX	1	3407	7/7	0.98	0.31	106,106,107,107	0
84	OHX	6	1920	7/7	0.98	0.14	133,133,134,134	0
84	OHX	A	1984	7/7	0.98	0.10	130,130,131,131	0
85	MG	1	4063	1/1	0.98	0.09	38,38,38,38	0
84	OHX	1	3465	7/7	0.98	0.18	117,117,117,117	0
84	OHX	AR	3523	7/7	0.98	0.15	107,108,108,108	0
85	MG	z	202	1/1	0.98	0.28	59,59,59,59	0
85	MG	AR	3818	1/1	0.98	0.78	37,37,37,37	0
85	MG	AR	3819	1/1	0.98	0.36	37,37,37,37	0
84	OHX	6	1922	7/7	0.98	0.18	121,122,122,122	0
85	MG	1	4067	1/1	0.98	0.09	40,40,40,40	0
84	OHX	AR	3525	7/7	0.98	0.06	119,119,120,120	0
84	OHX	6	1923	7/7	0.98	0.17	121,121,122,122	0
84	OHX	6	1924	7/7	0.98	0.15	134,135,135,135	0
84	OHX	1	3570	7/7	0.98	0.09	144,144,145,145	0
84	OHX	AR	3529	7/7	0.98	0.12	108,109,109,109	0
84	OHX	6	1926	7/7	0.98	0.12	120,121,121,121	0
84	OHX	1	3697	7/7	0.98	0.25	119,119,120,120	0
84	OHX	6	1928	7/7	0.98	0.08	126,126,127,127	0
85	MG	AR	3830	1/1	0.98	0.46	42,42,42,42	0
84	OHX	1	3511	7/7	0.98	0.14	109,109,109,109	0
85	MG	1	4078	1/1	0.98	0.29	24,24,24,24	0
84	OHX	6	1930	7/7	0.98	0.21	121,121,122,122	0
85	MG	AR	4081	1/1	0.98	0.24	55,55,55,55	0
84	OHX	6	1931	7/7	0.98	0.10	115,116,116,116	0
84	OHX	1	3512	7/7	0.98	0.17	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3513	7/7	0.98	0.11	113,113,114,114	0
84	OHX	1	3410	7/7	0.98	0.32	112,112,112,112	0
84	OHX	1	3515	7/7	0.98	0.10	110,110,110,110	0
84	OHX	1	3516	7/7	0.98	0.12	116,117,117,117	0
84	OHX	6	1937	7/7	0.98	0.11	119,120,120,120	0
84	OHX	1	3467	7/7	0.98	0.17	123,123,124,124	0
84	OHX	1	3468	7/7	0.98	0.20	116,117,117,117	0
84	OHX	1	3439	7/7	0.98	0.19	109,109,109,109	0
84	OHX	1	3470	7/7	0.98	0.18	115,115,115,115	0
85	MG	1	3875	1/1	0.98	0.46	23,23,23,23	0
84	OHX	6	1942	7/7	0.98	0.16	135,135,136,136	0
84	OHX	A	2010	7/7	0.98	0.14	157,158,158,159	0
84	OHX	1	3521	7/7	0.98	0.14	116,117,117,117	0
84	OHX	6	1944	7/7	0.98	0.10	143,143,144,144	0
84	OHX	6	1945	7/7	0.98	0.17	126,127,127,128	0
84	OHX	AR	3550	7/7	0.98	0.14	107,107,107,107	0
84	OHX	1	3522	7/7	0.98	0.13	120,121,121,121	0
84	OHX	1	3523	7/7	0.98	0.19	119,119,120,120	0
85	MG	1	3885	1/1	0.98	0.49	20,20,20,20	0
84	OHX	6	1948	7/7	0.98	0.13	127,128,128,128	0
84	OHX	1	3524	7/7	0.98	0.21	116,117,117,117	0
85	MG	1	3888	1/1	0.98	0.40	29,29,29,29	0
85	MG	AR	4106	1/1	0.98	0.07	46,46,46,46	0
85	MG	AR	3858	1/1	0.98	0.32	36,36,36,36	0
85	MG	1	3889	1/1	0.98	0.54	23,23,23,23	0
85	MG	AR	3860	1/1	0.98	0.51	23,23,23,23	0
84	OHX	1	3440	7/7	0.98	0.22	110,110,111,111	0
85	MG	1	3891	1/1	0.98	0.60	17,17,17,17	0
85	MG	AR	3863	1/1	0.98	0.57	21,21,21,21	0
84	OHX	6	1951	7/7	0.98	0.14	134,134,135,135	0
85	MG	1	3893	1/1	0.98	0.26	26,26,26,26	0
84	OHX	1	3472	7/7	0.98	0.17	110,111,111,111	0
84	OHX	1	3587	7/7	0.98	0.23	133,133,133,134	0
84	OHX	1	3441	7/7	0.98	0.20	116,116,116,117	0
85	MG	AR	3870	1/1	0.98	0.70	33,33,33,33	0
84	OHX	1	3474	7/7	0.98	0.16	122,122,123,123	0
85	MG	6	2098	1/1	0.98	0.52	68,68,68,68	0
84	OHX	1	3590	7/7	0.98	0.12	137,138,138,138	0
84	OHX	1	3475	7/7	0.98	0.14	117,117,118,118	0
84	OHX	6	1958	7/7	0.98	0.15	126,127,127,127	0
85	MG	AR	3876	1/1	0.98	0.55	27,27,27,27	0
84	OHX	1	3530	7/7	0.98	0.13	138,138,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3415	7/7	0.98	0.32	123,124,124,124	0
85	MG	1	3904	1/1	0.98	0.53	25,25,25,25	0
84	OHX	1	3532	7/7	0.98	0.07	159,159,159,159	0
85	MG	1	4121	1/1	0.98	0.10	64,64,64,64	0
84	OHX	1	3533	7/7	0.98	0.13	149,149,150,150	0
85	MG	AR	4131	1/1	0.98	0.09	39,39,39,39	0
85	MG	AR	3884	1/1	0.98	0.45	22,22,22,22	0
84	OHX	AC	101	7/7	0.98	0.30	114,115,115,115	0
84	OHX	6	1963	7/7	0.98	0.16	125,125,126,126	0
84	OHX	1	3477	7/7	0.98	0.12	109,109,109,109	0
85	MG	1	3910	1/1	0.98	0.58	19,19,19,19	0
84	OHX	1	3535	7/7	0.98	0.17	111,111,111,112	0
84	OHX	AR	3572	7/7	0.98	0.28	118,119,119,119	0
84	OHX	AR	3573	7/7	0.98	0.21	123,123,123,123	0
84	OHX	3	201	7/7	0.98	0.19	121,121,121,122	0
84	OHX	1	3479	7/7	0.98	0.17	108,109,109,109	0
85	MG	1	4132	1/1	0.98	0.13	86,86,86,86	0
85	MG	1	4133	1/1	0.98	0.09	51,51,51,51	0
85	MG	6	2119	1/1	0.98	0.47	74,74,74,74	0
84	OHX	AR	3401	7/7	0.98	0.39	121,121,121,122	0
84	OHX	AR	3406	7/7	0.98	0.34	112,112,113,113	0
84	OHX	AR	3407	7/7	0.98	0.34	113,113,113,113	0
84	OHX	AR	3411	7/7	0.98	0.30	106,106,106,106	0
84	OHX	AR	3412	7/7	0.98	0.28	109,109,109,109	0
84	OHX	AR	3582	7/7	0.98	0.27	114,114,114,114	0
84	OHX	AR	3414	7/7	0.98	0.30	113,113,114,114	0
85	MG	1	4142	1/1	0.98	0.26	38,38,38,38	0
84	OHX	AR	3415	7/7	0.98	0.35	109,109,110,110	0
84	OHX	AR	3417	7/7	0.98	0.26	111,112,112,112	0
84	OHX	AR	3425	7/7	0.98	0.23	105,106,106,106	0
85	MG	6	2131	1/1	0.98	0.24	44,44,44,44	0
84	OHX	1	3443	7/7	0.98	0.19	119,120,120,120	0
84	OHX	AR	3430	7/7	0.98	0.14	107,107,107,107	0
84	OHX	AR	3589	7/7	0.98	0.13	109,110,110,110	0
85	MG	1	4149	1/1	0.98	0.18	54,54,54,54	0
84	OHX	1	3444	7/7	0.98	0.23	116,116,117,117	0
84	OHX	AR	3744	7/7	0.98	0.17	109,110,110,110	0
84	OHX	AR	3433	7/7	0.98	0.21	110,110,110,111	0
84	OHX	AS	201	7/7	0.98	0.24	119,119,119,120	0
84	OHX	AS	202	7/7	0.98	0.22	124,124,125,125	0
85	MG	1	3935	1/1	0.98	0.23	47,47,47,47	0
84	OHX	AS	203	7/7	0.98	0.16	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	sR	401	7/7	0.98	0.22	161,161,162,162	0
84	OHX	AS	204	7/7	0.98	0.15	113,113,113,113	0
84	OHX	AS	205	7/7	0.98	0.12	113,113,114,114	0
84	OHX	AR	3435	7/7	0.98	0.22	112,113,113,113	0
84	OHX	AS	207	7/7	0.98	0.16	122,122,122,123	0
84	OHX	AR	3436	7/7	0.98	0.24	109,109,109,109	0
84	OHX	AR	3437	7/7	0.98	0.23	108,108,108,108	0
84	OHX	AR	3439	7/7	0.98	0.25	119,120,120,120	0
84	OHX	6	1970	7/7	0.98	0.26	126,126,127,127	0
84	OHX	AT	202	7/7	0.98	0.30	106,106,106,106	0
84	OHX	1	3482	7/7	0.98	0.18	117,117,117,117	0
84	OHX	AT	204	7/7	0.98	0.11	105,105,105,106	0
84	OHX	AR	3443	7/7	0.98	0.14	116,116,117,117	0
84	OHX	AR	3444	7/7	0.98	0.15	112,112,112,112	0
84	OHX	1	3417	7/7	0.98	0.31	116,117,117,117	0
84	OHX	1	3484	7/7	0.98	0.10	125,126,126,126	0
84	OHX	AR	3448	7/7	0.98	0.17	115,115,115,115	0
84	OHX	AR	3450	7/7	0.98	0.16	127,127,127,128	0
84	OHX	AR	3451	7/7	0.98	0.20	114,114,114,114	0
84	OHX	AR	3452	7/7	0.98	0.18	121,121,122,122	0
85	MG	AR	4190	1/1	0.98	0.19	30,30,30,30	0
84	OHX	AR	3453	7/7	0.98	0.10	106,106,107,107	0
84	OHX	AR	3454	7/7	0.98	0.17	112,112,113,113	0
85	MG	1	4180	1/1	0.98	0.35	45,45,45,45	0
84	OHX	1	3420	7/7	0.98	0.29	118,118,118,118	0
84	OHX	1	3486	7/7	0.98	0.14	116,117,117,117	0
84	OHX	AR	3457	7/7	0.98	0.18	108,108,108,109	0
84	OHX	CE	401	7/7	0.98	0.17	114,114,115,115	0
85	MG	6	2170	1/1	0.98	0.17	64,64,64,64	0
84	OHX	4	201	7/7	0.98	0.35	108,108,108,108	0
84	OHX	1	3447	7/7	0.98	0.20	113,113,113,113	0
84	OHX	1	3448	7/7	0.98	0.21	117,117,117,117	0
84	OHX	AR	3461	7/7	0.98	0.14	110,111,111,111	0
84	OHX	1	3403	7/7	0.98	0.30	113,113,113,114	0
84	OHX	AR	3464	7/7	0.98	0.17	106,106,106,106	0
84	OHX	AR	3465	7/7	0.98	0.17	118,118,118,118	0
85	MG	AR	4208	1/1	0.98	0.21	57,57,57,57	0
84	OHX	1	3491	7/7	0.98	0.18	120,120,121,121	0
84	OHX	CP	501	7/7	0.98	0.20	126,126,126,127	0
85	MG	6	2182	1/1	0.98	0.14	83,83,83,83	0
84	OHX	CX	201	7/7	0.98	0.17	116,116,116,116	0
85	MG	6	2184	1/1	0.98	0.22	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	6	1981	7/7	0.98	0.29	139,140,140,140	0
85	MG	1	4196	1/1	0.98	0.42	30,30,30,30	0
84	OHX	DD	101	7/7	0.98	0.29	113,114,114,114	0
84	OHX	DH	201	7/7	0.98	0.13	113,113,113,113	0
84	OHX	DQ	201	7/7	0.98	0.15	111,111,111,111	0
84	OHX	A	1901	7/7	0.98	0.29	127,127,127,128	0
84	OHX	A	1903	7/7	0.98	0.35	149,149,150,150	0
84	OHX	A	1908	7/7	0.98	0.24	141,142,143,143	0
84	OHX	AR	3468	7/7	0.98	0.16	124,124,125,125	0
84	OHX	4	207	7/7	0.98	0.12	118,119,119,119	0
84	OHX	AR	3470	7/7	0.98	0.17	115,116,116,116	0
84	OHX	A	1912	7/7	0.98	0.19	137,137,138,138	0
84	OHX	AR	3471	7/7	0.98	0.13	109,109,109,109	0
84	OHX	A	1914	7/7	0.98	0.23	126,127,127,127	0
84	OHX	1	3430	7/7	0.98	0.19	110,110,110,110	0
84	OHX	A	1916	7/7	0.98	0.18	136,137,137,138	0
84	OHX	1	3493	7/7	0.98	0.17	115,116,116,116	0
84	OHX	1	3452	7/7	0.98	0.16	109,109,109,109	0
84	OHX	A	1919	7/7	0.98	0.17	121,122,122,122	0
85	MG	1	3991	1/1	0.98	0.17	66,66,66,66	0
85	MG	1	4215	1/1	0.98	0.62	27,27,27,27	0
84	OHX	AR	3475	7/7	0.98	0.14	116,116,116,116	0
84	OHX	A	1922	7/7	0.98	0.11	123,124,124,124	0
85	MG	1	3783	1/1	0.98	0.46	18,18,18,18	0
84	OHX	A	1923	7/7	0.98	0.13	124,125,125,125	0
84	OHX	AR	3476	7/7	0.98	0.17	109,109,109,109	0
84	OHX	AR	3477	7/7	0.98	0.20	112,112,113,113	0
84	OHX	1	3453	7/7	0.98	0.14	120,120,120,120	0
84	OHX	A	1929	7/7	0.98	0.14	123,123,124,124	0
84	OHX	1	3408	7/7	0.99	0.32	112,112,112,113	0
85	MG	AR	4172	1/1	0.99	0.12	65,65,65,65	0
84	OHX	1	3450	7/7	0.99	0.17	121,122,122,123	0
84	OHX	AR	3402	7/7	0.99	0.39	113,113,113,113	0
85	MG	AR	3866	1/1	0.99	0.23	34,34,34,34	0
84	OHX	AR	3403	7/7	0.99	0.28	110,110,110,110	0
84	OHX	AR	3404	7/7	0.99	0.33	112,112,112,112	0
84	OHX	AR	3405	7/7	0.99	0.34	119,119,120,120	0
84	OHX	2	201	7/7	0.99	0.31	119,119,120,120	0
84	OHX	6	1901	7/7	0.99	0.34	119,120,120,120	0
84	OHX	AR	3609	7/7	0.99	0.16	107,107,107,107	0
84	OHX	AR	3408	7/7	0.99	0.33	107,107,107,107	0
84	OHX	AR	3409	7/7	0.99	0.34	120,120,120,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AR	3410	7/7	0.99	0.31	109,109,109,110	0
84	OHX	6	1902	7/7	0.99	0.34	136,136,137,137	0
84	OHX	6	1903	7/7	0.99	0.29	117,118,118,118	0
85	MG	AR	3878	1/1	0.99	0.36	31,31,31,31	0
84	OHX	AR	3413	7/7	0.99	0.26	107,107,107,107	0
84	OHX	6	1904	7/7	0.99	0.27	124,124,124,125	0
84	OHX	1	3426	7/7	0.99	0.28	120,120,120,120	0
85	MG	AR	4191	1/1	0.99	0.17	58,58,58,58	0
85	MG	AR	3983	1/1	0.99	0.12	33,33,33,33	0
84	OHX	AR	3416	7/7	0.99	0.29	114,114,115,115	0
84	OHX	AT	201	7/7	0.99	0.33	109,109,110,110	0
85	MG	AR	4195	1/1	0.99	0.18	63,63,63,63	0
85	MG	1	4031	1/1	0.99	0.55	21,21,21,21	0
84	OHX	6	1906	7/7	0.99	0.29	122,123,123,124	0
85	MG	1	3858	1/1	0.99	0.37	25,25,25,25	0
85	MG	AR	3887	1/1	0.99	0.46	21,21,21,21	0
84	OHX	AR	3418	7/7	0.99	0.30	116,116,117,117	0
84	OHX	AR	3419	7/7	0.99	0.27	122,122,123,123	0
84	OHX	AR	3420	7/7	0.99	0.29	113,114,114,114	0
84	OHX	AR	3421	7/7	0.99	0.25	113,113,113,113	0
84	OHX	AR	3422	7/7	0.99	0.28	112,112,112,112	0
84	OHX	AR	3423	7/7	0.99	0.28	110,111,111,111	0
84	OHX	AR	3424	7/7	0.99	0.27	112,112,113,113	0
84	OHX	1	3478	7/7	0.99	0.14	125,125,125,126	0
84	OHX	AR	3426	7/7	0.99	0.27	111,112,112,112	0
85	MG	AR	3799	1/1	0.99	0.36	22,22,22,22	0
84	OHX	6	1908	7/7	0.99	0.25	120,120,121,121	0
85	MG	1	4134	1/1	0.99	0.20	63,63,63,63	0
84	OHX	AR	3428	7/7	0.99	0.21	115,115,115,116	0
84	OHX	AR	3429	7/7	0.99	0.19	112,112,112,112	0
85	MG	6	2175	1/1	0.99	0.10	118,118,118,118	0
84	OHX	1	3427	7/7	0.99	0.26	112,113,113,113	0
84	OHX	AR	3431	7/7	0.99	0.24	109,109,110,110	0
84	OHX	1	3428	7/7	0.99	0.28	126,126,127,127	0
84	OHX	1	3429	7/7	0.99	0.22	110,110,110,110	0
84	OHX	AR	3434	7/7	0.99	0.22	111,111,111,111	0
85	MG	6	2181	1/1	0.99	0.11	95,95,95,95	0
85	MG	AR	3909	1/1	0.99	0.57	25,25,25,25	0
85	MG	AR	3910	1/1	0.99	0.32	23,23,23,23	0
84	OHX	6	1912	7/7	0.99	0.18	122,122,123,123	0
84	OHX	1	3409	7/7	0.99	0.30	116,116,117,117	0
84	OHX	6	1914	7/7	0.99	0.20	133,133,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3438	7/7	0.99	0.22	108,108,108,108	0
84	OHX	6	1915	7/7	0.99	0.17	119,119,120,120	0
85	MG	A	2141	1/1	0.99	0.31	101,101,101,101	0
84	OHX	AR	3440	7/7	0.99	0.18	125,125,125,126	0
85	MG	1	3882	1/1	0.99	0.45	32,32,32,32	0
84	OHX	4	202	7/7	0.99	0.33	112,112,112,113	0
85	MG	A	2145	1/1	0.99	0.21	92,92,92,92	0
84	OHX	6	1917	7/7	0.99	0.16	131,131,132,132	0
84	OHX	CV	201	7/7	0.99	0.31	117,117,117,117	0
84	OHX	AR	3509	7/7	0.99	0.10	106,106,106,106	0
84	OHX	1	3402	7/7	0.99	0.35	114,115,115,115	0
84	OHX	AR	3578	7/7	0.99	0.14	109,109,110,110	0
84	OHX	1	3411	7/7	0.99	0.29	111,112,112,112	0
84	OHX	1	3433	7/7	0.99	0.26	118,119,119,119	0
84	OHX	AR	3446	7/7	0.99	0.17	112,113,113,113	0
85	MG	1	3725	1/1	0.99	0.38	34,34,34,34	0
84	OHX	A	1902	7/7	0.99	0.26	122,122,123,123	0
85	MG	AR	4241	1/1	0.99	0.39	17,17,17,17	0
84	OHX	1	3412	7/7	0.99	0.30	114,114,115,115	0
84	OHX	A	1904	7/7	0.99	0.23	133,134,134,134	0
84	OHX	A	1905	7/7	0.99	0.29	128,129,129,129	0
84	OHX	A	1906	7/7	0.99	0.23	142,143,143,143	0
85	MG	1	4164	1/1	0.99	0.22	58,58,58,58	0
84	OHX	A	1907	7/7	0.99	0.19	133,134,134,134	0
84	OHX	1	3413	7/7	0.99	0.32	112,113,113,113	0
84	OHX	AR	3449	7/7	0.99	0.14	116,117,117,117	0
85	MG	1	4076	1/1	0.99	0.24	64,64,64,64	0
84	OHX	1	3436	7/7	0.99	0.28	115,115,115,115	0
84	OHX	1	3437	7/7	0.99	0.24	116,117,117,117	0
85	MG	AR	3940	1/1	0.99	0.49	21,21,21,21	0
85	MG	1	3903	1/1	0.99	0.67	21,21,21,21	0
84	OHX	1	3490	7/7	0.99	0.17	113,113,113,113	0
84	OHX	1	3414	7/7	0.99	0.27	109,109,109,109	0
84	OHX	1	3464	7/7	0.99	0.20	109,109,109,109	0
84	OHX	1	3405	7/7	0.99	0.37	124,125,125,125	0
84	OHX	1	3416	7/7	0.99	0.24	109,109,109,109	0
84	OHX	1	3406	7/7	0.99	0.33	108,108,108,108	0
84	OHX	1	3418	7/7	0.99	0.27	114,115,115,115	0
85	MG	1	3911	1/1	0.99	0.65	21,21,21,21	0
85	MG	AR	4052	1/1	0.99	0.12	86,86,86,86	0
85	MG	1	3825	1/1	0.99	0.41	31,31,31,31	0
84	OHX	1	3419	7/7	0.99	0.26	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	A	1920	7/7	0.99	0.14	128,128,129,129	0
85	MG	1	3745	1/1	0.99	0.67	31,31,31,31	0
84	OHX	1	3401	7/7	0.99	0.38	114,114,115,115	0
84	OHX	1	3421	7/7	0.99	0.29	115,115,116,116	0
85	MG	1	3748	1/1	0.99	0.34	44,44,44,44	0
84	OHX	AR	3462	7/7	0.99	0.16	116,116,116,116	0
84	OHX	A	1924	7/7	0.99	0.09	132,132,133,133	0
88	ZN	AP	501	1/1	0.99	0.04	61,61,61,61	0
88	ZN	DL	101	1/1	0.99	0.20	41,41,41,41	0
88	ZN	DO	201	1/1	0.99	0.15	32,32,32,32	0
88	ZN	DQ	202	1/1	0.99	0.03	63,63,63,63	0
88	ZN	DR	501	1/1	0.99	0.15	59,59,59,59	0
88	ZN	b	102	1/1	0.99	0.16	71,71,71,71	0
85	MG	1	4097	1/1	0.99	0.22	70,70,70,70	0
88	ZN	e	102	1/1	0.99	0.08	79,79,79,79	0
84	OHX	A	1925	7/7	0.99	0.12	136,137,137,137	0
84	OHX	1	3422	7/7	0.99	0.26	116,116,117,117	0
84	OHX	1	3423	7/7	0.99	0.26	120,120,121,121	0
84	OHX	1	3424	7/7	0.99	0.23	115,115,115,115	0
88	ZN	AQ	501	1/1	1.00	0.13	56,56,56,56	0
88	ZN	d6	103	1/1	1.00	0.13	53,53,53,53	0
88	ZN	AK	101	1/1	1.00	0.15	34,34,34,34	0
88	ZN	AN	500	1/1	1.00	0.13	38,38,38,38	0
85	MG	AR	4168	1/1	1.00	0.19	65,65,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.