



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 1, 2020 – 11:59 AM BST

PDB ID : 5DC3  
Title : Complex of yeast 80S ribosome with non-modified eIF5A  
Authors : Melnikov, S.; Mailliot, J.; Shin, B.-S.; Rigger, L.; Yusupova, G.; Micura, R.;  
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Deposited on : 2015-08-23  
Resolution : 3.25 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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.14.1
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)	:	2.14.1

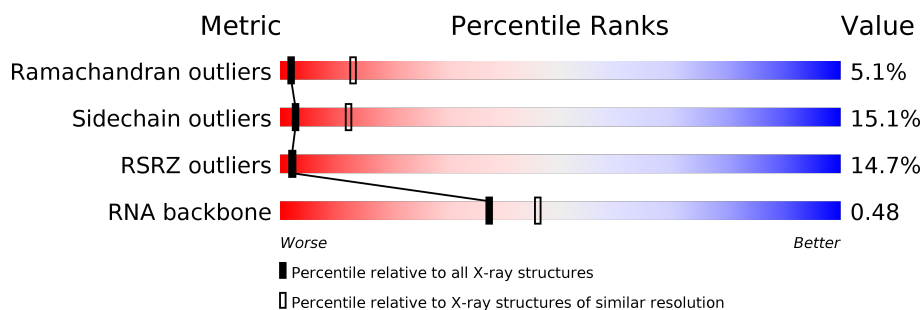
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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))
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)
RNA backbone	3102	1072 (3.62-2.90)

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 on 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	2	1800	<div> <div>12%</div> <div>72%</div> <div>25%</div> <div>..</div> </div>
1	6	1800	<div> <div>5%</div> <div>74%</div> <div>24%</div> <div>.</div> </div>
2	S0	251	<div> <div>48%</div> <div>65%</div> <div>18%</div> <div>18%</div> </div>
2	s0	251	<div> <div>31%</div> <div>68%</div> <div>14%</div> <div>18%</div> </div>
3	S1	254	<div> <div>13%</div> <div>64%</div> <div>20%</div> <div>16%</div> </div>
3	s1	254	<div> <div>12%</div> <div>67%</div> <div>17%</div> <div>15%</div> </div>
4	S2	253	<div> <div>25%</div> <div>72%</div> <div>13%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
4	s2	253	
5	S3	239	
5	s3	239	
6	S4	260	
6	s4	260	
7	S5	224	
7	s5	224	
8	S6	236	
8	s6	236	
9	S7	189	
9	s7	189	
10	S8	200	
10	s8	200	
11	S9	196	
11	s9	196	
12	C0	105	
13	C1	155	
13	c1	155	
14	C2	142	
14	c2	142	
15	C3	150	
15	c3	150	
16	C4	136	
16	c4	136	
17	C5	141	

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Mol	Chain	Length	Quality of chain
17	c5	141	
18	C6	142	
18	c6	142	
19	C7	136	
19	c7	136	
20	C8	145	
20	c8	145	
21	C9	143	
21	c9	143	
22	D0	120	
22	d0	120	
23	D1	87	
23	d1	87	
24	D2	129	
24	d2	129	
25	D3	144	
25	d3	144	
26	D4	134	
26	d4	134	
27	D5	107	
27	d5	107	
28	D6	97	
28	d6	97	
29	D7	81	
29	d7	81	

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Mol	Chain	Length	Quality of chain
30	D8	66	
30	d8	66	
31	D9	55	
31	d9	55	
32	E0	62	
32	e0	62	
33	E1	76	
33	e1	76	
34	SR	318	
34	sR	318	
35	SM	273	
35	sM	273	
36	1	3396	
36	5	3396	
37	3	121	
37	7	121	
38	4	158	
38	8	158	
39	L2	253	
39	l2	253	
40	L3	386	
40	l3	386	
41	L4	361	
41	l4	361	
42	L5	296	

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Mol	Chain	Length	Quality of chain
42	l5	296	
43	L6	175	
43	l6	175	
44	L7	243	
44	l7	243	
45	L8	255	
45	l8	255	
46	L9	191	
46	l9	191	
47	M0	220	
47	m0	220	
48	M1	173	
48	m1	173	
49	M3	198	
49	m3	198	
50	M4	137	
50	m4	137	
51	M5	203	
51	m5	203	
52	M6	198	
52	m6	198	
53	M7	183	
53	m7	183	
54	M8	185	
54	m8	185	

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Mol	Chain	Length	Quality of chain
55	M9	188	
55	m9	188	
56	N0	172	
56	n0	172	
57	N1	159	
57	n1	159	
58	N2	120	
58	n2	120	
59	N3	136	
59	n3	136	
60	N4	155	
60	n4	155	
61	N5	141	
61	n5	141	
62	N6	126	
62	n6	126	
63	N7	135	
63	n7	135	
64	N8	148	
64	n8	148	
65	N9	58	
65	n9	58	
66	O0	104	
66	o0	104	
67	O1	112	

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Mol	Chain	Length	Quality of chain
67	o1	112	
68	O2	129	
68	o2	129	
69	O3	106	
69	o3	106	
70	O4	119	
70	o4	119	
71	O5	119	
71	o5	119	
72	O6	99	
72	o6	99	
73	O7	87	
73	o7	87	
74	O8	77	
74	o8	77	
75	O9	50	
75	o9	50	
76	Q0	52	
76	q0	52	
77	Q1	25	
77	q1	25	
78	Q2	105	
78	q2	105	
79	Q3	91	
79	q3	91	

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Mol	Chain	Length	Quality of chain
80	c0	105	<div><div></div><div>59%</div><div>71%</div><div>17%</div><div>9%</div></div>
81	m2	150	<div><div></div><div>100%</div></div>
82	p0	311	<div><div></div><div>6%</div><div>40%</div><div>5%</div><div>54%</div></div>
83	p1	47	<div><div></div><div>100%</div></div>
84	p2	46	<div><div></div><div>100%</div></div>
85	f	157	<div><div></div><div>61%</div><div>74%</div><div>18%</div><div>6%</div></div>

## 2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 404042 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2	1781	Total	C	N	O	P	0	1	0
			37970	16975	6720	12493	1782			
1	6	1795	Total	C	N	O	P	0	1	0
			38260	17105	6763	12596	1796			

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S0	206	Total	C	N	O	S	0	0	0
			1577	1014	278	283	2			
2	s0	206	Total	C	N	O	S	0	0	0
			1583	1017	281	283	2			

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S1	214	Total	C	N	O	S	0	0	0
			1709	1084	310	311	4			
3	s1	216	Total	C	N	O	S	0	0	0
			1722	1091	312	315	4			

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	S2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			
4	s2	217	Total	C	N	O	S	0	0	0
			1635	1047	289	297	2			

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	S3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			
5	s3	223	Total	C	N	O	S	0	0	0
			1734	1101	313	314	6			

- Molecule 6 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	S4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			
6	s4	260	Total	C	N	O	S	0	0	0
			2068	1316	389	360	3			

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	S5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
7	s5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

- Molecule 8 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	S6	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
8	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 9 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	S7	184	Total	C	N	O	0	0	0
			1481	951	265	265			
9	s7	186	Total	C	N	O	0	0	0
			1491	957	267	267			

- Molecule 10 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	S8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

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

- Molecule 11 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	S9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
11	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 12 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	C0	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			

- Molecule 13 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	C1	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
13	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	C2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			
14	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- Molecule 15 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	C3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
15	c3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

- Molecule 16 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	C4	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
16	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 17 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	C5	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			
17	c5	135	Total	C	N	O	S	0	0	0
			1039	658	196	178	7			

- Molecule 18 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	C6	141	Total	C	N	O		0	0	0
			1105	708	203	194				
18	c6	142	Total	C	N	O		0	0	0
			1111	711	204	196				

- Molecule 19 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	C7	120	Total	C	N	O	S	0	0	0
			926	577	177	170	2			
19	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 20 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	C8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			
20	c8	145	Total	C	N	O	S	0	0	0
			1192	743	237	210	2			

- Molecule 21 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	C9	143	Total	C	N	O	S	0	0	0
			1112	694	208	208	2			

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

- Molecule 22 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	D0	107	Total	C	N	O	S	0	0	0
			855	539	156	159	1			
22	d0	110	Total	C	N	O	S	0	0	0
			882	554	161	166	1			

- Molecule 23 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	D1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
23	d1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

- Molecule 24 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	D2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
24	d2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

- Molecule 25 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	D3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
25	d3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

- Molecule 26 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	D4	134	Total	C	N	O	0	0	0
			1073	676	208	189			
26	d4	134	Total	C	N	O	0	0	0
			1073	676	208	189			

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	D5	70	Total	C	N	O	0	0	0
			563	360	104	99			
27	d5	69	Total	C	N	O	0	0	0
			558	357	103	98			

- Molecule 28 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	D6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			
28	d6	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

- Molecule 29 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	D7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			
29	d7	81	Total	C	N	O	S	0	0	0
			610	382	110	113	5			

- Molecule 30 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	D8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			
30	d8	63	Total	C	N	O	S	0	0	0
			497	306	99	91	1			

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			
31	d9	53	Total	C	N	O	S	0	0	0
			442	274	92	72	4			

- Molecule 32 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	E0	60	Total	C	N	O	S	0	0	0
			475	299	98	77	1			
32	e0	62	Total	C	N	O	S	0	0	0
			491	309	101	80	1			

- Molecule 33 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	E1	71	Total	C	N	O	S	0	0	0
			566	362	106	94	4			
33	e1	76	Total	C	N	O	S	0	0	0
			608	388	117	99	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E1	77	ALA	GLY	conflict	UNP P05759
e1	77	ALA	GLY	conflict	UNP P05759

- Molecule 34 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	SR	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			
34	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

- Molecule 35 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	SM	159	Total	C	N	O		0	0	0
			1104	652	221	231				
35	sM	104	Total	C	N	O		0	0	0
			679	402	140	137				

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1	3149	Total	C	N	O	P	0	0	0
			67355	30086	12142	21978	3149			
36	5	3169	Total	C	N	O	P	0	0	0
			67780	30276	12216	22120	3168			



- Molecule 37 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	3	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			
37	7	121	Total	C	N	O	P	0	0	0
			2579	1152	461	845	121			

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	4	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			
38	8	158	Total	C	N	O	P	0	0	0
			3353	1500	586	1109	158			

- Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	L2	252	Total	C	N	O	S	0	0	0
			1914	1191	388	334	1			
39	l2	252	Total	C	N	O	S	0	0	0
			1912	1190	388	333	1			

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	L3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
40	l3	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	L4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
41	l4	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	L5	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
42	l5	294	Total	C	N	O	S	0	0	0
			2359	1489	412	456	2			

- Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	L6	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
43	l6	157	Total	C	N	O	S	0	0	0
			1248	806	224	217	1			

- Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	L7	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
44	l7	223	Total	C	N	O	S	0	0	0
			1791	1155	325	310	1			

- Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	L8	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			
45	l8	231	Total	C	N	O	S	0	0	0
			1763	1130	316	314	3			

- Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	L9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			
46	l9	191	Total	C	N	O	S	0	0	0
			1518	963	274	277	4			

- Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	M0	211	Total	C	N	O	S	0	0	0
			1705	1083	322	294	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	m0	213	Total	C	N	O	S	0	0	0
			1722	1094	325	297	6			

- Molecule 48 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	M1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			
48	m1	169	Total	C	N	O	S	0	0	0
			1353	847	253	249	4			

- Molecule 49 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	M3	193	Total	C	N	O	S	0	0	0
			1543	962	315	266				
49	m3	194	Total	C	N	O	S	0	0	0
			1548	965	316	267				

- Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	M4	136	Total	C	N	O	S	0	0	0
			1053	675	199	177	2			
50	m4	137	Total	C	N	O	S	0	0	0
			1059	678	200	179	2			

- Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	M5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
51	m5	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
52	m6	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	M7	183	Total	C	N	O	0	0	0
			1420	882	281	257			
53	m7	155	Total	C	N	O	0	0	0
			1227	764	238	225			

- Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	M8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
54	m8	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	M9	188	Total	C	N	O	0	0	0
			1521	935	326	260			
55	m9	188	Total	C	N	O	0	0	0
			1521	935	326	260			

- Molecule 56 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	N0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
56	n0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	N1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
57	n1	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
58	N2	100	Total	C	N	O	0	0	0
			796	516	131	149			
58	n2	98	Total	C	N	O	0	0	0
			778	505	127	146			

- Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	N3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
59	n3	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	N4	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			
60	n4	135	Total	C	N	O	S	0	0	0
			1038	651	206	180	1			

- Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N5	121	Total	C	N	O	S	0	0	0
			964	620	169	173	2			
61	n5	120	Total	C	N	O	S	0	0	0
			959	617	168	172	2			

- Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
62	N6	126	Total	C	N	O	0	0	0
			993	625	192	176			
62	n6	126	Total	C	N	O	0	0	0
			993	625	192	176			

- Molecule 63 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
63	N7	135	Total	C	N	O	0	0	0
			1092	710	202	180			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
63	n7	135	Total	C	N	O	0	0	0
			1092	710	202	180			

- Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	N8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			
64	n8	148	Total	C	N	O	S	0	0	0
			1173	749	231	190	3			

- Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
65	N9	58	Total	C	N	O	0	0	0
			462	289	100	73			
65	n9	58	Total	C	N	O	0	0	0
			462	289	100	73			

- Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
66	O0	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
66	o0	100	Total	C	N	O	S	0	0	0
			767	492	128	146	1			

- Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
67	O1	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
67	o1	109	Total	C	N	O	S	0	0	0
			883	559	167	156	1			

- Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
68	O2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
68	o2	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	O3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
69	o3	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	O4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
70	o4	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O4	?	-	LYS	deletion	UNP P87262
o4	?	-	LYS	deletion	UNP P87262

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	O5	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
71	o5	119	Total	C	N	O	S	0	0	0
			965	612	185	167	1			

- Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	O6	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
72	o6	99	Total	C	N	O	S	0	0	0
			770	481	156	131	2			

- Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	O7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	o7	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	O8	77	Total	C	N	O		0	0	0
			612	391	115	106				
74	o8	77	Total	C	N	O		0	0	0
			608	388	114	106				

- Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	O9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
75	o9	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
76	Q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			
76	q0	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 77 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	Q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
77	q1	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	Q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
78	q2	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			



- Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	Q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
79	q3	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

- Molecule 80 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	c0	96	Total	C	N	O	S	0	0	0
			762	491	125	144	2			

- Molecule 81 is a protein called 60S ribosomal protein L12-A (uL11).

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

- Molecule 82 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 83 is a protein called 60S ribosomal protein P1 alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	p1	47	Total	C	N	O	S	0	0	0
			235	141	47	47				

- Molecule 84 is a protein called 60S ribosomal P2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
84	p2	46	Total	C	N	O	S	0	0	0
			230	138	46	46				

- Molecule 85 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
85	f	148	Total	C	N	O	S	0	0	0
			1116	692	188	227	9			

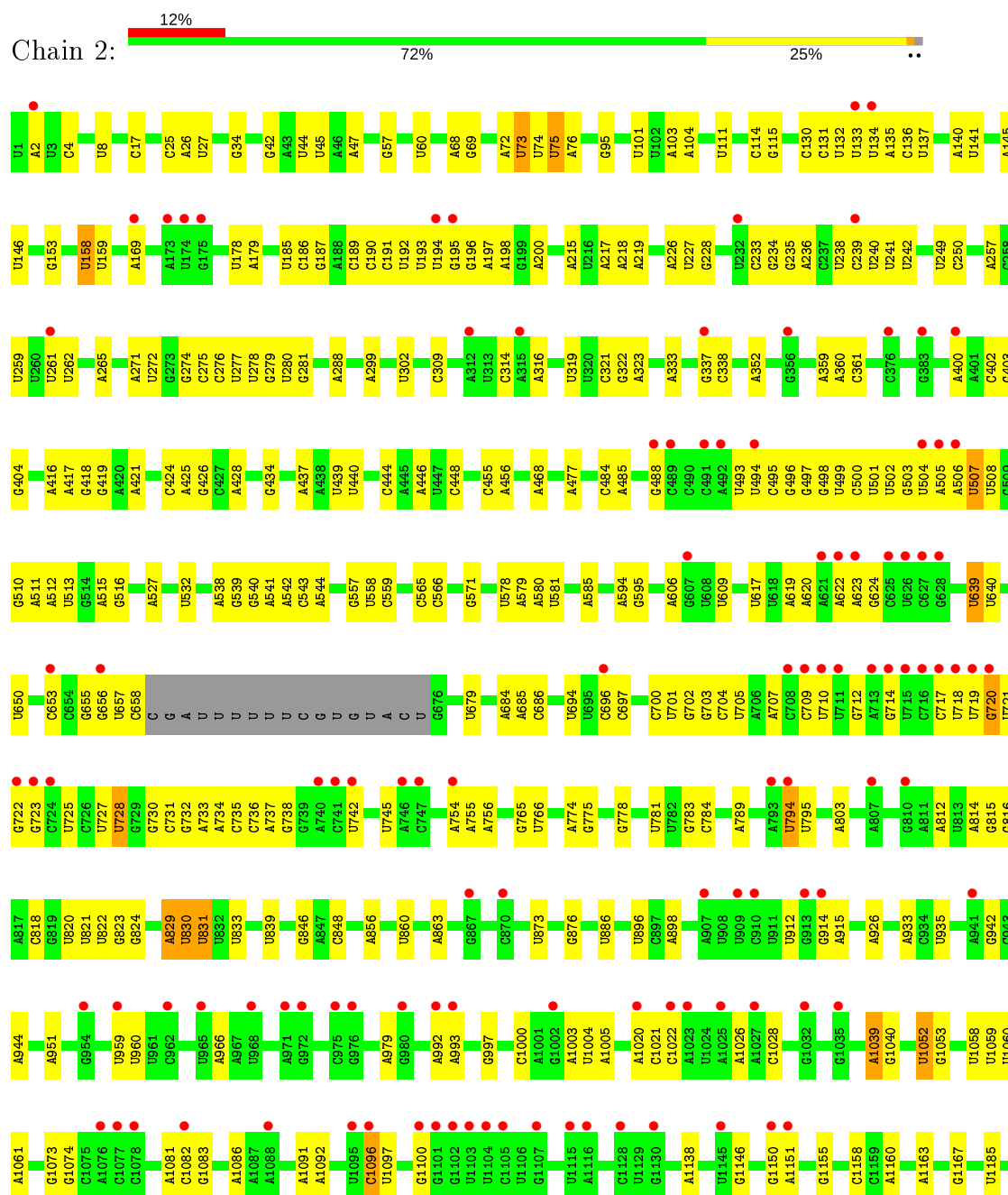
- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

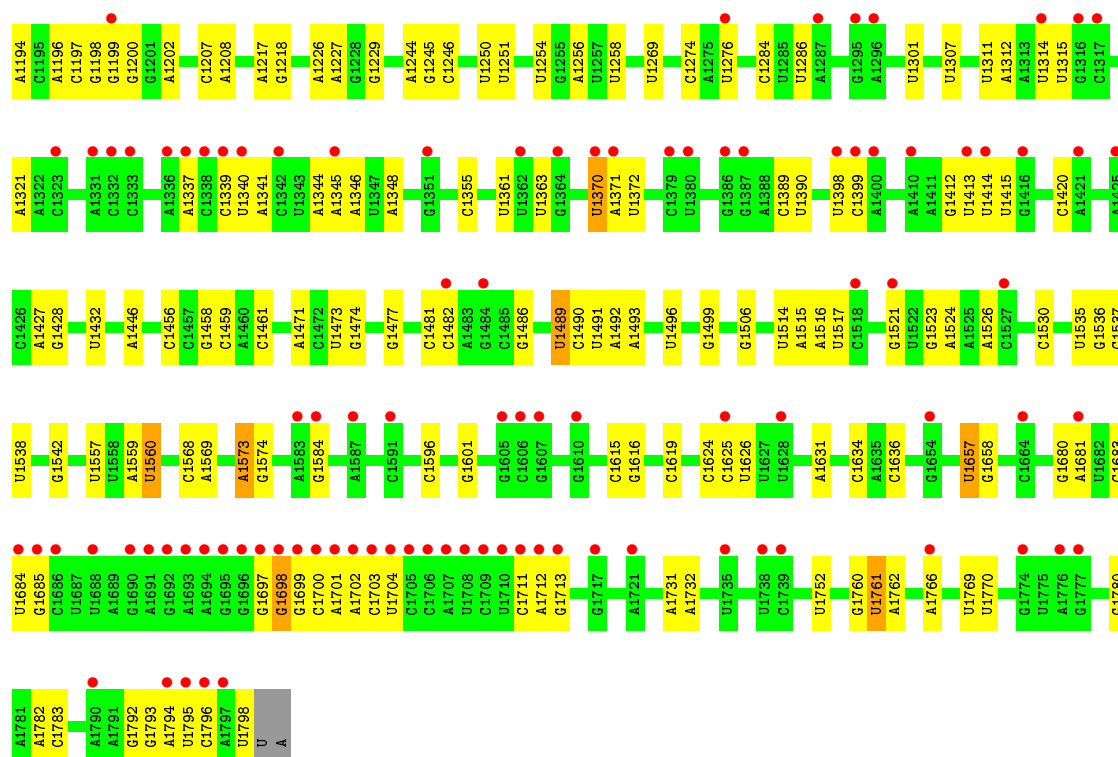
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86	q0	1	Total 1	Zn 1	0	0
86	D6	1	Total 1	Zn 1	0	0
86	Q2	1	Total 1	Zn 1	0	0
86	e1	1	Total 1	Zn 1	0	0
86	Q3	1	Total 1	Zn 1	0	0
86	D9	1	Total 1	Zn 1	0	0
86	E1	1	Total 1	Zn 1	0	0
86	Q0	1	Total 1	Zn 1	0	0
86	d7	1	Total 1	Zn 1	0	0
86	q3	1	Total 1	Zn 1	0	0
86	d9	1	Total 1	Zn 1	0	0
86	D7	1	Total 1	Zn 1	0	0
86	d6	1	Total 1	Zn 1	0	0
86	o7	1	Total 1	Zn 1	0	0
86	O7	1	Total 1	Zn 1	0	0
86	q2	1	Total 1	Zn 1	0	0

### 3 Residue-property plots [i](#)

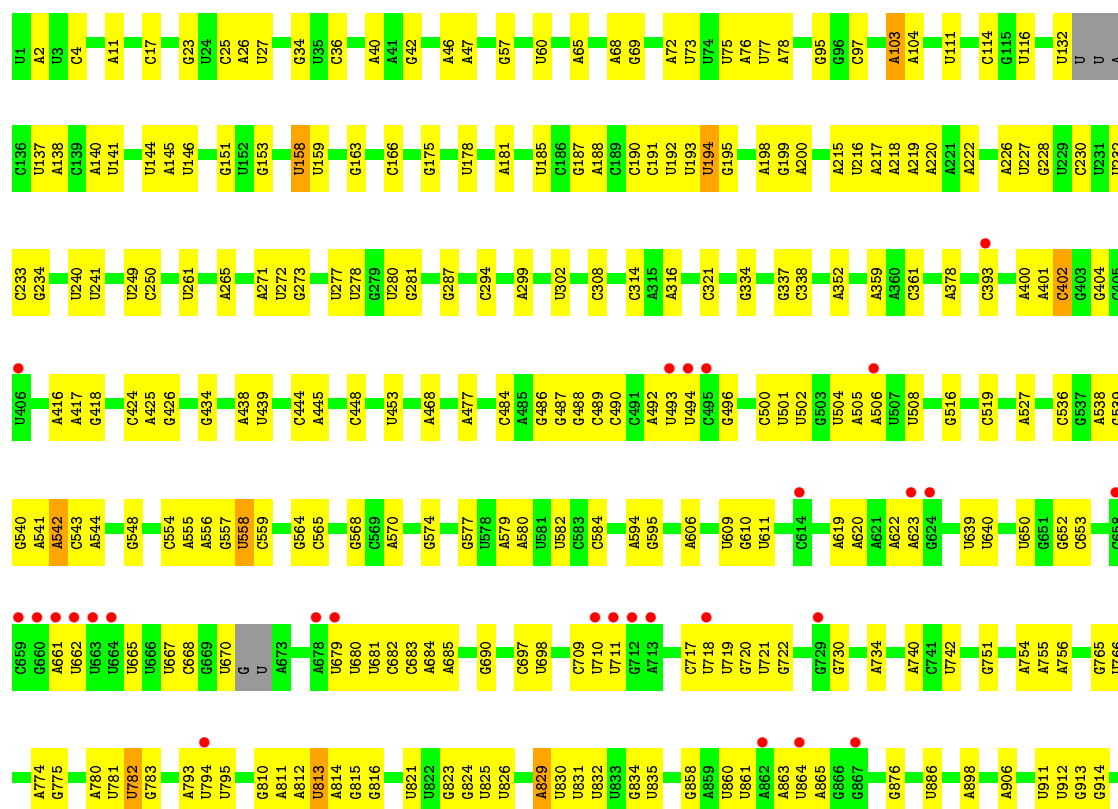
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

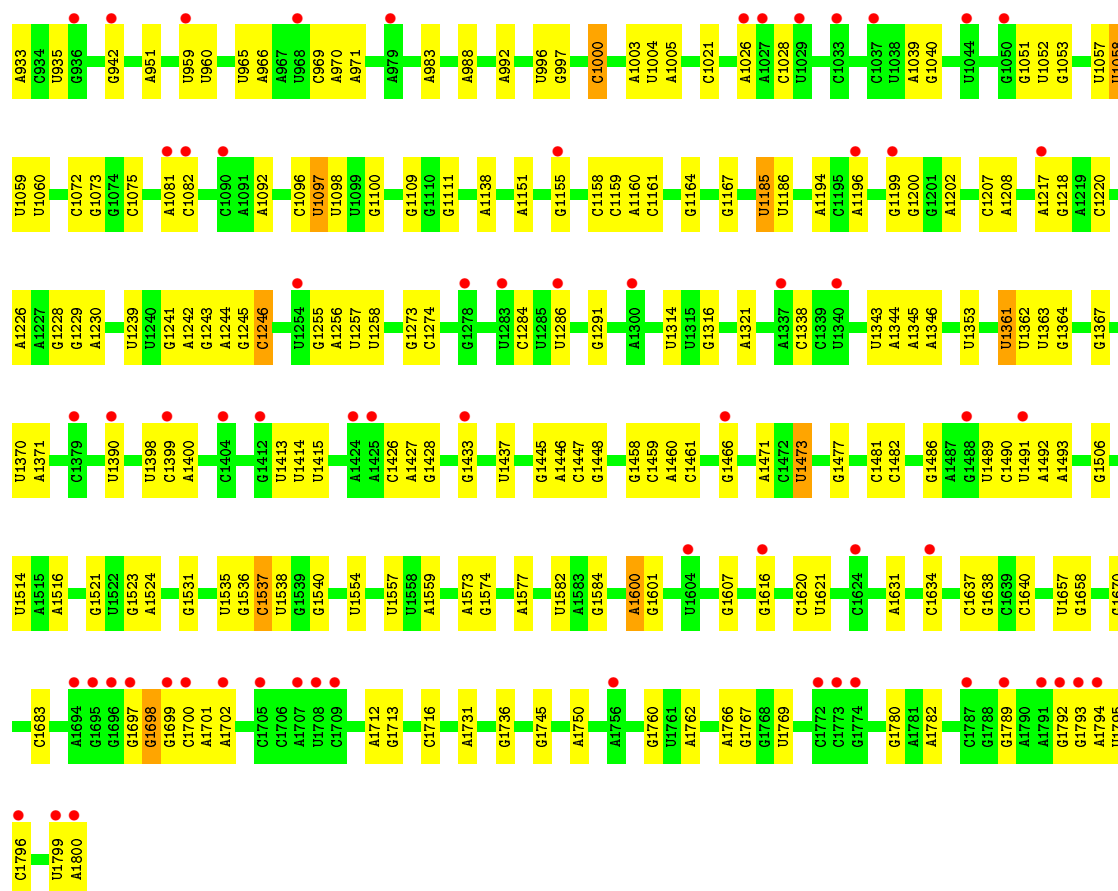
- Molecule 1: 18S ribosomal RNA



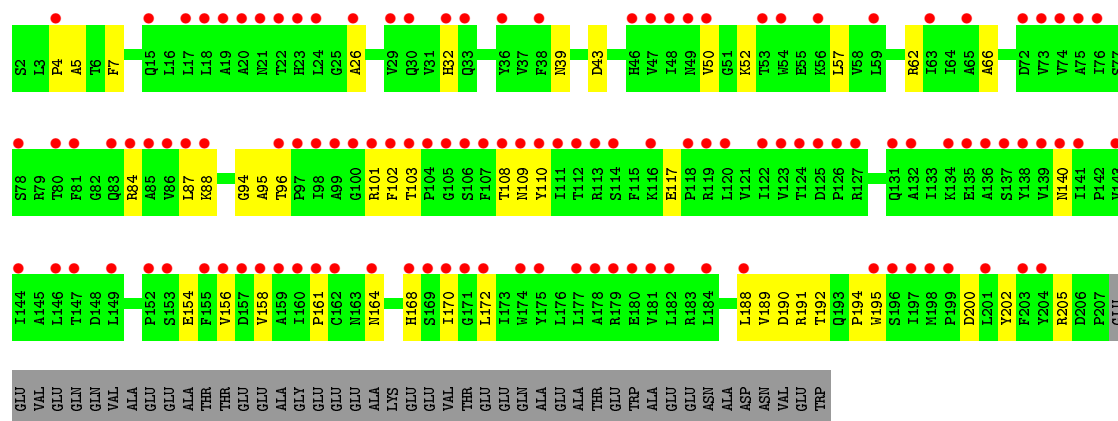


- Molecule 1: 18S ribosomal RNA

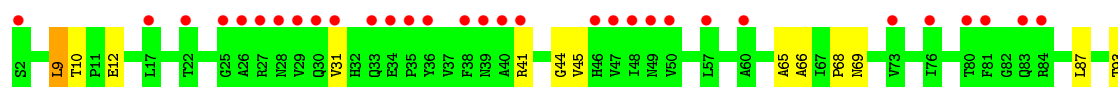


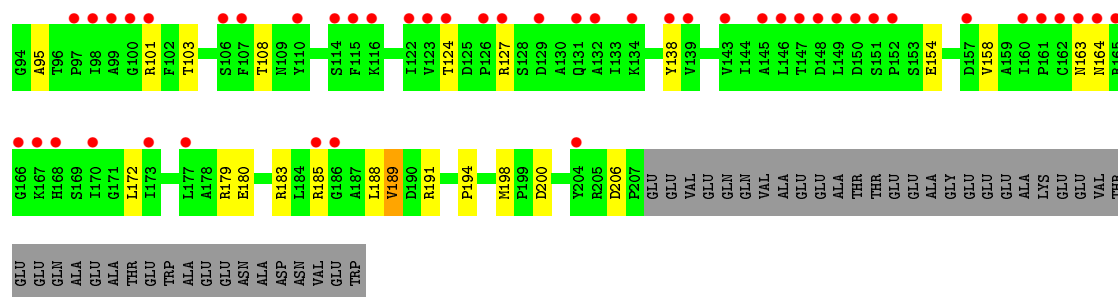


• Molecule 2: 40S ribosomal protein S0-A

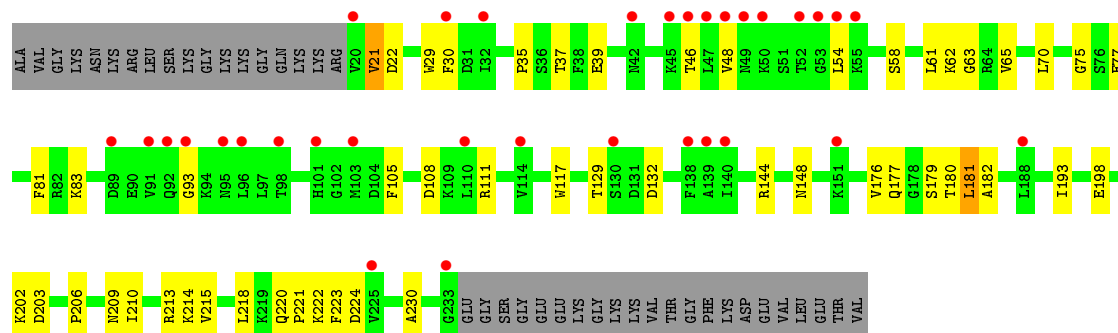


• Molecule 2: 40S ribosomal protein S0-A

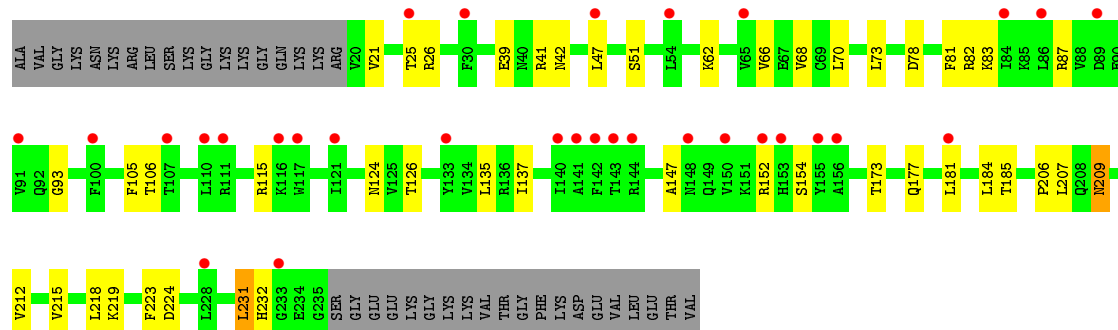




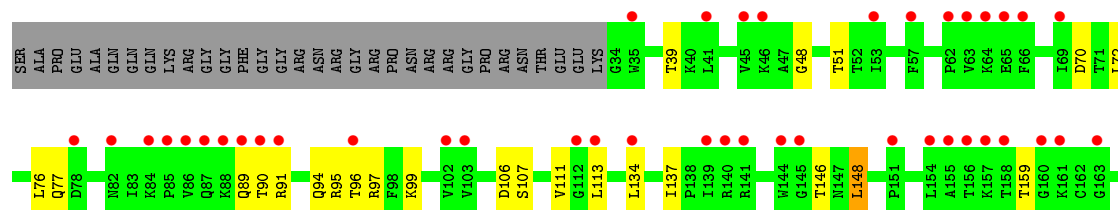
• Molecule 3: 40S ribosomal protein S1-A

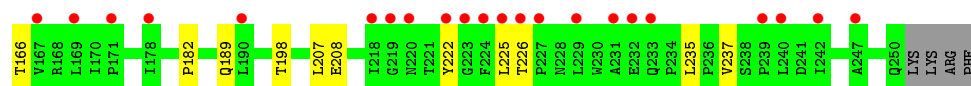


• Molecule 3: 40S ribosomal protein S1-A

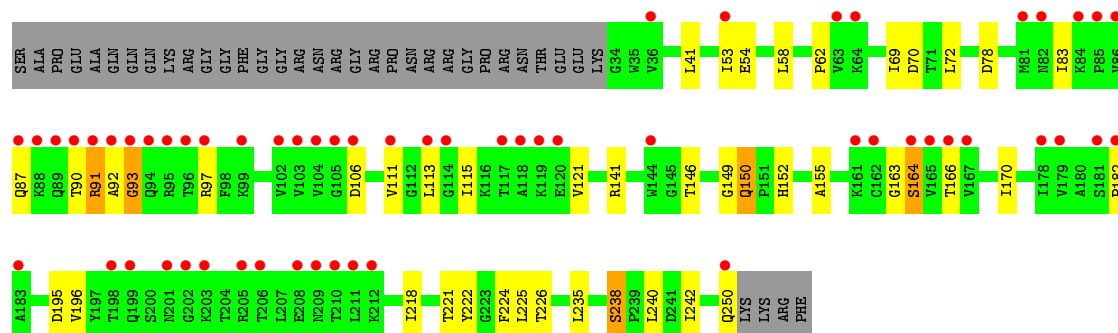


• Molecule 4: 40S ribosomal protein S2

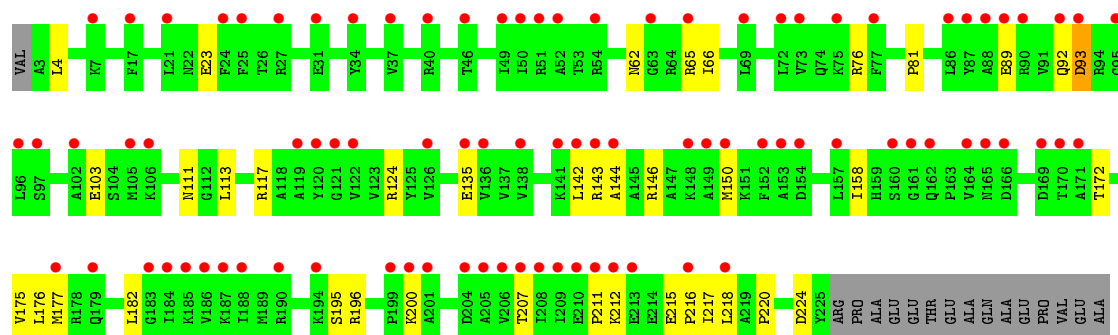
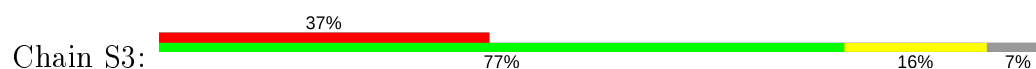




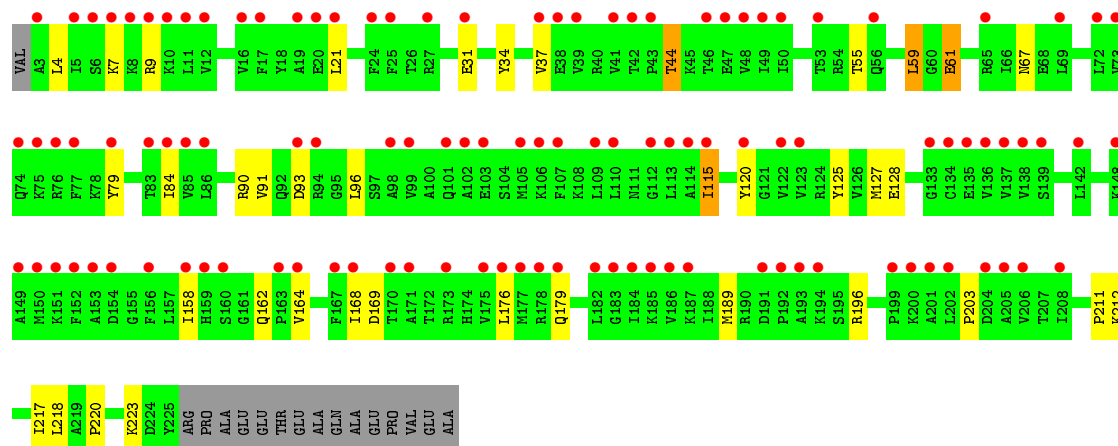
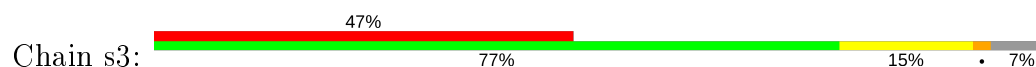
- Molecule 4: 40S ribosomal protein S2



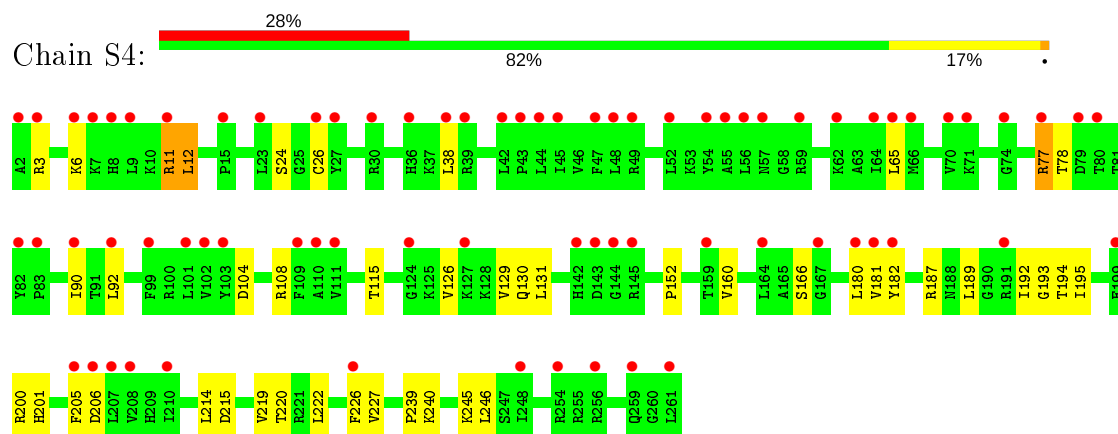
- Molecule 5: 40S ribosomal protein S3



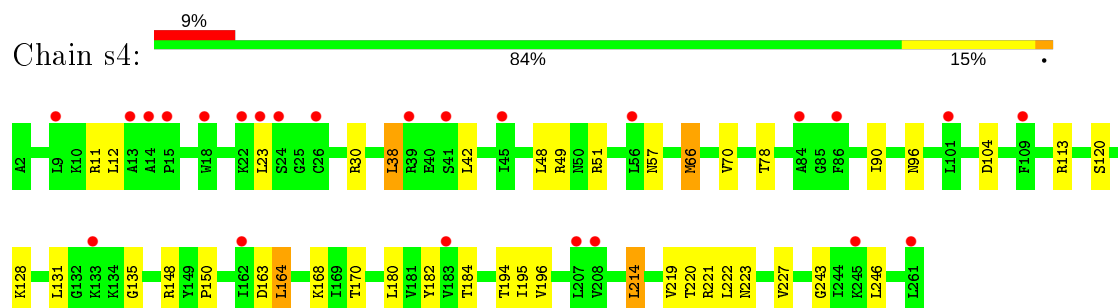
- Molecule 5: 40S ribosomal protein S3



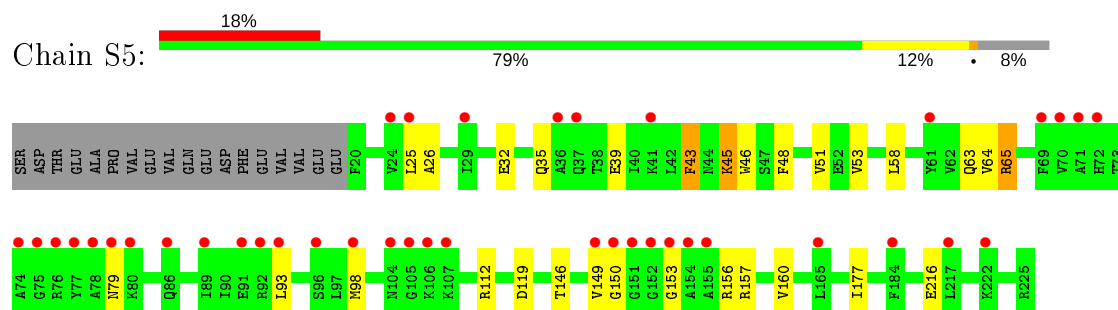
- Molecule 6: 40S ribosomal protein S4-A



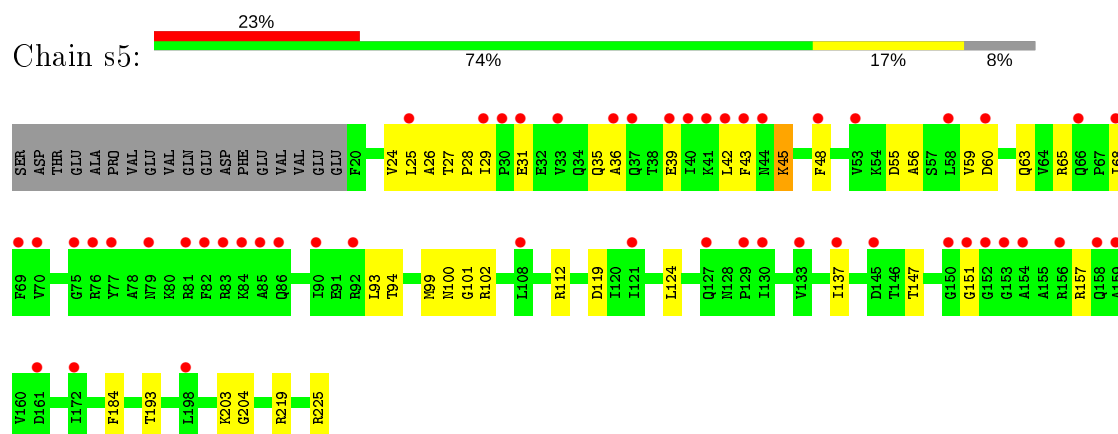
- Molecule 6: 40S ribosomal protein S4-A



- Molecule 7: 40S ribosomal protein S5

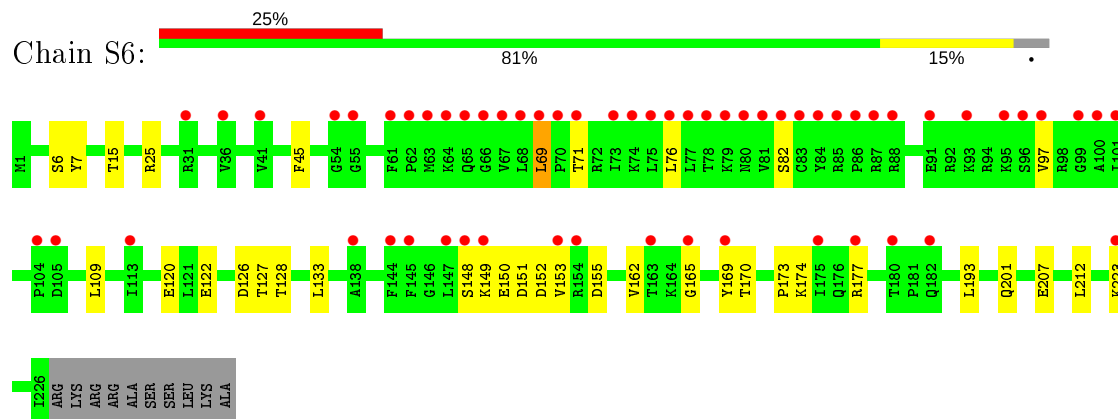


- Molecule 7: 40S ribosomal protein S5

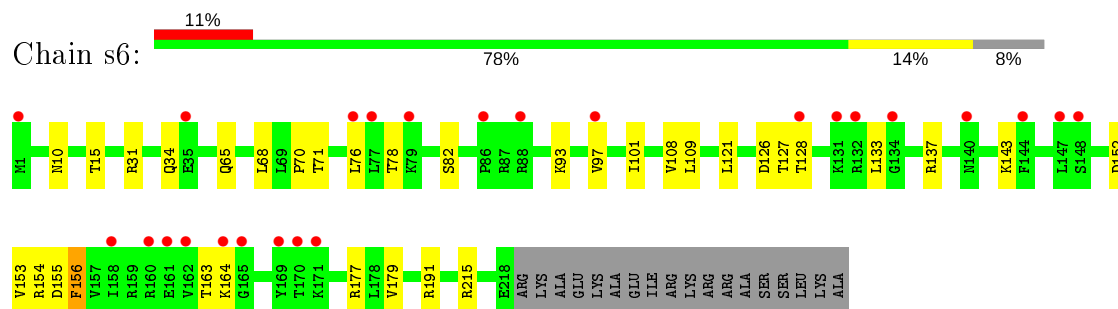




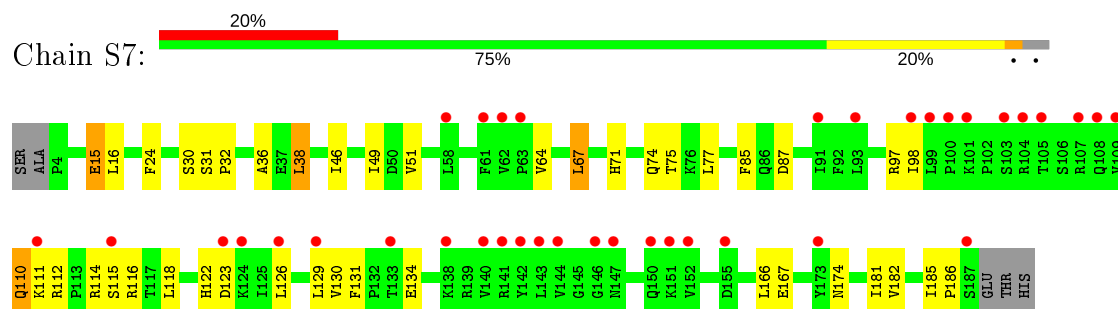
- Molecule 8: 40S ribosomal protein S6-A



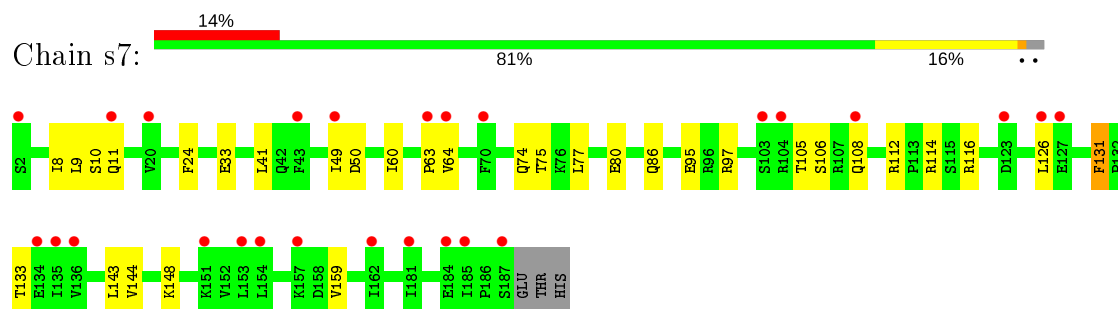
- Molecule 8: 40S ribosomal protein S6-A



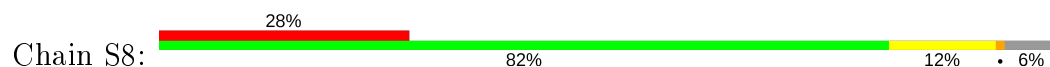
- Molecule 9: 40S ribosomal protein S7-A

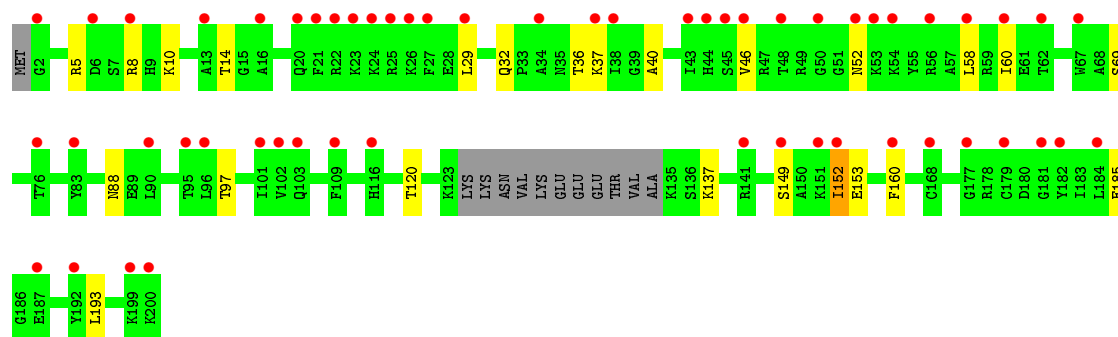


- Molecule 9: 40S ribosomal protein S7-A

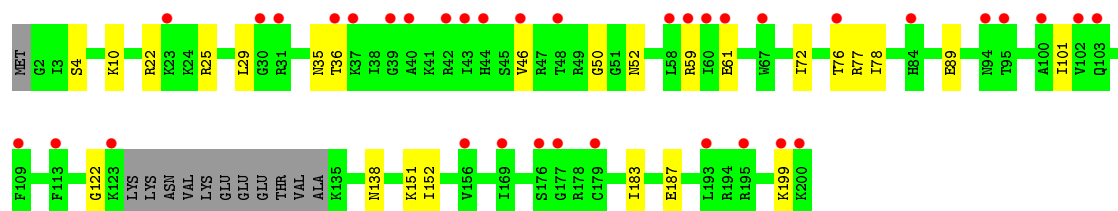
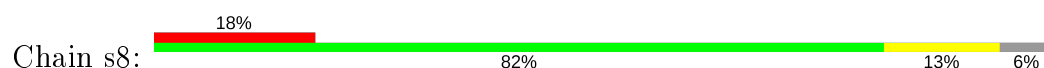


- Molecule 10: 40S ribosomal protein S8-A

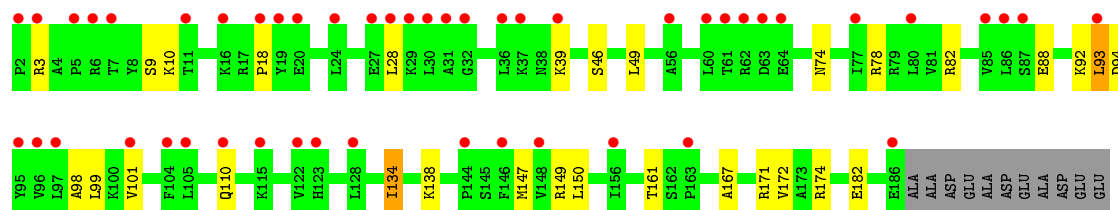
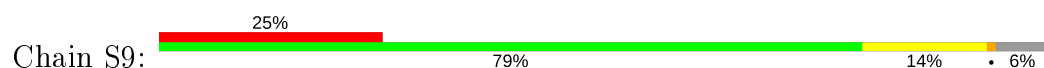




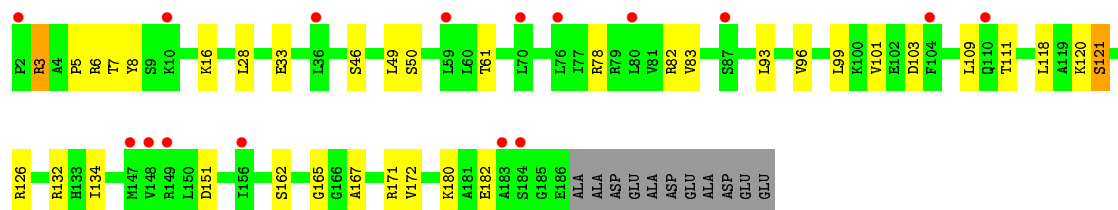
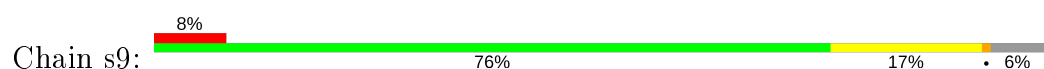
• Molecule 10: 40S ribosomal protein S8-A



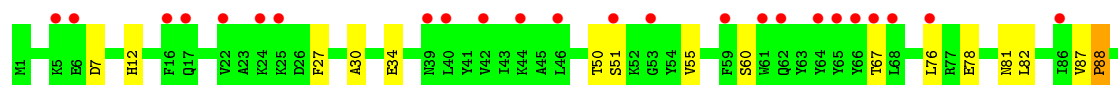
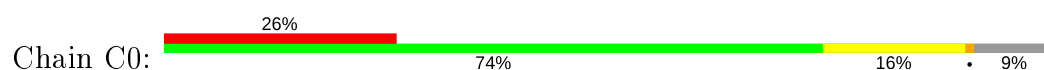
• Molecule 11: 40S ribosomal protein S9-A

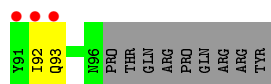


• Molecule 11: 40S ribosomal protein S9-A

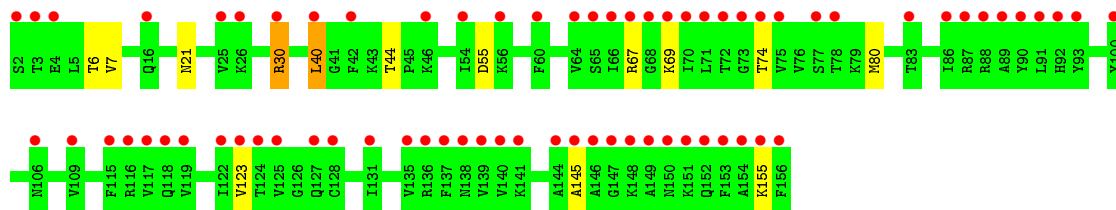
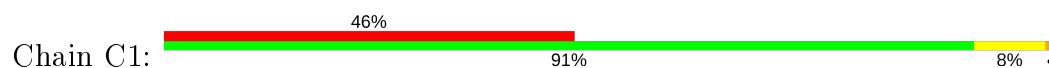


• Molecule 12: 40S ribosomal protein S10-A

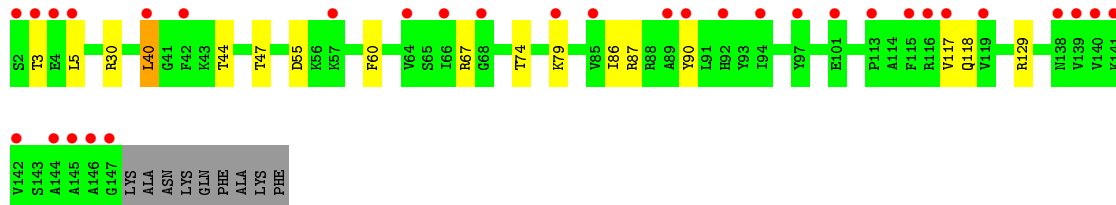
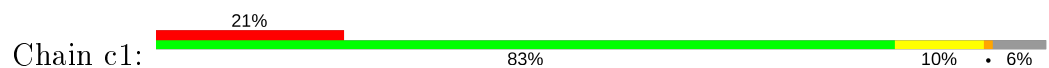




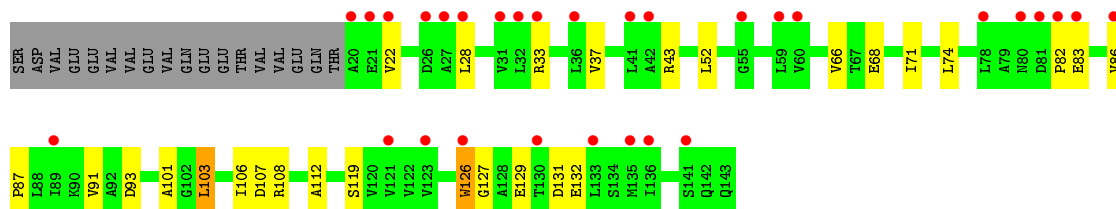
- Molecule 13: 40S ribosomal protein S11-A



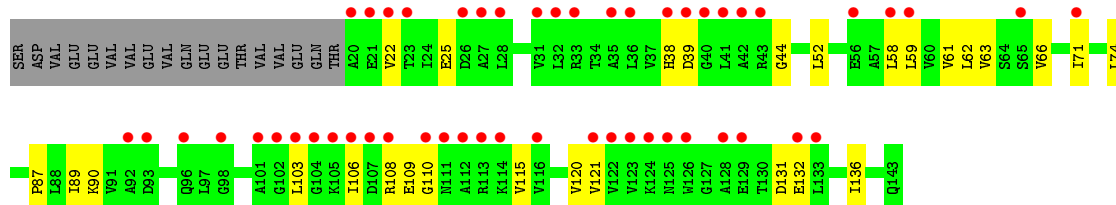
- Molecule 13: 40S ribosomal protein S11-A



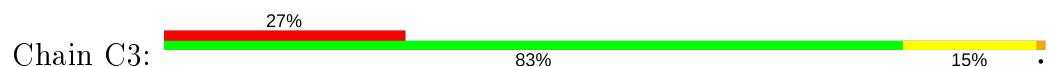
- Molecule 14: 40S ribosomal protein S12

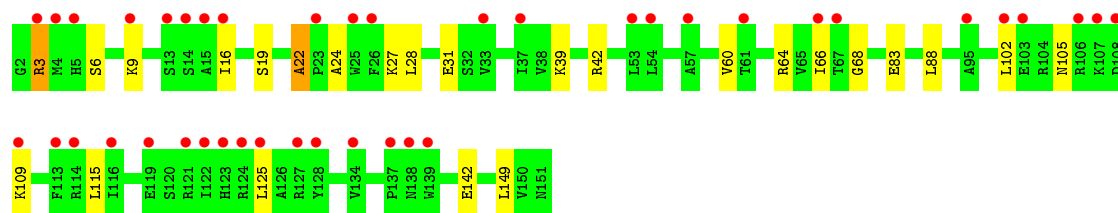


- Molecule 14: 40S ribosomal protein S12

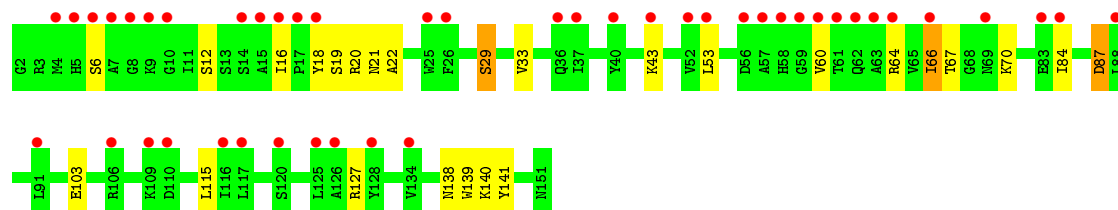
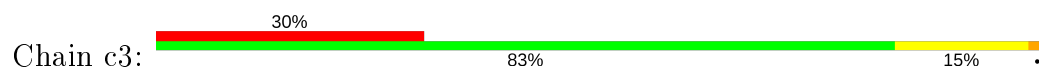


- Molecule 15: 40S ribosomal protein S13

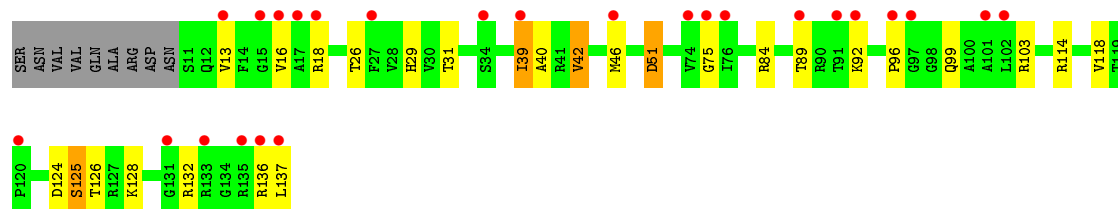
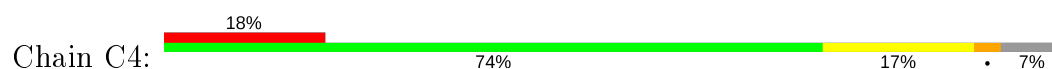




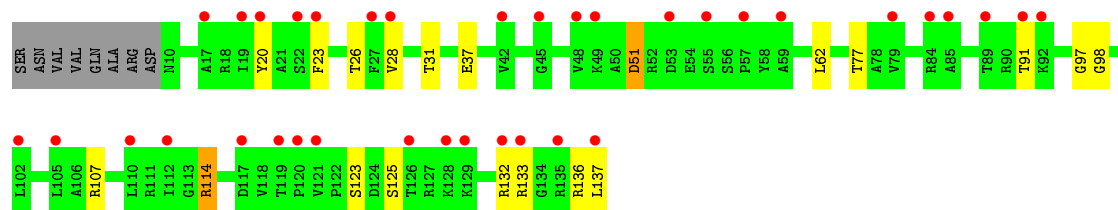
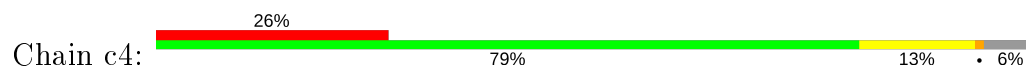
- Molecule 15: 40S ribosomal protein S13



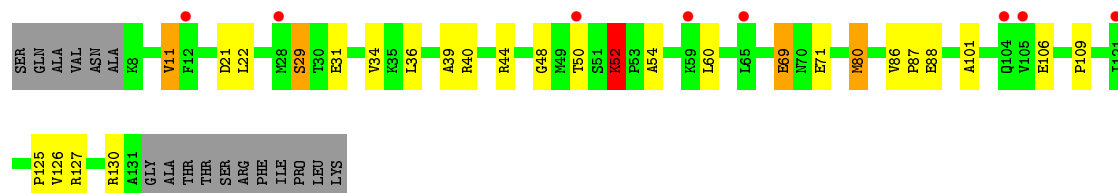
- Molecule 16: 40S ribosomal protein S14-A



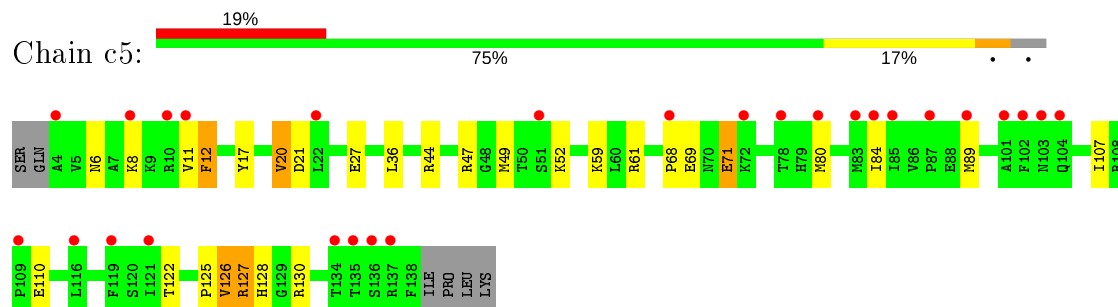
- Molecule 16: 40S ribosomal protein S14-A



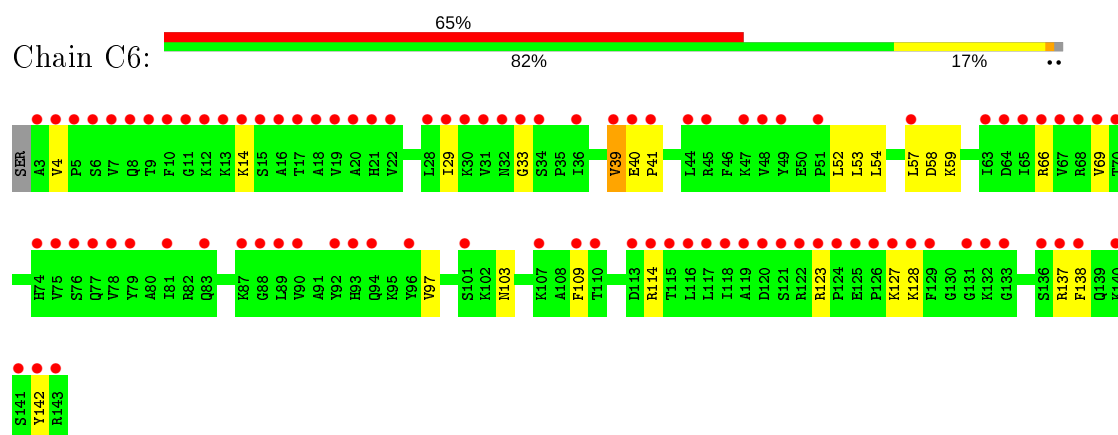
- Molecule 17: 40S ribosomal protein S15



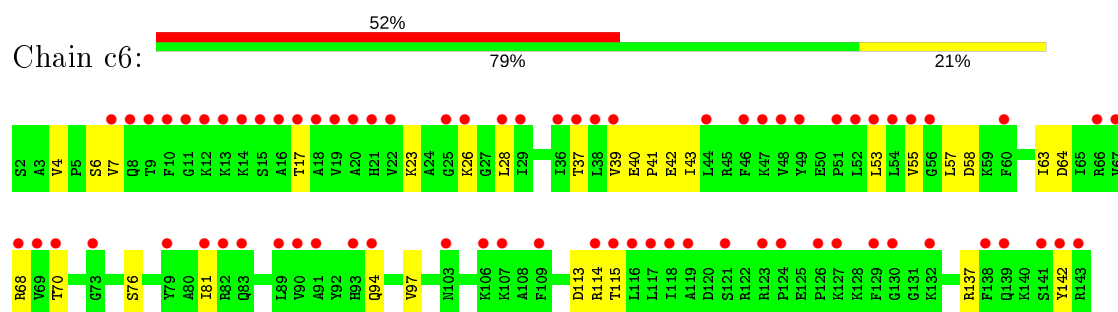
- Molecule 17: 40S ribosomal protein S15



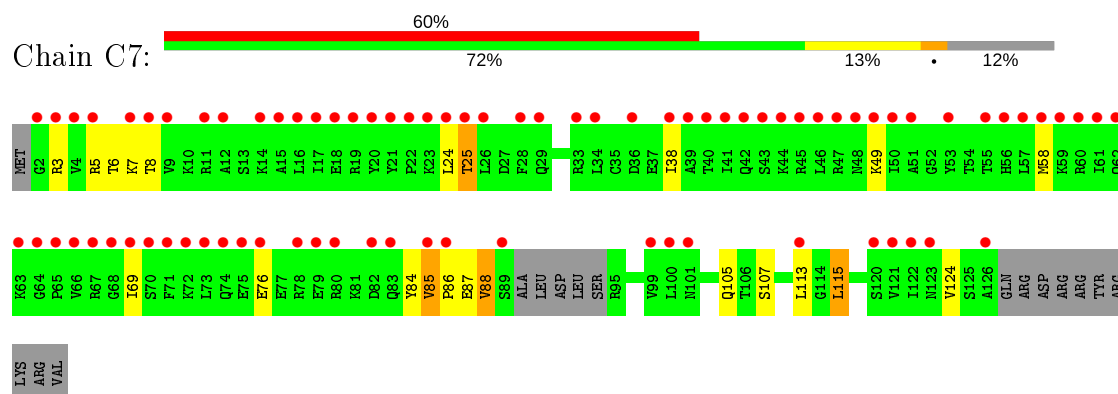
- Molecule 18: 40S ribosomal protein S16-A



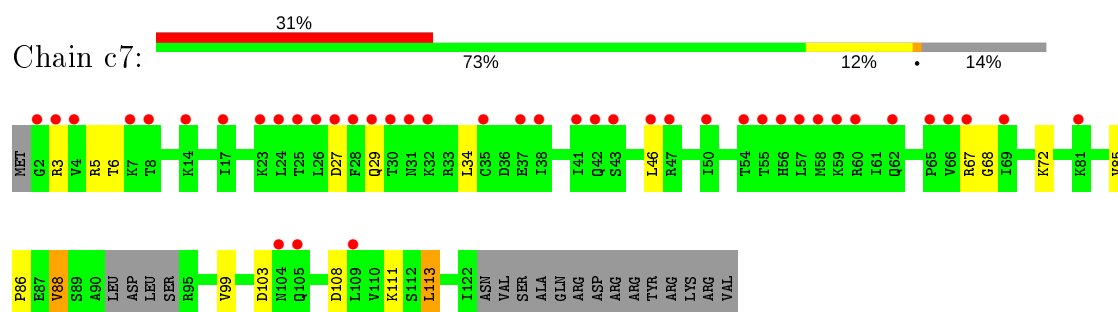
- Molecule 18: 40S ribosomal protein S16-A



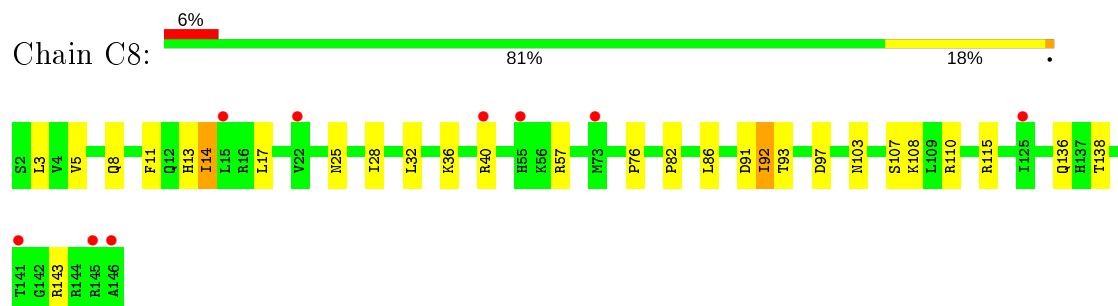
- Molecule 19: 40S ribosomal protein S17-A



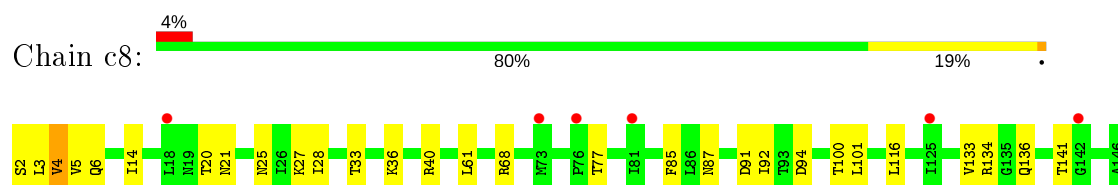
- Molecule 19: 40S ribosomal protein S17-A



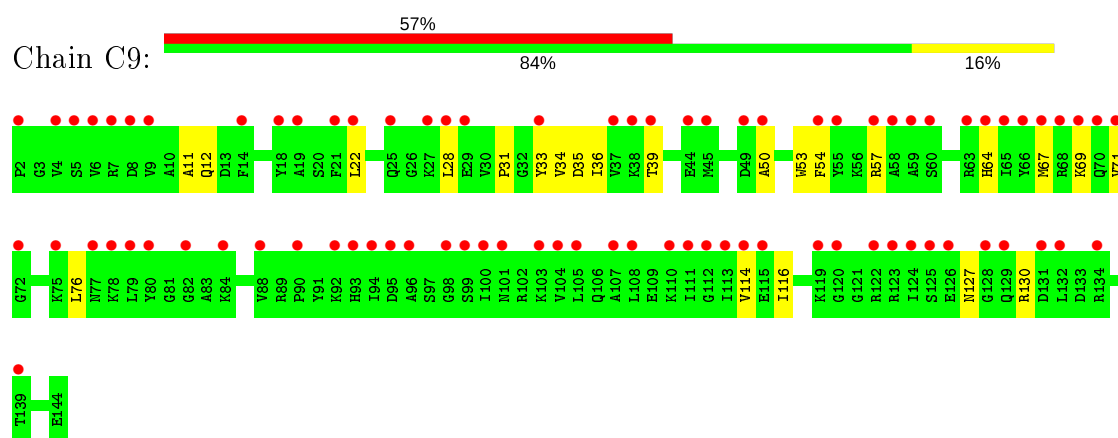
- Molecule 20: 40S ribosomal protein S18-A



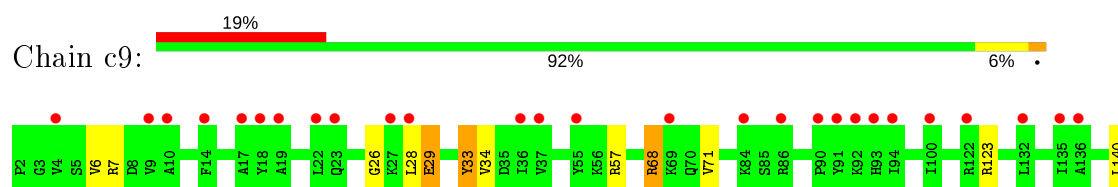
- Molecule 20: 40S ribosomal protein S18-A



- Molecule 21: 40S ribosomal protein S19-A

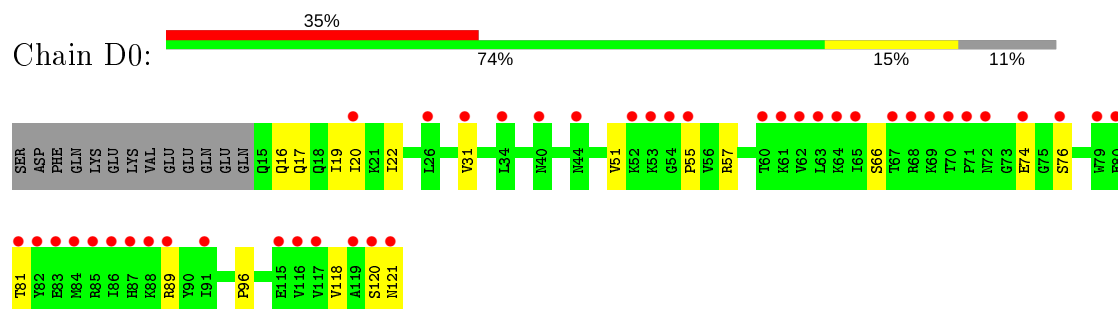


- Molecule 21: 40S ribosomal protein S19-A

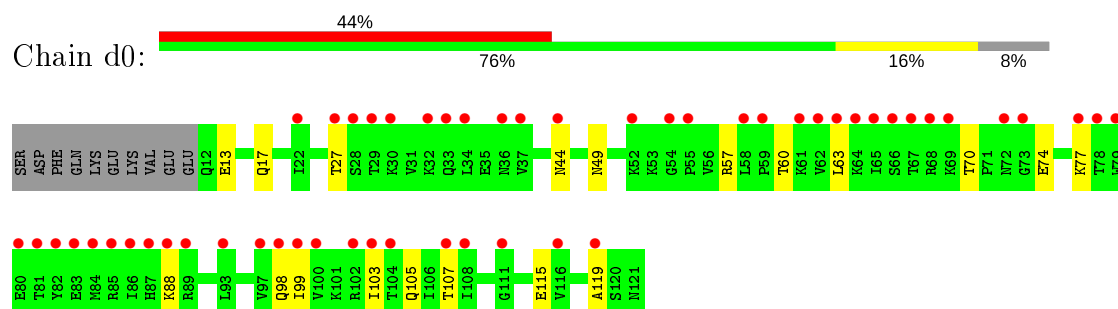




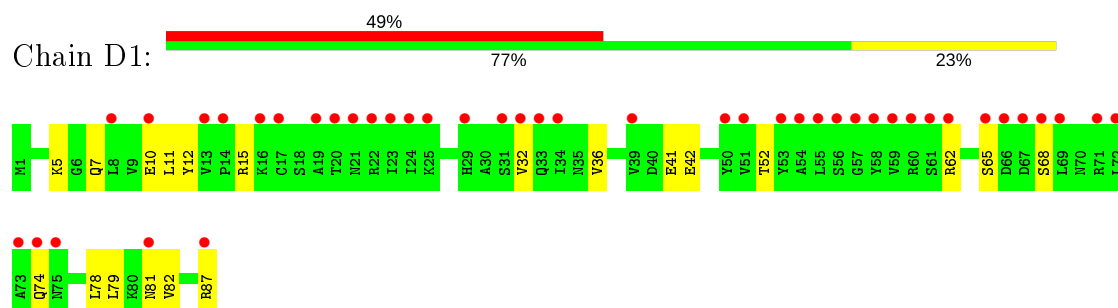
- Molecule 22: 40S ribosomal protein S20



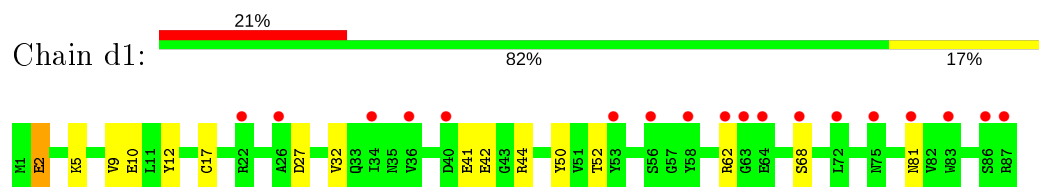
- Molecule 22: 40S ribosomal protein S20



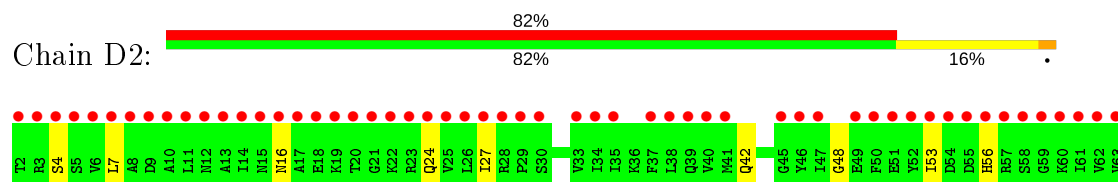
- Molecule 23: 40S ribosomal protein S21-A

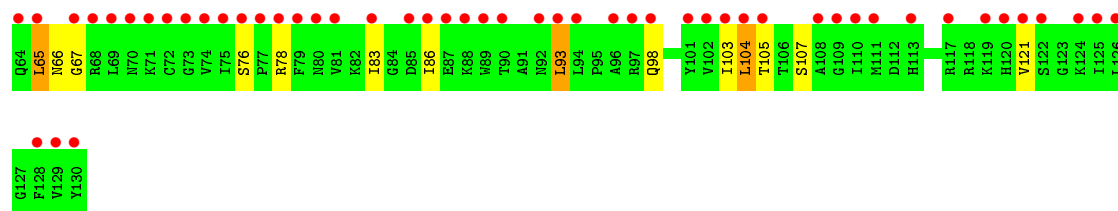


- Molecule 23: 40S ribosomal protein S21-A

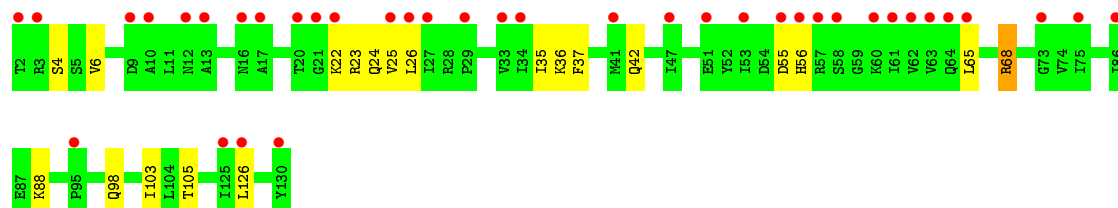
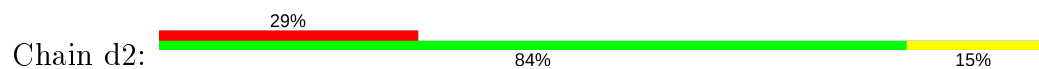


- Molecule 24: 40S ribosomal protein S22-A

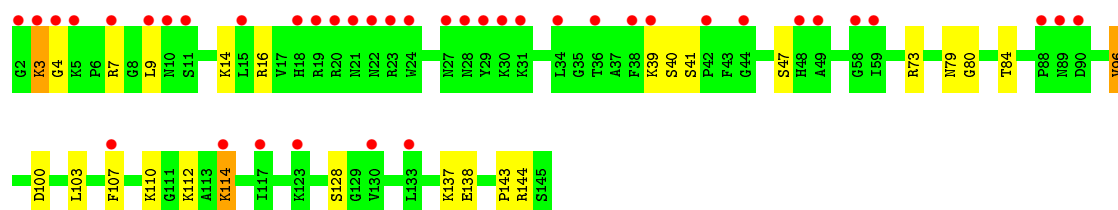
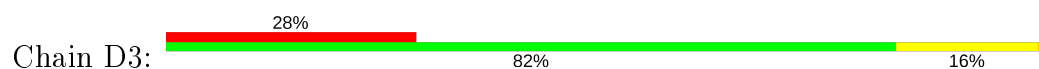




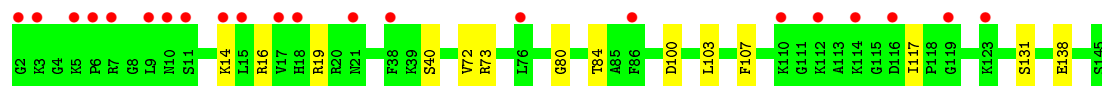
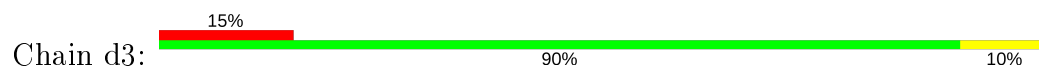
• Molecule 24: 40S ribosomal protein S22-A



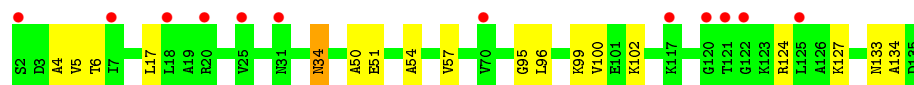
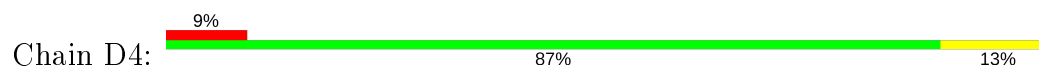
• Molecule 25: 40S ribosomal protein S23-A



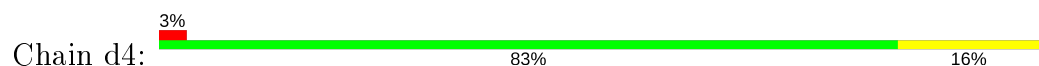
• Molecule 25: 40S ribosomal protein S23-A



• Molecule 26: 40S ribosomal protein S24-A

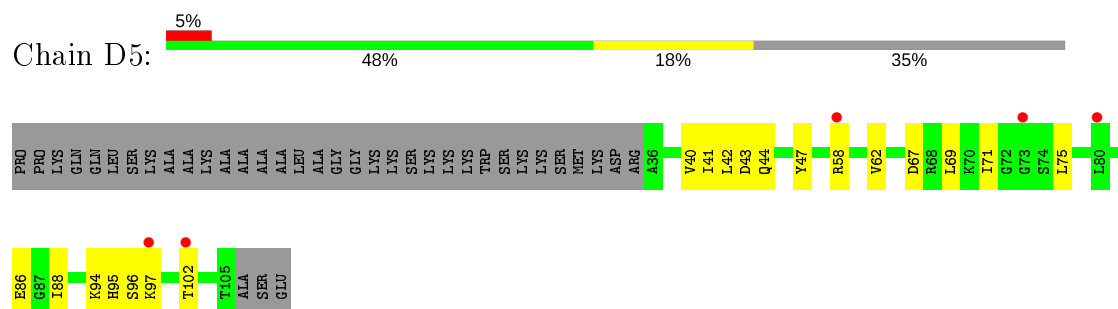


• Molecule 26: 40S ribosomal protein S24-A

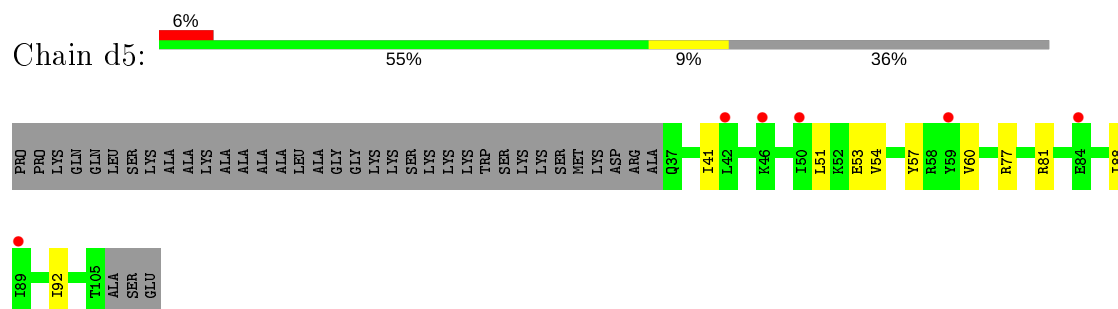




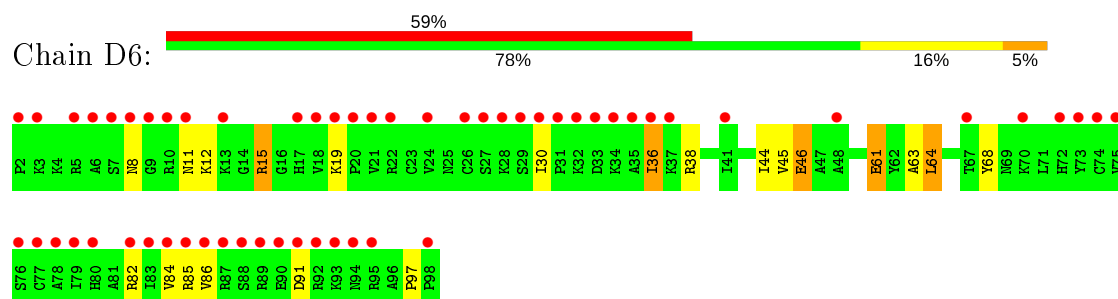
- Molecule 27: 40S ribosomal protein S25-A



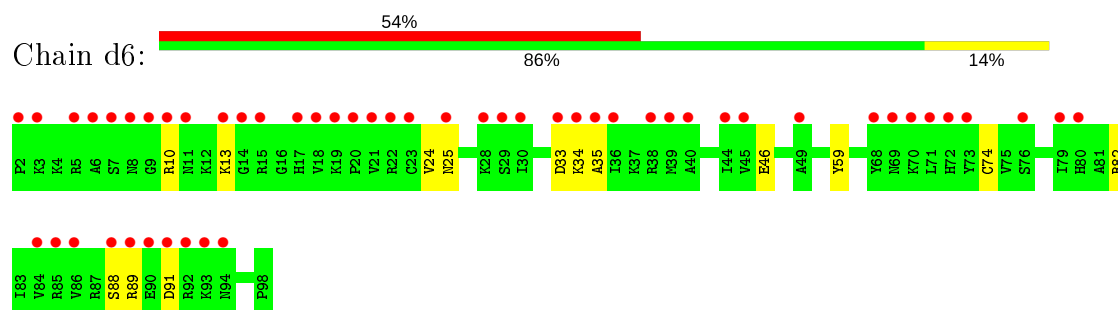
- Molecule 27: 40S ribosomal protein S25-A



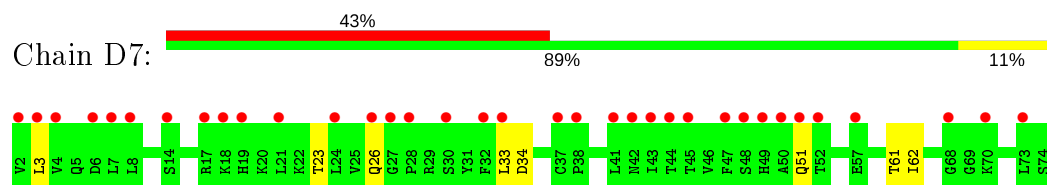
- Molecule 28: 40S ribosomal protein S26-B



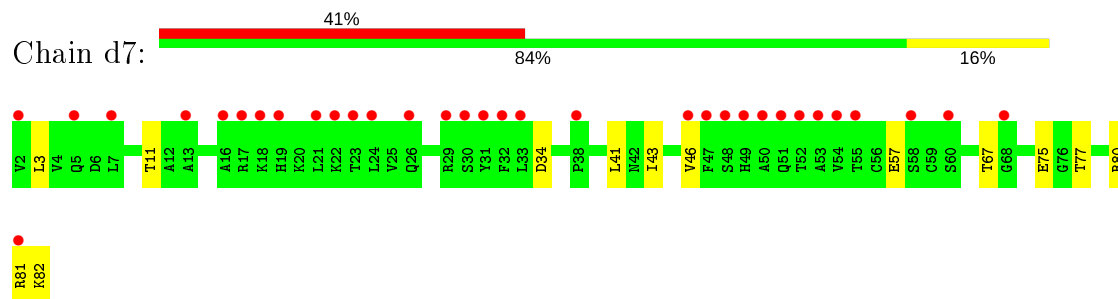
- Molecule 28: 40S ribosomal protein S26-B



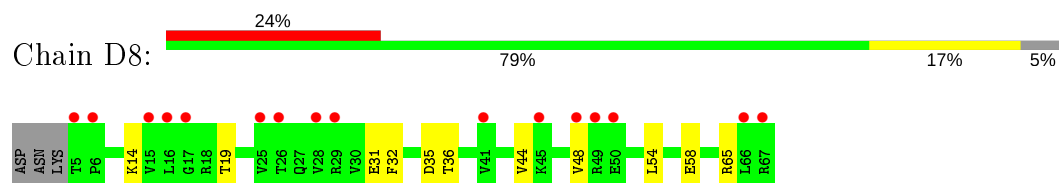
- Molecule 29: 40S ribosomal protein S27-A



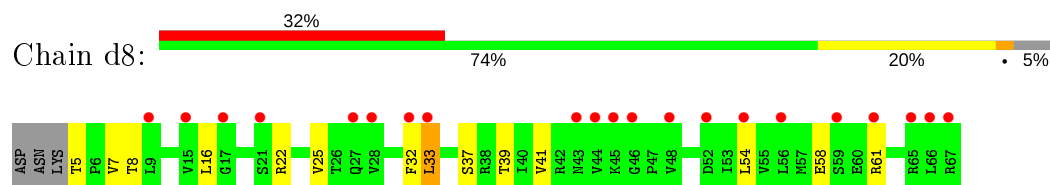
- Molecule 29: 40S ribosomal protein S27-A



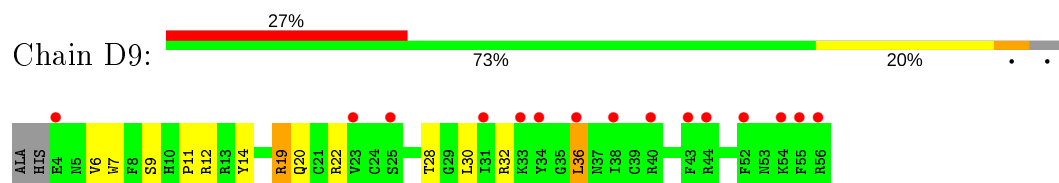
- Molecule 30: 40S ribosomal protein S28-A



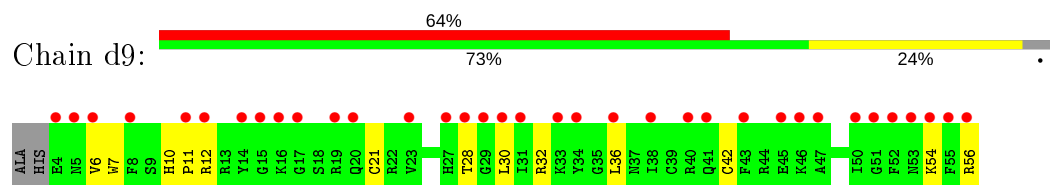
- Molecule 30: 40S ribosomal protein S28-A



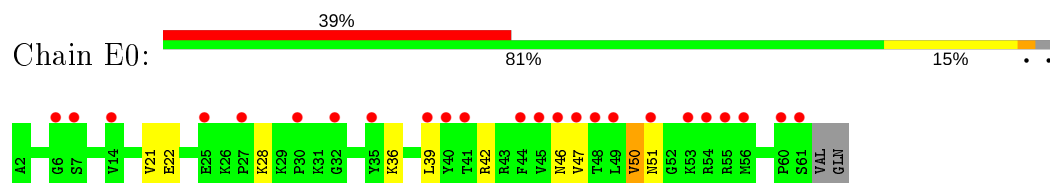
- Molecule 31: 40S ribosomal protein S29-A



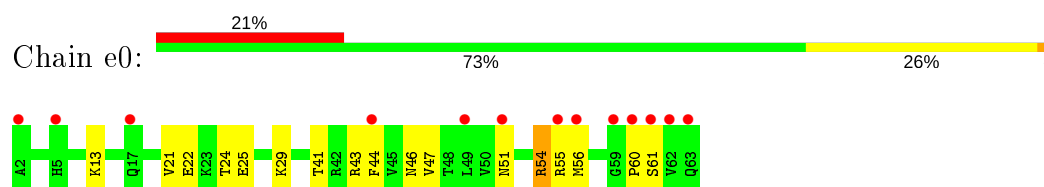
- Molecule 31: 40S ribosomal protein S29-A



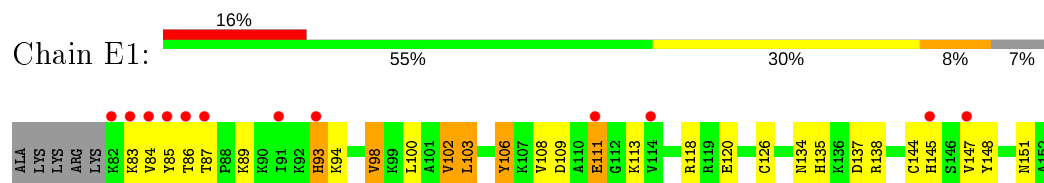
- Molecule 32: 40S ribosomal protein S30-A



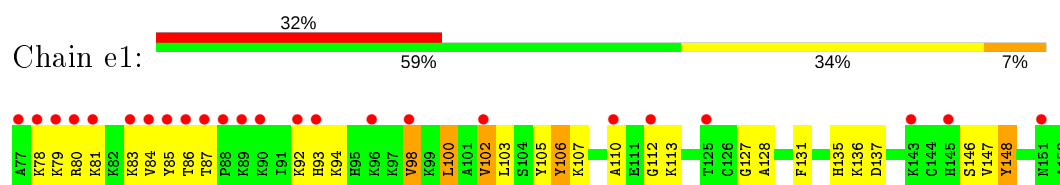
- Molecule 32: 40S ribosomal protein S30-A



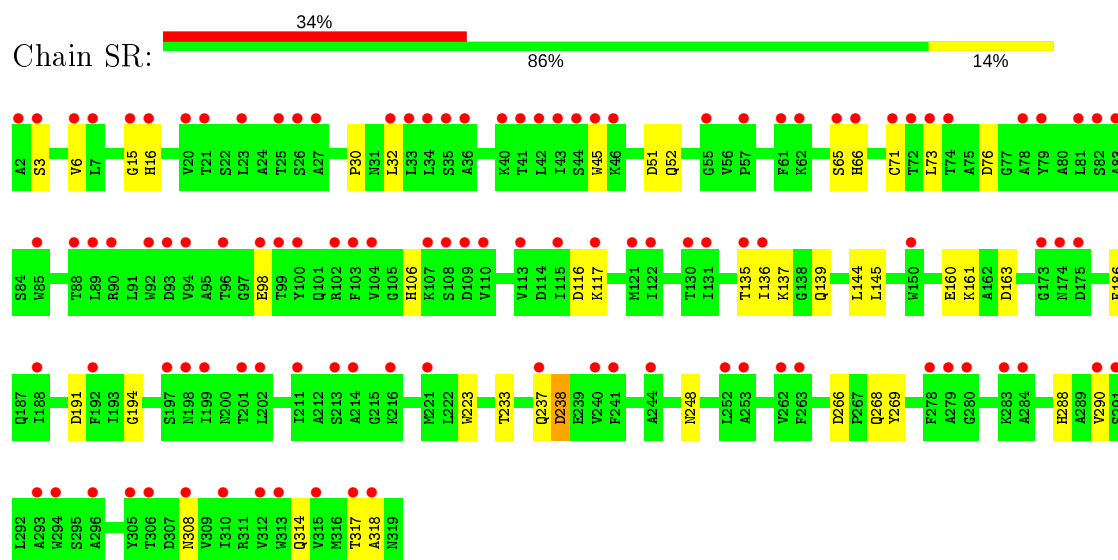
• Molecule 33: Ubiquitin-40S ribosomal protein S31



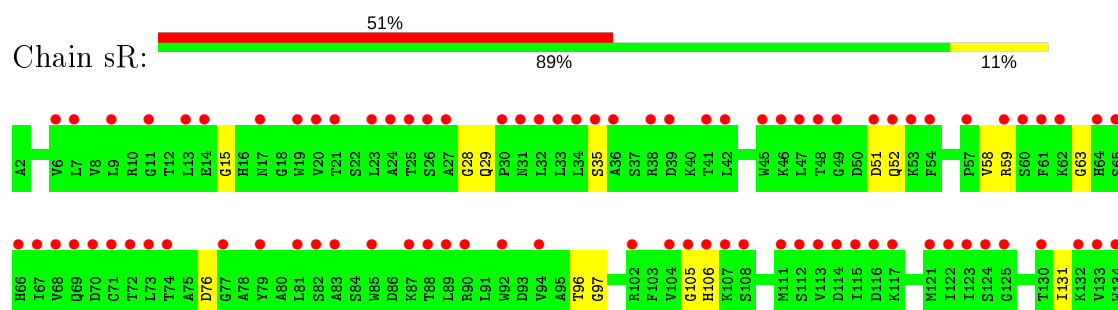
• Molecule 33: Ubiquitin-40S ribosomal protein S31

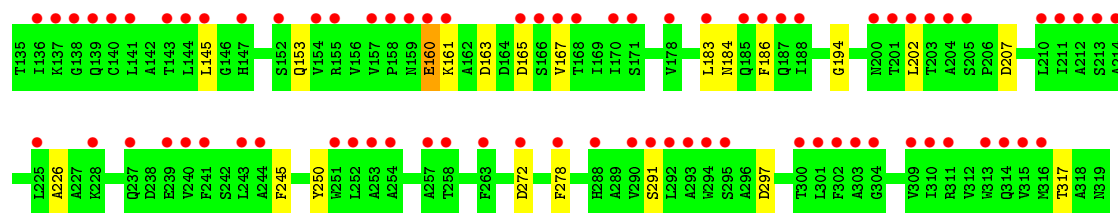


• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

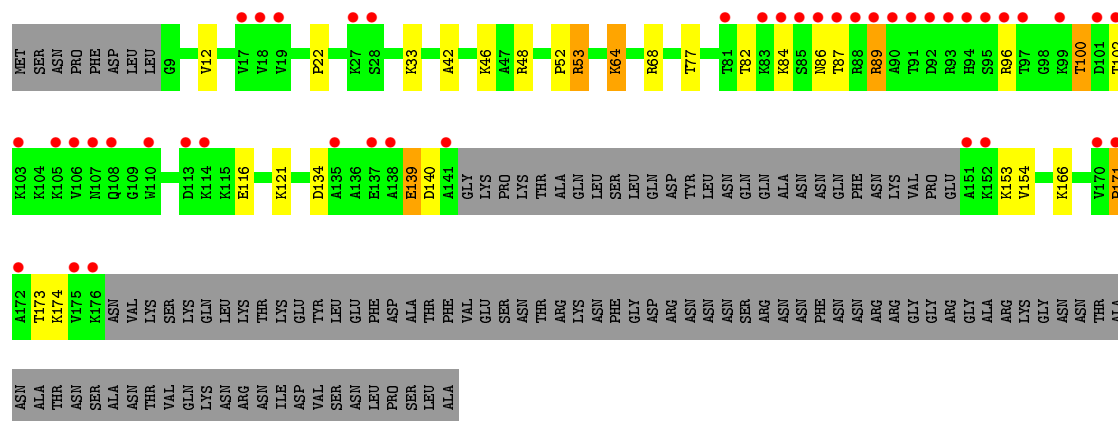


• Molecule 34: Guanine nucleotide-binding protein subunit beta-like protein

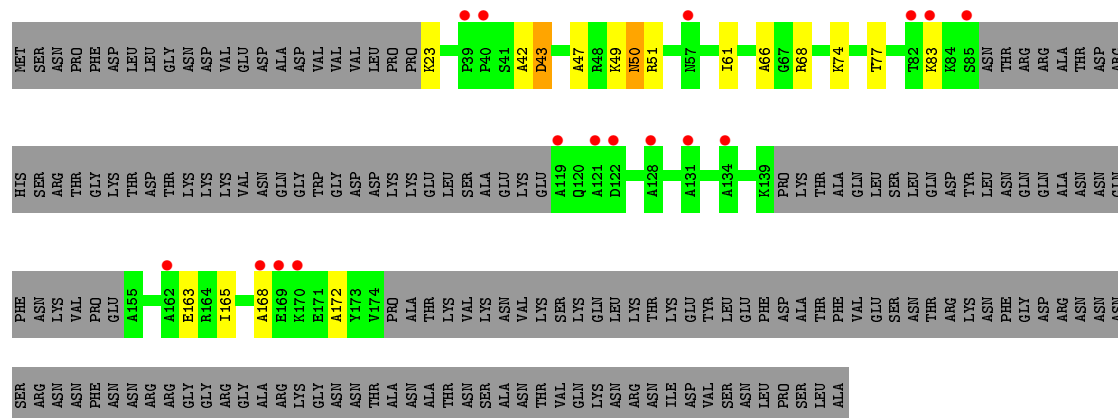




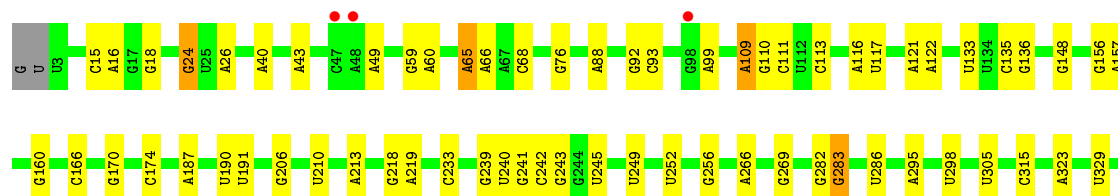
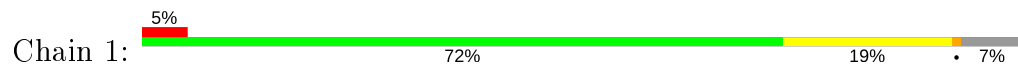
• Molecule 35: Suppressor protein STM1



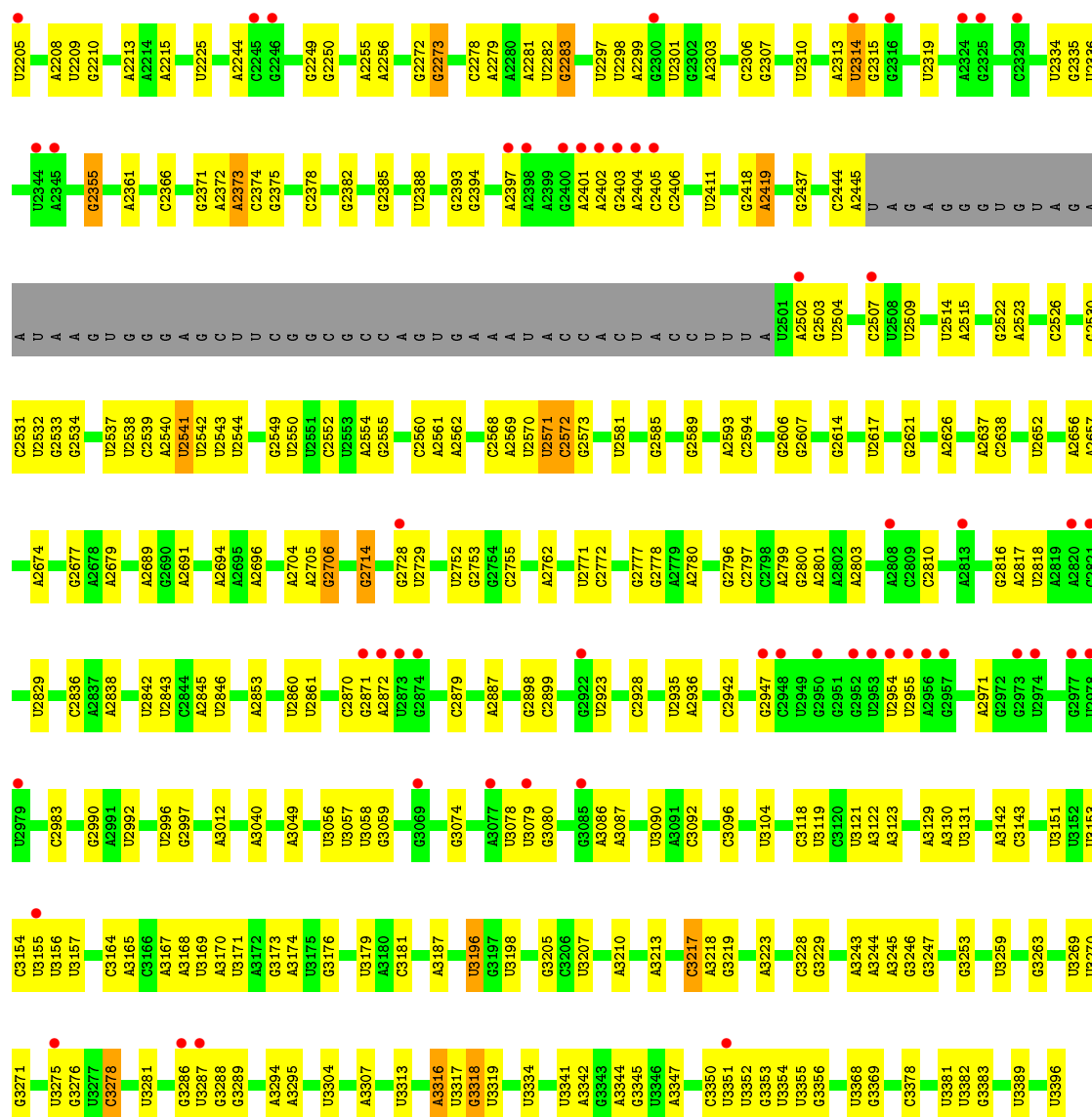
• Molecule 35: Suppressor protein STM1



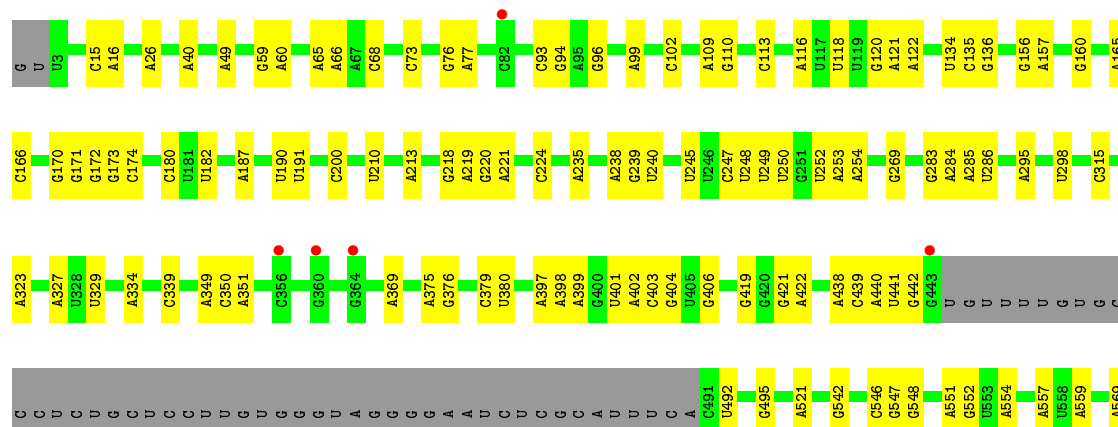
• Molecule 36: 25S ribosomal RNA

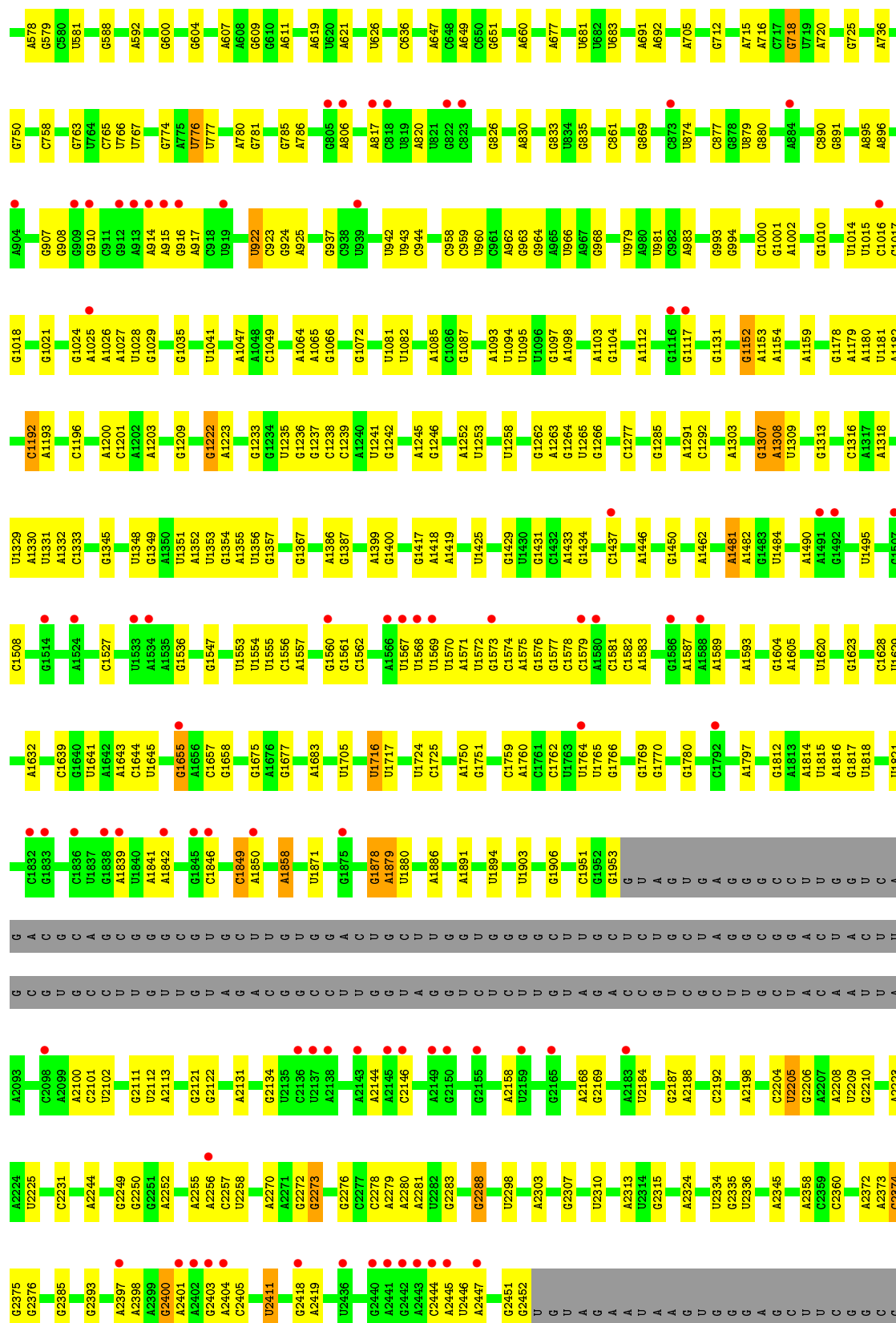


[illegible]



• Molecule 36: 25S ribosomal RNA

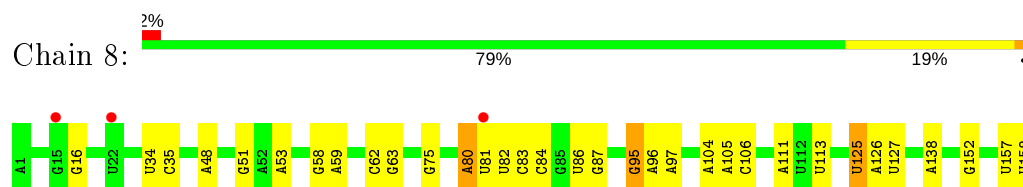




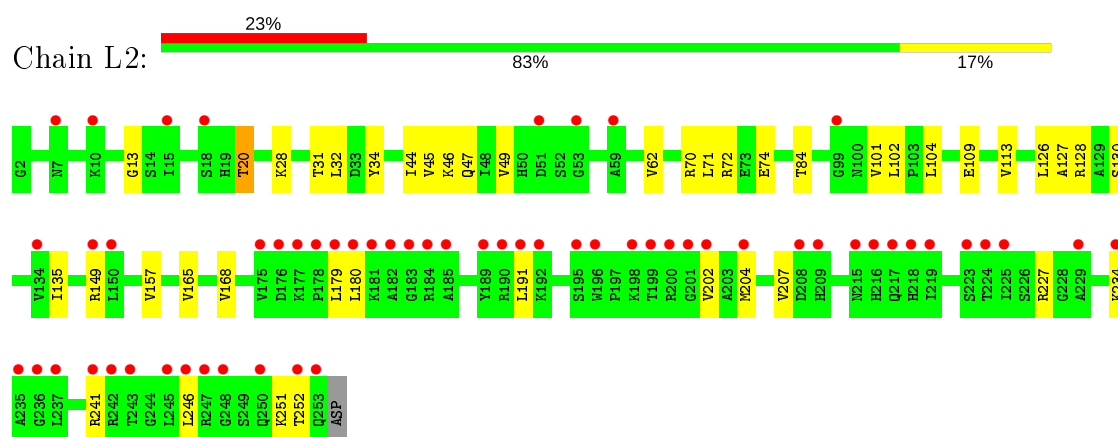




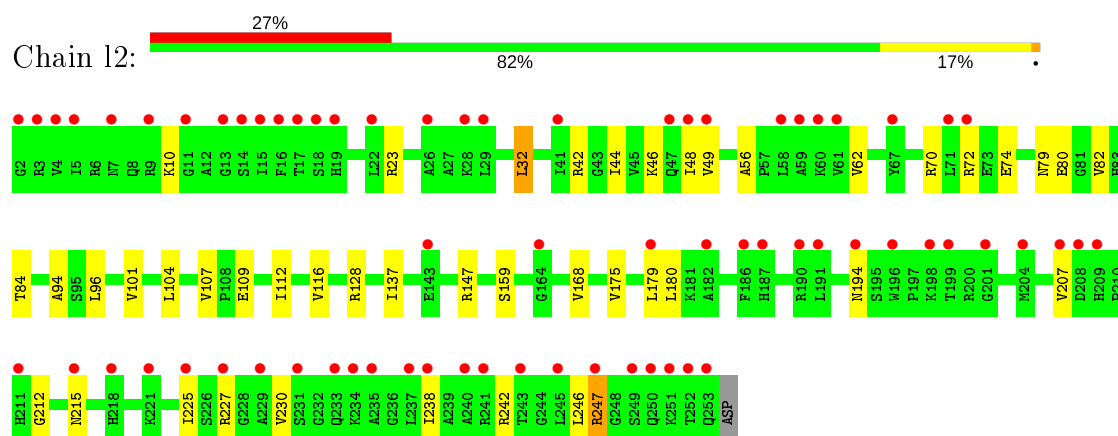
- Molecule 38: 5.8S ribosomal RNA



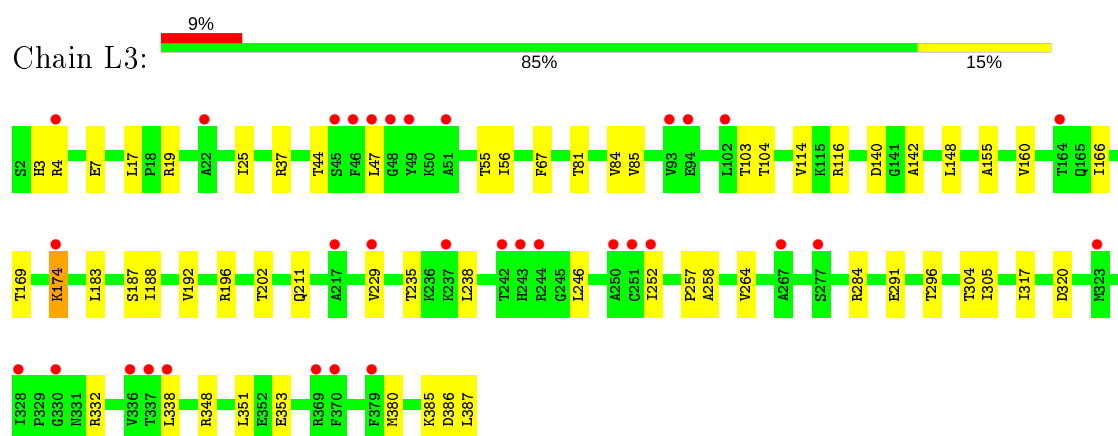
- Molecule 39: 60S ribosomal protein L2-A



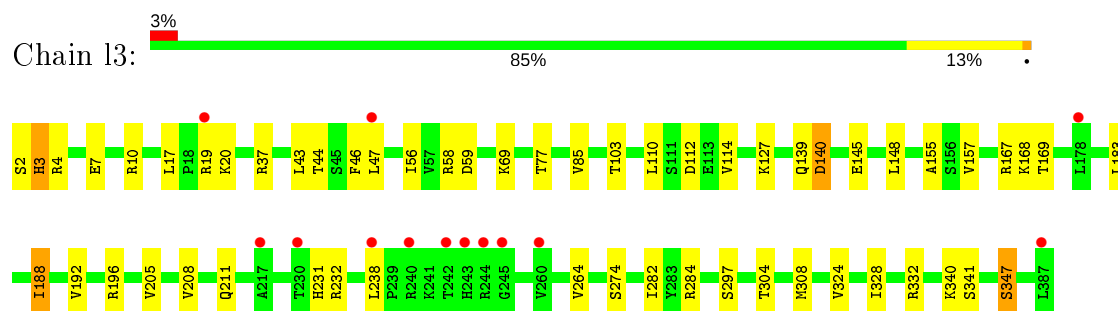
- Molecule 39: 60S ribosomal protein L2-A



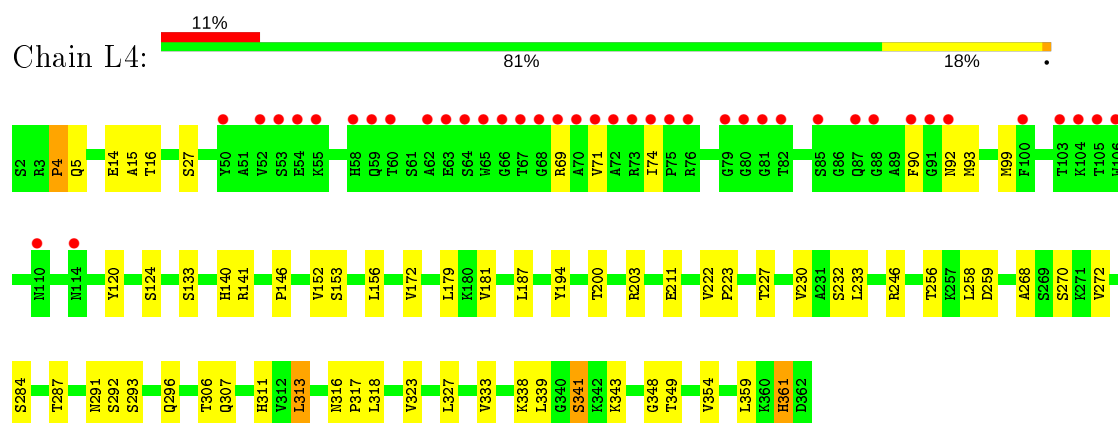
- Molecule 40: 60S ribosomal protein L3



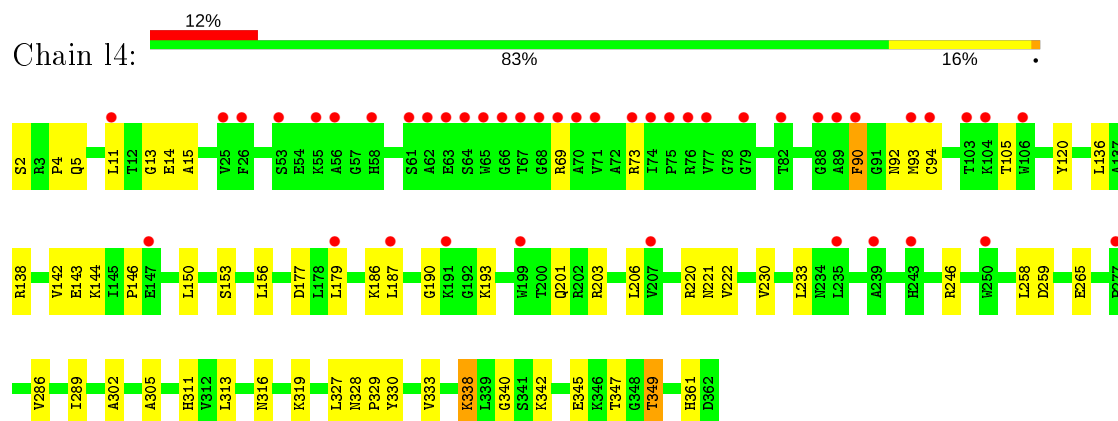
- Molecule 40: 60S ribosomal protein L3



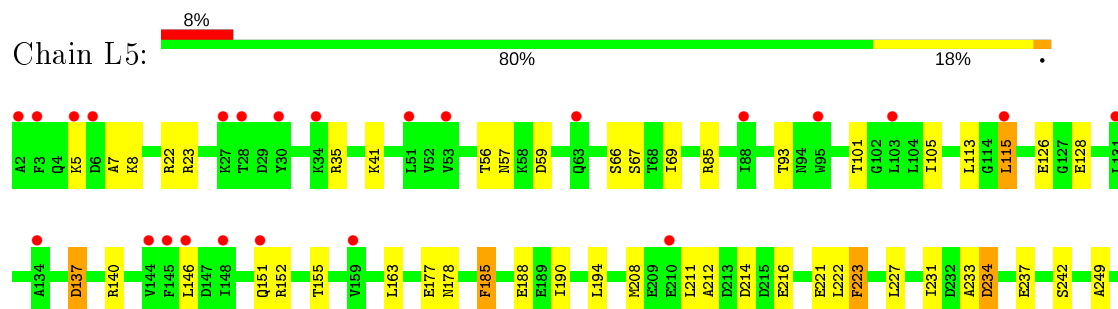
- Molecule 41: 60S ribosomal protein L4-A



- Molecule 41: 60S ribosomal protein L4-A

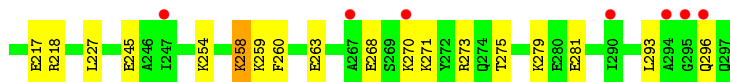
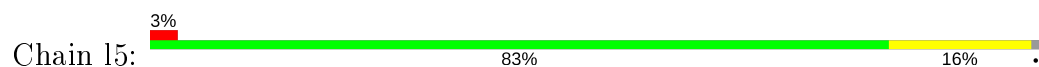


- Molecule 42: 60S ribosomal protein L5

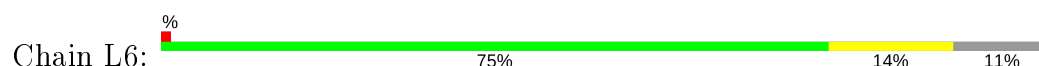




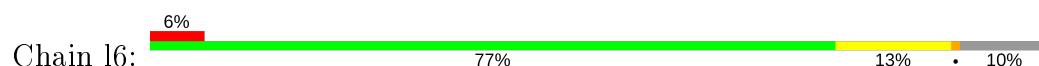
- Molecule 42: 60S ribosomal protein L5



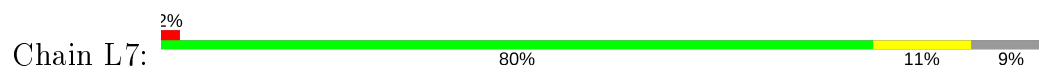
- Molecule 43: 60S ribosomal protein L6-A



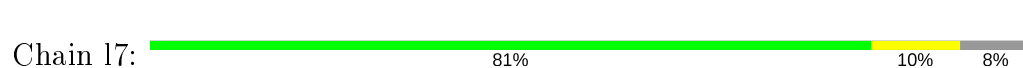
- Molecule 43: 60S ribosomal protein L6-A

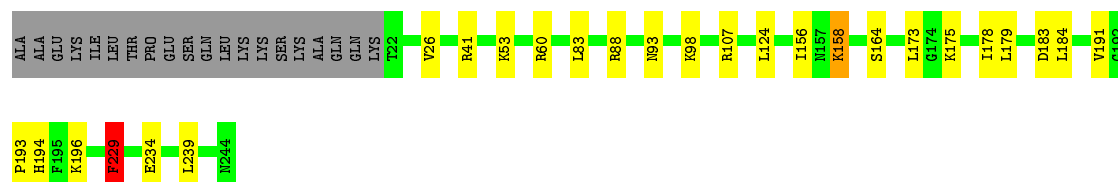


- Molecule 44: 60S ribosomal protein L7-A

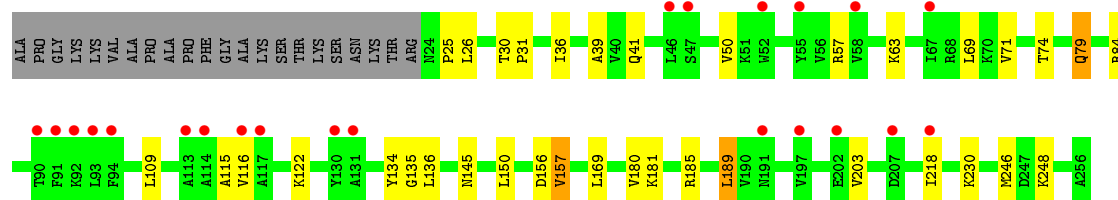
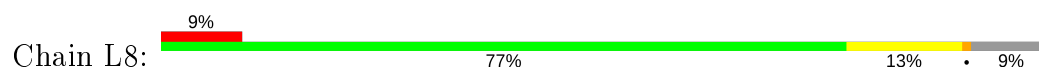


- Molecule 44: 60S ribosomal protein L7-A

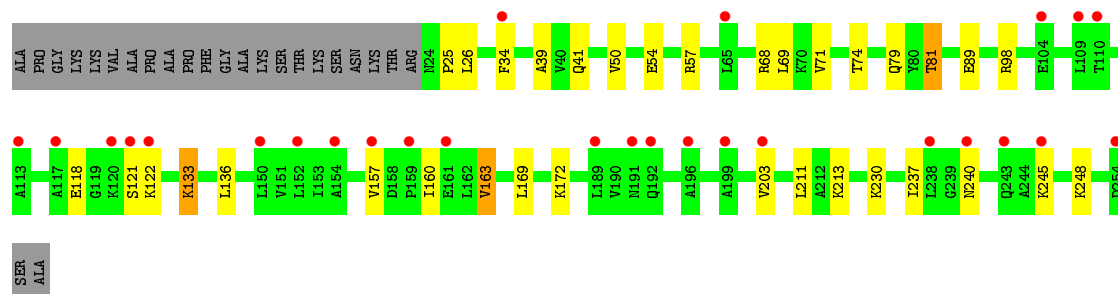
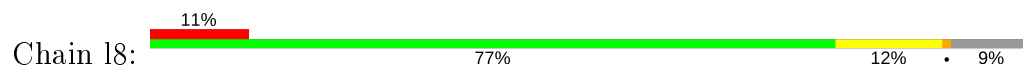




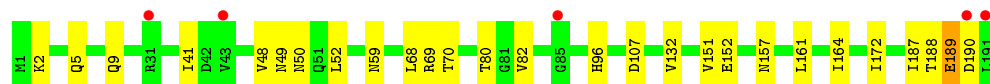
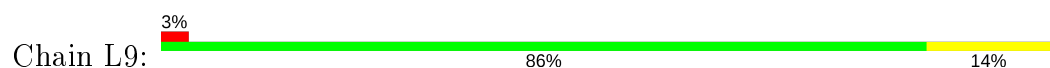
- Molecule 45: 60S ribosomal protein L8-A



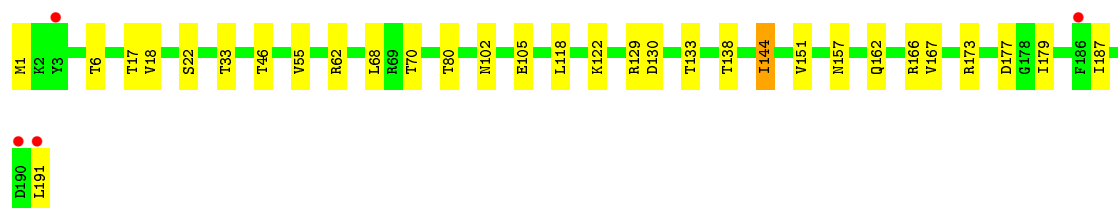
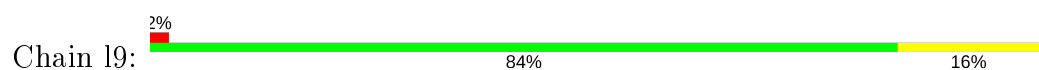
- Molecule 45: 60S ribosomal protein L8-A



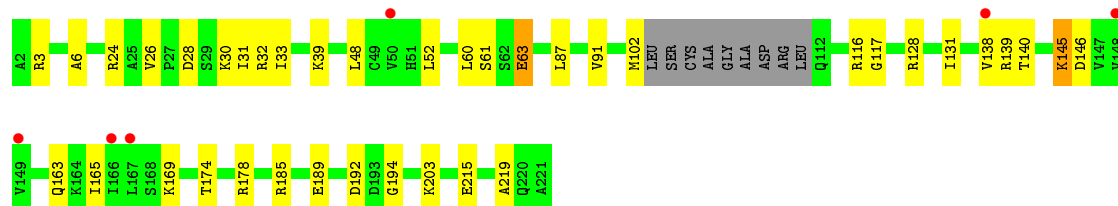
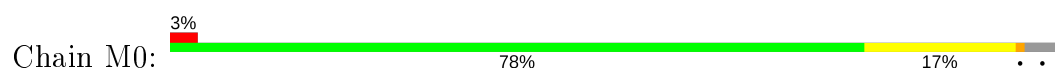
- Molecule 46: 60S ribosomal protein L9-A



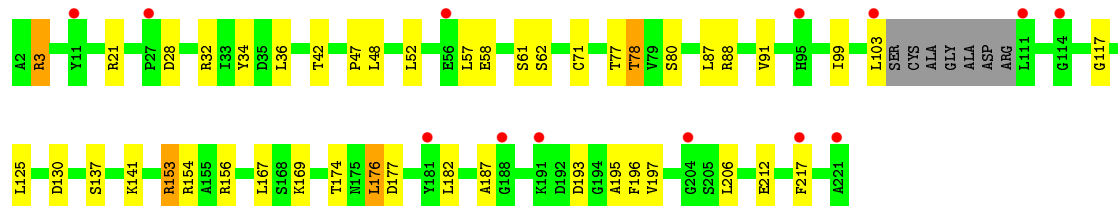
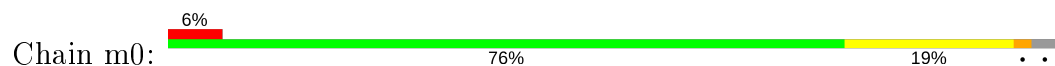
- Molecule 46: 60S ribosomal protein L9-A



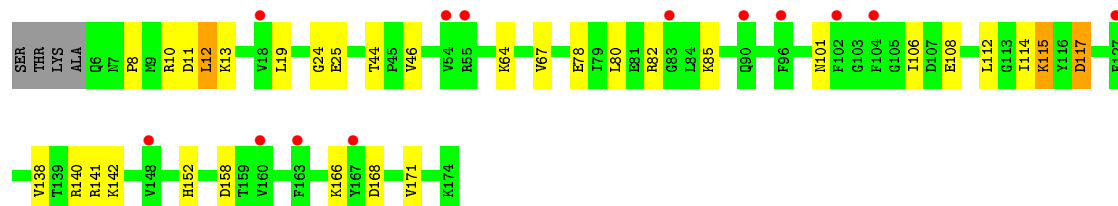
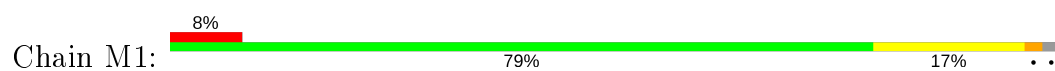
- Molecule 47: 60S ribosomal protein L10



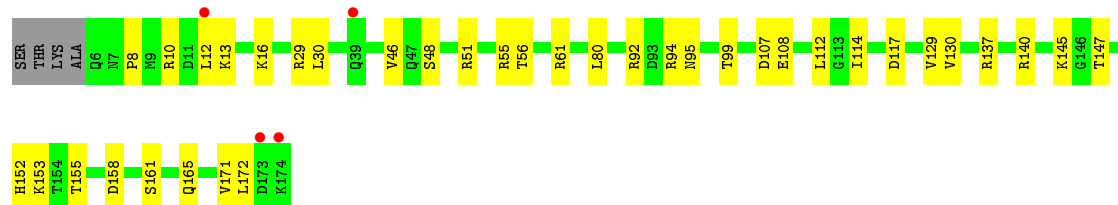
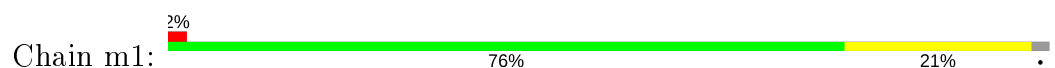
- Molecule 47: 60S ribosomal protein L10



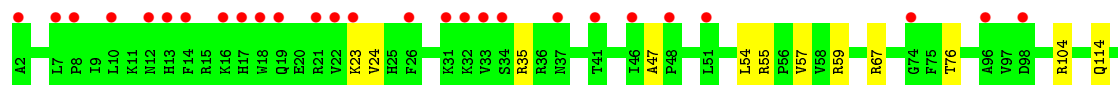
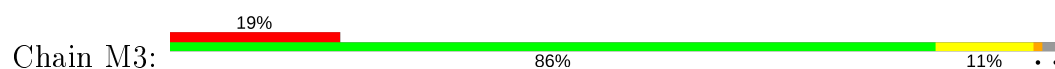
- Molecule 48: 60S ribosomal protein L11-B

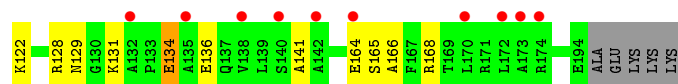


- Molecule 48: 60S ribosomal protein L11-B

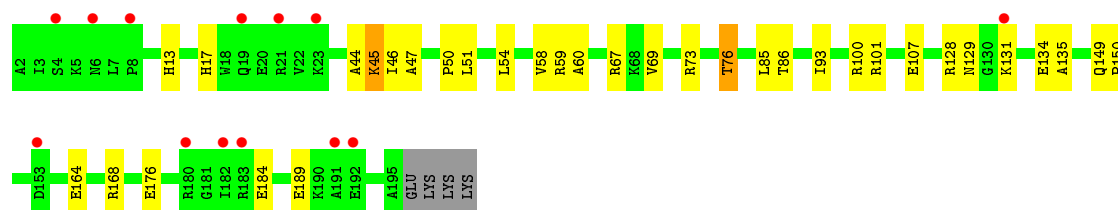
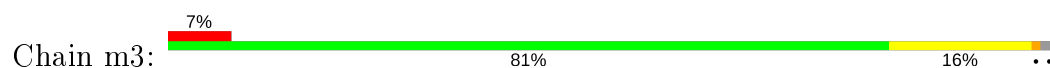


- Molecule 49: 60S ribosomal protein L13-A

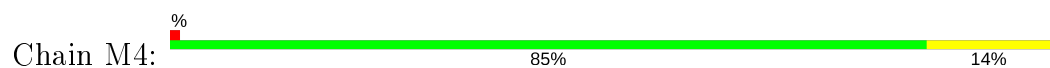




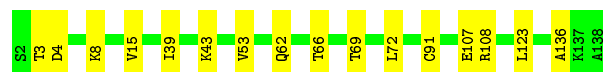
- Molecule 49: 60S ribosomal protein L13-A



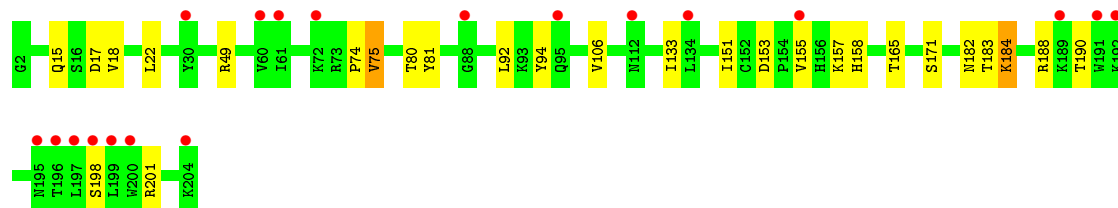
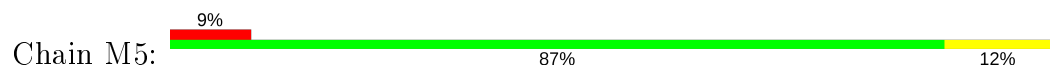
- Molecule 50: 60S ribosomal protein L14-A



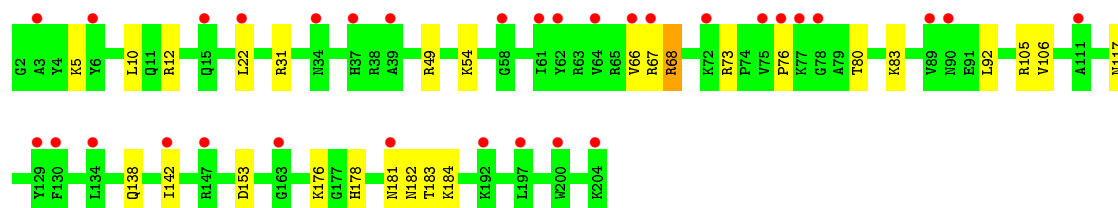
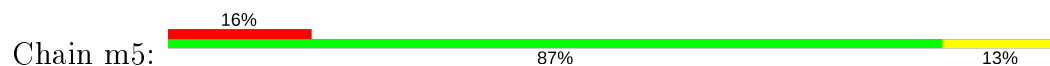
- Molecule 50: 60S ribosomal protein L14-A



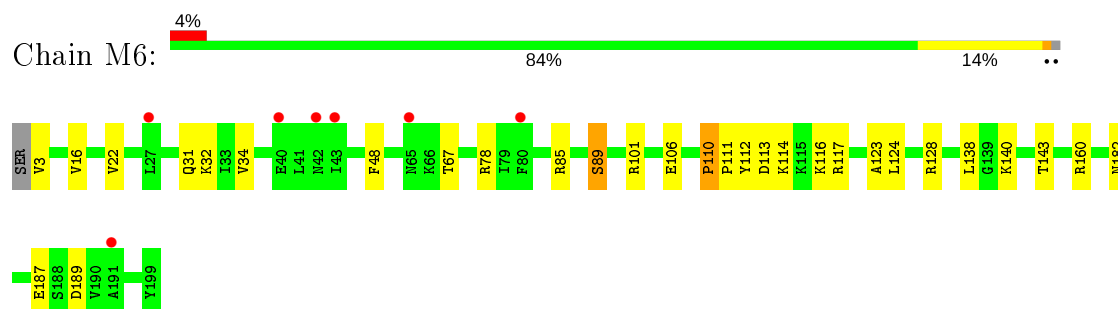
- Molecule 51: 60S ribosomal protein L15-A



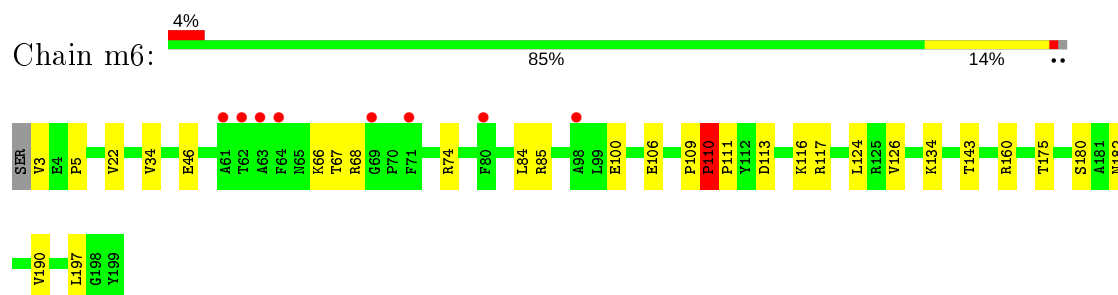
- Molecule 51: 60S ribosomal protein L15-A



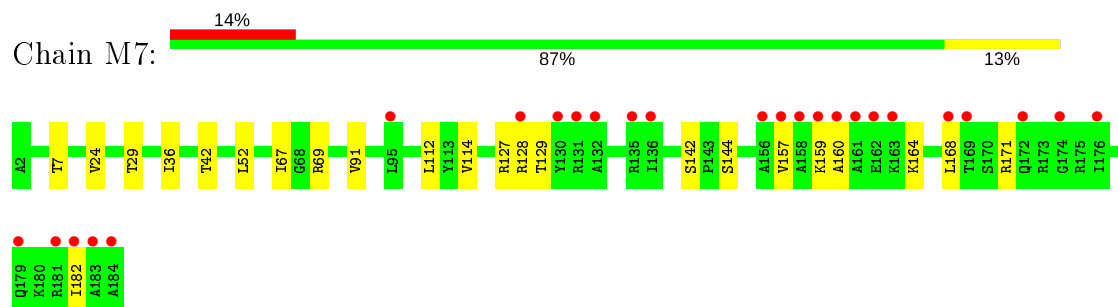
- Molecule 52: 60S ribosomal protein L16-A



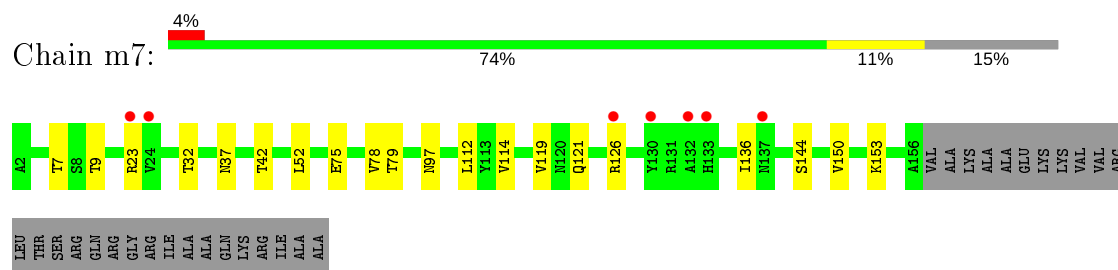
- Molecule 52: 60S ribosomal protein L16-A



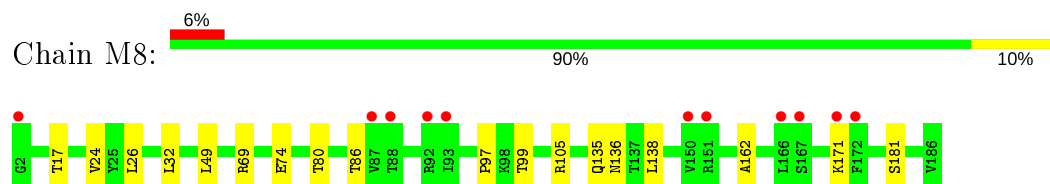
- Molecule 53: 60S ribosomal protein L17-A



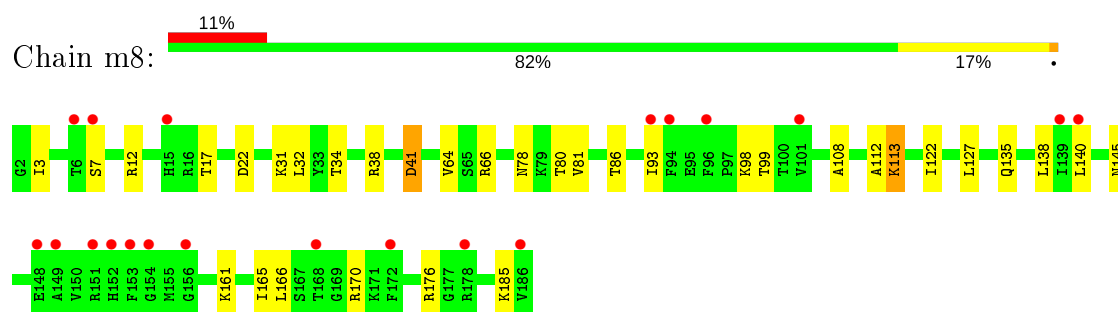
- Molecule 53: 60S ribosomal protein L17-A



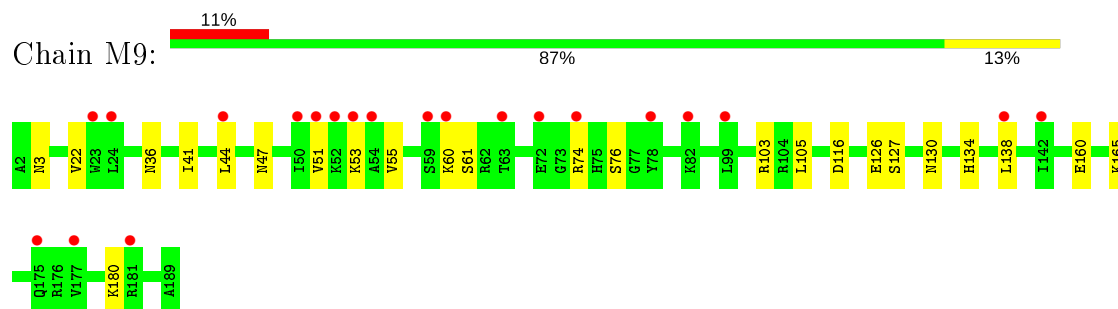
- Molecule 54: 60S ribosomal protein L18-A



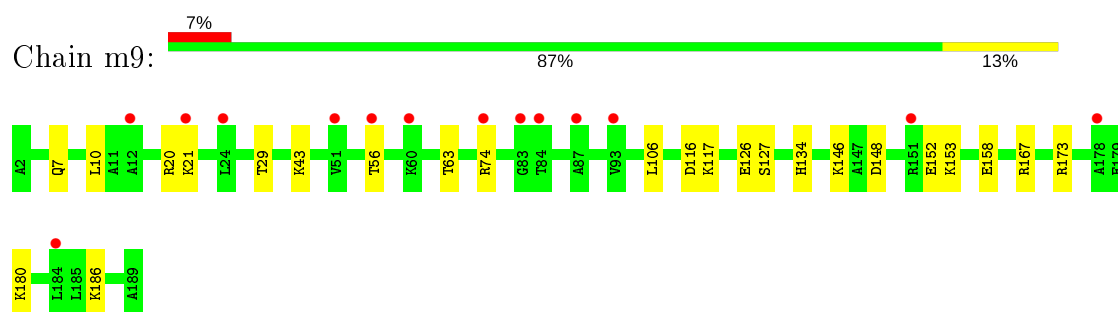
- Molecule 54: 60S ribosomal protein L18-A



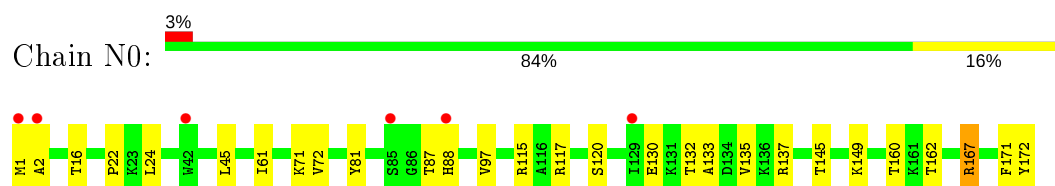
- Molecule 55: 60S ribosomal protein L19-A



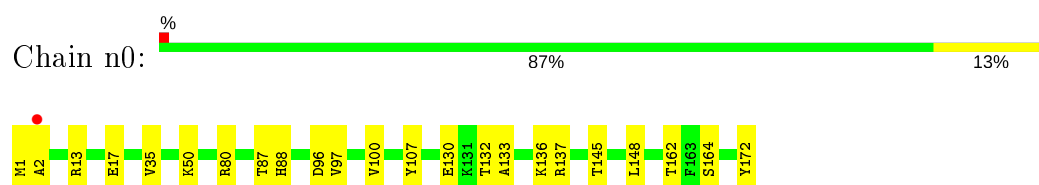
- Molecule 55: 60S ribosomal protein L19-A



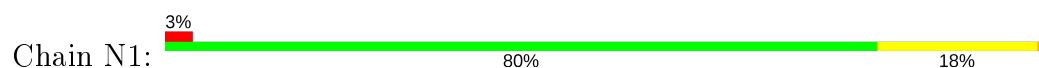
- Molecule 56: 60S ribosomal protein L20-A



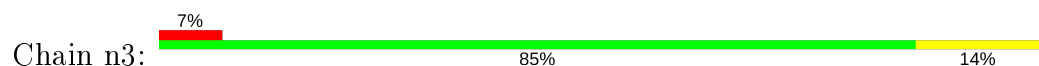
- Molecule 56: 60S ribosomal protein L20-A

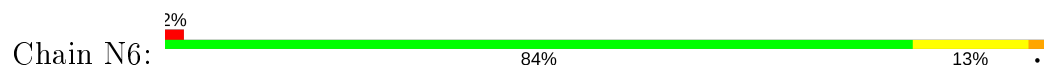


- Molecule 57: 60S ribosomal protein L21-A



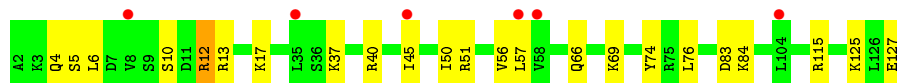
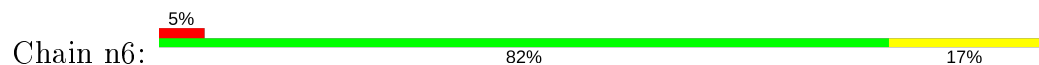




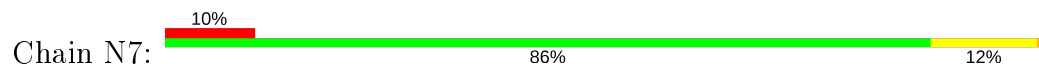




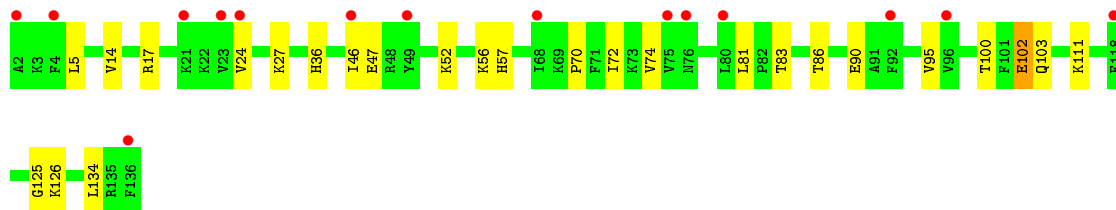
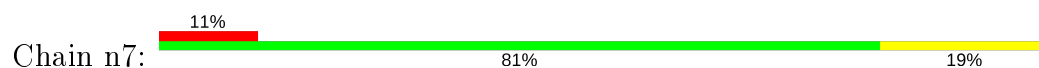
- Molecule 62: 60S ribosomal protein L26-A



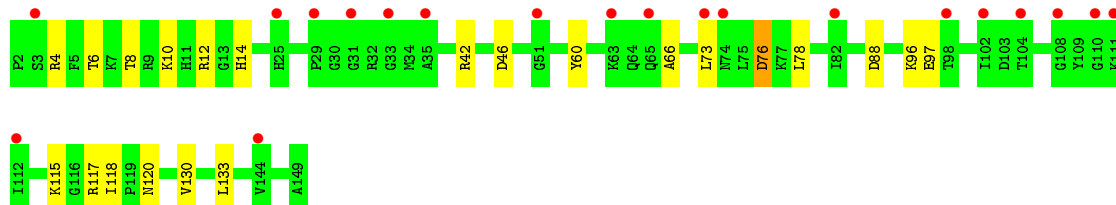
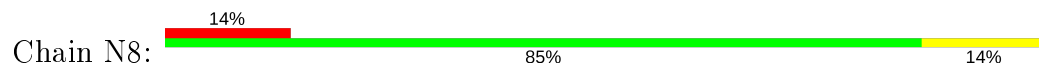
- Molecule 63: 60S ribosomal protein L27-A



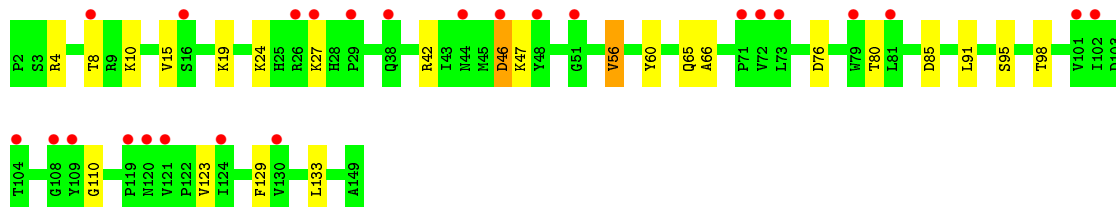
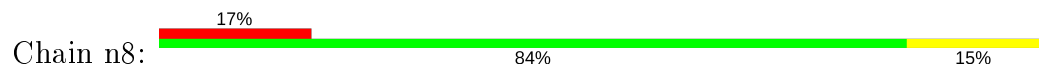
- Molecule 63: 60S ribosomal protein L27-A



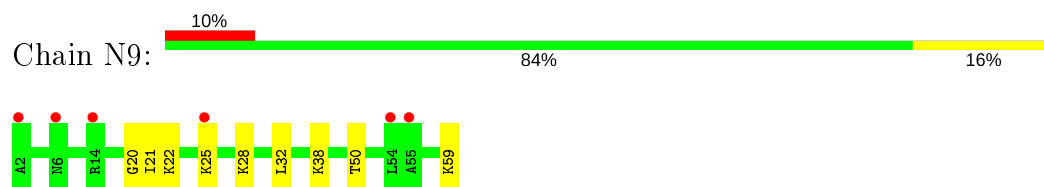
- Molecule 64: 60S ribosomal protein L28



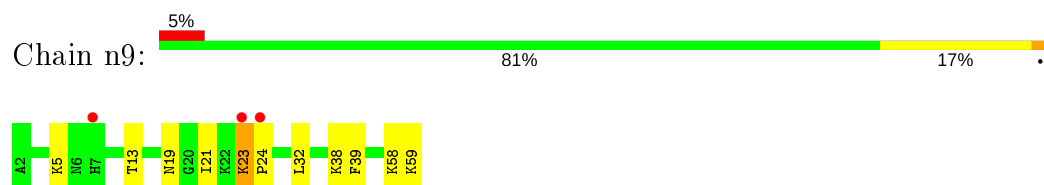
- Molecule 64: 60S ribosomal protein L28



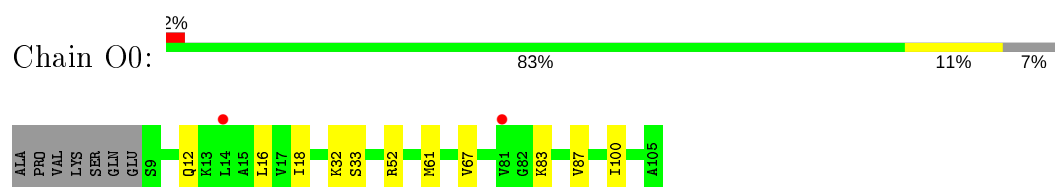
- Molecule 65: 60S ribosomal protein L29



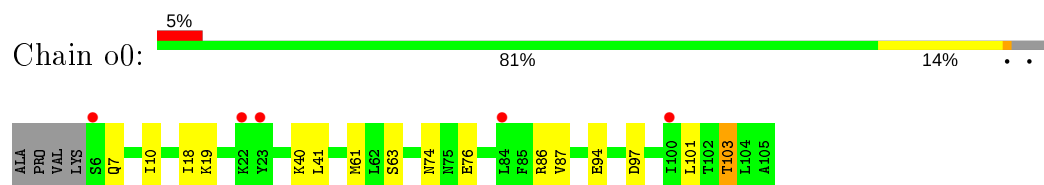
- Molecule 65: 60S ribosomal protein L29



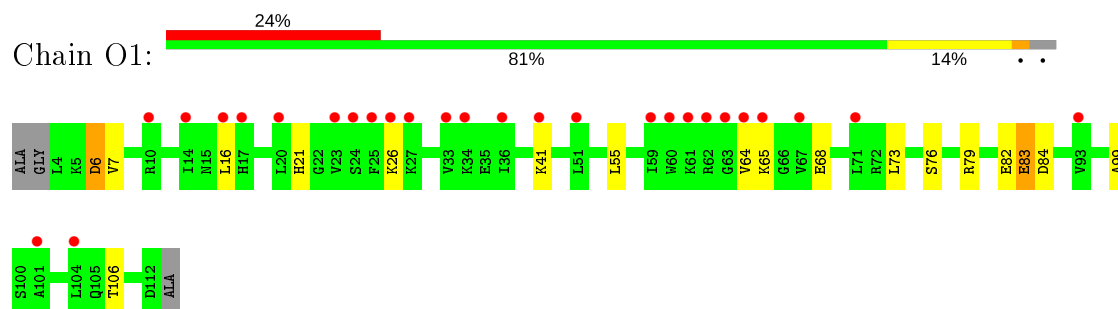
- Molecule 66: 60S ribosomal protein L30



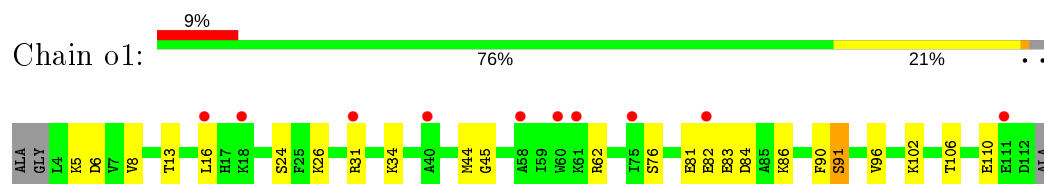
- Molecule 66: 60S ribosomal protein L30



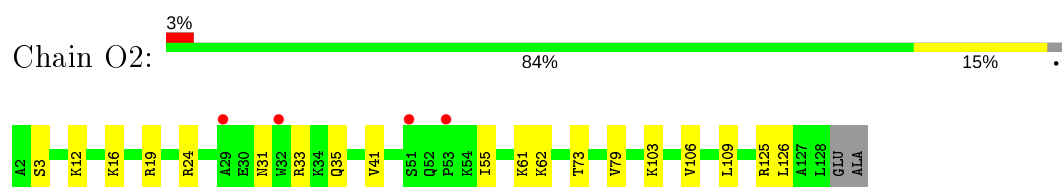
- Molecule 67: 60S ribosomal protein L31-A



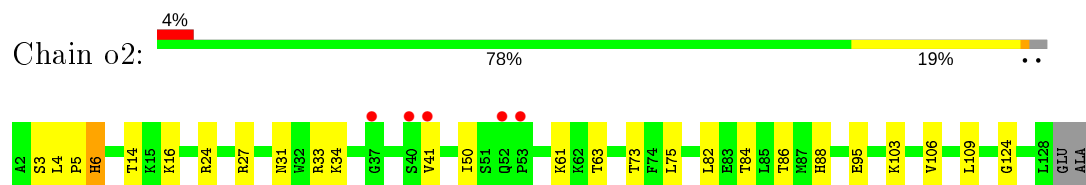
- Molecule 67: 60S ribosomal protein L31-A



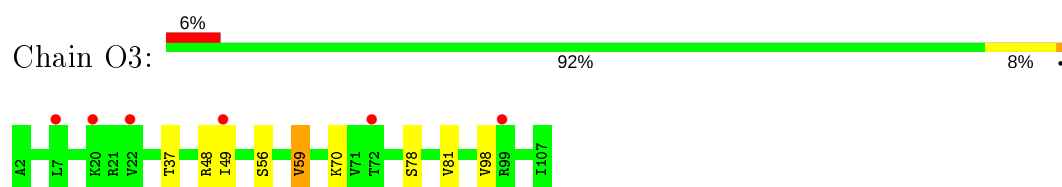
- Molecule 68: 60S ribosomal protein L32



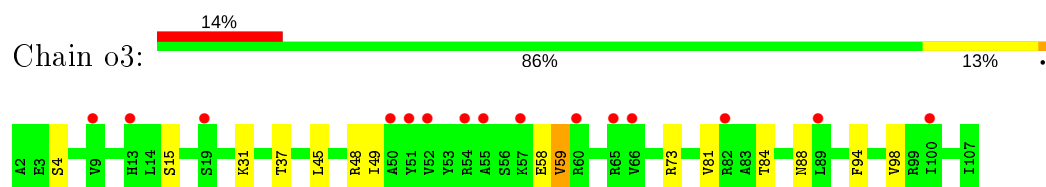
- Molecule 68: 60S ribosomal protein L32



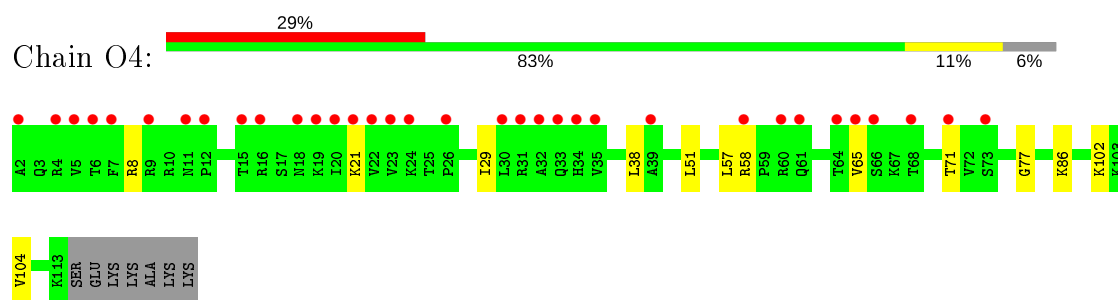
- Molecule 69: 60S ribosomal protein L33-A



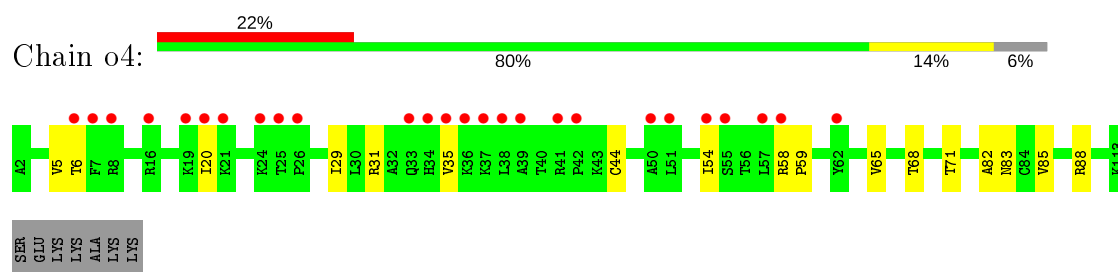
- Molecule 69: 60S ribosomal protein L33-A



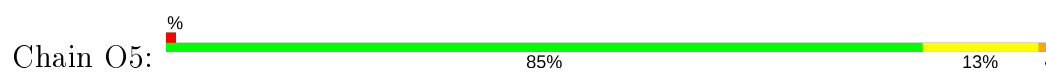
- Molecule 70: 60S ribosomal protein L34-A



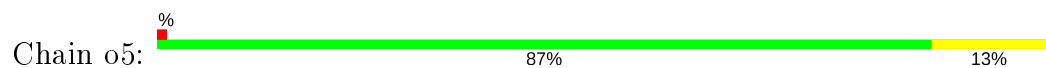
- Molecule 70: 60S ribosomal protein L34-A



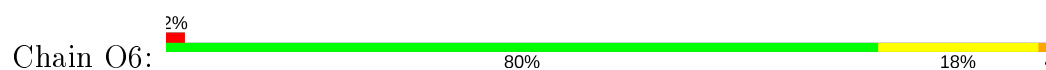
- Molecule 71: 60S ribosomal protein L35-A



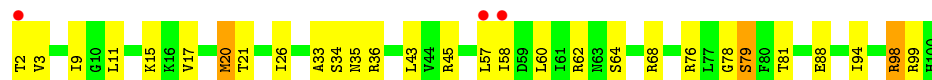
- Molecule 71: 60S ribosomal protein L35-A



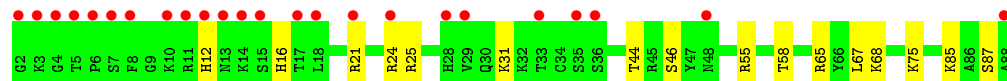
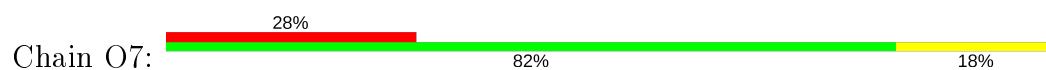
- Molecule 72: 60S ribosomal protein L36-A



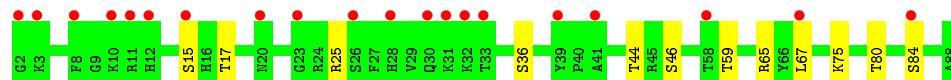
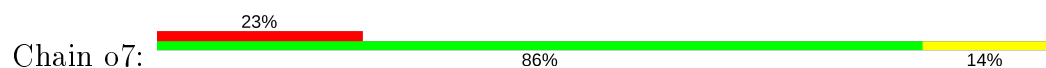
- Molecule 72: 60S ribosomal protein L36-A



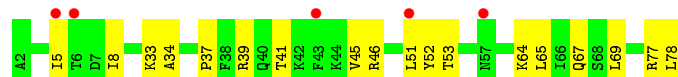
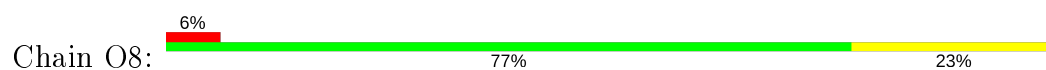
- Molecule 73: 60S ribosomal protein L37-A



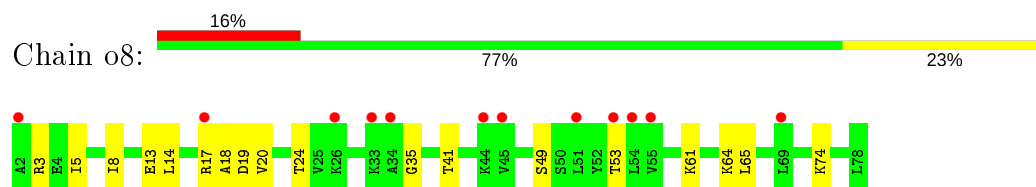
- Molecule 73: 60S ribosomal protein L37-A



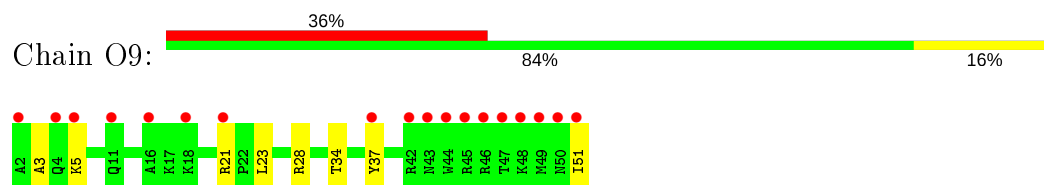
- Molecule 74: 60S ribosomal protein L38



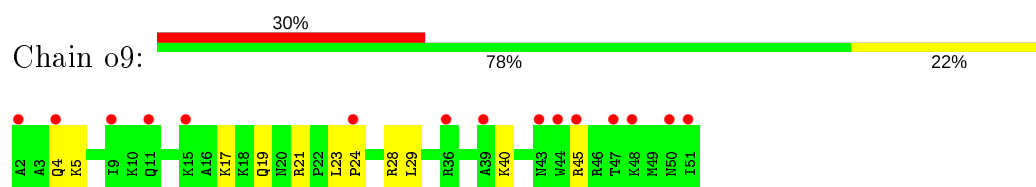
## • Molecule 74: 60S ribosomal protein L38



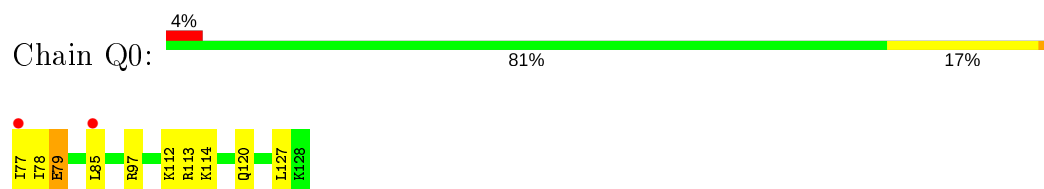
## • Molecule 75: 60S ribosomal protein L39



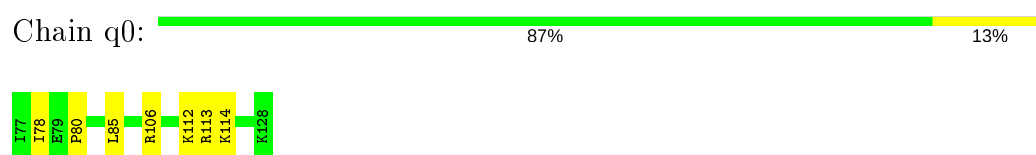
## • Molecule 75: 60S ribosomal protein L39



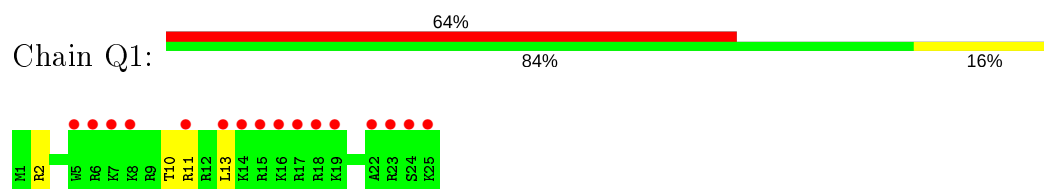
## • Molecule 76: Ubiquitin-60S ribosomal protein L40



## • Molecule 76: Ubiquitin-60S ribosomal protein L40



## • Molecule 77: 60S ribosomal protein L41-A

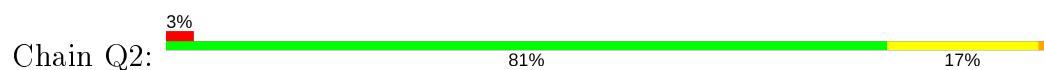


## • Molecule 77: 60S ribosomal protein L41-A

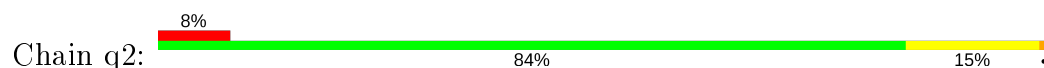




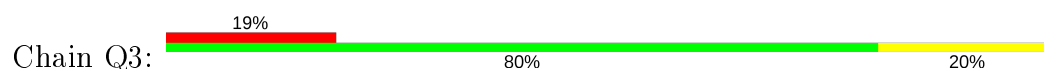
- Molecule 78: 60S ribosomal protein L42-A



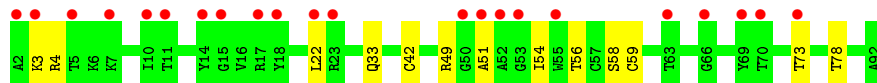
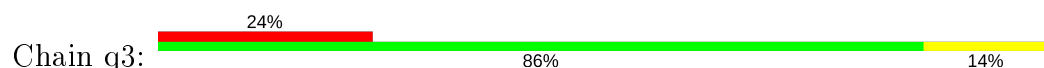
- Molecule 78: 60S ribosomal protein L42-A



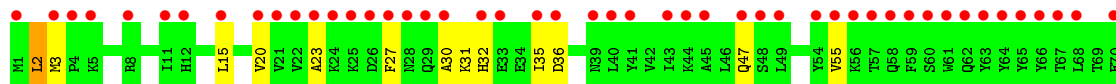
- Molecule 79: 60S ribosomal protein L43-A



- Molecule 79: 60S ribosomal protein L43-A



- Molecule 80: 40S ribosomal protein S10-A



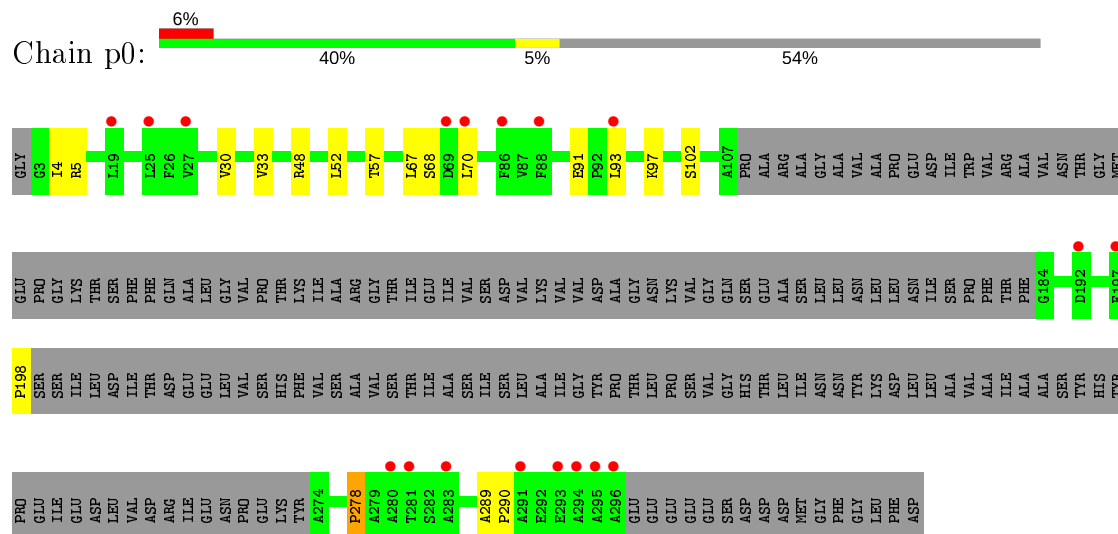
- Molecule 81: 60S ribosomal protein L12-A (uL11)



There are no outlier residues recorded for this chain.



- Molecule 82: 60S acidic ribosomal protein P0



- Molecule 83: 60S ribosomal protein P1 alpha



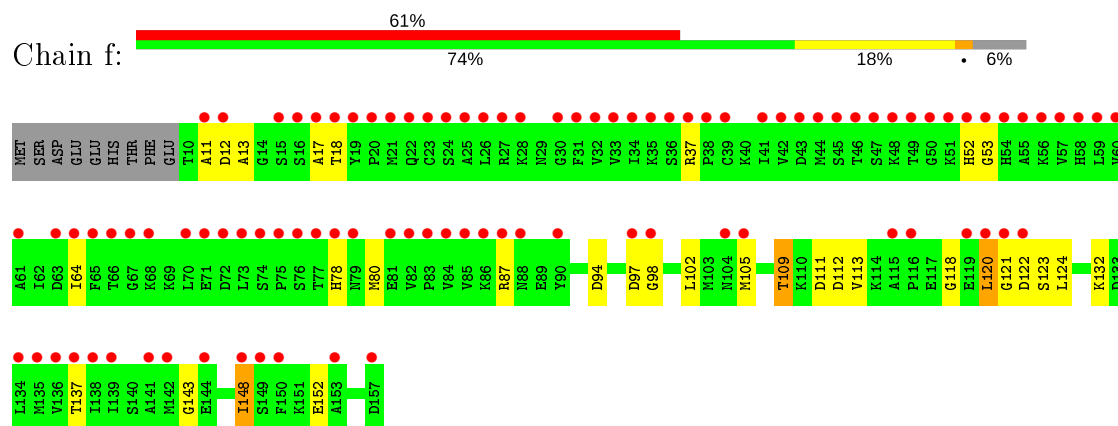
There are no outlier residues recorded for this chain.

- Molecule 84: 60S ribosomal P2 beta



There are no outlier residues recorded for this chain.

- Molecule 85: Eukaryotic translation initiation factor 5A-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	438.23 Å   289.33 Å   305.47 Å 90.00°   98.95°   90.00°	Depositor
Resolution (Å)	190.48 – 3.25 196.56 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (190.48-3.25) 99.9 (196.56-3.25)	Depositor EDS
$R_{merge}$	0.41	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 3.26 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.252 ,   0.301 0.257 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.7	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 78.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	404042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.52% 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:  
ZN

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	2	0.37	0/42467	0.89	53/66169 (0.1%)
1	6	0.43	0/42790	0.93	47/66673 (0.1%)
2	S0	0.28	0/1617	0.51	0/2215
2	s0	0.30	0/1623	0.52	0/2222
3	S1	0.27	0/1735	0.53	0/2335
3	s1	0.29	0/1748	0.52	0/2352
4	S2	0.30	0/1665	0.52	0/2263
4	s2	0.33	0/1665	0.57	1/2263 (0.0%)
5	S3	0.31	0/1759	0.49	0/2368
5	s3	0.29	0/1759	0.47	0/2368
6	S4	0.29	0/2109	0.53	0/2839
6	s4	0.34	0/2109	0.57	1/2839 (0.0%)
7	S5	0.27	0/1629	0.49	0/2202
7	s5	0.28	0/1629	0.50	0/2202
8	S6	0.29	0/1823	0.48	0/2439
8	s6	0.33	0/1779	0.52	0/2379
9	S7	0.29	0/1506	0.54	0/2028
9	s7	0.29	0/1516	0.53	1/2043 (0.0%)
10	S8	0.32	0/1514	0.51	0/2021
10	s8	0.35	0/1514	0.51	0/2021
11	S9	0.29	0/1519	0.49	0/2035
11	s9	0.31	0/1519	0.51	0/2035
12	C0	0.29	0/789	0.48	1/1067 (0.1%)
13	C1	0.32	0/1239	0.51	0/1673
13	c1	0.36	0/1194	0.52	0/1610
14	C2	0.28	0/898	0.52	1/1220 (0.1%)
14	c2	0.24	0/898	0.49	0/1220
15	C3	0.31	0/1215	0.51	1/1638 (0.1%)
15	c3	0.33	0/1215	0.53	0/1638
16	C4	0.28	0/901	0.54	0/1217
16	c4	0.30	0/960	0.55	0/1290
17	C5	0.31	0/998	0.55	1/1341 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	c5	0.31	0/1060	0.50	0/1426
18	C6	0.29	0/1125	0.56	2/1510 (0.1%)
18	c6	0.29	0/1131	0.51	0/1518
19	C7	0.31	0/935	0.54	0/1254
19	c7	0.29	0/914	0.52	0/1224
20	C8	0.30	0/1211	0.52	0/1628
20	c8	0.29	0/1211	0.51	0/1628
21	C9	0.28	0/1130	0.48	0/1517
21	c9	0.29	0/1130	0.47	0/1517
22	D0	0.30	0/865	0.55	0/1169
22	d0	0.28	0/892	0.52	0/1205
23	D1	0.28	0/693	0.51	0/935
23	d1	0.30	0/693	0.49	0/935
24	D2	0.31	0/1038	0.58	3/1395 (0.2%)
24	d2	0.34	0/1038	0.56	0/1395
25	D3	0.34	0/1139	0.54	0/1518
25	d3	0.38	0/1139	0.59	0/1518
26	D4	0.29	0/1087	0.46	0/1449
26	d4	0.31	0/1087	0.52	0/1449
27	D5	0.28	0/571	0.57	0/768
27	d5	0.27	0/566	0.47	0/761
28	D6	0.30	0/782	0.53	0/1047
28	d6	0.35	0/782	0.52	0/1047
29	D7	0.28	0/620	0.51	0/838
29	d7	0.28	0/620	0.50	0/838
30	D8	0.28	0/499	0.48	0/670
30	d8	0.28	0/499	0.54	0/670
31	D9	0.30	0/452	0.53	1/600 (0.2%)
31	d9	0.32	0/452	0.51	0/600
32	E0	0.28	0/483	0.47	0/643
32	e0	0.32	0/499	0.54	0/665
33	E1	0.30	0/577	0.60	0/770
33	e1	0.30	0/619	0.64	0/822
34	SR	0.26	0/2490	0.49	0/3389
34	sR	0.26	0/2495	0.45	0/3395
35	SM	0.32	0/1113	0.55	2/1502 (0.1%)
35	sM	0.32	0/682	0.50	0/921
36	1	0.55	0/75394	1.02	101/117545 (0.1%)
36	5	0.58	2/75865 (0.0%)	1.04	122/118275 (0.1%)
37	3	0.47	0/2883	0.88	0/4491
37	7	0.55	0/2883	1.03	4/4491 (0.1%)
38	4	0.51	0/3746	0.99	5/5832 (0.1%)
38	8	0.50	0/3746	0.95	4/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	L2	0.37	0/1948	0.58	0/2617
39	l2	0.39	0/1946	0.60	0/2614
40	L3	0.39	0/3146	0.57	0/4228
40	l3	0.43	0/3146	0.58	0/4228
41	L4	0.41	0/2800	0.60	0/3790
41	l4	0.40	1/2800 (0.0%)	0.62	1/3790 (0.0%)
42	L5	0.34	0/2425	0.53	0/3271
42	l5	0.40	0/2408	0.56	0/3248
43	L6	0.38	0/1260	0.56	0/1694
43	l6	0.41	0/1269	0.58	0/1705
44	L7	0.42	0/1821	0.59	0/2451
44	l7	0.44	0/1828	0.63	2/2461 (0.1%)
45	L8	0.31	0/1836	0.52	1/2481 (0.0%)
45	l8	0.33	0/1795	0.52	0/2429
46	L9	0.37	0/1539	0.55	0/2073
46	l9	0.40	0/1539	0.56	0/2073
47	M0	0.41	0/1741	0.55	0/2335
47	m0	0.43	0/1758	0.61	0/2358
48	M1	0.31	0/1374	0.50	0/1842
48	m1	0.34	0/1374	0.56	0/1842
49	M3	0.40	0/1568	0.59	0/2106
49	m3	0.40	0/1573	0.57	0/2113
50	M4	0.40	0/1068	0.54	0/1438
50	m4	0.41	0/1074	0.57	0/1446
51	M5	0.38	0/1757	0.57	0/2354
51	m5	0.37	0/1757	0.56	0/2354
52	M6	0.43	0/1585	0.58	0/2128
52	m6	0.50	0/1585	0.61	0/2128
53	M7	0.42	0/1443	0.55	0/1944
53	m7	0.44	0/1250	0.61	0/1683
54	M8	0.39	0/1465	0.60	0/1965
54	m8	0.40	0/1465	0.62	0/1965
55	M9	0.30	0/1538	0.48	0/2050
55	m9	0.34	0/1538	0.51	0/2050
56	N0	0.39	0/1481	0.59	0/1990
56	n0	0.43	0/1481	0.57	0/1990
57	N1	0.41	0/1300	0.56	0/1743
57	n1	0.44	0/1300	0.55	0/1743
58	N2	0.29	0/812	0.48	0/1099
58	n2	0.32	0/794	0.54	0/1076
59	N3	0.38	0/1018	0.56	0/1369
59	n3	0.45	0/1018	0.64	0/1369
60	N4	0.31	0/712	0.47	0/958

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
60	n4	0.36	0/1052	0.53	0/1398
61	N5	0.34	0/979	0.57	1/1321 (0.1%)
61	n5	0.34	0/974	0.56	0/1314
62	N6	0.37	0/1004	0.63	2/1341 (0.1%)
62	n6	0.34	0/1004	0.56	0/1341
63	N7	0.31	0/1118	0.51	0/1497
63	n7	0.31	0/1118	0.51	0/1497
64	N8	0.41	0/1204	0.64	0/1612
64	n8	0.42	0/1204	0.63	0/1612
65	N9	0.38	0/473	0.57	0/629
65	n9	0.45	0/473	0.71	1/629 (0.2%)
66	O0	0.30	0/751	0.46	0/1008
66	o0	0.32	0/775	0.51	0/1040
67	O1	0.36	0/890	0.53	0/1196
67	o1	0.43	0/897	0.59	0/1205
68	O2	0.42	0/1041	0.61	0/1394
68	o2	0.42	0/1041	0.59	0/1394
69	O3	0.44	0/868	0.52	0/1168
69	o3	0.47	0/868	0.58	0/1168
70	O4	0.33	0/890	0.53	1/1189 (0.1%)
70	o4	0.35	0/890	0.56	0/1189
71	O5	0.38	0/978	0.56	0/1301
71	o5	0.33	0/974	0.53	0/1297
72	O6	0.35	0/778	0.57	0/1034
72	o6	0.34	0/777	0.53	0/1033
73	O7	0.41	0/696	0.62	0/923
73	o7	0.39	0/696	0.61	0/923
74	O8	0.31	0/618	0.51	0/826
74	o8	0.32	0/614	0.51	0/822
75	O9	0.38	0/443	0.60	0/588
75	o9	0.37	0/443	0.56	0/588
76	Q0	0.44	0/423	0.60	0/562
76	q0	0.46	0/423	0.62	0/562
77	Q1	0.35	0/234	0.61	0/300
77	q1	0.43	0/234	0.58	0/300
78	Q2	0.51	1/860 (0.1%)	0.64	0/1136
78	q2	0.52	1/860 (0.1%)	0.64	1/1136 (0.1%)
79	Q3	0.38	0/701	0.58	0/934
79	q3	0.42	0/701	0.60	0/934
80	c0	0.28	0/777	0.53	2/1049 (0.2%)
82	p0	0.27	0/1091	0.53	2/1472 (0.1%)
85	f	0.31	0/1131	0.59	1/1522 (0.1%)
All	All	0.45	5/432438 (0.0%)	0.84	366/634802 (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
7	s5	0	1
18	c6	0	2
19	C7	0	1
27	D5	0	1
52	M6	0	1
52	m6	0	1
56	n0	0	1
64	n8	0	2
65	N9	0	1
All	All	0	11

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	q2	17	CYS	CB-SG	8.72	1.97	1.82
78	Q2	17	CYS	CB-SG	8.11	1.96	1.82
36	5	1152	G	N9-C4	-7.24	1.32	1.38
36	5	2971	A	N9-C4	6.37	1.41	1.37
41	l4	94	CYS	CB-SG	-5.72	1.72	1.81

All (366) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	1152	G	N3-C4-C5	13.24	135.22	128.60
36	5	1152	G	N3-C4-N9	-12.64	118.41	126.00
36	5	1152	G	C2-N3-C4	-10.83	106.48	111.90
36	5	2726	C	C6-N1-C2	-9.83	116.37	120.30
36	1	3217	C	N1-C2-O2	8.77	124.16	118.90
36	1	3217	C	C2-N1-C1'	8.69	128.36	118.80
36	5	2572	C	N1-C2-O2	8.67	124.10	118.90
36	1	1307	G	P-O3'-C3'	8.61	130.03	119.70
36	1	3217	C	N3-C2-O2	-8.04	116.27	121.90
36	1	406	G	O4'-C1'-N9	8.04	114.63	108.20
36	1	2572	C	N1-C2-O2	7.91	123.64	118.90
1	2	1096	C	N1-C2-O2	7.86	123.61	118.90
36	1	1269	U	C2-N1-C1'	7.83	127.10	117.70
36	5	1152	G	N3-C2-N2	-7.79	114.45	119.90
36	5	3245	A	N7-C8-N9	7.79	117.69	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1367	G	C5-C6-N1	-7.71	107.64	111.50
36	1	2306	C	C2-N1-C1'	7.68	127.25	118.80
36	1	2572	C	N3-C2-O2	-7.68	116.53	121.90
1	2	959	U	C2-N1-C1'	7.66	126.90	117.70
37	7	101	G	N1-C6-O6	7.64	124.49	119.90
38	4	125	U	C2-N1-C1'	7.58	126.80	117.70
1	2	1096	C	C2-N1-C1'	7.55	127.11	118.80
1	6	1473	U	C2-N1-C1'	7.55	126.76	117.70
36	1	637	C	C6-N1-C2	7.53	123.31	120.30
1	6	1274	C	N1-C2-O2	7.53	123.42	118.90
36	5	2572	C	C2-N1-C1'	7.51	127.06	118.80
36	5	1903	U	C5-C6-N1	7.45	126.42	122.70
36	5	3197	G	N3-C4-N9	-7.43	121.54	126.00
36	1	2714	G	N3-C4-C5	7.42	132.31	128.60
36	5	1152	G	N1-C6-O6	7.41	124.35	119.90
1	6	1185	U	N1-C2-O2	7.37	127.96	122.80
36	5	3154	C	C2-N1-C1'	7.31	126.84	118.80
1	6	1000	C	C2-N1-C1'	7.25	126.77	118.80
36	5	2278	C	N1-C2-O2	7.19	123.22	118.90
1	2	959	U	N3-C2-O2	-7.19	117.17	122.20
36	1	343	U	O5'-P-OP2	-7.19	99.23	105.70
36	1	1556	C	N3-C2-O2	-7.18	116.87	121.90
36	1	2572	C	C2-N1-C1'	7.17	126.69	118.80
1	2	728	U	C2-N1-C1'	7.17	126.30	117.70
36	1	3278	C	N1-C2-O2	7.16	123.20	118.90
36	1	2617	U	C5-C4-O4	7.16	130.19	125.90
36	5	3154	C	N1-C2-O2	7.15	123.19	118.90
36	5	2283	G	N1-C6-O6	7.14	124.19	119.90
1	2	1274	C	N1-C2-O2	7.13	123.18	118.90
36	5	1152	G	C8-N9-C1'	7.12	136.26	127.00
36	1	2278	C	N1-C2-O2	7.12	123.17	118.90
44	17	229	PHE	CB-CG-CD1	7.12	125.78	120.80
36	1	1269	U	N1-C2-O2	7.11	127.78	122.80
1	2	959	U	N1-C2-O2	7.10	127.77	122.80
36	1	2572	C	C6-N1-C2	-7.07	117.47	120.30
38	4	125	U	N1-C2-O2	7.06	127.74	122.80
36	1	24	G	O5'-P-OP2	-7.04	99.36	105.70
36	5	1903	U	N3-C4-O4	6.98	124.29	119.40
36	1	2306	C	N1-C2-O2	6.98	123.09	118.90
1	2	1370	U	P-O3'-C3'	6.96	128.05	119.70
36	1	1367	G	N1-C6-O6	6.95	124.07	119.90
1	2	728	U	N1-C2-O2	6.93	127.65	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	2572	C	N3-C2-O2	-6.92	117.06	121.90
36	5	1152	G	C4-N9-C1'	-6.92	117.51	126.50
1	6	1473	U	N3-C2-O2	-6.91	117.36	122.20
1	6	813	U	C2-N1-C1'	6.88	125.96	117.70
36	1	439	C	C2-N1-C1'	6.88	126.37	118.80
36	5	1307	G	P-O3'-C3'	6.83	127.89	119.70
36	5	1200	A	N1-C6-N6	6.82	122.69	118.60
36	5	2283	G	C5-C6-O6	-6.81	124.51	128.60
36	1	439	C	N1-C2-O2	6.74	122.94	118.90
36	1	583	G	O5'-P-OP1	-6.73	99.64	105.70
36	5	3245	A	C8-N9-C4	-6.73	103.11	105.80
1	2	507	U	C2-N1-C1'	6.72	125.77	117.70
1	2	1698	G	P-O3'-C3'	6.69	127.73	119.70
1	6	453	U	C2-N1-C1'	6.69	125.72	117.70
36	1	2714	G	N3-C4-N9	-6.68	121.99	126.00
36	1	1201	C	C6-N1-C2	-6.68	117.63	120.30
36	1	3278	C	N3-C2-O2	-6.66	117.24	121.90
62	N6	57	LEU	CA-CB-CG	6.66	130.61	115.30
36	1	1269	U	N3-C2-O2	-6.66	117.54	122.20
1	6	1473	U	N1-C2-O2	6.66	127.46	122.80
36	1	3057	U	N3-C2-O2	-6.64	117.55	122.20
36	5	3197	G	N3-C4-C5	6.62	131.91	128.60
36	1	3217	C	C6-N1-C1'	-6.60	112.88	120.80
38	8	80	A	N7-C8-N9	6.59	117.09	113.80
36	1	2283	G	N1-C6-O6	6.58	123.85	119.90
36	5	2526	C	N1-C2-O2	6.51	122.81	118.90
36	5	2524	A	O4'-C1'-N9	6.50	113.40	108.20
36	5	2376	G	O5'-P-OP2	-6.46	99.89	105.70
36	5	1192	C	N1-C2-O2	6.45	122.77	118.90
1	2	507	U	N1-C2-O2	6.43	127.30	122.80
36	5	2272	G	O4'-C1'-N9	6.43	113.34	108.20
1	2	728	U	N3-C2-O2	-6.40	117.72	122.20
36	1	1604	G	C4-N9-C1'	6.40	134.82	126.50
37	7	101	G	C5-C6-O6	-6.40	124.76	128.60
1	2	73	U	O4'-C1'-N1	6.39	113.31	108.20
36	5	2231	C	C2-N1-C1'	6.39	125.83	118.80
38	8	80	A	C8-N9-C4	-6.39	103.25	105.80
36	5	3049	A	C8-N9-C4	6.36	108.34	105.80
36	1	917	A	O5'-P-OP2	-6.36	99.98	105.70
36	1	1556	C	N1-C2-O2	6.33	122.70	118.90
1	2	831	U	C2-N1-C1'	6.32	125.28	117.70
36	5	922	U	N3-C2-O2	-6.31	117.78	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	813	U	N1-C2-O2	6.30	127.21	122.80
12	C0	88	PRO	N-CA-CB	6.29	110.85	103.30
36	1	922	U	C2-N1-C1'	6.29	125.25	117.70
36	5	3245	A	C5-N7-C8	-6.29	100.76	103.90
1	2	1039	A	O4'-C1'-N9	6.27	113.22	108.20
36	1	1903	U	N3-C4-O4	6.27	123.79	119.40
36	1	2829	U	N3-C4-O4	6.26	123.78	119.40
36	5	2273	G	C8-N9-C4	6.26	108.91	106.40
1	6	36	C	C5-C4-N4	-6.26	115.82	120.20
18	C6	40	GLU	C-N-CD	-6.25	106.85	120.60
36	5	3309	G	N3-C4-C5	-6.25	125.47	128.60
1	2	794	U	P-O3'-C3'	6.24	127.19	119.70
1	2	1274	C	N3-C2-O2	-6.22	117.55	121.90
1	2	639	U	N3-C2-O2	-6.22	117.84	122.20
36	5	1495	U	C2-N1-C1'	6.22	125.16	117.70
1	2	1052	U	C2-N1-C1'	6.22	125.16	117.70
36	5	718	G	O4'-C1'-N9	6.21	113.16	108.20
36	5	1903	U	N3-C4-C5	-6.20	110.88	114.60
36	5	968	G	O5'-P-OP1	-6.19	100.13	105.70
82	p0	290	PRO	N-CA-CB	6.18	110.72	103.30
36	1	2617	U	N1-C2-N3	6.18	118.61	114.90
80	c0	83	PRO	N-CA-CB	6.16	110.69	103.30
36	1	2355	G	N1-C6-O6	6.15	123.59	119.90
36	5	1849	C	C6-N1-C2	6.15	122.76	120.30
36	5	2728	G	C8-N9-C4	-6.15	103.94	106.40
1	6	1274	C	N3-C2-O2	-6.13	117.61	121.90
6	s4	38	LEU	CA-CB-CG	6.11	129.36	115.30
82	p0	278	PRO	N-CA-CB	6.09	110.61	103.30
36	1	2617	U	N3-C2-O2	-6.08	117.94	122.20
37	7	73	C	C2-N1-C1'	6.08	125.49	118.80
36	5	776	U	C5-C6-N1	-6.07	119.66	122.70
36	5	2971	A	C2-N3-C4	6.04	113.62	110.60
1	6	542	A	P-O3'-C3'	6.04	126.95	119.70
36	5	2996	U	C2-N1-C1'	6.04	124.95	117.70
36	5	1878	G	C4-N9-C1'	6.04	134.35	126.50
1	2	1389	C	N1-C2-O2	6.01	122.50	118.90
36	1	1581	C	N1-C2-O2	6.00	122.50	118.90
36	1	2419	A	O5'-P-OP1	-5.99	100.31	105.70
36	5	2726	C	N3-C2-O2	-5.99	117.70	121.90
36	5	406	G	O4'-C1'-N9	5.99	112.99	108.20
36	1	2846	U	N3-C2-O2	-5.97	118.02	122.20
36	5	1481	A	P-O3'-C3'	5.97	126.86	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1604	G	N3-C4-C5	-5.96	125.62	128.60
36	1	2273	G	C8-N9-C4	5.96	108.78	106.40
1	2	158	U	P-O3'-C3'	5.94	126.83	119.70
1	2	1657	U	C6-N1-C1'	5.94	129.52	121.20
36	5	1903	U	C6-N1-C2	-5.93	117.44	121.00
36	5	1879	A	O5'-P-OP1	5.93	117.82	110.70
65	n9	23	LYS	C-N-CD	5.93	140.85	128.40
1	6	163	G	C8-N9-C4	-5.93	104.03	106.40
36	5	1367	G	N1-C6-O6	5.92	123.45	119.90
36	1	1820	U	OP2-P-O3'	5.91	118.20	105.20
36	5	2205	U	O4'-C1'-N1	5.89	112.91	108.20
1	6	1097	U	P-O3'-C3'	5.87	126.75	119.70
36	5	2996	U	N1-C2-O2	5.85	126.90	122.80
35	SM	171	PRO	N-CA-CB	5.85	110.32	103.30
36	5	3309	G	C4-N9-C1'	5.85	134.10	126.50
1	2	1269	U	C2-N1-C1'	5.84	124.70	117.70
36	1	952	A	N1-C6-N6	5.84	122.10	118.60
36	1	3344	A	O4'-C1'-N9	5.84	112.87	108.20
1	2	1389	C	C2-N1-C1'	5.83	125.21	118.80
36	1	1556	C	C6-N1-C2	-5.79	117.98	120.30
36	5	3309	G	N3-C4-N9	5.78	129.47	126.00
1	6	1600	A	OP1-P-O3'	5.76	117.88	105.20
36	1	1903	U	C5-C6-N1	5.76	125.58	122.70
1	6	558	U	C2-N1-C1'	5.76	124.61	117.70
36	1	2273	G	C4-N9-C1'	-5.75	119.02	126.50
17	C5	52	LYS	C-N-CD	5.75	140.48	128.40
36	5	942	U	N3-C4-O4	5.74	123.42	119.40
80	c0	90	PRO	N-CA-CB	5.72	110.17	103.30
1	2	720	G	OP1-P-O3'	5.72	117.78	105.20
1	6	795	U	N3-C2-O2	-5.72	118.20	122.20
36	5	2617	U	N1-C2-O2	-5.70	118.81	122.80
36	5	3195	U	P-O3'-C3'	5.70	126.54	119.70
9	s7	131	PHE	C-N-CD	5.69	140.35	128.40
1	6	1274	C	C2-N1-C1'	5.69	125.06	118.80
36	1	1484	U	P-O3'-C3'	5.68	126.52	119.70
36	5	1308	A	C8-N9-C4	-5.67	103.53	105.80
36	5	1308	A	N7-C8-N9	5.66	116.63	113.80
1	6	158	U	P-O3'-C3'	5.66	126.49	119.70
1	2	1274	C	C2-N1-C1'	5.66	125.03	118.80
36	1	2870	C	O4'-C1'-N1	5.66	112.73	108.20
36	1	3057	U	N1-C2-O2	5.66	126.76	122.80
38	4	125	U	N3-C2-O2	-5.65	118.25	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1096	C	C6-N1-C1'	-5.65	114.02	120.80
36	5	2552	C	C2-N1-C1'	5.65	125.01	118.80
1	6	1698	G	P-O3'-C3'	5.64	126.47	119.70
36	5	1152	G	C5-N7-C8	-5.64	101.48	104.30
15	C3	22	ALA	C-N-CD	-5.63	108.21	120.60
36	5	869	G	N1-C6-O6	-5.63	116.52	119.90
36	1	910	G	C8-N9-C4	-5.63	104.15	106.40
36	5	1303	A	C8-N9-C4	5.60	108.04	105.80
1	6	795	U	C2-N1-C1'	5.60	124.42	117.70
36	5	1222	G	P-O3'-C3'	5.59	126.41	119.70
36	5	943	U	N1-C2-O2	-5.59	118.89	122.80
36	1	65	A	P-O3'-C3'	5.58	126.40	119.70
36	5	2943	G	C6-C5-N7	-5.58	127.05	130.40
31	D9	36	LEU	CA-CB-CG	5.57	128.11	115.30
1	2	1657	U	C5-C4-O4	5.57	129.24	125.90
36	5	1655	G	N7-C8-N9	5.56	115.88	113.10
36	1	1333	C	C6-N1-C2	-5.55	118.08	120.30
36	5	2374	C	C2-N1-C1'	5.55	124.91	118.80
36	5	3154	C	N3-C2-O2	-5.55	118.01	121.90
61	N5	34	LEU	CA-CB-CG	5.55	128.06	115.30
36	5	3092	C	O4'-C1'-N1	5.54	112.64	108.20
36	5	880	G	O4'-C1'-N9	5.54	112.63	108.20
78	q2	17	CYS	CA-CB-SG	5.54	123.97	114.00
1	2	639	U	N1-C2-O2	5.53	126.67	122.80
1	6	453	U	N1-C2-O2	5.53	126.67	122.80
36	5	3169	U	N1-C2-O2	5.53	126.67	122.80
36	1	1604	G	N3-C4-N9	5.52	129.31	126.00
1	6	965	U	C2-N1-C1'	5.52	124.32	117.70
1	6	402	C	O5'-P-OP2	-5.51	100.74	105.70
1	6	1745	G	N3-C4-N9	5.51	129.30	126.00
1	2	617	U	C2-N1-C1'	5.50	124.30	117.70
1	2	1000	C	C2-N1-C1'	5.50	124.85	118.80
36	1	2679	A	O4'-C1'-N9	5.50	112.60	108.20
24	D2	104	LEU	CA-CB-CG	5.50	127.94	115.30
36	5	2146	C	N1-C2-O2	5.48	122.19	118.90
36	5	2833	A	C8-N9-C4	5.48	107.99	105.80
1	2	1246	C	C2-N1-C1'	5.47	124.82	118.80
36	1	835	G	O4'-C1'-N9	5.47	112.57	108.20
36	1	718	G	C4-C5-N7	5.46	112.98	110.80
36	1	1556	C	C2-N1-C1'	5.45	124.79	118.80
36	5	1655	G	C8-N9-C4	-5.45	104.22	106.40
1	2	720	G	P-O3'-C3'	5.44	126.23	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	830	U	N1-C2-O2	5.44	126.61	122.80
36	5	2572	C	C6-N1-C1'	-5.44	114.28	120.80
36	1	2373	A	O5'-P-OP1	-5.43	100.82	105.70
1	6	144	U	C2-N1-C1'	5.43	124.21	117.70
1	2	1657	U	C2-N1-C1'	-5.42	111.19	117.70
36	1	1368	U	C5-C4-O4	-5.42	122.65	125.90
36	5	1316	C	C6-N1-C2	-5.42	118.13	120.30
1	2	581	U	C2-N1-C1'	5.42	124.20	117.70
36	1	3344	A	N7-C8-N9	5.41	116.51	113.80
1	2	507	U	N3-C2-O2	-5.40	118.42	122.20
38	8	95	G	C4-N9-C1'	-5.40	119.48	126.50
36	1	1604	G	C8-N9-C1'	-5.40	119.98	127.00
24	D2	65	LEU	CA-CB-CG	5.39	127.71	115.30
36	1	2571	U	N3-C2-O2	-5.39	118.43	122.20
36	5	833	G	N1-C6-O6	-5.39	116.67	119.90
1	2	1560	U	N3-C2-O2	-5.39	118.43	122.20
36	1	1716	U	P-O3'-C3'	5.38	126.16	119.70
24	D2	93	LEU	CA-CB-CG	5.38	127.66	115.30
44	17	229	PHE	CB-CG-CD2	-5.36	117.05	120.80
36	1	2836	C	N3-C2-O2	-5.36	118.15	121.90
36	5	891	G	N1-C6-O6	-5.35	116.69	119.90
36	1	2541	U	P-O3'-C3'	5.35	126.12	119.70
36	1	1434	G	C5-C6-N1	5.34	114.17	111.50
36	1	2306	C	N3-C2-O2	-5.34	118.16	121.90
1	6	558	U	P-O3'-C3'	5.34	126.11	119.70
1	6	1000	C	N3-C2-O2	-5.34	118.16	121.90
36	5	922	U	C5-C6-N1	-5.34	120.03	122.70
1	6	813	U	N3-C2-O2	-5.34	118.46	122.20
36	5	3311	C	C6-N1-C2	-5.33	118.17	120.30
1	2	1761	U	P-O3'-C3'	5.33	126.10	119.70
36	5	1481	A	C8-N9-C4	-5.33	103.67	105.80
36	5	2943	G	N1-C6-O6	5.33	123.10	119.90
1	2	831	U	N1-C2-O2	5.33	126.53	122.80
1	2	1096	C	N3-C2-O2	-5.33	118.17	121.90
36	1	2306	C	C6-N1-C1'	-5.33	114.41	120.80
1	2	1657	U	N1-C2-N3	5.32	118.09	114.90
1	6	1745	G	C5-C6-O6	-5.30	125.42	128.60
1	2	1370	U	OP2-P-O3'	5.29	116.85	105.20
36	5	1367	G	C5-C6-N1	-5.29	108.86	111.50
36	5	3214	U	N3-C2-O2	-5.29	118.50	122.20
1	6	858	G	O4'-C1'-N9	5.28	112.42	108.20
1	2	75	U	N1-C2-O2	5.28	126.49	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1820	U	P-O3'-C3'	5.28	126.03	119.70
1	6	864	U	C2-N1-C1'	5.28	124.03	117.70
1	6	453	U	C5-C6-N1	5.27	125.34	122.70
1	2	1573	A	OP2-P-O3'	5.27	116.79	105.20
36	5	2376	G	C8-N9-C1'	-5.26	120.16	127.00
36	1	2371	G	N3-C2-N2	5.26	123.58	119.90
36	1	283	G	C4-C5-N7	5.26	112.90	110.80
36	5	1604	G	C4-N9-C1'	5.25	133.33	126.50
36	5	3197	G	N3-C2-N2	-5.25	116.22	119.90
36	1	3318	G	C4-N9-C1'	5.25	133.32	126.50
1	2	831	U	C5-C6-N1	5.24	125.32	122.70
35	SM	134	ASP	CB-CG-OD2	5.24	123.02	118.30
36	1	857	G	N1-C6-O6	5.23	123.04	119.90
36	1	959	C	O5'-P-OP2	-5.23	100.99	105.70
36	5	2400	G	N1-C6-O6	5.23	123.04	119.90
38	4	125	U	C6-N1-C1'	-5.23	113.88	121.20
36	5	776	U	C4-C5-C6	5.23	122.84	119.70
36	1	3096	C	C6-N1-C2	-5.23	118.21	120.30
1	6	1361	U	C2-N1-C1'	5.22	123.97	117.70
36	1	1349	G	O4'-C1'-N9	5.22	112.37	108.20
36	5	2584	G	C4-N9-C1'	5.22	133.28	126.50
36	5	3197	G	C4-N9-C1'	-5.22	119.72	126.50
36	5	835	G	O4'-C1'-N9	5.21	112.37	108.20
36	5	3195	U	OP1-P-O3'	5.21	116.66	105.20
36	5	1200	A	C6-C5-N7	-5.21	128.65	132.30
38	8	125	U	C2-N1-C1'	5.21	123.95	117.70
36	1	2550	U	N1-C2-O2	5.21	126.44	122.80
36	5	1716	U	P-O3'-C3'	5.20	125.94	119.70
1	2	1573	A	P-O3'-C3'	5.20	125.94	119.70
1	6	1246	C	C2-N1-C1'	5.20	124.52	118.80
1	2	1489	U	N3-C2-O2	-5.19	118.57	122.20
36	5	2942	C	N1-C2-O2	-5.19	115.78	118.90
36	5	2531	C	C2-N1-C1'	5.19	124.51	118.80
36	1	776	U	C4-C5-C6	5.18	122.81	119.70
1	6	1537	C	C6-N1-C2	-5.18	118.23	120.30
1	6	829	A	OP1-P-O3'	5.17	116.56	105.20
36	5	1154	A	N1-C6-N6	-5.17	115.50	118.60
1	6	1058	U	OP1-P-O3'	5.16	116.54	105.20
36	5	283	G	C4-C5-N7	5.14	112.86	110.80
14	C2	103	LEU	CA-CB-CG	5.14	127.13	115.30
36	1	2371	G	N1-C2-N2	-5.14	111.57	116.20
36	1	2314	U	C2-N1-C1'	5.14	123.87	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	1	1444	G	C4-C5-N7	5.13	112.85	110.80
1	6	194	U	C2-N1-C1'	5.13	123.86	117.70
36	1	1858	A	C2-N3-C4	5.13	113.16	110.60
36	5	1203	A	N1-C6-N6	5.13	121.68	118.60
36	5	915	A	C2-N3-C4	5.12	113.16	110.60
36	5	2726	C	C5-C4-N4	5.12	123.79	120.20
36	5	776	U	N1-C2-N3	5.12	117.97	114.90
36	5	2231	C	C6-N1-C1'	-5.12	114.66	120.80
36	5	1858	A	O4'-C1'-N9	5.12	112.29	108.20
36	5	2843	U	N1-C2-O2	5.12	126.38	122.80
1	6	151	G	N3-C4-N9	-5.11	122.93	126.00
36	5	915	A	N3-C4-C5	-5.11	123.22	126.80
36	1	3316	A	OP2-P-O3'	5.11	116.44	105.20
36	5	2288	G	N1-C6-O6	5.11	122.96	119.90
36	1	2829	U	C5-C4-O4	-5.10	122.84	125.90
38	4	103	G	N3-C4-C5	-5.10	126.05	128.60
36	5	2411	U	C5-C4-O4	5.10	128.96	125.90
36	5	966	U	N3-C2-O2	-5.09	118.63	122.20
1	6	1000	C	C6-N1-C1'	-5.09	114.69	120.80
36	1	1201	C	C5-C6-N1	5.09	123.55	121.00
36	1	2706	G	N3-C4-N9	5.09	129.05	126.00
36	1	3196	U	N3-C2-O2	-5.09	118.64	122.20
85	f	53	GLY	N-CA-C	5.09	125.82	113.10
36	5	2950	G	O4'-C1'-N9	5.09	112.27	108.20
1	6	782	U	N3-C2-O2	-5.09	118.64	122.20
36	5	3377	G	C5-C6-O6	-5.09	125.55	128.60
18	C6	40	GLU	C-N-CA	5.08	143.35	122.00
36	1	1581	C	N3-C2-O2	-5.08	118.34	121.90
62	N6	126	LEU	CA-CB-CG	5.08	126.99	115.30
1	6	453	U	N3-C2-O2	-5.08	118.64	122.20
36	5	2552	C	N1-C2-O2	5.08	121.95	118.90
36	5	1628	C	C6-N1-C2	-5.08	118.27	120.30
70	O4	51	LEU	CA-CB-CG	5.08	126.98	115.30
41	14	340	GLY	N-CA-C	-5.08	100.40	113.10
36	5	419	G	N7-C8-N9	-5.07	110.56	113.10
45	L8	189	LEU	CA-CB-CG	5.07	126.96	115.30
4	s2	93	GLY	N-CA-C	5.07	125.78	113.10
36	5	2772	C	P-O3'-C3'	5.07	125.78	119.70
1	2	959	U	C6-N1-C1'	-5.07	114.10	121.20
36	1	2132	C	N1-C2-O2	5.07	121.94	118.90
36	5	2725	U	O5'-P-OP2	-5.07	101.14	105.70
37	7	115	G	N3-C4-C5	-5.06	126.07	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	1640	C	C2-N1-C1'	5.04	124.35	118.80
36	1	1351	U	N1-C2-O2	5.04	126.33	122.80
1	2	1389	C	N3-C2-O2	-5.03	118.38	121.90
36	1	1367	G	C4-C5-C6	5.02	121.81	118.80
1	6	103	A	P-O3'-C3'	5.02	125.73	119.70
1	2	1052	U	N1-C2-O2	5.02	126.31	122.80
36	1	2112	U	P-O3'-C3'	5.02	125.72	119.70
36	5	1429	G	C6-C5-N7	-5.02	127.39	130.40
1	2	829	A	P-O3'-C3'	5.02	125.72	119.70
36	1	776	U	N3-C2-O2	-5.01	118.69	122.20
1	6	610	G	C4-N9-C1'	5.01	133.02	126.50
1	6	1058	U	P-O3'-C3'	5.01	125.72	119.70
36	1	109	A	OP1-P-O3'	5.01	116.22	105.20
36	5	2345	A	N1-C6-N6	5.00	121.60	118.60
36	5	3154	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	C7	85	VAL	Peptide
27	D5	94	LYS	Peptide
52	M6	110	PRO	Peptide
65	N9	20	GLY	Peptide
18	c6	40	GLU	Peptide
18	c6	41	PRO	Peptide
52	m6	110	PRO	Peptide
56	n0	133	ALA	Peptide
64	n8	46	ASP	Peptide
64	n8	66	ALA	Peptide
7	s5	99	MET	Peptide

## 5.2 Too-close contacts

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



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	
2	S0	204/251 (81%)	156 (76%)	30 (15%)	18 (9%)	1	5
2	s0	204/251 (81%)	158 (78%)	31 (15%)	15 (7%)	1	7
3	S1	212/254 (84%)	154 (73%)	36 (17%)	22 (10%)	0	3
3	s1	214/254 (84%)	165 (77%)	37 (17%)	12 (6%)	2	11
4	S2	215/253 (85%)	174 (81%)	33 (15%)	8 (4%)	3	19
4	s2	215/253 (85%)	175 (81%)	26 (12%)	14 (6%)	1	9
5	S3	221/239 (92%)	189 (86%)	21 (10%)	11 (5%)	2	13
5	s3	221/239 (92%)	183 (83%)	27 (12%)	11 (5%)	2	13
6	S4	258/260 (99%)	205 (80%)	37 (14%)	16 (6%)	1	10
6	s4	258/260 (99%)	198 (77%)	44 (17%)	16 (6%)	1	10
7	S5	204/224 (91%)	163 (80%)	28 (14%)	13 (6%)	1	9
7	s5	204/224 (91%)	157 (77%)	30 (15%)	17 (8%)	1	5
8	S6	224/236 (95%)	198 (88%)	17 (8%)	9 (4%)	3	17
8	s6	216/236 (92%)	186 (86%)	24 (11%)	6 (3%)	5	25
9	S7	182/189 (96%)	137 (75%)	27 (15%)	18 (10%)	0	3
9	s7	184/189 (97%)	146 (79%)	25 (14%)	13 (7%)	1	7
10	S8	184/200 (92%)	159 (86%)	18 (10%)	7 (4%)	3	19
10	s8	184/200 (92%)	156 (85%)	21 (11%)	7 (4%)	3	19
11	S9	183/196 (93%)	148 (81%)	28 (15%)	7 (4%)	3	19
11	s9	183/196 (93%)	151 (82%)	24 (13%)	8 (4%)	2	15
12	C0	94/105 (90%)	74 (79%)	13 (14%)	7 (7%)	1	7
13	C1	153/155 (99%)	123 (80%)	23 (15%)	7 (5%)	2	15
13	c1	144/155 (93%)	122 (85%)	20 (14%)	2 (1%)	11	40
14	C2	122/142 (86%)	73 (60%)	32 (26%)	17 (14%)	0	1
14	c2	122/142 (86%)	76 (62%)	30 (25%)	16 (13%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	C3	148/150 (99%)	122 (82%)	20 (14%)	6 (4%)	3	17
15	c3	148/150 (99%)	117 (79%)	21 (14%)	10 (7%)	1	8
16	C4	125/136 (92%)	92 (74%)	21 (17%)	12 (10%)	0	4
16	c4	126/136 (93%)	98 (78%)	19 (15%)	9 (7%)	1	7
17	C5	122/141 (86%)	90 (74%)	17 (14%)	15 (12%)	0	2
17	c5	133/141 (94%)	98 (74%)	19 (14%)	16 (12%)	0	2
18	C6	139/142 (98%)	111 (80%)	19 (14%)	9 (6%)	1	9
18	c6	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	2	16
19	C7	116/136 (85%)	89 (77%)	20 (17%)	7 (6%)	1	10
19	c7	113/136 (83%)	89 (79%)	16 (14%)	8 (7%)	1	7
20	C8	143/145 (99%)	109 (76%)	27 (19%)	7 (5%)	2	14
20	c8	143/145 (99%)	116 (81%)	21 (15%)	6 (4%)	3	16
21	C9	141/143 (99%)	115 (82%)	19 (14%)	7 (5%)	2	13
21	c9	141/143 (99%)	119 (84%)	17 (12%)	5 (4%)	3	21
22	D0	105/120 (88%)	90 (86%)	9 (9%)	6 (6%)	1	11
22	d0	108/120 (90%)	87 (81%)	18 (17%)	3 (3%)	5	25
23	D1	85/87 (98%)	61 (72%)	17 (20%)	7 (8%)	1	6
23	d1	85/87 (98%)	71 (84%)	8 (9%)	6 (7%)	1	7
24	D2	127/129 (98%)	111 (87%)	12 (9%)	4 (3%)	4	24
24	d2	127/129 (98%)	117 (92%)	7 (6%)	3 (2%)	6	28
25	D3	142/144 (99%)	109 (77%)	20 (14%)	13 (9%)	1	4
25	d3	142/144 (99%)	125 (88%)	14 (10%)	3 (2%)	7	32
26	D4	132/134 (98%)	114 (86%)	8 (6%)	10 (8%)	1	6
26	d4	132/134 (98%)	110 (83%)	14 (11%)	8 (6%)	1	10
27	D5	68/107 (64%)	47 (69%)	15 (22%)	6 (9%)	1	5
27	d5	67/107 (63%)	52 (78%)	14 (21%)	1 (2%)	10	39
28	D6	95/97 (98%)	62 (65%)	19 (20%)	14 (15%)	0	1
28	d6	95/97 (98%)	70 (74%)	20 (21%)	5 (5%)	2	12
29	D7	79/81 (98%)	58 (73%)	18 (23%)	3 (4%)	3	19
29	d7	79/81 (98%)	62 (78%)	15 (19%)	2 (2%)	5	28
30	D8	61/66 (92%)	53 (87%)	6 (10%)	2 (3%)	4	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	d8	61/66 (92%)	47 (77%)	10 (16%)	4 (7%)	1	9
31	D9	51/55 (93%)	42 (82%)	6 (12%)	3 (6%)	1	10
31	d9	51/55 (93%)	41 (80%)	7 (14%)	3 (6%)	1	10
32	E0	58/62 (94%)	48 (83%)	7 (12%)	3 (5%)	2	12
32	e0	60/62 (97%)	46 (77%)	8 (13%)	6 (10%)	0	3
33	E1	69/76 (91%)	39 (56%)	12 (17%)	18 (26%)	0	0
33	e1	74/76 (97%)	38 (51%)	12 (16%)	24 (32%)	0	0
34	SR	316/318 (99%)	266 (84%)	34 (11%)	16 (5%)	2	13
34	sR	316/318 (99%)	264 (84%)	39 (12%)	13 (4%)	3	17
35	SM	155/273 (57%)	114 (74%)	22 (14%)	19 (12%)	0	2
35	sM	98/273 (36%)	59 (60%)	28 (29%)	11 (11%)	0	2
39	L2	250/253 (99%)	216 (86%)	25 (10%)	9 (4%)	3	20
39	l2	250/253 (99%)	208 (83%)	32 (13%)	10 (4%)	3	17
40	L3	384/386 (100%)	332 (86%)	39 (10%)	13 (3%)	3	22
40	l3	384/386 (100%)	341 (89%)	38 (10%)	5 (1%)	12	41
41	L4	359/361 (99%)	296 (82%)	38 (11%)	25 (7%)	1	7
41	l4	359/361 (99%)	295 (82%)	42 (12%)	22 (6%)	1	10
42	L5	294/296 (99%)	231 (79%)	38 (13%)	25 (8%)	1	5
42	l5	292/296 (99%)	253 (87%)	31 (11%)	8 (3%)	5	26
43	L6	152/175 (87%)	135 (89%)	13 (9%)	4 (3%)	5	27
43	l6	153/175 (87%)	125 (82%)	24 (16%)	4 (3%)	5	27
44	L7	220/243 (90%)	190 (86%)	24 (11%)	6 (3%)	5	26
44	l7	221/243 (91%)	199 (90%)	17 (8%)	5 (2%)	6	29
45	L8	231/255 (91%)	190 (82%)	30 (13%)	11 (5%)	2	14
45	l8	229/255 (90%)	178 (78%)	37 (16%)	14 (6%)	1	10
46	L9	189/191 (99%)	161 (85%)	20 (11%)	8 (4%)	3	16
46	l9	189/191 (99%)	170 (90%)	16 (8%)	3 (2%)	9	37
47	M0	207/220 (94%)	169 (82%)	32 (16%)	6 (3%)	4	25
47	m0	209/220 (95%)	161 (77%)	35 (17%)	13 (6%)	1	10
48	M1	167/173 (96%)	130 (78%)	25 (15%)	12 (7%)	1	7
48	m1	167/173 (96%)	139 (83%)	18 (11%)	10 (6%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	M3	191/198 (96%)	149 (78%)	34 (18%)	8 (4%)	3	16
49	m3	192/198 (97%)	148 (77%)	30 (16%)	14 (7%)	1	7
50	M4	134/137 (98%)	116 (87%)	14 (10%)	4 (3%)	4	24
50	m4	135/137 (98%)	120 (89%)	13 (10%)	2 (2%)	10	39
51	M5	201/203 (99%)	178 (89%)	16 (8%)	7 (4%)	3	21
51	m5	201/203 (99%)	178 (89%)	18 (9%)	5 (2%)	5	28
52	M6	195/198 (98%)	171 (88%)	17 (9%)	7 (4%)	3	20
52	m6	195/198 (98%)	173 (89%)	18 (9%)	4 (2%)	7	32
53	M7	181/183 (99%)	149 (82%)	26 (14%)	6 (3%)	4	22
53	m7	153/183 (84%)	140 (92%)	11 (7%)	2 (1%)	12	41
54	M8	183/185 (99%)	157 (86%)	22 (12%)	4 (2%)	6	31
54	m8	183/185 (99%)	152 (83%)	25 (14%)	6 (3%)	4	22
55	M9	186/188 (99%)	164 (88%)	19 (10%)	3 (2%)	9	37
55	m9	186/188 (99%)	166 (89%)	20 (11%)	0	100	100
56	N0	170/172 (99%)	150 (88%)	13 (8%)	7 (4%)	3	17
56	n0	170/172 (99%)	156 (92%)	13 (8%)	1 (1%)	25	59
57	N1	157/159 (99%)	135 (86%)	16 (10%)	6 (4%)	3	19
57	n1	157/159 (99%)	138 (88%)	14 (9%)	5 (3%)	4	23
58	N2	98/120 (82%)	73 (74%)	21 (21%)	4 (4%)	3	17
58	n2	96/120 (80%)	84 (88%)	8 (8%)	4 (4%)	3	16
59	N3	134/136 (98%)	117 (87%)	11 (8%)	6 (4%)	2	15
59	n3	134/136 (98%)	121 (90%)	7 (5%)	6 (4%)	2	15
60	N4	96/155 (62%)	76 (79%)	15 (16%)	5 (5%)	2	12
60	n4	133/155 (86%)	109 (82%)	16 (12%)	8 (6%)	1	10
61	N5	119/141 (84%)	101 (85%)	16 (13%)	2 (2%)	9	36
61	n5	118/141 (84%)	101 (86%)	13 (11%)	4 (3%)	3	22
62	N6	124/126 (98%)	109 (88%)	13 (10%)	2 (2%)	9	37
62	n6	124/126 (98%)	104 (84%)	16 (13%)	4 (3%)	4	23
63	N7	133/135 (98%)	106 (80%)	16 (12%)	11 (8%)	1	5
63	n7	133/135 (98%)	111 (84%)	15 (11%)	7 (5%)	2	12
64	N8	146/148 (99%)	121 (83%)	20 (14%)	5 (3%)	3	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
64	n8	146/148 (99%)	122 (84%)	18 (12%)	6 (4%)	3	17
65	N9	56/58 (97%)	47 (84%)	7 (12%)	2 (4%)	3	20
65	n9	56/58 (97%)	40 (71%)	10 (18%)	6 (11%)	0	3
66	O0	95/104 (91%)	84 (88%)	11 (12%)	0	100	100
66	o0	98/104 (94%)	85 (87%)	9 (9%)	4 (4%)	3	17
67	O1	107/112 (96%)	92 (86%)	9 (8%)	6 (6%)	2	11
67	o1	107/112 (96%)	91 (85%)	9 (8%)	7 (6%)	1	9
68	O2	125/129 (97%)	111 (89%)	13 (10%)	1 (1%)	19	52
68	o2	125/129 (97%)	112 (90%)	10 (8%)	3 (2%)	6	28
69	O3	104/106 (98%)	98 (94%)	5 (5%)	1 (1%)	15	47
69	o3	104/106 (98%)	90 (86%)	11 (11%)	3 (3%)	4	25
70	O4	110/119 (92%)	94 (86%)	15 (14%)	1 (1%)	17	50
70	o4	110/119 (92%)	93 (84%)	15 (14%)	2 (2%)	8	35
71	O5	117/119 (98%)	97 (83%)	14 (12%)	6 (5%)	2	13
71	o5	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	9	36
72	O6	97/99 (98%)	78 (80%)	12 (12%)	7 (7%)	1	7
72	o6	97/99 (98%)	76 (78%)	13 (13%)	8 (8%)	1	6
73	O7	85/87 (98%)	73 (86%)	11 (13%)	1 (1%)	13	43
73	o7	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
74	O8	75/77 (97%)	63 (84%)	9 (12%)	3 (4%)	3	17
74	o8	75/77 (97%)	59 (79%)	10 (13%)	6 (8%)	1	6
75	O9	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	7	32
75	o9	48/50 (96%)	39 (81%)	7 (15%)	2 (4%)	3	16
76	Q0	50/52 (96%)	42 (84%)	5 (10%)	3 (6%)	1	10
76	q0	50/52 (96%)	47 (94%)	1 (2%)	2 (4%)	3	17
77	Q1	23/25 (92%)	19 (83%)	4 (17%)	0	100	100
77	q1	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
78	Q2	103/105 (98%)	84 (82%)	12 (12%)	7 (7%)	1	8
78	q2	103/105 (98%)	88 (85%)	11 (11%)	4 (4%)	3	18
79	Q3	89/91 (98%)	77 (86%)	6 (7%)	6 (7%)	1	8
79	q3	89/91 (98%)	80 (90%)	7 (8%)	2 (2%)	6	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	c0	92/105 (88%)	63 (68%)	16 (17%)	13 (14%)	0	1
82	p0	139/311 (45%)	113 (81%)	20 (14%)	6 (4%)	2	16
85	f	146/157 (93%)	98 (67%)	30 (20%)	18 (12%)	0	2
All	All	22479/24300 (92%)	18504 (82%)	2828 (13%)	1147 (5%)	2	13

All (1147) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S0	4	PRO
2	S0	158	VAL
2	S0	190	ASP
2	S0	191	ARG
2	S0	192	THR
3	S1	37	THR
3	S1	132	ASP
3	S1	181	LEU
3	S1	182	ALA
3	S1	206	PRO
3	S1	213	ARG
4	S2	48	GLY
5	S3	195	SER
5	S3	211	PRO
5	S3	220	PRO
6	S4	12	LEU
7	S5	26	ALA
7	S5	39	GLU
7	S5	51	VAL
7	S5	63	GLN
7	S5	98	MET
8	S6	122	GLU
8	S6	149	LYS
8	S6	173	PRO
8	S6	174	LYS
9	S7	31	SER
9	S7	32	PRO
9	S7	64	VAL
9	S7	74	GLN
9	S7	112	ARG
9	S7	131	PHE
9	S7	186	PRO
11	S9	93	LEU

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Mol	Chain	Res	Type
11	S9	134	ILE
12	C0	87	VAL
12	C0	88	PRO
12	C0	92	ILE
13	C1	7	VAL
13	C1	55	ASP
13	C1	155	LYS
14	C2	91	VAL
15	C3	68	GLY
16	C4	42	VAL
16	C4	125	SER
17	C5	11	VAL
17	C5	52	LYS
17	C5	54	ALA
17	C5	80	MET
17	C5	87	PRO
17	C5	125	PRO
18	C6	41	PRO
18	C6	58	ASP
18	C6	114	ARG
18	C6	138	PHE
19	C7	85	VAL
19	C7	86	PRO
19	C7	88	VAL
21	C9	11	ALA
21	C9	31	PRO
21	C9	53	TRP
21	C9	69	LYS
24	D2	78	ARG
24	D2	83	ILE
25	D3	114	LYS
27	D5	43	ASP
27	D5	44	GLN
28	D6	45	VAL
28	D6	82	ARG
28	D6	84	VAL
28	D6	85	ARG
28	D6	86	VAL
29	D7	62	ILE
33	E1	93	HIS
33	E1	98	VAL
33	E1	102	VAL

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Mol	Chain	Res	Type
33	E1	103	LEU
34	SR	318	ALA
35	SM	140	ASP
35	SM	153	LYS
35	SM	171	PRO
39	L2	20	THR
39	L2	130	SER
40	L3	3	HIS
40	L3	4	ARG
40	L3	140	ASP
41	L4	15	ALA
41	L4	146	PRO
41	L4	232	SER
41	L4	233	LEU
41	L4	270	SER
41	L4	291	ASN
41	L4	317	PRO
41	L4	318	LEU
41	L4	341	SER
42	L5	57	ASN
42	L5	178	ASN
42	L5	221	GLU
42	L5	223	PHE
42	L5	233	ALA
42	L5	234	ASP
42	L5	257	GLU
42	L5	258	LYS
42	L5	292	ALA
42	L5	293	LEU
44	L7	163	LEU
45	L8	25	PRO
45	L8	31	PRO
45	L8	116	VAL
45	L8	122	LYS
45	L8	157	VAL
46	L9	50	ASN
47	M0	145	LYS
47	M0	219	ALA
48	M1	8	PRO
48	M1	11	ASP
49	M3	129	ASN
50	M4	9	ALA

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Mol	Chain	Res	Type
51	M5	74	PRO
52	M6	16	VAL
52	M6	110	PRO
52	M6	111	PRO
52	M6	112	TYR
56	N0	133	ALA
56	N0	167	ARG
57	N1	126	VAL
58	N2	51	GLY
60	N4	81	PRO
63	N7	30	ASP
63	N7	128	GLN
67	O1	21	HIS
67	O1	99	ALA
71	O5	71	LYS
71	O5	119	LYS
72	O6	33	ALA
74	O8	33	LYS
78	Q2	30	ALA
78	Q2	100	LYS
2	s0	65	ALA
2	s0	66	ALA
2	s0	95	ALA
2	s0	164	ASN
2	s0	189	VAL
2	s0	194	PRO
2	s0	206	ASP
3	s1	147	ALA
3	s1	206	PRO
3	s1	231	LEU
4	s2	91	ARG
5	s3	211	PRO
5	s3	217	ILE
5	s3	220	PRO
6	s4	104	ASP
6	s4	163	ASP
6	s4	195	ILE
6	s4	196	VAL
7	s5	36	ALA
7	s5	184	PHE
7	s5	204	GLY
8	s6	154	ARG

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Mol	Chain	Res	Type
9	s7	63	PRO
9	s7	106	SER
9	s7	131	PHE
11	s9	118	LEU
11	s9	121	SER
80	c0	2	LEU
80	c0	83	PRO
80	c0	94	ILE
13	c1	40	LEU
14	c2	22	VAL
14	c2	89	ILE
14	c2	131	ASP
15	c3	12	SER
15	c3	66	ILE
15	c3	87	ASP
16	c4	91	THR
16	c4	98	GLY
16	c4	132	ARG
17	c5	11	VAL
17	c5	52	LYS
17	c5	68	PRO
17	c5	125	PRO
18	c6	42	GLU
18	c6	97	VAL
19	c7	67	ARG
19	c7	88	VAL
19	c7	99	VAL
20	c8	92	ILE
21	c9	33	TYR
24	d2	68	ARG
25	d3	138	GLU
26	d4	52	LYS
28	d6	34	LYS
30	d8	32	PHE
30	d8	61	ARG
31	d9	6	VAL
32	e0	60	PRO
33	e1	79	LYS
33	e1	83	LYS
33	e1	87	THR
33	e1	92	LYS
33	e1	98	VAL

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Mol	Chain	Res	Type
33	e1	102	VAL
34	sR	163	ASP
35	sM	83	LYS
40	l3	140	ASP
40	l3	188	ILE
41	l4	142	VAL
41	l4	233	LEU
41	l4	305	ALA
41	l4	329	PRO
41	l4	349	THR
41	l4	361	HIS
42	l5	178	ASN
44	l7	193	PRO
45	l8	25	PRO
45	l8	26	LEU
45	l8	34	PHE
45	l8	122	LYS
47	m0	153	ARG
48	m1	8	PRO
48	m1	108	GLU
49	m3	51	LEU
49	m3	134	GLU
51	m5	76	PRO
51	m5	183	THR
52	m6	110	PRO
52	m6	111	PRO
53	m7	37	ASN
54	m8	41	ASP
54	m8	112	ALA
54	m8	113	LYS
57	n1	135	PRO
60	n4	63	ILE
60	n4	76	VAL
61	n5	44	PRO
62	n6	84	LYS
63	n7	5	LEU
65	n9	23	LYS
65	n9	24	PRO
65	n9	39	PHE
67	o1	5	LYS
67	o1	84	ASP
67	o1	86	LYS

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Mol	Chain	Res	Type
68	o2	6	HIS
69	o3	88	ASN
71	o5	99	GLN
72	o6	33	ALA
72	o6	79	SER
72	o6	98	ARG
74	o8	17	ARG
85	f	64	ILE
85	f	109	THR
85	f	111	ASP
85	f	148	ILE
2	S0	39	ASN
2	S0	66	ALA
2	S0	95	ALA
2	S0	194	PRO
3	S1	21	VAL
3	S1	58	SER
3	S1	62	LYS
3	S1	63	GLY
3	S1	93	GLY
3	S1	177	GLN
4	S2	91	ARG
5	S3	144	ALA
5	S3	216	PRO
6	S4	24	SER
6	S4	104	ASP
6	S4	195	ILE
7	S5	35	GLN
7	S5	43	PHE
7	S5	150	GLY
7	S5	153	GLY
8	S6	148	SER
8	S6	152	ASP
9	S7	110	GLN
9	S7	111	LYS
9	S7	116	ARG
10	S8	149	SER
11	S9	150	LEU
11	S9	167	ALA
13	C1	40	LEU
13	C1	145	ALA
14	C2	101	ALA

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Mol	Chain	Res	Type
14	C2	119	SER
14	C2	126	TRP
14	C2	127	GLY
14	C2	131	ASP
15	C3	19	SER
15	C3	22	ALA
15	C3	24	ALA
16	C4	96	PRO
16	C4	126	THR
17	C5	48	GLY
18	C6	59	LYS
18	C6	97	VAL
19	C7	124	VAL
20	C8	14	ILE
20	C8	91	ASP
20	C8	92	ILE
21	C9	50	ALA
22	D0	55	PRO
23	D1	81	ASN
25	D3	4	GLY
25	D3	110	LYS
25	D3	112	LYS
25	D3	137	LYS
26	D4	5	VAL
26	D4	100	VAL
27	D5	41	ILE
27	D5	71	ILE
28	D6	36	ILE
31	D9	20	GLN
32	E0	51	ASN
33	E1	83	LYS
33	E1	106	TYR
33	E1	144	CYS
34	SR	51	ASP
34	SR	163	ASP
35	SM	12	VAL
35	SM	42	ALA
35	SM	52	PRO
35	SM	166	LYS
39	L2	13	GLY
39	L2	34	TYR
39	L2	246	LEU

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Mol	Chain	Res	Type
39	L2	251	LYS
40	L3	351	LEU
40	L3	385	LYS
41	L4	268	ALA
41	L4	311	HIS
41	L4	313	LEU
41	L4	338	LYS
42	L5	59	ASP
42	L5	93	THR
42	L5	252	ALA
42	L5	253	PHE
44	L7	26	VAL
45	L8	36	ILE
45	L8	39	ALA
45	L8	115	ALA
46	L9	188	THR
47	M0	63	GLU
47	M0	117	GLY
48	M1	12	LEU
48	M1	24	GLY
48	M1	114	ILE
48	M1	115	LYS
49	M3	47	ALA
49	M3	141	ALA
49	M3	166	ALA
51	M5	184	LYS
53	M7	67	ILE
55	M9	53	LYS
55	M9	130	ASN
56	N0	24	LEU
58	N2	11	ILE
58	N2	60	GLY
59	N3	82	ALA
61	N5	24	LEU
62	N6	126	LEU
63	N7	3	LYS
63	N7	17	ARG
63	N7	125	GLY
64	N8	66	ALA
64	N8	76	ASP
64	N8	96	LYS
67	O1	6	ASP

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Mol	Chain	Res	Type
67	O1	83	GLU
67	O1	84	ASP
71	O5	35	LYS
72	O6	80	PHE
78	Q2	34	SER
78	Q2	94	GLY
79	Q3	59	CYS
2	s0	44	GLY
2	s0	68	PRO
3	s1	41	ARG
3	s1	82	ARG
3	s1	93	GLY
3	s1	106	THR
4	s2	92	ALA
4	s2	121	VAL
4	s2	149	GLY
4	s2	163	GLY
5	s3	93	ASP
5	s3	115	ILE
5	s3	179	GLN
6	s4	164	LEU
7	s5	26	ALA
7	s5	35	GLN
7	s5	43	PHE
7	s5	100	ASN
8	s6	156	PHE
8	s6	164	LYS
9	s7	10	SER
10	s8	35	ASN
10	s8	122	GLY
80	c0	23	ALA
80	c0	32	HIS
80	c0	88	ILE
15	c3	18	TYR
15	c3	19	SER
15	c3	60	VAL
16	c4	97	GLY
17	c5	8	LYS
17	c5	17	TYR
17	c5	20	VAL
17	c5	47	ARG
17	c5	71	GLU

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Mol	Chain	Res	Type
17	c5	80	MET
18	c6	39	VAL
18	c6	113	ASP
20	c8	14	ILE
20	c8	91	ASP
21	c9	26	GLY
21	c9	34	VAL
22	d0	17	GLN
22	d0	49	ASN
23	d1	2	GLU
26	d4	33	ALA
26	d4	35	VAL
26	d4	53	ASP
26	d4	68	LYS
27	d5	53	GLU
28	d6	13	LYS
29	d7	57	GLU
30	d8	33	LEU
31	d9	7	TRP
31	d9	11	PRO
32	e0	51	ASN
33	e1	84	VAL
33	e1	100	LEU
33	e1	107	LYS
33	e1	110	ALA
33	e1	127	GLY
34	sR	160	GLU
35	sM	42	ALA
35	sM	47	ALA
35	sM	50	ASN
35	sM	66	ALA
35	sM	163	GLU
39	l2	80	GLU
39	l2	94	ALA
39	l2	194	ASN
39	l2	212	GLY
40	l3	155	ALA
40	l3	347	SER
41	l4	15	ALA
41	l4	90	PHE
41	l4	221	ASN
41	l4	311	HIS

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Mol	Chain	Res	Type
41	l4	330	TYR
41	l4	338	LYS
42	l5	260	PHE
44	l7	191	VAL
45	l8	69	LEU
45	l8	118	GLU
45	l8	237	ILE
46	l9	130	ASP
46	l9	144	ILE
47	m0	57	LEU
47	m0	77	THR
47	m0	78	THR
47	m0	195	ALA
48	m1	94	ARG
48	m1	114	ILE
48	m1	152	HIS
49	m3	44	ALA
49	m3	47	ALA
49	m3	76	THR
49	m3	93	ILE
49	m3	150	PRO
51	m5	181	ASN
51	m5	184	LYS
58	n2	51	GLY
59	n3	4	ASN
60	n4	25	ASP
60	n4	26	SER
61	n5	45	LYS
61	n5	62	VAL
62	n6	6	LEU
63	n7	56	LYS
63	n7	125	GLY
64	n8	76	ASP
65	n9	5	LYS
65	n9	21	ILE
66	o0	7	GLN
66	o0	101	LEU
67	o1	45	GLY
68	o2	5	PRO
68	o2	124	GLY
71	o5	119	LYS
72	o6	34	SER

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Mol	Chain	Res	Type
72	o6	64	SER
74	o8	18	ALA
76	q0	78	ILE
82	p0	68	SER
82	p0	278	PRO
2	S0	5	ALA
2	S0	109	ASN
2	S0	161	PRO
2	S0	195	TRP
2	S0	202	TYR
3	S1	54	LEU
3	S1	209	ASN
4	S2	106	ASP
5	S3	217	ILE
5	S3	218	LEU
6	S4	26	CYS
7	S5	45	LYS
8	S6	69	LEU
8	S6	165	GLY
9	S7	36	ALA
9	S7	98	ILE
9	S7	129	LEU
9	S7	134	GLU
10	S8	40	ALA
10	S8	120	THR
10	S8	152	ILE
10	S8	153	GLU
11	S9	147	MET
12	C0	30	ALA
12	C0	34	GLU
12	C0	60	SER
14	C2	22	VAL
14	C2	93	ASP
14	C2	106	ILE
14	C2	107	ASP
14	C2	112	ALA
15	C3	28	LEU
16	C4	18	ARG
16	C4	40	ALA
16	C4	114	ARG
16	C4	124	ASP
17	C5	109	PRO

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Mol	Chain	Res	Type
17	C5	127	ARG
19	C7	115	LEU
20	C8	76	PRO
20	C8	103	ASN
22	D0	17	GLN
22	D0	96	PRO
22	D0	120	SER
23	D1	7	GLN
23	D1	15	ARG
25	D3	39	LYS
25	D3	41	SER
25	D3	80	GLY
25	D3	96	VAL
25	D3	138	GLU
26	D4	4	ALA
26	D4	54	ALA
26	D4	95	GLY
28	D6	8	ASN
28	D6	11	ASN
28	D6	46	GLU
29	D7	75	GLU
30	D8	36	THR
32	E0	47	VAL
33	E1	87	THR
33	E1	111	GLU
33	E1	118	ARG
33	E1	145	HIS
34	SR	3	SER
34	SR	15	GLY
34	SR	16	HIS
34	SR	135	THR
34	SR	186	PHE
35	SM	64	LYS
35	SM	82	THR
35	SM	86	ASN
35	SM	87	THR
35	SM	139	GLU
35	SM	173	THR
39	L2	47	GLN
39	L2	127	ALA
40	L3	142	ALA
40	L3	155	ALA

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Mol	Chain	Res	Type
40	L3	174	LYS
40	L3	291	GLU
40	L3	348	ARG
41	L4	4	PRO
41	L4	14	GLU
42	L5	7	ALA
42	L5	137	ASP
42	L5	212	ALA
42	L5	259	LYS
42	L5	289	LYS
43	L6	20	LYS
46	L9	2	LYS
46	L9	59	ASN
46	L9	107	ASP
46	L9	189	GLU
46	L9	190	ASP
48	M1	108	GLU
48	M1	152	HIS
49	M3	134	GLU
49	M3	136	GLU
50	M4	10	SER
50	M4	29	ALA
51	M5	158	HIS
52	M6	123	ALA
52	M6	182	ASN
53	M7	159	LYS
53	M7	160	ALA
53	M7	164	LYS
54	M8	74	GLU
57	N1	122	GLN
59	N3	134	GLY
60	N4	76	VAL
60	N4	97	LYS
61	N5	48	SER
63	N7	16	GLY
63	N7	102	GLU
63	N7	124	ALA
64	N8	97	GLU
64	N8	117	ARG
71	O5	90	ARG
71	O5	91	ALA
72	O6	78	GLY

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Mol	Chain	Res	Type
75	O9	3	ALA
76	Q0	120	GLN
78	Q2	17	CYS
78	Q2	60	LYS
78	Q2	102	GLN
79	Q3	60	CYS
2	s0	191	ARG
3	s1	207	LEU
3	s1	209	ASN
3	s1	224	ASP
5	s3	44	THR
5	s3	196	ARG
6	s4	23	LEU
6	s4	66	MET
6	s4	168	LYS
6	s4	214	LEU
7	s5	28	PRO
7	s5	39	GLU
8	s6	152	ASP
9	s7	41	LEU
10	s8	199	LYS
11	s9	3	ARG
11	s9	5	PRO
11	s9	120	LYS
11	s9	167	ALA
80	c0	30	ALA
80	c0	82	LEU
80	c0	95	GLN
13	c1	55	ASP
14	c2	58	LEU
15	c3	43	LYS
15	c3	140	LYS
16	c4	51	ASP
17	c5	6	ASN
17	c5	127	ARG
19	c7	103	ASP
20	c8	77	THR
21	c9	29	GLU
21	c9	68	ARG
22	d0	119	ALA
23	d1	44	ARG
26	d4	58	PHE

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Mol	Chain	Res	Type
28	d6	46	GLU
32	e0	61	SER
33	e1	81	LYS
33	e1	85	TYR
33	e1	103	LEU
33	e1	105	TYR
33	e1	112	GLY
33	e1	128	ALA
33	e1	136	LYS
34	sR	15	GLY
34	sR	28	GLY
34	sR	63	GLY
34	sR	226	ALA
35	sM	165	ILE
35	sM	172	ALA
40	l3	3	HIS
41	l4	4	PRO
41	l4	5	GLN
41	l4	146	PRO
41	l4	302	ALA
41	l4	342	LYS
42	l5	119	TYR
42	l5	245	GLU
42	l5	258	LYS
43	l6	11	PRO
43	l6	173	MET
44	l7	158	LYS
45	l8	39	ALA
45	l8	81	THR
45	l8	203	VAL
45	l8	230	LYS
47	m0	3	ARG
47	m0	130	ASP
47	m0	154	ARG
47	m0	176	LEU
47	m0	187	ALA
47	m0	196	PHE
48	m1	95	ASN
48	m1	145	LYS
49	m3	50	PRO
49	m3	135	ALA
52	m6	5	PRO

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Mol	Chain	Res	Type
54	m8	99	THR
54	m8	108	ALA
57	n1	136	ARG
58	n2	105	LEU
59	n3	42	SER
59	n3	106	LYS
60	n4	64	THR
60	n4	83	THR
61	n5	55	ASN
62	n6	125	LYS
63	n7	36	HIS
63	n7	103	GLN
64	n8	47	LYS
64	n8	129	PHE
67	o1	82	GLU
69	o3	94	PHE
70	o4	82	ALA
72	o6	99	ARG
74	o8	74	LYS
75	o9	40	LYS
82	p0	102	SER
85	f	132	LYS
2	S0	26	ALA
2	S0	94	GLY
2	S0	205	ARG
3	S1	35	PRO
3	S1	224	ASP
3	S1	230	ALA
4	S2	39	THR
4	S2	107	SER
4	S2	148	LEU
4	S2	182	PRO
5	S3	62	ASN
5	S3	81	PRO
6	S4	11	ARG
6	S4	77	ARG
6	S4	200	ARG
6	S4	201	HIS
6	S4	205	PHE
6	S4	245	LYS
7	S5	58	LEU
7	S5	64	VAL

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Mol	Chain	Res	Type
9	S7	15	GLU
9	S7	30	SER
10	S8	10	LYS
10	S8	52	ASN
11	S9	98	ALA
13	C1	6	THR
14	C2	83	GLU
14	C2	87	PRO
16	C4	39	ILE
17	C5	29	SER
17	C5	69	GLU
17	C5	101	ALA
18	C6	33	GLY
18	C6	142	TYR
19	C7	87	GLU
22	D0	16	GLN
23	D1	10	GLU
23	D1	42	GLU
25	D3	3	LYS
25	D3	40	SER
26	D4	34	ASN
26	D4	134	ALA
27	D5	88	ILE
28	D6	15	ARG
33	E1	84	VAL
33	E1	94	LYS
33	E1	109	ASP
33	E1	148	TYR
34	SR	98	GLU
34	SR	139	GLN
34	SR	161	LYS
34	SR	237	GLN
35	SM	53	ARG
35	SM	174	LYS
39	L2	234	LYS
40	L3	258	ALA
41	L4	16	THR
41	L4	140	HIS
41	L4	361	HIS
42	L5	185	PHE
42	L5	214	ASP
42	L5	295	GLY

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
43	L6	58	LEU
44	L7	72	ALA
44	L7	178	ILE
45	L8	79	GLN
46	L9	96	HIS
48	M1	117	ASP
49	M3	76	THR
51	M5	94	TYR
51	M5	165	THR
54	M8	99	THR
54	M8	162	ALA
55	M9	3	ASN
56	N0	2	ALA
57	N1	124	VAL
59	N3	81	GLN
59	N3	132	ASN
60	N4	86	SER
63	N7	7	ALA
63	N7	103	GLN
65	N9	32	LEU
71	O5	118	ILE
72	O6	3	VAL
76	Q0	79	GLU
79	Q3	7	LYS
79	Q3	58	SER
79	Q3	91	GLU
2	s0	10	THR
2	s0	163	ASN
3	s1	218	LEU
3	s1	223	PHE
4	s2	93	GLY
4	s2	150	GLN
4	s2	235	LEU
4	s2	238	SER
6	s4	11	ARG
6	s4	57	ASN
6	s4	90	ILE
7	s5	55	ASP
7	s5	56	ALA
7	s5	60	ASP
9	s7	9	LEU
9	s7	11	GLN

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Mol	Chain	Res	Type
9	s7	64	VAL
9	s7	74	GLN
9	s7	105	THR
9	s7	133	THR
10	s8	52	ASN
80	c0	3	MET
80	c0	31	LYS
14	c2	39	ASP
14	c2	106	ILE
14	c2	108	ARG
15	c3	29	SER
16	c4	37	GLU
16	c4	114	ARG
16	c4	125	SER
17	c5	49	MET
18	c6	4	VAL
19	c7	113	LEU
23	d1	10	GLU
23	d1	42	GLU
24	d2	56	HIS
26	d4	54	ALA
28	d6	35	ALA
30	d8	16	LEU
32	e0	47	VAL
32	e0	54	ARG
33	e1	94	LYS
33	e1	137	ASP
34	sR	161	LYS
34	sR	165	ASP
35	sM	43	ASP
35	sM	168	ALA
39	l2	56	ALA
41	l4	11	LEU
41	l4	143	GLU
41	l4	328	ASN
44	l7	229	PHE
45	l8	133	LYS
47	m0	117	GLY
48	m1	165	GLN
49	m3	60	ALA
49	m3	101	ARG
49	m3	129	ASN

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Mol	Chain	Res	Type
50	m4	8	LYS
50	m4	136	ALA
51	m5	68	ARG
52	m6	109	PRO
54	m8	145	ASN
56	n0	2	ALA
57	n1	127	GLN
58	n2	60	GLY
59	n3	16	GLY
59	n3	107	GLY
60	n4	72	SER
64	n8	110	GLY
67	o1	91	SER
69	o3	59	VAL
72	o6	20	MET
74	o8	3	ARG
74	o8	20	VAL
78	q2	33	ALA
78	q2	78	LYS
79	q3	4	ARG
82	p0	33	VAL
82	p0	289	ALA
85	f	97	ASP
85	f	113	VAL
85	f	120	LEU
85	f	122	ASP
85	f	152	GLU
2	S0	102	PHE
3	S1	210	ILE
3	S1	221	PRO
5	S3	93	ASP
5	S3	196	ARG
6	S4	193	GLY
6	S4	194	THR
7	S5	65	ARG
9	S7	38	LEU
13	C1	30	ARG
14	C2	68	GLU
14	C2	82	PRO
14	C2	108	ARG
15	C3	3	ARG
16	C4	51	ASP

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Mol	Chain	Res	Type
16	C4	75	GLY
17	C5	130	ARG
18	C6	39	VAL
19	C7	25	THR
20	C8	36	LYS
20	C8	82	PRO
25	D3	143	PRO
26	D4	6	THR
26	D4	50	ALA
28	D6	97	PRO
29	D7	51	GLN
31	D9	19	ARG
33	E1	85	TYR
33	E1	100	LEU
35	SM	89	ARG
35	SM	100	THR
40	L3	317	ILE
41	L4	90	PHE
41	L4	223	PRO
42	L5	85	ARG
44	L7	164	SER
44	L7	191	VAL
48	M1	64	LYS
48	M1	141	ARG
49	M3	165	SER
50	M4	6	ILE
51	M5	81	TYR
52	M6	89	SER
53	M7	182	ILE
57	N1	18	ASP
57	N1	159	PHE
59	N3	109	MET
68	O2	12	LYS
72	O6	21	THR
72	O6	34	SER
72	O6	99	ARG
73	O7	68	LYS
74	O8	34	ALA
2	s0	103	THR
2	s0	127	ARG
4	s2	164	SER
5	s3	59	LEU

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Mol	Chain	Res	Type
5	s3	61	GLU
5	s3	203	PRO
6	s4	30	ARG
7	s5	29	ILE
7	s5	45	LYS
8	s6	68	LEU
8	s6	70	PRO
9	s7	112	ARG
10	s8	78	ILE
10	s8	101	ILE
80	c0	35	ILE
80	c0	90	PRO
14	c2	25	GLU
14	c2	63	VAL
14	c2	87	PRO
14	c2	109	GLU
14	c2	115	VAL
16	c4	77	THR
17	c5	12	PHE
17	c5	130	ARG
18	c6	142	TYR
19	c7	111	LYS
20	c8	61	LEU
23	d1	41	GLU
25	d3	131	SER
26	d4	30	PRO
28	d6	59	TYR
29	d7	75	GLU
32	e0	43	ARG
33	e1	106	TYR
33	e1	131	PHE
33	e1	146	SER
33	e1	148	TYR
34	sR	97	GLY
34	sR	105	GLY
34	sR	186	PHE
34	sR	250	TYR
39	l2	32	LEU
39	l2	70	ARG
39	l2	215	ASN
42	l5	98	ALA
42	l5	270	LYS

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Mol	Chain	Res	Type
43	l6	10	TYR
44	l7	178	ILE
45	l8	121	SER
46	l9	167	VAL
48	m1	12	LEU
49	m3	45	LYS
53	m7	75	GLU
57	n1	148	PRO
63	n7	102	GLU
65	n9	32	LEU
66	o0	10	ILE
66	o0	103	THR
67	o1	83	GLU
76	q0	80	PRO
78	q2	76	LYS
79	q3	51	ALA
82	p0	198	PRO
85	f	13	ALA
85	f	121	GLY
6	S4	152	PRO
6	S4	214	LEU
9	S7	67	LEU
11	S9	18	PRO
12	C0	93	GLN
17	C5	39	ALA
21	C9	39	THR
23	D1	12	TYR
24	D2	67	GLY
26	D4	133	ASN
27	D5	86	GLU
28	D6	61	GLU
28	D6	63	ALA
33	E1	86	THR
34	SR	160	GLU
34	SR	238	ASP
35	SM	22	PRO
41	L4	5	GLN
41	L4	141	ARG
42	L5	115	LEU
42	L5	249	ALA
43	L6	98	VAL
47	M0	6	ALA

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Mol	Chain	Res	Type
57	N1	155	PRO
69	O3	59	VAL
79	Q3	51	ALA
2	s0	9	LEU
4	s2	106	ASP
4	s2	155	ALA
4	s2	182	PRO
11	s9	165	GLY
14	c2	90	LYS
19	c7	86	PRO
39	l2	247	ARG
41	l4	13	GLY
42	l5	125	VAL
59	n3	28	ASN
62	n6	12	ARG
63	n7	70	PRO
64	n8	24	LYS
64	n8	56	VAL
70	o4	59	PRO
75	o9	24	PRO
78	q2	74	CYS
85	f	11	ALA
85	f	17	ALA
85	f	18	THR
85	f	98	GLY
3	S1	176	VAL
17	C5	126	VAL
21	C9	116	ILE
43	L6	36	PRO
51	M5	75	VAL
58	N2	19	VAL
63	N7	37	PRO
67	O1	7	VAL
6	s4	243	GLY
7	s5	59	VAL
7	s5	151	GLY
9	s7	8	ILE
11	s9	162	SER
17	c5	126	VAL
20	c8	4	VAL
35	sM	51	ARG
39	l2	175	VAL

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Mol	Chain	Res	Type
43	l6	36	PRO
48	m1	117	ASP
60	n4	132	GLY
74	o8	35	GLY
85	f	143	GLY
3	S1	75	GLY
24	D2	48	GLY
32	E0	50	VAL
34	SR	194	GLY
35	SM	154	VAL
41	L4	272	VAL
45	L8	135	GLY
53	M7	157	VAL
56	N0	22	PRO
56	N0	72	VAL
60	N4	80	ARG
65	N9	21	ILE
70	O4	77	GLY
74	O8	37	PRO
4	s2	62	PRO
6	s4	135	GLY
7	s5	101	GLY
14	c2	44	GLY
14	c2	66	VAL
15	c3	22	ALA
25	d3	80	GLY
34	sR	194	GLY
47	m0	47	PRO
72	o6	78	GLY
3	S1	48	VAL
4	S2	235	LEU
8	S6	162	VAL
28	D6	64	LEU
31	D9	11	PRO
41	L4	181	VAL
45	L8	30	THR
48	M1	67	VAL
56	N0	135	VAL
10	s8	50	GLY
19	c7	68	GLY
24	d2	6	VAL
41	l4	190	GLY

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Mol	Chain	Res	Type
57	n1	124	VAL
85	f	118	GLY
6	S4	239	PRO
14	C2	66	VAL
16	C4	118	VAL
30	D8	44	VAL
34	SR	30	PRO
41	L4	348	GLY
47	M0	194	GLY
54	M8	97	PRO
59	N3	3	GLY
62	N6	45	ILE
6	s4	150	PRO
14	c2	110	GLY
45	l8	163	VAL
58	n2	30	PRO
22	D0	118	VAL
23	D1	82	VAL
76	Q0	78	ILE
23	d1	9	VAL
49	m3	46	ILE
40	L3	257	PRO

### 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	
2	S0	164/209 (78%)	138 (84%)	26 (16%)	2	11
2	s0	165/209 (79%)	142 (86%)	23 (14%)	3	15
3	S1	191/223 (86%)	159 (83%)	32 (17%)	2	9
3	s1	192/223 (86%)	157 (82%)	35 (18%)	1	7
4	S2	176/204 (86%)	148 (84%)	28 (16%)	2	11
4	s2	176/204 (86%)	141 (80%)	35 (20%)	1	5
5	S3	182/194 (94%)	153 (84%)	29 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	s3	182/194 (94%)	150 (82%)	32 (18%)	2	8
6	S4	221/221 (100%)	188 (85%)	33 (15%)	3	12
6	s4	221/221 (100%)	192 (87%)	29 (13%)	4	17
7	S5	173/190 (91%)	154 (89%)	19 (11%)	6	24
7	s5	173/190 (91%)	150 (87%)	23 (13%)	4	16
8	S6	188/201 (94%)	160 (85%)	28 (15%)	3	12
8	s6	187/201 (93%)	158 (84%)	29 (16%)	2	11
9	S7	165/169 (98%)	137 (83%)	28 (17%)	2	9
9	s7	165/169 (98%)	146 (88%)	19 (12%)	5	22
10	S8	150/161 (93%)	132 (88%)	18 (12%)	5	20
10	s8	150/161 (93%)	132 (88%)	18 (12%)	5	20
11	S9	158/165 (96%)	133 (84%)	25 (16%)	2	11
11	s9	158/165 (96%)	128 (81%)	30 (19%)	1	6
12	C0	77/98 (79%)	66 (86%)	11 (14%)	3	14
13	C1	129/136 (95%)	120 (93%)	9 (7%)	15	43
13	c1	129/136 (95%)	113 (88%)	16 (12%)	4	19
14	C2	88/118 (75%)	76 (86%)	12 (14%)	3	16
14	c2	88/118 (75%)	76 (86%)	12 (14%)	3	16
15	C3	127/127 (100%)	107 (84%)	20 (16%)	2	11
15	c3	127/127 (100%)	108 (85%)	19 (15%)	3	12
16	C4	81/104 (78%)	62 (76%)	19 (24%)	1	3
16	c4	97/104 (93%)	84 (87%)	13 (13%)	4	16
17	C5	101/117 (86%)	83 (82%)	18 (18%)	2	7
17	c5	103/117 (88%)	85 (82%)	18 (18%)	2	8
18	C6	117/118 (99%)	101 (86%)	16 (14%)	3	16
18	c6	118/118 (100%)	96 (81%)	22 (19%)	1	6
19	C7	94/124 (76%)	76 (81%)	18 (19%)	1	6
19	c7	92/124 (74%)	80 (87%)	12 (13%)	4	17
20	C8	128/128 (100%)	105 (82%)	23 (18%)	1	7
20	c8	128/128 (100%)	104 (81%)	24 (19%)	1	6
21	C9	115/115 (100%)	99 (86%)	16 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	c9	115/115 (100%)	105 (91%)	10 (9%)	10	34
22	D0	100/113 (88%)	88 (88%)	12 (12%)	5	20
22	d0	103/113 (91%)	87 (84%)	16 (16%)	2	11
23	D1	74/74 (100%)	61 (82%)	13 (18%)	2	8
23	d1	74/74 (100%)	63 (85%)	11 (15%)	3	12
24	D2	110/110 (100%)	91 (83%)	19 (17%)	2	8
24	d2	110/110 (100%)	92 (84%)	18 (16%)	2	10
25	D3	119/119 (100%)	103 (87%)	16 (13%)	4	16
25	d3	119/119 (100%)	108 (91%)	11 (9%)	9	31
26	D4	112/112 (100%)	103 (92%)	9 (8%)	12	37
26	d4	112/112 (100%)	96 (86%)	16 (14%)	3	14
27	D5	61/88 (69%)	49 (80%)	12 (20%)	1	5
27	d5	61/88 (69%)	52 (85%)	9 (15%)	3	13
28	D6	83/83 (100%)	71 (86%)	12 (14%)	3	14
28	d6	83/83 (100%)	74 (89%)	9 (11%)	6	24
29	D7	70/70 (100%)	64 (91%)	6 (9%)	10	34
29	d7	70/70 (100%)	59 (84%)	11 (16%)	2	11
30	D8	56/59 (95%)	47 (84%)	9 (16%)	2	10
30	d8	56/59 (95%)	45 (80%)	11 (20%)	1	5
31	D9	47/48 (98%)	36 (77%)	11 (23%)	1	3
31	d9	47/48 (98%)	37 (79%)	10 (21%)	1	4
32	E0	51/53 (96%)	43 (84%)	8 (16%)	2	11
32	e0	53/53 (100%)	41 (77%)	12 (23%)	1	3
33	E1	62/66 (94%)	45 (73%)	17 (27%)	0	1
33	e1	66/66 (100%)	54 (82%)	12 (18%)	1	7
34	SR	259/261 (99%)	230 (89%)	29 (11%)	6	23
34	sR	260/261 (100%)	236 (91%)	24 (9%)	9	31
35	SM	97/228 (42%)	82 (84%)	15 (16%)	2	11
35	sM	54/228 (24%)	46 (85%)	8 (15%)	3	13
39	L2	193/195 (99%)	158 (82%)	35 (18%)	1	7
39	l2	192/195 (98%)	156 (81%)	36 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	L3	320/322 (99%)	274 (86%)	46 (14%)	3	14
40	l3	319/322 (99%)	264 (83%)	55 (17%)	2	9
41	L4	288/288 (100%)	241 (84%)	47 (16%)	2	10
41	l4	288/288 (100%)	247 (86%)	41 (14%)	3	15
42	L5	244/244 (100%)	203 (83%)	41 (17%)	2	9
42	l5	243/244 (100%)	201 (83%)	42 (17%)	2	8
43	L6	134/152 (88%)	114 (85%)	20 (15%)	3	12
43	l6	135/152 (89%)	115 (85%)	20 (15%)	3	13
44	L7	186/204 (91%)	164 (88%)	22 (12%)	5	21
44	l7	187/204 (92%)	164 (88%)	23 (12%)	4	20
45	L8	187/207 (90%)	160 (86%)	27 (14%)	3	14
45	l8	177/207 (86%)	154 (87%)	23 (13%)	4	17
46	L9	171/171 (100%)	151 (88%)	20 (12%)	5	21
46	l9	171/171 (100%)	142 (83%)	29 (17%)	2	9
47	M0	177/186 (95%)	142 (80%)	35 (20%)	1	5
47	m0	179/186 (96%)	143 (80%)	36 (20%)	1	5
48	M1	147/150 (98%)	124 (84%)	23 (16%)	2	11
48	m1	147/150 (98%)	120 (82%)	27 (18%)	1	7
49	M3	154/158 (98%)	138 (90%)	16 (10%)	7	25
49	m3	154/158 (98%)	132 (86%)	22 (14%)	3	14
50	M4	107/108 (99%)	92 (86%)	15 (14%)	3	15
50	m4	108/108 (100%)	94 (87%)	14 (13%)	4	17
51	M5	175/175 (100%)	153 (87%)	22 (13%)	4	18
51	m5	175/175 (100%)	152 (87%)	23 (13%)	4	17
52	M6	160/161 (99%)	136 (85%)	24 (15%)	3	12
52	m6	160/161 (99%)	134 (84%)	26 (16%)	2	10
53	M7	140/145 (97%)	123 (88%)	17 (12%)	5	20
53	m7	125/145 (86%)	107 (86%)	18 (14%)	3	14
54	M8	150/150 (100%)	136 (91%)	14 (9%)	9	30
54	m8	150/150 (100%)	120 (80%)	30 (20%)	1	5
55	M9	153/153 (100%)	132 (86%)	21 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	m9	153/153 (100%)	129 (84%)	24 (16%)	2	11
56	N0	156/156 (100%)	134 (86%)	22 (14%)	3	15
56	n0	156/156 (100%)	135 (86%)	21 (14%)	4	16
57	N1	136/136 (100%)	107 (79%)	29 (21%)	1	4
57	n1	136/136 (100%)	113 (83%)	23 (17%)	2	9
58	N2	87/106 (82%)	79 (91%)	8 (9%)	9	31
58	n2	85/106 (80%)	72 (85%)	13 (15%)	2	12
59	N3	104/104 (100%)	90 (86%)	14 (14%)	4	16
59	n3	104/104 (100%)	89 (86%)	15 (14%)	3	14
60	N4	57/129 (44%)	50 (88%)	7 (12%)	4	20
60	n4	100/129 (78%)	88 (88%)	12 (12%)	5	20
61	N5	104/117 (89%)	86 (83%)	18 (17%)	2	8
61	n5	104/117 (89%)	92 (88%)	12 (12%)	5	22
62	N6	109/109 (100%)	90 (83%)	19 (17%)	2	8
62	n6	109/109 (100%)	89 (82%)	20 (18%)	1	7
63	N7	115/115 (100%)	104 (90%)	11 (10%)	8	29
63	n7	115/115 (100%)	95 (83%)	20 (17%)	2	8
64	N8	118/118 (100%)	100 (85%)	18 (15%)	2	12
64	n8	118/118 (100%)	100 (85%)	18 (15%)	2	12
65	N9	46/46 (100%)	40 (87%)	6 (13%)	4	17
65	n9	46/46 (100%)	41 (89%)	5 (11%)	6	24
66	O0	81/87 (93%)	70 (86%)	11 (14%)	3	16
66	o0	84/87 (97%)	71 (84%)	13 (16%)	2	11
67	O1	92/96 (96%)	78 (85%)	14 (15%)	3	12
67	o1	94/96 (98%)	76 (81%)	18 (19%)	1	6
68	O2	109/110 (99%)	91 (84%)	18 (16%)	2	10
68	o2	109/110 (99%)	85 (78%)	24 (22%)	1	3
69	O3	90/90 (100%)	81 (90%)	9 (10%)	7	27
69	o3	90/90 (100%)	77 (86%)	13 (14%)	3	14
70	O4	95/101 (94%)	84 (88%)	11 (12%)	5	22
70	o4	95/101 (94%)	80 (84%)	15 (16%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	O5	104/104 (100%)	90 (86%)	14 (14%)	4	16
71	o5	103/104 (99%)	90 (87%)	13 (13%)	4	18
72	O6	81/81 (100%)	66 (82%)	15 (18%)	1	6
72	o6	80/81 (99%)	56 (70%)	24 (30%)	0	1
73	O7	70/70 (100%)	55 (79%)	15 (21%)	1	4
73	o7	70/70 (100%)	58 (83%)	12 (17%)	2	9
74	O8	68/68 (100%)	53 (78%)	15 (22%)	1	3
74	o8	67/68 (98%)	55 (82%)	12 (18%)	2	7
75	O9	45/45 (100%)	38 (84%)	7 (16%)	2	11
75	o9	45/45 (100%)	36 (80%)	9 (20%)	1	5
76	Q0	47/47 (100%)	39 (83%)	8 (17%)	2	9
76	q0	47/47 (100%)	42 (89%)	5 (11%)	6	25
77	Q1	23/23 (100%)	19 (83%)	4 (17%)	2	8
77	q1	23/23 (100%)	15 (65%)	8 (35%)	0	0
78	Q2	90/90 (100%)	76 (84%)	14 (16%)	2	11
78	q2	90/90 (100%)	77 (86%)	13 (14%)	3	14
79	Q3	71/71 (100%)	59 (83%)	12 (17%)	2	9
79	q3	71/71 (100%)	60 (84%)	11 (16%)	2	11
80	c0	73/98 (74%)	64 (88%)	9 (12%)	4	20
82	p0	105/253 (42%)	94 (90%)	11 (10%)	7	25
85	f	124/133 (93%)	108 (87%)	16 (13%)	4	18
All	All	18850/20374 (92%)	15999 (85%)	2851 (15%)	3	12

All (2851) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S0	7	PHE
2	S0	32	HIS
2	S0	43	ASP
2	S0	50	VAL
2	S0	52	LYS
2	S0	57	LEU
2	S0	62	ARG
2	S0	84	ARG
2	S0	87	LEU

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Mol	Chain	Res	Type
2	S0	88	LYS
2	S0	96	THR
2	S0	101	ARG
2	S0	103	THR
2	S0	108	THR
2	S0	110	TYR
2	S0	117	GLU
2	S0	140	ASN
2	S0	154	GLU
2	S0	156	VAL
2	S0	164	ASN
2	S0	168	HIS
2	S0	170	ILE
2	S0	172	LEU
2	S0	188	LEU
2	S0	189	VAL
2	S0	200	ASP
3	S1	21	VAL
3	S1	22	ASP
3	S1	29	TRP
3	S1	30	PHE
3	S1	39	GLU
3	S1	46	THR
3	S1	61	LEU
3	S1	65	VAL
3	S1	70	LEU
3	S1	77	GLU
3	S1	81	PHE
3	S1	83	LYS
3	S1	105	PHE
3	S1	108	ASP
3	S1	111	ARG
3	S1	117	TRP
3	S1	129	THR
3	S1	144	ARG
3	S1	148	ASN
3	S1	179	SER
3	S1	180	THR
3	S1	181	LEU
3	S1	193	ILE
3	S1	198	GLU
3	S1	202	LYS

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Mol	Chain	Res	Type
3	S1	203	ASP
3	S1	214	LYS
3	S1	215	VAL
3	S1	218	LEU
3	S1	220	GLN
3	S1	222	LYS
3	S1	223	PHE
4	S2	51	THR
4	S2	70	ASP
4	S2	72	LEU
4	S2	76	LEU
4	S2	77	GLN
4	S2	89	GLN
4	S2	90	THR
4	S2	94	GLN
4	S2	95	ARG
4	S2	96	THR
4	S2	97	ARG
4	S2	99	LYS
4	S2	111	VAL
4	S2	113	LEU
4	S2	134	LEU
4	S2	137	ILE
4	S2	146	THR
4	S2	148	LEU
4	S2	159	THR
4	S2	166	THR
4	S2	189	GLN
4	S2	198	THR
4	S2	207	LEU
4	S2	208	GLU
4	S2	222	TYR
4	S2	225	LEU
4	S2	226	THR
4	S2	237	VAL
5	S3	4	LEU
5	S3	23	GLU
5	S3	65	ARG
5	S3	66	ILE
5	S3	76	ARG
5	S3	89	GLU
5	S3	92	GLN

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Mol	Chain	Res	Type
5	S3	93	ASP
5	S3	103	GLU
5	S3	111	ASN
5	S3	113	LEU
5	S3	117	ARG
5	S3	124	ARG
5	S3	135	GLU
5	S3	142	LEU
5	S3	143	ARG
5	S3	146	ARG
5	S3	150	MET
5	S3	158	ILE
5	S3	172	THR
5	S3	175	VAL
5	S3	176	LEU
5	S3	177	MET
5	S3	182	LEU
5	S3	200	LYS
5	S3	207	THR
5	S3	212	LYS
5	S3	215	GLU
5	S3	224	ASP
6	S4	3	ARG
6	S4	6	LYS
6	S4	11	ARG
6	S4	12	LEU
6	S4	38	LEU
6	S4	65	LEU
6	S4	77	ARG
6	S4	78	THR
6	S4	90	ILE
6	S4	92	LEU
6	S4	108	ARG
6	S4	115	THR
6	S4	126	VAL
6	S4	129	VAL
6	S4	130	GLN
6	S4	131	LEU
6	S4	160	VAL
6	S4	166	SER
6	S4	180	LEU
6	S4	181	VAL

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Mol	Chain	Res	Type
6	S4	182	TYR
6	S4	187	ARG
6	S4	189	LEU
6	S4	192	ILE
6	S4	206	ASP
6	S4	215	ASP
6	S4	219	VAL
6	S4	220	THR
6	S4	222	LEU
6	S4	226	PHE
6	S4	227	VAL
6	S4	240	LYS
6	S4	246	LEU
7	S5	25	LEU
7	S5	32	GLU
7	S5	43	PHE
7	S5	45	LYS
7	S5	46	TRP
7	S5	48	PHE
7	S5	53	VAL
7	S5	65	ARG
7	S5	79	ASN
7	S5	93	LEU
7	S5	112	ARG
7	S5	119	ASP
7	S5	146	THR
7	S5	149	VAL
7	S5	156	ARG
7	S5	157	ARG
7	S5	160	VAL
7	S5	177	ILE
7	S5	216	GLU
8	S6	6	SER
8	S6	7	TYR
8	S6	15	THR
8	S6	25	ARG
8	S6	45	PHE
8	S6	69	LEU
8	S6	71	THR
8	S6	76	LEU
8	S6	82	SER
8	S6	97	VAL

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Mol	Chain	Res	Type
8	S6	109	LEU
8	S6	120	GLU
8	S6	126	ASP
8	S6	127	THR
8	S6	128	THR
8	S6	133	LEU
8	S6	150	GLU
8	S6	151	ASP
8	S6	153	VAL
8	S6	155	ASP
8	S6	169	TYR
8	S6	170	THR
8	S6	177	ARG
8	S6	193	LEU
8	S6	201	GLN
8	S6	207	GLU
8	S6	212	LEU
8	S6	223	LYS
9	S7	15	GLU
9	S7	16	LEU
9	S7	24	PHE
9	S7	38	LEU
9	S7	46	ILE
9	S7	49	ILE
9	S7	51	VAL
9	S7	67	LEU
9	S7	71	HIS
9	S7	75	THR
9	S7	77	LEU
9	S7	85	PHE
9	S7	87	ASP
9	S7	97	ARG
9	S7	110	GLN
9	S7	114	ARG
9	S7	115	SER
9	S7	118	LEU
9	S7	122	HIS
9	S7	123	ASP
9	S7	126	LEU
9	S7	130	VAL
9	S7	166	LEU
9	S7	167	GLU

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Mol	Chain	Res	Type
9	S7	174	ASN
9	S7	181	ILE
9	S7	182	VAL
9	S7	185	ILE
10	S8	5	ARG
10	S8	8	ARG
10	S8	14	THR
10	S8	29	LEU
10	S8	32	GLN
10	S8	36	THR
10	S8	37	LYS
10	S8	46	VAL
10	S8	58	LEU
10	S8	60	ILE
10	S8	69	SER
10	S8	88	ASN
10	S8	97	THR
10	S8	137	LYS
10	S8	152	ILE
10	S8	160	PHE
10	S8	185	GLU
10	S8	193	LEU
11	S9	3	ARG
11	S9	9	SER
11	S9	10	LYS
11	S9	28	LEU
11	S9	39	LYS
11	S9	46	SER
11	S9	49	LEU
11	S9	74	ASN
11	S9	78	ARG
11	S9	82	ARG
11	S9	88	GLU
11	S9	92	LYS
11	S9	93	LEU
11	S9	94	ASP
11	S9	99	LEU
11	S9	101	VAL
11	S9	110	GLN
11	S9	134	ILE
11	S9	138	LYS
11	S9	149	ARG

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Mol	Chain	Res	Type
11	S9	161	THR
11	S9	171	ARG
11	S9	172	VAL
11	S9	174	ARG
11	S9	182	GLU
12	C0	7	ASP
12	C0	12	HIS
12	C0	27	PHE
12	C0	50	THR
12	C0	51	SER
12	C0	55	VAL
12	C0	67	THR
12	C0	76	LEU
12	C0	78	GLU
12	C0	81	ASN
12	C0	82	LEU
13	C1	21	ASN
13	C1	30	ARG
13	C1	40	LEU
13	C1	44	THR
13	C1	67	ARG
13	C1	69	LYS
13	C1	74	THR
13	C1	80	MET
13	C1	123	VAL
14	C2	28	LEU
14	C2	33	ARG
14	C2	37	VAL
14	C2	43	ARG
14	C2	52	LEU
14	C2	71	ILE
14	C2	74	LEU
14	C2	86	VAL
14	C2	103	LEU
14	C2	126	TRP
14	C2	129	GLU
14	C2	132	GLU
15	C3	3	ARG
15	C3	6	SER
15	C3	9	LYS
15	C3	16	ILE
15	C3	27	LYS

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Mol	Chain	Res	Type
15	C3	31	GLU
15	C3	39	LYS
15	C3	42	ARG
15	C3	60	VAL
15	C3	64	ARG
15	C3	66	ILE
15	C3	83	GLU
15	C3	88	LEU
15	C3	102	LEU
15	C3	105	ASN
15	C3	109	LYS
15	C3	115	LEU
15	C3	125	LEU
15	C3	142	GLU
15	C3	149	LEU
16	C4	13	VAL
16	C4	16	VAL
16	C4	26	THR
16	C4	29	HIS
16	C4	31	THR
16	C4	39	ILE
16	C4	42	VAL
16	C4	46	MET
16	C4	51	ASP
16	C4	84	ARG
16	C4	89	THR
16	C4	92	LYS
16	C4	99	GLN
16	C4	103	ARG
16	C4	125	SER
16	C4	128	LYS
16	C4	132	ARG
16	C4	136	ARG
16	C4	137	LEU
17	C5	11	VAL
17	C5	21	ASP
17	C5	22	LEU
17	C5	29	SER
17	C5	31	GLU
17	C5	34	VAL
17	C5	36	LEU
17	C5	40	ARG

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Mol	Chain	Res	Type
17	C5	44	ARG
17	C5	50	THR
17	C5	52	LYS
17	C5	60	LEU
17	C5	69	GLU
17	C5	71	GLU
17	C5	80	MET
17	C5	86	VAL
17	C5	88	GLU
17	C5	106	GLU
18	C6	4	VAL
18	C6	14	LYS
18	C6	29	ILE
18	C6	39	VAL
18	C6	52	LEU
18	C6	53	LEU
18	C6	54	LEU
18	C6	57	LEU
18	C6	66	ARG
18	C6	69	VAL
18	C6	103	ASN
18	C6	109	PHE
18	C6	123	ARG
18	C6	127	LYS
18	C6	128	LYS
18	C6	137	ARG
19	C7	3	ARG
19	C7	5	ARG
19	C7	6	THR
19	C7	7	LYS
19	C7	8	THR
19	C7	24	LEU
19	C7	25	THR
19	C7	38	ILE
19	C7	49	LYS
19	C7	58	MET
19	C7	69	ILE
19	C7	76	GLU
19	C7	84	TYR
19	C7	88	VAL
19	C7	105	GLN
19	C7	107	SER

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Mol	Chain	Res	Type
19	C7	113	LEU
19	C7	115	LEU
20	C8	3	LEU
20	C8	5	VAL
20	C8	8	GLN
20	C8	11	PHE
20	C8	13	HIS
20	C8	14	ILE
20	C8	17	LEU
20	C8	25	ASN
20	C8	28	ILE
20	C8	32	LEU
20	C8	40	ARG
20	C8	57	ARG
20	C8	86	LEU
20	C8	92	ILE
20	C8	93	THR
20	C8	97	ASP
20	C8	107	SER
20	C8	108	LYS
20	C8	110	ARG
20	C8	115	ARG
20	C8	136	GLN
20	C8	138	THR
20	C8	143	ARG
21	C9	12	GLN
21	C9	22	LEU
21	C9	28	LEU
21	C9	33	TYR
21	C9	34	VAL
21	C9	35	ASP
21	C9	36	ILE
21	C9	54	PHE
21	C9	57	ARG
21	C9	64	HIS
21	C9	67	MET
21	C9	71	VAL
21	C9	76	LEU
21	C9	114	VAL
21	C9	127	ASN
21	C9	130	ARG
22	D0	19	ILE

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Mol	Chain	Res	Type
22	D0	20	ILE
22	D0	22	ILE
22	D0	31	VAL
22	D0	51	VAL
22	D0	57	ARG
22	D0	66	SER
22	D0	74	GLU
22	D0	76	SER
22	D0	81	THR
22	D0	89	ARG
22	D0	121	ASN
23	D1	5	LYS
23	D1	11	LEU
23	D1	32	VAL
23	D1	36	VAL
23	D1	41	GLU
23	D1	52	THR
23	D1	62	ARG
23	D1	65	SER
23	D1	68	SER
23	D1	74	GLN
23	D1	78	LEU
23	D1	79	LEU
23	D1	87	ARG
24	D2	4	SER
24	D2	7	LEU
24	D2	16	ASN
24	D2	24	GLN
24	D2	27	ILE
24	D2	42	GLN
24	D2	53	ILE
24	D2	56	HIS
24	D2	65	LEU
24	D2	66	ASN
24	D2	76	SER
24	D2	86	ILE
24	D2	93	LEU
24	D2	98	GLN
24	D2	103	ILE
24	D2	104	LEU
24	D2	105	THR
24	D2	107	SER

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Mol	Chain	Res	Type
24	D2	121	VAL
25	D3	3	LYS
25	D3	7	ARG
25	D3	9	LEU
25	D3	14	LYS
25	D3	16	ARG
25	D3	47	SER
25	D3	73	ARG
25	D3	79	ASN
25	D3	84	THR
25	D3	96	VAL
25	D3	100	ASP
25	D3	103	LEU
25	D3	107	PHE
25	D3	114	LYS
25	D3	128	SER
25	D3	144	ARG
26	D4	17	LEU
26	D4	34	ASN
26	D4	51	GLU
26	D4	57	VAL
26	D4	96	LEU
26	D4	99	LYS
26	D4	102	LYS
26	D4	124	ARG
26	D4	127	LYS
27	D5	40	VAL
27	D5	42	LEU
27	D5	47	TYR
27	D5	58	ARG
27	D5	62	VAL
27	D5	67	ASP
27	D5	69	LEU
27	D5	75	LEU
27	D5	95	HIS
27	D5	96	SER
27	D5	97	LYS
27	D5	102	THR
28	D6	12	LYS
28	D6	15	ARG
28	D6	19	LYS
28	D6	30	ILE

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Mol	Chain	Res	Type
28	D6	36	ILE
28	D6	38	ARG
28	D6	44	ILE
28	D6	46	GLU
28	D6	61	GLU
28	D6	64	LEU
28	D6	68	TYR
28	D6	91	ASP
29	D7	3	LEU
29	D7	23	THR
29	D7	26	GLN
29	D7	33	LEU
29	D7	34	ASP
29	D7	61	THR
30	D8	14	LYS
30	D8	19	THR
30	D8	31	GLU
30	D8	32	PHE
30	D8	35	ASP
30	D8	48	VAL
30	D8	54	LEU
30	D8	58	GLU
30	D8	65	ARG
31	D9	6	VAL
31	D9	7	TRP
31	D9	9	SER
31	D9	12	ARG
31	D9	14	TYR
31	D9	19	ARG
31	D9	22	ARG
31	D9	28	THR
31	D9	30	LEU
31	D9	32	ARG
31	D9	36	LEU
32	E0	21	VAL
32	E0	22	GLU
32	E0	28	LYS
32	E0	36	LYS
32	E0	39	LEU
32	E0	42	ARG
32	E0	46	ASN
32	E0	50	VAL

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Mol	Chain	Res	Type
33	E1	89	LYS
33	E1	93	HIS
33	E1	98	VAL
33	E1	102	VAL
33	E1	103	LEU
33	E1	106	TYR
33	E1	108	VAL
33	E1	111	GLU
33	E1	113	LYS
33	E1	120	GLU
33	E1	126	CYS
33	E1	134	ASN
33	E1	135	HIS
33	E1	137	ASP
33	E1	138	ARG
33	E1	147	VAL
33	E1	151	ASN
34	SR	6	VAL
34	SR	32	LEU
34	SR	45	TRP
34	SR	52	GLN
34	SR	65	SER
34	SR	66	HIS
34	SR	71	CYS
34	SR	73	LEU
34	SR	76	ASP
34	SR	106	HIS
34	SR	116	ASP
34	SR	117	LYS
34	SR	136	ILE
34	SR	137	LYS
34	SR	144	LEU
34	SR	145	LEU
34	SR	191	ASP
34	SR	223	TRP
34	SR	233	THR
34	SR	238	ASP
34	SR	248	ASN
34	SR	266	ASP
34	SR	268	GLN
34	SR	269	TYR
34	SR	288	HIS

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Mol	Chain	Res	Type
34	SR	290	VAL
34	SR	308	ASN
34	SR	314	GLN
34	SR	317	THR
35	SM	33	LYS
35	SM	46	LYS
35	SM	48	ARG
35	SM	53	ARG
35	SM	64	LYS
35	SM	68	ARG
35	SM	77	THR
35	SM	84	LYS
35	SM	89	ARG
35	SM	96	ARG
35	SM	100	THR
35	SM	102	THR
35	SM	116	GLU
35	SM	121	LYS
35	SM	139	GLU
39	L2	20	THR
39	L2	28	LYS
39	L2	31	THR
39	L2	32	LEU
39	L2	44	ILE
39	L2	45	VAL
39	L2	46	LYS
39	L2	49	VAL
39	L2	62	VAL
39	L2	70	ARG
39	L2	71	LEU
39	L2	72	ARG
39	L2	74	GLU
39	L2	84	THR
39	L2	101	VAL
39	L2	102	LEU
39	L2	104	LEU
39	L2	109	GLU
39	L2	113	VAL
39	L2	126	LEU
39	L2	128	ARG
39	L2	135	ILE
39	L2	149	ARG

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Mol	Chain	Res	Type
39	L2	157	VAL
39	L2	165	VAL
39	L2	168	VAL
39	L2	179	LEU
39	L2	180	LEU
39	L2	191	LEU
39	L2	202	VAL
39	L2	204	MET
39	L2	207	VAL
39	L2	227	ARG
39	L2	241	ARG
39	L2	252	THR
40	L3	7	GLU
40	L3	17	LEU
40	L3	19	ARG
40	L3	25	ILE
40	L3	37	ARG
40	L3	44	THR
40	L3	47	LEU
40	L3	55	THR
40	L3	56	ILE
40	L3	67	PHE
40	L3	81	THR
40	L3	84	VAL
40	L3	85	VAL
40	L3	103	THR
40	L3	104	THR
40	L3	114	VAL
40	L3	116	ARG
40	L3	148	LEU
40	L3	160	VAL
40	L3	166	ILE
40	L3	169	THR
40	L3	174	LYS
40	L3	183	LEU
40	L3	187	SER
40	L3	188	ILE
40	L3	192	VAL
40	L3	196	ARG
40	L3	202	THR
40	L3	211	GLN
40	L3	229	VAL

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Mol	Chain	Res	Type
40	L3	235	THR
40	L3	238	LEU
40	L3	246	LEU
40	L3	252	ILE
40	L3	264	VAL
40	L3	284	ARG
40	L3	296	THR
40	L3	304	THR
40	L3	305	ILE
40	L3	320	ASP
40	L3	332	ARG
40	L3	338	LEU
40	L3	353	GLU
40	L3	380	MET
40	L3	386	ASP
40	L3	387	LEU
41	L4	4	PRO
41	L4	27	SER
41	L4	69	ARG
41	L4	71	VAL
41	L4	74	ILE
41	L4	92	ASN
41	L4	93	MET
41	L4	99	MET
41	L4	120	TYR
41	L4	124	SER
41	L4	133	SER
41	L4	152	VAL
41	L4	153	SER
41	L4	156	LEU
41	L4	172	VAL
41	L4	179	LEU
41	L4	187	LEU
41	L4	194	TYR
41	L4	200	THR
41	L4	203	ARG
41	L4	211	GLU
41	L4	222	VAL
41	L4	227	THR
41	L4	230	VAL
41	L4	246	ARG
41	L4	256	THR

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Mol	Chain	Res	Type
41	L4	258	LEU
41	L4	259	ASP
41	L4	284	SER
41	L4	287	THR
41	L4	292	SER
41	L4	293	SER
41	L4	296	GLN
41	L4	306	THR
41	L4	307	GLN
41	L4	313	LEU
41	L4	316	ASN
41	L4	323	VAL
41	L4	327	LEU
41	L4	333	VAL
41	L4	339	LEU
41	L4	341	SER
41	L4	343	LYS
41	L4	349	THR
41	L4	354	VAL
41	L4	359	LEU
41	L4	361	HIS
42	L5	5	LYS
42	L5	8	LYS
42	L5	22	ARG
42	L5	23	ARG
42	L5	35	ARG
42	L5	41	LYS
42	L5	56	THR
42	L5	66	SER
42	L5	67	SER
42	L5	69	ILE
42	L5	101	THR
42	L5	105	ILE
42	L5	113	LEU
42	L5	115	LEU
42	L5	126	GLU
42	L5	128	GLU
42	L5	137	ASP
42	L5	140	ARG
42	L5	146	LEU
42	L5	151	GLN
42	L5	152	ARG

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Mol	Chain	Res	Type
42	L5	155	THR
42	L5	163	LEU
42	L5	177	GLU
42	L5	185	PHE
42	L5	188	GLU
42	L5	190	ILE
42	L5	194	LEU
42	L5	208	MET
42	L5	211	LEU
42	L5	216	GLU
42	L5	222	LEU
42	L5	223	PHE
42	L5	227	LEU
42	L5	231	ILE
42	L5	234	ASP
42	L5	237	GLU
42	L5	242	SER
42	L5	272	TYR
42	L5	278	SER
42	L5	293	LEU
43	L6	5	LYS
43	L6	14	ASP
43	L6	15	VAL
43	L6	21	THR
43	L6	31	ARG
43	L6	35	VAL
43	L6	48	ARG
43	L6	52	VAL
43	L6	57	HIS
43	L6	64	LEU
43	L6	65	ILE
43	L6	76	LEU
43	L6	78	ARG
43	L6	84	VAL
43	L6	89	THR
43	L6	93	VAL
43	L6	134	ARG
43	L6	152	THR
43	L6	154	LEU
43	L6	160	SER
44	L7	24	GLU
44	L7	25	GLN

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Mol	Chain	Res	Type
44	L7	26	VAL
44	L7	38	LYS
44	L7	60	ARG
44	L7	78	GLU
44	L7	82	LYS
44	L7	93	ASN
44	L7	98	LYS
44	L7	100	ARG
44	L7	107	ARG
44	L7	110	ARG
44	L7	115	THR
44	L7	124	LEU
44	L7	127	LEU
44	L7	143	THR
44	L7	157	ASN
44	L7	173	LEU
44	L7	179	LEU
44	L7	182	ASP
44	L7	184	LEU
44	L7	239	LEU
45	L8	26	LEU
45	L8	41	GLN
45	L8	50	VAL
45	L8	57	ARG
45	L8	63	LYS
45	L8	69	LEU
45	L8	71	VAL
45	L8	74	THR
45	L8	79	GLN
45	L8	84	ARG
45	L8	109	LEU
45	L8	134	TYR
45	L8	136	LEU
45	L8	145	ASN
45	L8	150	LEU
45	L8	156	ASP
45	L8	157	VAL
45	L8	169	LEU
45	L8	180	VAL
45	L8	181	LYS
45	L8	185	ARG
45	L8	189	LEU

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Mol	Chain	Res	Type
45	L8	203	VAL
45	L8	218	ILE
45	L8	230	LYS
45	L8	246	MET
45	L8	248	LYS
46	L9	5	GLN
46	L9	9	GLN
46	L9	41	ILE
46	L9	48	VAL
46	L9	49	ASN
46	L9	52	LEU
46	L9	68	LEU
46	L9	69	ARG
46	L9	70	THR
46	L9	80	THR
46	L9	82	VAL
46	L9	132	VAL
46	L9	151	VAL
46	L9	152	GLU
46	L9	157	ASN
46	L9	161	LEU
46	L9	164	ILE
46	L9	172	ILE
46	L9	187	ILE
46	L9	189	GLU
47	M0	3	ARG
47	M0	24	ARG
47	M0	26	VAL
47	M0	28	ASP
47	M0	30	LYS
47	M0	31	ILE
47	M0	32	ARG
47	M0	33	ILE
47	M0	39	LYS
47	M0	48	LEU
47	M0	52	LEU
47	M0	60	LEU
47	M0	61	SER
47	M0	63	GLU
47	M0	87	LEU
47	M0	91	VAL
47	M0	102	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
47	M0	116	ARG
47	M0	128	ARG
47	M0	131	ILE
47	M0	138	VAL
47	M0	139	ARG
47	M0	140	THR
47	M0	145	LYS
47	M0	146	ASP
47	M0	163	GLN
47	M0	165	ILE
47	M0	169	LYS
47	M0	174	THR
47	M0	178	ARG
47	M0	185	ARG
47	M0	189	GLU
47	M0	192	ASP
47	M0	203	LYS
47	M0	215	GLU
48	M1	10	ARG
48	M1	12	LEU
48	M1	13	LYS
48	M1	19	LEU
48	M1	25	GLU
48	M1	44	THR
48	M1	46	VAL
48	M1	78	GLU
48	M1	80	LEU
48	M1	82	ARG
48	M1	85	LYS
48	M1	101	ASN
48	M1	106	ILE
48	M1	112	LEU
48	M1	115	LYS
48	M1	117	ASP
48	M1	138	VAL
48	M1	140	ARG
48	M1	142	LYS
48	M1	158	ASP
48	M1	166	LYS
48	M1	168	ASP
48	M1	171	VAL
49	M3	23	LYS

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Mol	Chain	Res	Type
49	M3	24	VAL
49	M3	35	ARG
49	M3	54	LEU
49	M3	55	ARG
49	M3	57	VAL
49	M3	59	ARG
49	M3	67	ARG
49	M3	104	ARG
49	M3	114	GLN
49	M3	122	LYS
49	M3	128	ARG
49	M3	131	LYS
49	M3	134	GLU
49	M3	164	GLU
49	M3	168	ARG
50	M4	5	SER
50	M4	8	LYS
50	M4	15	VAL
50	M4	20	VAL
50	M4	43	LYS
50	M4	53	VAL
50	M4	58	ILE
50	M4	63	VAL
50	M4	64	VAL
50	M4	65	LEU
50	M4	74	ARG
50	M4	90	VAL
50	M4	92	GLU
50	M4	105	GLN
50	M4	130	THR
51	M5	15	GLN
51	M5	17	ASP
51	M5	18	VAL
51	M5	22	LEU
51	M5	49	ARG
51	M5	75	VAL
51	M5	80	THR
51	M5	92	LEU
51	M5	106	VAL
51	M5	133	ILE
51	M5	151	ILE
51	M5	153	ASP

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Mol	Chain	Res	Type
51	M5	155	VAL
51	M5	157	LYS
51	M5	171	SER
51	M5	182	ASN
51	M5	183	THR
51	M5	184	LYS
51	M5	188	ARG
51	M5	190	THR
51	M5	198	SER
51	M5	201	ARG
52	M6	3	VAL
52	M6	22	VAL
52	M6	31	GLN
52	M6	32	LYS
52	M6	34	VAL
52	M6	48	PHE
52	M6	67	THR
52	M6	78	ARG
52	M6	85	ARG
52	M6	89	SER
52	M6	101	ARG
52	M6	106	GLU
52	M6	113	ASP
52	M6	114	LYS
52	M6	116	LYS
52	M6	117	ARG
52	M6	124	LEU
52	M6	128	ARG
52	M6	138	LEU
52	M6	140	LYS
52	M6	143	THR
52	M6	160	ARG
52	M6	187	GLU
52	M6	189	ASP
53	M7	7	THR
53	M7	24	VAL
53	M7	29	THR
53	M7	36	ILE
53	M7	42	THR
53	M7	52	LEU
53	M7	69	ARG
53	M7	91	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
53	M7	112	LEU
53	M7	114	VAL
53	M7	127	ARG
53	M7	128	ARG
53	M7	129	THR
53	M7	142	SER
53	M7	144	SER
53	M7	168	LEU
53	M7	171	ARG
54	M8	17	THR
54	M8	24	VAL
54	M8	26	LEU
54	M8	32	LEU
54	M8	49	LEU
54	M8	69	ARG
54	M8	80	THR
54	M8	86	THR
54	M8	105	ARG
54	M8	135	GLN
54	M8	136	ASN
54	M8	138	LEU
54	M8	171	LYS
54	M8	181	SER
55	M9	22	VAL
55	M9	36	ASN
55	M9	41	ILE
55	M9	44	LEU
55	M9	47	ASN
55	M9	51	VAL
55	M9	55	VAL
55	M9	60	LYS
55	M9	61	SER
55	M9	74	ARG
55	M9	76	SER
55	M9	103	ARG
55	M9	105	LEU
55	M9	116	ASP
55	M9	126	GLU
55	M9	127	SER
55	M9	134	HIS
55	M9	138	LEU
55	M9	160	GLU

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Mol	Chain	Res	Type
55	M9	165	LYS
55	M9	180	LYS
56	N0	1	MET
56	N0	16	THR
56	N0	45	LEU
56	N0	61	ILE
56	N0	71	LYS
56	N0	81	TYR
56	N0	87	THR
56	N0	88	HIS
56	N0	97	VAL
56	N0	115	ARG
56	N0	117	ARG
56	N0	120	SER
56	N0	130	GLU
56	N0	132	THR
56	N0	137	ARG
56	N0	145	THR
56	N0	149	LYS
56	N0	160	THR
56	N0	162	THR
56	N0	167	ARG
56	N0	171	PHE
56	N0	172	TYR
57	N1	12	ARG
57	N1	14	MET
57	N1	18	ASP
57	N1	25	VAL
57	N1	26	HIS
57	N1	27	LEU
57	N1	32	LYS
57	N1	39	ILE
57	N1	55	LYS
57	N1	75	ILE
57	N1	78	LYS
57	N1	79	MET
57	N1	83	ARG
57	N1	88	ARG
57	N1	89	LEU
57	N1	101	CYS
57	N1	104	GLU
57	N1	106	LEU

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Mol	Chain	Res	Type
57	N1	118	GLU
57	N1	122	GLN
57	N1	126	VAL
57	N1	127	GLN
57	N1	131	GLN
57	N1	139	ARG
57	N1	141	VAL
57	N1	143	THR
57	N1	154	VAL
57	N1	157	GLU
57	N1	158	THR
58	N2	10	LYS
58	N2	16	THR
58	N2	38	ILE
58	N2	50	LEU
58	N2	52	ASN
58	N2	70	LYS
58	N2	99	LYS
58	N2	100	THR
59	N3	9	THR
59	N3	13	ILE
59	N3	44	SER
59	N3	54	LEU
59	N3	69	LEU
59	N3	73	VAL
59	N3	83	LYS
59	N3	84	SER
59	N3	86	ARG
59	N3	102	ILE
59	N3	106	LYS
59	N3	108	GLU
59	N3	115	THR
59	N3	124	ASP
60	N4	4	GLU
60	N4	5	ILE
60	N4	17	ARG
60	N4	19	THR
60	N4	41	LYS
60	N4	43	ARG
60	N4	45	ASN
61	N5	27	ARG
61	N5	28	THR

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Mol	Chain	Res	Type
61	N5	34	LEU
61	N5	36	LYS
61	N5	37	THR
61	N5	38	LEU
61	N5	63	ILE
61	N5	71	THR
61	N5	73	MET
61	N5	74	LYS
61	N5	108	LEU
61	N5	115	ARG
61	N5	125	ARG
61	N5	127	THR
61	N5	133	LEU
61	N5	135	ILE
61	N5	139	ILE
61	N5	142	ILE
62	N6	3	LYS
62	N6	10	SER
62	N6	14	LYS
62	N6	37	LYS
62	N6	40	ARG
62	N6	45	ILE
62	N6	50	ILE
62	N6	51	ARG
62	N6	56	VAL
62	N6	57	LEU
62	N6	59	VAL
62	N6	71	SER
62	N6	74	TYR
62	N6	76	LEU
62	N6	89	LYS
62	N6	111	LEU
62	N6	113	LYS
62	N6	115	ARG
62	N6	127	GLU
63	N7	17	ARG
63	N7	30	ASP
63	N7	34	LYS
63	N7	46	ILE
63	N7	60	LYS
63	N7	64	LYS
63	N7	75	VAL

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Mol	Chain	Res	Type
63	N7	83	THR
63	N7	102	GLU
63	N7	109	GLU
63	N7	134	LEU
64	N8	4	ARG
64	N8	6	THR
64	N8	8	THR
64	N8	10	LYS
64	N8	12	ARG
64	N8	14	HIS
64	N8	42	ARG
64	N8	46	ASP
64	N8	60	TYR
64	N8	73	LEU
64	N8	76	ASP
64	N8	78	LEU
64	N8	88	ASP
64	N8	115	LYS
64	N8	118	ILE
64	N8	120	ASN
64	N8	130	VAL
64	N8	133	LEU
65	N9	22	LYS
65	N9	25	LYS
65	N9	28	LYS
65	N9	38	LYS
65	N9	50	THR
65	N9	59	LYS
66	O0	12	GLN
66	O0	16	LEU
66	O0	18	ILE
66	O0	32	LYS
66	O0	33	SER
66	O0	52	ARG
66	O0	61	MET
66	O0	67	VAL
66	O0	83	LYS
66	O0	87	VAL
66	O0	100	ILE
67	O1	6	ASP
67	O1	16	LEU
67	O1	26	LYS

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Mol	Chain	Res	Type
67	O1	41	LYS
67	O1	55	LEU
67	O1	64	VAL
67	O1	65	LYS
67	O1	68	GLU
67	O1	73	LEU
67	O1	76	SER
67	O1	79	ARG
67	O1	82	GLU
67	O1	83	GLU
67	O1	106	THR
68	O2	3	SER
68	O2	16	LYS
68	O2	19	ARG
68	O2	24	ARG
68	O2	31	ASN
68	O2	33	ARG
68	O2	35	GLN
68	O2	41	VAL
68	O2	55	ILE
68	O2	61	LYS
68	O2	62	LYS
68	O2	73	THR
68	O2	79	VAL
68	O2	103	LYS
68	O2	106	VAL
68	O2	109	LEU
68	O2	125	ARG
68	O2	126	LEU
69	O3	37	THR
69	O3	48	ARG
69	O3	49	ILE
69	O3	56	SER
69	O3	59	VAL
69	O3	70	LYS
69	O3	78	SER
69	O3	81	VAL
69	O3	98	VAL
70	O4	8	ARG
70	O4	21	LYS
70	O4	29	ILE
70	O4	38	LEU

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Mol	Chain	Res	Type
70	O4	57	LEU
70	O4	58	ARG
70	O4	65	VAL
70	O4	71	THR
70	O4	86	LYS
70	O4	102	LYS
70	O4	104	VAL
71	O5	7	TYR
71	O5	13	SER
71	O5	15	GLU
71	O5	21	LEU
71	O5	22	VAL
71	O5	28	LEU
71	O5	47	VAL
71	O5	48	ARG
71	O5	71	LYS
71	O5	89	ARG
71	O5	90	ARG
71	O5	96	GLU
71	O5	101	THR
71	O5	102	GLU
72	O6	11	LEU
72	O6	21	THR
72	O6	26	ILE
72	O6	36	ARG
72	O6	53	TYR
72	O6	57	LEU
72	O6	58	ILE
72	O6	62	ARG
72	O6	68	ARG
72	O6	76	ARG
72	O6	81	THR
72	O6	90	MET
72	O6	91	ASN
72	O6	98	ARG
72	O6	99	ARG
73	O7	12	HIS
73	O7	16	HIS
73	O7	21	ARG
73	O7	24	ARG
73	O7	25	ARG
73	O7	31	LYS

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Mol	Chain	Res	Type
73	O7	44	THR
73	O7	46	SER
73	O7	55	ARG
73	O7	58	THR
73	O7	65	ARG
73	O7	67	LEU
73	O7	75	LYS
73	O7	85	LYS
73	O7	87	SER
74	O8	5	ILE
74	O8	8	ILE
74	O8	39	ARG
74	O8	41	THR
74	O8	45	VAL
74	O8	46	ARG
74	O8	51	LEU
74	O8	52	TYR
74	O8	53	THR
74	O8	64	LYS
74	O8	65	LEU
74	O8	67	GLN
74	O8	69	LEU
74	O8	77	ARG
74	O8	78	LEU
75	O9	5	LYS
75	O9	21	ARG
75	O9	23	LEU
75	O9	28	ARG
75	O9	34	THR
75	O9	37	TYR
75	O9	51	ILE
76	Q0	77	ILE
76	Q0	79	GLU
76	Q0	85	LEU
76	Q0	97	ARG
76	Q0	112	LYS
76	Q0	113	ARG
76	Q0	114	LYS
76	Q0	127	LEU
77	Q1	2	ARG
77	Q1	10	THR
77	Q1	11	ARG

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Mol	Chain	Res	Type
77	Q1	13	LEU
78	Q2	8	ARG
78	Q2	9	LYS
78	Q2	20	HIS
78	Q2	26	THR
78	Q2	45	ARG
78	Q2	47	GLN
78	Q2	80	ARG
78	Q2	83	LEU
78	Q2	84	THR
78	Q2	92	GLU
78	Q2	93	LEU
78	Q2	100	LYS
78	Q2	104	LEU
78	Q2	105	GLN
79	Q3	5	THR
79	Q3	11	THR
79	Q3	25	GLN
79	Q3	28	LYS
79	Q3	33	GLN
79	Q3	36	ARG
79	Q3	40	SER
79	Q3	45	LYS
79	Q3	49	ARG
79	Q3	64	VAL
79	Q3	70	THR
79	Q3	84	ARG
2	s0	9	LEU
2	s0	12	GLU
2	s0	31	VAL
2	s0	41	ARG
2	s0	45	VAL
2	s0	69	ASN
2	s0	87	LEU
2	s0	93	THR
2	s0	101	ARG
2	s0	108	THR
2	s0	124	THR
2	s0	138	TYR
2	s0	154	GLU
2	s0	158	VAL
2	s0	172	LEU

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Mol	Chain	Res	Type
2	s0	179	ARG
2	s0	180	GLU
2	s0	183	ARG
2	s0	185	ARG
2	s0	188	LEU
2	s0	189	VAL
2	s0	198	MET
2	s0	200	ASP
3	s1	21	VAL
3	s1	25	THR
3	s1	26	ARG
3	s1	39	GLU
3	s1	42	ASN
3	s1	47	LEU
3	s1	51	SER
3	s1	62	LYS
3	s1	66	VAL
3	s1	68	VAL
3	s1	70	LEU
3	s1	73	LEU
3	s1	78	ASP
3	s1	81	PHE
3	s1	83	LYS
3	s1	87	ARG
3	s1	105	PHE
3	s1	115	ARG
3	s1	124	ASN
3	s1	126	THR
3	s1	135	LEU
3	s1	137	ILE
3	s1	152	ARG
3	s1	154	SER
3	s1	173	THR
3	s1	177	GLN
3	s1	181	LEU
3	s1	184	LEU
3	s1	185	THR
3	s1	209	ASN
3	s1	212	VAL
3	s1	215	VAL
3	s1	219	LYS
3	s1	231	LEU

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Mol	Chain	Res	Type
3	s1	232	HIS
4	s2	41	LEU
4	s2	53	ILE
4	s2	54	GLU
4	s2	58	LEU
4	s2	69	ILE
4	s2	70	ASP
4	s2	72	LEU
4	s2	78	ASP
4	s2	83	ILE
4	s2	87	GLN
4	s2	90	THR
4	s2	91	ARG
4	s2	97	ARG
4	s2	111	VAL
4	s2	113	LEU
4	s2	115	ILE
4	s2	141	ARG
4	s2	146	THR
4	s2	150	GLN
4	s2	152	HIS
4	s2	164	SER
4	s2	166	THR
4	s2	170	ILE
4	s2	195	ASP
4	s2	196	VAL
4	s2	218	ILE
4	s2	221	THR
4	s2	222	TYR
4	s2	224	PHE
4	s2	225	LEU
4	s2	226	THR
4	s2	238	SER
4	s2	240	LEU
4	s2	242	ILE
4	s2	250	GLN
5	s3	4	LEU
5	s3	7	LYS
5	s3	9	ARG
5	s3	21	LEU
5	s3	31	GLU
5	s3	34	TYR

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Mol	Chain	Res	Type
5	s3	37	VAL
5	s3	44	THR
5	s3	55	THR
5	s3	59	LEU
5	s3	61	GLU
5	s3	67	ASN
5	s3	79	TYR
5	s3	84	ILE
5	s3	90	ARG
5	s3	91	VAL
5	s3	96	LEU
5	s3	115	ILE
5	s3	120	TYR
5	s3	125	TYR
5	s3	127	MET
5	s3	128	GLU
5	s3	158	ILE
5	s3	162	GLN
5	s3	164	VAL
5	s3	168	ILE
5	s3	169	ASP
5	s3	176	LEU
5	s3	189	MET
5	s3	212	LYS
5	s3	218	LEU
5	s3	223	LYS
6	s4	12	LEU
6	s4	38	LEU
6	s4	42	LEU
6	s4	48	LEU
6	s4	49	ARG
6	s4	51	ARG
6	s4	66	MET
6	s4	70	VAL
6	s4	78	THR
6	s4	96	ASN
6	s4	113	ARG
6	s4	120	SER
6	s4	128	LYS
6	s4	131	LEU
6	s4	148	ARG
6	s4	164	LEU

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Mol	Chain	Res	Type
6	s4	170	THR
6	s4	180	LEU
6	s4	182	TYR
6	s4	184	THR
6	s4	194	THR
6	s4	214	LEU
6	s4	219	VAL
6	s4	220	THR
6	s4	221	ARG
6	s4	222	LEU
6	s4	223	ASN
6	s4	227	VAL
6	s4	246	LEU
7	s5	24	VAL
7	s5	25	LEU
7	s5	27	THR
7	s5	31	GLU
7	s5	42	LEU
7	s5	45	LYS
7	s5	48	PHE
7	s5	63	GLN
7	s5	65	ARG
7	s5	68	ILE
7	s5	93	LEU
7	s5	94	THR
7	s5	102	ARG
7	s5	112	ARG
7	s5	119	ASP
7	s5	124	LEU
7	s5	137	ILE
7	s5	147	THR
7	s5	157	ARG
7	s5	193	THR
7	s5	203	LYS
7	s5	219	ARG
7	s5	225	ARG
8	s6	10	ASN
8	s6	15	THR
8	s6	31	ARG
8	s6	34	GLN
8	s6	65	GLN
8	s6	71	THR

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Mol	Chain	Res	Type
8	s6	76	LEU
8	s6	78	THR
8	s6	82	SER
8	s6	93	LYS
8	s6	97	VAL
8	s6	101	ILE
8	s6	108	VAL
8	s6	109	LEU
8	s6	121	LEU
8	s6	126	ASP
8	s6	127	THR
8	s6	128	THR
8	s6	133	LEU
8	s6	137	ARG
8	s6	143	LYS
8	s6	153	VAL
8	s6	155	ASP
8	s6	156	PHE
8	s6	163	THR
8	s6	177	ARG
8	s6	179	VAL
8	s6	191	ARG
8	s6	215	ARG
9	s7	24	PHE
9	s7	33	GLU
9	s7	49	ILE
9	s7	50	ASP
9	s7	60	ILE
9	s7	75	THR
9	s7	77	LEU
9	s7	80	GLU
9	s7	86	GLN
9	s7	95	GLU
9	s7	97	ARG
9	s7	108	GLN
9	s7	114	ARG
9	s7	116	ARG
9	s7	126	LEU
9	s7	143	LEU
9	s7	144	VAL
9	s7	148	LYS
9	s7	159	VAL

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Mol	Chain	Res	Type
10	s8	4	SER
10	s8	10	LYS
10	s8	22	ARG
10	s8	25	ARG
10	s8	29	LEU
10	s8	36	THR
10	s8	46	VAL
10	s8	59	ARG
10	s8	61	GLU
10	s8	72	ILE
10	s8	76	THR
10	s8	77	ARG
10	s8	89	GLU
10	s8	138	ASN
10	s8	151	LYS
10	s8	152	ILE
10	s8	183	ILE
10	s8	187	GLU
11	s9	3	ARG
11	s9	6	ARG
11	s9	7	THR
11	s9	8	TYR
11	s9	16	LYS
11	s9	28	LEU
11	s9	33	GLU
11	s9	46	SER
11	s9	49	LEU
11	s9	50	SER
11	s9	61	THR
11	s9	78	ARG
11	s9	82	ARG
11	s9	83	VAL
11	s9	93	LEU
11	s9	96	VAL
11	s9	99	LEU
11	s9	101	VAL
11	s9	103	ASP
11	s9	109	LEU
11	s9	111	THR
11	s9	121	SER
11	s9	126	ARG
11	s9	132	ARG

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Mol	Chain	Res	Type
11	s9	134	ILE
11	s9	151	ASP
11	s9	171	ARG
11	s9	172	VAL
11	s9	180	LYS
11	s9	182	GLU
80	c0	2	LEU
80	c0	15	LEU
80	c0	20	VAL
80	c0	27	PHE
80	c0	36	ASP
80	c0	47	GLN
80	c0	55	VAL
80	c0	71	GLU
80	c0	77	ARG
13	c1	3	THR
13	c1	5	LEU
13	c1	30	ARG
13	c1	40	LEU
13	c1	44	THR
13	c1	47	THR
13	c1	60	PHE
13	c1	67	ARG
13	c1	74	THR
13	c1	79	LYS
13	c1	86	ILE
13	c1	87	ARG
13	c1	90	TYR
13	c1	117	VAL
13	c1	118	GLN
13	c1	129	ARG
14	c2	38	HIS
14	c2	52	LEU
14	c2	59	LEU
14	c2	61	VAL
14	c2	62	LEU
14	c2	71	ILE
14	c2	74	LEU
14	c2	103	LEU
14	c2	120	VAL
14	c2	121	VAL
14	c2	132	GLU

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Mol	Chain	Res	Type
14	c2	136	ILE
15	c3	6	SER
15	c3	16	ILE
15	c3	20	ARG
15	c3	21	ASN
15	c3	29	SER
15	c3	33	VAL
15	c3	53	LEU
15	c3	64	ARG
15	c3	66	ILE
15	c3	67	THR
15	c3	70	LYS
15	c3	84	ILE
15	c3	87	ASP
15	c3	103	GLU
15	c3	115	LEU
15	c3	127	ARG
15	c3	138	ASN
15	c3	139	TRP
15	c3	141	TYR
16	c4	20	TYR
16	c4	23	PHE
16	c4	26	THR
16	c4	28	VAL
16	c4	31	THR
16	c4	51	ASP
16	c4	62	LEU
16	c4	107	ARG
16	c4	114	ARG
16	c4	123	SER
16	c4	133	ARG
16	c4	136	ARG
16	c4	137	LEU
17	c5	12	PHE
17	c5	20	VAL
17	c5	21	ASP
17	c5	27	GLU
17	c5	36	LEU
17	c5	44	ARG
17	c5	59	LYS
17	c5	61	ARG
17	c5	69	GLU

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Mol	Chain	Res	Type
17	c5	71	GLU
17	c5	84	ILE
17	c5	89	MET
17	c5	107	ILE
17	c5	110	GLU
17	c5	122	THR
17	c5	126	VAL
17	c5	127	ARG
17	c5	128	HIS
18	c6	6	SER
18	c6	7	VAL
18	c6	17	THR
18	c6	23	LYS
18	c6	26	LYS
18	c6	28	LEU
18	c6	37	THR
18	c6	43	ILE
18	c6	53	LEU
18	c6	55	VAL
18	c6	57	LEU
18	c6	58	ASP
18	c6	63	ILE
18	c6	64	ASP
18	c6	68	ARG
18	c6	70	THR
18	c6	76	SER
18	c6	81	ILE
18	c6	94	GLN
18	c6	114	ARG
18	c6	115	THR
18	c6	137	ARG
19	c7	3	ARG
19	c7	5	ARG
19	c7	6	THR
19	c7	27	ASP
19	c7	29	GLN
19	c7	34	LEU
19	c7	46	LEU
19	c7	72	LYS
19	c7	85	VAL
19	c7	88	VAL
19	c7	108	ASP

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Mol	Chain	Res	Type
19	c7	113	LEU
20	c8	2	SER
20	c8	3	LEU
20	c8	4	VAL
20	c8	5	VAL
20	c8	6	GLN
20	c8	20	THR
20	c8	21	ASN
20	c8	25	ASN
20	c8	27	LYS
20	c8	28	ILE
20	c8	33	THR
20	c8	36	LYS
20	c8	40	ARG
20	c8	68	ARG
20	c8	85	PHE
20	c8	87	ASN
20	c8	94	ASP
20	c8	100	THR
20	c8	101	LEU
20	c8	116	LEU
20	c8	133	VAL
20	c8	134	ARG
20	c8	136	GLN
20	c8	141	THR
21	c9	6	VAL
21	c9	7	ARG
21	c9	28	LEU
21	c9	29	GLU
21	c9	33	TYR
21	c9	57	ARG
21	c9	68	ARG
21	c9	71	VAL
21	c9	123	ARG
21	c9	140	LEU
22	d0	13	GLU
22	d0	27	THR
22	d0	44	ASN
22	d0	57	ARG
22	d0	60	THR
22	d0	63	LEU
22	d0	70	THR

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Mol	Chain	Res	Type
22	d0	74	GLU
22	d0	77	LYS
22	d0	88	LYS
22	d0	98	GLN
22	d0	99	ILE
22	d0	103	ILE
22	d0	105	GLN
22	d0	107	THR
22	d0	115	GLU
23	d1	2	GLU
23	d1	5	LYS
23	d1	12	TYR
23	d1	17	CYS
23	d1	27	ASP
23	d1	32	VAL
23	d1	50	TYR
23	d1	52	THR
23	d1	62	ARG
23	d1	68	SER
23	d1	81	ASN
24	d2	4	SER
24	d2	22	LYS
24	d2	23	ARG
24	d2	24	GLN
24	d2	25	VAL
24	d2	26	LEU
24	d2	35	ILE
24	d2	36	LYS
24	d2	37	PHE
24	d2	42	GLN
24	d2	55	ASP
24	d2	65	LEU
24	d2	68	ARG
24	d2	88	LYS
24	d2	98	GLN
24	d2	103	ILE
24	d2	105	THR
24	d2	126	LEU
25	d3	14	LYS
25	d3	16	ARG
25	d3	19	ARG
25	d3	40	SER

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Mol	Chain	Res	Type
25	d3	72	VAL
25	d3	73	ARG
25	d3	84	THR
25	d3	100	ASP
25	d3	103	LEU
25	d3	107	PHE
25	d3	117	ILE
26	d4	5	VAL
26	d4	10	ARG
26	d4	21	LYS
26	d4	26	ASP
26	d4	34	ASN
26	d4	43	LYS
26	d4	44	LEU
26	d4	49	LYS
26	d4	58	PHE
26	d4	62	THR
26	d4	74	LEU
26	d4	88	THR
26	d4	98	GLU
26	d4	104	SER
26	d4	116	LYS
26	d4	133	ASN
27	d5	41	ILE
27	d5	51	LEU
27	d5	54	VAL
27	d5	57	TYR
27	d5	60	VAL
27	d5	77	ARG
27	d5	81	ARG
27	d5	88	ILE
27	d5	92	ILE
28	d6	10	ARG
28	d6	24	VAL
28	d6	25	ASN
28	d6	33	ASP
28	d6	74	CYS
28	d6	82	ARG
28	d6	88	SER
28	d6	89	ARG
28	d6	91	ASP
29	d7	3	LEU

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Mol	Chain	Res	Type
29	d7	11	THR
29	d7	34	ASP
29	d7	41	LEU
29	d7	43	ILE
29	d7	46	VAL
29	d7	67	THR
29	d7	77	THR
29	d7	80	ARG
29	d7	81	ARG
29	d7	82	LYS
30	d8	5	THR
30	d8	7	VAL
30	d8	8	THR
30	d8	22	ARG
30	d8	25	VAL
30	d8	33	LEU
30	d8	37	SER
30	d8	39	THR
30	d8	41	VAL
30	d8	54	LEU
30	d8	58	GLU
31	d9	10	HIS
31	d9	12	ARG
31	d9	21	CYS
31	d9	28	THR
31	d9	30	LEU
31	d9	32	ARG
31	d9	36	LEU
31	d9	42	CYS
31	d9	54	LYS
31	d9	56	ARG
32	e0	13	LYS
32	e0	21	VAL
32	e0	22	GLU
32	e0	24	THR
32	e0	25	GLU
32	e0	29	LYS
32	e0	41	THR
32	e0	44	PHE
32	e0	46	ASN
32	e0	54	ARG
32	e0	55	ARG

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Mol	Chain	Res	Type
32	e0	56	MET
33	e1	78	LYS
33	e1	80	ARG
33	e1	86	THR
33	e1	93	HIS
33	e1	98	VAL
33	e1	100	LEU
33	e1	102	VAL
33	e1	106	TYR
33	e1	113	LYS
33	e1	135	HIS
33	e1	147	VAL
33	e1	148	TYR
34	sR	29	GLN
34	sR	35	SER
34	sR	51	ASP
34	sR	52	GLN
34	sR	58	VAL
34	sR	59	ARG
34	sR	76	ASP
34	sR	96	THR
34	sR	106	HIS
34	sR	131	ILE
34	sR	145	LEU
34	sR	153	GLN
34	sR	160	GLU
34	sR	167	VAL
34	sR	183	LEU
34	sR	184	ASN
34	sR	202	LEU
34	sR	207	ASP
34	sR	245	PHE
34	sR	272	ASP
34	sR	278	PHE
34	sR	291	SER
34	sR	297	ASP
34	sR	317	THR
35	sM	23	LYS
35	sM	43	ASP
35	sM	49	LYS
35	sM	50	ASN
35	sM	61	ILE

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Mol	Chain	Res	Type
35	sM	68	ARG
35	sM	74	LYS
35	sM	77	THR
39	l2	10	LYS
39	l2	23	ARG
39	l2	32	LEU
39	l2	42	ARG
39	l2	44	ILE
39	l2	46	LYS
39	l2	48	ILE
39	l2	49	VAL
39	l2	62	VAL
39	l2	72	ARG
39	l2	74	GLU
39	l2	79	ASN
39	l2	82	VAL
39	l2	84	THR
39	l2	96	LEU
39	l2	101	VAL
39	l2	104	LEU
39	l2	107	VAL
39	l2	109	GLU
39	l2	112	ILE
39	l2	116	VAL
39	l2	128	ARG
39	l2	137	ILE
39	l2	147	ARG
39	l2	159	SER
39	l2	168	VAL
39	l2	179	LEU
39	l2	180	LEU
39	l2	207	VAL
39	l2	225	ILE
39	l2	227	ARG
39	l2	230	VAL
39	l2	238	ILE
39	l2	242	ARG
39	l2	246	LEU
39	l2	247	ARG
40	l3	2	SER
40	l3	3	HIS
40	l3	4	ARG

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Mol	Chain	Res	Type
40	l3	7	GLU
40	l3	10	ARG
40	l3	17	LEU
40	l3	19	ARG
40	l3	20	LYS
40	l3	37	ARG
40	l3	43	LEU
40	l3	44	THR
40	l3	46	PHE
40	l3	47	LEU
40	l3	56	ILE
40	l3	58	ARG
40	l3	59	ASP
40	l3	69	LYS
40	l3	77	THR
40	l3	85	VAL
40	l3	103	THR
40	l3	110	LEU
40	l3	112	ASP
40	l3	114	VAL
40	l3	127	LYS
40	l3	139	GLN
40	l3	140	ASP
40	l3	145	GLU
40	l3	148	LEU
40	l3	157	VAL
40	l3	167	ARG
40	l3	168	LYS
40	l3	169	THR
40	l3	183	LEU
40	l3	188	ILE
40	l3	192	VAL
40	l3	196	ARG
40	l3	205	VAL
40	l3	208	VAL
40	l3	211	GLN
40	l3	231	HIS
40	l3	232	ARG
40	l3	238	LEU
40	l3	264	VAL
40	l3	274	SER
40	l3	282	ILE

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Mol	Chain	Res	Type
40	l3	284	ARG
40	l3	297	SER
40	l3	304	THR
40	l3	308	MET
40	l3	324	VAL
40	l3	328	ILE
40	l3	332	ARG
40	l3	340	LYS
40	l3	341	SER
40	l3	347	SER
41	l4	2	SER
41	l4	14	GLU
41	l4	69	ARG
41	l4	73	ARG
41	l4	90	PHE
41	l4	92	ASN
41	l4	93	MET
41	l4	105	THR
41	l4	120	TYR
41	l4	136	LEU
41	l4	138	ARG
41	l4	144	LYS
41	l4	150	LEU
41	l4	153	SER
41	l4	156	LEU
41	l4	177	ASP
41	l4	179	LEU
41	l4	186	LYS
41	l4	187	LEU
41	l4	193	LYS
41	l4	201	GLN
41	l4	203	ARG
41	l4	206	LEU
41	l4	220	ARG
41	l4	222	VAL
41	l4	230	VAL
41	l4	246	ARG
41	l4	258	LEU
41	l4	259	ASP
41	l4	265	GLU
41	l4	286	VAL
41	l4	289	ILE

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Mol	Chain	Res	Type
41	14	313	LEU
41	14	316	ASN
41	14	319	LYS
41	14	327	LEU
41	14	333	VAL
41	14	338	LYS
41	14	345	GLU
41	14	347	THR
41	14	349	THR
42	15	4	GLN
42	15	14	SER
42	15	15	ARG
42	15	34	LYS
42	15	35	ARG
42	15	51	LEU
42	15	65	ILE
42	15	74	VAL
42	15	75	LEU
42	15	89	THR
42	15	110	LEU
42	15	112	LYS
42	15	113	LEU
42	15	118	THR
42	15	122	VAL
42	15	132	THR
42	15	133	GLU
42	15	136	GLU
42	15	140	ARG
42	15	144	VAL
42	15	146	LEU
42	15	148	ILE
42	15	152	ARG
42	15	155	THR
42	15	185	PHE
42	15	194	LEU
42	15	210	GLU
42	15	217	GLU
42	15	218	ARG
42	15	227	LEU
42	15	254	LYS
42	15	258	LYS
42	15	259	LYS

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Mol	Chain	Res	Type
42	15	263	GLU
42	15	268	GLU
42	15	271	LYS
42	15	273	ARG
42	15	275	THR
42	15	279	LYS
42	15	281	GLU
42	15	293	LEU
42	15	296	GLN
43	16	13	GLU
43	16	20	LYS
43	16	21	THR
43	16	26	ARG
43	16	29	LYS
43	16	48	ARG
43	16	52	VAL
43	16	64	LEU
43	16	78	ARG
43	16	79	VAL
43	16	89	THR
43	16	91	VAL
43	16	104	GLU
43	16	131	LYS
43	16	152	THR
43	16	155	LEU
43	16	162	SER
43	16	166	LYS
43	16	173	MET
43	16	175	LYS
44	17	26	VAL
44	17	41	ARG
44	17	53	LYS
44	17	60	ARG
44	17	83	LEU
44	17	88	ARG
44	17	93	ASN
44	17	98	LYS
44	17	107	ARG
44	17	124	LEU
44	17	156	ILE
44	17	158	LYS
44	17	164	SER

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Mol	Chain	Res	Type
44	17	173	LEU
44	17	175	LYS
44	17	179	LEU
44	17	183	ASP
44	17	184	LEU
44	17	194	HIS
44	17	196	LYS
44	17	229	PHE
44	17	234	GLU
44	17	239	LEU
45	18	41	GLN
45	18	50	VAL
45	18	54	GLU
45	18	57	ARG
45	18	68	ARG
45	18	71	VAL
45	18	74	THR
45	18	79	GLN
45	18	81	THR
45	18	89	GLU
45	18	98	ARG
45	18	133	LYS
45	18	136	LEU
45	18	157	VAL
45	18	160	ILE
45	18	163	VAL
45	18	169	LEU
45	18	172	LYS
45	18	211	LEU
45	18	213	LYS
45	18	240	ASN
45	18	245	LYS
45	18	248	LYS
46	19	1	MET
46	19	6	THR
46	19	17	THR
46	19	18	VAL
46	19	22	SER
46	19	33	THR
46	19	46	THR
46	19	55	VAL
46	19	62	ARG

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Mol	Chain	Res	Type
46	l9	68	LEU
46	l9	70	THR
46	l9	80	THR
46	l9	102	ASN
46	l9	105	GLU
46	l9	118	LEU
46	l9	122	LYS
46	l9	129	ARG
46	l9	133	THR
46	l9	138	THR
46	l9	144	ILE
46	l9	151	VAL
46	l9	157	ASN
46	l9	162	GLN
46	l9	166	ARG
46	l9	173	ARG
46	l9	177	ASP
46	l9	179	ILE
46	l9	187	ILE
46	l9	191	LEU
47	m0	3	ARG
47	m0	21	ARG
47	m0	28	ASP
47	m0	32	ARG
47	m0	34	TYR
47	m0	36	LEU
47	m0	42	THR
47	m0	48	LEU
47	m0	52	LEU
47	m0	58	GLU
47	m0	61	SER
47	m0	62	SER
47	m0	71	CYS
47	m0	78	THR
47	m0	80	SER
47	m0	87	LEU
47	m0	88	ARG
47	m0	91	VAL
47	m0	99	ILE
47	m0	103	LEU
47	m0	125	LEU
47	m0	137	SER

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Mol	Chain	Res	Type
47	m0	141	LYS
47	m0	153	ARG
47	m0	156	ARG
47	m0	167	LEU
47	m0	169	LYS
47	m0	174	THR
47	m0	176	LEU
47	m0	177	ASP
47	m0	182	LEU
47	m0	193	ASP
47	m0	197	VAL
47	m0	206	LEU
47	m0	212	GLU
47	m0	217	PHE
48	m1	10	ARG
48	m1	13	LYS
48	m1	16	LYS
48	m1	29	ARG
48	m1	30	LEU
48	m1	46	VAL
48	m1	48	SER
48	m1	51	ARG
48	m1	55	ARG
48	m1	56	THR
48	m1	61	ARG
48	m1	80	LEU
48	m1	92	ARG
48	m1	99	THR
48	m1	107	ASP
48	m1	112	LEU
48	m1	129	VAL
48	m1	130	VAL
48	m1	137	ARG
48	m1	140	ARG
48	m1	147	THR
48	m1	153	LYS
48	m1	155	THR
48	m1	158	ASP
48	m1	161	SER
48	m1	171	VAL
48	m1	172	LEU
49	m3	13	HIS

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Mol	Chain	Res	Type
49	m3	17	HIS
49	m3	45	LYS
49	m3	54	LEU
49	m3	58	VAL
49	m3	59	ARG
49	m3	67	ARG
49	m3	69	VAL
49	m3	73	ARG
49	m3	76	THR
49	m3	85	LEU
49	m3	86	THR
49	m3	100	ARG
49	m3	107	GLU
49	m3	128	ARG
49	m3	131	LYS
49	m3	149	GLN
49	m3	164	GLU
49	m3	168	ARG
49	m3	176	GLU
49	m3	184	GLU
49	m3	189	GLU
50	m4	3	THR
50	m4	4	ASP
50	m4	15	VAL
50	m4	39	ILE
50	m4	43	LYS
50	m4	53	VAL
50	m4	62	GLN
50	m4	66	THR
50	m4	69	THR
50	m4	72	LEU
50	m4	91	CYS
50	m4	107	GLU
50	m4	108	ARG
50	m4	123	LEU
51	m5	5	LYS
51	m5	10	LEU
51	m5	12	ARG
51	m5	22	LEU
51	m5	31	ARG
51	m5	49	ARG
51	m5	54	LYS

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Mol	Chain	Res	Type
51	m5	66	VAL
51	m5	67	ARG
51	m5	68	ARG
51	m5	73	ARG
51	m5	80	THR
51	m5	83	LYS
51	m5	92	LEU
51	m5	105	ARG
51	m5	106	VAL
51	m5	117	ASN
51	m5	138	GLN
51	m5	142	ILE
51	m5	153	ASP
51	m5	176	LYS
51	m5	178	HIS
51	m5	182	ASN
52	m6	3	VAL
52	m6	22	VAL
52	m6	34	VAL
52	m6	46	GLU
52	m6	66	LYS
52	m6	67	THR
52	m6	68	ARG
52	m6	74	ARG
52	m6	84	LEU
52	m6	85	ARG
52	m6	100	GLU
52	m6	106	GLU
52	m6	110	PRO
52	m6	113	ASP
52	m6	116	LYS
52	m6	117	ARG
52	m6	124	LEU
52	m6	126	VAL
52	m6	134	LYS
52	m6	143	THR
52	m6	160	ARG
52	m6	175	THR
52	m6	180	SER
52	m6	182	ASN
52	m6	190	VAL
52	m6	197	LEU

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Mol	Chain	Res	Type
53	m7	7	THR
53	m7	9	THR
53	m7	23	ARG
53	m7	32	THR
53	m7	42	THR
53	m7	52	LEU
53	m7	78	VAL
53	m7	79	THR
53	m7	97	ASN
53	m7	112	LEU
53	m7	114	VAL
53	m7	119	VAL
53	m7	121	GLN
53	m7	126	ARG
53	m7	136	ILE
53	m7	144	SER
53	m7	150	VAL
53	m7	153	LYS
54	m8	3	ILE
54	m8	7	SER
54	m8	12	ARG
54	m8	17	THR
54	m8	22	ASP
54	m8	31	LYS
54	m8	32	LEU
54	m8	34	THR
54	m8	38	ARG
54	m8	41	ASP
54	m8	64	VAL
54	m8	66	ARG
54	m8	78	ASN
54	m8	80	THR
54	m8	81	VAL
54	m8	86	THR
54	m8	93	ILE
54	m8	98	LYS
54	m8	113	LYS
54	m8	122	ILE
54	m8	127	LEU
54	m8	135	GLN
54	m8	138	LEU
54	m8	140	LEU

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Mol	Chain	Res	Type
54	m8	161	LYS
54	m8	165	ILE
54	m8	166	LEU
54	m8	170	ARG
54	m8	176	ARG
54	m8	185	LYS
55	m9	7	GLN
55	m9	10	LEU
55	m9	20	ARG
55	m9	21	LYS
55	m9	29	THR
55	m9	43	LYS
55	m9	56	THR
55	m9	63	THR
55	m9	74	ARG
55	m9	106	LEU
55	m9	116	ASP
55	m9	117	LYS
55	m9	126	GLU
55	m9	127	SER
55	m9	134	HIS
55	m9	146	LYS
55	m9	148	ASP
55	m9	152	GLU
55	m9	153	LYS
55	m9	158	GLU
55	m9	167	ARG
55	m9	173	ARG
55	m9	180	LYS
55	m9	186	LYS
56	n0	1	MET
56	n0	13	ARG
56	n0	17	GLU
56	n0	35	VAL
56	n0	50	LYS
56	n0	80	ARG
56	n0	87	THR
56	n0	88	HIS
56	n0	96	ASP
56	n0	97	VAL
56	n0	100	VAL
56	n0	107	TYR

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Mol	Chain	Res	Type
56	n0	130	GLU
56	n0	132	THR
56	n0	136	LYS
56	n0	137	ARG
56	n0	145	THR
56	n0	148	LEU
56	n0	162	THR
56	n0	164	SER
56	n0	172	TYR
57	n1	9	SER
57	n1	12	ARG
57	n1	18	ASP
57	n1	25	VAL
57	n1	35	LYS
57	n1	47	SER
57	n1	71	SER
57	n1	78	LYS
57	n1	80	VAL
57	n1	83	ARG
57	n1	88	ARG
57	n1	89	LEU
57	n1	96	ILE
57	n1	102	ARG
57	n1	104	GLU
57	n1	118	GLU
57	n1	124	VAL
57	n1	126	VAL
57	n1	130	ARG
57	n1	139	ARG
57	n1	141	VAL
57	n1	150	THR
57	n1	159	PHE
58	n2	27	VAL
58	n2	37	LEU
58	n2	38	ILE
58	n2	43	VAL
58	n2	49	ASN
58	n2	57	THR
58	n2	58	GLU
58	n2	61	THR
58	n2	66	VAL
58	n2	75	TYR

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Mol	Chain	Res	Type
58	n2	96	VAL
58	n2	98	THR
58	n2	100	THR
59	n3	4	ASN
59	n3	7	GLN
59	n3	9	THR
59	n3	13	ILE
59	n3	32	ARG
59	n3	48	ARG
59	n3	74	MET
59	n3	83	LYS
59	n3	88	ARG
59	n3	93	LEU
59	n3	98	ASN
59	n3	108	GLU
59	n3	124	ASP
59	n3	125	LEU
59	n3	136	VAL
60	n4	1	MET
60	n4	5	ILE
60	n4	12	LYS
60	n4	19	THR
60	n4	39	LEU
60	n4	59	HIS
60	n4	63	ILE
60	n4	96	LEU
60	n4	99	GLU
60	n4	107	GLU
60	n4	127	LYS
60	n4	134	GLN
61	n5	27	ARG
61	n5	56	ARG
61	n5	57	LEU
61	n5	63	ILE
61	n5	65	GLN
61	n5	69	SER
61	n5	108	LEU
61	n5	115	ARG
61	n5	125	ARG
61	n5	135	ILE
61	n5	137	ASN
61	n5	142	ILE

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Mol	Chain	Res	Type
62	n6	4	GLN
62	n6	5	SER
62	n6	10	SER
62	n6	12	ARG
62	n6	13	ARG
62	n6	17	LYS
62	n6	37	LYS
62	n6	40	ARG
62	n6	45	ILE
62	n6	50	ILE
62	n6	51	ARG
62	n6	56	VAL
62	n6	57	LEU
62	n6	66	GLN
62	n6	69	LYS
62	n6	74	TYR
62	n6	76	LEU
62	n6	83	ASP
62	n6	115	ARG
62	n6	127	GLU
63	n7	14	VAL
63	n7	17	ARG
63	n7	24	VAL
63	n7	27	LYS
63	n7	46	ILE
63	n7	47	GLU
63	n7	52	LYS
63	n7	57	HIS
63	n7	72	ILE
63	n7	74	VAL
63	n7	81	LEU
63	n7	83	THR
63	n7	86	THR
63	n7	90	GLU
63	n7	95	VAL
63	n7	100	THR
63	n7	102	GLU
63	n7	111	LYS
63	n7	126	LYS
63	n7	134	LEU
64	n8	4	ARG
64	n8	8	THR

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Mol	Chain	Res	Type
64	n8	10	LYS
64	n8	15	VAL
64	n8	19	LYS
64	n8	27	LYS
64	n8	42	ARG
64	n8	46	ASP
64	n8	56	VAL
64	n8	60	TYR
64	n8	65	GLN
64	n8	80	THR
64	n8	85	ASP
64	n8	91	LEU
64	n8	95	SER
64	n8	98	THR
64	n8	123	VAL
64	n8	133	LEU
65	n9	13	THR
65	n9	19	ASN
65	n9	38	LYS
65	n9	58	LYS
65	n9	59	LYS
66	o0	18	ILE
66	o0	19	LYS
66	o0	40	LYS
66	o0	41	LEU
66	o0	61	MET
66	o0	63	SER
66	o0	74	ASN
66	o0	76	GLU
66	o0	86	ARG
66	o0	87	VAL
66	o0	94	GLU
66	o0	97	ASP
66	o0	103	THR
67	o1	6	ASP
67	o1	8	VAL
67	o1	13	THR
67	o1	16	LEU
67	o1	24	SER
67	o1	26	LYS
67	o1	31	ARG
67	o1	34	LYS

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Mol	Chain	Res	Type
67	o1	44	MET
67	o1	62	ARG
67	o1	76	SER
67	o1	81	GLU
67	o1	90	PHE
67	o1	91	SER
67	o1	96	VAL
67	o1	102	LYS
67	o1	106	THR
67	o1	110	GLU
68	o2	3	SER
68	o2	4	LEU
68	o2	6	HIS
68	o2	14	THR
68	o2	16	LYS
68	o2	24	ARG
68	o2	27	ARG
68	o2	31	ASN
68	o2	33	ARG
68	o2	34	LYS
68	o2	41	VAL
68	o2	50	ILE
68	o2	61	LYS
68	o2	63	THR
68	o2	73	THR
68	o2	75	LEU
68	o2	82	LEU
68	o2	84	THR
68	o2	86	THR
68	o2	88	HIS
68	o2	95	GLU
68	o2	103	LYS
68	o2	106	VAL
68	o2	109	LEU
69	o3	4	SER
69	o3	15	SER
69	o3	31	LYS
69	o3	37	THR
69	o3	45	LEU
69	o3	48	ARG
69	o3	49	ILE
69	o3	58	GLU

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Mol	Chain	Res	Type
69	o3	59	VAL
69	o3	73	ARG
69	o3	81	VAL
69	o3	84	THR
69	o3	98	VAL
70	o4	5	VAL
70	o4	6	THR
70	o4	20	ILE
70	o4	29	ILE
70	o4	31	ARG
70	o4	35	VAL
70	o4	44	CYS
70	o4	54	ILE
70	o4	58	ARG
70	o4	65	VAL
70	o4	68	THR
70	o4	71	THR
70	o4	83	ASN
70	o4	85	VAL
70	o4	88	ARG
71	o5	20	GLN
71	o5	21	LEU
71	o5	37	SER
71	o5	38	ARG
71	o5	47	VAL
71	o5	59	ASN
71	o5	62	GLN
71	o5	69	LEU
71	o5	79	ASP
71	o5	84	LYS
71	o5	85	THR
71	o5	89	ARG
71	o5	100	VAL
72	o6	2	THR
72	o6	3	VAL
72	o6	9	ILE
72	o6	11	LEU
72	o6	15	LYS
72	o6	17	VAL
72	o6	20	MET
72	o6	21	THR
72	o6	26	ILE

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Mol	Chain	Res	Type
72	o6	35	ASN
72	o6	36	ARG
72	o6	43	LEU
72	o6	45	ARG
72	o6	57	LEU
72	o6	58	ILE
72	o6	60	LEU
72	o6	62	ARG
72	o6	68	ARG
72	o6	76	ARG
72	o6	79	SER
72	o6	81	THR
72	o6	88	GLU
72	o6	94	ILE
72	o6	98	ARG
73	o7	15	SER
73	o7	17	THR
73	o7	25	ARG
73	o7	36	SER
73	o7	44	THR
73	o7	46	SER
73	o7	59	THR
73	o7	65	ARG
73	o7	67	LEU
73	o7	75	LYS
73	o7	80	THR
73	o7	84	SER
74	o8	5	ILE
74	o8	8	ILE
74	o8	13	GLU
74	o8	14	LEU
74	o8	19	ASP
74	o8	24	THR
74	o8	41	THR
74	o8	49	SER
74	o8	53	THR
74	o8	61	LYS
74	o8	64	LYS
74	o8	65	LEU
75	o9	4	GLN
75	o9	5	LYS
75	o9	17	LYS

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Mol	Chain	Res	Type
75	o9	19	GLN
75	o9	21	ARG
75	o9	23	LEU
75	o9	28	ARG
75	o9	29	LEU
75	o9	45	ARG
76	q0	85	LEU
76	q0	106	ARG
76	q0	112	LYS
76	q0	113	ARG
76	q0	114	LYS
77	q1	2	ARG
77	q1	9	ARG
77	q1	13	LEU
77	q1	15	ARG
77	q1	21	ARG
77	q1	23	ARG
77	q1	24	SER
77	q1	25	LYS
78	q2	7	THR
78	q2	8	ARG
78	q2	26	THR
78	q2	35	LEU
78	q2	61	LYS
78	q2	71	ARG
78	q2	78	LYS
78	q2	80	ARG
78	q2	84	THR
78	q2	85	LEU
78	q2	93	LEU
78	q2	105	GLN
78	q2	106	PHE
79	q3	3	LYS
79	q3	22	LEU
79	q3	33	GLN
79	q3	42	CYS
79	q3	49	ARG
79	q3	54	ILE
79	q3	56	THR
79	q3	58	SER
79	q3	59	CYS
79	q3	73	THR

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Mol	Chain	Res	Type
79	q3	78	THR
82	p0	4	ILE
82	p0	5	ARG
82	p0	30	VAL
82	p0	48	ARG
82	p0	52	LEU
82	p0	57	THR
82	p0	67	LEU
82	p0	70	LEU
82	p0	91	GLU
82	p0	93	LEU
82	p0	97	LYS
85	f	12	ASP
85	f	37	ARG
85	f	52	HIS
85	f	78	HIS
85	f	80	MET
85	f	87	ARG
85	f	94	ASP
85	f	102	LEU
85	f	105	MET
85	f	109	THR
85	f	112	ASP
85	f	120	LEU
85	f	123	SER
85	f	124	LEU
85	f	137	THR
85	f	148	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
3	S1	95	ASN
5	S3	159	HIS
6	S4	142	HIS
7	S5	116	HIS
10	S8	32	GLN
10	S8	52	ASN
11	S9	110	GLN
12	C0	81	ASN
20	C8	127	HIS
22	D0	44	ASN

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Mol	Chain	Res	Type
25	D3	79	ASN
27	D5	95	HIS
30	D8	27	GLN
33	E1	134	ASN
35	SM	94	HIS
40	L3	211	GLN
42	L5	40	HIS
46	L9	139	ASN
47	M0	14	ASN
47	M0	144	ASN
51	M5	15	GLN
52	M6	193	GLN
54	M8	135	GLN
63	N7	57	HIS
3	s1	149	GLN
3	s1	209	ASN
6	s4	142	HIS
10	s8	32	GLN
11	s9	133	HIS
80	c0	62	GLN
24	d2	56	HIS
27	d5	38	HIS
34	sR	106	HIS
34	sR	182	ASN
41	l4	296	GLN
41	l4	328	ASN
44	l7	48	ASN
49	m3	99	HIS
52	m6	29	ASN
55	m9	7	GLN
56	n0	8	GLN
60	n4	58	HIS
61	n5	137	ASN
64	n8	44	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1776/1800 (98%)	454 (25%)	49 (2%)
1	6	1791/1800 (99%)	436 (24%)	35 (1%)
36	1	3145/3396 (92%)	652 (20%)	49 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
36	5	3163/3396 (93%)	650 (20%)	49 (1%)
37	3	120/121 (99%)	11 (9%)	0
37	7	120/121 (99%)	16 (13%)	1 (0%)
38	4	157/158 (99%)	36 (22%)	1 (0%)
38	8	157/158 (99%)	33 (21%)	1 (0%)
All	All	10429/10950 (95%)	2288 (21%)	185 (1%)

All (2288) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	8	U
1	2	17	C
1	2	25	C
1	2	26	A
1	2	27	U
1	2	34	G
1	2	42	G
1	2	44	U
1	2	45	U
1	2	47	A
1	2	57	G
1	2	60	U
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	95	G
1	2	101	U
1	2	104	A
1	2	111	U
1	2	114	C
1	2	115	G
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A

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Mol	Chain	Res	Type
1	2	136	C
1	2	137	U
1	2	140	A
1	2	141	U
1	2	145	A
1	2	146	U
1	2	153	G
1	2	158	U
1	2	159	U
1	2	169	A
1	2	178	U
1	2	179	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	189	C
1	2	190	C
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	196	G
1	2	197	A
1	2	198	A
1	2	200	A
1	2	215	A
1	2	217	A
1	2	218	A
1	2	219	A
1	2	226	A
1	2	227	U
1	2	228	G
1	2	233	C
1	2	234	G
1	2	235	G
1	2	238	U
1	2	239	C
1	2	240	U
1	2	241	U
1	2	242	U
1	2	249	U

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Mol	Chain	Res	Type
1	2	250	C
1	2	257	A
1	2	259	U
1	2	261	U
1	2	262	U
1	2	265	A
1	2	271	A
1	2	272	U
1	2	274	G
1	2	275	C
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	288	A
1	2	299	A
1	2	302	U
1	2	309	C
1	2	314	C
1	2	316	A
1	2	319	U
1	2	321	C
1	2	322	G
1	2	323	A
1	2	333	A
1	2	337	G
1	2	338	C
1	2	352	A
1	2	359	A
1	2	360	A
1	2	361	C
1	2	400	A
1	2	402	C
1	2	403	G
1	2	404	G
1	2	416	A
1	2	418	G
1	2	419	G
1	2	421	A
1	2	424	C

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Mol	Chain	Res	Type
1	2	425	A
1	2	426	G
1	2	428	A
1	2	434	G
1	2	437	A
1	2	439	U
1	2	440	U
1	2	444	C
1	2	446	A
1	2	448	C
1	2	455	C
1	2	456	A
1	2	468	A
1	2	477	A
1	2	484	C
1	2	485	A
1	2	488	G
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	497	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	503	G
1	2	504	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	508	U
1	2	510	G
1	2	511	A
1	2	513	U
1	2	515	A
1	2	516	G
1	2	527	A
1	2	532	U
1	2	538	A
1	2	539	G
1	2	540	G

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Mol	Chain	Res	Type
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	566	C
1	2	571	G
1	2	578	U
1	2	579	A
1	2	580	A
1	2	585	A
1	2	594	A
1	2	595	G
1	2	606	A
1	2	609	U
1	2	619	A
1	2	620	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	639	U
1	2	640	U
1	2	650	U
1	2	653	C
1	2	655	G
1	2	656	G
1	2	657	U
1	2	658	C
1	2	679	U
1	2	684	A
1	2	686	C
1	2	694	U
1	2	696	C
1	2	697	C
1	2	700	C
1	2	701	U
1	2	702	G
1	2	703	G
1	2	704	C

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Mol	Chain	Res	Type
1	2	705	U
1	2	707	A
1	2	709	C
1	2	710	U
1	2	712	G
1	2	714	G
1	2	717	C
1	2	718	U
1	2	719	U
1	2	720	G
1	2	721	U
1	2	722	G
1	2	723	G
1	2	725	U
1	2	727	U
1	2	728	U
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	735	C
1	2	736	C
1	2	737	A
1	2	738	G
1	2	742	U
1	2	745	U
1	2	754	A
1	2	755	A
1	2	756	A
1	2	765	G
1	2	766	U
1	2	774	A
1	2	775	G
1	2	778	G
1	2	781	U
1	2	783	G
1	2	784	C
1	2	789	A
1	2	794	U
1	2	795	U
1	2	803	A

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Mol	Chain	Res	Type
1	2	812	A
1	2	814	A
1	2	815	G
1	2	816	G
1	2	818	C
1	2	820	U
1	2	821	U
1	2	822	U
1	2	823	G
1	2	824	G
1	2	829	A
1	2	830	U
1	2	831	U
1	2	833	U
1	2	839	U
1	2	846	G
1	2	848	C
1	2	856	A
1	2	860	U
1	2	863	A
1	2	873	U
1	2	876	G
1	2	886	U
1	2	896	U
1	2	898	A
1	2	912	U
1	2	914	G
1	2	915	A
1	2	926	A
1	2	933	A
1	2	935	U
1	2	942	G
1	2	944	A
1	2	951	A
1	2	960	U
1	2	966	A
1	2	979	A
1	2	992	A
1	2	993	A
1	2	997	G
1	2	1003	A
1	2	1004	U

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Mol	Chain	Res	Type
1	2	1005	A
1	2	1020	A
1	2	1021	C
1	2	1022	C
1	2	1026	A
1	2	1028	C
1	2	1039	A
1	2	1040	G
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1073	G
1	2	1074	G
1	2	1082	C
1	2	1083	G
1	2	1086	A
1	2	1091	A
1	2	1092	A
1	2	1096	C
1	2	1097	U
1	2	1100	G
1	2	1138	A
1	2	1146	G
1	2	1151	A
1	2	1155	G
1	2	1158	C
1	2	1160	A
1	2	1163	A
1	2	1167	G
1	2	1185	U
1	2	1194	A
1	2	1196	A
1	2	1197	C
1	2	1198	G
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1208	A
1	2	1217	A

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Mol	Chain	Res	Type
1	2	1218	G
1	2	1227	A
1	2	1229	G
1	2	1244	A
1	2	1245	G
1	2	1250	U
1	2	1251	U
1	2	1254	U
1	2	1256	A
1	2	1258	U
1	2	1276	U
1	2	1284	C
1	2	1286	U
1	2	1301	U
1	2	1307	U
1	2	1311	U
1	2	1312	A
1	2	1314	U
1	2	1315	U
1	2	1321	A
1	2	1337	A
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1344	A
1	2	1345	A
1	2	1346	A
1	2	1348	A
1	2	1355	C
1	2	1361	U
1	2	1363	U
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1412	G
1	2	1413	U
1	2	1414	U
1	2	1415	U
1	2	1420	C

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Mol	Chain	Res	Type
1	2	1427	A
1	2	1428	G
1	2	1432	U
1	2	1446	A
1	2	1456	C
1	2	1458	G
1	2	1459	C
1	2	1461	C
1	2	1471	A
1	2	1473	U
1	2	1474	G
1	2	1477	G
1	2	1482	C
1	2	1486	G
1	2	1489	U
1	2	1490	C
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1496	U
1	2	1499	G
1	2	1506	G
1	2	1514	U
1	2	1515	A
1	2	1516	A
1	2	1517	U
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1526	A
1	2	1530	C
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1542	G
1	2	1557	U
1	2	1559	A
1	2	1560	U
1	2	1569	A
1	2	1574	G
1	2	1584	G

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Mol	Chain	Res	Type
1	2	1596	C
1	2	1601	G
1	2	1616	G
1	2	1619	C
1	2	1624	C
1	2	1625	C
1	2	1626	U
1	2	1631	A
1	2	1634	C
1	2	1636	C
1	2	1657	U
1	2	1658	G
1	2	1680	G
1	2	1681	A
1	2	1683	C
1	2	1684	U
1	2	1685	G
1	2	1697	G
1	2	1698	G
1	2	1699	G
1	2	1700	C
1	2	1701	A
1	2	1702	A
1	2	1703	C
1	2	1704	U
1	2	1712	A
1	2	1713	G
1	2	1731	A
1	2	1732	A
1	2	1752	U
1	2	1760	G
1	2	1762	A
1	2	1766	A
1	2	1769	U
1	2	1770	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U

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Mol	Chain	Res	Type
1	2	1796	C
1	2	1798	U
36	1	15	C
36	1	16	A
36	1	18	G
36	1	24	G
36	1	26	A
36	1	40	A
36	1	43	A
36	1	49	A
36	1	59	G
36	1	60	A
36	1	65	A
36	1	66	A
36	1	68	C
36	1	76	G
36	1	88	A
36	1	92	G
36	1	93	C
36	1	99	A
36	1	109	A
36	1	110	G
36	1	111	C
36	1	113	C
36	1	116	A
36	1	117	U
36	1	121	A
36	1	122	A
36	1	133	U
36	1	135	C
36	1	136	G
36	1	148	G
36	1	156	G
36	1	157	A
36	1	160	G
36	1	166	C
36	1	170	G
36	1	174	C
36	1	187	A
36	1	190	U
36	1	191	U
36	1	206	G

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Mol	Chain	Res	Type
36	1	210	U
36	1	213	A
36	1	218	G
36	1	219	A
36	1	233	C
36	1	240	U
36	1	241	G
36	1	242	C
36	1	243	G
36	1	245	U
36	1	249	U
36	1	252	U
36	1	256	G
36	1	266	A
36	1	269	G
36	1	282	G
36	1	283	G
36	1	286	U
36	1	295	A
36	1	298	U
36	1	305	U
36	1	315	C
36	1	323	A
36	1	329	U
36	1	334	A
36	1	338	A
36	1	339	C
36	1	343	U
36	1	349	A
36	1	350	C
36	1	376	G
36	1	391	A
36	1	398	A
36	1	399	A
36	1	401	U
36	1	402	A
36	1	403	C
36	1	404	G
36	1	412	G
36	1	421	G
36	1	422	A
36	1	438	A

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Mol	Chain	Res	Type
36	1	440	A
36	1	495	G
36	1	498	A
36	1	520	U
36	1	521	A
36	1	530	G
36	1	535	G
36	1	543	C
36	1	544	C
36	1	546	C
36	1	547	G
36	1	548	G
36	1	551	A
36	1	552	G
36	1	555	U
36	1	557	A
36	1	558	U
36	1	559	A
36	1	578	A
36	1	579	G
36	1	588	G
36	1	591	G
36	1	592	A
36	1	604	G
36	1	609	G
36	1	611	A
36	1	620	U
36	1	621	A
36	1	622	A
36	1	636	C
36	1	649	A
36	1	660	A
36	1	677	A
36	1	681	U
36	1	682	U
36	1	689	U
36	1	691	A
36	1	705	A
36	1	708	G
36	1	709	A
36	1	712	G
36	1	715	A

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Mol	Chain	Res	Type
36	1	716	A
36	1	720	A
36	1	725	G
36	1	736	A
36	1	764	U
36	1	765	C
36	1	766	U
36	1	767	U
36	1	768	C
36	1	776	U
36	1	777	U
36	1	781	G
36	1	785	G
36	1	806	A
36	1	816	A
36	1	817	A
36	1	830	A
36	1	837	A
36	1	849	C
36	1	861	C
36	1	874	U
36	1	879	U
36	1	885	U
36	1	890	C
36	1	896	A
36	1	907	G
36	1	908	G
36	1	910	G
36	1	914	A
36	1	916	G
36	1	917	A
36	1	921	A
36	1	923	C
36	1	924	G
36	1	937	G
36	1	938	C
36	1	944	C
36	1	959	C
36	1	960	U
36	1	963	G
36	1	978	G
36	1	979	U

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Mol	Chain	Res	Type
36	1	980	A
36	1	981	U
36	1	982	C
36	1	987	U
36	1	994	G
36	1	1000	C
36	1	1001	G
36	1	1002	A
36	1	1006	A
36	1	1010	G
36	1	1013	G
36	1	1015	U
36	1	1017	C
36	1	1018	G
36	1	1020	G
36	1	1024	G
36	1	1025	A
36	1	1029	G
36	1	1036	A
36	1	1047	A
36	1	1049	C
36	1	1052	U
36	1	1064	A
36	1	1065	A
36	1	1071	U
36	1	1072	G
36	1	1081	U
36	1	1083	G
36	1	1090	G
36	1	1093	A
36	1	1094	U
36	1	1095	U
36	1	1096	U
36	1	1097	G
36	1	1098	A
36	1	1103	A
36	1	1104	G
36	1	1117	G
36	1	1131	G
36	1	1153	A
36	1	1159	A
36	1	1160	C

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Mol	Chain	Res	Type
36	1	1162	U
36	1	1174	G
36	1	1179	A
36	1	1180	A
36	1	1181	U
36	1	1182	A
36	1	1192	C
36	1	1201	C
36	1	1209	G
36	1	1212	A
36	1	1213	G
36	1	1217	A
36	1	1222	G
36	1	1225	A
36	1	1227	C
36	1	1232	C
36	1	1233	G
36	1	1235	U
36	1	1236	G
36	1	1237	G
36	1	1241	U
36	1	1243	G
36	1	1245	A
36	1	1246	G
36	1	1248	C
36	1	1249	G
36	1	1254	C
36	1	1258	U
36	1	1262	G
36	1	1263	A
36	1	1264	G
36	1	1266	G
36	1	1269	U
36	1	1270	A
36	1	1271	A
36	1	1274	A
36	1	1278	A
36	1	1279	C
36	1	1285	G
36	1	1287	A
36	1	1305	U
36	1	1307	G

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Mol	Chain	Res	Type
36	1	1308	A
36	1	1309	U
36	1	1318	A
36	1	1320	C
36	1	1330	A
36	1	1331	U
36	1	1332	A
36	1	1348	U
36	1	1349	G
36	1	1350	A
36	1	1351	U
36	1	1352	A
36	1	1353	U
36	1	1355	A
36	1	1356	U
36	1	1357	G
36	1	1386	A
36	1	1392	G
36	1	1398	U
36	1	1399	A
36	1	1400	G
36	1	1418	A
36	1	1419	A
36	1	1433	A
36	1	1434	G
36	1	1437	C
36	1	1446	A
36	1	1449	A
36	1	1450	G
36	1	1481	A
36	1	1482	A
36	1	1485	G
36	1	1508	C
36	1	1527	C
36	1	1533	U
36	1	1535	A
36	1	1556	C
36	1	1560	G
36	1	1561	G
36	1	1562	C
36	1	1563	C
36	1	1564	U

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Mol	Chain	Res	Type
36	1	1566	A
36	1	1567	U
36	1	1568	U
36	1	1569	U
36	1	1570	U
36	1	1571	A
36	1	1572	U
36	1	1576	G
36	1	1579	C
36	1	1580	A
36	1	1582	C
36	1	1583	A
36	1	1587	A
36	1	1589	A
36	1	1605	A
36	1	1620	U
36	1	1629	U
36	1	1639	C
36	1	1641	U
36	1	1643	A
36	1	1644	C
36	1	1645	U
36	1	1657	C
36	1	1677	G
36	1	1683	A
36	1	1688	U
36	1	1689	U
36	1	1716	U
36	1	1717	U
36	1	1724	U
36	1	1729	A
36	1	1736	G
36	1	1742	U
36	1	1746	U
36	1	1749	A
36	1	1750	A
36	1	1751	G
36	1	1752	A
36	1	1763	U
36	1	1764	U
36	1	1765	U
36	1	1766	G

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Mol	Chain	Res	Type
36	1	1767	C
36	1	1770	G
36	1	1780	G
36	1	1797	A
36	1	1798	A
36	1	1808	G
36	1	1810	A
36	1	1814	A
36	1	1815	U
36	1	1816	A
36	1	1817	G
36	1	1819	U
36	1	1820	U
36	1	1821	U
36	1	1839	A
36	1	1841	A
36	1	1842	A
36	1	1846	C
36	1	1849	C
36	1	1850	A
36	1	1864	A
36	1	1866	C
36	1	1879	A
36	1	1880	U
36	1	1906	G
36	1	1927	G
36	1	1934	G
36	1	1948	G
36	1	1951	C
36	1	1952	G
36	1	1953	G
36	1	1954	G
36	1	2094	C
36	1	2101	C
36	1	2102	U
36	1	2111	G
36	1	2113	A
36	1	2114	C
36	1	2121	G
36	1	2122	G
36	1	2131	A
36	1	2140	U

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Mol	Chain	Res	Type
36	1	2144	A
36	1	2158	A
36	1	2168	A
36	1	2169	G
36	1	2170	U
36	1	2187	G
36	1	2188	A
36	1	2195	C
36	1	2198	A
36	1	2205	U
36	1	2208	A
36	1	2209	U
36	1	2210	G
36	1	2213	A
36	1	2215	A
36	1	2225	U
36	1	2244	A
36	1	2249	G
36	1	2250	G
36	1	2255	A
36	1	2256	A
36	1	2272	G
36	1	2273	G
36	1	2279	A
36	1	2281	A
36	1	2282	U
36	1	2283	G
36	1	2298	U
36	1	2299	A
36	1	2301	U
36	1	2303	A
36	1	2307	G
36	1	2310	U
36	1	2313	A
36	1	2314	U
36	1	2315	G
36	1	2319	U
36	1	2334	U
36	1	2335	G
36	1	2336	U
36	1	2355	G
36	1	2361	A

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Mol	Chain	Res	Type
36	1	2366	C
36	1	2372	A
36	1	2373	A
36	1	2374	C
36	1	2375	G
36	1	2378	C
36	1	2382	G
36	1	2385	G
36	1	2388	U
36	1	2393	G
36	1	2394	G
36	1	2397	A
36	1	2401	A
36	1	2402	A
36	1	2403	G
36	1	2404	A
36	1	2405	C
36	1	2406	C
36	1	2411	U
36	1	2418	G
36	1	2419	A
36	1	2437	G
36	1	2444	C
36	1	2445	A
36	1	2502	A
36	1	2503	G
36	1	2504	U
36	1	2507	C
36	1	2509	U
36	1	2514	U
36	1	2515	A
36	1	2522	G
36	1	2523	A
36	1	2526	C
36	1	2530	G
36	1	2531	C
36	1	2532	U
36	1	2533	G
36	1	2534	G
36	1	2537	U
36	1	2538	U
36	1	2539	C

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Mol	Chain	Res	Type
36	1	2540	A
36	1	2541	U
36	1	2542	U
36	1	2543	U
36	1	2544	U
36	1	2549	G
36	1	2552	C
36	1	2554	A
36	1	2555	G
36	1	2560	C
36	1	2561	A
36	1	2562	A
36	1	2568	C
36	1	2569	A
36	1	2570	U
36	1	2571	U
36	1	2572	C
36	1	2573	G
36	1	2581	U
36	1	2585	G
36	1	2589	G
36	1	2593	A
36	1	2594	C
36	1	2606	G
36	1	2607	G
36	1	2614	G
36	1	2621	G
36	1	2626	A
36	1	2637	A
36	1	2638	C
36	1	2652	U
36	1	2656	A
36	1	2657	A
36	1	2674	A
36	1	2677	G
36	1	2689	A
36	1	2691	A
36	1	2694	A
36	1	2696	A
36	1	2704	A
36	1	2705	A
36	1	2706	G

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Mol	Chain	Res	Type
36	1	2714	G
36	1	2728	G
36	1	2729	U
36	1	2752	U
36	1	2753	G
36	1	2755	C
36	1	2762	A
36	1	2771	U
36	1	2772	C
36	1	2777	G
36	1	2778	G
36	1	2780	A
36	1	2796	G
36	1	2797	C
36	1	2799	A
36	1	2800	G
36	1	2801	A
36	1	2803	A
36	1	2810	C
36	1	2816	G
36	1	2817	A
36	1	2818	U
36	1	2838	A
36	1	2842	U
36	1	2843	U
36	1	2845	A
36	1	2853	A
36	1	2860	U
36	1	2861	U
36	1	2871	G
36	1	2872	A
36	1	2879	C
36	1	2887	A
36	1	2898	G
36	1	2899	C
36	1	2923	U
36	1	2928	C
36	1	2935	U
36	1	2936	A
36	1	2942	C
36	1	2947	G
36	1	2954	U

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Mol	Chain	Res	Type
36	1	2955	U
36	1	2971	A
36	1	2983	C
36	1	2990	G
36	1	2992	U
36	1	2996	U
36	1	2997	G
36	1	3012	A
36	1	3040	A
36	1	3049	A
36	1	3056	U
36	1	3058	U
36	1	3059	G
36	1	3074	G
36	1	3078	U
36	1	3079	U
36	1	3080	G
36	1	3086	A
36	1	3087	A
36	1	3090	U
36	1	3092	C
36	1	3104	U
36	1	3118	C
36	1	3119	U
36	1	3122	A
36	1	3123	A
36	1	3129	A
36	1	3130	A
36	1	3131	U
36	1	3142	A
36	1	3143	C
36	1	3151	U
36	1	3153	U
36	1	3154	C
36	1	3155	U
36	1	3156	U
36	1	3157	U
36	1	3164	C
36	1	3165	A
36	1	3167	A
36	1	3168	A
36	1	3169	U

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Mol	Chain	Res	Type
36	1	3170	A
36	1	3171	U
36	1	3173	G
36	1	3174	A
36	1	3176	G
36	1	3179	U
36	1	3181	C
36	1	3187	A
36	1	3196	U
36	1	3198	U
36	1	3205	G
36	1	3207	U
36	1	3210	A
36	1	3213	A
36	1	3217	C
36	1	3218	A
36	1	3219	G
36	1	3223	A
36	1	3228	C
36	1	3229	G
36	1	3243	A
36	1	3244	A
36	1	3245	A
36	1	3246	G
36	1	3247	G
36	1	3253	G
36	1	3259	U
36	1	3263	G
36	1	3269	U
36	1	3270	U
36	1	3271	G
36	1	3276	G
36	1	3278	C
36	1	3281	U
36	1	3286	G
36	1	3287	U
36	1	3288	G
36	1	3289	G
36	1	3294	A
36	1	3295	A
36	1	3304	U
36	1	3307	A

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Mol	Chain	Res	Type
36	1	3313	U
36	1	3316	A
36	1	3317	U
36	1	3318	G
36	1	3319	U
36	1	3334	U
36	1	3341	U
36	1	3342	A
36	1	3345	G
36	1	3347	A
36	1	3351	U
36	1	3352	U
36	1	3353	G
36	1	3354	U
36	1	3355	U
36	1	3356	G
36	1	3368	U
36	1	3369	G
36	1	3378	C
36	1	3381	U
36	1	3382	U
36	1	3383	G
36	1	3389	U
36	1	3396	U
37	3	7	G
37	3	11	A
37	3	22	A
37	3	41	G
37	3	54	U
37	3	65	G
37	3	74	C
37	3	76	A
37	3	102	A
37	3	112	G
37	3	121	U
38	4	18	U
38	4	20	U
38	4	34	U
38	4	35	C
38	4	48	A
38	4	51	G
38	4	53	A

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Mol	Chain	Res	Type
38	4	59	A
38	4	62	C
38	4	63	G
38	4	75	G
38	4	80	A
38	4	81	U
38	4	82	U
38	4	83	C
38	4	84	C
38	4	85	G
38	4	86	U
38	4	87	G
38	4	90	U
38	4	95	G
38	4	98	U
38	4	102	U
38	4	104	A
38	4	105	A
38	4	106	C
38	4	111	A
38	4	113	U
38	4	125	U
38	4	126	A
38	4	128	U
38	4	138	A
38	4	152	G
38	4	155	A
38	4	157	U
38	4	158	U
1	6	2	A
1	6	4	C
1	6	11	A
1	6	17	C
1	6	23	G
1	6	25	C
1	6	26	A
1	6	27	U
1	6	34	G
1	6	40	A
1	6	42	G
1	6	46	A
1	6	47	A

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Mol	Chain	Res	Type
1	6	57	G
1	6	60	U
1	6	65	A
1	6	68	A
1	6	69	G
1	6	72	A
1	6	73	U
1	6	75	U
1	6	76	A
1	6	77	U
1	6	78	A
1	6	95	G
1	6	97	C
1	6	104	A
1	6	111	U
1	6	114	C
1	6	116	U
1	6	132	U
1	6	137	U
1	6	138	A
1	6	140	A
1	6	141	U
1	6	145	A
1	6	146	U
1	6	153	G
1	6	158	U
1	6	159	U
1	6	166	C
1	6	175	G
1	6	178	U
1	6	181	A
1	6	185	U
1	6	188	A
1	6	190	C
1	6	191	C
1	6	192	U
1	6	193	U
1	6	194	U
1	6	195	G
1	6	198	A
1	6	199	G
1	6	200	A

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Mol	Chain	Res	Type
1	6	215	A
1	6	216	U
1	6	217	A
1	6	218	A
1	6	219	A
1	6	220	A
1	6	222	A
1	6	226	A
1	6	227	U
1	6	228	G
1	6	230	C
1	6	232	U
1	6	233	C
1	6	234	G
1	6	240	U
1	6	241	U
1	6	249	U
1	6	250	C
1	6	261	U
1	6	265	A
1	6	271	A
1	6	272	U
1	6	273	G
1	6	277	U
1	6	278	U
1	6	280	U
1	6	281	G
1	6	287	G
1	6	294	C
1	6	299	A
1	6	302	U
1	6	308	C
1	6	314	C
1	6	316	A
1	6	321	C
1	6	334	G
1	6	337	G
1	6	338	C
1	6	352	A
1	6	359	A
1	6	361	C
1	6	378	A

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Mol	Chain	Res	Type
1	6	393	C
1	6	400	A
1	6	401	A
1	6	402	C
1	6	404	G
1	6	416	A
1	6	418	G
1	6	424	C
1	6	425	A
1	6	426	G
1	6	434	G
1	6	438	A
1	6	439	U
1	6	444	C
1	6	445	A
1	6	448	C
1	6	468	A
1	6	477	A
1	6	484	C
1	6	486	G
1	6	487	G
1	6	488	G
1	6	489	C
1	6	490	C
1	6	492	A
1	6	493	U
1	6	494	U
1	6	496	G
1	6	500	C
1	6	501	U
1	6	502	U
1	6	504	U
1	6	505	A
1	6	506	A
1	6	508	U
1	6	516	G
1	6	519	C
1	6	527	A
1	6	536	C
1	6	538	A
1	6	539	G
1	6	540	G

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Mol	Chain	Res	Type
1	6	541	A
1	6	542	A
1	6	543	C
1	6	544	A
1	6	548	G
1	6	554	C
1	6	555	A
1	6	556	A
1	6	557	G
1	6	558	U
1	6	559	C
1	6	564	G
1	6	565	C
1	6	568	G
1	6	570	A
1	6	574	G
1	6	577	G
1	6	579	A
1	6	580	A
1	6	582	U
1	6	584	C
1	6	594	A
1	6	595	G
1	6	606	A
1	6	609	U
1	6	611	U
1	6	619	A
1	6	620	A
1	6	622	A
1	6	623	A
1	6	639	U
1	6	640	U
1	6	650	U
1	6	652	G
1	6	653	C
1	6	661	A
1	6	662	U
1	6	665	U
1	6	667	U
1	6	668	C
1	6	670	U
1	6	679	U

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Mol	Chain	Res	Type
1	6	680	U
1	6	681	U
1	6	682	C
1	6	683	C
1	6	684	A
1	6	685	A
1	6	690	G
1	6	697	C
1	6	698	U
1	6	709	C
1	6	710	U
1	6	711	U
1	6	718	U
1	6	719	U
1	6	720	G
1	6	721	U
1	6	722	G
1	6	730	G
1	6	734	A
1	6	740	A
1	6	742	U
1	6	751	G
1	6	754	A
1	6	755	A
1	6	756	A
1	6	765	G
1	6	766	U
1	6	774	A
1	6	775	G
1	6	780	A
1	6	781	U
1	6	782	U
1	6	783	G
1	6	793	A
1	6	794	U
1	6	810	G
1	6	811	A
1	6	812	A
1	6	813	U
1	6	814	A
1	6	815	G
1	6	816	G

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Mol	Chain	Res	Type
1	6	821	U
1	6	823	G
1	6	824	G
1	6	825	U
1	6	826	U
1	6	829	A
1	6	830	U
1	6	831	U
1	6	832	U
1	6	834	G
1	6	835	U
1	6	860	U
1	6	861	U
1	6	863	A
1	6	865	A
1	6	876	G
1	6	886	U
1	6	898	A
1	6	906	A
1	6	911	U
1	6	912	U
1	6	913	G
1	6	914	G
1	6	933	A
1	6	935	U
1	6	942	G
1	6	951	A
1	6	959	U
1	6	960	U
1	6	966	A
1	6	969	C
1	6	970	A
1	6	971	A
1	6	983	A
1	6	988	A
1	6	992	A
1	6	996	U
1	6	997	G
1	6	1000	C
1	6	1003	A
1	6	1004	U
1	6	1005	A

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Mol	Chain	Res	Type
1	6	1021	C
1	6	1026	A
1	6	1028	C
1	6	1039	A
1	6	1040	G
1	6	1052	U
1	6	1053	G
1	6	1057	U
1	6	1058	U
1	6	1059	U
1	6	1060	U
1	6	1072	C
1	6	1073	G
1	6	1075	C
1	6	1081	A
1	6	1082	C
1	6	1092	A
1	6	1096	C
1	6	1097	U
1	6	1098	U
1	6	1100	G
1	6	1109	G
1	6	1111	G
1	6	1138	A
1	6	1151	A
1	6	1155	G
1	6	1158	C
1	6	1159	C
1	6	1160	A
1	6	1161	C
1	6	1164	G
1	6	1167	G
1	6	1185	U
1	6	1186	U
1	6	1194	A
1	6	1196	A
1	6	1199	G
1	6	1200	G
1	6	1202	A
1	6	1207	C
1	6	1208	A
1	6	1217	A

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Mol	Chain	Res	Type
1	6	1218	G
1	6	1220	C
1	6	1226	A
1	6	1228	G
1	6	1229	G
1	6	1230	A
1	6	1239	U
1	6	1241	G
1	6	1242	A
1	6	1243	G
1	6	1244	A
1	6	1245	G
1	6	1246	C
1	6	1255	G
1	6	1256	A
1	6	1257	U
1	6	1258	U
1	6	1273	G
1	6	1284	C
1	6	1286	U
1	6	1291	G
1	6	1314	U
1	6	1316	G
1	6	1321	A
1	6	1338	C
1	6	1343	U
1	6	1344	A
1	6	1345	A
1	6	1346	A
1	6	1353	U
1	6	1361	U
1	6	1362	U
1	6	1363	U
1	6	1364	G
1	6	1367	G
1	6	1370	U
1	6	1371	A
1	6	1390	U
1	6	1398	U
1	6	1399	C
1	6	1400	A
1	6	1413	U

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Mol	Chain	Res	Type
1	6	1414	U
1	6	1415	U
1	6	1426	C
1	6	1427	A
1	6	1428	G
1	6	1433	G
1	6	1437	U
1	6	1445	G
1	6	1446	A
1	6	1447	C
1	6	1448	G
1	6	1458	G
1	6	1459	C
1	6	1460	A
1	6	1461	C
1	6	1466	G
1	6	1471	A
1	6	1473	U
1	6	1477	G
1	6	1481	C
1	6	1482	C
1	6	1486	G
1	6	1489	U
1	6	1490	C
1	6	1491	U
1	6	1492	A
1	6	1493	A
1	6	1506	G
1	6	1514	U
1	6	1516	A
1	6	1521	G
1	6	1523	G
1	6	1524	A
1	6	1531	G
1	6	1535	U
1	6	1536	G
1	6	1537	C
1	6	1538	U
1	6	1540	G
1	6	1554	U
1	6	1557	U
1	6	1559	A

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Mol	Chain	Res	Type
1	6	1573	A
1	6	1574	G
1	6	1577	A
1	6	1582	U
1	6	1584	G
1	6	1600	A
1	6	1601	G
1	6	1607	G
1	6	1616	G
1	6	1621	U
1	6	1631	A
1	6	1634	C
1	6	1637	C
1	6	1638	G
1	6	1657	U
1	6	1658	G
1	6	1670	G
1	6	1683	C
1	6	1697	G
1	6	1698	G
1	6	1699	G
1	6	1700	C
1	6	1701	A
1	6	1702	A
1	6	1712	A
1	6	1713	G
1	6	1716	C
1	6	1731	A
1	6	1736	G
1	6	1750	A
1	6	1760	G
1	6	1762	A
1	6	1766	A
1	6	1767	G
1	6	1769	U
1	6	1780	G
1	6	1782	A
1	6	1789	G
1	6	1792	G
1	6	1793	G
1	6	1794	A
1	6	1795	U

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Mol	Chain	Res	Type
1	6	1796	C
1	6	1799	U
1	6	1800	A
36	5	15	C
36	5	16	A
36	5	26	A
36	5	40	A
36	5	49	A
36	5	59	G
36	5	60	A
36	5	65	A
36	5	66	A
36	5	68	C
36	5	73	C
36	5	76	G
36	5	77	A
36	5	93	C
36	5	94	G
36	5	96	G
36	5	99	A
36	5	102	C
36	5	109	A
36	5	110	G
36	5	113	C
36	5	116	A
36	5	118	U
36	5	120	G
36	5	121	A
36	5	122	A
36	5	134	U
36	5	135	C
36	5	136	G
36	5	156	G
36	5	157	A
36	5	160	G
36	5	165	A
36	5	166	C
36	5	170	G
36	5	171	G
36	5	172	G
36	5	173	G
36	5	174	C

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Mol	Chain	Res	Type
36	5	180	C
36	5	182	U
36	5	187	A
36	5	190	U
36	5	191	U
36	5	200	C
36	5	210	U
36	5	213	A
36	5	218	G
36	5	219	A
36	5	220	G
36	5	221	A
36	5	224	C
36	5	235	A
36	5	239	G
36	5	240	U
36	5	245	U
36	5	247	C
36	5	248	U
36	5	249	U
36	5	250	U
36	5	252	U
36	5	253	A
36	5	254	A
36	5	269	G
36	5	284	A
36	5	286	U
36	5	295	A
36	5	298	U
36	5	315	C
36	5	323	A
36	5	327	A
36	5	329	U
36	5	334	A
36	5	339	C
36	5	349	A
36	5	350	C
36	5	351	A
36	5	369	A
36	5	375	A
36	5	376	G
36	5	379	C

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Mol	Chain	Res	Type
36	5	380	U
36	5	398	A
36	5	399	A
36	5	401	U
36	5	402	A
36	5	403	C
36	5	404	G
36	5	421	G
36	5	422	A
36	5	438	A
36	5	439	C
36	5	440	A
36	5	441	U
36	5	442	G
36	5	492	U
36	5	495	G
36	5	521	A
36	5	542	G
36	5	546	C
36	5	547	G
36	5	548	G
36	5	551	A
36	5	552	G
36	5	554	A
36	5	557	A
36	5	559	A
36	5	569	A
36	5	578	A
36	5	579	G
36	5	581	U
36	5	592	A
36	5	600	G
36	5	604	G
36	5	607	A
36	5	609	G
36	5	611	A
36	5	619	A
36	5	621	A
36	5	626	U
36	5	636	C
36	5	647	A
36	5	649	A

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Mol	Chain	Res	Type
36	5	651	G
36	5	660	A
36	5	677	A
36	5	681	U
36	5	683	U
36	5	691	A
36	5	692	A
36	5	705	A
36	5	712	G
36	5	715	A
36	5	716	A
36	5	718	G
36	5	720	A
36	5	725	G
36	5	736	A
36	5	750	G
36	5	758	C
36	5	763	G
36	5	766	U
36	5	767	U
36	5	774	G
36	5	776	U
36	5	777	U
36	5	780	A
36	5	781	G
36	5	785	G
36	5	786	A
36	5	806	A
36	5	817	A
36	5	820	A
36	5	826	G
36	5	830	A
36	5	861	C
36	5	874	U
36	5	877	C
36	5	879	U
36	5	890	C
36	5	895	A
36	5	896	A
36	5	907	G
36	5	908	G
36	5	910	G

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Mol	Chain	Res	Type
36	5	914	A
36	5	916	G
36	5	917	A
36	5	922	U
36	5	923	C
36	5	924	G
36	5	925	A
36	5	937	G
36	5	944	C
36	5	958	C
36	5	959	C
36	5	960	U
36	5	962	A
36	5	963	G
36	5	964	G
36	5	979	U
36	5	981	U
36	5	983	A
36	5	994	G
36	5	1000	C
36	5	1001	G
36	5	1002	A
36	5	1010	G
36	5	1014	U
36	5	1015	U
36	5	1016	C
36	5	1017	C
36	5	1018	G
36	5	1021	G
36	5	1024	G
36	5	1025	A
36	5	1026	A
36	5	1028	U
36	5	1029	G
36	5	1035	G
36	5	1041	U
36	5	1047	A
36	5	1049	C
36	5	1064	A
36	5	1065	A
36	5	1066	G
36	5	1072	G

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Mol	Chain	Res	Type
36	5	1081	U
36	5	1082	U
36	5	1085	A
36	5	1087	G
36	5	1093	A
36	5	1094	U
36	5	1095	U
36	5	1097	G
36	5	1098	A
36	5	1103	A
36	5	1104	G
36	5	1112	A
36	5	1117	G
36	5	1131	G
36	5	1152	G
36	5	1153	A
36	5	1159	A
36	5	1178	G
36	5	1179	A
36	5	1180	A
36	5	1181	U
36	5	1182	A
36	5	1192	C
36	5	1193	A
36	5	1196	C
36	5	1201	C
36	5	1209	G
36	5	1222	G
36	5	1223	A
36	5	1233	G
36	5	1235	U
36	5	1236	G
36	5	1237	G
36	5	1239	C
36	5	1241	U
36	5	1242	G
36	5	1245	A
36	5	1246	G
36	5	1252	A
36	5	1253	U
36	5	1258	U
36	5	1262	G

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Mol	Chain	Res	Type
36	5	1263	A
36	5	1264	G
36	5	1265	U
36	5	1266	G
36	5	1277	C
36	5	1285	G
36	5	1291	A
36	5	1292	C
36	5	1307	G
36	5	1308	A
36	5	1309	U
36	5	1313	G
36	5	1318	A
36	5	1330	A
36	5	1331	U
36	5	1332	A
36	5	1333	C
36	5	1345	G
36	5	1348	U
36	5	1349	G
36	5	1351	U
36	5	1352	A
36	5	1353	U
36	5	1354	G
36	5	1355	A
36	5	1356	U
36	5	1357	G
36	5	1386	A
36	5	1387	G
36	5	1399	A
36	5	1400	G
36	5	1417	G
36	5	1418	A
36	5	1419	A
36	5	1425	U
36	5	1431	G
36	5	1433	A
36	5	1434	G
36	5	1437	C
36	5	1446	A
36	5	1450	G
36	5	1462	A

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Mol	Chain	Res	Type
36	5	1481	A
36	5	1482	A
36	5	1484	U
36	5	1490	A
36	5	1508	C
36	5	1527	C
36	5	1536	G
36	5	1547	G
36	5	1553	U
36	5	1554	U
36	5	1555	U
36	5	1556	C
36	5	1557	A
36	5	1560	G
36	5	1561	G
36	5	1562	C
36	5	1567	U
36	5	1568	U
36	5	1569	U
36	5	1570	U
36	5	1571	A
36	5	1572	U
36	5	1573	G
36	5	1574	C
36	5	1575	A
36	5	1576	G
36	5	1577	G
36	5	1578	C
36	5	1579	C
36	5	1581	C
36	5	1582	C
36	5	1583	A
36	5	1587	A
36	5	1589	A
36	5	1593	A
36	5	1605	A
36	5	1620	U
36	5	1623	G
36	5	1629	U
36	5	1632	A
36	5	1639	C
36	5	1641	U

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Mol	Chain	Res	Type
36	5	1643	A
36	5	1644	C
36	5	1645	U
36	5	1655	G
36	5	1657	C
36	5	1658	G
36	5	1675	G
36	5	1677	G
36	5	1683	A
36	5	1705	U
36	5	1716	U
36	5	1717	U
36	5	1724	U
36	5	1725	C
36	5	1750	A
36	5	1751	G
36	5	1759	C
36	5	1760	A
36	5	1762	C
36	5	1764	U
36	5	1765	U
36	5	1766	G
36	5	1769	G
36	5	1770	G
36	5	1780	G
36	5	1797	A
36	5	1812	G
36	5	1814	A
36	5	1815	U
36	5	1816	A
36	5	1817	G
36	5	1818	U
36	5	1821	U
36	5	1839	A
36	5	1841	A
36	5	1842	A
36	5	1846	C
36	5	1849	C
36	5	1850	A
36	5	1858	A
36	5	1871	U
36	5	1878	G

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Mol	Chain	Res	Type
36	5	1879	A
36	5	1880	U
36	5	1886	A
36	5	1891	A
36	5	1894	U
36	5	1906	G
36	5	1951	C
36	5	1953	G
36	5	2100	A
36	5	2101	C
36	5	2102	U
36	5	2111	G
36	5	2112	U
36	5	2113	A
36	5	2121	G
36	5	2122	G
36	5	2131	A
36	5	2134	G
36	5	2144	A
36	5	2158	A
36	5	2168	A
36	5	2169	G
36	5	2184	U
36	5	2187	G
36	5	2188	A
36	5	2192	C
36	5	2198	A
36	5	2205	U
36	5	2206	G
36	5	2208	A
36	5	2210	G
36	5	2223	A
36	5	2225	U
36	5	2244	A
36	5	2250	G
36	5	2252	A
36	5	2255	A
36	5	2256	A
36	5	2258	U
36	5	2270	A
36	5	2273	G
36	5	2276	G

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Mol	Chain	Res	Type
36	5	2279	A
36	5	2280	A
36	5	2281	A
36	5	2288	G
36	5	2298	U
36	5	2303	A
36	5	2307	G
36	5	2310	U
36	5	2313	A
36	5	2315	G
36	5	2324	A
36	5	2334	U
36	5	2335	G
36	5	2336	U
36	5	2358	A
36	5	2360	C
36	5	2372	A
36	5	2373	A
36	5	2374	C
36	5	2375	G
36	5	2385	G
36	5	2393	G
36	5	2397	A
36	5	2398	A
36	5	2400	G
36	5	2401	A
36	5	2403	G
36	5	2404	A
36	5	2405	C
36	5	2411	U
36	5	2418	G
36	5	2419	A
36	5	2444	C
36	5	2445	A
36	5	2446	U
36	5	2447	A
36	5	2451	G
36	5	2452	G
36	5	2493	U
36	5	2494	A
36	5	2495	C
36	5	2497	U

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Mol	Chain	Res	Type
36	5	2501	U
36	5	2502	A
36	5	2503	G
36	5	2504	U
36	5	2510	U
36	5	2513	U
36	5	2514	U
36	5	2515	A
36	5	2523	A
36	5	2526	C
36	5	2530	G
36	5	2536	A
36	5	2537	U
36	5	2538	U
36	5	2539	C
36	5	2540	A
36	5	2543	U
36	5	2549	G
36	5	2552	C
36	5	2555	G
36	5	2560	C
36	5	2566	C
36	5	2568	C
36	5	2569	A
36	5	2570	U
36	5	2571	U
36	5	2572	C
36	5	2573	G
36	5	2574	G
36	5	2584	G
36	5	2585	G
36	5	2593	A
36	5	2603	G
36	5	2606	G
36	5	2607	G
36	5	2614	G
36	5	2637	A
36	5	2652	U
36	5	2656	A
36	5	2674	A
36	5	2675	C
36	5	2677	G

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Mol	Chain	Res	Type
36	5	2689	A
36	5	2691	A
36	5	2694	A
36	5	2696	A
36	5	2705	A
36	5	2714	G
36	5	2719	U
36	5	2728	G
36	5	2729	U
36	5	2737	C
36	5	2739	A
36	5	2752	U
36	5	2753	G
36	5	2755	C
36	5	2762	A
36	5	2771	U
36	5	2772	C
36	5	2773	C
36	5	2777	G
36	5	2778	G
36	5	2796	G
36	5	2799	A
36	5	2800	G
36	5	2801	A
36	5	2810	C
36	5	2817	A
36	5	2818	U
36	5	2838	A
36	5	2843	U
36	5	2845	A
36	5	2847	A
36	5	2849	C
36	5	2851	A
36	5	2853	A
36	5	2861	U
36	5	2863	G
36	5	2871	G
36	5	2872	A
36	5	2886	U
36	5	2887	A
36	5	2889	C
36	5	2899	C

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Mol	Chain	Res	Type
36	5	2904	U
36	5	2911	A
36	5	2914	G
36	5	2923	U
36	5	2935	U
36	5	2936	A
36	5	2942	C
36	5	2945	G
36	5	2947	G
36	5	2954	U
36	5	2972	G
36	5	2979	U
36	5	2983	C
36	5	2990	G
36	5	2996	U
36	5	2997	G
36	5	3012	A
36	5	3028	G
36	5	3030	G
36	5	3054	U
36	5	3056	U
36	5	3059	G
36	5	3078	U
36	5	3079	U
36	5	3086	A
36	5	3087	A
36	5	3091	A
36	5	3092	C
36	5	3119	U
36	5	3122	A
36	5	3130	A
36	5	3131	U
36	5	3132	C
36	5	3142	A
36	5	3143	C
36	5	3150	A
36	5	3153	U
36	5	3156	U
36	5	3157	U
36	5	3158	G
36	5	3164	C
36	5	3165	A

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Mol	Chain	Res	Type
36	5	3167	A
36	5	3168	A
36	5	3171	U
36	5	3172	A
36	5	3173	G
36	5	3174	A
36	5	3176	G
36	5	3180	A
36	5	3181	C
36	5	3187	A
36	5	3188	G
36	5	3195	U
36	5	3196	U
36	5	3207	U
36	5	3217	C
36	5	3218	A
36	5	3219	G
36	5	3229	G
36	5	3233	C
36	5	3238	G
36	5	3239	G
36	5	3243	A
36	5	3244	A
36	5	3245	A
36	5	3246	G
36	5	3247	G
36	5	3252	G
36	5	3253	G
36	5	3259	U
36	5	3272	C
36	5	3275	U
36	5	3276	G
36	5	3277	U
36	5	3279	A
36	5	3281	U
36	5	3282	U
36	5	3285	C
36	5	3286	G
36	5	3288	G
36	5	3289	G
36	5	3290	G
36	5	3294	A

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Mol	Chain	Res	Type
36	5	3304	U
36	5	3313	U
36	5	3316	A
36	5	3317	U
36	5	3318	G
36	5	3319	U
36	5	3320	A
36	5	3342	A
36	5	3345	G
36	5	3348	G
36	5	3350	C
36	5	3351	U
36	5	3352	U
36	5	3354	U
36	5	3355	U
36	5	3356	G
36	5	3358	U
36	5	3368	U
36	5	3369	G
36	5	3378	C
36	5	3389	U
36	5	3390	G
36	5	3396	U
37	7	7	G
37	7	22	A
37	7	41	G
37	7	45	A
37	7	54	U
37	7	60	G
37	7	65	G
37	7	73	C
37	7	76	A
37	7	99	G
37	7	101	G
37	7	102	A
37	7	103	A
37	7	110	G
37	7	112	G
37	7	121	U
38	8	16	G
38	8	34	U
38	8	35	C

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Mol	Chain	Res	Type
38	8	48	A
38	8	51	G
38	8	53	A
38	8	58	G
38	8	59	A
38	8	62	C
38	8	63	G
38	8	75	G
38	8	80	A
38	8	81	U
38	8	82	U
38	8	83	C
38	8	84	C
38	8	86	U
38	8	87	G
38	8	95	G
38	8	96	A
38	8	97	A
38	8	104	A
38	8	105	A
38	8	106	C
38	8	111	A
38	8	113	U
38	8	125	U
38	8	126	A
38	8	127	U
38	8	138	A
38	8	152	G
38	8	157	U
38	8	158	U

All (185) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	25	C
1	2	45	U
1	2	103	A
1	2	114	C
1	2	130	C
1	2	131	C
1	2	136	C
1	2	158	U

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Mol	Chain	Res	Type
1	2	217	A
1	2	218	A
1	2	240	U
1	2	278	U
1	2	280	U
1	2	322	G
1	2	417	A
1	2	497	G
1	2	499	U
1	2	501	U
1	2	503	G
1	2	512	A
1	2	558	U
1	2	571	G
1	2	622	A
1	2	685	A
1	2	704	C
1	2	720	G
1	2	721	U
1	2	794	U
1	2	829	A
1	2	1058	U
1	2	1081	A
1	2	1150	G
1	2	1196	A
1	2	1207	C
1	2	1226	A
1	2	1244	A
1	2	1250	U
1	2	1344	A
1	2	1370	U
1	2	1481	C
1	2	1489	U
1	2	1490	C
1	2	1568	C
1	2	1573	A
1	2	1615	C
1	2	1657	U
1	2	1698	G
1	2	1711	C
1	2	1761	U
36	1	65	A

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Mol	Chain	Res	Type
36	1	109	A
36	1	239	G
36	1	282	G
36	1	619	A
36	1	715	A
36	1	763	G
36	1	873	C
36	1	916	G
36	1	981	U
36	1	993	G
36	1	1064	A
36	1	1094	U
36	1	1097	G
36	1	1103	A
36	1	1273	A
36	1	1307	G
36	1	1329	U
36	1	1331	U
36	1	1352	A
36	1	1355	A
36	1	1484	U
36	1	1562	C
36	1	1716	U
36	1	1820	U
36	1	2101	C
36	1	2112	U
36	1	2209	U
36	1	2249	G
36	1	2297	U
36	1	2372	A
36	1	2403	G
36	1	2418	G
36	1	2537	U
36	1	2541	U
36	1	2554	A
36	1	2585	G
36	1	2593	A
36	1	2817	A
36	1	3078	U
36	1	3121	U
36	1	3169	U
36	1	3228	C

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Mol	Chain	Res	Type
36	1	3269	U
36	1	3275	U
36	1	3316	A
36	1	3350	C
36	1	3351	U
36	1	3353	G
38	4	85	G
1	6	25	C
1	6	76	A
1	6	103	A
1	6	114	C
1	6	158	U
1	6	187	G
1	6	192	U
1	6	217	A
1	6	400	A
1	6	417	A
1	6	542	A
1	6	555	A
1	6	557	G
1	6	558	U
1	6	697	C
1	6	717	C
1	6	755	A
1	6	829	A
1	6	1051	G
1	6	1058	U
1	6	1097	U
1	6	1241	G
1	6	1244	A
1	6	1255	G
1	6	1344	A
1	6	1481	C
1	6	1489	U
1	6	1491	U
1	6	1535	U
1	6	1573	A
1	6	1600	A
1	6	1620	C
1	6	1657	U
1	6	1698	G
1	6	1700	C

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Mol	Chain	Res	Type
36	5	238	A
36	5	285	A
36	5	397	A
36	5	438	A
36	5	588	G
36	5	765	C
36	5	916	G
36	5	993	G
36	5	1027	A
36	5	1064	A
36	5	1081	U
36	5	1152	G
36	5	1222	G
36	5	1238	C
36	5	1241	U
36	5	1307	G
36	5	1329	U
36	5	1331	U
36	5	1352	A
36	5	1355	A
36	5	1481	A
36	5	1560	G
36	5	1572	U
36	5	1716	U
36	5	1816	A
36	5	1878	G
36	5	2101	C
36	5	2112	U
36	5	2168	A
36	5	2204	C
36	5	2209	U
36	5	2249	G
36	5	2255	A
36	5	2257	C
36	5	2372	A
36	5	2445	A
36	5	2446	U
36	5	2493	U
36	5	2500	A
36	5	2771	U
36	5	2772	C
36	5	2818	U

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Mol	Chain	Res	Type
36	5	2971	A
36	5	3078	U
36	5	3195	U
36	5	3275	U
36	5	3289	G
36	5	3317	U
36	5	3357	U
37	7	111	U
38	8	111	A

## 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 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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
1	2	2
81	m2	2
80	c0	1
36	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c0	84:GLU	C	87:HIS	N	7.38
1	2	1716:C	O3'	1717:G	P	5.29
1	5	2437:G	O3'	2438:A	P	3.76
1	m2	52:UNK	C	54:UNK	N	3.58
1	m2	23:UNK	C	28:UNK	N	3.14
1	2	1685:G	O3'	1686:C	P	3.04



## 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	2	1781/1800 (98%)	0.92	209 (11%) 4 4	60, 99, 172, 210	0
1	6	1795/1800 (99%)	0.61	93 (5%) 27 25	46, 86, 159, 201	0
2	S0	206/251 (82%)	2.50	120 (58%) 0 0	101, 114, 125, 133	0
2	s0	206/251 (82%)	1.66	78 (37%) 0 0	83, 99, 113, 119	0
3	S1	214/254 (84%)	0.78	33 (15%) 2 2	107, 142, 167, 173	0
3	s1	216/254 (85%)	0.84	31 (14%) 2 2	84, 98, 115, 123	0
4	S2	217/253 (85%)	1.54	64 (29%) 0 0	84, 97, 111, 115	0
4	s2	217/253 (85%)	1.43	58 (26%) 0 0	68, 81, 96, 103	0
5	S3	223/239 (93%)	1.74	89 (39%) 0 0	89, 100, 122, 129	0
5	s3	223/239 (93%)	2.19	112 (50%) 0 0	84, 111, 133, 137	0
6	S4	260/260 (100%)	1.35	74 (28%) 0 0	77, 102, 110, 125	0
6	s4	260/260 (100%)	0.69	24 (9%) 9 10	61, 83, 97, 119	0
7	S5	206/224 (91%)	1.02	40 (19%) 1 1	102, 123, 131, 134	0
7	s5	206/224 (91%)	1.26	52 (25%) 0 0	87, 108, 122, 128	0
8	S6	226/236 (95%)	1.16	59 (26%) 0 0	78, 110, 127, 139	0
8	s6	218/236 (92%)	0.77	25 (11%) 4 4	60, 89, 107, 116	0
9	S7	184/189 (97%)	0.93	37 (20%) 1 1	101, 123, 139, 142	0
9	s7	186/189 (98%)	0.79	26 (13%) 2 2	77, 105, 132, 137	0
10	S8	188/200 (94%)	1.50	56 (29%) 0 0	71, 89, 123, 135	0
10	s8	188/200 (94%)	1.08	36 (19%) 1 1	56, 75, 116, 133	0
11	S9	185/196 (94%)	1.33	49 (26%) 0 0	90, 107, 133, 150	0
11	s9	185/196 (94%)	0.82	16 (8%) 10 10	72, 90, 116, 130	0
12	C0	96/105 (91%)	1.39	27 (28%) 0 0	92, 113, 133, 141	0
13	C1	155/155 (100%)	2.03	71 (45%) 0 0	73, 85, 112, 127	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
13	c1	146/155 (94%)	1.48	32 (21%)	0	1	59, 72, 97, 121	0
14	C2	124/142 (87%)	1.09	30 (24%)	0	0	138, 146, 152, 159	0
14	c2	124/142 (87%)	2.36	51 (41%)	0	0	169, 184, 194, 196	0
15	C3	150/150 (100%)	1.39	41 (27%)	0	0	81, 94, 113, 116	0
15	c3	150/150 (100%)	1.37	45 (30%)	0	0	67, 80, 97, 102	0
16	C4	127/136 (93%)	1.03	25 (19%)	1	1	84, 139, 155, 159	0
16	c4	128/136 (94%)	1.36	36 (28%)	0	0	66, 102, 112, 119	0
17	C5	124/141 (87%)	0.54	8 (6%)	18	18	88, 100, 112, 119	0
17	c5	135/141 (95%)	1.00	27 (20%)	1	1	78, 105, 114, 118	0
18	C6	141/142 (99%)	3.40	93 (65%)	0	0	92, 112, 117, 120	0
18	c6	142/142 (100%)	2.38	74 (52%)	0	0	80, 101, 116, 125	0
19	C7	120/136 (88%)	2.78	81 (67%)	0	0	99, 108, 126, 129	0
19	c7	117/136 (86%)	1.45	42 (35%)	0	0	87, 102, 115, 118	0
20	C8	145/145 (100%)	0.41	9 (6%)	20	19	86, 110, 131, 137	0
20	c8	145/145 (100%)	0.50	6 (4%)	37	34	88, 100, 118, 127	0
21	C9	143/143 (100%)	2.22	82 (57%)	0	0	95, 110, 121, 126	0
21	c9	143/143 (100%)	1.21	27 (18%)	1	1	84, 96, 112, 121	0
22	D0	107/120 (89%)	1.91	42 (39%)	0	0	85, 112, 128, 130	0
22	d0	110/120 (91%)	2.21	53 (48%)	0	0	84, 114, 139, 156	0
23	D1	87/87 (100%)	2.09	43 (49%)	0	0	100, 106, 118, 127	0
23	d1	87/87 (100%)	0.99	18 (20%)	1	1	80, 88, 108, 116	0
24	D2	129/129 (100%)	3.56	106 (82%)	0	0	83, 94, 103, 112	0
24	d2	129/129 (100%)	1.40	38 (29%)	0	0	65, 75, 82, 89	0
25	D3	144/144 (100%)	1.43	40 (27%)	0	0	71, 77, 86, 97	0
25	d3	144/144 (100%)	1.04	22 (15%)	2	2	58, 63, 74, 82	0
26	D4	134/134 (100%)	0.52	12 (8%)	9	10	88, 111, 122, 128	0
26	d4	134/134 (100%)	0.37	4 (2%)	50	48	68, 92, 105, 108	0
27	D5	70/107 (65%)	0.28	5 (7%)	16	15	119, 131, 137, 138	0
27	d5	69/107 (64%)	0.60	6 (8%)	10	10	97, 115, 125, 126	0
28	D6	97/97 (100%)	2.66	57 (58%)	0	0	88, 104, 150, 154	0
28	d6	97/97 (100%)	2.43	52 (53%)	0	0	71, 86, 115, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
29	D7	81/81 (100%)	1.64	35 (43%)	0	0	98, 110, 134, 137	0
29	d7	81/81 (100%)	1.88	33 (40%)	0	0	80, 94, 124, 130	0
30	D8	63/66 (95%)	1.23	16 (25%)	0	0	110, 125, 137, 139	0
30	d8	63/66 (95%)	1.62	21 (33%)	0	0	103, 116, 125, 130	0
31	D9	53/55 (96%)	1.53	15 (28%)	0	0	86, 90, 106, 111	0
31	d9	53/55 (96%)	2.70	35 (66%)	0	0	81, 92, 128, 141	0
32	E0	60/62 (96%)	2.14	24 (40%)	0	0	77, 108, 128, 130	0
32	e0	62/62 (100%)	1.01	13 (20%)	1	1	66, 91, 110, 113	0
33	E1	71/76 (93%)	0.87	12 (16%)	1	1	105, 134, 149, 153	0
33	e1	76/76 (100%)	1.56	24 (31%)	0	0	112, 161, 175, 179	0
34	SR	318/318 (100%)	1.65	109 (34%)	0	0	108, 119, 131, 147	0
34	sR	318/318 (100%)	2.41	162 (50%)	0	0	110, 127, 139, 150	0
35	SM	159/273 (58%)	1.25	43 (27%)	0	0	62, 98, 144, 148	0
35	sM	104/273 (38%)	0.74	16 (15%)	2	2	56, 109, 181, 186	0
36	1	3149/3396 (92%)	0.62	160 (5%)	28	26	38, 61, 124, 213	0
36	5	3169/3396 (93%)	0.65	120 (3%)	40	37	37, 56, 124, 192	0
37	3	121/121 (100%)	0.22	0	100	100	44, 76, 91, 98	0
37	7	121/121 (100%)	0.31	1 (0%)	86	86	41, 62, 74, 80	0
38	4	158/158 (100%)	0.42	2 (1%)	77	75	47, 64, 94, 125	0
38	8	158/158 (100%)	0.45	3 (1%)	66	64	46, 66, 95, 118	0
39	L2	252/253 (99%)	1.22	59 (23%)	0	1	46, 64, 80, 86	0
39	l2	252/253 (99%)	1.40	69 (27%)	0	0	45, 61, 75, 85	0
40	L3	386/386 (100%)	0.64	33 (8%)	10	10	44, 64, 77, 87	0
40	l3	386/386 (100%)	0.43	13 (3%)	45	42	37, 51, 64, 79	0
41	L4	361/361 (100%)	0.57	40 (11%)	5	5	42, 57, 70, 74	0
41	l4	361/361 (100%)	0.77	44 (12%)	4	4	45, 60, 74, 82	0
42	L5	296/296 (100%)	0.47	24 (8%)	12	11	60, 83, 99, 107	0
42	l5	294/296 (99%)	0.36	10 (3%)	45	42	50, 64, 89, 105	0
43	L6	156/175 (89%)	0.48	2 (1%)	77	75	52, 59, 72, 82	0
43	l6	157/175 (89%)	0.50	10 (6%)	19	18	53, 60, 78, 87	0
44	L7	222/243 (91%)	0.55	5 (2%)	60	58	42, 52, 78, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	l7	223/243 (91%)	0.30	0 100 100	42, 51, 80, 105	0
45	L8	233/255 (91%)	0.65	22 (9%) 8 9	70, 86, 109, 117	0
45	l8	231/255 (90%)	0.79	27 (11%) 4 4	73, 86, 106, 114	0
46	L9	191/191 (100%)	0.30	5 (2%) 56 52	62, 72, 83, 92	0
46	l9	191/191 (100%)	0.37	4 (2%) 63 61	47, 57, 72, 82	0
47	M0	211/220 (95%)	0.55	6 (2%) 53 50	47, 61, 88, 110	0
47	m0	213/220 (96%)	0.72	13 (6%) 21 20	45, 64, 88, 97	0
48	M1	169/173 (97%)	0.66	13 (7%) 13 12	70, 88, 99, 102	0
48	m1	169/173 (97%)	0.31	4 (2%) 59 55	54, 71, 79, 83	0
49	M3	193/198 (97%)	1.06	37 (19%) 1 1	43, 68, 93, 114	0
49	m3	194/198 (97%)	0.56	13 (6%) 17 17	44, 71, 100, 112	0
50	M4	136/137 (99%)	0.23	1 (0%) 87 88	56, 62, 74, 86	0
50	m4	137/137 (100%)	0.12	0 100 100	51, 57, 70, 81	0
51	M5	203/203 (100%)	0.87	19 (9%) 8 9	45, 59, 70, 72	0
51	m5	203/203 (100%)	1.08	32 (15%) 2 2	46, 63, 73, 78	0
52	M6	197/198 (99%)	0.57	7 (3%) 42 39	44, 51, 67, 69	0
52	m6	197/198 (99%)	0.50	8 (4%) 37 34	37, 45, 64, 67	0
53	M7	183/183 (100%)	1.25	25 (13%) 3 3	49, 56, 93, 112	0
53	m7	155/183 (84%)	0.45	7 (4%) 33 31	42, 50, 63, 82	0
54	M8	185/185 (100%)	0.67	11 (5%) 22 21	45, 58, 71, 86	0
54	m8	185/185 (100%)	0.80	20 (10%) 5 6	44, 60, 70, 74	0
55	M9	188/188 (100%)	0.86	21 (11%) 5 5	67, 80, 140, 146	0
55	m9	188/188 (100%)	0.68	14 (7%) 14 14	53, 67, 127, 138	0
56	N0	172/172 (100%)	0.65	6 (3%) 44 40	51, 59, 70, 76	0
56	n0	172/172 (100%)	0.30	1 (0%) 89 89	45, 52, 62, 68	0
57	N1	159/159 (100%)	0.57	5 (3%) 49 47	46, 58, 95, 103	0
57	n1	159/159 (100%)	0.43	4 (2%) 57 53	43, 52, 86, 91	0
58	N2	100/120 (83%)	1.18	25 (25%) 0 0	95, 107, 121, 123	0
58	n2	98/120 (81%)	0.99	21 (21%) 0 1	78, 90, 97, 100	0
59	N3	136/136 (100%)	1.36	30 (22%) 0 1	54, 62, 72, 79	0
59	n3	136/136 (100%)	0.79	9 (6%) 18 17	38, 47, 57, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
60	N4	98/155 (63%)	2.95	38 (38%) 0 0	63, 75, 134, 138	0
60	n4	135/155 (87%)	1.08	19 (14%) 2 2	47, 94, 119, 124	0
61	N5	121/141 (85%)	0.87	11 (9%) 9 10	62, 73, 86, 99	0
61	n5	120/141 (85%)	0.66	9 (7%) 14 13	58, 72, 86, 98	0
62	N6	126/126 (100%)	0.39	3 (2%) 59 55	53, 66, 76, 81	0
62	n6	126/126 (100%)	0.66	6 (4%) 30 28	55, 68, 79, 85	0
63	N7	135/135 (100%)	0.60	13 (9%) 8 8	87, 98, 107, 111	0
63	n7	135/135 (100%)	0.61	15 (11%) 5 5	80, 92, 102, 106	0
64	N8	148/148 (100%)	1.15	20 (13%) 3 3	38, 60, 79, 86	0
64	n8	148/148 (100%)	1.13	25 (16%) 1 1	38, 61, 75, 78	0
65	N9	58/58 (100%)	0.80	6 (10%) 6 6	41, 63, 89, 95	0
65	n9	58/58 (100%)	0.49	3 (5%) 27 25	41, 60, 82, 89	0
66	O0	97/104 (93%)	0.23	2 (2%) 63 61	85, 93, 107, 109	0
66	o0	100/104 (96%)	0.41	5 (5%) 28 26	74, 83, 101, 111	0
67	O1	109/112 (97%)	1.07	27 (24%) 0 0	62, 73, 92, 98	0
67	o1	109/112 (97%)	0.86	10 (9%) 9 10	49, 60, 84, 98	0
68	O2	127/129 (98%)	0.53	4 (3%) 49 47	39, 53, 65, 71	0
68	o2	127/129 (98%)	0.48	5 (3%) 39 36	38, 56, 69, 72	0
69	O3	106/106 (100%)	0.86	6 (5%) 23 22	44, 49, 70, 78	0
69	o3	106/106 (100%)	1.12	15 (14%) 2 2	42, 49, 70, 78	0
70	O4	112/119 (94%)	1.27	34 (30%) 0 0	61, 78, 107, 113	0
70	o4	112/119 (94%)	1.04	26 (23%) 0 1	54, 72, 102, 107	0
71	O5	119/119 (100%)	0.35	1 (0%) 86 86	58, 74, 82, 87	0
71	o5	119/119 (100%)	0.20	1 (0%) 86 86	62, 75, 89, 98	0
72	O6	99/99 (100%)	0.19	2 (2%) 65 63	64, 72, 94, 105	0
72	o6	99/99 (100%)	0.31	3 (3%) 50 48	66, 75, 87, 101	0
73	O7	87/87 (100%)	1.55	24 (27%) 0 0	46, 53, 71, 76	0
73	o7	87/87 (100%)	1.43	20 (22%) 0 1	43, 52, 76, 93	0
74	O8	77/77 (100%)	0.38	5 (6%) 18 18	86, 97, 109, 114	0
74	o8	77/77 (100%)	0.81	12 (15%) 2 2	80, 91, 101, 103	0
75	O9	50/50 (100%)	1.81	18 (36%) 0 0	55, 60, 64, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
75	o9	50/50 (100%)	1.45	15 (30%) 0 0	52, 58, 66, 67	0
76	Q0	52/52 (100%)	0.38	2 (3%) 40 37	52, 60, 76, 79	0
76	q0	52/52 (100%)	0.22	0 100 100	43, 47, 56, 59	0
77	Q1	25/25 (100%)	2.55	16 (64%) 0 0	62, 66, 73, 73	0
77	q1	25/25 (100%)	1.58	7 (28%) 0 0	53, 58, 59, 59	0
78	Q2	105/105 (100%)	0.34	3 (2%) 51 50	46, 58, 78, 103	0
78	q2	105/105 (100%)	0.65	8 (7%) 13 12	45, 56, 71, 94	0
79	Q3	91/91 (100%)	1.02	17 (18%) 1 1	56, 68, 82, 90	0
79	q3	91/91 (100%)	1.08	22 (24%) 0 0	47, 60, 76, 85	0
80	c0	96/105 (91%)	2.71	62 (64%) 0 0	104, 135, 149, 151	0
81	m2	0/150	-	-	-	-
82	p0	143/311 (45%)	0.82	18 (12%) 3 3	102, 125, 192, 199	0
83	p1	0/47	-	-	-	-
84	p2	0/46	-	-	-	-
85	f	148/157 (94%)	3.43	96 (64%) 0 0	49, 95, 145, 147	148 (100%)
All	All	33261/35493 (93%)	0.94	4903 (14%) 2 2	37, 76, 134, 213	148 (0%)

All (4903) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
53	M7	161	ALA	23.1
1	2	1699	G	20.2
60	N4	86	SER	16.1
53	M7	160	ALA	14.7
60	N4	88	ASP	13.6
18	C6	21	HIS	12.6
53	M7	162	GLU	12.5
1	2	1696	G	12.4
85	f	120	LEU	12.3
13	c1	3	THR	12.0
19	C7	2	GLY	11.9
34	sR	303	ALA	11.8
1	2	1698	G	11.6
1	2	1708	U	11.5
60	N4	89	LEU	11.5
34	sR	213	SER	11.4
4	s2	87	GLN	11.2
80	c0	22	VAL	11.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
60	N4	83	THR	10.9
1	2	1709	C	10.8
18	C6	68	ARG	10.7
1	2	1694	A	10.7
28	D6	2	PRO	10.7
60	N4	84	GLY	10.6
18	C6	20	ALA	10.5
5	s3	151	LYS	10.5
16	C4	75	GLY	10.4
1	2	715	U	10.3
85	f	30	GLY	10.2
60	N4	85	ALA	10.1
60	N4	71	ARG	10.1
1	2	1695	G	10.0
14	c2	20	ALA	9.8
7	S5	152	GLY	9.7
85	f	18	THR	9.6
13	C1	146	ALA	9.5
14	c2	122	VAL	9.4
80	c0	23	ALA	9.4
2	S0	98	ILE	9.3
13	c1	2	SER	9.3
22	d0	64	LYS	9.3
18	C6	15	SER	9.2
1	2	718	U	9.2
18	C6	9	THR	9.2
32	E0	61	SER	9.1
19	C7	62	GLN	9.1
60	N4	90	ILE	9.0
4	s2	88	LYS	9.0
60	N4	75	THR	8.9
34	sR	72	THR	8.8
23	d1	87	ARG	8.8
1	2	1697	G	8.8
14	c2	105	LYS	8.6
14	c2	103	LEU	8.6
36	1	1570	U	8.6
14	c2	102	GLY	8.6
1	2	1707	A	8.6
34	sR	158	PRO	8.5
19	C7	65	PRO	8.5
85	f	71	GLU	8.4

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Mol	Chain	Res	Type	RSRZ
60	N4	70	LYS	8.3
16	C4	74	VAL	8.3
15	C3	15	ALA	8.3
17	c5	134	THR	8.3
24	D2	111	MET	8.2
3	S1	92	GLN	8.2
32	E0	46	ASN	8.1
1	2	1702	A	8.1
14	c2	112	ALA	8.1
35	SM	170	VAL	8.1
36	5	2873	U	8.1
7	S5	151	GLY	8.1
22	d0	67	THR	8.1
34	sR	67	ILE	8.0
31	D9	56	ARG	8.0
7	s5	37	GLN	8.0
8	S6	77	LEU	8.0
34	sR	81	LEU	7.9
2	s0	46	HIS	7.9
18	C6	6	SER	7.9
85	f	46	THR	7.8
34	sR	33	LEU	7.8
34	sR	122	ILE	7.8
14	c2	36	LEU	7.8
60	N4	72	SER	7.8
14	c2	32	LEU	7.8
22	D0	82	TYR	7.8
28	D6	3	LYS	7.7
24	D2	27	ILE	7.7
34	SR	25	THR	7.7
4	s2	105	GLY	7.7
60	N4	69	LYS	7.6
53	M7	184	ALA	7.6
9	S7	108	GLN	7.6
3	s1	54	LEU	7.6
18	C6	123	ARG	7.5
80	c0	25	LYS	7.5
19	C7	99	VAL	7.5
14	c2	133	LEU	7.5
4	s2	93	GLY	7.5
35	SM	85	SER	7.5
34	sR	24	ALA	7.4

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Mol	Chain	Res	Type	RSRZ
36	5	2403	G	7.4
1	2	1710	U	7.4
1	2	1706	C	7.4
34	sR	25	THR	7.4
22	D0	86	ILE	7.4
28	D6	31	PRO	7.4
32	E0	48	THR	7.4
1	2	1711	C	7.3
34	SR	284	ALA	7.3
85	f	42	VAL	7.3
36	5	2871	G	7.2
1	2	1705	C	7.2
13	C1	147	GLY	7.2
4	s2	89	GLN	7.2
24	D2	34	ILE	7.2
24	D2	71	LYS	7.2
1	2	716	C	7.2
14	c2	21	GLU	7.1
85	f	61	ALA	7.1
60	N4	68	ALA	7.1
24	D2	65	LEU	7.1
33	e1	81	LYS	7.1
1	2	1692	G	7.1
28	D6	20	PRO	7.1
34	SR	44	SER	7.1
34	sR	301	LEU	7.1
14	c2	106	ILE	7.1
28	D6	89	ARG	7.1
34	SR	32	LEU	7.0
21	C9	71	VAL	7.0
6	S4	54	TYR	7.0
14	C2	20	ALA	7.0
85	f	63	ASP	7.0
56	N0	1	MET	7.0
18	C6	13	LYS	7.0
18	C6	22	VAL	7.0
35	sM	119	ALA	7.0
1	2	913	G	7.0
18	C6	14	LYS	7.0
1	6	662	U	7.0
28	D6	8	ASN	7.0
60	N4	87	LEU	7.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
60	N4	98	PRO	7.0
41	L4	67	THR	7.0
18	C6	118	ILE	7.0
24	D2	25	VAL	6.9
85	f	38	PRO	6.9
31	d9	4	GLU	6.9
23	D1	69	LEU	6.9
22	D0	120	SER	6.9
7	s5	152	GLY	6.9
34	SR	33	LEU	6.9
18	C6	12	LYS	6.9
1	2	714	G	6.9
34	sR	170	ILE	6.9
34	sR	314	GLN	6.9
22	D0	87	HIS	6.9
13	C1	152	GLN	6.9
18	C6	17	THR	6.8
85	f	49	THR	6.8
36	5	2442	G	6.8
14	c2	123	VAL	6.8
60	N4	82	ILE	6.8
36	1	2402	A	6.8
80	c0	65	TYR	6.8
18	C6	7	VAL	6.8
60	n4	67	VAL	6.8
21	c9	18	TYR	6.8
73	O7	2	GLY	6.8
18	C6	8	GLN	6.8
70	O4	23	VAL	6.8
14	c2	41	LEU	6.8
85	f	31	PHE	6.8
1	2	709	C	6.8
21	c9	55	TYR	6.7
34	sR	26	SER	6.7
39	L2	253	GLN	6.7
8	S6	75	LEU	6.7
36	1	2871	G	6.7
29	d7	46	VAL	6.7
36	1	1569	U	6.7
5	s3	185	LYS	6.7
85	f	20	PRO	6.7
1	2	719	U	6.6

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Mol	Chain	Res	Type	RSRZ
2	S0	97	PRO	6.6
18	C6	10	PHE	6.6
18	C6	115	THR	6.6
1	2	1693	A	6.6
85	f	72	ASP	6.6
45	L8	116	VAL	6.6
23	D1	53	TYR	6.6
1	2	1701	A	6.6
33	e1	96	LYS	6.6
85	f	83	PRO	6.6
5	s3	69	LEU	6.6
16	C4	15	GLY	6.5
33	e1	85	TYR	6.5
8	S6	73	ILE	6.5
33	e1	77	ALA	6.5
4	S2	62	PRO	6.5
8	S6	78	THR	6.5
34	sR	202	LEU	6.5
71	O5	120	ALA	6.5
30	D8	66	LEU	6.5
85	f	59	LEU	6.5
5	s3	184	ILE	6.5
85	f	57	VAL	6.5
39	L2	252	THR	6.5
7	s5	158	GLN	6.5
1	2	1690	G	6.5
4	s2	118	ALA	6.5
5	s3	138	VAL	6.5
34	SR	253	ALA	6.5
80	c0	93	TYR	6.5
9	S7	105	THR	6.4
85	f	87	ARG	6.4
28	D6	76	SER	6.4
60	N4	74	LYS	6.4
85	f	73	LEU	6.4
4	S2	88	LYS	6.4
8	S6	66	GLY	6.4
19	C7	71	PHE	6.4
22	D0	81	THR	6.4
5	S3	186	VAL	6.4
35	SM	19	VAL	6.4
60	N4	73	ARG	6.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	S1	42	ASN	6.4
85	f	58	HIS	6.4
15	c3	8	GLY	6.4
11	S9	5	PRO	6.4
3	S1	46	THR	6.3
13	C1	145	ALA	6.3
28	d6	8	ASN	6.3
34	sR	241	PHE	6.3
41	L4	69	ARG	6.3
34	sR	157	VAL	6.3
28	D6	88	SER	6.3
16	C4	16	VAL	6.3
34	sR	65	SER	6.3
28	D6	18	VAL	6.3
1	2	1700	C	6.2
11	S9	2	PRO	6.2
75	O9	2	ALA	6.2
4	s2	90	THR	6.2
13	c1	4	GLU	6.2
85	f	45	SER	6.2
8	S6	74	LYS	6.2
21	C9	108	LEU	6.2
34	sR	23	LEU	6.2
1	6	659	C	6.2
4	S2	69	ILE	6.2
33	e1	87	THR	6.2
5	s3	139	SER	6.2
33	E1	86	THR	6.2
33	E1	87	THR	6.2
33	e1	80	ARG	6.2
34	sR	92	TRP	6.2
3	S1	151	LYS	6.2
24	D2	76	SER	6.2
23	D1	55	LEU	6.1
29	d7	24	LEU	6.1
77	Q1	25	LYS	6.1
80	c0	28	ASN	6.1
85	f	70	LEU	6.1
14	c2	39	ASP	6.1
14	c2	128	ALA	6.1
36	1	2401	A	6.1
23	D1	68	SER	6.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
24	D2	69	LEU	6.1
4	s2	86	VAL	6.1
8	S6	96	SER	6.1
41	l4	67	THR	6.1
5	s3	113	LEU	6.1
1	2	1370	U	6.1
85	f	41	ILE	6.1
14	C2	141	SER	6.0
24	D2	104	LEU	6.0
85	f	121	GLY	6.0
34	sR	302	PHE	6.0
10	S8	200	LYS	6.0
28	d6	93	LYS	6.0
15	c3	16	ILE	6.0
32	e0	63	GLN	6.0
53	M7	130	TYR	6.0
1	2	506	A	6.0
29	d7	21	LEU	6.0
30	D8	16	LEU	6.0
1	2	1703	C	6.0
1	6	658	C	6.0
2	s0	151	SER	6.0
35	SM	171	PRO	6.0
24	D2	60	LYS	6.0
2	S0	174	TRP	6.0
85	f	81	GLU	6.0
5	s3	152	PHE	6.0
19	c7	41	ILE	6.0
1	2	1686	C	6.0
19	C7	63	LYS	6.0
28	d6	73	TYR	6.0
18	C6	132	LYS	6.0
34	sR	21	THR	6.0
60	n4	68	ALA	6.0
24	D2	117	ARG	6.0
24	D2	46	TYR	5.9
10	s8	200	LYS	5.9
15	c3	83	GLU	5.9
2	S0	113	ARG	5.9
45	l8	192	GLN	5.9
85	f	35	LYS	5.9
16	C4	13	VAL	5.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
28	D6	83	ILE	5.9
34	sR	61	PHE	5.9
4	s2	96	THR	5.9
18	C6	117	LEU	5.9
36	5	2402	A	5.9
4	s2	84	LYS	5.9
24	D2	72	CYS	5.9
85	f	64	ILE	5.9
7	s5	153	GLY	5.9
31	d9	29	GLY	5.9
23	D1	32	VAL	5.9
2	S0	126	PRO	5.9
28	d6	69	ASN	5.8
85	f	84	VAL	5.8
53	M7	168	LEU	5.8
2	S0	138	TYR	5.8
18	c6	19	VAL	5.8
33	e1	86	THR	5.8
29	D7	7	LEU	5.8
28	D6	92	ARG	5.8
9	S7	150	GLN	5.8
85	f	142	MET	5.8
85	f	22	GLN	5.8
17	c5	4	ALA	5.8
2	s0	101	ARG	5.8
14	c2	111	ASN	5.8
11	S9	97	LEU	5.8
54	M8	167	SER	5.8
18	C6	29	ILE	5.8
29	d7	22	LYS	5.7
2	S0	139	VAL	5.7
18	C6	11	GLY	5.7
24	D2	6	VAL	5.7
24	D2	92	ASN	5.7
5	s3	153	ALA	5.7
15	c3	9	LYS	5.7
24	D2	11	LEU	5.7
18	C6	36	ILE	5.7
41	L4	68	GLY	5.7
7	S5	71	ALA	5.7
34	sR	32	LEU	5.7
34	SR	198	ASN	5.7

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Mol	Chain	Res	Type	RSRZ
45	l8	109	LEU	5.7
34	sR	34	LEU	5.7
24	D2	39	GLN	5.7
53	M7	158	ALA	5.7
80	c0	57	THR	5.7
18	c6	124	PRO	5.7
21	C9	67	MET	5.7
31	D9	55	PHE	5.6
31	d9	5	ASN	5.6
29	d7	60	SER	5.6
19	c7	28	PHE	5.6
24	D2	59	GLY	5.6
70	o4	39	ALA	5.6
7	S5	79	ASN	5.6
2	S0	17	LEU	5.6
3	s1	89	ASP	5.6
18	c6	52	LEU	5.6
34	sR	121	MET	5.6
2	S0	23	HIS	5.6
25	D3	2	GLY	5.6
85	f	47	SER	5.6
34	SR	79	TYR	5.6
7	s5	82	PHE	5.6
31	d9	52	PHE	5.6
60	N4	76	VAL	5.6
59	N3	32	ARG	5.6
4	S2	178	ILE	5.6
34	sR	62	LYS	5.6
21	C9	114	VAL	5.6
30	d8	44	VAL	5.6
79	q3	2	ALA	5.6
80	c0	64	TYR	5.5
2	S0	74	VAL	5.5
19	C7	89	SER	5.5
85	f	17	ALA	5.5
7	S5	153	GLY	5.5
21	C9	113	ILE	5.5
85	f	76	SER	5.5
24	D2	41	MET	5.5
1	2	711	U	5.5
60	N4	67	VAL	5.5
22	D0	71	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
19	C7	74	GLN	5.5
14	C2	83	GLU	5.5
53	M7	181	ARG	5.5
18	C6	3	ALA	5.5
4	S2	63	VAL	5.5
7	S5	37	GLN	5.5
18	c6	18	ALA	5.5
32	E0	47	VAL	5.5
10	S8	152	ILE	5.5
7	s5	36	ALA	5.5
18	c6	68	ARG	5.5
24	D2	62	VAL	5.5
7	S5	36	ALA	5.5
32	E0	56	MET	5.4
18	c6	44	LEU	5.4
18	C6	121	SER	5.4
49	m3	191	ALA	5.4
36	5	2494	A	5.4
18	C6	69	VAL	5.4
2	S0	110	TYR	5.4
24	D2	14	ILE	5.4
21	C9	28	LEU	5.4
85	f	115	ALA	5.4
15	C3	14	SER	5.4
19	C7	60	ARG	5.4
24	D2	85	ASP	5.4
34	sR	212	ALA	5.4
85	f	56	LYS	5.4
34	SR	72	THR	5.4
73	O7	12	HIS	5.4
2	s0	98	ILE	5.4
2	S0	170	ILE	5.4
21	C9	27	LYS	5.4
85	f	39	CYS	5.4
28	d6	11	ASN	5.4
23	D1	73	ALA	5.4
28	d6	88	SER	5.4
34	SR	305	TYR	5.4
13	C1	74	THR	5.3
35	SM	89	ARG	5.3
34	sR	20	VAL	5.3
85	f	60	VAL	5.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	d0	98	GLN	5.3
63	n7	68	ILE	5.3
18	C6	70	THR	5.3
19	C7	18	GLU	5.3
85	f	11	ALA	5.3
36	1	2874	G	5.3
1	2	717	C	5.3
33	e1	88	PRO	5.3
34	sR	14	GLU	5.3
23	D1	62	ARG	5.3
28	D6	17	HIS	5.3
28	d6	14	GLY	5.3
34	SR	131	ILE	5.3
34	sR	115	ILE	5.3
15	C3	123	HIS	5.3
18	C6	74	HIS	5.3
85	f	37	ARG	5.3
28	D6	90	GLU	5.3
24	D2	108	ALA	5.3
36	5	2443	A	5.3
24	D2	22	LYS	5.3
8	S6	97	VAL	5.3
28	d6	71	LEU	5.3
2	S0	100	GLY	5.2
18	C6	81	ILE	5.2
85	f	43	ASP	5.2
70	O4	6	THR	5.2
29	d7	32	PHE	5.2
36	1	1568	U	5.2
1	2	1794	A	5.2
2	S0	118	PRO	5.2
18	C6	16	ALA	5.2
24	D2	110	ILE	5.2
24	D2	129	VAL	5.2
11	S9	29	LYS	5.2
85	f	86	LYS	5.2
18	c6	20	ALA	5.2
2	S0	146	LEU	5.2
82	p0	280	ALA	5.2
85	f	149	SER	5.2
13	C1	127	GLN	5.2
36	1	2873	U	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	s3	115	ILE	5.2
85	f	85	VAL	5.2
34	SR	216	LYS	5.2
5	s3	8	LYS	5.2
2	S0	203	PHE	5.2
18	c6	90	VAL	5.2
19	C7	59	LYS	5.2
34	SR	61	PHE	5.1
18	C6	32	ASN	5.1
36	5	2539	C	5.1
60	n4	87	LEU	5.1
2	S0	99	ALA	5.1
22	D0	61	LYS	5.1
5	s3	182	LEU	5.1
8	S6	149	LYS	5.1
5	s3	137	VAL	5.1
18	c6	8	GLN	5.1
29	d7	54	VAL	5.1
32	E0	54	ARG	5.1
34	sR	77	GLY	5.1
2	S0	201	LEU	5.1
73	O7	5	THR	5.1
21	C9	119	LYS	5.1
4	S2	232	GLU	5.1
18	C6	79	TYR	5.1
24	D2	74	VAL	5.1
7	s5	68	ILE	5.1
22	d0	79	TRP	5.1
28	d6	76	SER	5.1
34	sR	186	PHE	5.1
24	D2	128	PHE	5.1
21	C9	95	ASP	5.1
39	L2	201	GLY	5.1
1	2	656	G	5.0
10	S8	22	ARG	5.0
13	c1	5	LEU	5.0
26	d4	2	SER	5.0
3	S1	95	ASN	5.0
41	l4	69	ARG	5.0
24	D2	120	HIS	5.0
58	N2	27	VAL	5.0
36	1	1567	U	5.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	d0	37	VAL	5.0
9	S7	142	TYR	5.0
29	D7	3	LEU	5.0
2	S0	198	MET	5.0
4	S2	155	ALA	5.0
5	s3	150	MET	5.0
15	C3	5	HIS	5.0
85	f	23	CYS	5.0
22	D0	72	ASN	5.0
2	S0	107	PHE	5.0
22	d0	83	GLU	5.0
2	S0	72	ASP	5.0
36	5	2874	G	5.0
2	s0	170	ILE	5.0
22	d0	29	THR	5.0
34	SR	40	LYS	5.0
34	sR	104	VAL	5.0
19	C7	101	ASN	4.9
21	C9	132	LEU	4.9
45	l8	120	LYS	4.9
29	D7	38	PRO	4.9
2	S0	153	SER	4.9
36	1	2403	G	4.9
55	M9	52	LYS	4.9
31	d9	20	GLN	4.9
34	sR	138	GLY	4.9
30	D8	67	ARG	4.9
23	D1	56	SER	4.9
10	S8	179	CYS	4.9
2	S0	122	ILE	4.9
8	S6	175	ILE	4.9
23	D1	34	ILE	4.9
2	s0	165	ARG	4.9
18	C6	40	GLU	4.9
55	M9	51	VAL	4.9
35	SM	151	ALA	4.9
43	l6	129	GLU	4.9
80	c0	24	LYS	4.9
11	S9	96	VAL	4.9
18	C6	142	TYR	4.9
19	C7	21	TYR	4.9
53	M7	179	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
6	S4	111	VAL	4.9
34	SR	115	ILE	4.9
70	O4	32	ALA	4.9
24	D2	81	VAL	4.9
22	d0	87	HIS	4.9
21	C9	90	PRO	4.9
8	S6	71	THR	4.9
7	S5	78	ALA	4.9
16	c4	28	VAL	4.8
19	c7	57	LEU	4.8
85	f	148	ILE	4.8
28	d6	9	GLY	4.8
18	C6	19	VAL	4.8
34	sR	113	VAL	4.8
5	s3	98	ALA	4.8
18	C6	143	ARG	4.8
32	E0	6	GLY	4.8
2	S0	188	LEU	4.8
2	s0	48	ILE	4.8
2	S0	137	SER	4.8
32	E0	45	VAL	4.8
5	s3	114	ALA	4.8
36	1	2404	A	4.8
18	C6	39	VAL	4.8
28	D6	73	TYR	4.8
18	C6	65	ILE	4.8
27	d5	89	ILE	4.8
28	D6	9	GLY	4.8
8	S6	153	VAL	4.8
14	c2	126	TRP	4.8
16	c4	92	LYS	4.8
34	sR	89	LEU	4.8
24	D2	37	PHE	4.8
28	d6	30	ILE	4.8
5	s3	202	LEU	4.8
9	s7	43	PHE	4.8
4	s2	95	ARG	4.8
34	sR	82	SER	4.8
85	f	33	VAL	4.8
1	2	134	U	4.8
14	c2	31	VAL	4.8
18	c6	28	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
34	sR	309	VAL	4.8
85	f	134	LEU	4.8
18	c6	49	TYR	4.8
1	2	793	A	4.8
24	D2	10	ALA	4.8
12	C0	93	GLN	4.8
85	f	153	ALA	4.8
32	E0	44	PHE	4.7
22	d0	30	LYS	4.7
51	M5	60	VAL	4.7
85	f	157	ASP	4.7
25	D3	7	ARG	4.7
19	C7	25	THR	4.7
29	d7	47	PHE	4.7
39	L2	224	THR	4.7
5	S3	161	GLY	4.7
6	S4	44	LEU	4.7
2	S0	156	VAL	4.7
4	s2	85	PRO	4.7
10	s8	95	THR	4.7
23	D1	10	GLU	4.7
2	S0	18	LEU	4.7
24	D2	121	VAL	4.7
28	d6	21	VAL	4.7
34	sR	116	ASP	4.7
24	d2	61	ILE	4.7
33	e1	89	LYS	4.7
34	sR	252	LEU	4.7
19	C7	57	LEU	4.7
28	D6	78	ALA	4.7
2	S0	161	PRO	4.7
2	S0	22	THR	4.7
18	c6	38	LEU	4.7
36	1	1572	U	4.7
32	e0	49	LEU	4.7
13	c1	139	VAL	4.7
36	1	2872	A	4.7
61	N5	124	VAL	4.7
19	c7	42	GLN	4.7
70	o4	38	LEU	4.7
2	S0	158	VAL	4.7
16	c4	91	THR	4.7

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Mol	Chain	Res	Type	RSRZ
8	S6	148	SER	4.7
25	d3	2	GLY	4.7
28	D6	29	SER	4.7
29	D7	19	HIS	4.7
4	s2	119	LYS	4.7
10	S8	8	ARG	4.7
11	s9	148	VAL	4.7
13	c1	117	VAL	4.7
5	S3	187	LYS	4.6
6	S4	38	LEU	4.6
19	C7	64	GLY	4.6
9	S7	104	ARG	4.6
75	O9	46	ARG	4.6
19	c7	4	VAL	4.6
11	S9	186	GLU	4.6
24	D2	124	LYS	4.6
34	SR	36	ALA	4.6
36	1	1564	U	4.6
3	S1	91	VAL	4.6
18	c6	55	VAL	4.6
58	N2	28	PHE	4.6
15	C3	121	ARG	4.6
2	S0	177	LEU	4.6
4	s2	117	THR	4.6
22	D0	70	THR	4.6
32	E0	60	PRO	4.6
34	sR	123	ILE	4.6
56	N0	2	ALA	4.6
14	C2	32	LEU	4.6
18	c6	83	GLN	4.6
18	C6	114	ARG	4.6
22	D0	64	LYS	4.6
5	S3	150	MET	4.6
85	f	44	MET	4.6
4	S2	157	LYS	4.6
34	SR	78	ALA	4.6
4	S2	66	PHE	4.6
13	C1	136	ARG	4.6
75	O9	45	ARG	4.6
31	d9	27	HIS	4.6
2	S0	30	GLN	4.6
82	p0	69	ASP	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	d0	77	LYS	4.6
33	e1	83	LYS	4.6
64	N8	108	GLY	4.6
2	s0	152	PRO	4.6
18	C6	90	VAL	4.6
24	D2	15	ASN	4.6
18	c6	29	ILE	4.6
2	s0	162	CYS	4.6
85	f	78	HIS	4.6
23	D1	23	ILE	4.5
24	D2	73	GLY	4.5
39	l2	194	ASN	4.5
74	o8	2	ALA	4.5
5	s3	186	VAL	4.5
60	N4	78	ALA	4.5
28	D6	77	CYS	4.5
4	S2	144	TRP	4.5
10	S8	62	THR	4.5
18	c6	51	PRO	4.5
39	L2	216	HIS	4.5
18	C6	120	ASP	4.5
21	C9	124	ILE	4.5
75	o9	51	ILE	4.5
34	sR	124	SER	4.5
34	SR	313	TRP	4.5
80	c0	68	LEU	4.5
18	C6	64	ASP	4.5
34	sR	45	TRP	4.5
80	c0	62	GLN	4.5
77	Q1	15	ARG	4.5
85	f	27	ARG	4.5
70	O4	64	THR	4.5
11	S9	101	VAL	4.5
18	c6	121	SER	4.5
8	S6	67	VAL	4.5
8	s6	162	VAL	4.5
34	SR	214	ALA	4.5
25	d3	11	SER	4.5
15	C3	53	LEU	4.5
28	D6	85	ARG	4.5
85	f	74	SER	4.5
19	c7	104	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
24	D2	51	GLU	4.5
3	s1	153	HIS	4.5
18	c6	54	LEU	4.5
18	c6	94	GLN	4.5
24	D2	103	ILE	4.5
2	S0	32	HIS	4.5
18	C6	126	PRO	4.5
74	o8	54	LEU	4.5
80	c0	94	ILE	4.5
2	S0	106	SER	4.5
13	c1	116	ARG	4.5
1	2	1096	C	4.5
30	d8	9	LEU	4.5
80	c0	79	TYR	4.5
3	S1	32	ILE	4.5
39	l2	18	SER	4.5
41	l4	62	ALA	4.5
53	M7	183	ALA	4.5
19	C7	53	TYR	4.5
30	d8	17	GLY	4.4
12	C0	91	TYR	4.4
33	e1	84	VAL	4.4
36	1	1762	C	4.4
63	N7	26	VAL	4.4
24	D2	70	ASN	4.4
75	O9	51	ILE	4.4
7	S5	70	VAL	4.4
34	SR	20	VAL	4.4
5	s3	148	LYS	4.4
35	SM	141	ALA	4.4
75	O9	47	THR	4.4
14	c2	43	ARG	4.4
24	D2	61	ILE	4.4
28	d6	2	PRO	4.4
18	C6	67	VAL	4.4
26	d4	99	LYS	4.4
28	D6	19	LYS	4.4
59	N3	137	VAL	4.4
34	SR	92	TRP	4.4
60	N4	66	GLU	4.4
28	D6	80	HIS	4.4
39	l2	60	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
2	S0	101	ARG	4.4
36	5	2441	A	4.4
61	n5	23	ALA	4.4
2	S0	105	GLY	4.4
24	D2	21	GLY	4.4
7	s5	42	LEU	4.4
2	s0	164	ASN	4.4
5	S3	152	PHE	4.4
7	s5	154	ALA	4.4
18	C6	119	ALA	4.4
80	c0	21	VAL	4.4
5	s3	167	PHE	4.4
21	C9	110	LYS	4.4
30	d8	21	SER	4.4
1	2	696	C	4.4
19	C7	50	ILE	4.4
2	S0	157	ASP	4.4
5	S3	218	LEU	4.4
14	c2	59	LEU	4.4
15	c3	125	LEU	4.4
28	D6	86	VAL	4.4
18	C6	92	TYR	4.4
8	s6	147	LEU	4.4
24	D2	126	LEU	4.4
31	d9	30	LEU	4.4
1	6	678	A	4.4
7	s5	44	ASN	4.4
8	S6	81	VAL	4.4
13	C1	91	LEU	4.4
19	C7	14	LYS	4.4
28	D6	84	VAL	4.4
34	SR	34	LEU	4.4
4	s2	92	ALA	4.4
19	c7	65	PRO	4.4
1	6	1695	G	4.3
14	c2	65	SER	4.3
18	C6	136	SER	4.3
1	2	1796	C	4.3
35	sM	83	LYS	4.3
80	c0	44	LYS	4.3
34	SR	108	SER	4.3
31	d9	55	PHE	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
35	SM	86	ASN	4.3
85	f	65	PHE	4.3
1	6	1199	G	4.3
1	6	1082	C	4.3
22	D0	62	VAL	4.3
34	SR	94	VAL	4.3
13	C1	4	GLU	4.3
34	sR	36	ALA	4.3
13	C1	64	VAL	4.3
19	c7	67	ARG	4.3
15	c3	40	TYR	4.3
39	L2	195	SER	4.3
6	S4	45	ILE	4.3
85	f	50	GLY	4.3
21	C9	38	LYS	4.3
31	D9	54	LYS	4.3
85	f	119	GLU	4.3
24	D2	35	ILE	4.3
25	D3	18	HIS	4.3
5	S3	208	ILE	4.3
18	C6	57	LEU	4.3
14	c2	121	VAL	4.3
34	sR	294	TRP	4.3
48	M1	104	PHE	4.3
1	2	1795	U	4.3
1	6	1799	U	4.3
22	D0	54	GLY	4.3
28	d6	18	VAL	4.3
28	d6	35	ALA	4.3
60	n4	95	SER	4.3
7	S5	61	TYR	4.3
34	SR	150	TRP	4.3
67	O1	27	LYS	4.3
11	S9	32	GLY	4.3
31	d9	36	LEU	4.3
19	c7	3	ARG	4.3
24	D2	50	PHE	4.3
34	SR	278	PHE	4.3
21	C9	80	TYR	4.3
80	c0	29	GLN	4.3
2	s0	17	LEU	4.3
34	SR	66	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
82	p0	70	LEU	4.3
25	D3	4	GLY	4.3
85	f	135	MET	4.3
1	2	1410	A	4.2
4	S2	87	GLN	4.2
5	S3	21	LEU	4.2
2	S0	47	VAL	4.2
2	S0	111	ILE	4.2
4	S2	224	PHE	4.2
18	C6	129	PHE	4.2
28	d6	13	LYS	4.2
36	5	1569	U	4.2
35	SM	88	ARG	4.2
10	S8	102	VAL	4.2
22	D0	84	MET	4.2
58	N2	33	TYR	4.2
36	5	1568	U	4.2
2	S0	199	PRO	4.2
18	c6	11	GLY	4.2
6	S4	110	ALA	4.2
14	c2	42	ALA	4.2
80	c0	3	MET	4.2
1	2	710	U	4.2
18	C6	63	ILE	4.2
31	D9	52	PHE	4.2
24	D2	68	ARG	4.2
85	f	55	ALA	4.2
34	sR	87	LYS	4.2
70	o4	21	LYS	4.2
2	S0	83	GLN	4.2
24	D2	3	ARG	4.2
28	d6	89	ARG	4.2
80	c0	74	GLU	4.2
5	S3	96	LEU	4.2
34	SR	81	LEU	4.2
1	6	1694	A	4.2
13	C1	137	PHE	4.2
7	s5	30	PRO	4.2
14	c2	107	ASP	4.2
24	d2	126	LEU	4.2
30	d8	66	LEU	4.2
59	n3	2	SER	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
60	N4	97	LYS	4.2
4	s2	162	CYS	4.2
85	f	66	THR	4.2
34	SR	291	SER	4.2
2	s0	150	ASP	4.2
31	d9	16	LYS	4.2
12	C0	66	TYR	4.2
30	d8	65	ARG	4.2
53	M7	157	VAL	4.2
60	n4	69	LYS	4.2
73	O7	29	VAL	4.2
18	c6	12	LYS	4.2
18	c6	39	VAL	4.2
78	Q2	106	PHE	4.2
5	s3	38	GLU	4.2
67	o1	82	GLU	4.2
7	S5	76	ARG	4.2
14	c2	22	VAL	4.2
2	S0	196	SER	4.2
28	d6	36	ILE	4.2
24	D2	24	GLN	4.1
6	S4	66	MET	4.1
34	SR	42	LEU	4.1
65	N9	2	ALA	4.1
59	N3	4	ASN	4.1
79	q3	3	LYS	4.1
13	C1	90	TYR	4.1
33	E1	147	VAL	4.1
80	c0	20	VAL	4.1
28	d6	10	ARG	4.1
10	s8	199	LYS	4.1
75	o9	11	GLN	4.1
80	c0	5	LYS	4.1
34	SR	7	LEU	4.1
9	S7	109	VAL	4.1
1	2	723	G	4.1
5	S3	184	ILE	4.1
64	n8	124	ILE	4.1
49	M3	140	SER	4.1
70	O4	5	VAL	4.1
1	6	506	A	4.1
33	e1	79	LYS	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
53	M7	176	ILE	4.1
21	C9	39	THR	4.1
7	S5	154	ALA	4.1
25	d3	15	LEU	4.1
34	sR	42	LEU	4.1
39	L2	223	SER	4.1
18	c6	69	VAL	4.1
58	N2	92	TRP	4.1
58	n2	70	LYS	4.1
39	l2	250	GLN	4.1
32	E0	55	ARG	4.1
34	SR	99	THR	4.1
2	s0	116	LYS	4.1
11	S9	20	GLU	4.1
2	S0	123	VAL	4.1
2	S0	175	TYR	4.1
68	O2	51	SER	4.1
80	c0	66	TYR	4.1
85	f	26	LEU	4.1
2	s0	134	LYS	4.1
4	s2	64	LYS	4.1
26	D4	25	VAL	4.1
34	sR	140	CYS	4.1
70	O4	35	VAL	4.1
23	D1	58	TYR	4.1
34	sR	171	SER	4.1
34	sR	272	ASP	4.1
39	l2	208	ASP	4.1
16	c4	129	LYS	4.1
14	c2	110	GLY	4.1
60	N4	65	GLU	4.1
10	S8	168	CYS	4.1
4	S2	113	LEU	4.1
7	S5	96	SER	4.1
19	C7	7	LYS	4.1
29	d7	17	ARG	4.1
24	D2	55	ASP	4.1
34	SR	62	LYS	4.1
39	l2	251	LYS	4.1
4	s2	82	ASN	4.1
22	d0	100	VAL	4.1
1	6	663	U	4.1

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Mol	Chain	Res	Type	RSRZ
6	S4	8	HIS	4.1
19	C7	38	ILE	4.1
48	M1	167	TYR	4.1
22	D0	53	LYS	4.1
70	O4	21	LYS	4.1
14	c2	56	GLU	4.1
34	SR	262	VAL	4.1
8	S6	95	LYS	4.1
19	C7	46	LEU	4.1
34	SR	199	ILE	4.1
18	c6	143	ARG	4.1
24	D2	18	GLU	4.1
34	sR	27	ALA	4.1
6	S4	65	LEU	4.1
47	m0	103	LEU	4.1
24	d2	20	THR	4.0
14	c2	104	GLY	4.0
18	c6	141	SER	4.0
34	sR	244	ALA	4.0
53	M7	136	ILE	4.0
79	Q3	24	ARG	4.0
18	C6	77	GLN	4.0
34	SR	43	ILE	4.0
39	l2	5	ILE	4.0
14	c2	33	ARG	4.0
31	d9	40	ARG	4.0
29	d7	55	THR	4.0
34	sR	257	ALA	4.0
36	5	2404	A	4.0
34	sR	166	SER	4.0
64	N8	73	LEU	4.0
11	S9	104	PHE	4.0
25	D3	24	TRP	4.0
27	d5	50	ILE	4.0
61	n5	113	LEU	4.0
85	f	90	TYR	4.0
66	o0	6	SER	4.0
80	c0	98	ASN	4.0
47	m0	221	ALA	4.0
5	S3	188	ILE	4.0
32	E0	49	LEU	4.0
85	f	68	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
2	S0	152	PRO	4.0
16	C4	92	LYS	4.0
39	l2	16	PHE	4.0
5	S3	206	VAL	4.0
7	S5	41	LYS	4.0
18	c6	119	ALA	4.0
34	sR	83	ALA	4.0
34	sR	243	LEU	4.0
5	S3	166	ASP	4.0
60	n4	27	LYS	4.0
17	c5	103	ASN	4.0
31	d9	56	ARG	4.0
58	n2	13	LYS	4.0
24	d2	55	ASP	4.0
5	S3	183	GLY	4.0
22	d0	63	LEU	4.0
26	D4	125	LEU	4.0
34	sR	112	SER	4.0
13	C1	122	ILE	4.0
36	5	2444	C	4.0
18	C6	66	ARG	4.0
34	sR	167	VAL	4.0
85	f	136	VAL	4.0
4	S2	156	THR	4.0
34	SR	41	THR	4.0
2	S0	102	PHE	4.0
24	D2	5	SER	4.0
39	L2	189	TYR	4.0
10	S8	20	GLN	4.0
2	S0	26	ALA	4.0
8	S6	154	ARG	4.0
9	s7	11	GLN	3.9
1	2	1777	G	3.9
2	S0	85	ALA	3.9
5	S3	25	PHE	3.9
15	c3	56	ASP	3.9
1	2	1151	A	3.9
11	S9	87	SER	3.9
24	D2	101	TYR	3.9
34	SR	65	SER	3.9
1	2	742	U	3.9
2	S0	149	LEU	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	s8	179	CYS	3.9
80	c0	55	VAL	3.9
7	s5	129	PRO	3.9
15	C3	122	ILE	3.9
85	f	77	THR	3.9
4	s2	161	LYS	3.9
7	s5	150	GLY	3.9
8	s6	160	ARG	3.9
28	D6	5	ARG	3.9
39	L2	250	GLN	3.9
77	Q1	14	LYS	3.9
2	S0	104	PRO	3.9
34	SR	85	TRP	3.9
24	D2	53	ILE	3.9
13	C1	93	TYR	3.9
25	D3	29	TYR	3.9
29	d7	18	LYS	3.9
34	sR	201	THR	3.9
39	L2	198	LYS	3.9
53	M7	163	LYS	3.9
11	S9	28	LEU	3.9
24	D2	58	SER	3.9
39	l2	253	GLN	3.9
73	o7	23	GLY	3.9
34	sR	134	TRP	3.9
32	e0	51	ASN	3.9
21	c9	9	VAL	3.9
70	O4	34	HIS	3.9
10	S8	58	LEU	3.9
10	s8	36	THR	3.9
34	sR	41	THR	3.9
7	S5	74	ALA	3.9
34	sR	30	PRO	3.9
2	s0	27	ARG	3.9
3	S1	140	ILE	3.9
13	C1	148	LYS	3.9
14	C2	136	ILE	3.9
34	SR	283	LYS	3.9
59	N3	2	SER	3.9
1	2	1338	C	3.9
75	o9	2	ALA	3.9
85	f	25	ALA	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	s2	203	LYS	3.9
36	1	2397	A	3.9
2	s0	145	ALA	3.9
14	C2	82	PRO	3.9
18	C6	41	PRO	3.9
18	c6	142	TYR	3.9
29	D7	2	VAL	3.9
5	S3	148	LYS	3.9
85	f	28	LYS	3.9
22	D0	85	ARG	3.9
5	s3	11	LEU	3.9
19	c7	24	LEU	3.9
21	C9	37	VAL	3.9
25	D3	34	LEU	3.9
46	l9	191	LEU	3.9
33	e1	78	LYS	3.9
2	S0	131	GLN	3.9
34	sR	139	GLN	3.9
59	N3	33	ASN	3.9
36	1	2205	U	3.9
5	s3	83	THR	3.9
28	D6	35	ALA	3.9
59	N3	52	ALA	3.9
11	s9	184	SER	3.9
1	2	195	G	3.9
9	S7	147	ASN	3.9
19	c7	69	ILE	3.9
22	D0	65	ILE	3.9
18	c6	130	GLY	3.9
33	E1	85	TYR	3.9
34	sR	310	ILE	3.9
43	l6	130	ILE	3.9
39	l2	234	LYS	3.9
4	s2	97	ARG	3.8
13	C1	117	VAL	3.8
55	M9	181	ARG	3.8
66	o0	23	TYR	3.8
34	sR	85	TRP	3.8
80	c0	60	SER	3.8
3	S1	49	ASN	3.8
5	s3	193	ALA	3.8
13	c1	115	PHE	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
18	C6	128	LYS	3.8
51	M5	198	SER	3.8
55	M9	72	GLU	3.8
60	N4	81	PRO	3.8
58	N2	93	ILE	3.8
85	f	138	ILE	3.8
39	l2	19	HIS	3.8
70	O4	2	ALA	3.8
25	d3	10	ASN	3.8
1	6	1800	A	3.8
28	d6	34	LYS	3.8
35	SM	152	LYS	3.8
36	5	2401	A	3.8
9	S7	91	ILE	3.8
15	C3	16	ILE	3.8
16	c4	22	SER	3.8
85	f	16	SER	3.8
3	S1	20	VAL	3.8
67	O1	33	VAL	3.8
9	S7	123	ASP	3.8
24	d2	27	ILE	3.8
1	2	1704	U	3.8
1	6	1340	U	3.8
21	c9	22	LEU	3.8
24	D2	93	LEU	3.8
11	S9	31	ALA	3.8
4	S2	64	LYS	3.8
18	C6	87	LYS	3.8
39	L2	99	GLY	3.8
24	D2	23	ARG	3.8
64	n8	120	ASN	3.8
9	S7	98	ILE	3.8
13	c1	142	VAL	3.8
16	c4	110	LEU	3.8
19	C7	58	MET	3.8
5	s3	183	GLY	3.8
16	c4	27	PHE	3.8
28	d6	68	TYR	3.8
39	l2	72	ARG	3.8
41	l4	66	GLY	3.8
85	f	52	HIS	3.8
6	S4	26	CYS	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	S6	64	LYS	3.8
34	sR	313	TRP	3.8
35	SM	175	VAL	3.8
85	f	32	VAL	3.8
18	c6	21	HIS	3.8
25	d3	18	HIS	3.8
36	5	1025	A	3.8
7	s5	145	ASP	3.8
18	C6	44	LEU	3.8
5	S3	143	ARG	3.8
35	sM	85	SER	3.8
2	s0	173	ILE	3.8
12	C0	92	ILE	3.8
2	s0	33	GLN	3.8
13	C1	153	PHE	3.8
18	c6	10	PHE	3.8
22	d0	84	MET	3.8
19	c7	2	GLY	3.8
10	s8	58	LEU	3.8
22	d0	97	VAL	3.8
28	D6	33	ASP	3.8
25	D3	28	ASN	3.8
36	5	2447	A	3.8
75	O9	49	MET	3.8
8	S6	80	ASN	3.8
22	d0	54	GLY	3.8
24	D2	13	ALA	3.8
2	s0	34	GLU	3.8
80	c0	78	GLU	3.8
34	SR	310	ILE	3.8
34	sR	73	LEU	3.8
72	o6	58	ILE	3.8
65	n9	23	LYS	3.8
1	6	1696	G	3.8
2	S0	135	GLU	3.8
1	6	1707	A	3.8
18	c6	114	ARG	3.8
2	S0	124	THR	3.8
4	s2	166	THR	3.8
22	d0	62	VAL	3.8
28	D6	21	VAL	3.8
14	c2	40	GLY	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	S0	195	TRP	3.7
4	s2	91	ARG	3.7
4	S2	41	LEU	3.7
22	d0	65	ILE	3.7
55	M9	24	LEU	3.7
5	s3	175	VAL	3.7
7	s5	133	VAL	3.7
8	S6	79	LYS	3.7
10	S8	44	HIS	3.7
18	c6	138	PHE	3.7
21	c9	93	HIS	3.7
22	d0	81	THR	3.7
2	s0	166	GLY	3.7
45	l8	113	ALA	3.7
23	D1	51	VAL	3.7
5	s3	9	ARG	3.7
34	sR	88	THR	3.7
21	C9	70	GLN	3.7
7	s5	58	LEU	3.7
8	s6	169	TYR	3.7
35	SM	99	LYS	3.7
45	L8	93	LEU	3.7
67	O1	67	VAL	3.7
9	s7	184	GLU	3.7
5	s3	160	SER	3.7
85	f	15	SER	3.7
7	s5	130	ILE	3.7
24	D2	75	ILE	3.7
34	sR	183	LEU	3.7
36	1	2139	A	3.7
2	S0	162	CYS	3.7
3	S1	110	LEU	3.7
16	C4	76	ILE	3.7
24	d2	86	ILE	3.7
26	D4	7	ILE	3.7
5	s3	48	VAL	3.7
24	D2	28	ARG	3.7
31	d9	12	ARG	3.7
34	SR	290	VAL	3.7
1	2	1107	G	3.7
21	C9	92	LYS	3.7
5	s3	208	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
25	D3	20	ARG	3.7
53	M7	135	ARG	3.7
70	O4	16	ARG	3.7
80	c0	48	SER	3.7
7	S5	149	VAL	3.7
4	s2	209	ASN	3.7
5	S3	142	LEU	3.7
13	C1	149	ALA	3.7
15	c3	53	LEU	3.7
3	S1	52	THR	3.7
34	sR	79	TYR	3.7
3	S1	114	VAL	3.7
35	SM	18	VAL	3.7
34	SR	45	TRP	3.7
5	s3	176	LEU	3.7
6	s4	23	LEU	3.7
35	sM	121	ALA	3.7
45	L8	191	ASN	3.7
45	L8	218	ILE	3.7
10	S8	53	LYS	3.7
21	C9	6	VAL	3.7
24	D2	102	VAL	3.7
34	sR	35	SER	3.7
6	S4	143	ASP	3.7
16	c4	53	ASP	3.7
21	C9	123	ARG	3.7
14	C2	41	LEU	3.7
8	s6	131	LYS	3.7
21	C9	18	TYR	3.7
30	d8	32	PHE	3.7
1	2	1399	C	3.7
28	D6	82	ARG	3.7
34	sR	292	LEU	3.7
14	c2	27	ALA	3.7
22	d0	88	LYS	3.7
24	D2	125	ILE	3.7
34	SR	188	ILE	3.7
21	C9	104	VAL	3.7
23	D1	87	ARG	3.7
34	SR	35	SER	3.7
53	M7	169	THR	3.7
6	S4	6	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
36	5	2540	A	3.7
31	d9	23	VAL	3.7
19	C7	83	GLN	3.7
21	C9	129	GLN	3.7
64	n8	104	THR	3.6
18	c6	60	PHE	3.6
15	C3	128	TYR	3.6
4	s2	211	LEU	3.6
5	s3	65	ARG	3.6
17	c5	135	THR	3.6
19	c7	60	ARG	3.6
34	SR	306	THR	3.6
82	p0	192	ASP	3.6
85	f	82	VAL	3.6
5	S3	157	LEU	3.6
13	C1	40	LEU	3.6
55	M9	44	LEU	3.6
5	s3	173	ARG	3.6
13	c1	145	ALA	3.6
18	c6	91	ALA	3.6
31	D9	38	ILE	3.6
11	S9	39	LYS	3.6
25	D3	30	LYS	3.6
26	D4	2	SER	3.6
28	D6	28	LYS	3.6
2	s0	146	LEU	3.6
29	d7	49	HIS	3.6
45	l8	65	LEU	3.6
53	M7	172	GLN	3.6
5	s3	134	CYS	3.6
11	s9	149	ARG	3.6
6	S4	47	PHE	3.6
7	S5	104	ASN	3.6
12	C0	39	ASN	3.6
2	S0	48	ILE	3.6
19	c7	8	THR	3.6
34	SR	55	GLY	3.6
5	s3	72	LEU	3.6
29	D7	26	GLN	3.6
41	L4	73	ARG	3.6
6	S4	15	PRO	3.6
11	S9	144	PRO	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
13	C1	88	ARG	3.6
5	s3	179	GLN	3.6
14	c2	26	ASP	3.6
24	D2	2	THR	3.6
29	d7	33	LEU	3.6
49	M3	34	SER	3.6
15	C3	9	LYS	3.6
18	c6	118	ILE	3.6
51	m5	111	ALA	3.6
23	D1	21	ASN	3.6
5	S3	90	ARG	3.6
19	C7	78	ARG	3.6
2	S0	114	SER	3.6
18	C6	141	SER	3.6
41	l4	103	THR	3.6
2	s0	123	VAL	3.6
63	N7	90	GLU	3.6
8	S6	76	LEU	3.6
18	C6	116	LEU	3.6
41	l4	65	TRP	3.6
59	N3	25	CYS	3.6
8	S6	180	THR	3.6
21	C9	139	THR	3.6
1	2	1077	C	3.6
29	d7	81	ARG	3.6
41	l4	73	ARG	3.6
10	S8	96	LEU	3.6
18	C6	133	GLY	3.6
24	D2	130	TYR	3.6
17	C5	104	GLN	3.6
5	s3	191	ASP	3.6
28	d6	90	GLU	3.6
39	l2	15	ILE	3.6
43	L6	130	ILE	3.6
85	f	139	ILE	3.6
10	S8	23	LYS	3.6
73	O7	88	ALA	3.6
2	S0	171	GLY	3.6
22	d0	82	TYR	3.6
34	sR	263	PHE	3.6
51	m5	76	PRO	3.6
34	sR	52	GLN	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	D0	119	ALA	3.6
24	d2	21	GLY	3.6
80	c0	76	LEU	3.6
1	2	1379	C	3.6
1	2	1691	A	3.6
41	L4	65	TRP	3.6
2	s0	49	ASN	3.6
22	D0	83	GLU	3.6
35	SM	84	LYS	3.6
61	n5	114	VAL	3.6
85	f	51	LYS	3.6
5	S3	201	ALA	3.6
6	S4	55	ALA	3.6
15	c3	5	HIS	3.6
22	d0	78	THR	3.6
32	e0	2	ALA	3.6
41	L4	105	THR	3.6
41	l4	79	GLY	3.6
42	L5	146	LEU	3.6
1	2	1340	U	3.5
5	s3	7	LYS	3.5
24	D2	119	LYS	3.5
10	S8	60	ILE	3.5
32	e0	62	VAL	3.5
34	SR	89	LEU	3.5
34	SR	201	THR	3.5
34	sR	13	LEU	3.5
39	L2	246	LEU	3.5
63	N7	2	ALA	3.5
5	S3	185	LYS	3.5
5	s3	164	VAL	3.5
6	s4	207	LEU	3.5
24	D2	12	ASN	3.5
24	D2	26	LEU	3.5
51	M5	197	LEU	3.5
1	2	1371	A	3.5
36	5	1580	A	3.5
60	n4	94	ARG	3.5
13	C1	3	THR	3.5
19	C7	28	PHE	3.5
34	sR	203	THR	3.5
48	M1	127	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
80	c0	54	TYR	3.5
24	D2	122	SER	3.5
7	s5	137	ILE	3.5
39	l2	196	TRP	3.5
2	S0	182	LEU	3.5
4	s2	113	LEU	3.5
5	s3	171	ALA	3.5
28	d6	15	ARG	3.5
13	c1	90	TYR	3.5
74	o8	33	LYS	3.5
39	l2	186	PHE	3.5
1	2	1337	A	3.5
22	d0	28	SER	3.5
2	S0	76	ILE	3.5
3	s1	111	ARG	3.5
29	D7	51	GLN	3.5
30	D8	45	LYS	3.5
63	N7	42	LEU	3.5
31	d9	43	PHE	3.5
55	M9	78	TYR	3.5
2	s0	129	ASP	3.5
34	sR	64	HIS	3.5
4	s2	165	VAL	3.5
41	l4	71	VAL	3.5
85	f	34	ILE	3.5
19	C7	26	LEU	3.5
21	c9	28	LEU	3.5
28	d6	20	PRO	3.5
34	sR	7	LEU	3.5
42	L5	51	LEU	3.5
8	S6	54	GLY	3.5
15	c3	15	ALA	3.5
34	sR	214	ALA	3.5
55	m9	83	GLY	3.5
13	C1	156	PHE	3.5
2	S0	49	ASN	3.5
28	d6	86	VAL	3.5
30	D8	41	VAL	3.5
22	D0	60	THR	3.5
33	e1	90	LYS	3.5
39	l2	13	GLY	3.5
4	S2	169	LEU	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	S3	169	ASP	3.5
21	C9	60	SER	3.5
24	d2	2	THR	3.5
51	M5	134	LEU	3.5
51	M5	196	THR	3.5
34	sR	254	ALA	3.5
21	C9	7	ARG	3.5
1	2	315	A	3.5
63	n7	75	VAL	3.5
5	s3	142	LEU	3.5
36	1	2954	U	3.5
49	m3	6	ASN	3.5
55	m9	184	LEU	3.5
16	c4	55	SER	3.5
18	c6	115	THR	3.5
21	C9	72	GLY	3.5
74	O8	43	PHE	3.5
80	c0	58	GLN	3.5
31	d9	14	TYR	3.5
70	o4	37	LYS	3.5
75	O9	48	LYS	3.5
4	S2	45	VAL	3.5
1	2	1766	A	3.5
25	D3	22	ASN	3.5
72	O6	100	HIS	3.5
14	C2	26	ASP	3.5
39	L2	208	ASP	3.5
9	s7	187	SER	3.5
14	c2	92	ALA	3.5
25	d3	6	PRO	3.5
40	l3	242	THR	3.5
55	m9	178	ALA	3.5
13	c1	97	TYR	3.5
70	O4	30	LEU	3.5
70	o4	57	LEU	3.5
3	S1	53	GLY	3.5
5	S3	190	ARG	3.5
16	C4	18	ARG	3.5
5	s3	10	LYS	3.5
8	S6	99	GLY	3.5
10	S8	151	LYS	3.5
34	sR	54	PHE	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2	713	A	3.5
2	S0	20	ALA	3.5
49	M3	7	LEU	3.5
61	N5	82	LEU	3.5
4	S2	57	PHE	3.5
19	C7	44	LYS	3.5
28	d6	70	LYS	3.5
32	E0	53	LYS	3.5
34	sR	161	LYS	3.5
2	s0	99	ALA	3.5
26	D4	31	ASN	3.4
34	SR	174	ASN	3.4
35	SM	137	GLU	3.4
8	S6	84	TYR	3.4
6	S4	102	VAL	3.4
18	C6	75	VAL	3.4
17	c5	8	LYS	3.4
18	c6	132	LYS	3.4
22	d0	58	LEU	3.4
24	d2	22	LYS	3.4
36	1	1605	A	3.4
36	1	2502	A	3.4
49	M3	26	PHE	3.4
15	C3	57	ALA	3.4
29	d7	50	ALA	3.4
82	p0	296	ALA	3.4
85	f	54	HIS	3.4
12	C0	64	TYR	3.4
1	6	1700	C	3.4
5	S3	54	ARG	3.4
5	S3	122	VAL	3.4
34	sR	200	ASN	3.4
2	s0	177	LEU	3.4
6	S4	159	THR	3.4
19	C7	69	ILE	3.4
23	D1	20	THR	3.4
23	D1	24	ILE	3.4
80	c0	43	ILE	3.4
2	s0	100	GLY	3.4
3	S1	233	GLY	3.4
20	c8	142	GLY	3.4
24	D2	17	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
28	D6	6	ALA	3.4
5	s3	101	GLN	3.4
18	c6	82	ARG	3.4
29	d7	51	GLN	3.4
60	n4	70	LYS	3.4
14	C2	28	LEU	3.4
34	SR	26	SER	3.4
80	c0	67	THR	3.4
85	f	24	SER	3.4
21	C9	57	ARG	3.4
7	s5	86	GLN	3.4
36	1	2808	A	3.4
19	C7	100	LEU	3.4
24	D2	52	TYR	3.4
73	o7	12	HIS	3.4
79	Q3	22	LEU	3.4
80	c0	39	ASN	3.4
32	E0	7	SER	3.4
57	n1	79	MET	3.4
59	N3	61	THR	3.4
1	2	1105	C	3.4
60	N4	94	ARG	3.4
18	C6	83	GLN	3.4
22	d0	33	GLN	3.4
34	sR	47	LEU	3.4
1	2	1712	A	3.4
77	Q1	18	ARG	3.4
2	S0	108	THR	3.4
70	O4	66	SER	3.4
5	s3	102	ALA	3.4
9	s7	154	LEU	3.4
2	S0	141	ILE	3.4
16	c4	23	PHE	3.4
19	C7	19	ARG	3.4
23	D1	17	CYS	3.4
28	D6	34	LYS	3.4
41	L4	81	GLY	3.4
59	n3	3	GLY	3.4
25	D3	21	ASN	3.4
5	s3	3	ALA	3.4
9	S7	103	SER	3.4
5	s3	86	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
16	c4	137	LEU	3.4
19	C7	9	VAL	3.4
49	M3	2	ALA	3.4
1	6	1491	U	3.4
79	Q3	36	ARG	3.4
21	C9	77	ASN	3.4
28	D6	11	ASN	3.4
34	sR	17	ASN	3.4
4	S2	231	ALA	3.4
6	S4	261	LEU	3.4
14	C2	86	VAL	3.4
22	d0	116	VAL	3.4
36	5	1566	A	3.4
2	S0	38	PHE	3.4
6	S4	49	ARG	3.4
18	c6	129	PHE	3.4
39	L2	219	ILE	3.4
80	c0	12	HIS	3.4
1	2	1774	G	3.4
1	6	1709	C	3.4
24	d2	60	LYS	3.4
58	N2	94	ARG	3.4
5	s3	168	ILE	3.4
1	2	492	A	3.4
23	D1	33	GLN	3.4
58	N2	9	GLN	3.4
58	n2	97	SER	3.4
16	c4	45	GLY	3.4
18	C6	88	GLY	3.4
41	L4	63	GLU	3.4
14	C2	33	ARG	3.4
1	2	1100	G	3.4
5	s3	16	VAL	3.4
35	sM	122	ASP	3.4
40	L3	217	ALA	3.4
58	n2	37	LEU	3.4
22	d0	86	ILE	3.4
29	D7	42	ASN	3.4
15	c3	14	SER	3.4
24	D2	19	LYS	3.4
1	2	626	U	3.4
6	S4	52	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
7	S5	165	LEU	3.4
19	C7	16	LEU	3.4
80	c0	49	LEU	3.4
19	C7	82	ASP	3.4
34	sR	70	ASP	3.4
39	l2	59	ALA	3.4
5	S3	120	TYR	3.4
24	D2	47	ILE	3.4
1	6	1033	C	3.4
3	s1	143	THR	3.4
18	C6	101	SER	3.4
15	C3	114	ARG	3.4
39	l2	17	THR	3.4
39	l2	199	THR	3.4
14	C2	31	VAL	3.3
58	n2	66	VAL	3.3
7	S5	155	ALA	3.3
13	c1	89	ALA	3.3
69	o3	55	ALA	3.3
2	s0	110	TYR	3.3
39	L2	225	ILE	3.3
53	M7	182	ILE	3.3
13	c1	138	ASN	3.3
34	SR	102	ARG	3.3
39	l2	28	LYS	3.3
41	L4	80	GLY	3.3
19	C7	120	SER	3.3
55	M9	177	VAL	3.3
55	m9	24	LEU	3.3
2	s0	115	PHE	3.3
2	s0	160	ILE	3.3
21	C9	66	TYR	3.3
35	SM	105	LYS	3.3
60	n4	73	ARG	3.3
19	C7	70	SER	3.3
34	SR	312	VAL	3.3
35	SM	106	VAL	3.3
41	l4	82	THR	3.3
7	S5	69	PHE	3.3
77	Q1	7	LYS	3.3
85	f	48	LYS	3.3
6	S4	199	GLU	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2	1681	A	3.3
23	D1	75	ASN	3.3
29	D7	4	VAL	3.3
49	M3	33	VAL	3.3
12	C0	24	LYS	3.3
25	D3	5	LYS	3.3
34	sR	143	THR	3.3
60	n4	75	THR	3.3
18	C6	124	PRO	3.3
34	sR	211	ILE	3.3
54	m8	148	GLU	3.3
58	N2	108	TYR	3.3
14	c2	28	LEU	3.3
22	D0	34	LEU	3.3
39	l2	191	LEU	3.3
49	M3	18	TRP	3.3
65	N9	54	LEU	3.3
73	o7	10	LYS	3.3
79	Q3	71	VAL	3.3
2	S0	159	ALA	3.3
2	S0	160	ILE	3.3
19	C7	75	GLU	3.3
24	d2	13	ALA	3.3
40	L3	277	SER	3.3
64	N8	82	ILE	3.3
24	d2	26	LEU	3.3
25	D3	39	LYS	3.3
5	S3	24	PHE	3.3
1	2	1342	C	3.3
6	s4	14	ALA	3.3
43	l6	149	ILE	3.3
51	m5	129	TYR	3.3
85	f	79	ASN	3.3
5	s3	187	LYS	3.3
11	S9	11	THR	3.3
28	d6	7	SER	3.3
11	S9	128	LEU	3.3
31	d9	11	PRO	3.3
39	L2	191	LEU	3.3
49	M3	10	LEU	3.3
1	6	1756[A]	A	3.3
4	s2	103	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
21	C9	14	PHE	3.3
67	O1	25	PHE	3.3
7	s5	92	ARG	3.3
11	S9	123	HIS	3.3
16	c4	20	TYR	3.3
25	d3	21	ASN	3.3
33	E1	145	HIS	3.3
2	s0	29	VAL	3.3
18	c6	9	THR	3.3
73	O7	7	SER	3.3
85	f	36	SER	3.3
24	D2	79	PHE	3.3
79	q3	55	TRP	3.3
17	c5	80	MET	3.3
2	s0	40	ALA	3.3
2	s0	41	ARG	3.3
9	S7	141	ARG	3.3
13	C1	154	ALA	3.3
29	D7	18	LYS	3.3
31	d9	45	GLU	3.3
67	O1	101	ALA	3.3
25	D3	48	HIS	3.3
78	q2	59	HIS	3.3
82	p0	25	LEU	3.3
1	6	794	U	3.3
2	s0	107	PHE	3.3
15	C3	4	MET	3.3
25	d3	110	LYS	3.3
7	S5	89	ILE	3.3
21	C9	8	ASP	3.3
34	sR	114	ASP	3.3
39	l2	225	ILE	3.3
24	d2	63	VAL	3.3
73	O7	8	PHE	3.3
5	S3	92	GLN	3.3
34	SR	213	SER	3.3
36	5	3276	G	3.3
5	S3	213	GLU	3.3
19	C7	45	ARG	3.3
30	d8	67	ARG	3.3
13	c1	144	ALA	3.3
23	D1	57	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
80	c0	11	ILE	3.3
60	n4	88	ASP	3.3
16	c4	48	VAL	3.3
21	c9	92	LYS	3.3
28	d6	17	HIS	3.3
51	M5	192	LYS	3.3
5	s3	105	MET	3.2
5	s3	135	GLU	3.2
19	C7	22	PRO	3.2
49	M3	37	ASN	3.2
11	s9	87	SER	3.2
34	sR	108	SER	3.2
49	m3	192	GLU	3.2
51	m5	200	TRP	3.2
79	Q3	25	GLN	3.2
39	l2	48	ILE	3.2
39	l2	243	THR	3.2
40	l3	245	GLY	3.2
6	S4	23	LEU	3.2
25	D3	15	LEU	3.2
2	S0	181	VAL	3.2
5	S3	200	LYS	3.2
5	s3	200	LYS	3.2
9	s7	70	PHE	3.2
69	O3	22	VAL	3.2
30	d8	61	ARG	3.2
9	s7	108	GLN	3.2
34	sR	239	GLU	3.2
24	D2	4	SER	3.2
24	D2	83	ILE	3.2
1	6	711	U	3.2
2	s0	25	GLY	3.2
28	d6	6	ALA	3.2
74	O8	6	THR	3.2
12	C0	65	TYR	3.2
41	l4	191	LYS	3.2
80	c0	41	TYR	3.2
8	S6	87	ARG	3.2
29	D7	32	PHE	3.2
48	M1	148	VAL	3.2
5	s3	177	MET	3.2
39	L2	204	MET	3.2

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Mol	Chain	Res	Type	RSRZ
41	l4	93	MET	3.2
68	o2	52	GLN	3.2
75	O9	43	ASN	3.2
2	S0	134	LYS	3.2
5	s3	109	LEU	3.2
22	D0	26	LEU	3.2
25	D3	133	LEU	3.2
28	D6	32	LYS	3.2
40	L3	47	LEU	3.2
61	N5	108	LEU	3.2
36	1	1955	U	3.2
41	L4	50	TYR	3.2
7	s5	161	ASP	3.2
18	c6	67	VAL	3.2
24	D2	63	VAL	3.2
41	L4	71	VAL	3.2
80	c0	59	PHE	3.2
1	2	1150	G	3.2
1	2	1584	G	3.2
4	S2	171	PRO	3.2
16	C4	97	GLY	3.2
60	N4	79	GLN	3.2
13	C1	144	ALA	3.2
16	c4	105	LEU	3.2
30	d8	43	ASN	3.2
32	e0	55	ARG	3.2
41	L4	72	ALA	3.2
45	L8	131	ALA	3.2
17	c5	78	THR	3.2
18	C6	78	VAL	3.2
34	sR	133	VAL	3.2
14	C2	21	GLU	3.2
28	d6	33	ASP	3.2
7	s5	108	LEU	3.2
2	S0	136	ALA	3.2
5	S3	144	ALA	3.2
5	s3	178	ARG	3.2
22	d0	85	ARG	3.2
34	sR	304	GLY	3.2
39	L2	179	LEU	3.2
2	s0	28	ASN	3.2
23	d1	53	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
30	D8	15	VAL	3.2
34	sR	159	ASN	3.2
39	L2	196	TRP	3.2
41	L4	106	TRP	3.2
85	f	19	TYR	3.2
5	S3	210	GLU	3.2
12	C0	25	LYS	3.2
3	s1	140	ILE	3.2
14	c2	98	GLY	3.2
22	d0	73	GLY	3.2
24	d2	3	ARG	3.2
63	n7	46	ILE	3.2
70	O4	33	GLN	3.2
73	O7	28	HIS	3.2
1	2	623	A	3.2
6	s4	15	PRO	3.2
36	5	2397	A	3.2
22	d0	32	LYS	3.2
28	d6	19	LYS	3.2
34	SR	82	SER	3.2
2	S0	144	ILE	3.2
1	6	712	G	3.2
7	s5	151	GLY	3.2
8	S6	69	LEU	3.2
34	sR	147	HIS	3.2
39	L2	180	LEU	3.2
1	2	1076	A	3.2
6	S4	181	VAL	3.2
19	C7	48	ASN	3.2
28	d6	22	ARG	3.2
73	O7	13	ASN	3.2
34	sR	205	SER	3.2
9	S7	146	GLY	3.2
22	d0	27	THR	3.2
32	E0	39	LEU	3.2
74	O8	5	ILE	3.2
2	S0	155	PHE	3.2
3	S1	225	VAL	3.2
33	E1	82	LYS	3.2
60	N4	41	LYS	3.2
5	S3	216	PRO	3.2
16	C4	120	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
16	C4	135	ARG	3.2
8	S6	101	ILE	3.2
19	C7	41	ILE	3.2
22	d0	66	SER	3.2
42	l5	290	ILE	3.2
77	Q1	24	SER	3.2
1	6	1705	C	3.2
3	S1	98	THR	3.2
19	c7	29	GLN	3.2
5	s3	37	VAL	3.2
34	SR	110	VAL	3.2
42	l5	267	ALA	3.2
1	2	1398	U	3.2
5	S3	211	PRO	3.2
1	6	660	G	3.2
10	s8	23	LYS	3.2
10	s8	177	GLY	3.2
54	M8	166	LEU	3.2
34	SR	318	ALA	3.2
36	1	1103	A	3.2
39	l2	249	SER	3.2
2	S0	127	ARG	3.2
4	s2	94	GLN	3.2
5	s3	123	VAL	3.2
21	c9	17	ALA	3.2
39	L2	235	ALA	3.2
39	L2	247	ARG	3.2
51	m5	15	GLN	3.2
5	S3	95	GLY	3.2
7	s5	84	LYS	3.2
8	s6	76	LEU	3.2
13	C1	46	LYS	3.2
39	L2	236	GLY	3.2
67	O1	71	LEU	3.2
28	D6	87	ARG	3.2
54	m8	94	PHE	3.2
19	C7	66	VAL	3.2
45	l8	104	GLU	3.2
36	5	1534	A	3.2
15	c3	88	LEU	3.1
1	6	679	U	3.1
23	d1	63	GLY	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
31	d9	50	ILE	3.1
39	l2	29	LEU	3.1
41	L4	74	ILE	3.1
13	C1	116	ARG	3.1
15	C3	124	ARG	3.1
70	O4	7	PHE	3.1
75	O9	21	ARG	3.1
14	c2	101	ALA	3.1
16	c4	59	ALA	3.1
29	D7	30	SER	3.1
10	s8	37	LYS	3.1
35	SM	97	THR	3.1
58	n2	100	THR	3.1
29	D7	8	LEU	3.1
1	6	1337	A	3.1
7	s5	40	ILE	3.1
35	sM	39	PRO	3.1
39	l2	164	GLY	3.1
1	2	708	C	3.1
13	C1	60	PHE	3.1
21	c9	4	VAL	3.1
49	M3	22	VAL	3.1
2	s0	83	GLN	3.1
27	d5	59	TYR	3.1
35	SM	103	LYS	3.1
55	m9	21	LYS	3.1
70	o4	19	LYS	3.1
73	O7	3	LYS	3.1
34	SR	197	SER	3.1
15	C3	54	LEU	3.1
16	C4	102	LEU	3.1
22	d0	93	LEU	3.1
28	D6	91	ASP	3.1
7	s5	75	GLY	3.1
21	C9	128	GLY	3.1
15	c3	4	MET	3.1
36	1	2143	A	3.1
36	5	2872	A	3.1
45	L8	114	ALA	3.1
60	n4	66	GLU	3.1
36	5	2496	C	3.1
59	N3	81	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
77	Q1	17	ARG	3.1
6	S4	167	GLY	3.1
19	C7	40	THR	3.1
28	d6	80	HIS	3.1
41	l4	75	PRO	3.1
5	s3	12	VAL	3.1
9	S7	151	LYS	3.1
27	D5	97	LYS	3.1
1	6	710	U	3.1
1	6	864	U	3.1
10	s8	103	GLN	3.1
39	L2	245	LEU	3.1
28	d6	3	LYS	3.1
36	1	1486	G	3.1
36	1	2187	G	3.1
41	L4	66	GLY	3.1
43	l6	66	SER	3.1
52	M6	42	ASN	3.1
57	n1	160	ILE	3.1
13	C1	155	LYS	3.1
18	C6	107	LYS	3.1
22	d0	107	THR	3.1
60	n4	85	ALA	3.1
3	s1	155	TYR	3.1
8	S6	182	GLN	3.1
13	C1	128	CYS	3.1
63	n7	49	TYR	3.1
10	S8	177	GLY	3.1
1	6	1424	A	3.1
18	C6	138	PHE	3.1
18	c6	106	LYS	3.1
34	SR	263	PHE	3.1
2	S0	147	THR	3.1
9	s7	134	GLU	3.1
10	S8	6	ASP	3.1
36	5	1016	C	3.1
34	SR	6	VAL	3.1
34	SR	90	ARG	3.1
35	SM	91	THR	3.1
45	L8	90	THR	3.1
61	n5	119	THR	3.1
73	O7	6	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
6	S4	180	LEU	3.1
12	C0	17	GLN	3.1
21	C9	103	LYS	3.1
3	s1	30	PHE	3.1
34	SR	211	ILE	3.1
64	N8	110	GLY	3.1
1	6	493	U	3.1
36	1	3079	U	3.1
5	s3	43	PRO	3.1
19	C7	121	VAL	3.1
39	l2	211	HIS	3.1
13	C1	56	LYS	3.1
25	D3	9	LEU	3.1
34	sR	187	GLN	3.1
64	N8	65	GLN	3.1
10	S8	101	ILE	3.1
21	c9	14	PHE	3.1
36	5	2440	G	3.1
76	Q0	77	ILE	3.1
17	c5	137	ARG	3.1
2	S0	29	VAL	3.1
5	S3	105	MET	3.1
5	s3	154	ASP	3.1
36	5	2538	U	3.1
34	sR	46	LYS	3.1
78	q2	34	SER	3.1
6	S4	80	THR	3.1
16	C4	89	THR	3.1
21	C9	107	ALA	3.1
45	L8	130	TYR	3.1
79	q3	11	THR	3.1
1	2	1078	C	3.1
1	2	1332	C	3.1
18	C6	94	GLN	3.1
42	L5	63	GLN	3.1
42	L5	148	ILE	3.1
4	S2	84	LYS	3.1
13	c1	57	LYS	3.1
33	e1	145	HIS	3.1
34	sR	132	LYS	3.1
5	S3	119	ALA	3.1
25	D3	11	SER	3.1

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Mol	Chain	Res	Type	RSRZ
39	l2	182	ALA	3.1
19	C7	8	THR	3.1
31	d9	46	LYS	3.1
70	o4	35	VAL	3.1
77	q1	25	LYS	3.1
2	s0	149	LEU	3.1
3	s1	110	LEU	3.1
9	S7	115	SER	3.1
25	D3	27	ASN	3.1
51	M5	200	TRP	3.1
56	N0	85	SER	3.1
10	s8	30	GLY	3.1
34	sR	71	CYS	3.1
36	1	2150	G	3.1
39	L2	199	THR	3.1
59	N3	3	GLY	3.1
82	p0	88	PHE	3.1
19	C7	72	LYS	3.1
73	o7	32	LYS	3.1
7	S5	98	MET	3.1
1	2	1776	A	3.1
7	S5	92	ARG	3.1
26	D4	18	LEU	3.1
30	d8	33	LEU	3.1
2	S0	164	ASN	3.0
3	S1	55	LYS	3.0
5	S3	50	ILE	3.0
8	s6	165	GLY	3.0
14	c2	125	ASN	3.0
18	C6	96	TYR	3.0
70	o4	42	PRO	3.0
80	c0	27	PHE	3.0
18	C6	140	LYS	3.0
29	D7	45	THR	3.0
30	d8	27	GLN	3.0
34	sR	185	GLN	3.0
56	N0	129	ILE	3.0
67	O1	14	ILE	3.0
5	s3	99	VAL	3.0
21	C9	29	GLU	3.0
40	l3	387	LEU	3.0
53	M7	131	ARG	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	S1	30	PHE	3.0
10	S8	26	LYS	3.0
10	s8	109	PHE	3.0
14	C2	27	ALA	3.0
17	c5	101	ALA	3.0
19	C7	12	ALA	3.0
63	N7	91	ALA	3.0
73	o7	41	ALA	3.0
15	C3	107	LYS	3.0
3	s1	117	TRP	3.0
13	C1	138	ASN	3.0
58	n2	11	ILE	3.0
6	s4	183	VAL	3.0
24	D2	64	GLN	3.0
35	sM	169	GLU	3.0
41	L4	54	GLU	3.0
29	D7	52	THR	3.0
30	d8	28	VAL	3.0
31	D9	40	ARG	3.0
85	f	21	MET	3.0
19	c7	59	LYS	3.0
31	d9	8	PHE	3.0
1	2	1416	G	3.0
29	D7	27	GLY	3.0
14	c2	113	ARG	3.0
34	sR	94	VAL	3.0
51	M5	95	GLN	3.0
51	M5	155	VAL	3.0
19	c7	25	THR	3.0
19	c7	55	THR	3.0
29	D7	24	LEU	3.0
25	D3	123	LYS	3.0
2	S0	178	ALA	3.0
22	d0	103	ILE	3.0
39	L2	15	ILE	3.0
5	s3	76	ARG	3.0
7	S5	24	VAL	3.0
18	c6	66	ARG	3.0
34	sR	19	TRP	3.0
34	sR	178	VAL	3.0
34	sR	141	LEU	3.0
64	n8	81	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
85	f	88	ASN	3.0
1	6	1217	A	3.0
1	6	1794	A	3.0
5	S3	153	ALA	3.0
18	C6	109	PHE	3.0
34	SR	83	ALA	3.0
3	S1	101	HIS	3.0
24	D2	86	ILE	3.0
24	d2	53	ILE	3.0
28	D6	26	CYS	3.0
32	E0	25	GLU	3.0
59	N3	35	TYR	3.0
34	sR	288	HIS	3.0
24	d2	25	VAL	3.0
33	E1	114	VAL	3.0
18	c6	89	LEU	3.0
25	D3	31	LYS	3.0
39	l2	179	LEU	3.0
35	SM	107	ASN	3.0
21	C9	21	PHE	3.0
85	f	150	PHE	3.0
1	2	1082	C	3.0
8	s6	88	ARG	3.0
34	sR	168	THR	3.0
40	l3	244	ARG	3.0
1	2	494	U	3.0
13	C1	66	ILE	3.0
36	1	2947	G	3.0
13	C1	123	VAL	3.0
19	C7	4	VAL	3.0
49	M3	8	PRO	3.0
77	Q1	19	LYS	3.0
9	S7	126	LEU	3.0
34	SR	93	ASP	3.0
80	c0	1	MET	3.0
4	s2	164	SER	3.0
10	s8	42	ARG	3.0
15	c3	6	SER	3.0
5	s3	53	THR	3.0
10	S8	192	TYR	3.0
63	n7	2	ALA	3.0
31	d9	33	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	2	491	C	3.0
9	S7	140	VAL	3.0
34	sR	66	HIS	3.0
70	O4	22	VAL	3.0
36	1	1565	G	3.0
36	5	2183	A	3.0
11	S9	6	ARG	3.0
24	D2	97	ARG	3.0
39	l2	3	ARG	3.0
49	M3	98	ASP	3.0
9	s7	49	ILE	3.0
16	c4	19	ILE	3.0
22	d0	36	ASN	3.0
41	L4	55	LYS	3.0
66	o0	22	LYS	3.0
13	c1	64	VAL	3.0
18	C6	48	VAL	3.0
79	Q3	70	THR	3.0
22	D0	68	ARG	3.0
32	e0	5	HIS	3.0
34	SR	57	PRO	3.0
38	4	158	U	3.0
39	L2	242	ARG	3.0
51	M5	191	TRP	3.0
58	N2	107	PHE	3.0
21	c9	19	ALA	3.0
22	d0	99	ILE	3.0
28	d6	49	ALA	3.0
5	s3	85	VAL	3.0
18	C6	4	VAL	3.0
29	d7	30	SER	3.0
15	C3	61	THR	3.0
39	l2	252	THR	3.0
2	S0	116	LYS	3.0
4	S2	151	PRO	3.0
6	S4	7	LYS	3.0
13	C1	151	LYS	3.0
85	f	105	MET	3.0
48	M1	83	GLY	3.0
21	c9	10	ALA	3.0
2	S0	143	VAL	3.0
5	s3	73	VAL	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	s1	181	LEU	3.0
16	C4	133	ARG	3.0
19	C7	34	LEU	3.0
23	D1	65	SER	3.0
34	SR	240	VAL	3.0
41	L4	53	SER	3.0
51	m5	75	VAL	3.0
44	L7	209	ASN	3.0
77	q1	13	LEU	3.0
4	S2	96	THR	3.0
5	s3	159	HIS	3.0
8	S6	145	PHE	3.0
10	S8	109	PHE	3.0
12	C0	5	LYS	3.0
42	L5	5	LYS	3.0
18	c6	126	PRO	3.0
34	SR	280	GLY	3.0
4	s2	178	ILE	3.0
28	d6	79	ILE	3.0
36	5	1567	U	3.0
80	c0	35	ILE	3.0
1	2	910	C	3.0
18	C6	28	LEU	3.0
23	D1	31	SER	3.0
74	o8	26	LYS	3.0
18	c6	46	PHE	3.0
34	sR	130	THR	3.0
39	L2	218	HIS	3.0
1	2	1685	G	2.9
39	l2	240	ALA	2.9
70	o4	41	ARG	2.9
11	S9	86	LEU	2.9
24	D2	38	LEU	2.9
39	L2	176	ASP	2.9
24	d2	12	ASN	2.9
36	1	1581	C	2.9
2	s0	80	THR	2.9
5	S3	207	THR	2.9
17	c5	83	MET	2.9
24	D2	109	GLY	2.9
39	L2	241	ARG	2.9
41	L4	88	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	S0	19	ALA	2.9
22	D0	91	ILE	2.9
22	d0	108	ILE	2.9
16	C4	137	LEU	2.9
19	C7	20	TYR	2.9
51	m5	6	TYR	2.9
64	N8	35	ALA	2.9
70	o4	36	LYS	2.9
4	s2	208	GLU	2.9
28	d6	85	ARG	2.9
39	L2	209	HIS	2.9
75	O9	4	GLN	2.9
2	s0	76	ILE	2.9
6	S4	127	LYS	2.9
28	d6	45	VAL	2.9
34	SR	135	THR	2.9
2	S0	75	ALA	2.9
5	S3	102	ALA	2.9
67	O1	51	LEU	2.9
19	C7	67	ARG	2.9
59	N3	70	ARG	2.9
7	S5	80	LYS	2.9
18	c6	13	LYS	2.9
19	C7	29	GLN	2.9
28	D6	27	SER	2.9
28	d6	39	MET	2.9
4	S2	218	ILE	2.9
5	S3	88	ALA	2.9
5	s3	39	VAL	2.9
6	S4	2	ALA	2.9
14	c2	116	VAL	2.9
30	D8	28	VAL	2.9
70	O4	20	ILE	2.9
34	sR	145	LEU	2.9
31	d9	34	TYR	2.9
58	N2	80	THR	2.9
61	n5	123	TYR	2.9
5	s3	77	PHE	2.9
6	S4	226	PHE	2.9
7	s5	48	PHE	2.9
8	S6	144	PHE	2.9
58	n2	15	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
36	1	884	A	2.9
31	d9	38	ILE	2.9
36	1	2978	U	2.9
13	C1	65	SER	2.9
60	N4	95	SER	2.9
2	s0	60	ALA	2.9
5	S3	34	TYR	2.9
85	f	141	ALA	2.9
1	2	1295	G	2.9
6	S4	77	ARG	2.9
8	s6	170	THR	2.9
28	d6	38	ARG	2.9
36	1	2185	G	2.9
42	L5	3	PHE	2.9
55	m9	84	THR	2.9
74	o8	53	THR	2.9
1	2	489	C	2.9
13	C1	69	LYS	2.9
13	c1	79	LYS	2.9
79	q3	7	LYS	2.9
39	L2	183	GLY	2.9
6	S4	101	LEU	2.9
12	C0	42	VAL	2.9
17	c5	104	GLN	2.9
29	D7	43	ILE	2.9
30	d8	48	VAL	2.9
67	O1	16	LEU	2.9
21	c9	90	PRO	2.9
22	d0	68	ARG	2.9
23	D1	81	ASN	2.9
29	D7	48	SER	2.9
34	SR	27	ALA	2.9
39	L2	149	ARG	2.9
40	l3	240	ARG	2.9
19	c7	81	LYS	2.9
58	N2	95	PHE	2.9
60	N4	40	PHE	2.9
1	2	810	G	2.9
1	2	1339	C	2.9
24	D2	67	GLY	2.9
10	s8	60	ILE	2.9
16	C4	39	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
19	c7	17	ILE	2.9
24	d2	62	VAL	2.9
41	L4	87	GLN	2.9
58	n2	54	VAL	2.9
5	s3	106	LYS	2.9
21	C9	19	ALA	2.9
33	e1	93	HIS	2.9
45	l8	245	LYS	2.9
5	S3	199	PRO	2.9
23	d1	83	TRP	2.9
4	S2	242	ILE	2.9
19	C7	11	ARG	2.9
40	l3	47	LEU	2.9
5	s3	120	TYR	2.9
15	C3	113	PHE	2.9
39	L2	229	ALA	2.9
51	m5	39	ALA	2.9
18	c6	93	HIS	2.9
2	S0	21	ASN	2.9
22	D0	121	ASN	2.9
6	S4	124	GLY	2.9
18	C6	122	ARG	2.9
22	d0	102	ARG	2.9
34	sR	38	ARG	2.9
35	sM	82	THR	2.9
39	L2	184	ARG	2.9
41	L4	103	THR	2.9
46	L9	85	GLY	2.9
49	M3	41	THR	2.9
59	N3	115	THR	2.9
75	O9	44	TRP	2.9
4	S2	103	VAL	2.9
39	L2	202	VAL	2.9
51	M5	204	LYS	2.9
7	s5	85	ALA	2.9
34	sR	69	GLN	2.9
45	l8	196	ALA	2.9
51	m5	3	ALA	2.9
41	L4	58	HIS	2.9
7	s5	83	ARG	2.9
31	d9	17	GLY	2.9
35	SM	93	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	2	1413	U	2.9
2	s0	147	THR	2.9
3	s1	121	ILE	2.9
6	S4	9	LEU	2.9
9	S7	62	VAL	2.9
9	s7	153	LEU	2.9
13	C1	119	VAL	2.9
22	D0	63	LEU	2.9
36	1	870	G	2.9
36	1	896	A	2.9
40	L3	164	THR	2.9
40	L3	242	THR	2.9
49	m3	182	ILE	2.9
70	O4	71	THR	2.9
11	s9	110	GLN	2.9
19	C7	42	GLN	2.9
58	N2	15	PHE	2.9
3	S1	89	ASP	2.9
64	n8	46	ASP	2.9
11	S9	3	ARG	2.9
2	s0	161	PRO	2.9
4	S2	85	PRO	2.9
4	s2	182	PRO	2.9
9	S7	124	LYS	2.9
16	c4	120	PRO	2.9
41	L4	75	PRO	2.9
64	N8	31	GLY	2.9
29	d7	2	VAL	2.9
34	sR	240	VAL	2.9
36	5	3166	C	2.9
1	6	494	U	2.9
45	L8	52	TRP	2.9
54	m8	186	VAL	2.9
29	d7	52	THR	2.9
31	D9	43	PHE	2.9
52	m6	62	THR	2.9
1	2	1654	G	2.9
1	6	1697	G	2.9
39	L2	185	ALA	2.9
17	c5	10	ARG	2.9
14	c2	124	LYS	2.9
23	D1	25	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
6	S4	43	PRO	2.9
7	S5	75	GLY	2.9
2	S0	197	ILE	2.8
2	s0	31	VAL	2.8
3	s1	91	VAL	2.8
18	C6	76	SER	2.8
34	SR	113	VAL	2.8
34	SR	121	MET	2.8
39	L2	215	ASN	2.8
49	M3	14	PHE	2.8
77	Q1	5	TRP	2.8
36	1	818	C	2.8
78	Q2	50	PHE	2.8
5	s3	205	ALA	2.8
18	C6	110	THR	2.8
23	D1	22	ARG	2.8
35	SM	176	LYS	2.8
1	6	1433	G	2.8
13	C1	71	LEU	2.8
24	d2	73	GLY	2.8
36	1	3085	G	2.8
36	5	1524	A	2.8
42	L5	6	ASP	2.8
4	s2	104	VAL	2.8
5	s3	49	ILE	2.8
49	M3	46	ILE	2.8
85	f	75	PRO	2.8
2	s0	106	SER	2.8
21	C9	125	SER	2.8
48	M1	96	PHE	2.8
24	D2	16	ASN	2.8
34	SR	46	LYS	2.8
1	6	664	U	2.8
2	S0	53	THR	2.8
18	c6	79	TYR	2.8
9	s7	126	LEU	2.8
30	D8	17	GLY	2.8
34	sR	210	LEU	2.8
39	l2	2	GLY	2.8
4	S2	140	ARG	2.8
5	S3	17	PHE	2.8
8	S6	63	MET	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
16	c4	84	ARG	2.8
17	c5	89	MET	2.8
19	C7	61	ILE	2.8
22	D0	20	ILE	2.8
29	d7	19	HIS	2.8
59	N3	36	ILE	2.8
59	N3	114	ILE	2.8
22	D0	69	LYS	2.8
4	S2	220	ASN	2.8
49	M3	19	GLN	2.8
7	S5	105	GLY	2.8
49	M3	51	LEU	2.8
1	2	1606	C	2.8
6	s4	45	ILE	2.8
9	S7	111	LYS	2.8
23	d1	36	VAL	2.8
51	M5	61	ILE	2.8
65	N9	25	LYS	2.8
70	o4	26	PRO	2.8
2	S0	180	GLU	2.8
7	s5	31	GLU	2.8
9	s7	127	GLU	2.8
5	s3	79	TYR	2.8
9	S7	173	TYR	2.8
14	c2	96	GLN	2.8
18	C6	18	ALA	2.8
36	1	914	A	2.8
36	1	2145	A	2.8
55	m9	12	ALA	2.8
77	Q1	22	ALA	2.8
2	S0	84	ARG	2.8
2	s0	22	THR	2.8
3	s1	152	ARG	2.8
4	s2	205	ARG	2.8
7	S5	150	GLY	2.8
7	S5	107	LYS	2.8
34	SR	96	THR	2.8
36	1	805	G	2.8
5	s3	103	GLU	2.8
8	s6	35	GLU	2.8
10	S8	34	ALA	2.8
40	L3	22	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
61	N5	122	ALA	2.8
12	C0	53	GLY	2.8
18	c6	47	LYS	2.8
19	c7	26	LEU	2.8
17	C5	105	VAL	2.8
28	D6	75	VAL	2.8
36	5	2143	A	2.8
28	d6	44	ILE	2.8
34	sR	68	VAL	2.8
54	M8	93	ILE	2.8
1	2	628	G	2.8
1	2	1130	G	2.8
1	2	1145	U	2.8
1	2	1199	G	2.8
1	2	1738	U	2.8
1	6	942	G	2.8
6	S4	36	HIS	2.8
15	c3	110	ASP	2.8
10	S8	13	ALA	2.8
18	C6	137	ARG	2.8
24	d2	57	ARG	2.8
34	sR	253	ALA	2.8
4	S2	134	LEU	2.8
33	E1	83	LYS	2.8
70	o4	33	GLN	2.8
73	O7	14	LYS	2.8
80	c0	73	VAL	2.8
19	C7	79	GLU	2.8
20	C8	73	MET	2.8
19	C7	3	ARG	2.8
35	SM	96	ARG	2.8
36	1	1765	U	2.8
24	D2	7	LEU	2.8
31	D9	36	LEU	2.8
39	L2	182	ALA	2.8
1	2	722	G	2.8
6	s4	162	ILE	2.8
7	s5	29	ILE	2.8
9	s7	136	VAL	2.8
36	1	963	G	2.8
36	1	1349	G	2.8
36	1	3069	G	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	S8	21	PHE	2.8
36	5	2495	C	2.8
39	l2	61	VAL	2.8
41	L4	85	SER	2.8
2	S0	112	THR	2.8
6	S4	254	ARG	2.8
29	D7	44	THR	2.8
31	d9	28	THR	2.8
41	L4	82	THR	2.8
54	M8	151	ARG	2.8
61	n5	112	THR	2.8
18	C6	49	TYR	2.8
18	c6	117	LEU	2.8
19	C7	126	ALA	2.8
29	d7	31	TYR	2.8
41	l4	243	HIS	2.8
47	m0	111	LEU	2.8
70	o4	50	ALA	2.8
35	SM	110	TRP	2.8
1	2	1713	G	2.8
7	S5	106	LYS	2.8
11	S9	64	GLU	2.8
22	D0	88	LYS	2.8
22	D0	89	ARG	2.8
23	d1	22	ARG	2.8
28	d6	29	SER	2.8
67	O1	34	LYS	2.8
68	o2	40	SER	2.8
79	Q3	21	SER	2.8
36	1	363	G	2.8
2	S0	103	THR	2.8
15	c3	61	THR	2.8
7	S5	72	HIS	2.8
11	S9	36	LEU	2.8
58	N2	84	LEU	2.8
19	C7	68	GLY	2.8
29	D7	68	GLY	2.8
79	Q3	18	TYR	2.8
1	6	661	A	2.8
1	6	1425	A	2.8
19	C7	85	VAL	2.8
22	D0	117	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
34	SR	315	VAL	2.8
2	s0	185	ARG	2.8
18	c6	36	ILE	2.8
21	C9	134	ARG	2.8
57	n1	76	ILE	2.8
75	o9	36	ARG	2.8
77	q1	11	ARG	2.8
35	SM	95	SER	2.8
2	S0	184	LEU	2.8
3	s1	141	ALA	2.8
11	S9	24	LEU	2.8
29	d7	7	LEU	2.8
41	L4	114	ASN	2.8
19	C7	15	ALA	2.8
1	2	980	G	2.8
1	2	1605	G	2.8
19	c7	27	ASP	2.8
24	D2	29	PRO	2.8
36	1	2134	G	2.8
5	s3	75	LYS	2.8
8	s6	79	LYS	2.8
14	c2	108	ARG	2.8
15	C3	106	ARG	2.8
18	c6	127	LYS	2.8
39	l2	227	ARG	2.8
77	Q1	6	ARG	2.8
14	C2	59	LEU	2.8
16	c4	85	ALA	2.8
5	s3	42	THR	2.8
1	2	1482	C	2.8
13	C1	87	ARG	2.8
17	c5	109	PRO	2.8
25	D3	23	ARG	2.8
49	M3	23	LYS	2.8
64	N8	29	PRO	2.8
70	o4	58	ARG	2.8
73	O7	17	THR	2.8
5	s3	5	ILE	2.7
5	s3	50	ILE	2.7
14	c2	132	GLU	2.7
36	5	2950	G	2.7
61	N5	24	LEU	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	S2	46	LYS	2.7
6	S4	208	VAL	2.7
24	d2	130	TYR	2.7
36	1	1842	A	2.7
41	l4	70	ALA	2.7
49	m3	183	ARG	2.7
57	N1	62	GLY	2.7
58	n2	106	ALA	2.7
70	O4	4	ARG	2.7
77	Q1	16	LYS	2.7
39	l2	7	ASN	2.7
85	f	53	GLY	2.7
47	M0	148	VAL	2.7
7	S5	86	GLN	2.7
29	D7	37	CYS	2.7
60	n4	79	GLN	2.7
1	2	1664	C	2.7
1	6	1772	C	2.7
36	1	1857	C	2.7
36	1	2821	C	2.7
7	s5	76	ARG	2.7
19	C7	73	LEU	2.7
73	O7	10	LYS	2.7
24	D2	45	GLY	2.7
35	SM	172	ALA	2.7
55	m9	93	VAL	2.7
4	s2	250	GLN	2.7
5	s3	158	ILE	2.7
5	s3	163	PRO	2.7
32	E0	41	THR	2.7
34	sR	74	THR	2.7
36	1	1535	A	2.7
69	o3	100	ILE	2.7
5	s3	170	THR	2.7
11	S9	61	THR	2.7
58	n2	14	THR	2.7
6	S4	39	ARG	2.7
9	S7	107	ARG	2.7
10	s8	59	ARG	2.7
11	S9	60	LEU	2.7
25	d3	5	LYS	2.7
1	2	741	C	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
34	SR	173	GLY	2.7
2	S0	204	TYR	2.7
69	o3	51	TYR	2.7
5	S3	31	GLU	2.7
5	S3	97	SER	2.7
5	s3	47	GLU	2.7
9	s7	2	SER	2.7
73	o7	84	SER	2.7
5	s3	199	PRO	2.7
45	l8	159	PRO	2.7
80	c0	33	GLU	2.7
5	s3	94	ARG	2.7
18	c6	14	LYS	2.7
28	d6	72	HIS	2.7
36	5	2957	G	2.7
48	m1	174	LYS	2.7
64	N8	111	LYS	2.7
82	p0	281	THR	2.7
5	s3	17	PHE	2.7
53	M7	174	GLY	2.7
7	s5	33	VAL	2.7
58	n2	33	TYR	2.7
67	O1	64	VAL	2.7
1	2	965	U	2.7
5	s3	84	ILE	2.7
7	S5	91	GLU	2.7
12	C0	6	GLU	2.7
36	5	2146	C	2.7
18	c6	26	LYS	2.7
21	C9	63	ARG	2.7
31	D9	33	LYS	2.7
34	sR	60	SER	2.7
69	o3	19	SER	2.7
4	S2	82	ASN	2.7
18	c6	53	LEU	2.7
23	d1	75	ASN	2.7
24	D2	98	GLN	2.7
30	d8	56	LEU	2.7
39	l2	218	HIS	2.7
49	M3	17	HIS	2.7
70	O4	60	ARG	2.7
24	d2	65	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
14	c2	93	ASP	2.7
22	D0	79	TRP	2.7
1	2	914	G	2.7
1	6	1702	A	2.7
21	C9	50	ALA	2.7
63	N7	95	VAL	2.7
80	c0	75	TYR	2.7
7	s5	81	ARG	2.7
14	c2	129	GLU	2.7
24	D2	78	ARG	2.7
31	D9	31	ILE	2.7
1	2	747	C	2.7
2	s0	126	PRO	2.7
5	S3	69	LEU	2.7
6	s4	261	LEU	2.7
34	sR	106	HIS	2.7
36	1	1495	U	2.7
36	1	2148	U	2.7
59	N3	7	GLN	2.7
23	D1	29	HIS	2.7
59	N3	54	LEU	2.7
5	S3	204	ASP	2.7
5	s3	133	GLY	2.7
11	S9	7	THR	2.7
15	c3	25	TRP	2.7
35	SM	101	ASP	2.7
60	N4	21	PHE	2.7
69	O3	72	THR	2.7
4	s2	111	VAL	2.7
6	S4	191	ARG	2.7
16	c4	128	LYS	2.7
23	D1	19	ALA	2.7
39	L2	177	LYS	2.7
41	l4	55	LYS	2.7
45	L8	202	GLU	2.7
49	m3	23	LYS	2.7
51	m5	66	VAL	2.7
18	c6	81	ILE	2.7
31	d9	31	ILE	2.7
1	2	173	A	2.7
36	5	3167	A	2.7
1	2	976	G	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	S0	24	LEU	2.7
5	s3	6	SER	2.7
8	S6	147	LEU	2.7
9	s7	103	SER	2.7
15	c3	62	GLN	2.7
17	c5	22	LEU	2.7
36	1	2130	G	2.7
69	O3	7	LEU	2.7
2	s0	38	PHE	2.7
10	S8	27	PHE	2.7
36	1	1866	C	2.7
38	8	22	U	2.7
28	D6	93	LYS	2.7
47	m0	204	GLY	2.7
52	m6	64	PHE	2.7
59	N3	132	ASN	2.7
74	O8	57	ASN	2.7
9	s7	20	VAL	2.7
15	C3	127	ARG	2.7
23	d1	62	ARG	2.7
35	SM	138	ALA	2.7
4	S2	139	ILE	2.7
79	q3	18	TYR	2.7
80	c0	15	LEU	2.7
16	C4	96	PRO	2.7
31	D9	25	SER	2.7
34	SR	71	CYS	2.7
1	2	1717	G	2.7
1	6	718	U	2.7
5	S3	51	ARG	2.7
42	l5	295	GLY	2.7
51	M5	189	LYS	2.7
15	C3	25	TRP	2.7
54	M8	87	VAL	2.7
16	c4	126	THR	2.7
24	D2	96	ALA	2.7
36	1	1923	C	2.7
46	L9	190	ASP	2.7
49	M3	142	ALA	2.7
39	L2	237	LEU	2.7
17	C5	59	LYS	2.7
19	c7	32	LYS	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
41	l4	88	GLY	2.7
46	l9	186	PHE	2.7
80	c0	97	ARG	2.7
7	s5	70	VAL	2.7
12	C0	22	VAL	2.7
19	c7	35	CYS	2.7
19	c7	66	VAL	2.7
41	L4	64	SER	2.7
59	N3	84	SER	2.7
67	O1	23	VAL	2.7
45	L8	117	ALA	2.7
49	M3	96	ALA	2.7
4	S2	90	THR	2.7
4	S2	229	LEU	2.7
4	s2	212	LYS	2.7
11	s9	80	LEU	2.7
24	D2	20	THR	2.7
36	5	2418	G	2.7
3	s1	142	PHE	2.7
54	m8	178	ARG	2.7
49	M3	74	GLY	2.7
85	f	98	GLY	2.7
3	S1	139	ALA	2.7
5	S3	171	ALA	2.7
13	C1	86	ILE	2.7
23	d1	86	SER	2.7
1	2	133	U	2.7
1	2	1380	U	2.7
10	S8	90	LEU	2.7
14	C2	36	LEU	2.7
15	c3	69	ASN	2.7
42	L5	131	LEU	2.7
70	O4	24	LYS	2.7
54	m8	6	THR	2.7
60	n4	83	THR	2.7
85	f	12	ASP	2.7
18	C6	45	ARG	2.7
19	C7	5	ARG	2.7
28	d6	92	ARG	2.7
80	c0	8	ARG	2.7
5	s3	156	PHE	2.7
1	6	1792	G	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
20	c8	73	MET	2.7
2	s0	35	PRO	2.7
2	s0	73	VAL	2.7
9	S7	144	VAL	2.7
32	e0	59	GLY	2.7
34	sR	315	VAL	2.7
64	n8	121	VAL	2.7
2	s0	122	ILE	2.7
5	S3	87	TYR	2.6
6	s4	245	LYS	2.6
8	S6	93	LYS	2.6
14	c2	35	ALA	2.7
19	C7	39	ALA	2.7
21	C9	64	HIS	2.7
21	c9	136	ALA	2.7
67	o1	16	LEU	2.6
24	d2	9	ASP	2.6
5	S3	170	THR	2.6
22	D0	67	THR	2.6
34	sR	300	THR	2.6
45	L8	91	PHE	2.6
60	N4	29	PHE	2.6
3	S1	93	GLY	2.6
4	s2	63	VAL	2.6
31	d9	15	GLY	2.6
1	2	1739	C	2.6
4	S2	53	ILE	2.6
7	s5	90	ILE	2.6
11	s9	183	ALA	2.6
13	C1	30	ARG	2.6
13	C1	67	ARG	2.6
21	C9	55	TYR	2.6
21	C9	65	ILE	2.6
58	N2	11	ILE	2.6
10	s8	176	SER	2.6
34	sR	9	LEU	2.6
18	c6	103	ASN	2.6
1	2	1095	U	2.6
36	1	3155	U	2.6
45	L8	58	VAL	2.6
36	1	913	A	2.6
36	1	1800	A	2.6

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Mol	Chain	Res	Type	RSRZ
49	M3	172	LEU	2.6
49	m3	8	PRO	2.6
58	N2	41	ILE	2.6
64	n8	29	PRO	2.6
64	n8	102	ILE	2.6
75	o9	45	ARG	2.6
21	C9	93	HIS	2.6
25	d3	76	LEU	2.6
10	S8	67	TRP	2.6
30	d8	59	SER	2.6
2	S0	73	VAL	2.6
2	S0	125	ASP	2.6
5	S3	138	VAL	2.6
5	s3	194	LYS	2.6
8	s6	171	LYS	2.6
16	c4	79	VAL	2.6
34	sR	107	LYS	2.6
36	1	2400	G	2.6
47	m0	191	LYS	2.6
58	N2	54	VAL	2.6
64	N8	63	LYS	2.6
16	c4	133	ARG	2.6
19	c7	47	ARG	2.6
21	c9	122	ARG	2.6
41	l4	76	ARG	2.6
85	f	137	THR	2.6
36	5	3277	U	2.6
6	S4	92	LEU	2.6
16	C4	17	ALA	2.6
39	l2	238	ILE	2.6
42	L5	2	ALA	2.6
45	l8	152	LEU	2.6
57	N1	42	ILE	2.6
18	C6	51	PRO	2.6
1	2	754	A	2.6
36	1	2813	A	2.6
62	N6	116	LYS	2.6
64	n8	79	TRP	2.6
18	C6	131	GLY	2.6
18	c6	48	VAL	2.6
21	C9	115	GLU	2.6
21	C9	126	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
24	D2	40	VAL	2.6
26	D4	120	GLY	2.6
41	l4	147	GLU	2.6
63	n7	96	VAL	2.6
65	N9	14	ARG	2.6
4	s2	199	GLN	2.6
51	M5	195	ASN	2.6
6	S4	48	LEU	2.6
19	c7	109	LEU	2.6
21	c9	94	ILE	2.6
24	D2	90	THR	2.6
34	sR	144	LEU	2.6
39	L2	150	LEU	2.6
58	n2	41	ILE	2.6
11	S9	163	PRO	2.6
53	m7	130	TYR	2.6
31	d9	19	ARG	2.6
40	L3	369	ARG	2.6
2	s0	2	SER	2.6
15	C3	13	SER	2.6
36	5	2971	A	2.6
45	l8	121	SER	2.6
85	f	144	GLU	2.6
4	s2	201	ASN	2.6
24	D2	94	LEU	2.6
36	1	1761	C	2.6
45	l8	238	LEU	2.6
58	N2	89	LEU	2.6
63	N7	46	ILE	2.6
74	o8	51	LEU	2.6
14	c2	114	LYS	2.6
39	l2	67	TYR	2.6
1	2	194	U	2.6
1	2	1688	U	2.6
1	6	1708	U	2.6
5	s3	107	PHE	2.6
22	D0	55	PRO	2.6
41	l4	104	LYS	2.6
53	M7	159	LYS	2.6
36	1	2344	U	2.6
1	6	1699	G	2.6
30	D8	25	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
34	sR	160	GLU	2.6
36	1	2950	G	2.6
36	5	1507	G	2.6
55	M9	23	TRP	2.6
80	c0	61	TRP	2.6
2	s0	30	GLN	2.6
59	N3	53	SER	2.6
3	s1	116	LYS	2.6
7	s5	60	ASP	2.6
15	C3	102	LEU	2.6
17	c5	85	ILE	2.6
8	S6	169	TYR	2.6
11	S9	19	TYR	2.6
21	C9	69	LYS	2.6
36	1	1588	A	2.6
39	l2	22	LEU	2.6
51	M5	199	LEU	2.6
80	c0	26	ASP	2.6
82	p0	19	LEU	2.6
22	d0	72	ASN	2.6
16	C4	91	THR	2.6
34	sR	90	ARG	2.6
25	D3	42	PRO	2.6
2	s0	143	VAL	2.6
4	S2	223	GLY	2.6
4	s2	202	GLY	2.6
15	C3	119	GLU	2.6
15	C3	139	TRP	2.6
3	s1	47	LEU	2.6
4	s2	99	LYS	2.6
6	s4	133	LYS	2.6
8	s6	164	LYS	2.6
15	C3	37	ILE	2.6
21	C9	100	ILE	2.6
22	D0	76	SER	2.6
63	n7	80	LEU	2.6
75	O9	5	LYS	2.6
3	s1	100	PHE	2.6
6	s4	39	ARG	2.6
8	S6	138	ALA	2.6
77	Q1	11	ARG	2.6
1	6	1196	A	2.6

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Mol	Chain	Res	Type	RSRZ
30	D8	26	THR	2.6
36	5	2256	A	2.6
36	5	2969	A	2.6
73	o7	20	ASN	2.6
1	6	495	C	2.6
11	S9	27	GLU	2.6
15	c3	10	GLY	2.6
2	S0	168	HIS	2.6
5	S3	164	VAL	2.6
18	c6	7	VAL	2.6
70	o4	34	HIS	2.6
26	d4	18	LEU	2.6
28	D6	10	ARG	2.6
5	S3	149	ALA	2.6
8	S6	105	ASP	2.6
8	s6	144	PHE	2.6
41	L4	70	ALA	2.6
49	m3	153	ASP	2.6
63	n7	136	PHE	2.6
73	O7	15	SER	2.6
25	D3	10	ASN	2.6
54	M8	2	GLY	2.6
59	N3	98	ASN	2.6
2	S0	80	THR	2.6
3	S1	50	LYS	2.6
5	S3	212	LYS	2.6
21	C9	78	LYS	2.6
25	d3	3	LYS	2.6
27	D5	102	THR	2.6
36	1	2957	G	2.6
39	L2	175	VAL	2.6
36	5	1850	A	2.6
1	2	870	C	2.6
5	s3	21	LEU	2.6
10	S8	56	ARG	2.6
1	6	1390	U	2.6
14	C2	126	TRP	2.6
15	C3	125	LEU	2.6
19	c7	38	ILE	2.6
25	D3	59	ILE	2.6
40	L3	252	ILE	2.6
67	O1	104	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
6	S4	259	GLN	2.6
7	s5	69	PHE	2.6
21	C9	59	ALA	2.6
2	s0	157	ASP	2.6
4	s2	181	SER	2.6
82	p0	291	ALA	2.6
2	s0	186	GLY	2.6
21	c9	37	VAL	2.6
21	c9	84	LYS	2.6
29	D7	6	ASP	2.6
40	L3	336	VAL	2.6
61	N5	107	VAL	2.6
64	N8	51	GLY	2.6
8	s6	1	MET	2.6
16	C4	136	ARG	2.6
6	S4	90	ILE	2.6
15	c3	58	HIS	2.6
20	c8	18	LEU	2.6
24	D2	56	HIS	2.6
24	d2	41	MET	2.6
28	d6	5	ARG	2.6
72	o6	2	THR	2.6
73	o7	11	ARG	2.6
10	s8	67	TRP	2.6
28	D6	30	ILE	2.6
79	Q3	83	ILE	2.6
36	1	830	A	2.6
36	5	817	A	2.6
36	5	915	A	2.6
1	2	1333	C	2.6
34	SR	296	ALA	2.6
36	1	47	C	2.6
41	l4	26	PHE	2.6
39	L2	59	ALA	2.6
11	S9	37	LYS	2.6
18	C6	127	LYS	2.6
22	d0	61	LYS	2.6
4	S2	112	GLY	2.6
4	S2	160	GLY	2.6
23	D1	59	VAL	2.6
24	D2	33	VAL	2.6
33	E1	84	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
8	S6	68	LEU	2.6
4	S2	226	THR	2.6
11	s9	147	MET	2.6
19	C7	113	LEU	2.6
24	d2	29	PRO	2.6
29	D7	21	LEU	2.6
47	m0	27	PRO	2.6
51	m5	22	LEU	2.6
53	m7	137	ASN	2.6
14	C2	89	ILE	2.6
15	C3	67	THR	2.6
21	C9	94	ILE	2.6
34	sR	188	ILE	2.6
42	l5	247	ILE	2.6
47	M0	166	ILE	2.6
15	c3	26	PHE	2.5
48	M1	102	PHE	2.5
5	S3	205	ALA	2.5
5	s3	19	ALA	2.5
45	L8	92	LYS	2.5
45	l8	122	LYS	2.5
59	n3	38	ALA	2.5
1	2	720	G	2.5
1	2	1610	G	2.5
8	s6	134	GLY	2.5
60	N4	39	LEU	2.5
13	C1	54	ILE	2.5
13	c1	113	PRO	2.5
15	C3	23	PRO	2.5
21	C9	101	ASN	2.5
32	E0	51	ASN	2.5
80	c0	4	PRO	2.5
6	S4	71	LYS	2.5
13	c1	92	HIS	2.5
34	sR	228	LYS	2.5
13	C1	89	ALA	2.5
29	D7	50	ALA	2.5
34	sR	102	ARG	2.5
67	o1	58	ALA	2.5
5	s3	122	VAL	2.5
10	s8	102	VAL	2.5
31	d9	6	VAL	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
49	M3	138	VAL	2.5
63	N7	96	VAL	2.5
73	O7	4	GLY	2.5
1	2	627	C	2.5
1	2	993	A	2.5
1	6	1634	C	2.5
17	c5	51	SER	2.5
34	SR	252	LEU	2.5
34	sR	291	SER	2.5
36	1	919	U	2.5
36	5	1839	A	2.5
57	N1	85	LEU	2.5
1	2	1316	G	2.5
18	C6	5	PRO	2.5
18	C6	47	LYS	2.5
24	D2	80	ASN	2.5
36	5	1492	G	2.5
8	S6	88	ARG	2.5
22	d0	104	THR	2.5
6	s4	18	TRP	2.5
23	D1	54	ALA	2.5
39	L2	243	THR	2.5
45	l8	154	ALA	2.5
70	o4	25	THR	2.5
73	o7	33	THR	2.5
67	o1	60	TRP	2.5
39	L2	248	GLY	2.5
2	S0	87	LEU	2.5
4	S2	154	LEU	2.5
42	L5	34	LYS	2.5
6	S4	205	PHE	2.5
6	s4	109	PHE	2.5
14	C2	81	ASP	2.5
64	N8	112	ILE	2.5
78	q2	106	PHE	2.5
31	D9	44	ARG	2.5
36	1	1566	A	2.5
36	1	2398	A	2.5
63	N7	65	ARG	2.5
2	S0	132	ALA	2.5
13	C1	92	HIS	2.5
19	c7	105	GLN	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
51	M5	112	ASN	2.5
21	C9	112	GLY	2.5
39	l2	49	VAL	2.5
40	l3	230	THR	2.5
2	S0	88	LYS	2.5
3	S1	96	LEU	2.5
9	S7	99	LEU	2.5
11	S9	30	LEU	2.5
27	d5	42	LEU	2.5
28	d6	23	CYS	2.5
30	d8	45	LYS	2.5
17	c5	84	ILE	2.5
1	2	1414	U	2.5
8	S6	104	PRO	2.5
9	s7	63	PRO	2.5
49	M3	48	PRO	2.5
3	s1	133	TYR	2.5
17	c5	11	VAL	2.5
22	D0	40	ASN	2.5
36	1	931	C	2.5
36	1	2149	A	2.5
36	5	2812	C	2.5
39	L2	181	LYS	2.5
39	l2	215	ASN	2.5
41	l4	239	ALA	2.5
69	o3	52	VAL	2.5
79	q3	14	TYR	2.5
58	n2	79	LEU	2.5
6	S4	3	ARG	2.5
15	c3	106	ARG	2.5
21	C9	111	ILE	2.5
28	D6	36	ILE	2.5
36	1	364	G	2.5
4	S2	65	GLU	2.5
24	D2	9	ASP	2.5
21	C9	75	LYS	2.5
30	D8	6	PRO	2.5
33	e1	112	GLY	2.5
34	SR	104	VAL	2.5
35	sM	170	LYS	2.5
36	1	939	U	2.5
36	1	1436	U	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
40	L3	250	ALA	2.5
7	s5	156	ARG	2.5
20	C8	40	ARG	2.5
73	O7	33	THR	2.5
1	2	1721	A	2.5
5	s3	24	PHE	2.5
12	C0	59	PHE	2.5
21	C9	54	PHE	2.5
28	D6	41	ILE	2.5
36	1	1563	C	2.5
36	1	1667	A	2.5
18	c6	107	LYS	2.5
25	d3	112	LYS	2.5
40	L3	251	CYS	2.5
6	S4	103	TYR	2.5
8	S6	62	PRO	2.5
8	S6	165	GLY	2.5
13	C1	100	TYR	2.5
16	c4	42	VAL	2.5
34	SR	3	SER	2.5
35	sM	168	ALA	2.5
36	5	805	G	2.5
36	5	1655	G	2.5
41	l4	56	ALA	2.5
47	m0	114	GLY	2.5
1	2	174	U	2.5
2	S0	119	ARG	2.5
6	S4	142	HIS	2.5
23	D1	8	LEU	2.5
36	1	2953	U	2.5
85	f	104	ASN	2.5
2	s0	124	THR	2.5
16	c4	89	THR	2.5
33	E1	91	ILE	2.5
34	SR	21	THR	2.5
67	O1	36	ILE	2.5
75	o9	47	THR	2.5
8	s6	161	GLU	2.5
55	M9	60	LYS	2.5
36	5	2145	A	2.5
80	c0	70	GLU	2.5
2	s0	57	LEU	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	S4	182	TYR	2.5
6	s4	9	LEU	2.5
11	s9	36	LEU	2.5
13	C1	77	SER	2.5
21	C9	49	ASP	2.5
34	SR	2	ALA	2.5
41	l4	89	ALA	2.5
64	n8	109	TYR	2.5
70	o4	8	ARG	2.5
85	f	116	PRO	2.5
10	S8	160	PHE	2.5
1	2	1032	G	2.5
2	s0	39	ASN	2.5
8	s6	158	ILE	2.5
10	S8	38	ILE	2.5
19	C7	23	LYS	2.5
36	5	1560	G	2.5
43	l6	146	ILE	2.5
51	M5	72	LYS	2.5
51	m5	90	ASN	2.5
70	o4	54	ILE	2.5
10	s8	195	ARG	2.5
13	c1	147	GLY	2.5
21	c9	86	ARG	2.5
20	C8	146	ALA	2.5
21	C9	4	VAL	2.5
28	d6	84	VAL	2.5
31	d9	51	GLY	2.5
34	sR	155	ARG	2.5
32	E0	40	TYR	2.5
34	sR	6	VAL	2.5
47	m0	188	GLY	2.5
70	o4	51	LEU	2.5
1	2	312	A	2.5
1	2	1331	A	2.5
5	S3	194	LYS	2.5
41	L4	90	PHE	2.5
55	M9	59	SER	2.5
64	N8	3	SER	2.5
1	2	794	U	2.5
24	d2	51	GLU	2.5
4	s2	206	THR	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
18	c6	17	THR	2.5
34	sR	258	THR	2.5
36	5	2508	U	2.5
1	2	1351	G	2.5
2	S0	120	LEU	2.5
7	S5	217	LEU	2.5
21	C9	88	VAL	2.5
23	D1	72	LEU	2.5
24	d2	10	ALA	2.5
34	sR	225	LEU	2.5
36	1	2165	G	2.5
36	1	2977	G	2.5
36	5	916	G	2.5
55	M9	54	ALA	2.5
66	O0	14	LEU	2.5
74	o8	34	ALA	2.5
13	C1	26	LYS	2.5
25	d3	116	ASP	2.5
75	O9	18	LYS	2.5
3	s1	84	ILE	2.5
18	C6	93	HIS	2.5
28	D6	72	HIS	2.5
36	1	877	C	2.5
36	1	2192	C	2.5
36	5	1792	C	2.5
42	L5	88	ILE	2.5
41	l4	94	CYS	2.5
70	o4	16	ARG	2.5
5	s3	112	GLY	2.5
12	C0	40	LEU	2.5
13	C1	125	VAL	2.5
20	C8	141	THR	2.5
25	D3	44	GLY	2.5
15	c3	18	TYR	2.5
21	c9	91	TYR	2.5
34	sR	53	LYS	2.5
35	SM	27	LYS	2.5
53	M7	132	ALA	2.5
61	n5	90	ALA	2.5
80	c0	63	TYR	2.5
7	s5	43	PHE	2.5
8	S6	65	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
13	C1	42	PHE	2.5
25	D3	107	PHE	2.5
36	1	800	G	2.5
40	L3	243	HIS	2.5
67	O1	17	HIS	2.5
1	2	1027	A	2.4
10	S8	199	LYS	2.4
12	C0	44	LYS	2.4
12	C0	68	LEU	2.4
14	C2	133	LEU	2.4
34	SR	73	LEU	2.4
10	s8	76	THR	2.4
34	sR	204	ALA	2.4
82	p0	197	PHE	2.4
2	S0	63	ILE	2.4
5	s3	27	ARG	2.4
6	S4	11	ARG	2.4
6	S4	30	ARG	2.4
15	c3	37	ILE	2.4
34	SR	122	ILE	2.4
73	O7	24	ARG	2.4
24	D2	87	GLU	2.4
12	C0	51	SER	2.4
14	C2	135	MET	2.4
29	d7	48	SER	2.4
40	L3	45	SER	2.4
49	m3	4	SER	2.4
1	2	488	G	2.4
1	2	1386	G	2.4
6	s4	101	LEU	2.4
10	s8	193	LEU	2.4
11	S9	93	LEU	2.4
1	6	1037	C	2.4
1	6	1774	G	2.4
41	L4	52	VAL	2.4
79	q3	66	GLY	2.4
8	S6	61	PHE	2.4
12	C0	16	PHE	2.4
18	c6	109	PHE	2.4
27	D5	58	ARG	2.4
58	N2	64	THR	2.4
64	N8	98	THR	2.4

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Mol	Chain	Res	Type	RSRZ
73	o7	8	PHE	2.4
36	5	2981	U	2.4
8	S6	113	ILE	2.4
15	C3	116	ILE	2.4
44	L7	25	GLN	2.4
2	s0	148	ASP	2.4
13	c1	141	LYS	2.4
28	d6	28	LYS	2.4
39	l2	204	MET	2.4
10	S8	46	VAL	2.4
14	C2	78	LEU	2.4
34	SR	202	LEU	2.4
40	l3	243	HIS	2.4
41	l4	68	GLY	2.4
47	M0	149	VAL	2.4
51	m5	37	HIS	2.4
40	L3	330	GLY	2.4
64	n8	16	SER	2.4
79	q3	50	GLY	2.4
6	S4	27	TYR	2.4
10	S8	83	TYR	2.4
28	D6	22	ARG	2.4
29	d7	16	ALA	2.4
32	E0	35	TYR	2.4
34	SR	279	ALA	2.4
41	L4	62	ALA	2.4
75	O9	16	ALA	2.4
5	S3	165	ASN	2.4
36	5	873	C	2.4
58	N2	87	ASN	2.4
75	o9	43	ASN	2.4
1	2	1002	G	2.4
5	S3	89	GLU	2.4
8	S6	91	GLU	2.4
11	S9	156	ILE	2.4
36	5	2159	U	2.4
9	S7	93	LEU	2.4
24	d2	33	VAL	2.4
32	E0	14	VAL	2.4
34	SR	16	HIS	2.4
34	SR	175	ASP	2.4
39	l2	58	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
54	m8	154	GLY	2.4
64	N8	144	VAL	2.4
69	o3	89	LEU	2.4
8	S6	85	ARG	2.4
23	d1	56	SER	2.4
7	S5	222	LYS	2.4
26	D4	117	LYS	2.4
67	o1	61	LYS	2.4
16	c4	119	THR	2.4
54	M8	88	THR	2.4
79	q3	10	ILE	2.4
1	2	653	C	2.4
1	2	1102	G	2.4
5	S3	93	ASP	2.4
15	c3	59	GLY	2.4
25	D3	19	ARG	2.4
36	1	926	A	2.4
36	1	2922	G	2.4
40	L3	48	GLY	2.4
58	n2	76	LEU	2.4
58	n2	89	LEU	2.4
74	o8	45	VAL	2.4
85	f	67	GLY	2.4
10	S8	182	TYR	2.4
41	L4	100	PHE	2.4
11	S9	115	LYS	2.4
29	d7	58	SER	2.4
39	l2	14	SER	2.4
6	S4	64	ILE	2.4
51	m5	61	ILE	2.4
2	S0	96	THR	2.4
3	s1	148	ASN	2.4
15	C3	137	PRO	2.4
15	c3	91	LEU	2.4
18	c6	73	GLY	2.4
22	d0	59	PRO	2.4
35	sM	40	PRO	2.4
39	L2	178	PRO	2.4
59	N3	34	LEU	2.4
1	2	909	U	2.4
1	2	1527	C	2.4
5	S3	7	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
10	S8	116	HIS	2.4
39	l2	198	LYS	2.4
51	m5	130	PHE	2.4
22	d0	119	ALA	2.4
75	o9	39	ALA	2.4
5	s3	31	GLU	2.4
7	s5	121	ILE	2.4
18	C6	125	GLU	2.4
22	D0	74	GLU	2.4
41	l4	63	GLU	2.4
41	l4	64	SER	2.4
67	O1	59	ILE	2.4
82	p0	293	GLU	2.4
20	C8	145	ARG	2.4
35	SM	108	GLN	2.4
75	O9	42	ARG	2.4
10	S8	24	LYS	2.4
10	S8	181	GLY	2.4
19	C7	123	ASN	2.4
21	C9	9	VAL	2.4
28	D6	67	THR	2.4
29	D7	28	PRO	2.4
34	sR	31	ASN	2.4
39	L2	53	GLY	2.4
41	L4	91	GLY	2.4
48	M1	54	VAL	2.4
48	M1	160	VAL	2.4
54	M8	150	VAL	2.4
64	n8	72	VAL	2.4
1	2	261	U	2.4
2	s0	204	TYR	2.4
19	C7	51	ALA	2.4
75	o9	44	TRP	2.4
29	d7	26	GLN	2.4
36	5	1588	A	2.4
35	SM	17	VAL	2.4
41	L4	59	GLN	2.4
45	l8	157	VAL	2.4
49	M3	170	LEU	2.4
53	M7	95	LEU	2.4
1	6	936	G	2.4
1	6	1488	G	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	S2	219	GLY	2.4
58	N2	81	LYS	2.4
62	n6	8	VAL	2.4
2	s0	81	PHE	2.4
3	S1	138	PHE	2.4
8	S6	86	PRO	2.4
36	5	1845	G	2.4
36	5	1875	G	2.4
13	C1	83	THR	2.4
13	C1	124	THR	2.4
19	c7	30	THR	2.4
40	L3	337	THR	2.4
54	m8	168	THR	2.4
21	C9	33	TYR	2.4
33	E1	93	HIS	2.4
52	m6	61	ALA	2.4
79	q3	52	ALA	2.4
12	C0	61	TRP	2.4
36	5	2137	U	2.4
1	2	1317	C	2.4
3	S1	45	LYS	2.4
3	S1	48	VAL	2.4
3	s1	233	GLY	2.4
5	s3	41	VAL	2.4
14	C2	60	VAL	2.4
17	C5	65	LEU	2.4
19	c7	46	LEU	2.4
23	D1	39	VAL	2.4
25	d3	17	VAL	2.4
62	n6	57	LEU	2.4
63	n7	21	LYS	2.4
29	d7	38	PRO	2.4
34	sR	57	PRO	2.4
36	5	914	A	2.4
36	5	2941	A	2.4
40	L3	370	PHE	2.4
61	N5	32	PHE	2.4
73	o7	2	GLY	2.4
1	2	1425	A	2.4
24	D2	77	PRO	2.4
4	S2	222	TYR	2.4
10	s8	48	THR	2.4

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Mol	Chain	Res	Type	RSRZ
16	c4	132	ARG	2.4
55	M9	63	THR	2.4
64	N8	74	ASN	2.4
69	o3	65	ARG	2.4
70	o4	62	TYR	2.4
7	s5	172	ILE	2.4
15	c3	66	ILE	2.4
25	d3	14	LYS	2.4
34	SR	136	ILE	2.4
35	SM	83	LYS	2.4
39	l2	41	ILE	2.4
39	l2	209	HIS	2.4
7	S5	25	LEU	2.4
20	C8	15	LEU	2.4
36	5	2980	U	2.4
55	M9	138	LEU	2.4
4	S2	163	GLY	2.4
17	c5	136	SER	2.4
34	SR	237	GLN	2.4
52	m6	69	GLY	2.4
1	2	1518	C	2.4
1	6	1090	C	2.4
16	c4	57	PRO	2.4
64	n8	26	ARG	2.4
19	C7	76	GLU	2.4
45	L8	113	ALA	2.4
45	l8	161	GLU	2.4
10	S8	54	LYS	2.4
18	C6	30	LYS	2.4
33	e1	125	THR	2.4
36	1	920	A	2.4
36	5	1842	A	2.4
41	l4	74	ILE	2.4
56	N0	88	HIS	2.4
66	o0	100	ILE	2.4
70	o4	20	ILE	2.4
3	S1	47	LEU	2.4
6	S4	206	ASP	2.4
21	C9	105	LEU	2.4
42	L5	103	LEU	2.4
58	N2	76	LEU	2.4
58	n2	17	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	2	1607	G	2.4
1	6	959	U	2.4
1	6	1286	U	2.4
1	6	1616	G	2.4
5	s3	74	GLN	2.4
73	o7	15	SER	2.4
7	s5	41	LYS	2.4
8	S6	83	CYS	2.4
34	sR	137	LYS	2.4
39	l2	143	GLU	2.4
47	m0	56	GLU	2.4
1	2	1128	C	2.4
2	s0	163	ASN	2.4
16	c4	112	ILE	2.4
35	SM	90	ALA	2.4
36	1	2507	C	2.4
34	SR	130	THR	2.4
4	S2	35	TRP	2.3
13	c1	68	GLY	2.3
18	c6	22	VAL	2.3
30	D8	49	ARG	2.3
34	sR	154	VAL	2.3
36	1	1571	A	2.3
41	l4	207	VAL	2.3
45	L8	94	PHE	2.3
63	N7	92	PHE	2.3
68	o2	37	GLY	2.3
39	l2	47	GLN	2.3
39	l2	233	GLN	2.3
70	o4	7	PHE	2.3
10	s8	61	GLU	2.3
19	c7	23	LYS	2.3
21	C9	99	SER	2.3
31	D9	4	GLU	2.3
80	c0	71	GLU	2.3
2	s0	26	ALA	2.3
2	s0	132	ALA	2.3
5	S3	49	ILE	2.3
15	c3	7	ALA	2.3
17	c5	116	LEU	2.3
21	c9	132	LEU	2.3
1	2	1625	C	2.3

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Mol	Chain	Res	Type	RSRZ
2	S0	109	ASN	2.3
2	s0	127	ARG	2.3
3	s1	150	VAL	2.3
5	S3	27	ARG	2.3
24	d2	16	ASN	2.3
46	L9	191	LEU	2.3
67	O1	20	LEU	2.3
75	o9	50	ASN	2.3
79	Q3	86	LEU	2.3
13	C1	68	GLY	2.3
13	c1	140	VAL	2.3
31	D9	23	VAL	2.3
49	M3	174	ARG	2.3
11	s9	10	LYS	2.3
35	SM	92	ASP	2.3
67	O1	26	LYS	2.3
77	Q1	8	LYS	2.3
85	f	97	ASP	2.3
1	2	621	A	2.3
36	1	48	A	2.3
36	1	1575	A	2.3
10	S8	16	ALA	2.3
15	c3	84	ILE	2.3
16	c4	17	ALA	2.3
28	D6	7	SER	2.3
36	5	2978	U	2.3
70	o4	55	SER	2.3
73	O7	36	SER	2.3
9	s7	104	ARG	2.3
39	L2	190	ARG	2.3
39	l2	247	ARG	2.3
13	C1	75	VAL	2.3
28	D6	94	ASN	2.3
36	5	2155	G	2.3
42	l5	55	PHE	2.3
49	m3	131	LYS	2.3
59	N3	64	LYS	2.3
62	N6	124	GLY	2.3
75	O9	50	ASN	2.3
2	S0	54	TRP	2.3
2	S0	33	GLN	2.3
46	l9	190	ASP	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	2	1116	A	2.3
3	s1	86	LEU	2.3
5	S3	160	SER	2.3
28	d6	40	ALA	2.3
32	E0	27	PRO	2.3
36	1	2142	A	2.3
36	1	2147	A	2.3
39	l2	9	ARG	2.3
49	M3	132	ALA	2.3
58	N2	105	LEU	2.3
80	c0	40	LEU	2.3
5	S3	136	VAL	2.3
11	S9	122	VAL	2.3
13	c1	119	VAL	2.3
27	D5	73	GLY	2.3
39	l2	207	VAL	2.3
46	L9	43	VAL	2.3
49	M3	31	LYS	2.3
59	N3	8	GLY	2.3
69	o3	9	VAL	2.3
14	c2	38	HIS	2.3
4	S2	158	THR	2.3
19	C7	55	THR	2.3
34	SR	88	THR	2.3
68	O2	32	TRP	2.3
5	S3	154	ASP	2.3
1	6	1624	C	2.3
69	o3	54	ARG	2.3
24	d2	47	ILE	2.3
34	SR	244	ALA	2.3
35	sM	162	ALA	2.3
59	N3	13	ILE	2.3
9	S7	138	LYS	2.3
9	s7	64	VAL	2.3
13	C1	2	SER	2.3
15	c3	120	SER	2.3
18	C6	34	SER	2.3
42	L5	53	VAL	2.3
52	m6	80	PHE	2.3
63	n7	23	VAL	2.3
1	2	1583	A	2.3
30	d8	46	GLY	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
54	m8	156	GLY	2.3
40	L3	323	MET	2.3
8	S6	31	ARG	2.3
30	D8	29	ARG	2.3
39	l2	241	ARG	2.3
40	L3	4	ARG	2.3
65	N9	6	ASN	2.3
4	S2	225	LEU	2.3
6	s4	22	LYS	2.3
6	s4	84	ALA	2.3
9	S7	143	LEU	2.3
13	c1	94	ILE	2.3
15	c3	109	LYS	2.3
21	C9	22	LEU	2.3
48	m1	173	ASP	2.3
59	N3	49	LEU	2.3
80	c0	45	ALA	2.3
1	2	376	C	2.3
2	S0	50	VAL	2.3
4	S2	86	VAL	2.3
5	s3	25	PHE	2.3
1	2	1484	G	2.3
2	s0	114	SER	2.3
21	C9	2	PRO	2.3
22	d0	111	GLY	2.3
24	D2	30	SER	2.3
52	M6	80	PHE	2.3
36	5	360	G	2.3
36	5	1833	G	2.3
75	o9	24	PRO	2.3
36	1	2955	U	2.3
40	l3	19	ARG	2.3
1	2	169	A	2.3
1	2	1025	A	2.3
5	S3	179	GLN	2.3
10	s8	94	ASN	2.3
36	1	2956	A	2.3
12	C0	46	LEU	2.3
41	L4	92	ASN	2.3
41	L4	110	ASN	2.3
40	L3	49	TYR	2.3
40	L3	328	ILE	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
44	L7	136	TYR	2.3
52	m6	98	ALA	2.3
67	o1	75	ILE	2.3
71	o5	118	ILE	2.3
6	S4	109	PHE	2.3
15	c3	52	VAL	2.3
26	D4	70	VAL	2.3
32	e0	44	PHE	2.3
42	L5	144	VAL	2.3
2	S0	179	ARG	2.3
20	c8	76	PRO	2.3
34	sR	105	GLY	2.3
39	l2	201	GLY	2.3
1	2	724	C	2.3
1	6	1399	C	2.3
10	S8	45	SER	2.3
39	L2	18	SER	2.3
49	M3	164	GLU	2.3
54	m8	151	ARG	2.3
8	S6	223	LYS	2.3
1	2	1035	G	2.3
4	s2	144	TRP	2.3
6	S4	164	LEU	2.3
4	s2	183	ALA	2.3
17	c5	121	ILE	2.3
20	C8	125	ILE	2.3
28	d6	94	ASN	2.3
42	l5	294	ALA	2.3
54	m8	139	ILE	2.3
61	N5	60	TYR	2.3
79	Q3	69	TYR	2.3
80	c0	92	THR	2.3
8	S6	36	VAL	2.3
15	C3	26	PHE	2.3
22	D0	31	VAL	2.3
82	p0	283	ALA	2.3
2	s0	167	LYS	2.3
5	S3	135	GLU	2.3
25	D3	88	PRO	2.3
16	C4	46	MET	2.3
23	D1	61	SER	2.3
34	sR	152	SER	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
61	N5	100	LYS	2.3
61	n5	92	LYS	2.3
73	O7	35	SER	2.3
1	6	1773	C	2.3
3	s1	228	LEU	2.3
1	2	959	U	2.3
11	s9	156	ILE	2.3
15	c3	36	GLN	2.3
15	c3	117	LEU	2.3
36	1	1017	C	2.3
36	1	1907	C	2.3
74	O8	51	LEU	2.3
6	S4	99	PHE	2.3
11	S9	56	ALA	2.3
23	d1	58	TYR	2.3
24	D2	8	ALA	2.3
34	SR	241	PHE	2.3
35	sM	128	ALA	2.3
35	sM	131	ALA	2.3
36	5	2542	U	2.3
47	M0	50	VAL	2.3
66	O0	81	VAL	2.3
67	o1	31	ARG	2.3
70	O4	39	ALA	2.3
10	s8	39	GLY	2.3
12	C0	67	THR	2.3
15	C3	108	ASP	2.3
16	C4	131	GLY	2.3
24	D2	105	THR	2.3
58	n2	16	THR	2.3
1	2	400	A	2.3
1	2	505	A	2.3
15	C3	109	LYS	2.3
36	1	929	A	2.3
36	5	909	G	2.3
51	m5	77	LYS	2.3
69	o3	57	LYS	2.3
73	o7	3	LYS	2.3
15	c3	17	PRO	2.3
19	C7	86	PRO	2.3
65	n9	24	PRO	2.3
4	S2	190	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
5	S3	86	LEU	2.3
9	s7	185	ILE	2.3
10	s8	169	ILE	2.3
12	C0	62	GLN	2.3
19	c7	62	GLN	2.3
21	c9	23	GLN	2.3
2	s0	50	VAL	2.3
11	s9	104	PHE	2.3
19	C7	80	ARG	2.3
73	O7	21	ARG	2.3
75	o9	9	ILE	2.3
77	q1	5	TRP	2.3
80	c0	32	HIS	2.3
29	d7	53	ALA	2.3
40	L3	51	ALA	2.3
52	m6	63	ALA	2.3
1	2	968	U	2.3
1	2	1684	U	2.3
14	C2	130	THR	2.3
26	D4	122	GLY	2.3
28	d6	91	ASP	2.3
34	SR	74	THR	2.3
34	sR	39	ASP	2.3
36	1	2314	U	2.3
60	N4	24	GLY	2.3
67	o1	18	LYS	2.3
16	c4	117	ASP	2.3
19	c7	58	MET	2.3
1	2	1521	G	2.3
1	6	1789	G	2.3
6	S4	56	LEU	2.3
36	5	1514	G	2.3
2	S0	78	SER	2.3
11	S9	110	GLN	2.3
25	D3	38	PHE	2.3
39	L2	217	GLN	2.3
48	M1	55	ARG	2.3
67	O1	24	SER	2.3
80	c0	77	ARG	2.3
5	s3	149	ALA	2.3
5	s3	206	VAL	2.3
9	S7	61	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
27	d5	46	LYS	2.3
28	D6	24	VAL	2.3
33	e1	98	VAL	2.3
41	l4	199	TRP	2.3
45	L8	197	VAL	2.3
67	O1	60	TRP	2.3
1	2	1362	U	2.3
7	s5	79	ASN	2.3
23	D1	66	ASP	2.3
25	D3	90	ASP	2.3
36	1	2245	C	2.3
36	1	3351	U	2.3
36	5	823	C	2.3
36	5	1764	U	2.3
2	S0	4	PRO	2.3
29	D7	33	LEU	2.3
45	L8	46	LEU	2.3
53	m7	23	ARG	2.3
53	m7	126	ARG	2.3
60	N4	54	LEU	2.3
70	O4	31	ARG	2.3
79	Q3	29	LEU	2.3
19	C7	49	LYS	2.3
24	d2	34	ILE	2.3
55	M9	50	ILE	2.3
2	S0	36	TYR	2.3
8	s6	97	VAL	2.3
8	s6	148	SER	2.3
10	s8	100	ALA	2.3
11	S9	148	VAL	2.3
13	C1	140	VAL	2.3
29	d7	13	ALA	2.3
47	m0	11	TYR	2.3
70	O4	73	SER	2.3
73	o7	30	GLN	2.3
1	6	1466	G	2.2
67	O1	63	GLY	2.2
1	2	504	U	2.2
1	2	1735	U	2.2
14	c2	23	THR	2.2
29	D7	17	ARG	2.2
35	SM	81	THR	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
34	sR	117	LYS	2.2
36	1	1764	U	2.2
54	m8	140	LEU	2.2
70	o4	6	THR	2.2
1	2	1591	C	2.2
21	c9	69	LYS	2.2
34	SR	192	PHE	2.2
36	1	2405	C	2.2
36	5	1579	C	2.2
60	n4	90	ILE	2.2
62	n6	45	ILE	2.2
14	C2	22	VAL	2.2
40	l3	260	VAL	2.2
45	l8	203	VAL	2.2
69	o3	66	VAL	2.2
2	S0	169	SER	2.2
5	S3	52	ALA	2.2
15	C3	103	GLU	2.2
24	d2	56	HIS	2.2
24	d2	58	SER	2.2
25	D3	49	ALA	2.2
50	M4	138	ALA	2.2
79	q3	15	GLY	2.2
82	p0	294	ALA	2.2
41	l4	106	TRP	2.2
1	2	807	A	2.2
23	D1	71	ARG	2.2
36	5	806	A	2.2
55	M9	74	ARG	2.2
3	S1	54	LEU	2.2
25	d3	114	LYS	2.2
43	l6	43	LEU	2.2
58	N2	37	LEU	2.2
64	n8	73	LEU	2.2
1	2	175	G	2.2
13	C1	150	ASN	2.2
22	D0	44	ASN	2.2
51	m5	181	ASN	2.2
70	o4	24	LYS	2.2
73	o7	31	LYS	2.2
1	2	1115	U	2.2
11	S9	77	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
29	d7	23	THR	2.2
33	e1	102	VAL	2.2
36	5	2493	U	2.2
54	m8	153	PHE	2.2
54	m8	172	PHE	2.2
63	N7	82	PRO	2.2
1	6	1379	C	2.2
4	S2	233	GLN	2.2
6	s4	13	ALA	2.2
25	d3	119	GLY	2.2
29	d7	68	GLY	2.2
34	SR	293	ALA	2.2
58	N2	36	TYR	2.2
19	C7	56	HIS	2.2
21	C9	5	SER	2.2
24	D2	57	ARG	2.2
41	l4	53	SER	2.2
41	l4	58	HIS	2.2
67	O1	62	ARG	2.2
69	o3	82	ARG	2.2
9	S7	129	LEU	2.2
21	c9	27	LYS	2.2
23	d1	72	LEU	2.2
40	L3	237	LYS	2.2
41	l4	187	LEU	2.2
66	o0	84	LEU	2.2
1	2	740	A	2.2
1	6	1027	A	2.2
7	S5	29	ILE	2.2
13	C1	106	ASN	2.2
19	C7	36	ASP	2.2
25	D3	89	ASN	2.2
25	D3	117	ILE	2.2
26	D4	121	THR	2.2
34	SR	103	PHE	2.2
45	l8	110	THR	2.2
63	n7	92	PHE	2.2
64	N8	104	THR	2.2
82	p0	86	PHE	2.2
85	f	122	ASP	2.2
22	D0	116	VAL	2.2
64	n8	119	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	6	867	G	2.2
6	S4	82	TYR	2.2
13	C1	16	GLN	2.2
18	c6	16	ALA	2.2
21	C9	120	GLY	2.2
22	d0	89	ARG	2.2
36	1	909	G	2.2
36	1	2952	G	2.2
36	5	2952	G	2.2
42	L5	30	TYR	2.2
44	L7	135	ALA	2.2
51	m5	62	TYR	2.2
22	d0	69	LYS	2.2
25	D3	114	LYS	2.2
49	M3	16	LYS	2.2
1	2	975	C	2.2
4	S2	240	LEU	2.2
6	s4	24	SER	2.2
16	c4	102	LEU	2.2
36	5	1846	C	2.2
39	l2	71	LEU	2.2
43	l6	2	SER	2.2
76	Q0	85	LEU	2.2
10	s8	43	ILE	2.2
11	S9	85	VAL	2.2
13	C1	109	VAL	2.2
14	C2	121	VAL	2.2
18	C6	31	VAL	2.2
41	l4	25	VAL	2.2
55	m9	151	ARG	2.2
58	N2	91	ASP	2.2
79	Q3	26	VAL	2.2
2	S0	65	ALA	2.2
7	s5	39	GLU	2.2
9	S7	63	PRO	2.2
28	D6	95	ARG	2.2
18	c6	139	GLN	2.2
64	n8	27	LYS	2.2
69	O3	20	LYS	2.2
80	c0	30	ALA	2.2
36	1	1782	U	2.2
24	D2	113	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
42	L5	115	LEU	2.2
1	6	1155	G	2.2
36	1	1845	G	2.2
36	1	2316	G	2.2
36	1	2973	G	2.2
36	5	2165	G	2.2
73	o7	26	SER	2.2
10	S8	25	ARG	2.2
13	C1	135	VAL	2.2
21	c9	100	ILE	2.2
24	d2	75	ILE	2.2
39	L2	134	VAL	2.2
55	m9	51	VAL	2.2
57	n1	80	VAL	2.2
2	S0	56	LYS	2.2
14	C2	80	ASN	2.2
23	D1	50	TYR	2.2
28	D6	13	LYS	2.2
32	E0	32	GLY	2.2
33	E1	111	GLU	2.2
35	SM	114	LYS	2.2
55	M9	53	LYS	2.2
55	m9	60	LYS	2.2
61	n5	120	LYS	2.2
67	O1	61	LYS	2.2
40	l3	217	ALA	2.2
65	N9	55	ALA	2.2
68	O2	29	ALA	2.2
77	q1	22	ALA	2.2
78	q2	43	TYR	2.2
79	q3	51	ALA	2.2
1	2	1797	A	2.2
7	s5	25	LEU	2.2
30	d8	54	LEU	2.2
36	1	1491	A	2.2
41	l4	235	LEU	2.2
34	sR	251	TRP	2.2
36	1	2974	U	2.2
5	S3	77	PHE	2.2
17	c5	102	PHE	2.2
29	D7	14	SER	2.2
32	e0	56	MET	2.2

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Mol	Chain	Res	Type	RSRZ
34	SR	294	TRP	2.2
41	l4	250	TRP	2.2
19	C7	47	ARG	2.2
35	SM	28	SER	2.2
41	l4	61	SER	2.2
1	2	337	G	2.2
5	s3	192	PRO	2.2
6	S4	79	ASP	2.2
36	1	1547	G	2.2
36	1	1889	G	2.2
36	1	1954	G	2.2
36	5	912	G	2.2
36	5	1117	G	2.2
4	s2	210	THR	2.2
7	s5	127	GLN	2.2
15	C3	138	ASN	2.2
17	c5	87	PRO	2.2
22	d0	55	PRO	2.2
78	q2	47	GLN	2.2
80	c0	36	ASP	2.2
63	n7	76	ASN	2.2
13	c1	42	PHE	2.2
16	C4	27	PHE	2.2
18	c6	123	ARG	2.2
19	c7	7	LYS	2.2
21	C9	45	MET	2.2
24	D2	88	LYS	2.2
5	S3	126	VAL	2.2
9	s7	181	ILE	2.2
10	S8	37	LYS	2.2
25	d3	7	ARG	2.2
47	m0	95	HIS	2.2
60	N4	12	LYS	2.2
67	O1	10	ARG	2.2
69	O3	99	ARG	2.2
79	q3	23	ARG	2.2
36	1	665	A	2.2
36	1	2138	A	2.2
36	5	2954	U	2.2
8	S6	82	SER	2.2
10	S8	149	SER	2.2
5	S3	121	GLY	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
6	S4	74	GLY	2.2
27	d5	84	GLU	2.2
62	N6	127	GLU	2.2
35	SM	135	ALA	2.2
39	l2	235	ALA	2.2
2	S0	59	LEU	2.2
2	s0	97	PRO	2.2
6	S4	207	LEU	2.2
39	l2	237	LEU	2.2
62	n6	35	LEU	2.2
1	2	356	G	2.2
5	S3	65	ARG	2.2
5	s3	46	THR	2.2
25	d3	123	LYS	2.2
29	D7	47	PHE	2.2
36	5	2977	G	2.2
42	l5	109	THR	2.2
49	M3	21	ARG	2.2
73	O7	48	ASN	2.2
17	c5	119	PHE	2.2
47	m0	217	PHE	2.2
5	s3	136	VAL	2.2
15	c3	60	VAL	2.2
42	L5	95	TRP	2.2
51	m5	142	ILE	2.2
1	2	1628	U	2.2
18	c6	56	GLY	2.2
36	1	2979	U	2.2
1	2	1587	A	2.2
1	6	713	A	2.2
1	6	1081	A	2.2
7	s5	77	TYR	2.2
3	S1	188	LEU	2.2
7	s5	198	LEU	2.2
58	n2	53	ALA	2.2
5	S3	75	LYS	2.2
6	S4	59	ARG	2.2
23	D1	74	GLN	2.2
29	D7	70	LYS	2.2
31	d9	54	LYS	2.2
32	e0	60	PRO	2.2
34	sR	51	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
45	L8	207	ASP	2.2
55	m9	74	ARG	2.2
69	o3	60	ARG	2.2
75	o9	4	GLN	2.2
34	sR	278	PHE	2.2
1	2	1323	C	2.2
1	6	1796	C	2.2
4	s2	167	VAL	2.2
6	S4	70	VAL	2.2
16	c4	121	VAL	2.2
17	C5	28	MET	2.2
40	L3	229	VAL	2.2
54	m8	152	HIS	2.2
82	p0	27	VAL	2.2
1	2	954	G	2.2
1	2	1101	G	2.2
36	1	1493	G	2.2
36	1	2122	G	2.2
36	1	2246	G	2.2
64	n8	51	GLY	2.2
2	s0	84	ARG	2.2
3	s1	144	ARG	2.2
13	c1	40	LEU	2.2
21	C9	68	ARG	2.2
29	D7	73	LEU	2.2
34	sR	59	ARG	2.2
36	1	3287	U	2.2
39	l2	190	ARG	2.2
45	L8	55	TYR	2.2
51	m5	192	LYS	2.2
59	N3	51	ALA	2.2
59	n3	63	LYS	2.2
60	n4	96	LEU	2.2
78	q2	60	LYS	2.2
1	2	907	A	2.2
1	2	1088	A	2.2
7	S5	184	PHE	2.2
9	s7	123	ASP	2.2
23	D1	14	PRO	2.2
23	D1	67	ASP	2.2
24	D2	54	ASP	2.2
40	L3	46	PHE	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	s1	107	THR	2.2
4	s2	102	VAL	2.2
4	s2	179	VAL	2.2
6	s4	208	VAL	2.2
8	s6	128	THR	2.2
30	D8	5	THR	2.2
42	L5	159	VAL	2.2
53	m7	24	VAL	2.2
74	o8	55	VAL	2.2
1	6	1787	C	2.2
29	D7	49	HIS	2.2
34	sR	125	GLY	2.2
9	S7	101	LYS	2.2
11	S9	105	LEU	2.2
21	C9	84	LYS	2.2
26	D4	20	ARG	2.2
36	1	918	C	2.2
6	s4	41	SER	2.2
15	C3	95	ALA	2.2
16	C4	101	ALA	2.2
22	d0	34	LEU	2.2
39	L2	10	LYS	2.2
48	m1	12	LEU	2.2
75	O9	37	TYR	2.2
25	d3	86	PHE	2.2
38	8	81	U	2.2
1	6	624	G	2.2
1	6	1278	G	2.2
36	1	867	G	2.2
54	m8	96	PHE	2.2
3	s1	65	VAL	2.2
18	C6	113	ASP	2.2
30	d8	52	ASP	2.2
64	n8	71	PRO	2.2
20	c8	81	ILE	2.2
1	2	1023	A	2.2
1	2	1421	A	2.2
4	s2	81	MET	2.2
5	S3	209	ILE	2.2
22	D0	115	GLU	2.2
48	M1	18	VAL	2.2
14	C2	55	GLY	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
36	5	2149	A	2.2
23	D1	16	LYS	2.2
25	D3	3	LYS	2.2
39	L2	7	ASN	2.2
43	L6	134	ARG	2.2
64	n8	8	THR	2.2
70	O4	18	ASN	2.2
79	q3	70	THR	2.2
10	S8	29	LEU	2.1
14	c2	58	LEU	2.1
40	L3	338	LEU	2.1
47	M0	167	LEU	2.1
28	D6	48	ALA	2.1
59	N3	94	TYR	2.1
1	6	393	C	2.1
18	c6	15	SER	2.1
19	C7	43	SER	2.1
1	6	1029	U	2.1
5	s3	56	GLN	2.1
26	d4	72	PHE	2.1
40	L3	379	PHE	2.1
48	M1	90	GLN	2.1
2	s0	47	VAL	2.1
4	S2	141	ARG	2.1
11	S9	63	ASP	2.1
13	c1	66	ILE	2.1
30	D8	48	VAL	2.1
34	sR	136	ILE	2.1
28	D6	74	CYS	2.1
34	sR	316	MET	2.1
53	M7	128	ARG	2.1
62	n6	58	VAL	2.1
39	l2	221	LYS	2.1
67	O1	41	LYS	2.1
36	1	910	G	2.1
36	5	3080	G	2.1
38	8	15	G	2.1
79	Q3	19	GLY	2.1
6	S4	57	ASN	2.1
2	s0	36	TYR	2.1
10	S8	76	THR	2.1
19	C7	24	LEU	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
24	D2	89	TRP	2.1
45	l8	191	ASN	2.1
77	Q1	13	LEU	2.1
82	p0	93	LEU	2.1
35	sM	134	ALA	2.1
63	n7	118	PHE	2.1
2	S0	15	GLN	2.1
5	S3	162	GLN	2.1
7	s5	66	GLN	2.1
1	2	239	C	2.1
5	S3	106	LYS	2.1
10	s8	46	VAL	2.1
23	d1	34	ILE	2.1
36	1	1856	C	2.1
36	1	2151	C	2.1
36	5	2098	C	2.1
55	M9	142	ILE	2.1
59	n3	19	VAL	2.1
70	O4	9	ARG	2.1
1	2	1314	U	2.1
10	S8	50	GLY	2.1
36	5	2436	U	2.1
39	L2	51	ASP	2.1
6	S4	42	LEU	2.1
2	S0	46	HIS	2.1
2	s0	138	TYR	2.1
4	S2	247	ALA	2.1
10	s8	40	ALA	2.1
15	c3	128	TYR	2.1
22	d0	44	ASN	2.1
35	SM	87	THR	2.1
51	m5	34	ASN	2.1
59	n3	33	ASN	2.1
70	O4	68	THR	2.1
79	Q3	14	TYR	2.1
1	2	972	G	2.1
1	2	1020	A	2.1
1	2	1364	G	2.1
4	S2	91	ARG	2.1
5	S3	40	ARG	2.1
9	s7	151	LYS	2.1
19	c7	14	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
29	d7	5	GLN	2.1
42	l5	270	LYS	2.1
43	l6	70	LYS	2.1
51	m5	67	ARG	2.1
51	m5	72	LYS	2.1
54	M8	92	ARG	2.1
9	S7	187	SER	2.1
12	C0	86	ILE	2.1
14	c2	71	ILE	2.1
11	S9	18	PRO	2.1
1	2	1022	C	2.1
21	C9	82	GLY	2.1
24	d2	95	PRO	2.1
1	2	1104	U	2.1
4	S2	78	ASP	2.1
5	s3	204	ASP	2.1
11	s9	59	LEU	2.1
11	s9	70	LEU	2.1
29	D7	41	LEU	2.1
37	7	73	C	2.1
41	l4	11	LEU	2.1
59	N3	93	LEU	2.1
62	n6	104	LEU	2.1
78	q2	35	LEU	2.1
10	s8	84	HIS	2.1
11	S9	95	TYR	2.1
8	S6	163	THR	2.1
11	S9	16	LYS	2.1
18	c6	37	THR	2.1
19	C7	33	ARG	2.1
33	e1	92	LYS	2.1
39	l2	187	HIS	2.1
41	l4	90	PHE	2.1
65	n9	7	HIS	2.1
69	o3	13	HIS	2.1
79	q3	63	THR	2.1
4	S2	167	VAL	2.1
8	S6	41	VAL	2.1
13	C1	139	VAL	2.1
41	l4	77	VAL	2.1
70	O4	65	VAL	2.1
1	6	623	A	2.1

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Mol	Chain	Res	Type	RSRZ
1	6	1300	A	2.1
7	S5	93	LEU	2.1
18	c6	116	LEU	2.1
19	c7	43	SER	2.1
32	E0	30	PRO	2.1
36	1	651	G	2.1
36	1	921	A	2.1
36	1	924	G	2.1
36	1	1306	G	2.1
36	5	443	G	2.1
36	5	904	A	2.1
36	5	913	A	2.1
36	5	1573	G	2.1
36	5	2808	A	2.1
51	m5	78	GLY	2.1
64	n8	108	GLY	2.1
1	6	1283	U	2.1
5	s3	93	ASP	2.1
1	6	1404	C	2.1
8	S6	100	ALA	2.1
13	c1	146	ALA	2.1
16	c4	135	ARG	2.1
33	e1	110	ALA	2.1
36	5	1437	C	2.1
69	o3	50	ALA	2.1
70	O4	19	LYS	2.1
79	Q3	23	ARG	2.1
22	d0	80	GLU	2.1
6	S4	248	ILE	2.1
15	c3	116	ILE	2.1
17	C5	50	THR	2.1
35	sM	57	ASN	2.1
41	L4	60	THR	2.1
73	o7	58	THR	2.1
48	m1	39	GLN	2.1
2	S0	172	LEU	2.1
3	S1	103	MET	2.1
39	l2	11	GLY	2.1
39	l2	245	LEU	2.1
40	l3	178	LEU	2.1
17	c5	72	LYS	2.1
28	D6	37	LYS	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
39	L2	234	LYS	2.1
41	l4	277	PRO	2.1
63	N7	132	SER	2.1
68	O2	53	PRO	2.1
70	O4	26	PRO	2.1
75	o9	48	LYS	2.1
1	2	941	A	2.1
1	2	1296	A	2.1
6	s4	86	PHE	2.1
36	1	2345	A	2.1
42	L5	145	PHE	2.1
43	l6	142	ASP	2.1
45	l8	34	PHE	2.1
1	2	1387	G	2.1
1	6	968	U	2.1
1	6	1050	G	2.1
1	6	1793	G	2.1
36	1	912	G	2.1
4	s2	36	VAL	2.1
5	S3	37	VAL	2.1
5	s3	20	GLU	2.1
2	s0	131	GLN	2.1
5	S3	46	THR	2.1
13	C1	131	ILE	2.1
15	C3	134	VAL	2.1
17	C5	121	ILE	2.1
30	d8	15	VAL	2.1
31	d9	53	ASN	2.1
42	l5	4	GLN	2.1
49	m3	19	GLN	2.1
52	M6	65	ASN	2.1
68	o2	41	VAL	2.1
34	sR	237	GLN	2.1
39	L2	192	LYS	2.1
40	l3	238	LEU	2.1
41	L4	79	GLY	2.1
41	l4	179	LEU	2.1
57	N1	59	GLY	2.1
46	L9	31	ARG	2.1
51	m5	147	ARG	2.1
61	N5	40	LEU	2.1
74	o8	17	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	S0	81	PHE	2.1
4	S2	227	PRO	2.1
7	S5	77	TYR	2.1
4	s2	120	GLU	2.1
10	S8	187	GLU	2.1
15	c3	57	ALA	2.1
31	D9	34	TYR	2.1
34	SR	109	ASP	2.1
34	sR	165	ASP	2.1
45	l8	254	ASP	2.1
49	M3	135	ALA	2.1
52	M6	40	GLU	2.1
55	m9	87	ALA	2.1
67	o1	40	ALA	2.1
78	q2	33	ALA	2.1
1	2	746	A	2.1
1	2	992	A	2.1
20	C8	55	HIS	2.1
1	6	1044	U	2.1
21	c9	135	ILE	2.1
36	5	1491	A	2.1
57	N1	74	VAL	2.1
6	S4	62	LYS	2.1
1	2	625	C	2.1
1	2	867	G	2.1
8	s6	140	ASN	2.1
9	S7	133	THR	2.1
13	C1	72	THR	2.1
15	C3	3	ARG	2.1
18	C6	89	LEU	2.1
25	d3	9	LEU	2.1
36	1	2948	C	2.1
36	1	3286	G	2.1
36	5	910	G	2.1
36	5	1586	G	2.1
44	L7	124	LEU	2.1
45	l8	243	GLN	2.1
49	m3	180	ARG	2.1
51	m5	163	GLY	2.1
55	m9	56	THR	2.1
70	O4	61	GLN	2.1
73	o7	67	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
79	q3	5	THR	2.1
13	C1	115	PHE	2.1
21	C9	96	ALA	2.1
23	d1	68	SER	2.1
24	d2	17	ALA	2.1
42	L5	134	ALA	2.1
59	n3	35	TYR	2.1
61	N5	103	TYR	2.1
13	C1	25	VAL	2.1
8	s6	132	ARG	2.1
9	s7	162	ILE	2.1
13	C1	141	LYS	2.1
15	C3	66	ILE	2.1
21	c9	36	ILE	2.1
34	SR	107	LYS	2.1
34	sR	290	VAL	2.1
25	D3	58	GLY	2.1
39	L2	200	ARG	2.1
41	L4	104	LYS	2.1
59	N3	101	VAL	2.1
67	O1	93	VAL	2.1
75	o9	15	LYS	2.1
1	2	622	A	2.1
1	2	971	A	2.1
1	6	979	A	2.1
1	6	1604	U	2.1
10	S8	103	GLN	2.1
42	L5	151	GLN	2.1
51	M5	88	GLY	2.1
34	sR	111	MET	2.1
36	1	1028	U	2.1
4	s2	198	THR	2.1
34	sR	48	THR	2.1
36	1	1589	A	2.1
36	1	1858	A	2.1
1	6	614	C	2.1
1	6	729	G	2.1
9	S7	100	PRO	2.1
11	s9	2	PRO	2.1
17	c5	68	PRO	2.1
28	D6	98	PRO	2.1
36	1	2728	G	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
36	5	1832	C	2.1
15	c3	126	ALA	2.1
38	4	24	G	2.1
51	m5	89	VAL	2.1
54	M8	171	LYS	2.1
56	n0	2	ALA	2.1
4	S2	102	VAL	2.1
11	S9	62	ARG	2.1
15	C3	33	VAL	2.1
23	D1	13	VAL	2.1
23	D1	60	ARG	2.1
58	n2	65	VAL	2.1
60	n4	135	SER	2.1
73	O7	11	ARG	2.1
4	S2	145	GLY	2.1
10	S8	184	LEU	2.1
19	c7	56	HIS	2.1
27	D5	80	LEU	2.1
34	SR	23	LEU	2.1
32	e0	17	GLN	2.1
34	sR	49	GLY	2.1
74	o8	69	LEU	2.1
78	Q2	104	LEU	2.1
60	N4	1	MET	2.1
2	S0	140	ASN	2.1
10	S8	48	THR	2.1
10	S8	95	THR	2.1
18	c6	70	THR	2.1
28	d6	25	ASN	2.1
36	5	919	U	2.1
36	5	939	U	2.1
1	2	2	A	2.1
1	2	1336	A	2.1
1	2	1790	A	2.1
14	C2	123	VAL	2.1
15	c3	63	ALA	2.1
21	C9	58	ALA	2.1
22	d0	52	LYS	2.1
23	d1	64	GLU	2.1
36	1	846	A	2.1
36	5	884	A	2.1
36	5	2445	A	2.1

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Mol	Chain	Res	Type	RSRZ
46	l9	3	TYR	2.1
49	M3	32	LYS	2.1
47	M0	138	VAL	2.1
52	M6	191	ALA	2.1
54	m8	149	ALA	2.1
79	q3	17	ARG	2.1
8	S6	55	GLY	2.1
9	S7	155	ASP	2.1
12	C0	76	LEU	2.1
32	e0	61	SER	2.1
34	SR	15	GLY	2.1
51	m5	58	GLY	2.1
54	m8	7	SER	2.1
60	n4	72	SER	2.1
21	C9	131	ASP	2.1
36	1	2325	G	2.1
36	5	364	G	2.1
72	o6	57	LEU	2.1
73	O7	18	LEU	2.1
4	S2	89	GLN	2.1
5	S3	177	MET	2.1
55	M9	175	GLN	2.1
63	n7	4	PHE	2.1
80	c0	47	GLN	2.1
80	c0	95	GLN	2.1
6	S4	256	ARG	2.1
13	c1	101	GLU	2.1
28	D6	70	LYS	2.1
25	D3	36	THR	2.1
30	D8	50	GLU	2.1
34	SR	100	TYR	2.1
34	SR	308	ASN	2.1
34	SR	317	THR	2.1
49	m3	21	ARG	2.1
70	O4	15	THR	2.1
70	O4	58	ARG	2.1
5	s3	201	ALA	2.1
7	s5	53	VAL	2.1
14	C2	42	ALA	2.1
45	l8	199	ALA	2.1
49	M3	173	ALA	2.1
54	m8	101	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	2	1345	A	2.1
1	6	1791	A	2.1
9	s7	135	ILE	2.1
10	S8	43	ILE	2.1
21	C9	79	LEU	2.1
22	d0	22	ILE	2.1
28	D6	79	ILE	2.1
34	sR	11	GLY	2.1
36	1	2126	A	2.1
36	1	3077	A	2.1
45	L8	67	ILE	2.1
51	m5	197	LEU	2.1
69	O3	49	ILE	2.1
3	S1	130	SER	2.1
10	S8	2	GLY	2.1
21	C9	98	GLY	2.1
2	s0	168	HIS	2.1
11	S9	146	PHE	2.0
34	SR	221	MET	2.1
36	5	818	C	2.1
6	S4	145	ARG	2.0
10	s8	31	ARG	2.0
10	s8	123	LYS	2.0
48	M1	163	PHE	2.0
49	M3	13	HIS	2.1
54	M8	172	PHE	2.0
1	2	607	G	2.0
21	C9	44	GLU	2.0
21	C9	122	ARG	2.0
55	M9	82	LYS	2.0
74	o8	44	LYS	2.0
24	D2	49	GLU	2.0
34	SR	98	GLU	2.0
36	1	98	G	2.0
36	1	1905	G	2.0
36	1	2300	G	2.0
1	2	1276	U	2.0
1	6	1254	U	2.0
2	S0	86	VAL	2.0
3	s1	156	ALA	2.0
13	c1	85	VAL	2.0
4	s2	53	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
6	S4	83	PRO	2.0
6	S4	210	ILE	2.0
24	d2	125	ILE	2.0
4	s2	114	GLY	2.0
6	s4	56	LEU	2.0
8	s6	77	LEU	2.0
8	s6	86	PRO	2.0
53	m7	132	ALA	2.0
64	n8	44	ASN	2.0
79	q3	22	LEU	2.0
79	q3	53	GLY	2.0
33	e1	143	LYS	2.0
31	d9	41	GLN	2.0
35	SM	94	HIS	2.0
35	SM	113	ASP	2.0
36	1	2324	A	2.0
36	1	2820	A	2.0
36	5	2138	A	2.0
39	l2	231	SER	2.0
40	L3	174	LYS	2.0
8	S6	177	ARG	2.0
10	s8	44	HIS	2.0
40	L3	244	ARG	2.0
41	L4	76	ARG	2.0
42	l5	296	GLN	2.0
77	q1	6	ARG	2.0
79	Q3	32	GLN	2.0
19	c7	37	GLU	2.0
36	1	346	C	2.0
36	5	82	C	2.0
36	5	1836	C	2.0
39	l2	26	ALA	2.0
39	l2	229	ALA	2.0
51	M5	30	TYR	2.0
60	N4	22	VAL	2.0
64	n8	48	TYR	2.0
73	o7	39	TYR	2.0
82	p0	295	ALA	2.0
19	C7	122	ILE	2.0
23	d1	81	ASN	2.0
4	S2	161	LYS	2.0
5	S3	63	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
9	S7	58	LEU	2.0
10	S8	52	ASN	2.0
45	l8	150	LEU	2.0
45	l8	189	LEU	2.0
52	M6	27	LEU	2.0
52	M6	43	ILE	2.0
64	N8	102	ILE	2.0
70	O4	11	ASN	2.0
70	O4	12	PRO	2.0
36	1	880	G	2.0
36	5	822	G	2.0
36	5	1116	G	2.0
36	5	2814	G	2.0
43	l6	47	PHE	2.0
13	C1	118	GLN	2.0
22	D0	80	GLU	2.0
53	m7	133	HIS	2.0
56	N0	42	TRP	2.0
67	o1	111	GLU	2.0
9	S7	152	VAL	2.0
10	s8	156	VAL	2.0
15	c3	134	VAL	2.0
20	C8	22	VAL	2.0
36	1	1456	A	2.0
1	2	962	C	2.0
5	s3	110	LEU	2.0
13	C1	70	ILE	2.0
23	d1	26	ALA	2.0
31	d9	47	ALA	2.0
39	l2	4	VAL	2.0
40	L3	93	VAL	2.0
45	l8	117	ALA	2.0
51	m5	64	VAL	2.0
4	S2	239	PRO	2.0
8	S6	70	PRO	2.0
9	s7	157	LYS	2.0
34	SR	117	LYS	2.0
40	L3	102	LEU	2.0
15	c3	64	ARG	2.0
18	C6	33	GLY	2.0
19	c7	31	ASN	2.0
19	c7	54	THR	2.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
42	L5	28	THR	2.0
49	M3	12	ASN	2.0
77	q1	2	ARG	2.0
79	q3	73	THR	2.0
1	2	232	U	2.0
1	2	1103	U	2.0
36	5	1533	U	2.0
36	5	2975	U	2.0
1	6	1412	G	2.0
34	sR	295	SER	2.0
36	5	2947	G	2.0
42	L5	210	GLU	2.0
64	n8	38	GLN	2.0
16	C4	34	SER	2.0
23	d1	40	ASP	2.0
45	L8	47	SER	2.0
64	N8	25	HIS	2.0
5	S3	72	LEU	2.0
7	s5	159	ALA	2.0
15	c3	43	LYS	2.0
25	D3	130	VAL	2.0
51	m5	204	LYS	2.0
63	n7	24	VAL	2.0
34	sR	293	ALA	2.0
79	q3	69	TYR	2.0
19	c7	50	ILE	2.0
55	M9	99	LEU	2.0
1	2	1287	A	2.0
1	6	862	A	2.0
1	6	1026	A	2.0
6	S4	144	GLY	2.0
13	C1	73	GLY	2.0
64	N8	33	GLY	2.0
72	O6	14	GLY	2.0
35	SM	102	THR	2.0
36	1	2329	C	2.0
52	m6	71	PHE	2.0
68	o2	53	PRO	2.0
3	s1	25	THR	2.0
6	s4	26	CYS	2.0
13	C1	78	THR	2.0
58	n2	101	ASN	2.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
59	n3	4	ASN	2.0
1	6	406	U	2.0
21	C9	25	GLN	2.0
40	L3	94	GLU	2.0
4	s2	106	ASP	2.0
5	S3	73	VAL	2.0
5	S3	141	LYS	2.0
16	c4	49	LYS	2.0
22	D0	52	LYS	2.0
36	1	1512	U	2.0
36	1	1925	U	2.0
36	1	3275	U	2.0
42	L5	27	LYS	2.0
54	m8	15	HIS	2.0
67	O1	65	LYS	2.0
73	o7	28	HIS	2.0
80	c0	56	LYS	2.0
11	S9	80	LEU	2.0
11	s9	76	LEU	2.0
1	2	383	G	2.0
18	c6	25	GLY	2.0
19	C7	17	ILE	2.0
20	c8	125	ILE	2.0
34	sR	311	ARG	2.0
40	L3	267	ALA	2.0
53	M7	156	ALA	2.0
54	m8	93	ILE	2.0
59	n3	13	ILE	2.0
63	N7	72	ILE	2.0
10	s8	113	PHE	2.0
17	C5	12	PHE	2.0
25	d3	38	PHE	2.0
36	1	860	G	2.0
36	1	1488	G	2.0
36	1	1573	G	2.0
36	5	1838	G	2.0
36	5	2150	G	2.0
1	2	1400	A	2.0
29	D7	57	GLU	2.0
33	e1	151	ASN	2.0
36	1	806	A	2.0
36	1	883	A	2.0

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Mol	Chain	Res	Type	RSRZ
36	5	356	C	2.0
36	5	2136	C	2.0
45	l8	240	ASN	2.0
24	d2	64	GLN	2.0
75	O9	11	GLN	2.0
2	s0	139	VAL	2.0
10	S8	141	ARG	2.0
29	d7	29	ARG	2.0
47	m0	181	TYR	2.0
51	m5	134	LEU	2.0
64	n8	101	VAL	2.0
64	n8	130	VAL	2.0
77	Q1	23	ARG	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( $\text{\AA}^2$ )	Q<0.9
86	ZN	e1	501	1/1	0.72	0.15	165,165,165,165	0
86	ZN	D7	101	1/1	0.76	0.17	140,140,140,140	0
86	ZN	d7	101	1/1	0.78	0.31	134,134,134,134	0
86	ZN	E1	501	1/1	0.91	0.15	133,133,133,133	0
86	ZN	D6	500	1/1	0.94	0.06	99,99,99,99	0
86	ZN	d6	500	1/1	0.94	0.07	82,82,82,82	0
86	ZN	q2	501	1/1	0.95	0.07	74,74,74,74	0
86	ZN	d9	101	1/1	0.95	0.13	93,93,93,93	0
86	ZN	D9	101	1/1	0.97	0.11	89,89,89,89	0
86	ZN	Q2	501	1/1	0.97	0.08	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
86	ZN	Q0	500	1/1	0.98	0.20	57,57,57,57	0
86	ZN	q0	500	1/1	0.99	0.16	48,48,48,48	0
86	ZN	q3	501	1/1	0.99	0.18	64,64,64,64	0
86	ZN	Q3	501	1/1	0.99	0.14	74,74,74,74	0
86	ZN	o7	501	1/1	0.99	0.14	53,53,53,53	0
86	ZN	O7	100	1/1	1.00	0.13	53,53,53,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.