wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2023 – 08:12 AM EDT

PDB ID	:	7LH5
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with plazomicin, mRNA and tRNAs
Authors	:	Golkar, T.; Berghuis, A.M.; Schmeing, T.M.
Deposited on	:	2021-01-21
Resolution	:	3.27 Å(reported)

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

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

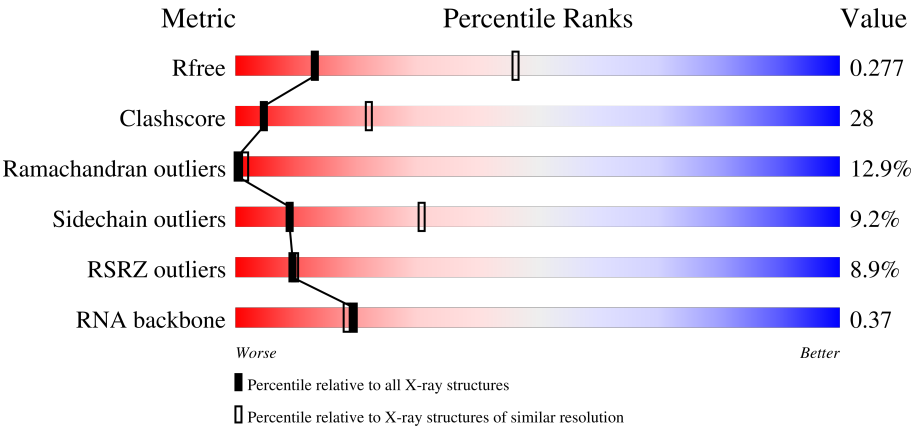
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)
RNA backbone	3102	1091 (3.66-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	AA	1520	2% 19% 40% 30% 9%
1	CA	1520	20% 46% 26% 7%
2	AB	256	26% 20% 52% 14% 15%
2	CB	256	2% 25% 59% 7% 9%

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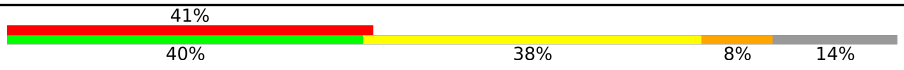
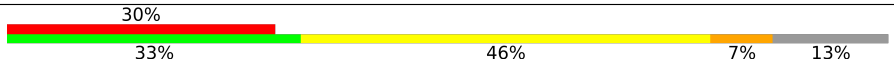
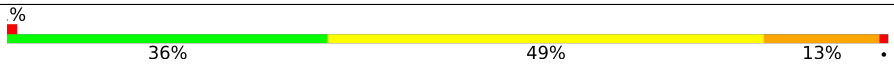
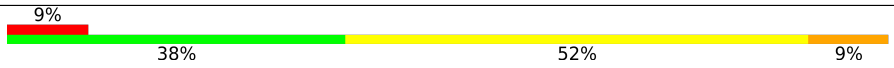
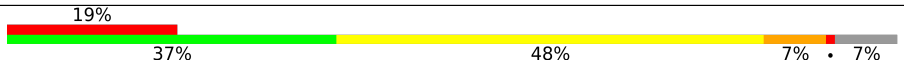
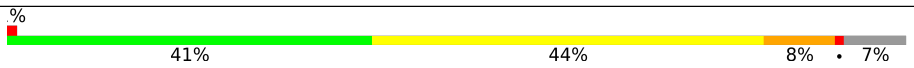
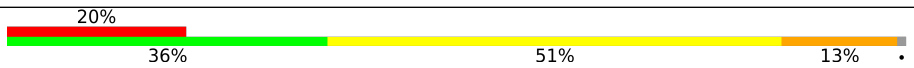
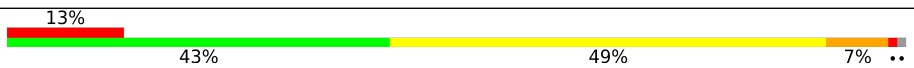
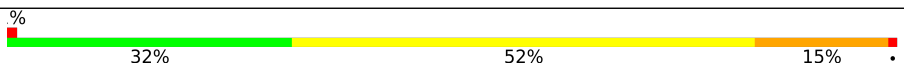
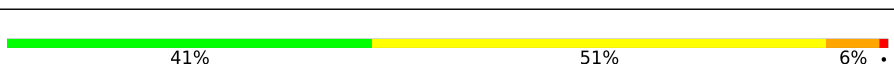
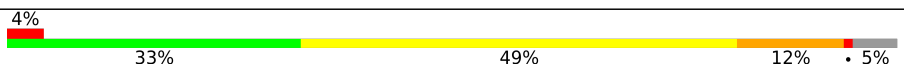
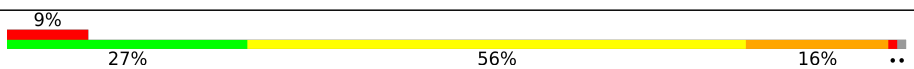
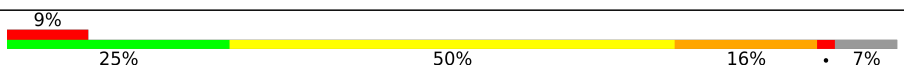
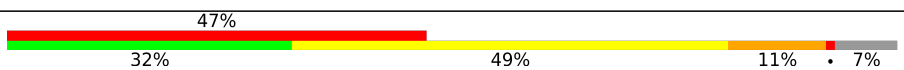
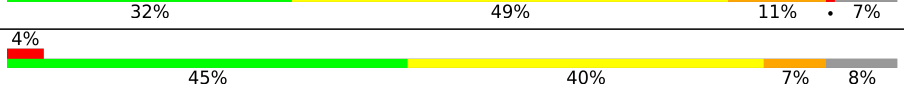
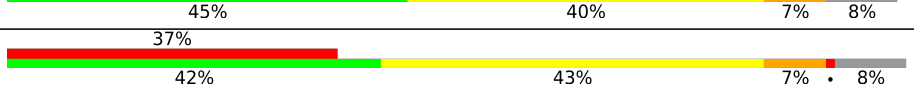
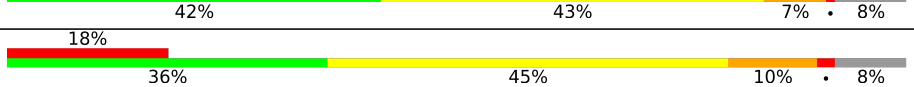
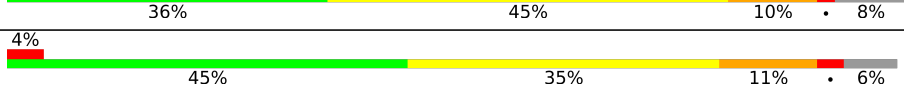
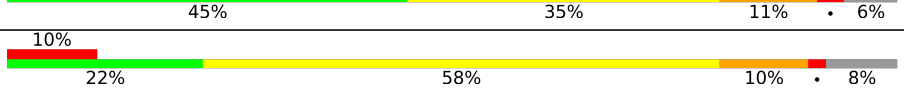
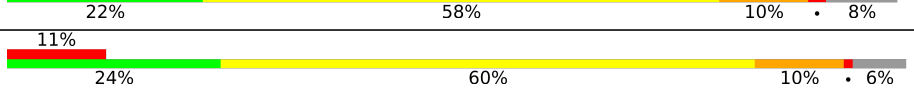
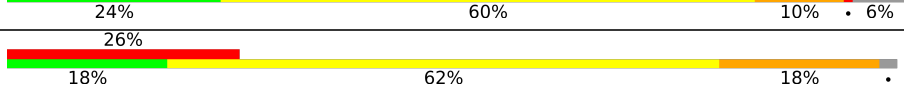
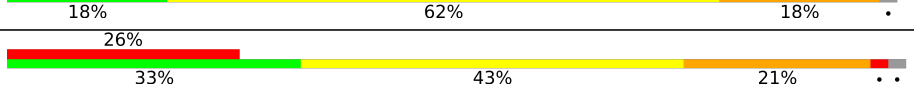
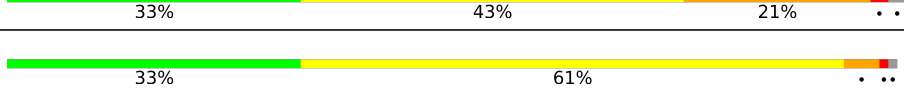
Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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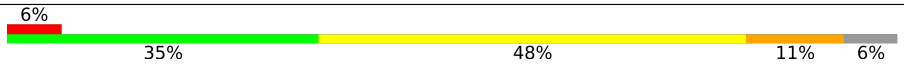
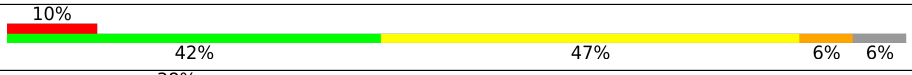
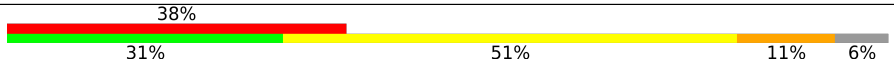
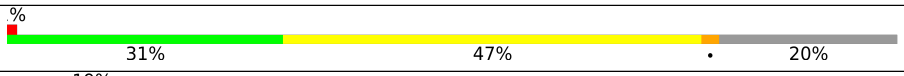
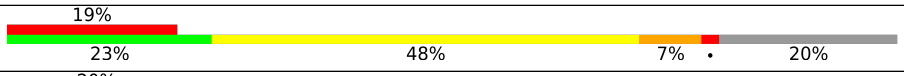
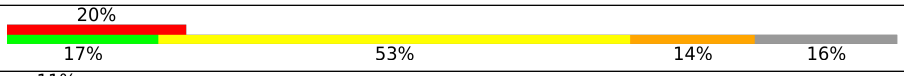
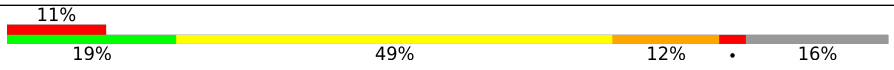
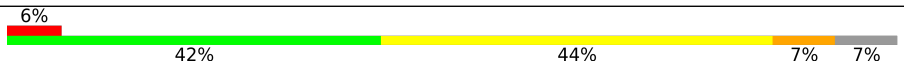
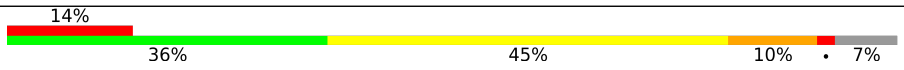
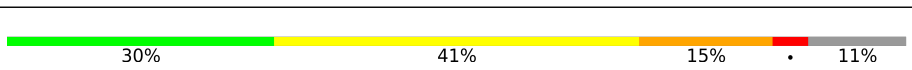
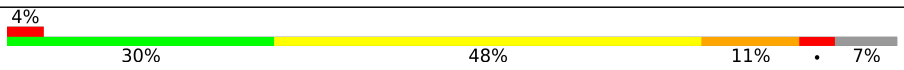
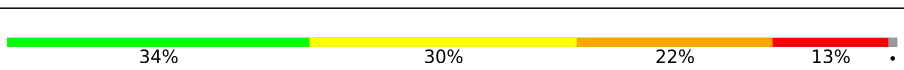
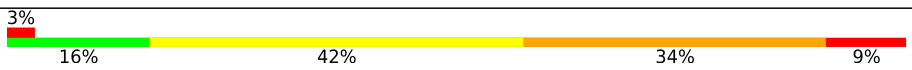
Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	CV	77	
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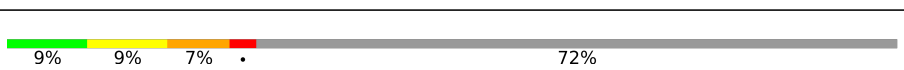
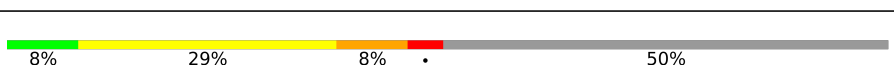
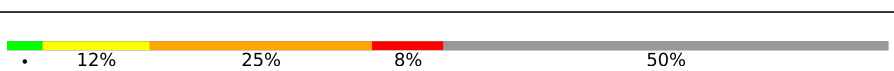
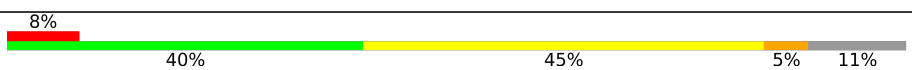
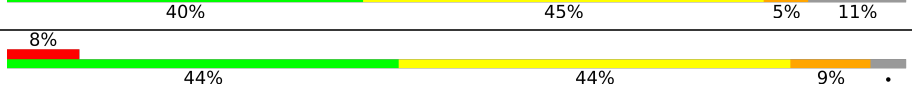
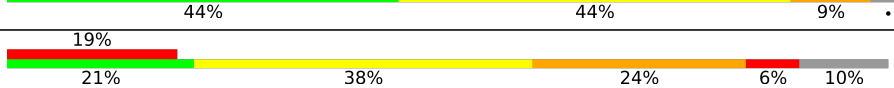
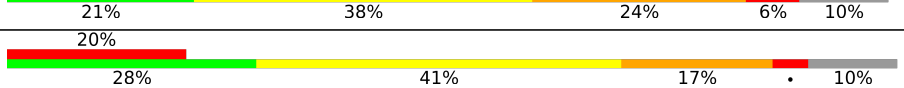
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	24	
24	CX	24	
25	B0	85	
25	D0	85	
26	B1	98	
26	D1	98	

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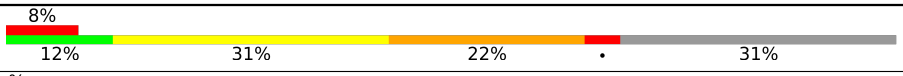
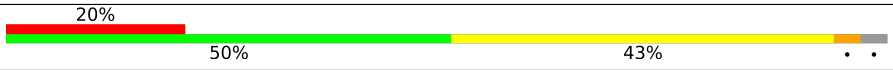
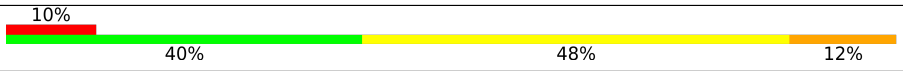
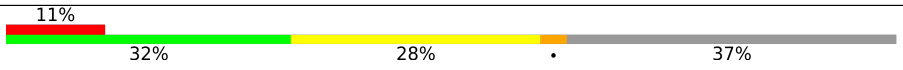
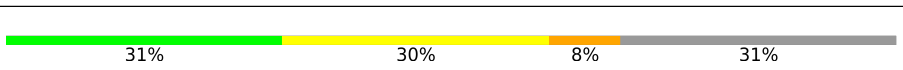
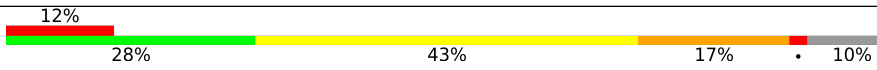
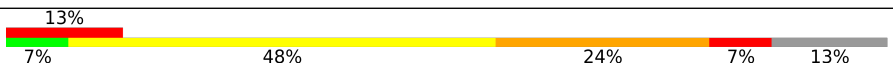
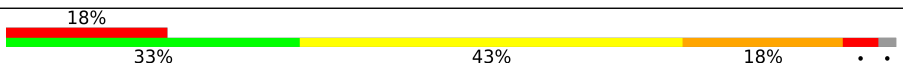
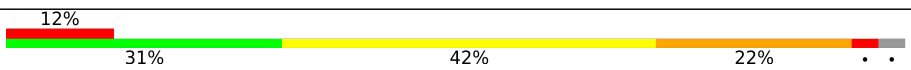
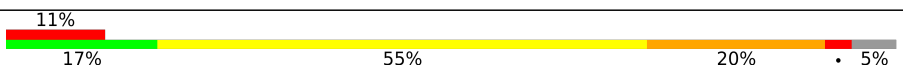
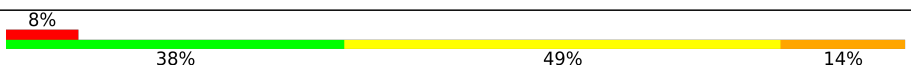
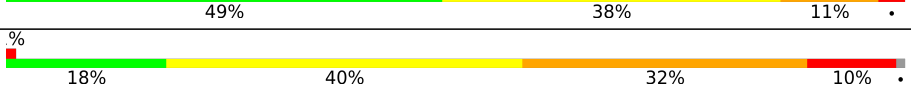
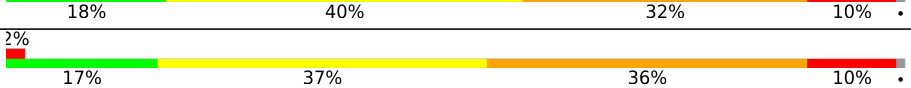
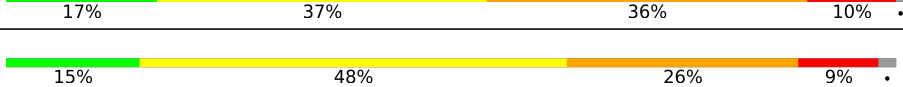
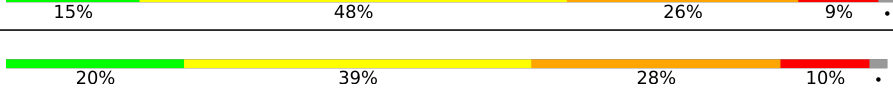
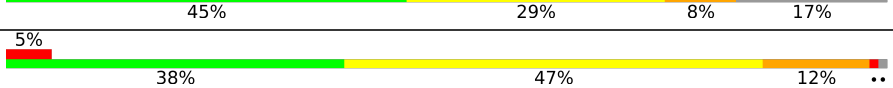
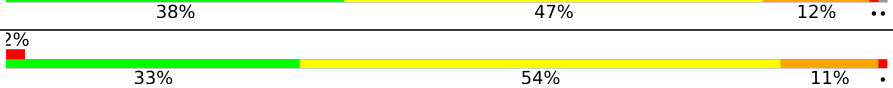
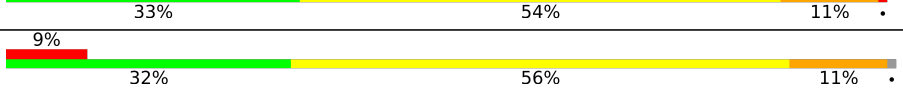
Mol	Chain	Length	Quality of chain
27	B2	72	
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2839	
35	DA	2839	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	

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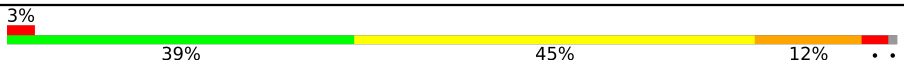
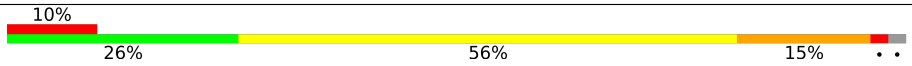
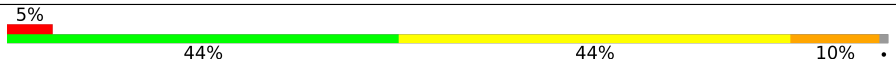
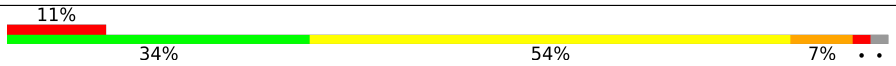
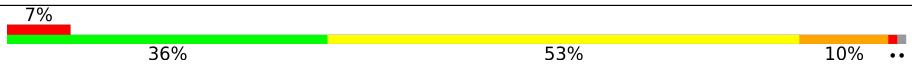
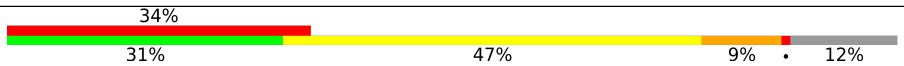
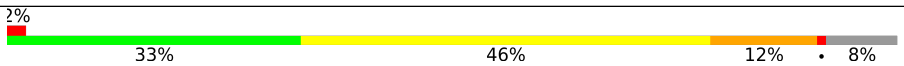
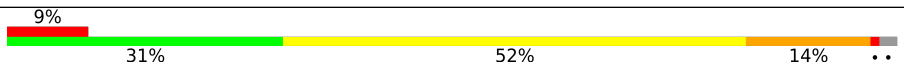
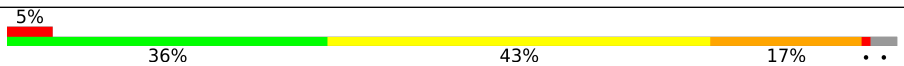
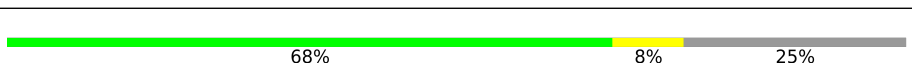
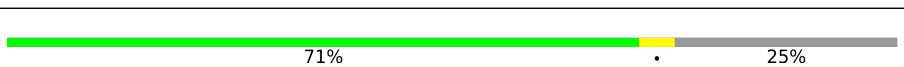
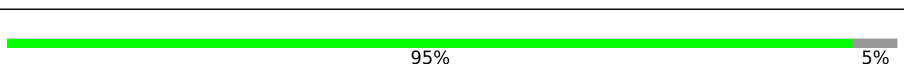
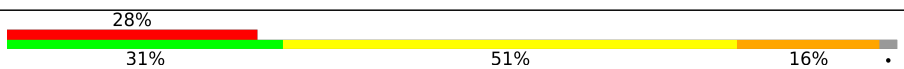
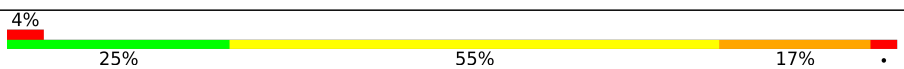
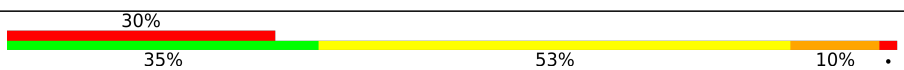
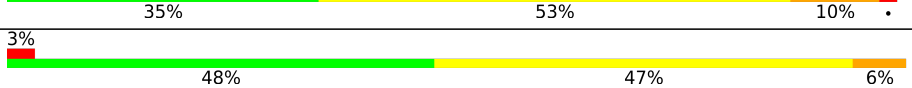
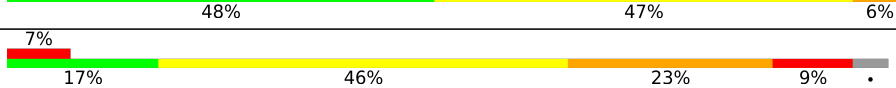
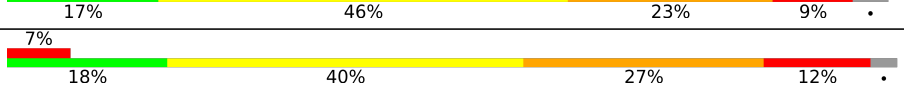
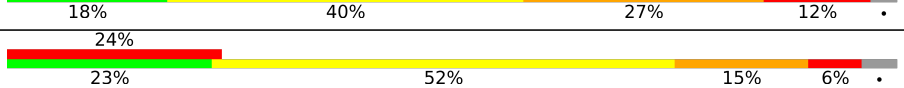
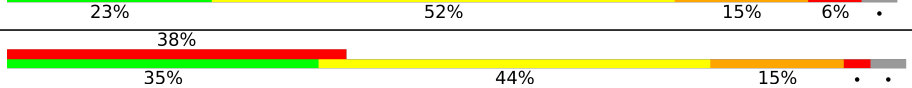
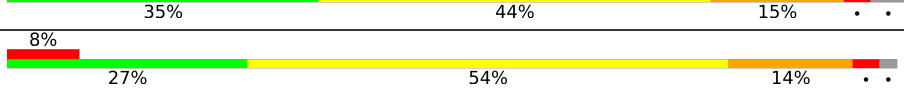
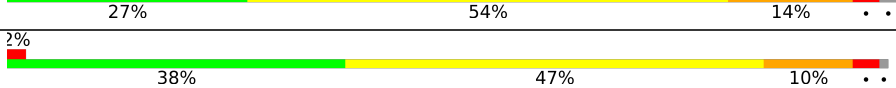
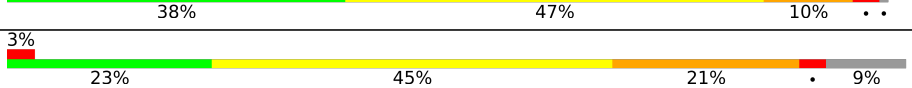
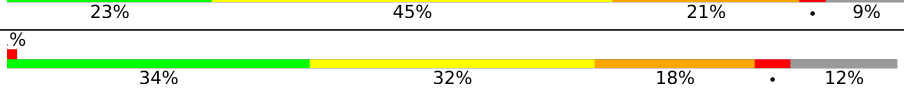
Mol	Chain	Length	Quality of chain
39	DE	206	
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BI	148	
43	DI	148	
44	BJ	173	
44	DJ	173	
45	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	

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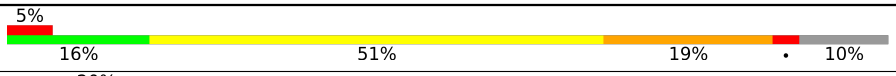
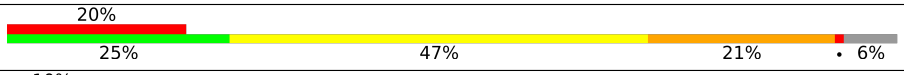
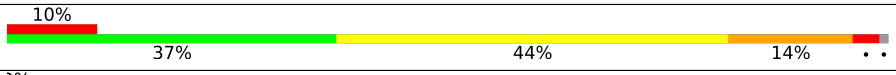
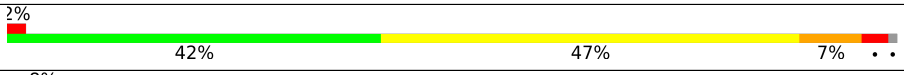
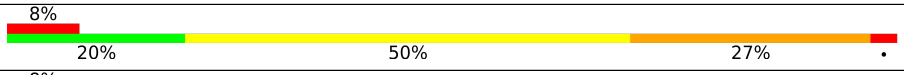
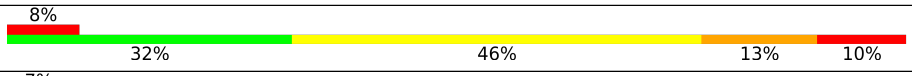
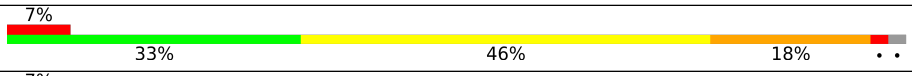
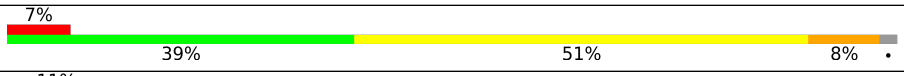
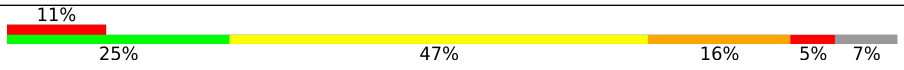
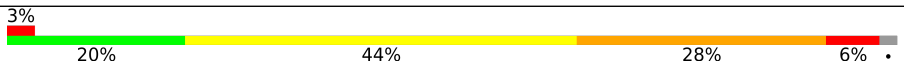
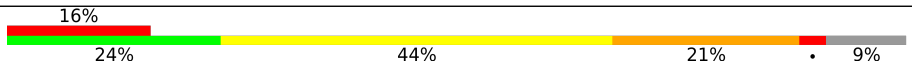
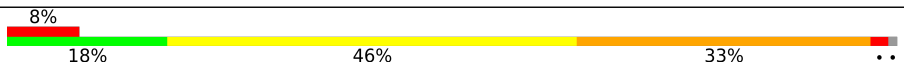
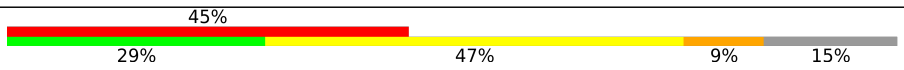
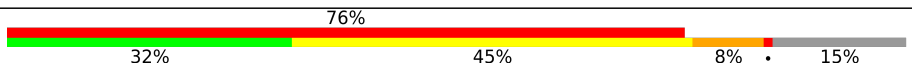
Mol	Chain	Length	Quality of chain
52	BT	146	
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	1619	-	-	-	X
59	MG	AA	1645	-	-	-	X
59	MG	AA	1660	-	-	-	X
59	MG	AA	1670	-	-	-	X
59	MG	AA	1674	-	-	-	X
59	MG	AA	1676	-	-	-	X
59	MG	AA	1681	-	-	-	X
59	MG	AA	1697	-	-	-	X
59	MG	AA	1743	-	-	-	X
59	MG	AA	1756	-	-	-	X
59	MG	AA	1760	-	-	-	X
59	MG	AA	1770	-	-	-	X
59	MG	AA	1777	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	AA	1804	-	-	-	X
59	MG	AA	1808	-	-	-	X
59	MG	AD	301	-	-	-	X
59	MG	AL	201	-	-	-	X
59	MG	AT	201	-	-	-	X
59	MG	AV	102	-	-	-	X
59	MG	AW	101	-	-	-	X
59	MG	AW	104	-	-	-	X
59	MG	AW	105	-	-	-	X
59	MG	AW	110	-	-	-	X
59	MG	AW	113	-	-	-	X
59	MG	AW	114	-	-	-	X
59	MG	AW	117	-	-	-	X
59	MG	AW	119	-	-	-	X
59	MG	BA	3011	-	-	-	X
59	MG	BA	3014	-	-	-	X
59	MG	BA	3108	-	-	-	X
59	MG	BA	3126	-	-	-	X
59	MG	BA	3132	-	-	-	X
59	MG	BA	3142	-	-	-	X
59	MG	BA	3145	-	-	-	X
59	MG	BA	3186	-	-	-	X
59	MG	BA	3224	-	-	-	X
59	MG	BA	3254	-	-	-	X
59	MG	BA	3257	-	-	-	X
59	MG	BA	3271	-	-	-	X
59	MG	BA	3285	-	-	-	X
59	MG	BA	3302	-	-	-	X
59	MG	BA	3306	-	-	-	X
59	MG	BA	3313	-	-	-	X
59	MG	BA	3344	-	-	-	X
59	MG	BA	3350	-	-	-	X
59	MG	BA	3353	-	-	-	X
59	MG	BA	3357	-	-	-	X
59	MG	BA	3364	-	-	-	X
59	MG	BA	3385	-	-	-	X
59	MG	BA	3389	-	-	-	X
59	MG	BA	3399	-	-	-	X
59	MG	BA	3400	-	-	-	X
59	MG	BA	3405	-	-	-	X
59	MG	BA	3427	-	-	-	X
59	MG	BA	3434	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	BA	3456	-	-	-	X
59	MG	BA	3457	-	-	-	X
59	MG	CA	1602	-	-	-	X
59	MG	CA	1619	-	-	-	X
59	MG	CA	1620	-	-	-	X
59	MG	CA	1627	-	-	-	X
59	MG	CA	1637	-	-	-	X
59	MG	CA	1646	-	-	-	X
59	MG	CA	1649	-	-	-	X
59	MG	CA	1652	-	-	-	X
59	MG	CA	1664	-	-	-	X
59	MG	CA	1674	-	-	-	X
59	MG	CA	1675	-	-	-	X
59	MG	CA	1677	-	-	-	X
59	MG	CA	1690	-	-	-	X
59	MG	CA	1695	-	-	-	X
59	MG	CA	1725	-	-	-	X
59	MG	CA	1742	-	-	-	X
59	MG	CA	1793	-	-	-	X
59	MG	CE	201	-	-	-	X
59	MG	CW	106	-	-	-	X
59	MG	CW	108	-	-	-	X
59	MG	CW	109	-	-	-	X
59	MG	CW	112	-	-	-	X
59	MG	DA	3005	-	-	-	X
59	MG	DA	3007	-	-	-	X
59	MG	DA	3008	-	-	-	X
59	MG	DA	3086	-	-	-	X
59	MG	DA	3105	-	-	-	X
59	MG	DA	3136	-	-	-	X
59	MG	DA	3152	-	-	-	X
59	MG	DA	3163	-	-	-	X
59	MG	DA	3203	-	-	-	X
59	MG	DA	3206	-	-	-	X
59	MG	DA	3224	-	-	-	X
59	MG	DA	3230	-	-	-	X
59	MG	DA	3246	-	-	-	X
59	MG	DA	3256	-	-	-	X
59	MG	DA	3258	-	-	-	X
59	MG	DA	3280	-	-	-	X
59	MG	DA	3307	-	-	-	X
59	MG	DA	3315	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	MG	DA	3316	-	-	-	X
59	MG	DA	3320	-	-	-	X
59	MG	DA	3342	-	-	-	X
59	MG	DA	3348	-	-	-	X
59	MG	DA	3356	-	-	-	X
59	MG	DA	3373	-	-	-	X
59	MG	DA	3382	-	-	-	X
59	MG	DB	207	-	-	-	X
59	MG	DB	211	-	-	-	X
59	MG	DO	202	-	-	-	X
59	MG	DV	201	-	-	-	X

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 296449 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32332	14390	5992	10446	1504			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1784	1139	321	319	5			
2	CB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			
3	CC	207	Total	C	N	O	S	0	0	0
			1620	1021	315	282	2			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			
5	CE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	121	Total	C	N	O	0	0	0
			947	599	186	162			
9	CI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
12	CL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	116	Total	C	N	O	S	0	0	0
			922	570	189	161	2			
13	CM	119	Total	C	N	O	S	0	0	0
			946	585	195	164	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			491	312	104	71	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	CP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			
19	CS	78	Total	C	N	O	S	0	0	0
			629	403	114	110	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	24	Total 208	C 128	N 50	O 30	0	0	0
21	CU	25	Total 217	C 134	N 52	O 31	0	0	0

- Molecule 22 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total 1622	C 723	N 294	O 529	P 76	0	0	0
22	CV	77	Total 1643	C 732	N 297	O 537	P 77	0	0	0

- Molecule 23 is a RNA chain called E-Site tRNA Phe and A-site tRNA Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	76	Total 1623	C 723	N 290	O 534	P 76	0	0	0
23	AY	19	Total 410	C 183	N 78	O 130	P 19	0	0	0
23	CW	76	Total 1623	C 723	N 290	O 534	P 76	0	0	0
23	CY	21	Total 453	C 202	N 86	O 144	P 21	0	0	0

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	12	Total 255	C 115	N 46	O 82	P 12	0	0	0
24	CX	12	Total 255	C 115	N 46	O 82	P 12	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	76	Total 607	C 376	N 128	O 102	S 1	0	0	0
25	D0	82	Total 645	C 401	N 136	O 107	S 1	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	B1	88	Total 692	C 435	N 139	O 118	0	0	0
26	D1	88	Total 692	C 435	N 139	O 118	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	50	Total 420	C 263	N 84	O 72	S 1	0	0	0
27	D2	53	Total 446	C 279	N 88	O 78	S 1	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	58	Total 459	C 293	N 89	O 77		0	0	0
28	D3	60	Total 476	C 303	N 91	O 81	S 1	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	B4	45	Total 222	C 132	N 45	O 45	0	0	0
29	D4	49	Total 241	C 143	N 49	O 49	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	54	Total 418	C 261	N 84	O 68	S 5	0	0	0
30	D5	60	Total 467	C 293	N 91	O 77	S 6	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	46	Total 398	C 247	N 81	O 66	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D6	47	Total	C	N	O	S	0	0	0
			408	253	84	67	4			

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
32	D7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			
33	D8	62	Total	C	N	O	S	0	0	0
			495	317	100	76	2			

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
34	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 35 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2824	Total	C	N	O	P	0	0	0
			60821	27070	11372	19556	2823			
35	DA	2824	Total	C	N	O	P	0	0	0
			60821	27070	11372	19556	2823			

- Molecule 36 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
36	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 37 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BC	190	Total	C	N	O	0	0	0
			1141	691	220	230			
37	DC	190	Total	C	N	O	0	0	0
			1141	691	220	230			

- Molecule 38 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	273	Total	C	N	O	S	0	0	0
			2126	1341	424	358	3			
38	DD	275	Total	C	N	O	S	0	0	0
			2144	1353	428	360	3			

- Molecule 39 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			
39	DE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 40 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	206	Total	C	N	O	S	0	0	0
			1615	1030	302	281	2			
40	DF	208	Total	C	N	O	S	0	0	0
			1627	1037	304	283	3			

- Molecule 41 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BG	178	Total	C	N	O	S	0	0	0
			1449	925	264	256	4			
41	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 42 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			
42	DH	165	Total	C	N	O	S	0	0	0
			1270	806	237	226	1			

- Molecule 43 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
43	DI	144	Total	C	N	O	S	0	0	0
			1124	718	199	206	1			

- Molecule 44 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O	0	0	0
			651	391	130	130			
44	DJ	130	Total	C	N	O	0	0	0
			651	391	130	130			

- Molecule 45 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BK	140	Total	C	N	O	0	0	0
			700	420	140	140			
45	DK	140	Total	C	N	O	0	0	0
			700	420	140	140			

- Molecule 46 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			
46	DN	140	Total	C	N	O	S	0	0	0
			1120	722	208	186	4			

- Molecule 47 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	DO	122	Total 933	C 588	N 171	O 170	S 4	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	144	Total 1099	C 684	N 225	O 188	S 2	0	0	0
48	DP	146	Total 1114	C 692	N 227	O 193	S 2	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	135	Total 1074	C 686	N 205	O 178	S 5	0	0	0
49	DQ	136	Total 1083	C 691	N 206	O 181	S 5	0	0	0

- Molecule 50 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
50	BR	116	Total 949	C 593	N 198	O 158	0	0	0
50	DR	117	Total 960	C 599	N 202	O 159	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	BS	102	Total 813	C 512	N 164	O 137	0	0	0
51	DS	99	Total 781	C 492	N 158	O 131	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	132	Total 1100	C 686	N 227	O 186	S 1	0	0	0
52	DT	137	Total 1141	C 710	N 234	O 196	S 1	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
53	DU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 54 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
54	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 55 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BW	111	Total	C	N	O	S	0	0	0
			886	558	174	152	2			
55	DW	111	Total	C	N	O	S	0	0	0
			886	558	174	152	2			

- Molecule 56 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BX	89	Total	C	N	O		0	0	0
			704	458	128	118				
56	DX	94	Total	C	N	O	S	0	0	0
			742	482	134	125	1			

- Molecule 57 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			
57	DY	109	Total	C	N	O	S	0	0	0
			835	534	157	139	5			

- Molecule 58 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	176	Total 1403	C 897	N 252	O 252	S 2	0	0	0
58	DZ	176	Total 1403	C 897	N 252	O 252	S 2	0	0	0

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	209	Total 209	Mg 209	0	0
59	AC	1	Total 1	Mg 1	0	0
59	AD	1	Total 1	Mg 1	0	0
59	AE	1	Total 1	Mg 1	0	0
59	AL	1	Total 1	Mg 1	0	0
59	AT	1	Total 1	Mg 1	0	0
59	AV	7	Total 7	Mg 7	0	0
59	AW	20	Total 20	Mg 20	0	0
59	AX	3	Total 3	Mg 3	0	0
59	B0	1	Total 1	Mg 1	0	0
59	B1	2	Total 2	Mg 2	0	0
59	B2	1	Total 1	Mg 1	0	0
59	B5	1	Total 1	Mg 1	0	0
59	B7	1	Total 1	Mg 1	0	0
59	B8	2	Total 2	Mg 2	0	0
59	BA	457	Total 457	Mg 457	0	0
59	BB	17	Total 17	Mg 17	0	0
59	BC	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	BE	2	Total Mg 2 2	0	0
59	BF	3	Total Mg 3 3	0	0
59	BQ	1	Total Mg 1 1	0	0
59	BS	1	Total Mg 1 1	0	0
59	BU	5	Total Mg 5 5	0	0
59	BV	1	Total Mg 1 1	0	0
59	BX	2	Total Mg 2 2	0	0
59	CA	195	Total Mg 195 195	0	0
59	CE	1	Total Mg 1 1	0	0
59	CF	1	Total Mg 1 1	0	0
59	CG	1	Total Mg 1 1	0	0
59	CI	1	Total Mg 1 1	0	0
59	CU	1	Total Mg 1 1	0	0
59	CV	4	Total Mg 4 4	0	0
59	CW	13	Total Mg 13 13	0	0
59	CX	2	Total Mg 2 2	0	0
59	D2	2	Total Mg 2 2	0	0
59	D5	1	Total Mg 1 1	0	0
59	DA	392	Total Mg 392 392	0	0
59	DB	12	Total Mg 12 12	0	0
59	DE	1	Total Mg 1 1	0	0

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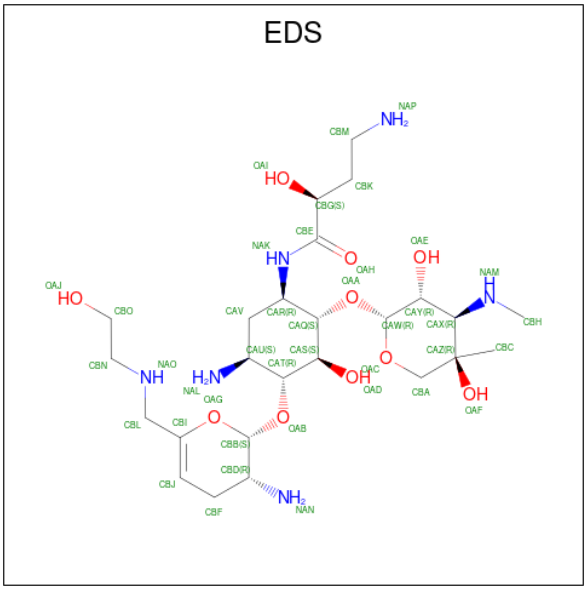
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	DF	2	Total Mg 2 2	0	0
59	DN	1	Total Mg 1 1	0	0
59	DO	2	Total Mg 2 2	0	0
59	DV	1	Total Mg 1 1	0	0

- Molecule 60 is (2S)-4-amino-N-[(1R,2S,3S,4R,5S)-5-amino-4-{[(2S,3R)-3-amino-6-{[(2-hydroxyethyl)amino]methyl}-3,4-dihydro-2H-pyran-2-y l]oxy}-2-{[3-deoxy-4-C-methyl-3-(methylamino)-beta-L-arabinopyranosyl]oxy}-3-hydroxycyclohexyl]-2-hydroxybutanamide (three-letter code: EDS) (formula: $C_{25}H_{48}N_6O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AA	1	Total C N O 41 25 6 10	0	0
60	CA	1	Total C N O 41 25 6 10	0	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AD	1	Total Zn 1 1	0	0
61	AN	1	Total Zn 1 1	0	0

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Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	B9	1	Total Zn 1 1	0	0
61	CD	1	Total Zn 1 1	0	0
61	CN	1	Total Zn 1 1	0	0
61	D9	1	Total Zn 1 1	0	0

- Molecule 62 is water.

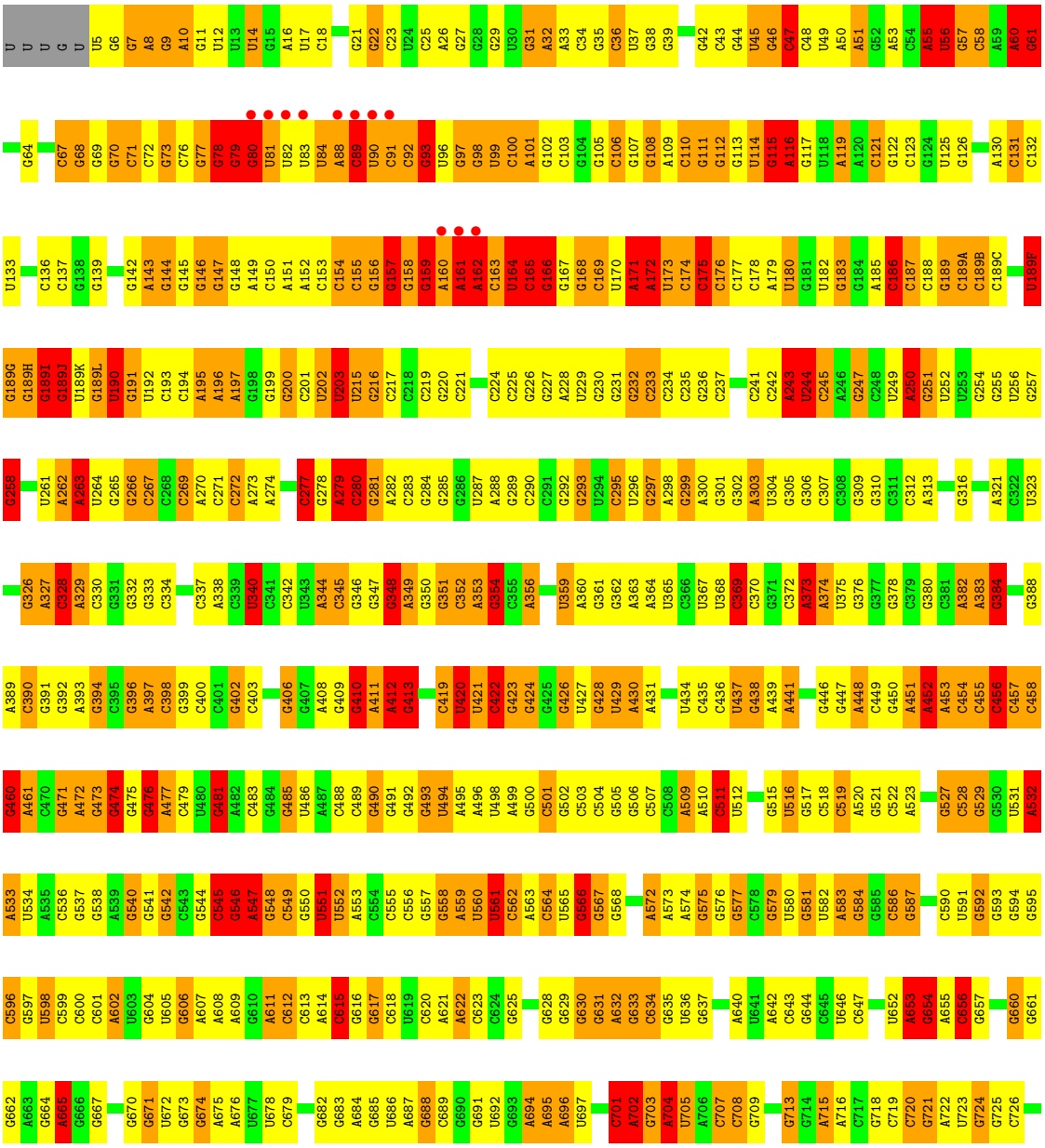
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	AA	2	Total O 2 2	0	0

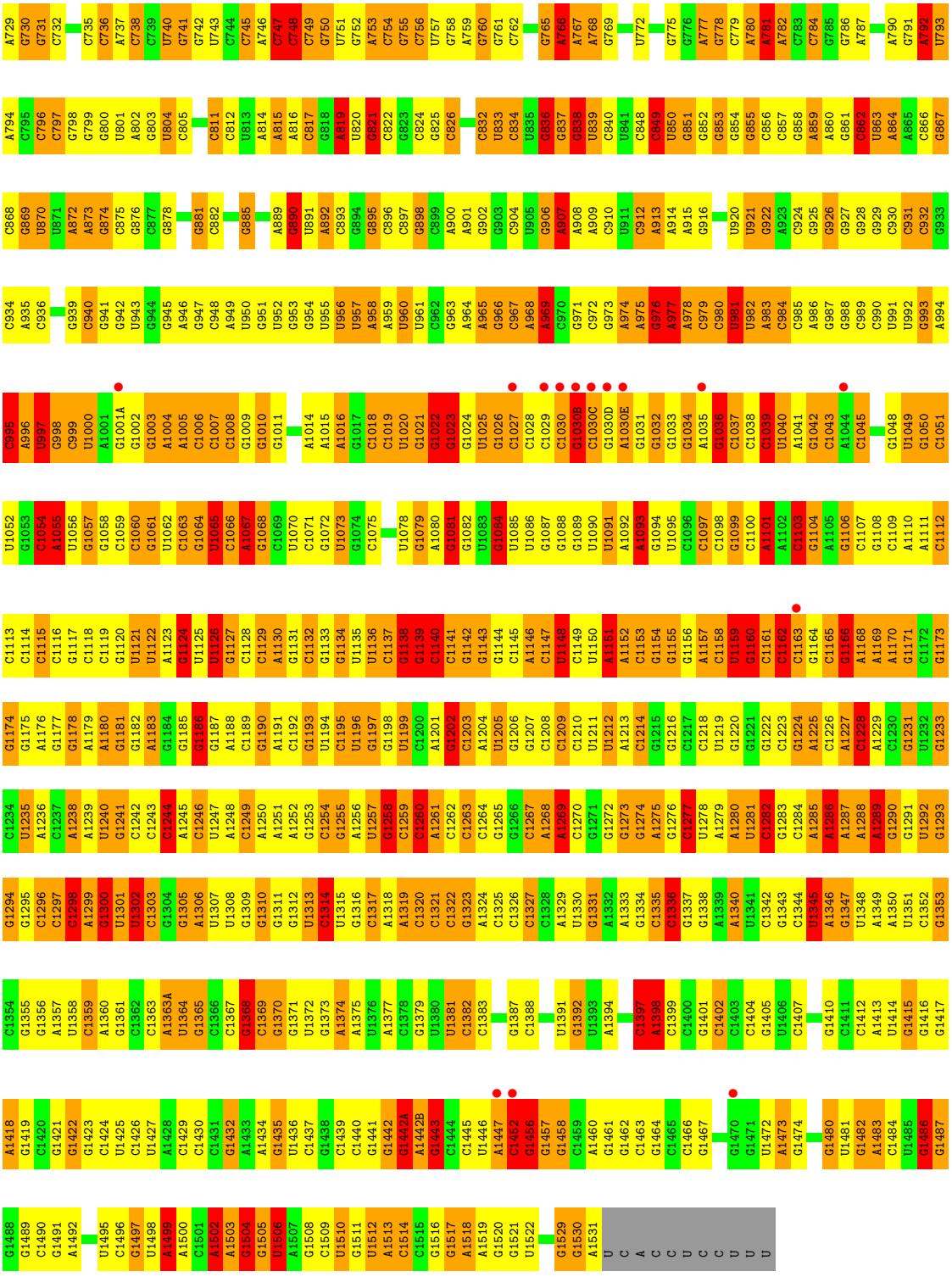
3 Residue-property plots (i)

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: 16S ribosomal RNA

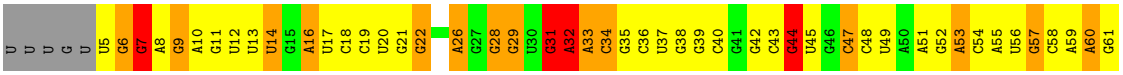
Chain AA: 

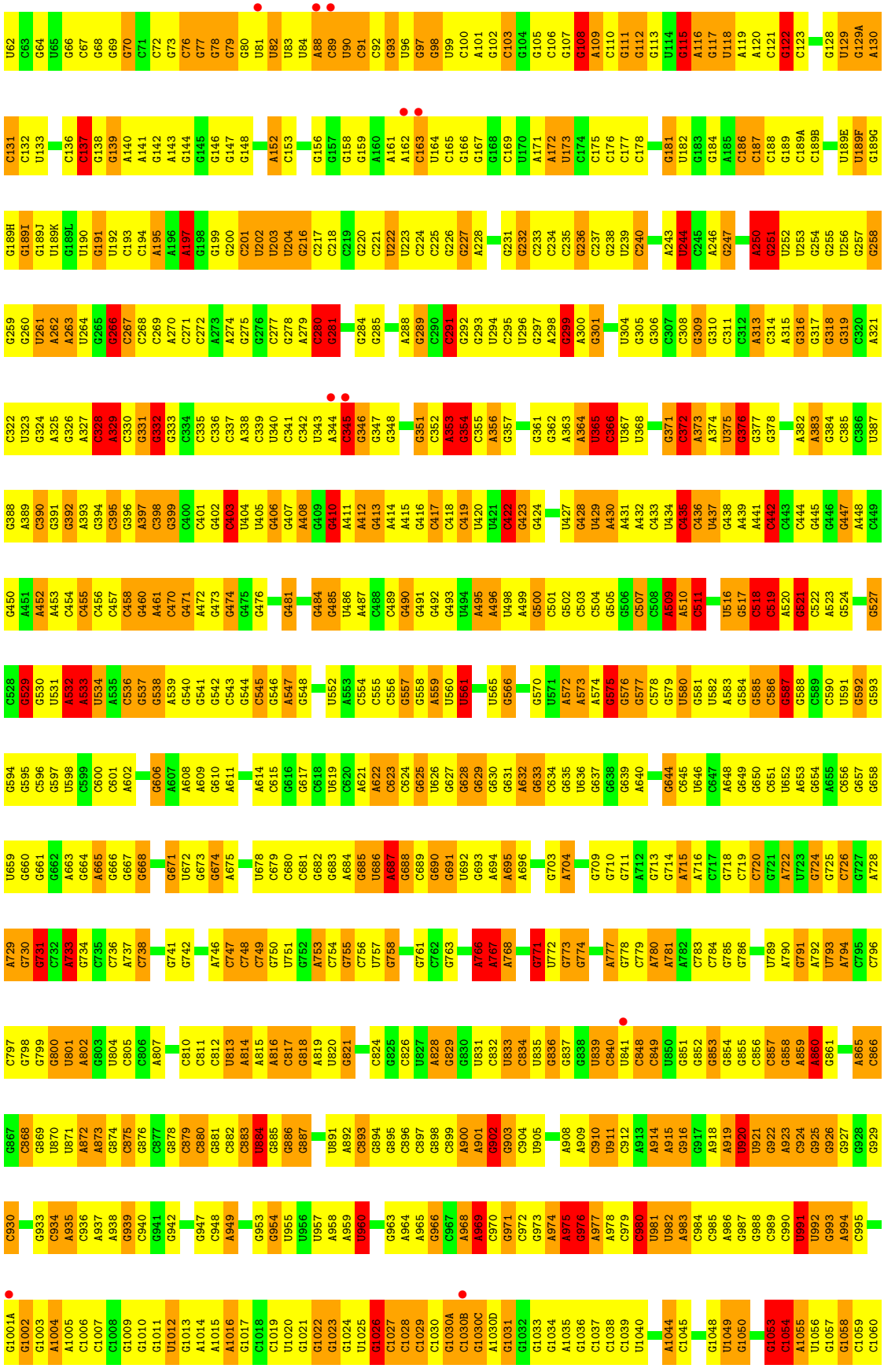


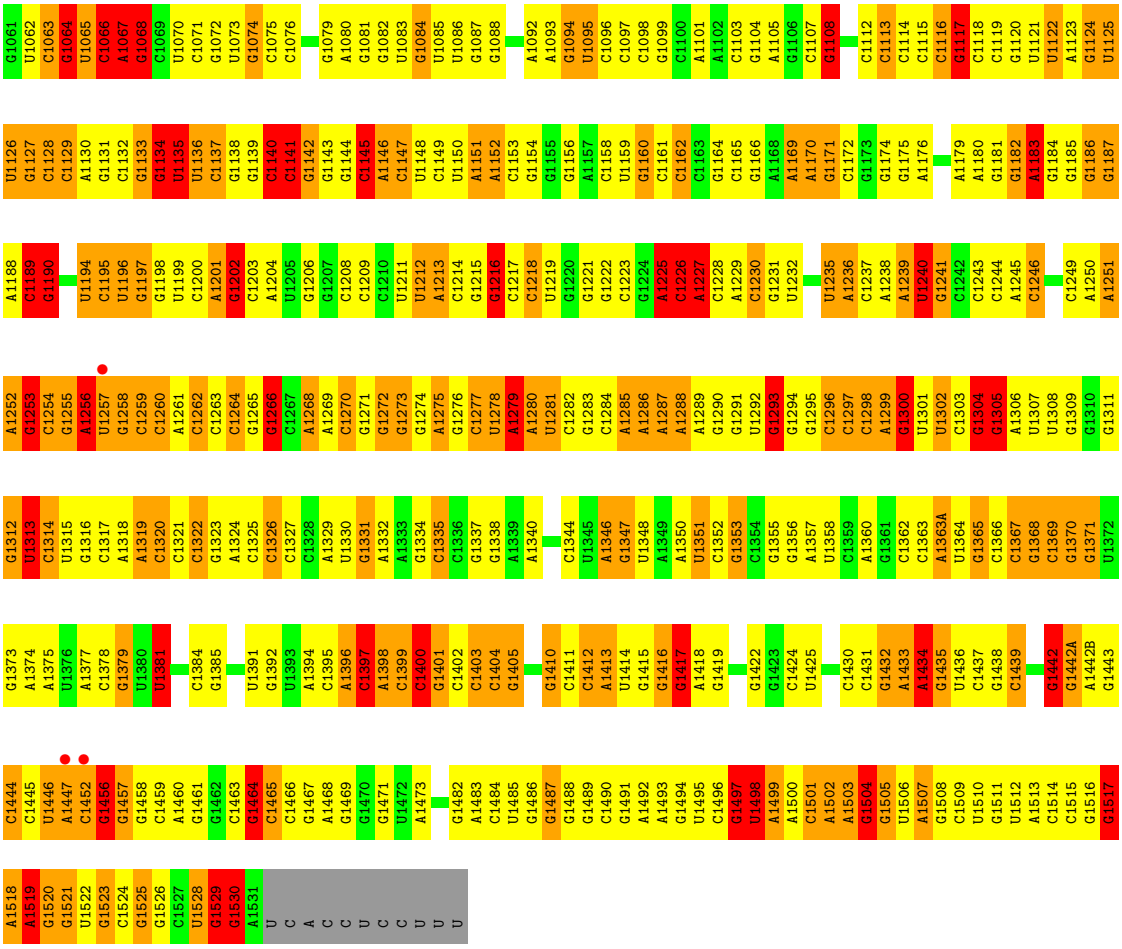


• Molecule 1: 16S ribosomal RNA

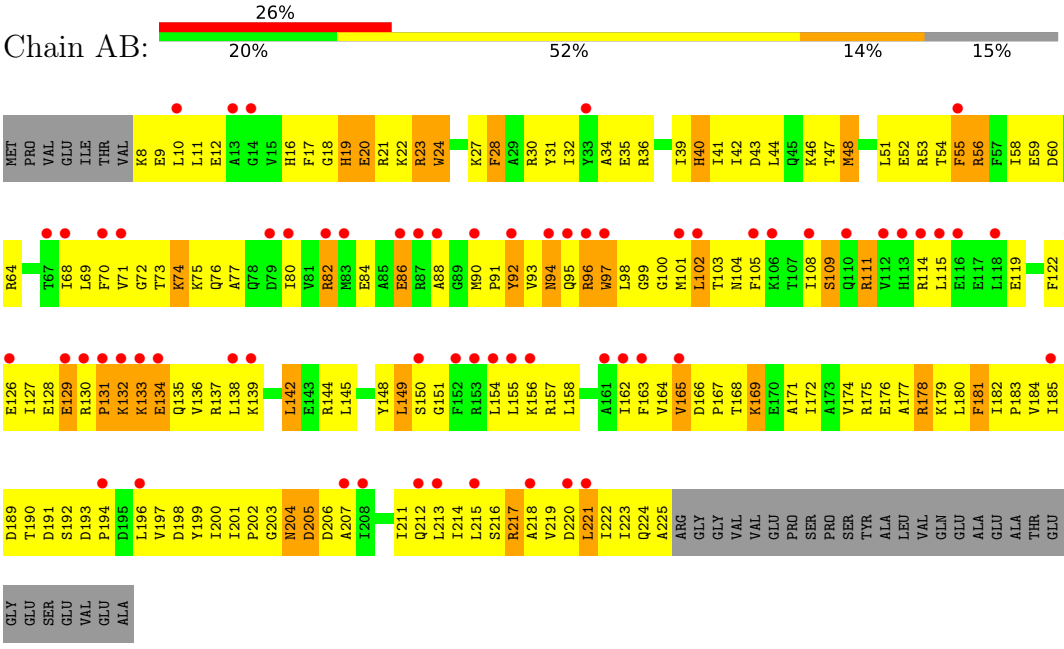
Chain CA:





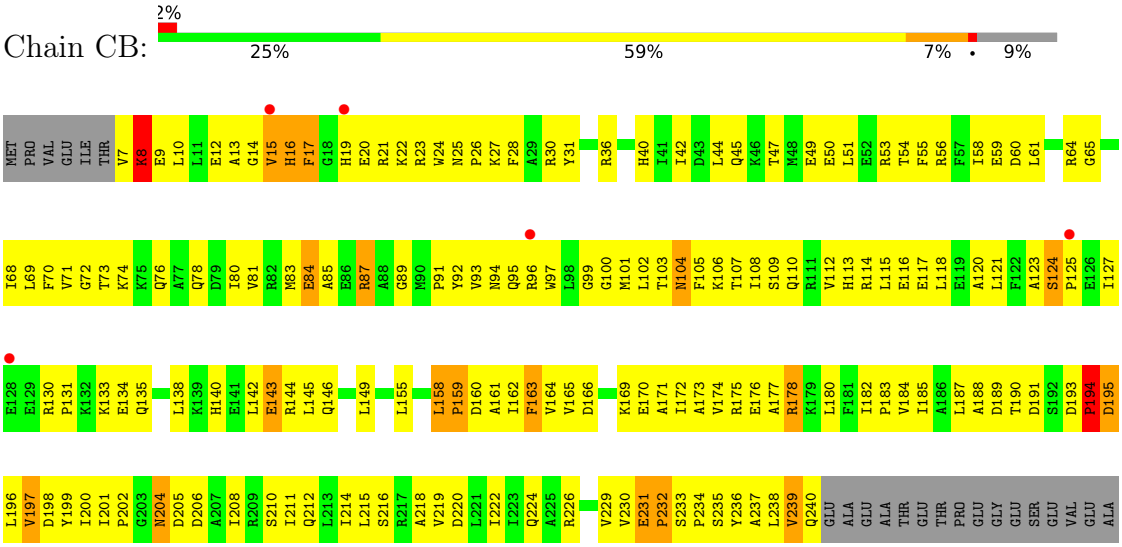


• Molecule 2: 30S ribosomal protein S2



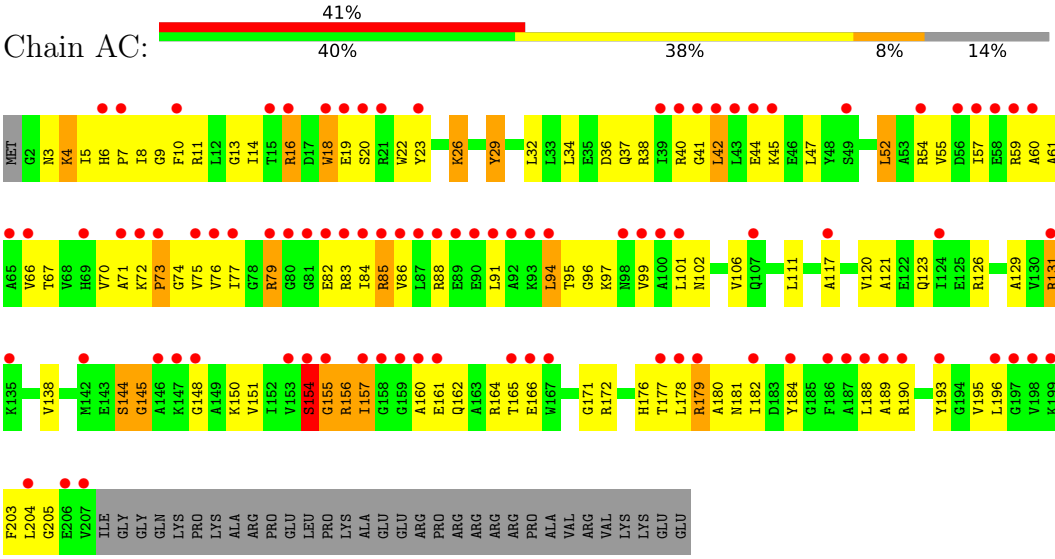
• Molecule 2: 30S ribosomal protein S2

Chain CB:



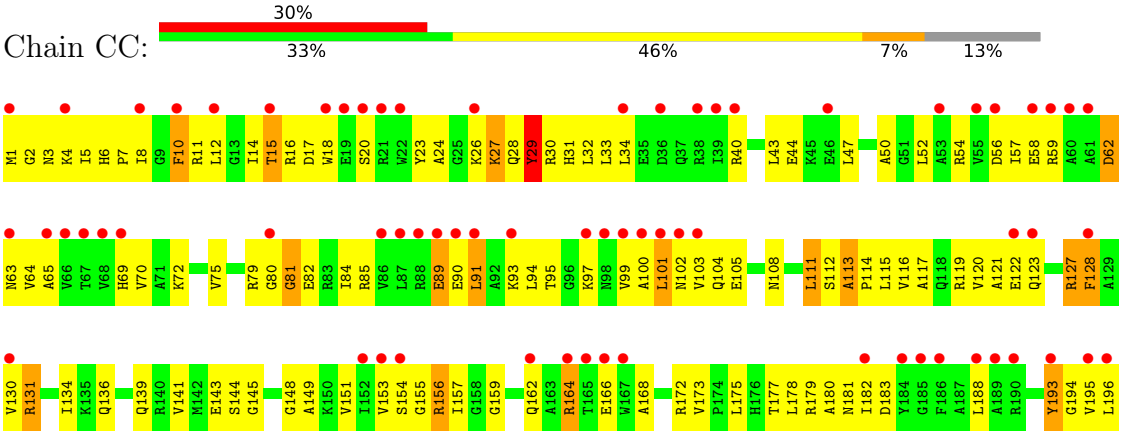
• Molecule 3: 30S ribosomal protein S3

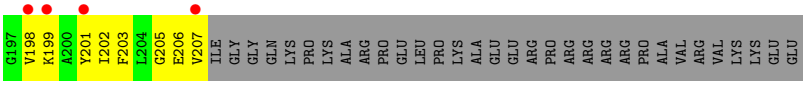
Chain AC:



• Molecule 3: 30S ribosomal protein S3

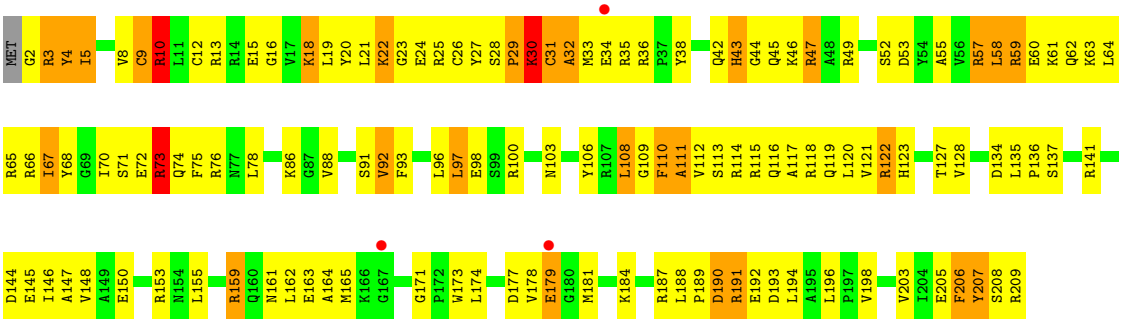
Chain CC:





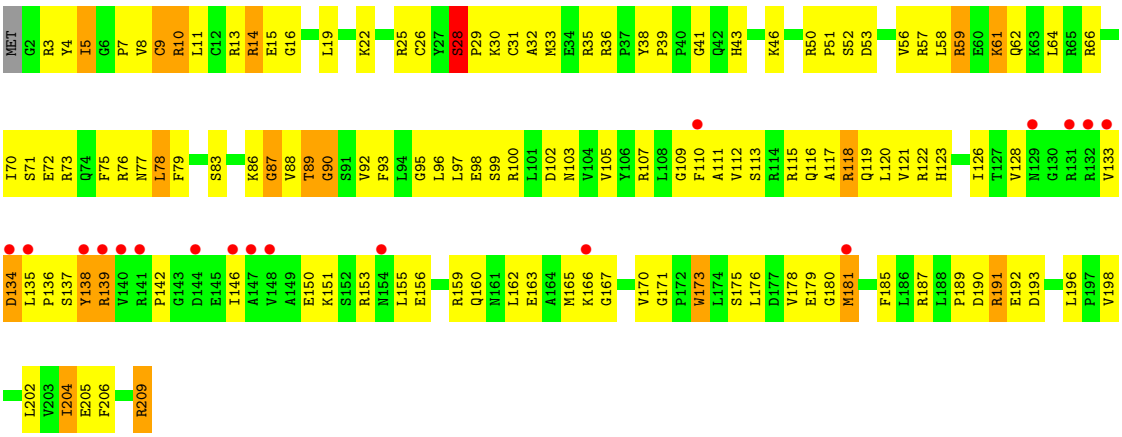
• Molecule 4: 30S ribosomal protein S4

Chain AD:



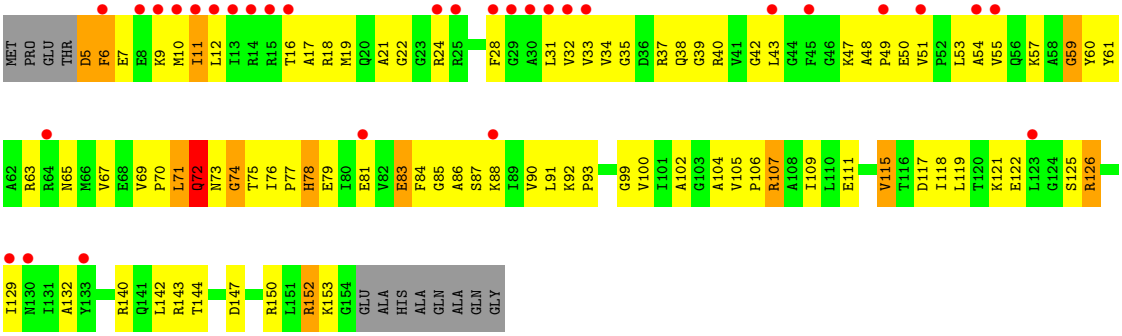
• Molecule 4: 30S ribosomal protein S4

Chain CD:



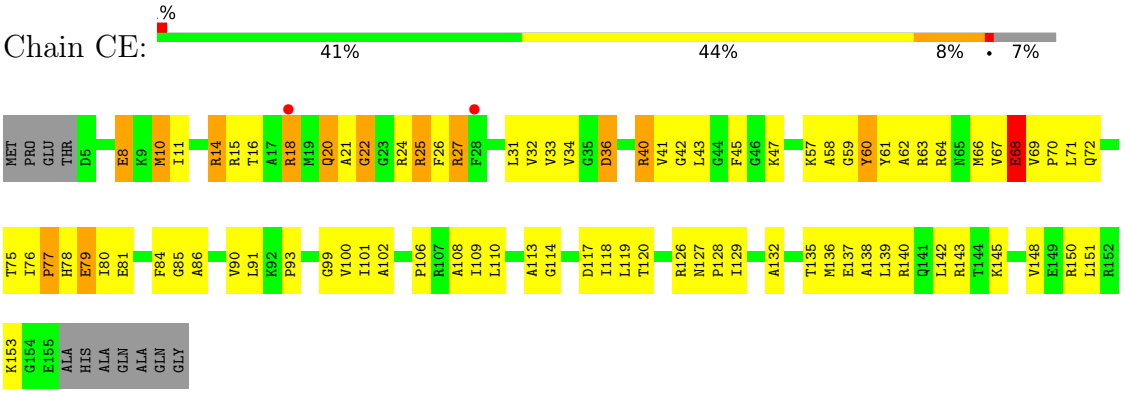
• Molecule 5: 30S ribosomal protein S5

Chain AE:



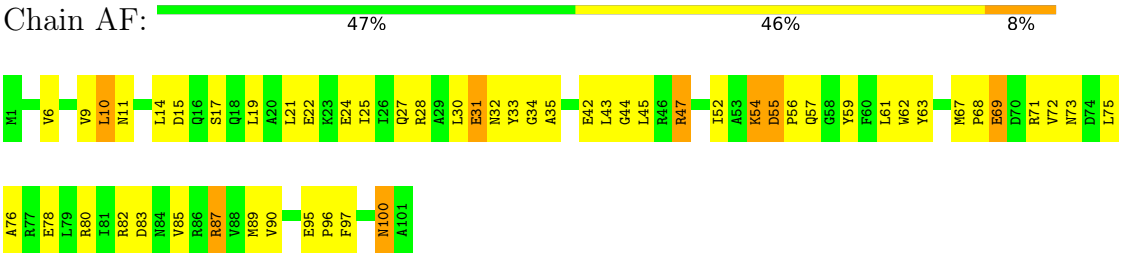
• Molecule 5: 30S ribosomal protein S5

Chain CE:



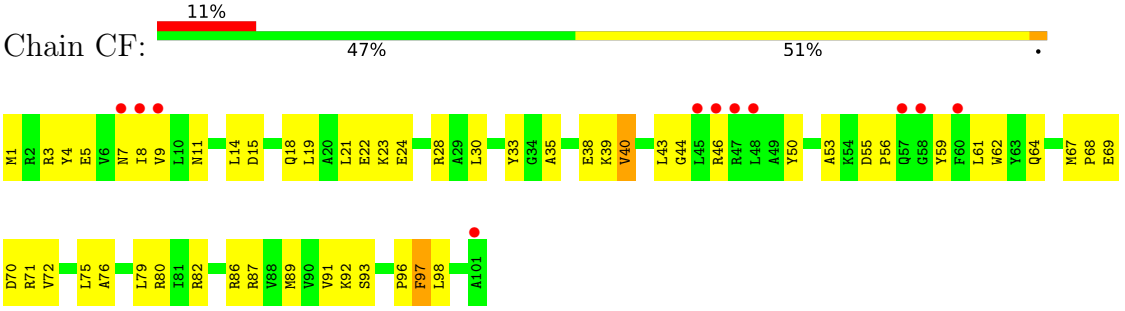
• Molecule 6: 30S ribosomal protein S6

Chain AF:



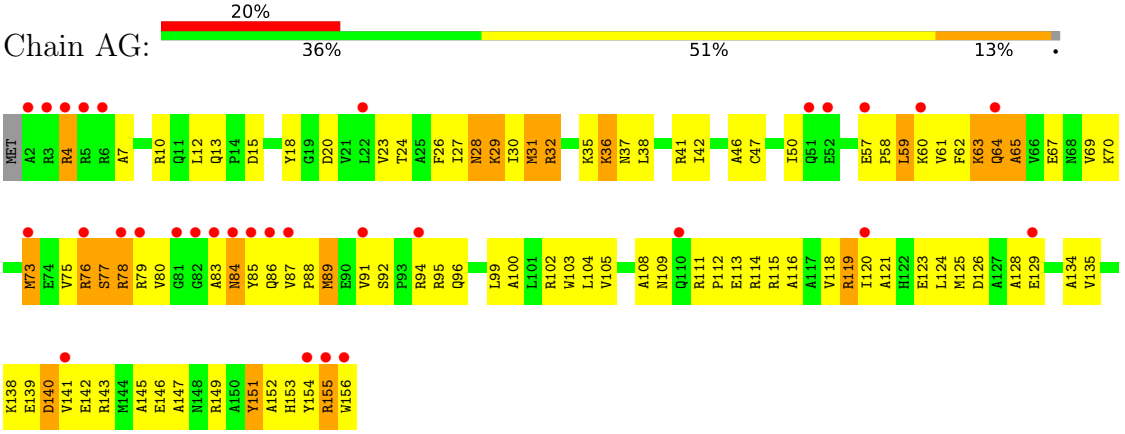
• Molecule 6: 30S ribosomal protein S6

Chain CF:



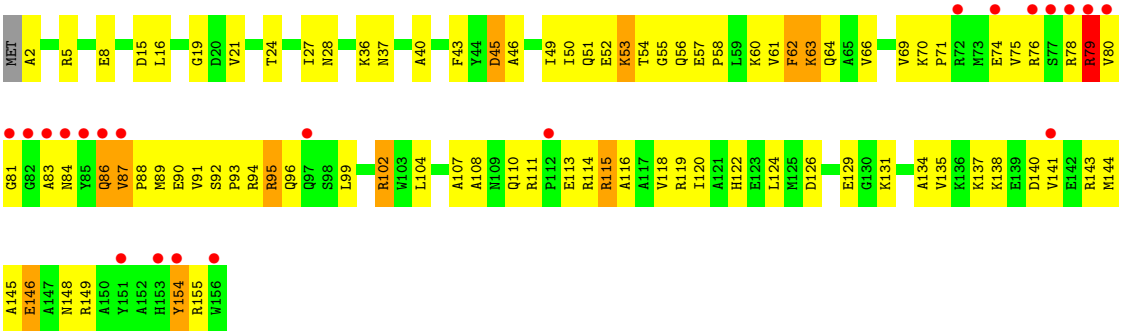
• Molecule 7: 30S ribosomal protein S7

Chain AG:

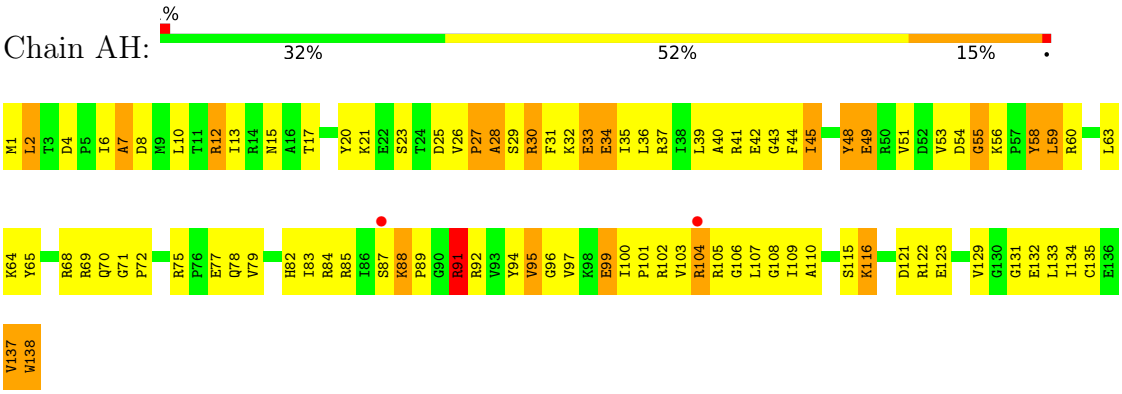


• Molecule 7: 30S ribosomal protein S7

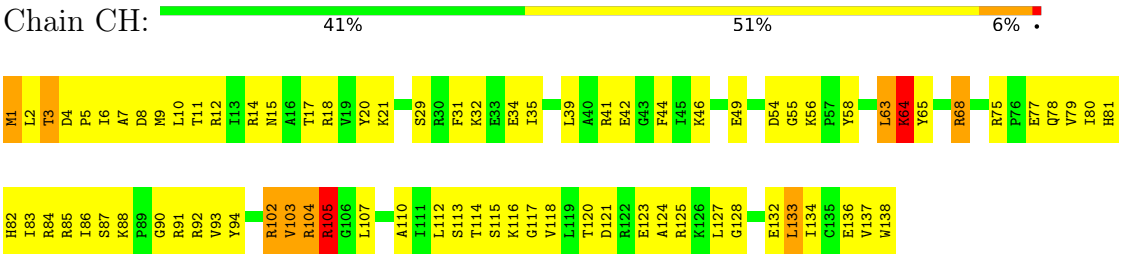
Chain CG:



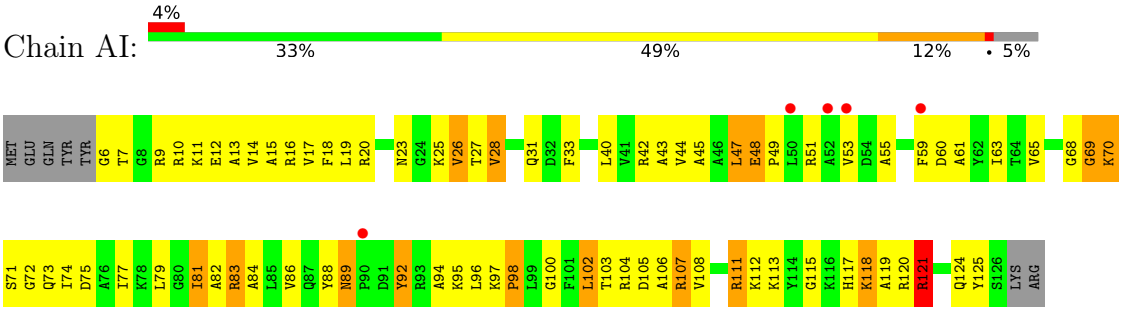
• Molecule 8: 30S ribosomal protein S8



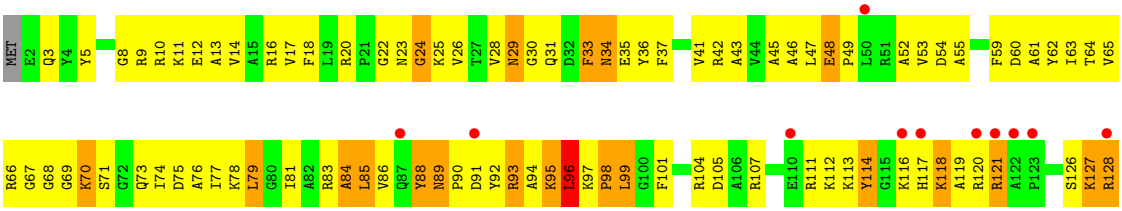
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9

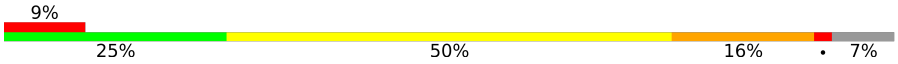


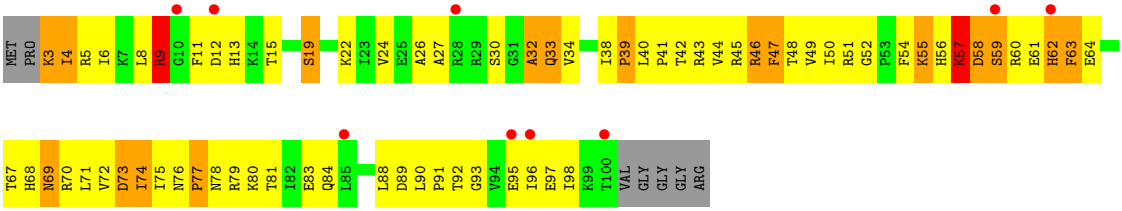
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10

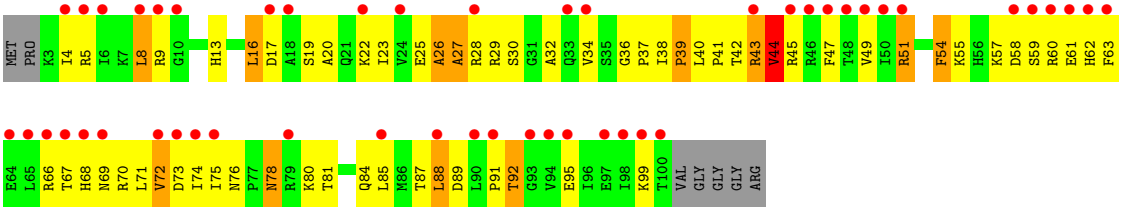
Chain AJ:





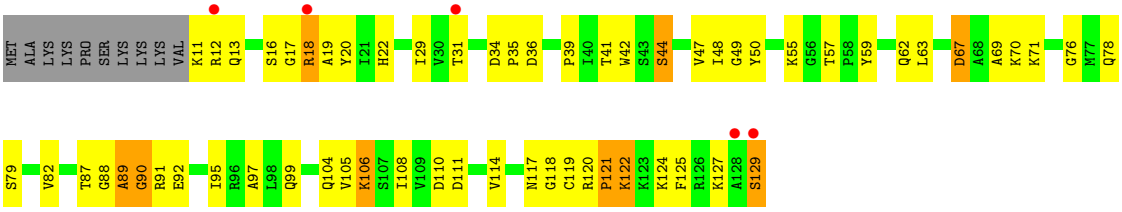
• Molecule 10: 30S ribosomal protein S10

Chain CJ:



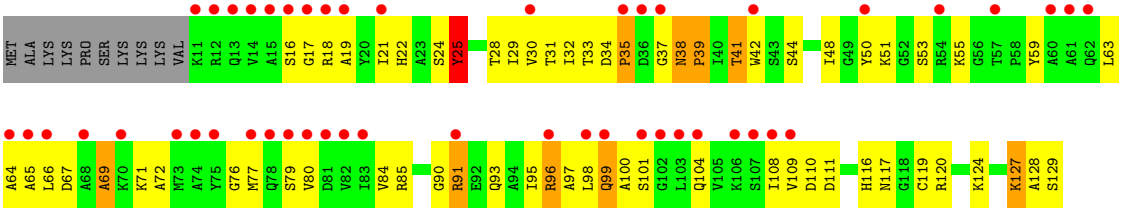
• Molecule 11: 30S ribosomal protein S11

Chain AK:



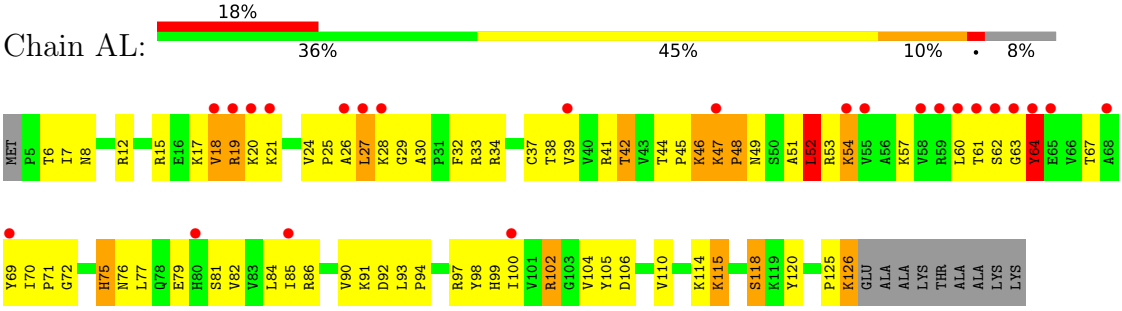
• Molecule 11: 30S ribosomal protein S11

Chain CK:



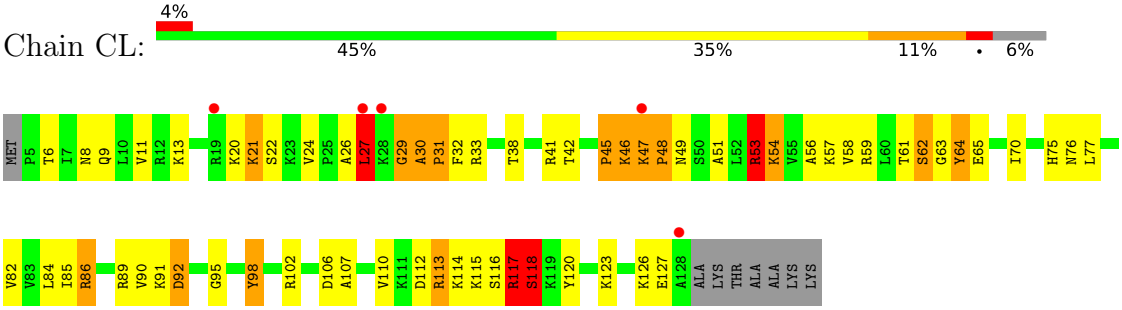
• Molecule 12: 30S ribosomal protein S12

Chain AL:



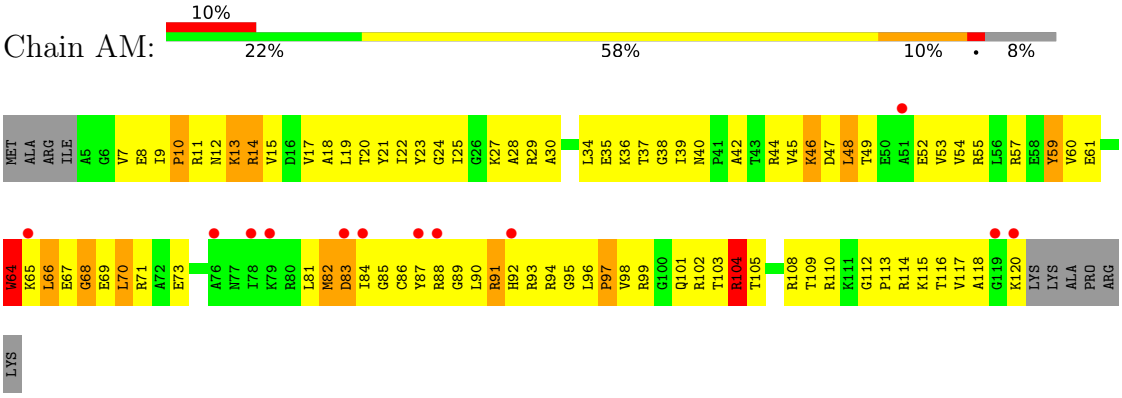
• Molecule 12: 30S ribosomal protein S12

Chain CL:



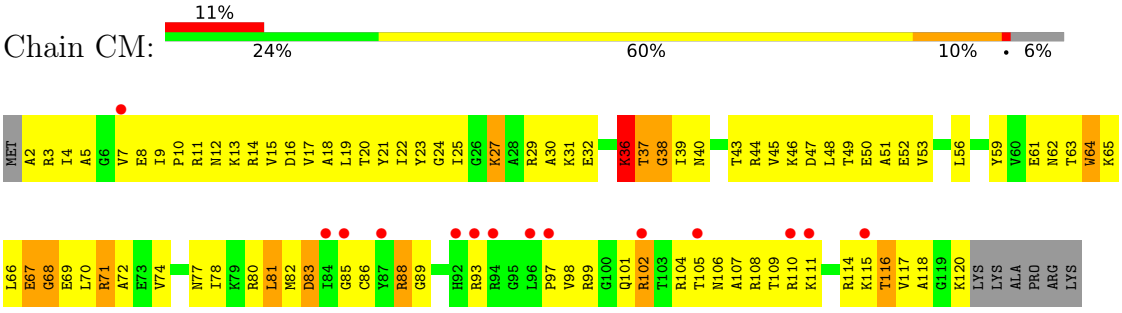
• Molecule 13: 30S ribosomal protein S13

Chain AM:



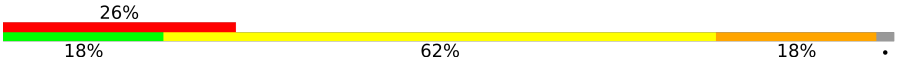
• Molecule 13: 30S ribosomal protein S13

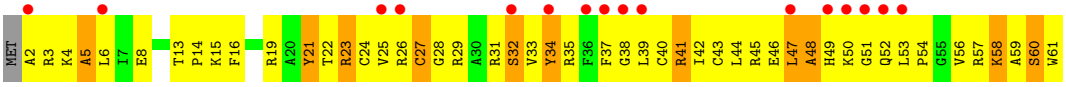
Chain CM:



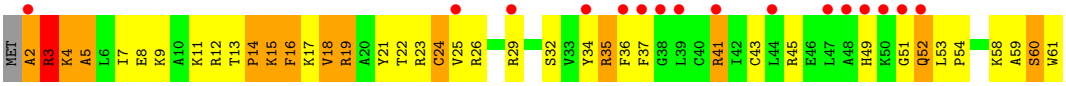
• Molecule 14: 30S ribosomal protein S14 type Z

Chain AN:



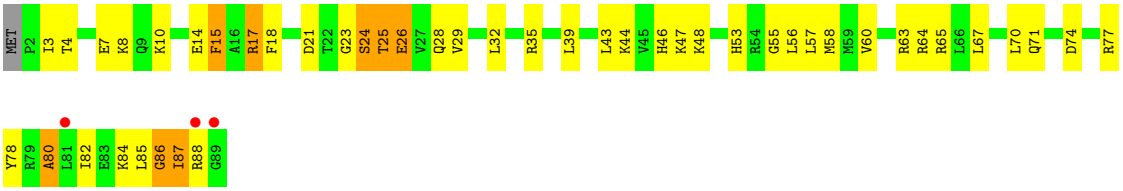


• Molecule 14: 30S ribosomal protein S14 type Z

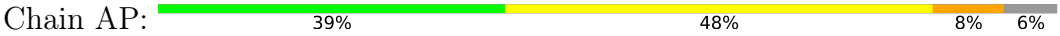


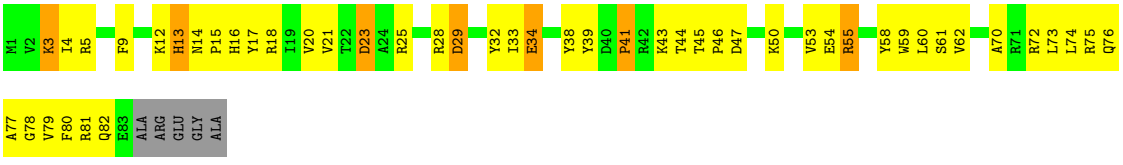
• Molecule 15: 30S ribosomal protein S15

• Molecule 15: 30S ribosomal protein S15



• Molecule 16: 30S ribosomal protein S16

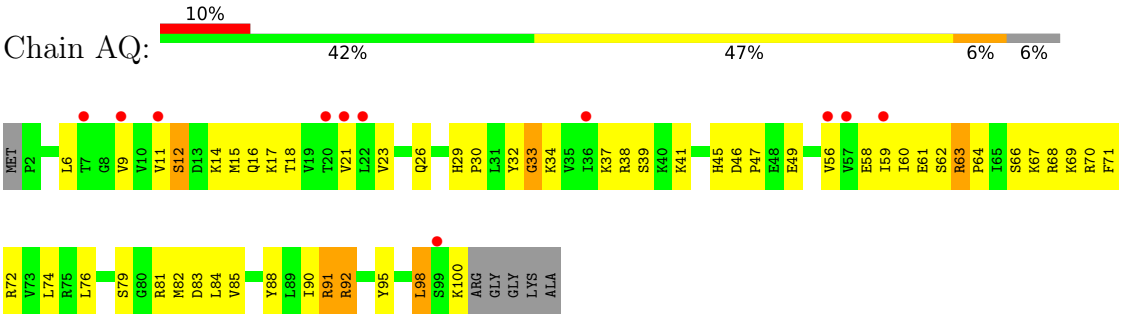




• Molecule 16: 30S ribosomal protein S16

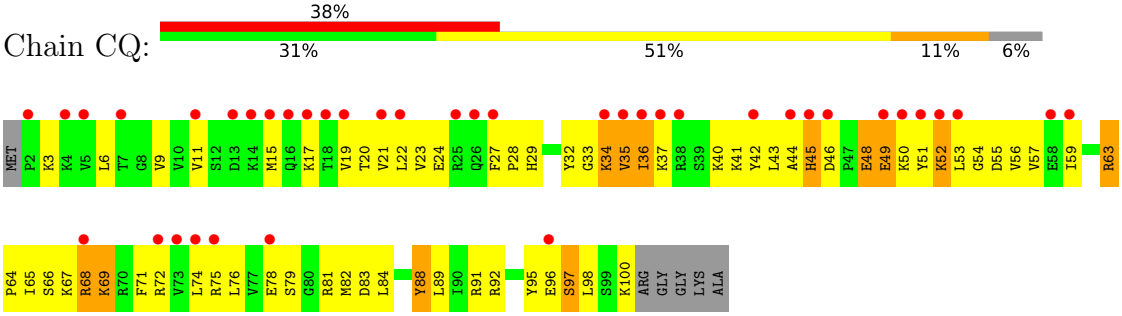
• Molecule 17: 30S ribosomal protein S17

Chain AQ:



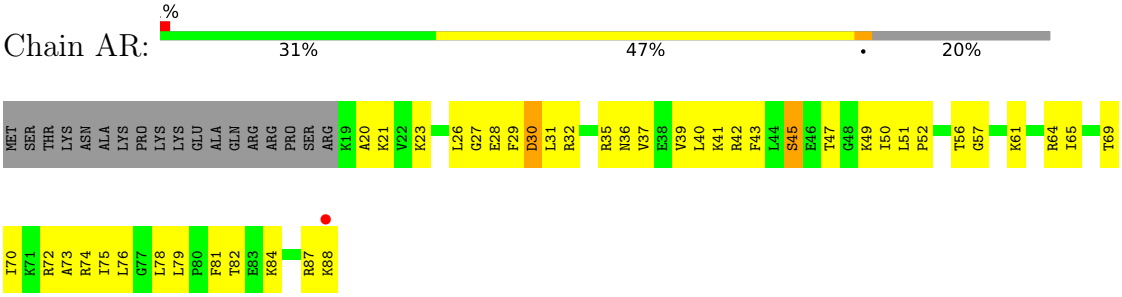
• Molecule 17: 30S ribosomal protein S17

Chain CQ:



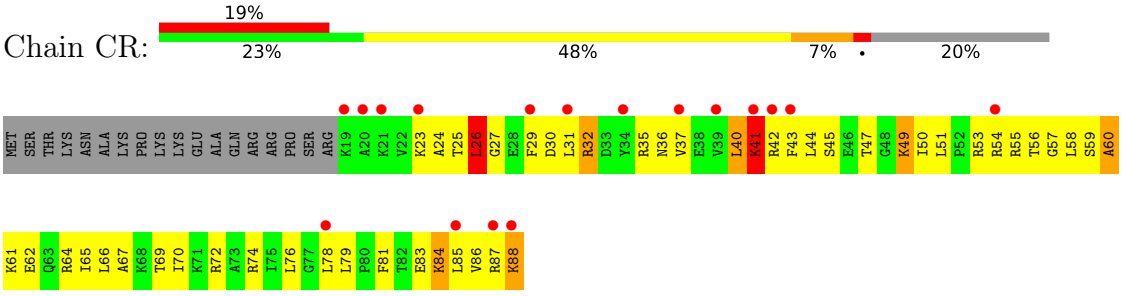
• Molecule 18: 30S ribosomal protein S18

Chain AR:



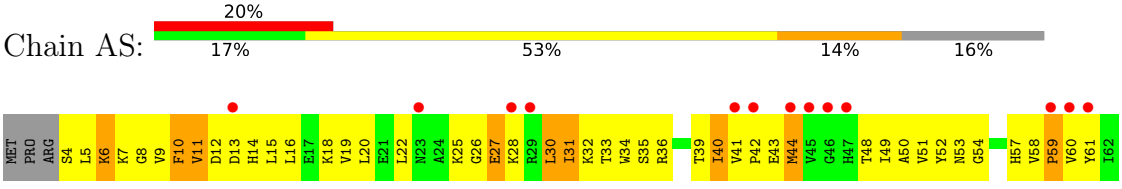
• Molecule 18: 30S ribosomal protein S18

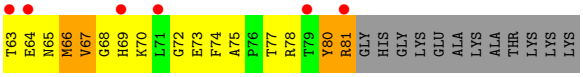
Chain CR:



• Molecule 19: 30S ribosomal protein S19

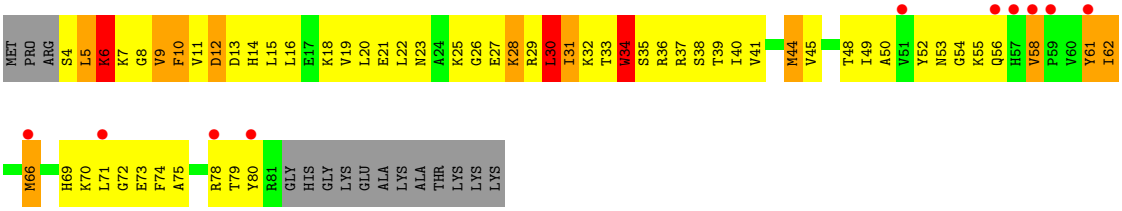
Chain AS:





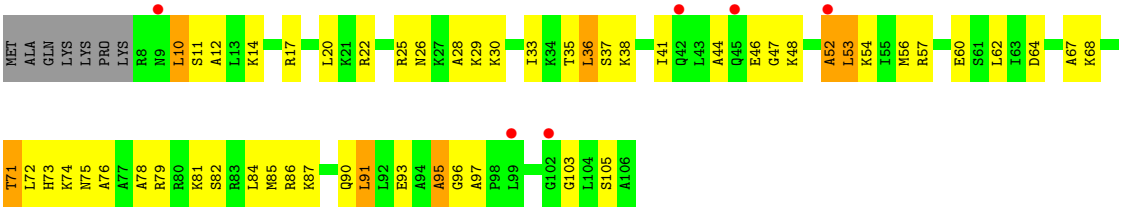
• Molecule 19: 30S ribosomal protein S19

Chain CS:



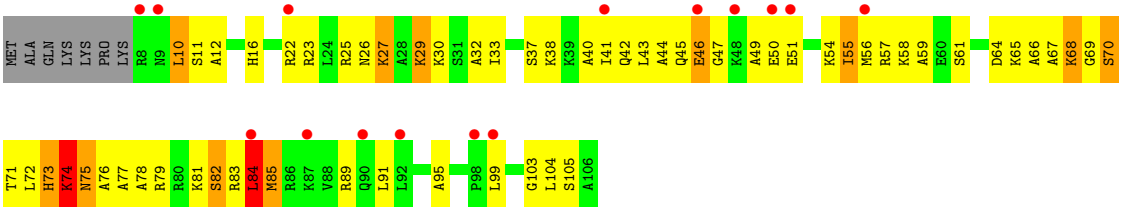
• Molecule 20: 30S ribosomal protein S20

Chain AT:



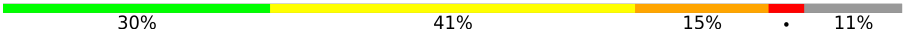
• Molecule 20: 30S ribosomal protein S20

Chain CT:



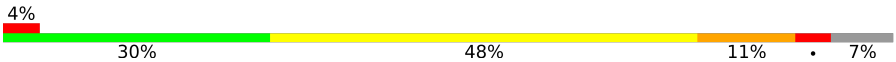
• Molecule 21: 30S ribosomal protein Thx

Chain AU:



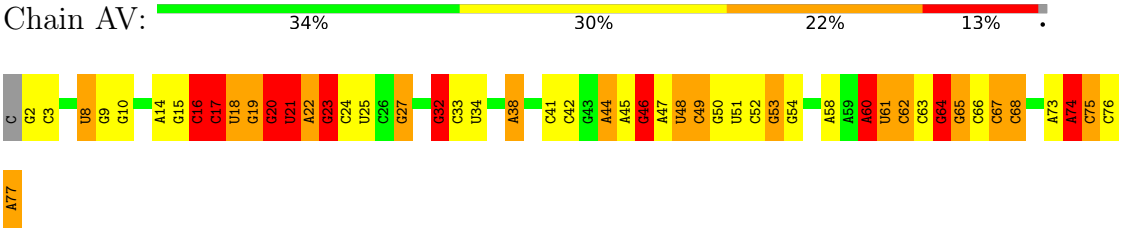
• Molecule 21: 30S ribosomal protein Thx

Chain CU:



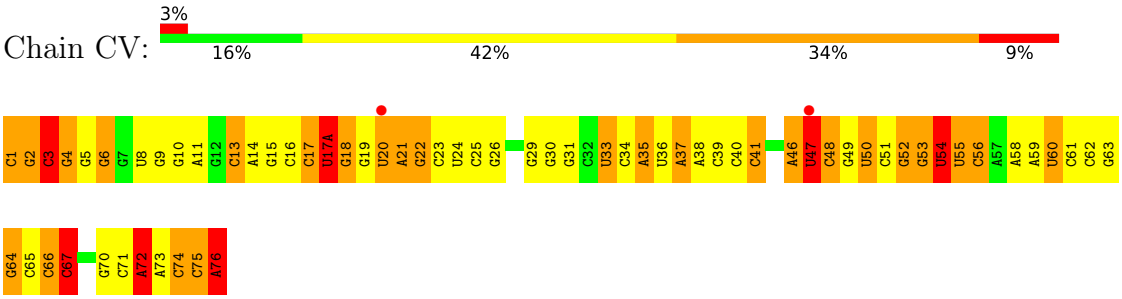
• Molecule 22: P-site tRNA fMet

Chain AV:



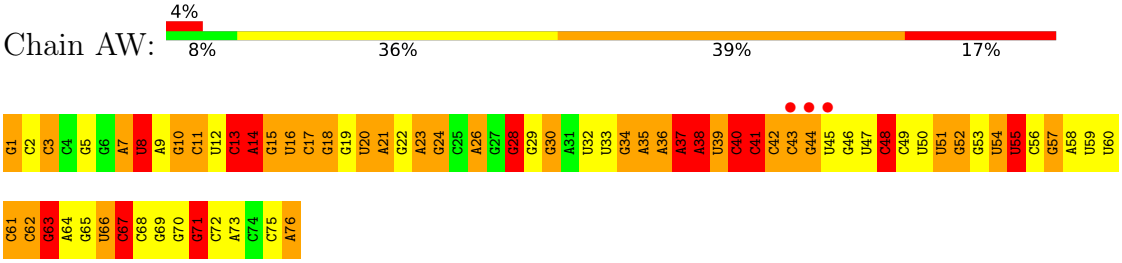
• Molecule 22: P-site tRNA fMet

Chain CV:



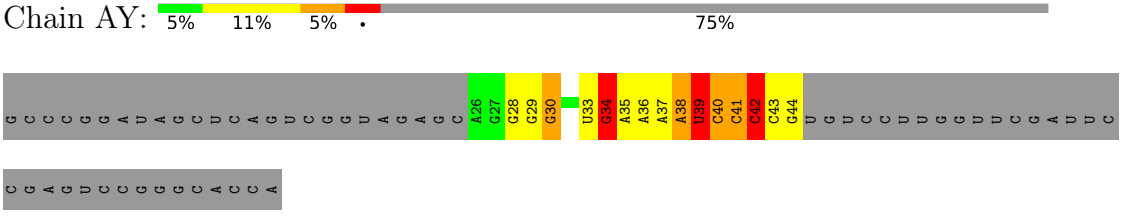
• Molecule 23: E-Site tRNA Phe and A-site tRNA Phe

Chain AW:



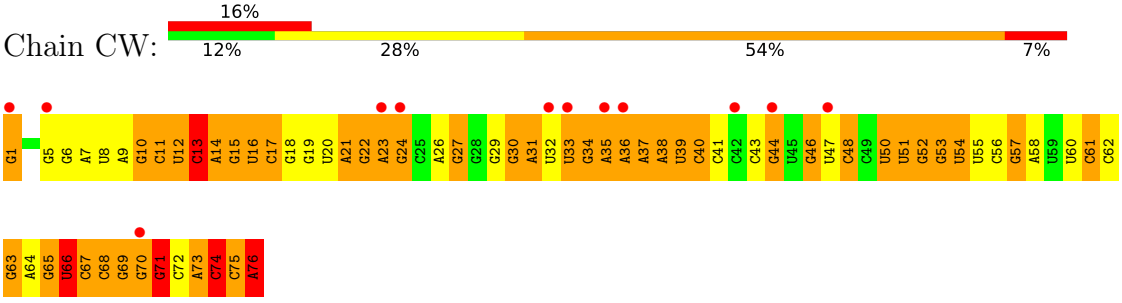
• Molecule 23: E-Site tRNA Phe and A-site tRNA Phe

Chain AY:



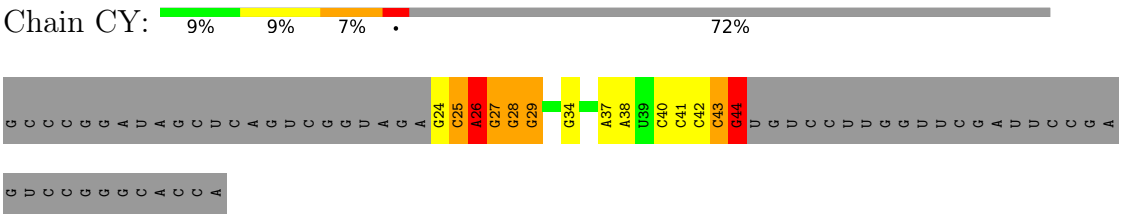
• Molecule 23: E-Site tRNA Phe and A-site tRNA Phe

Chain CW:



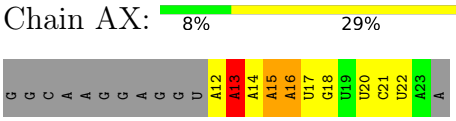
• Molecule 23: E-Site tRNA Phe and A-site tRNA Phe

Chain CY:



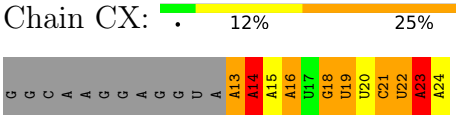
• Molecule 24: mRNA

Chain AX:



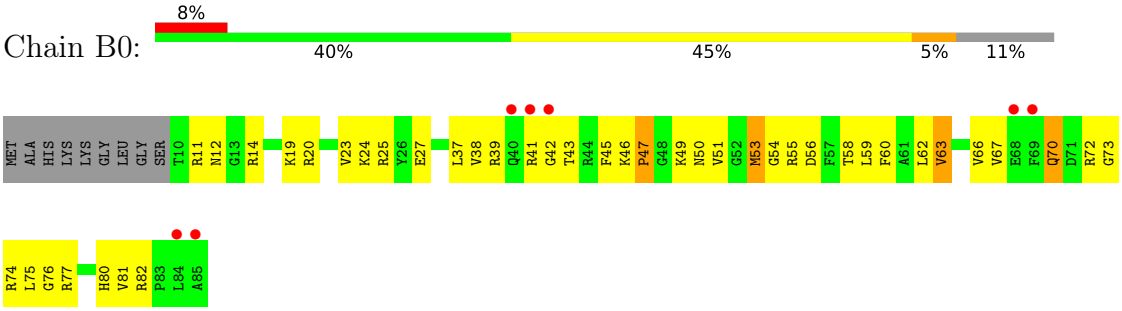
• Molecule 24: mRNA

Chain CX:



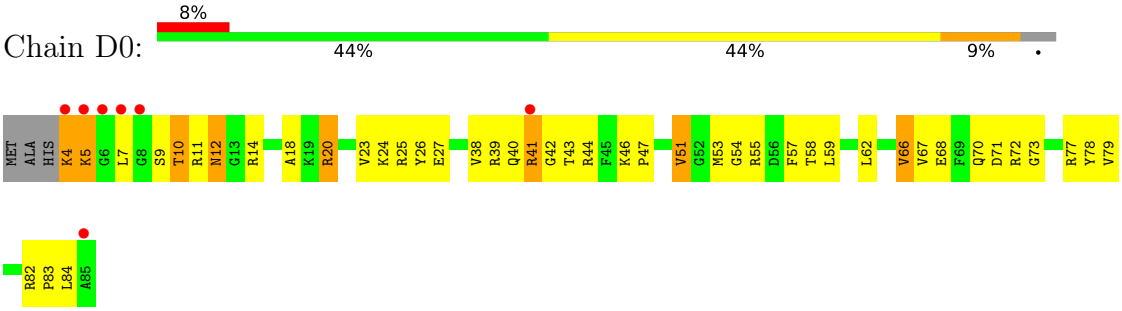
• Molecule 25: 50S ribosomal protein L27

Chain B0:



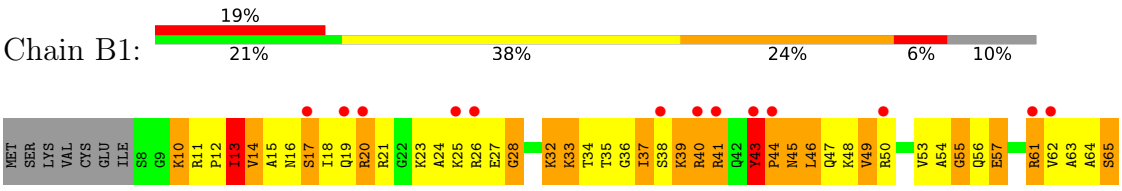
• Molecule 25: 50S ribosomal protein L27

Chain D0:



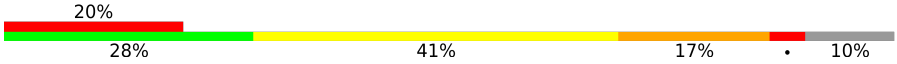
• Molecule 26: 50S ribosomal protein L28

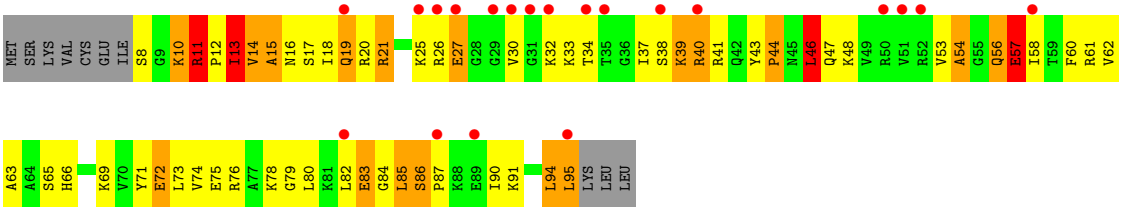
Chain B1:



• Molecule 26: 50S ribosomal protein L28

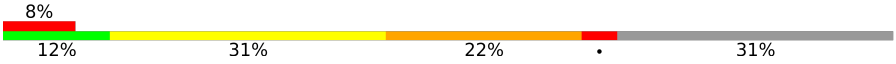
Chain D1:

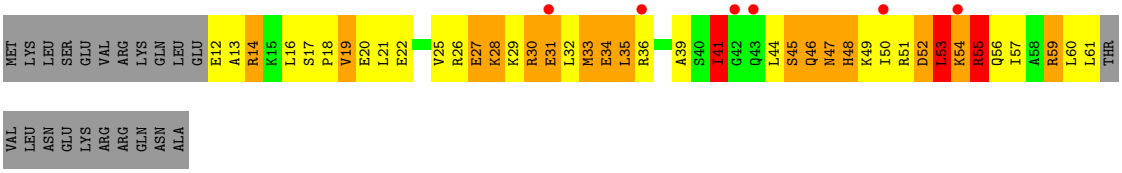




• Molecule 27: 50S ribosomal protein L29

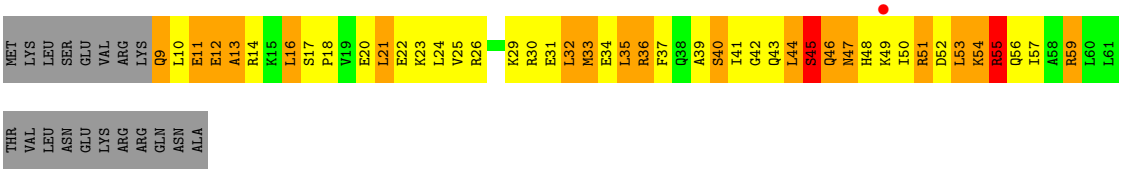
Chain B2:





• Molecule 27: 50S ribosomal protein L29

Chain D2:

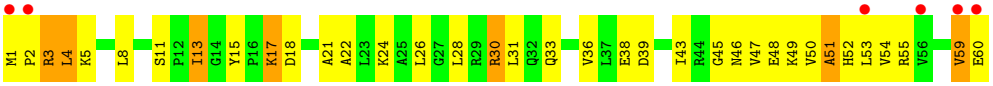


• Molecule 28: 50S ribosomal protein L30

Chain B3:

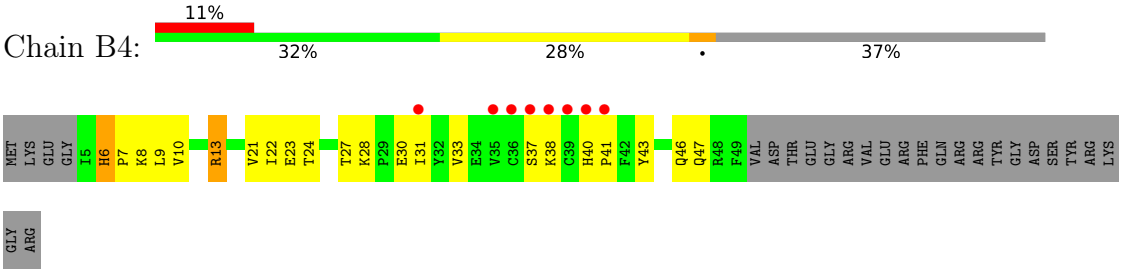
• Molecule 28: 50S ribosomal protein L30

Chain D3:



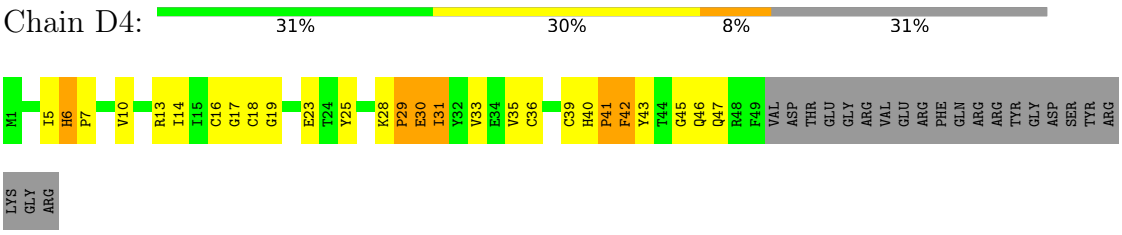
• Molecule 29: 50S ribosomal protein L31

Chain B4:



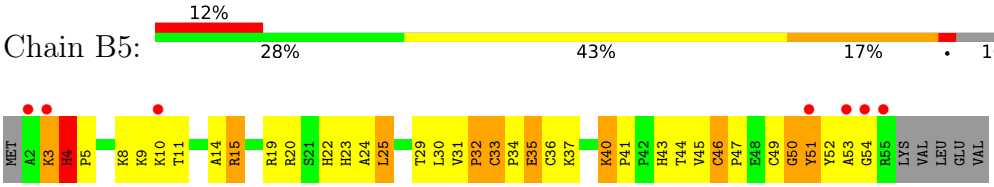
• Molecule 29: 50S ribosomal protein L31

Chain D4:



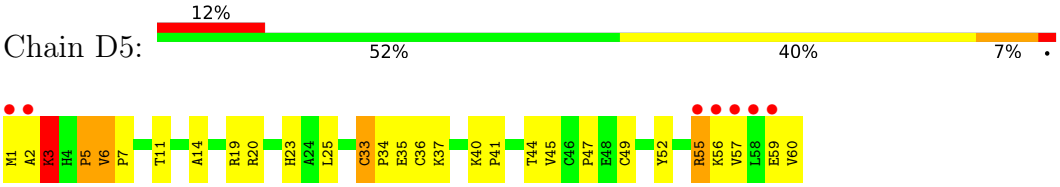
• Molecule 30: 50S ribosomal protein L32

Chain B5:



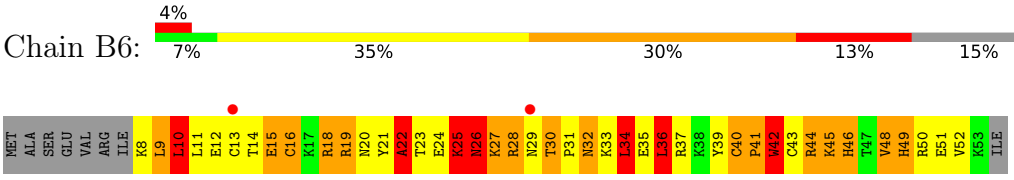
• Molecule 30: 50S ribosomal protein L32

Chain D5:



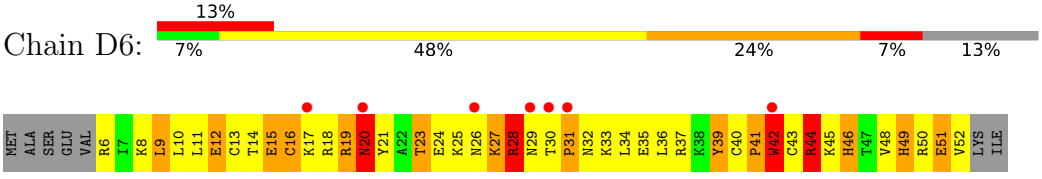
• Molecule 31: 50S ribosomal protein L33

Chain B6:



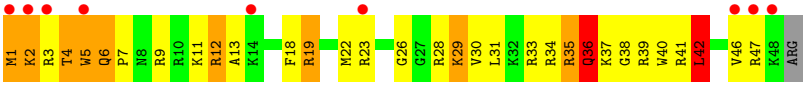
• Molecule 31: 50S ribosomal protein L33

Chain D6:



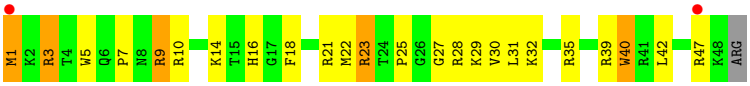
• Molecule 32: 50S ribosomal protein L34

Chain B7:



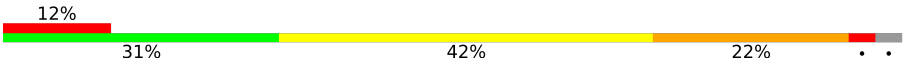
• Molecule 32: 50S ribosomal protein L34

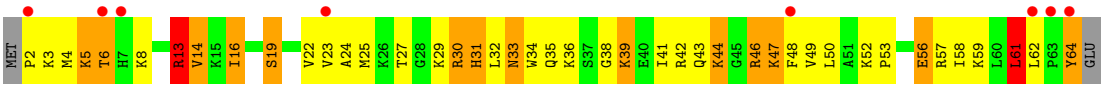
Chain D7:



• Molecule 33: 50S ribosomal protein L35

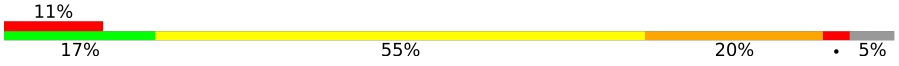
Chain B8:

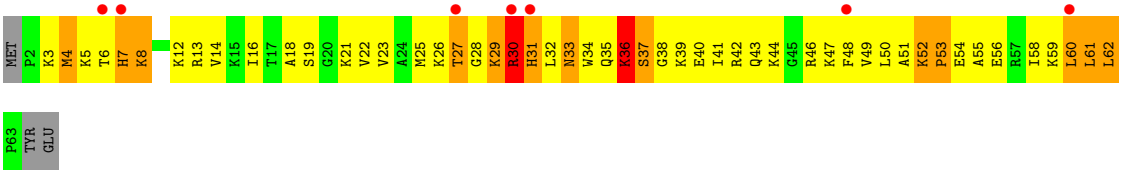




• Molecule 33: 50S ribosomal protein L35

Chain D8:



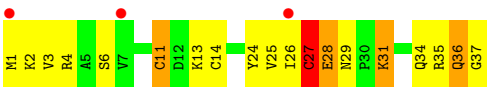


• Molecule 34: 50S ribosomal protein L36

Chain B9:

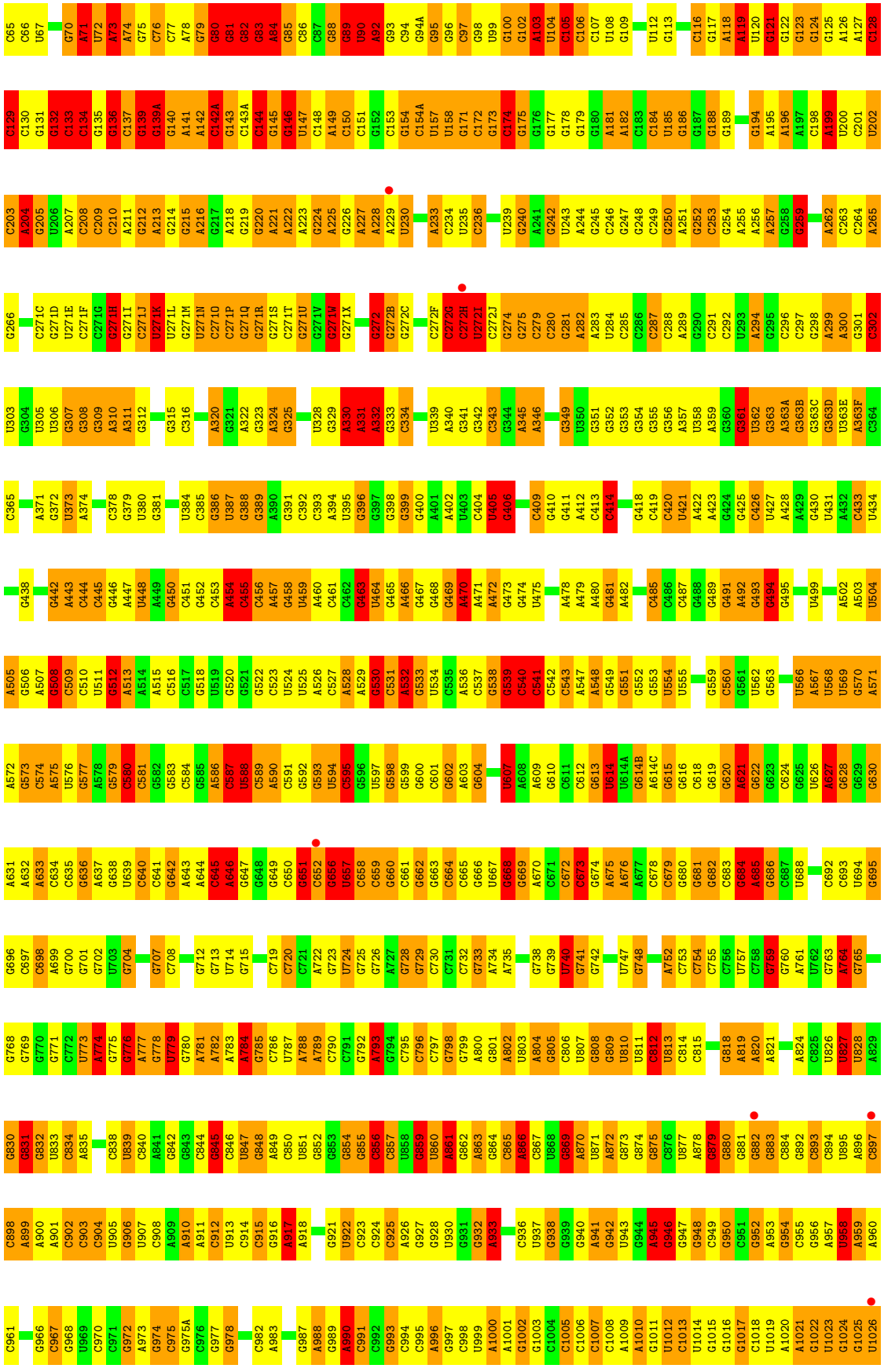
• Molecule 34: 50S ribosomal protein L36

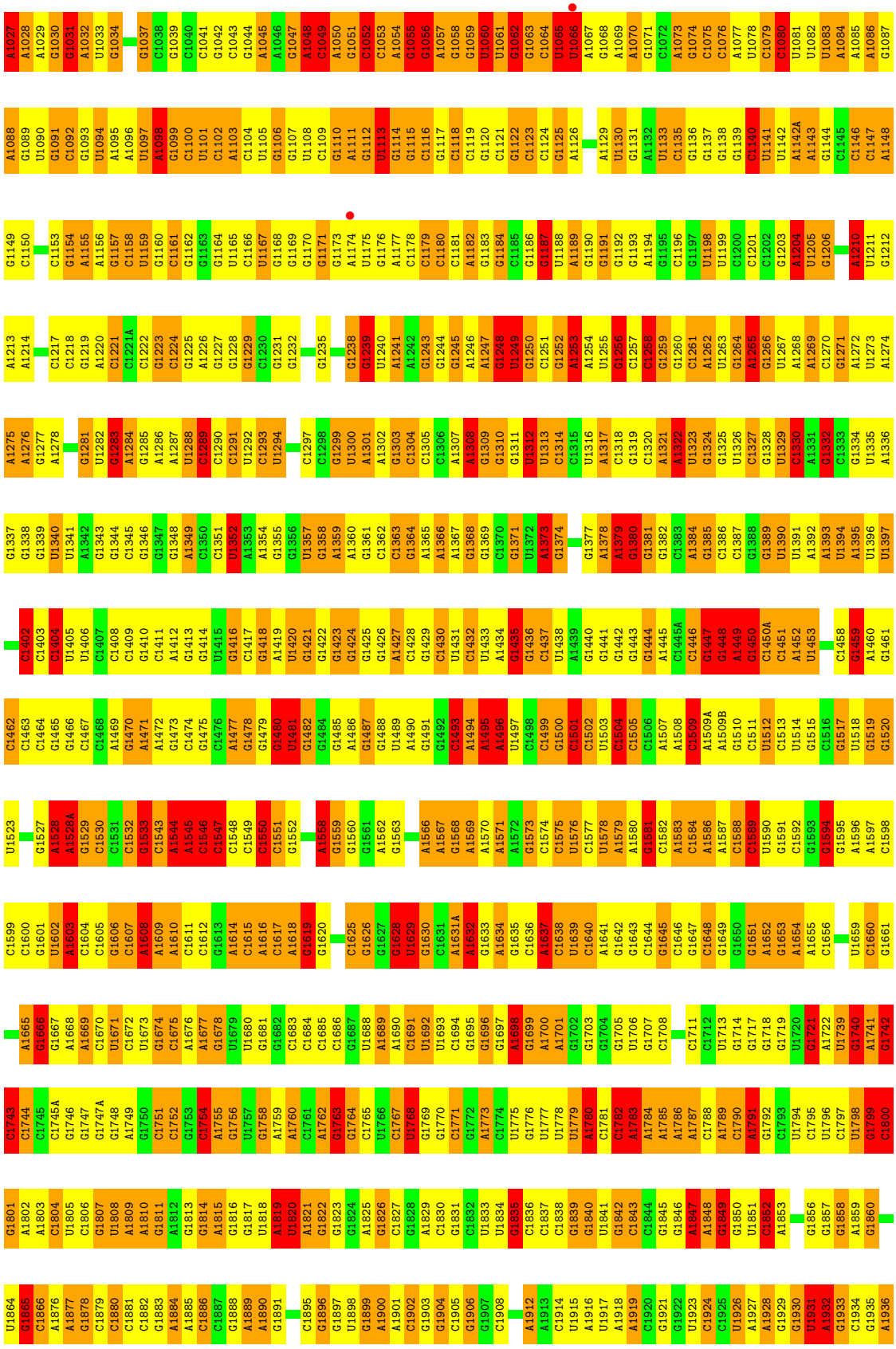
Chain D9:

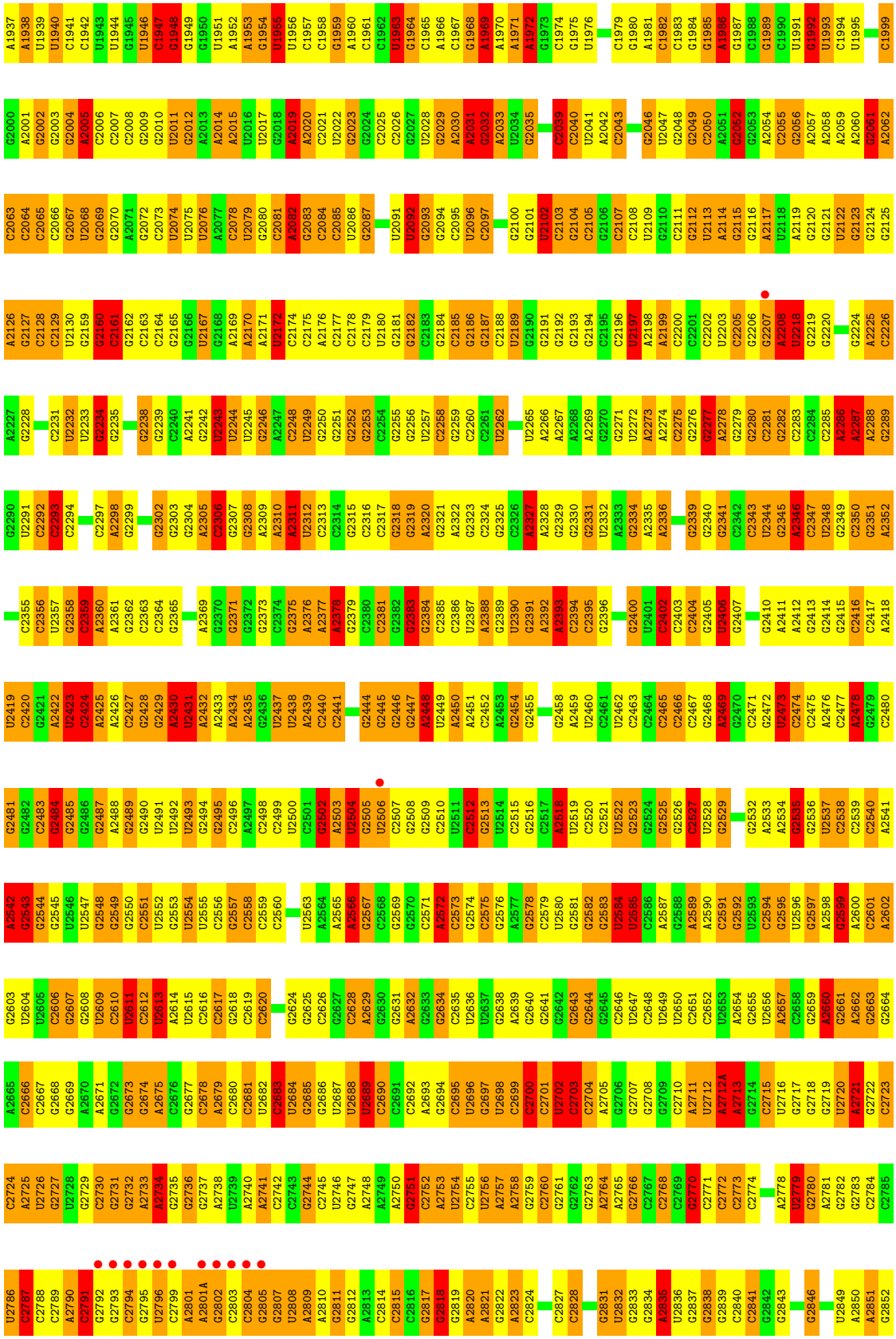


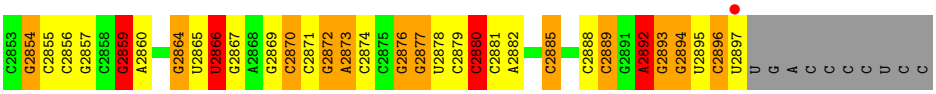
• Molecule 35: 23S ribosomal RNA

Chain BA:


C65 C66 U67 G70 A71 U72 A73 A74 G75 C76 C77 A78 G79 G80 G81 G82 G83 A84 G85 C86 C87 G88 G89 U90 A92 G93 C94 G94A G95 G96 C97 G98 U99 G100 G102 A103 U104 C105 C106 C107 U108 G109 U112 G113 C116 G117 A118 A119 U120 G121 G122 G123 G124 G125 A126 A127 C128
C129 C130 G131 G132 C133 C134 G135 G136 C137 G139 G139A G140 A141 A142 C142A G143 C143A C144 G145 G146 U147 C148 A149 C150 C151 G152 C153 G154 C154A U157 U158 G171 C172 G173 C174 G175 G176 G177 G178 G179 G180 A181 A182 C183 C184 U185 G186 G187 G188 G189 G194 A195 A196 A197 C198 A199 U200 C201 U202
C203 A204 G205 U206 A207 C208 C209 C210 A211 G212 A213 G214 G215 A216 G217 A218 G219 G220 A221 A222 A223 G224 A225 G226 A227 A228 A229 U230 A233 C234 U235 C236 U239 G240 A241 G242 U243 A244 G245 C246 G247 G248 C249 G250 A251 G252 C253 G254 A255 A256 A257 G258 G259 A262 C263 C264 A265
G266 C271C G271D U271E C271F C271G G271H G271I C271J U271K U271L G271M U271N C271O C271P G271Q G271R G271S C271T G271U G271V G271W G271X G272 G272B G272C C272F C272G C272H U272I C272J G274 G275 C279 C280 G281 A282 A283 U284 C285 C286 C287 C288 A289 G290 C291 C292 U293 A294 G295 C296 C297 G298 A299 A300 G301 C302
U303 G304 U305 U306 G307 G308 G309 A310 A311 G312 G315 C316 A320 G321 A322 G323 A324 G325 U328 G329 A330 A331 A332 G333 C334 U339 A340 G341 G342 C343 G344 A345 A346 G349 U350 G351 G352 G353 G354 G355 G356 A357 U358 A359 G360 C361 U362 G363 A363A G363B G363C G363D U363E A363F C364
C365 A371 G372 U373 A374 C378 G379 U380 G381 U384 C385 G386 U387 G388 G389 A390 G391 C392 G393 A394 U395 G396 G397 G398 G399 G400 A401 A402 U403 C404 U405 G406 C409 G410 G411 A412 C413 C414 G418 C419 C420 U421 A422 A423 G424 G425 C426 U427 A428 A429 G430 U431 A432 C433 U434
G438 G442 A443 C444 C445 G446 A447 U448 A449 G450 C451 G452 C453 A454 C455 C456 A457 G458 U459 A460 C461 C462 G463 U464 G465 A466 G467 G468 G469 A470 A471 A472 G473 G474 U475 A478 A479 A480 G481 A482 C485 C486 C487 G488 G489 G491 A492 G493 G494 G495 U499 A502 A503 U504
A505 G506 A507 G508 C509 C510 U511 G512 A513 A514 A515 C516 C517 G518 U519 G520 G521 G522 C523 U524 U525 A526 C527 A528 A529 G530 C531 A532 G533 U534 C535 A536 C537 G538 G539 C540 C541 C542 C543 A547 A548 G549 G551 G552 G553 U554 U555 G559 C560 G561 U562 G563 U566 A567 U568 U569 G570 A571
A572 G573 C574 A575 U576 G577 A578 G579 C580 C581 G582 G583 C584 G585 A586 C587 U588 C589 A590 C591 G592 G593 U594 C595 G596 U597 G598 G599 G600 C601 G602 A603 G604 U607 A608 A609 G610 C611 C612 G613 U614 U614A G614B A614C G615 G616 C618 G619 G620 A621 G622 G623 C624 G625 U626 A627 G628 G629 G630
A631 A632 A633 C634 C635 G636 A637 G638 U639 C640 C641 G642 A643 A644 C645 A646 G647 G648 G649 C650 G651 C652 G656 U657 C658 C659 G660 C661 G662 G663 C664 C665 G666 U667 G668 G669 A670 C671 C672 C673 G674 A675 A676 A677 C678 C679 G680 G681 G682 C683 G684 A685 G686 C687 U688 C692 C693 U694 G695
G696 C697 G698 A699 G700 G701 G702 U703 G704 G707 C708 G712 G713 U714 G715 C719 C720 G721 A722 G723 C790 U724 G725 G726 A727 G728 G729 C730 C731 C732 G733 A734 A735 G738 G739 U740 G741 G742 U747 G748 A752 C753 C754 C755 C756 U757 C758 G759 G760 A761 U762 G763 A764 G765
G768 G769 G770 G771 C772 U773 A774 G775 G776 A777 G778 U779 G780 A781 A782 A783 A784 G785 C786 U787 A788 A789 C790 G791 G792 A793 G794 C795 C796 C797 G798 G799 A800 G801 A802 U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 U813 C814 C815 G818 A819 A820 A821 A824 C825 U826 U827 U828 A829
G830 G831 G832 U833 C834 A835 C838 U839 C840 A841 C842 G843 C844 G845 C846 U847 C848 A849 C850 U851 G852 G853 C854 G855 C856 C857 U858 G859 U860 A861 C862 A863 G864 C865 A866 C867 U868 G869 A870 U871 A872 G873 G874 G875 C876 U877 A878 G879 G880 C881 G882 G883 C884 G892 C893 C894 U895 A896 C897
C898 A899 A900 A901 C902 C903 C904 U905 G906 U907 C908 A909 A910 A911 C912 U913 C914 C915 G916 A917 A918 G921 U922 C923 C924 G925 A926 G927 G928 U930 G931 G932 A933 C936 U937 G938 G939 G940 A941 G942 U943 G944 A945 G946 G947 G948 C949 G950 C951 G952 A953 G954 C955 G956 A957 U958 A959 A960
C961 G966 C967 G968 U969 C970 C971 G972 A973 G974 C975 G975A C976 G977 G978 C982 A983 G987 A988 G989 A990 C991 C992 G993 C994 C995 A996 G997 C998 U999 A1000 A1001 G1002 G1003 C1004 C1005 C1006 C1007 C1008 A1009 A1010 G1011 U1012 C1013 U1014 G1015 G1016 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026

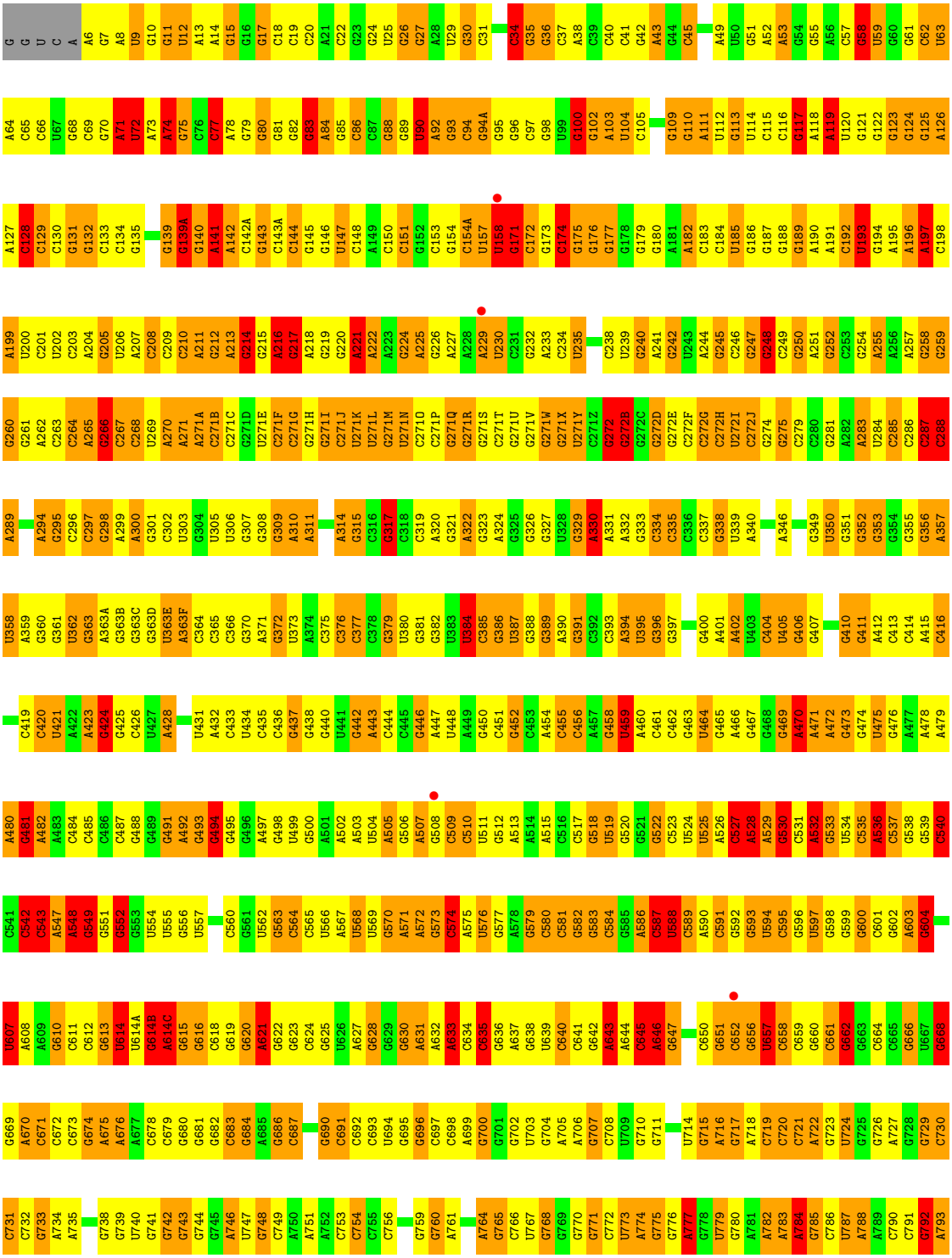


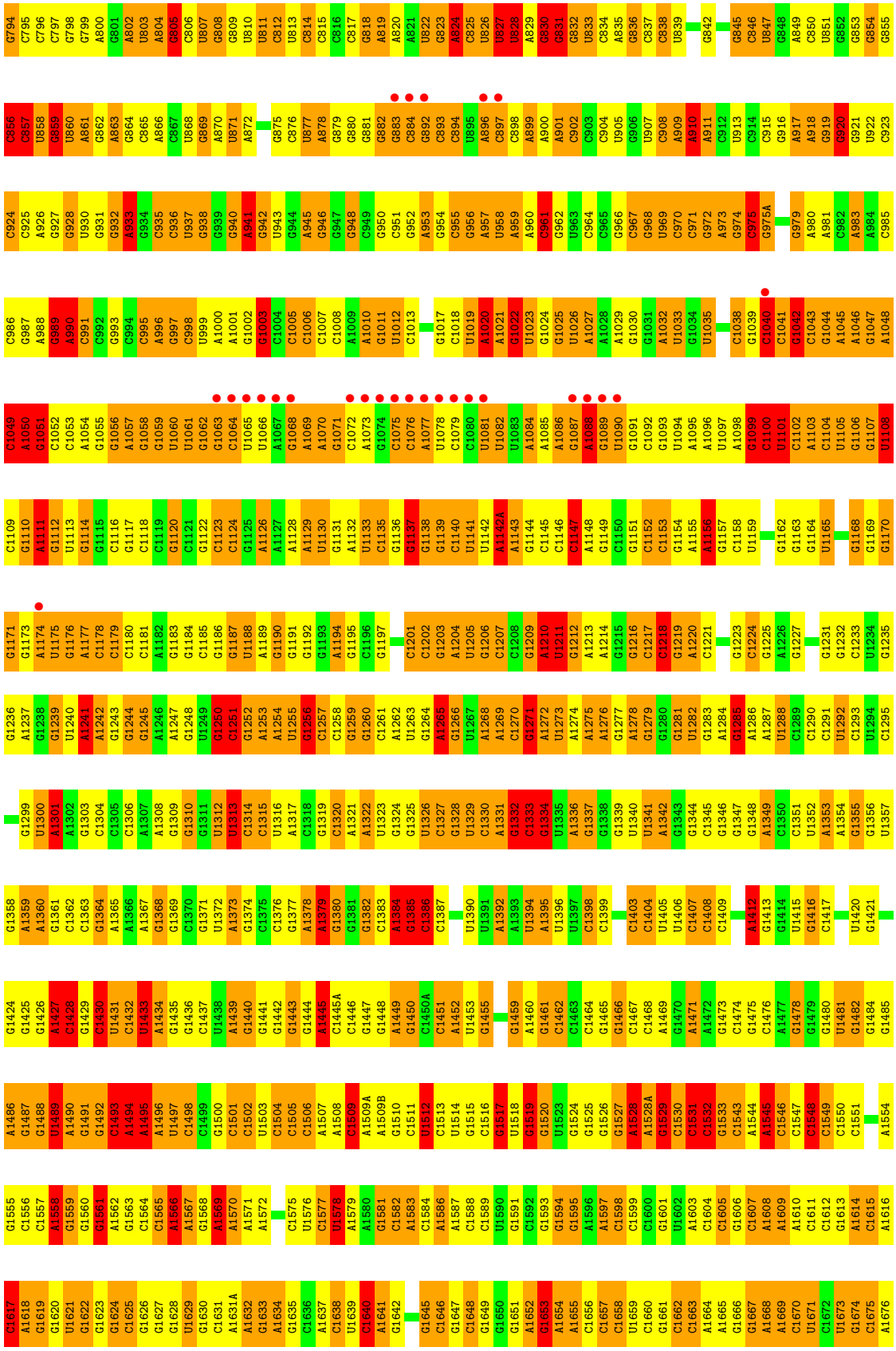


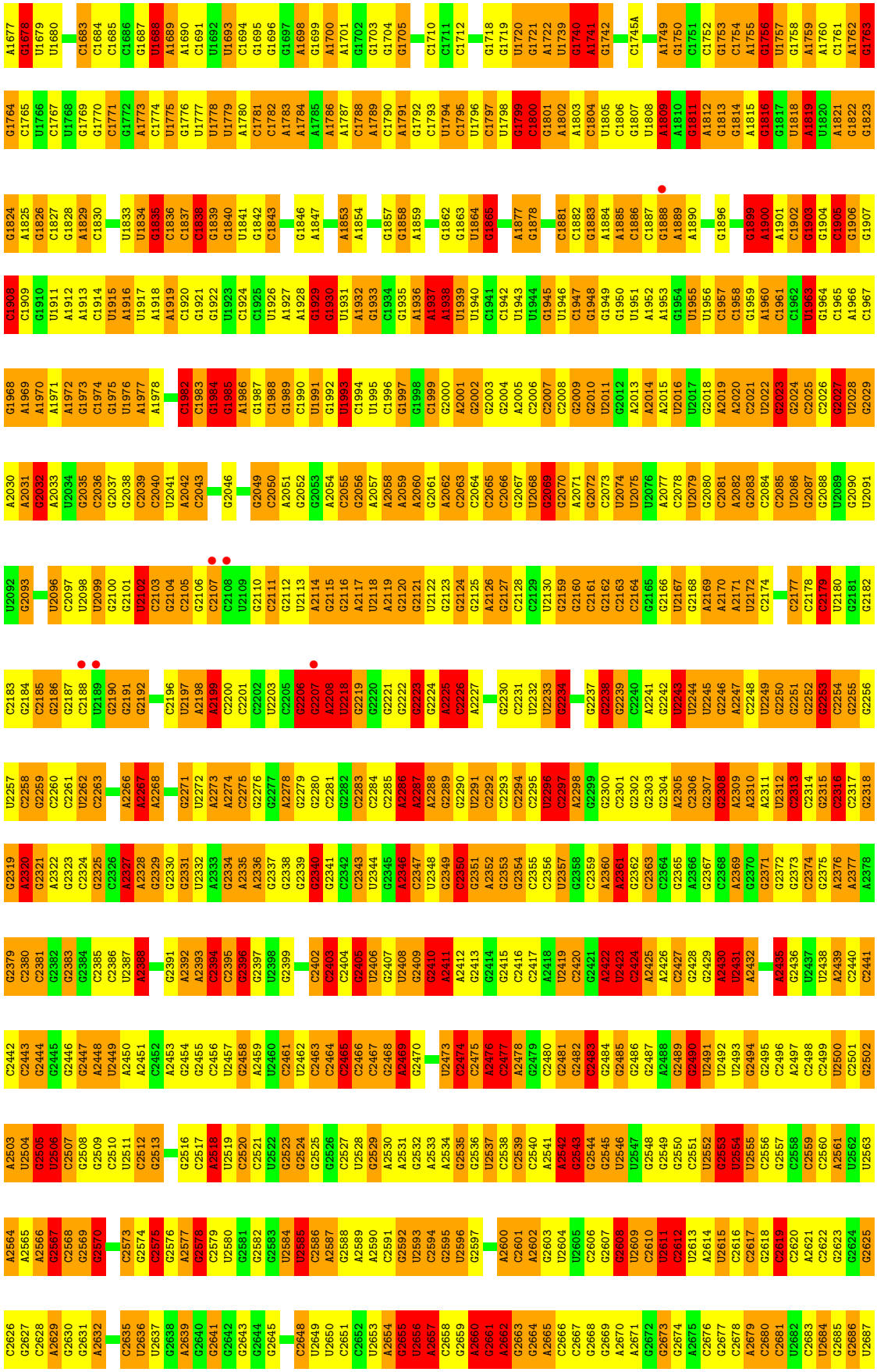


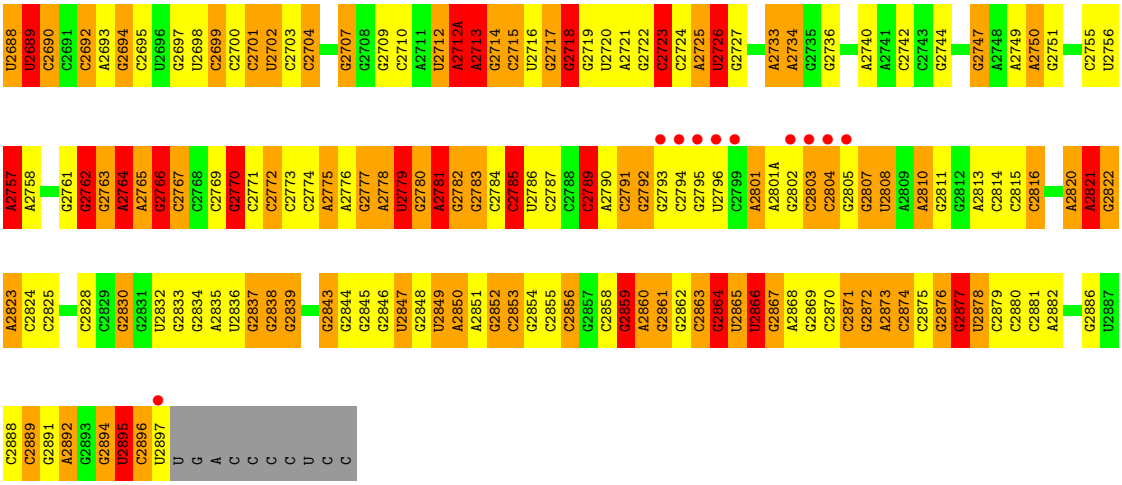
• Molecule 35: 23S ribosomal RNA

Chain DA:



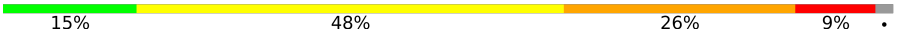


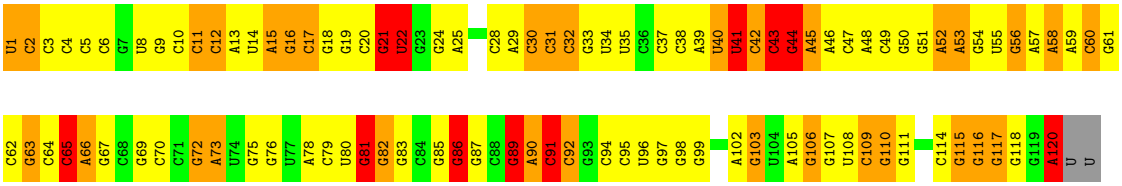




• Molecule 36: 5S ribosomal RNA

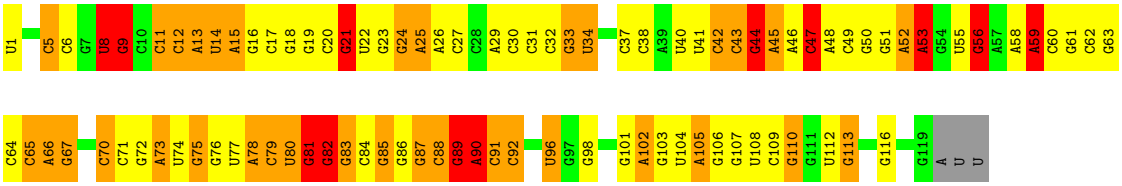
Chain BB:





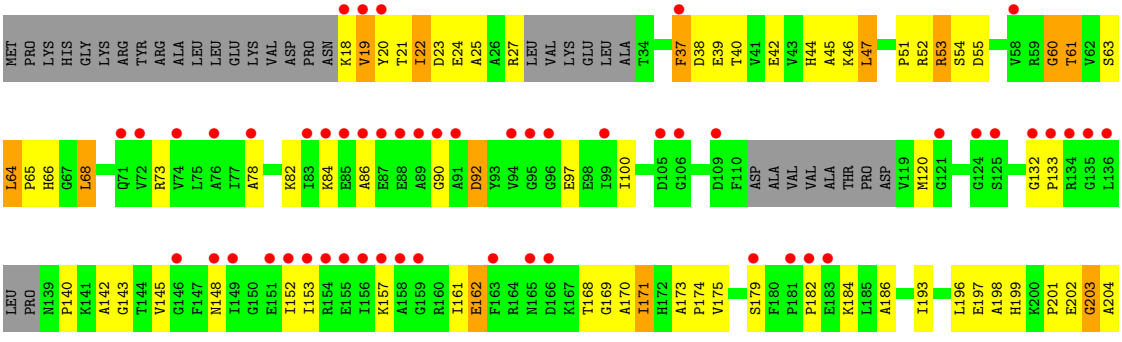
• Molecule 36: 5S ribosomal RNA

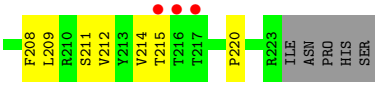
Chain DB:



• Molecule 37: 50S ribosomal protein L1

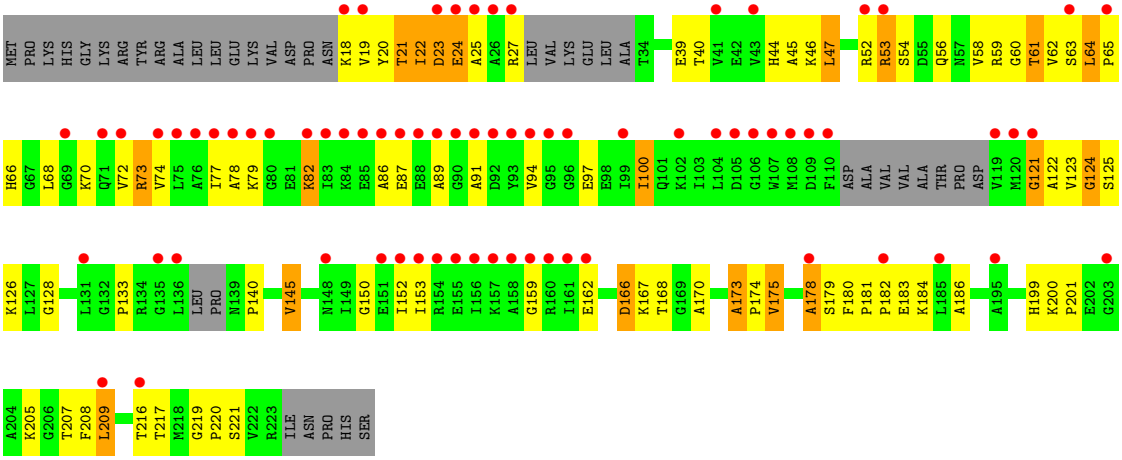
Chain BC:





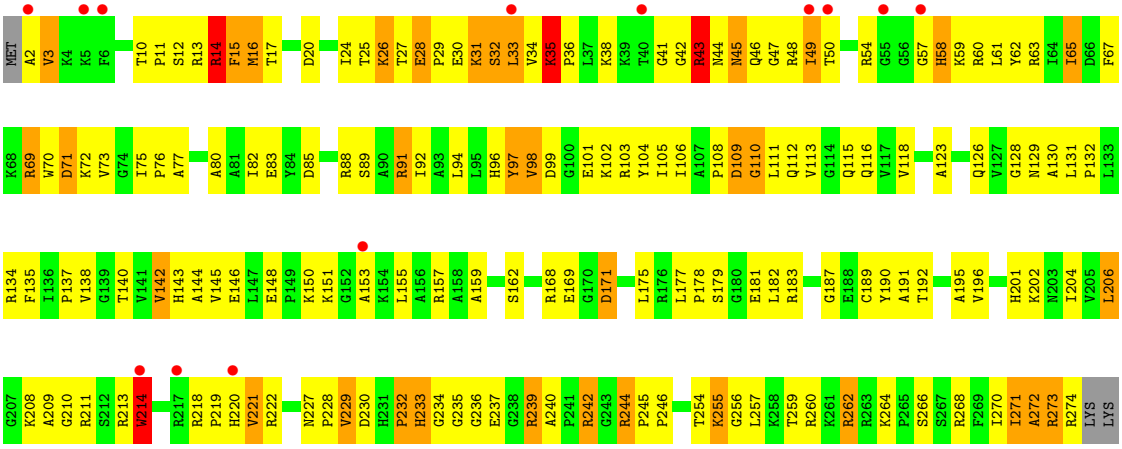
• Molecule 37: 50S ribosomal protein L1

Chain DC:



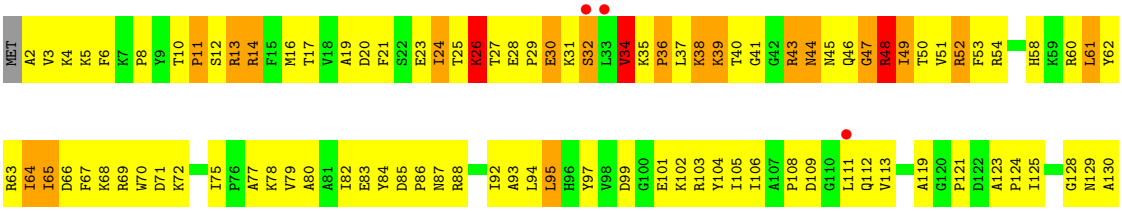
• Molecule 38: 50S ribosomal protein L2

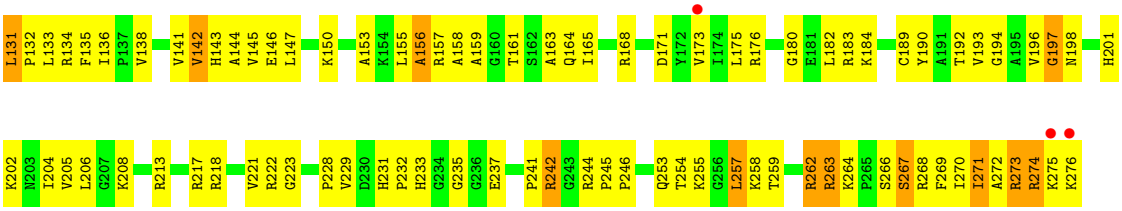
Chain BD:



• Molecule 38: 50S ribosomal protein L2

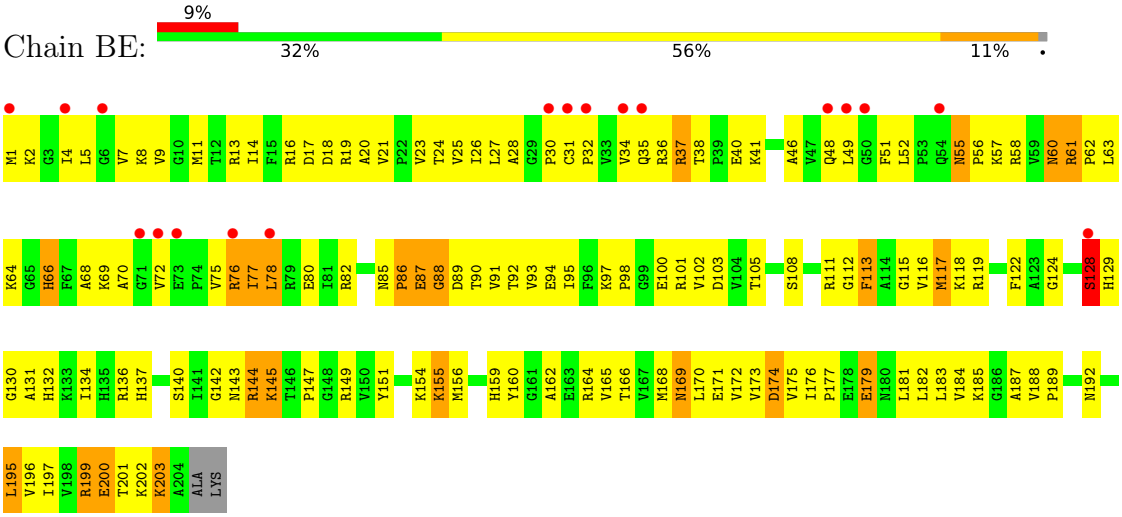
Chain DD:





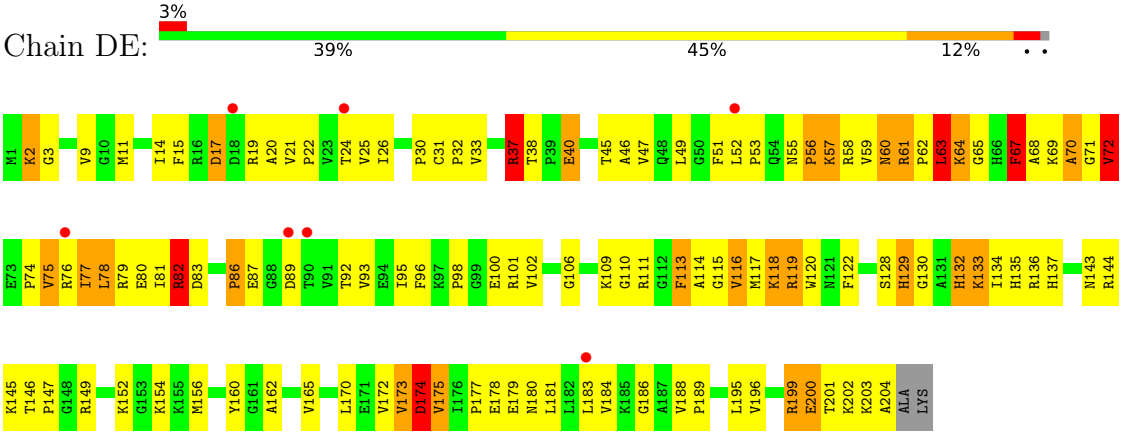
• Molecule 39: 50S ribosomal protein L3

Chain BE:



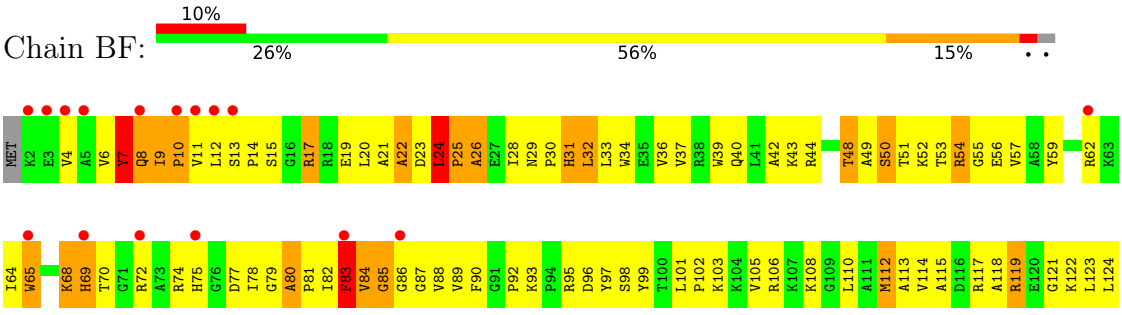
• Molecule 39: 50S ribosomal protein L3

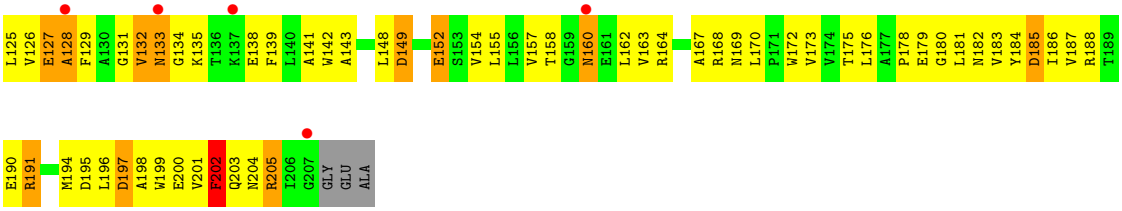
Chain DE:



• Molecule 40: 50S ribosomal protein L4

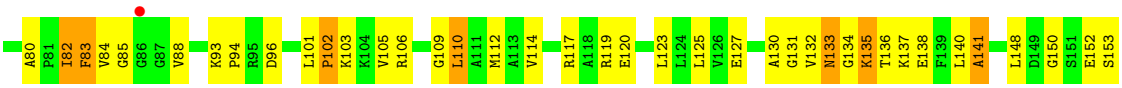
Chain BF:

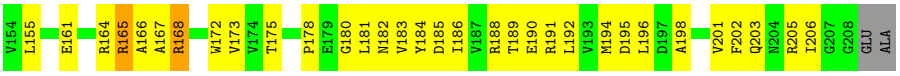




• Molecule 40: 50S ribosomal protein L4

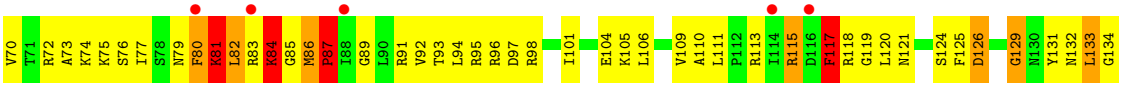
Chain DF:

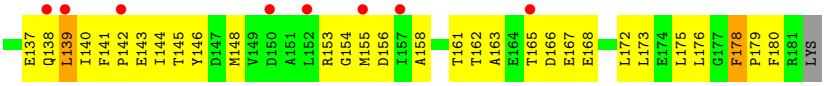




• Molecule 41: 50S ribosomal protein L5

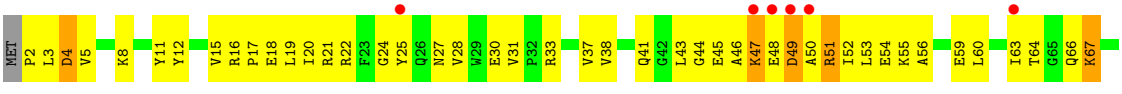
Chain BG:

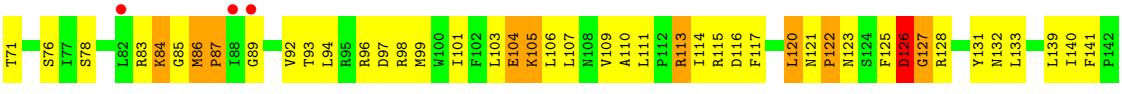


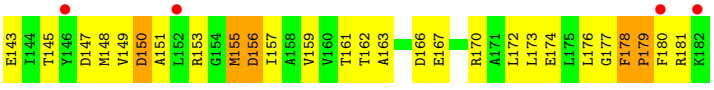


• Molecule 41: 50S ribosomal protein L5

Chain DG:

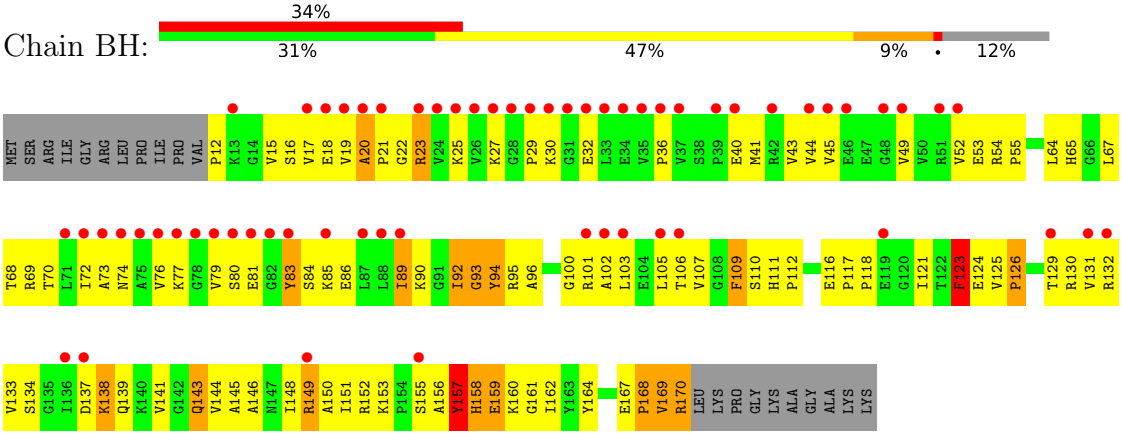






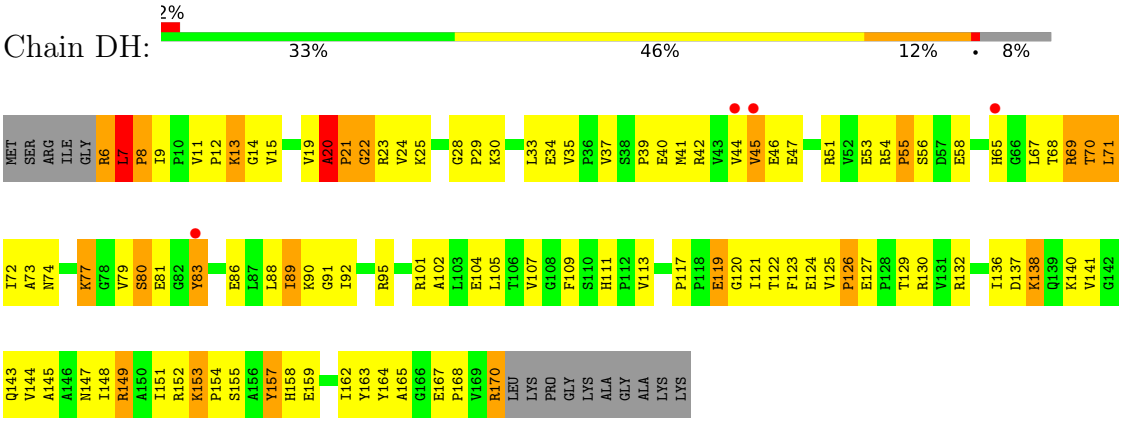
• Molecule 42: 50S ribosomal protein L6

Chain BH:



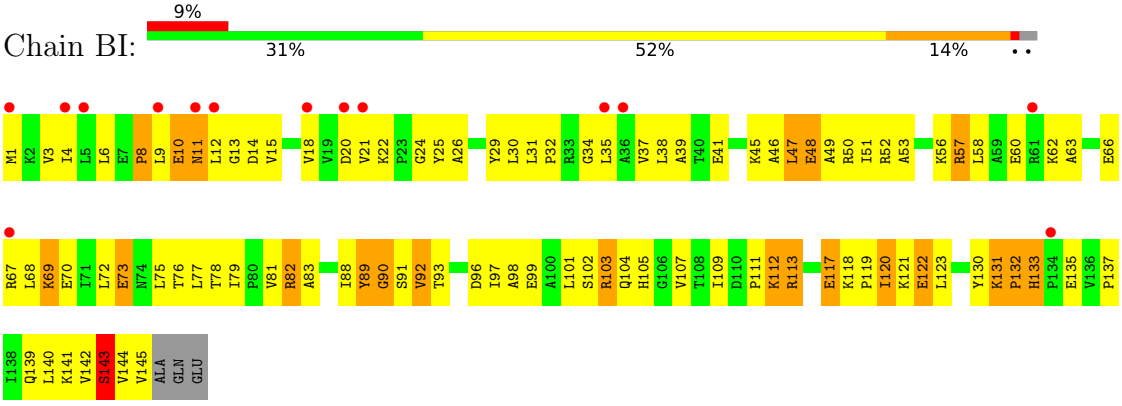
• Molecule 42: 50S ribosomal protein L6

Chain DH:



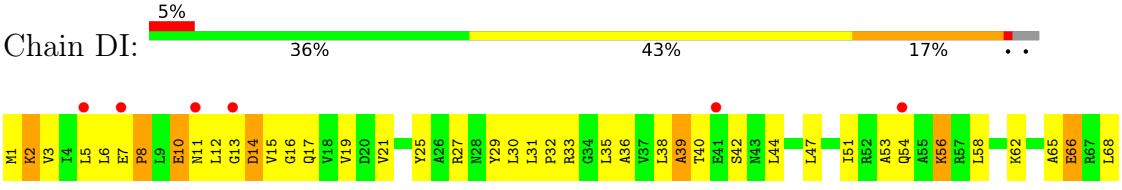
• Molecule 43: 50S ribosomal protein L9

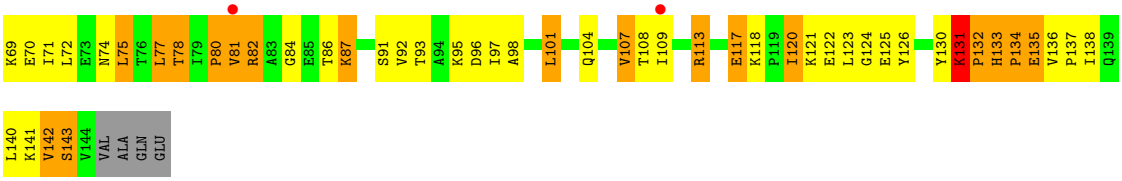
Chain BI:



• Molecule 43: 50S ribosomal protein L9

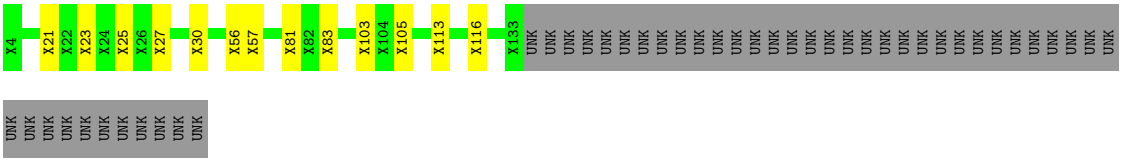
Chain DI:





• Molecule 44: 50S ribosomal protein L10

Chain BJ:

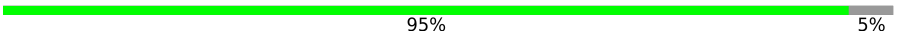


• Molecule 44: 50S ribosomal protein L10

Chain DJ:

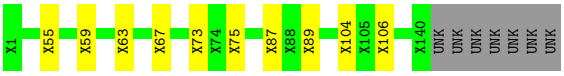
• Molecule 45: 50S ribosomal protein L11

Chain BK:



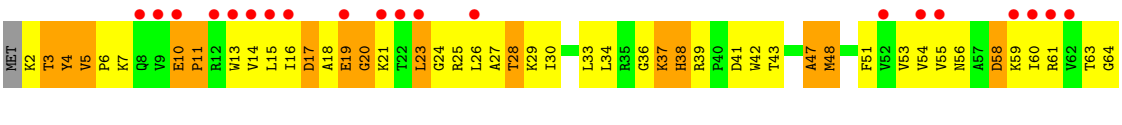
• Molecule 45: 50S ribosomal protein L11

Chain DK:



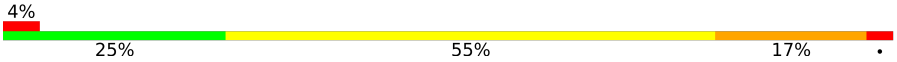
• Molecule 46: 50S ribosomal protein L13

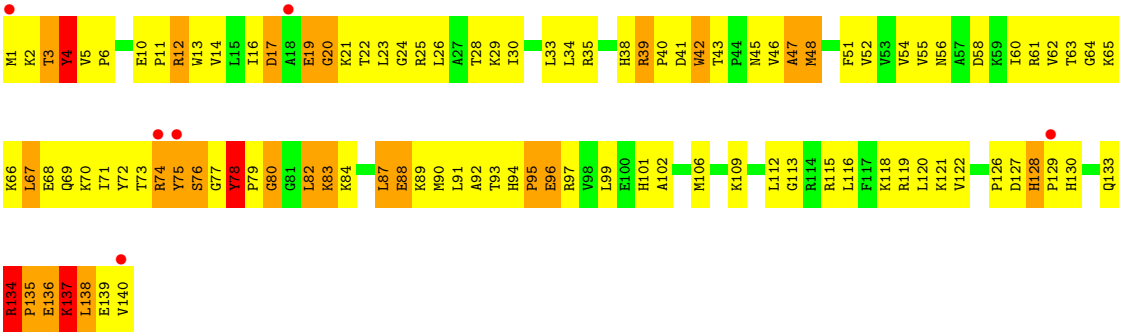
Chain BN:



• Molecule 46: 50S ribosomal protein L13

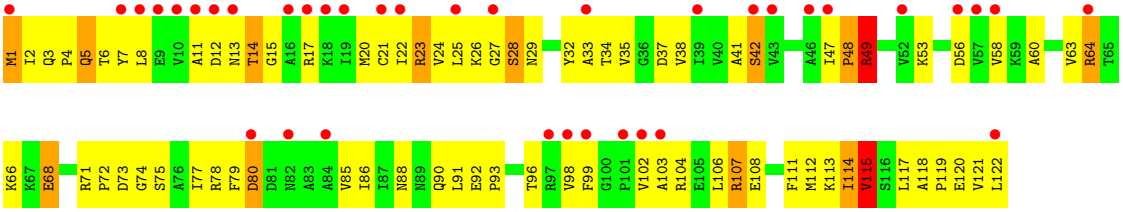
Chain DN:





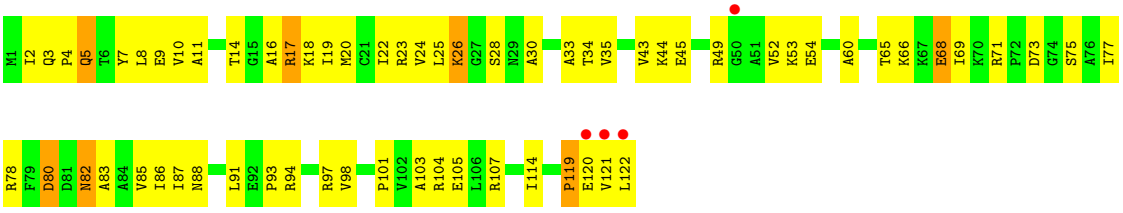
• Molecule 47: 50S ribosomal protein L14

Chain BO:



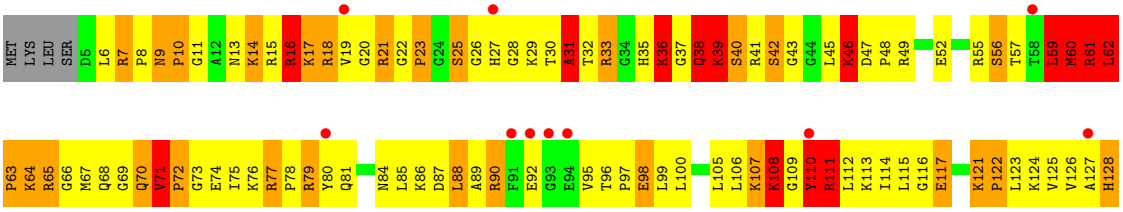
• Molecule 47: 50S ribosomal protein L14

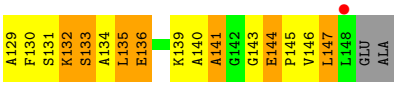
Chain DO:



• Molecule 48: 50S ribosomal protein L15

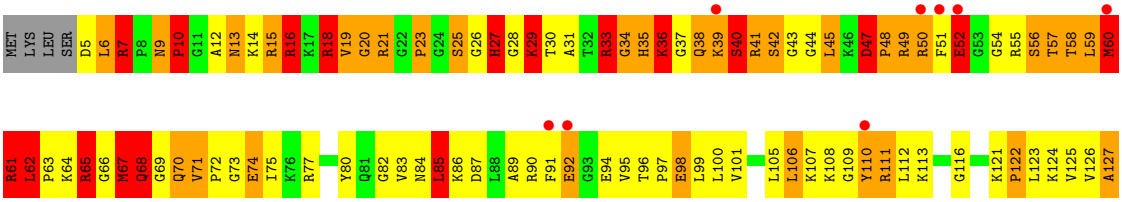
Chain BP:

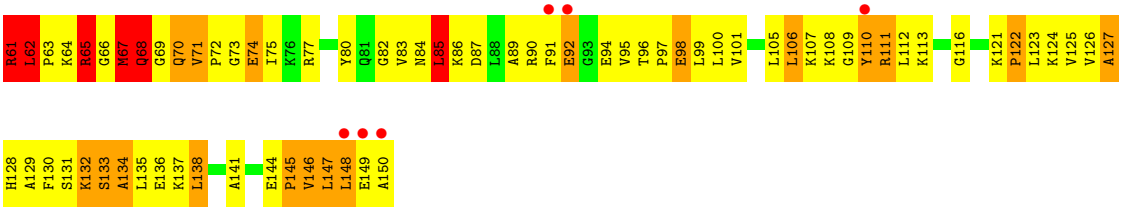




• Molecule 48: 50S ribosomal protein L15

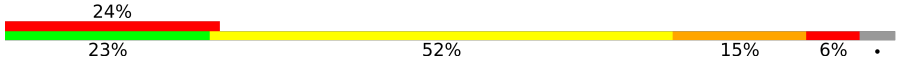
Chain DP:

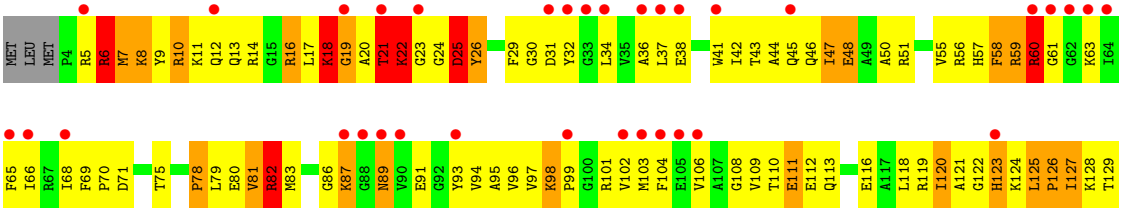




• Molecule 49: 50S ribosomal protein L16

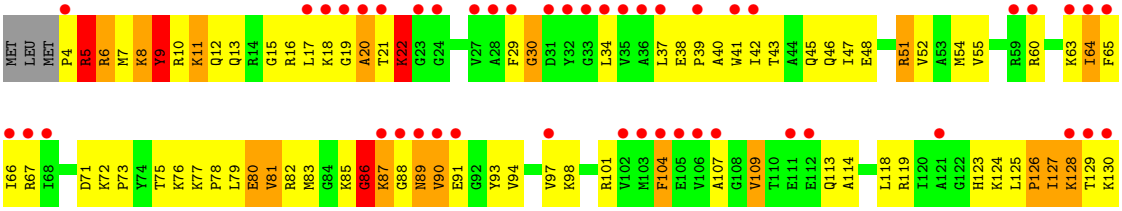
Chain BQ:

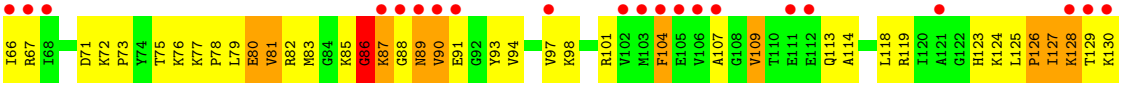


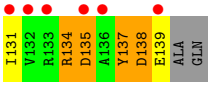


• Molecule 49: 50S ribosomal protein L16

Chain DQ:

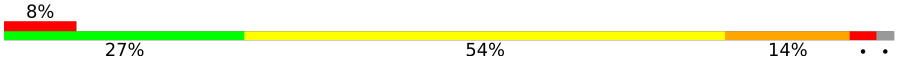


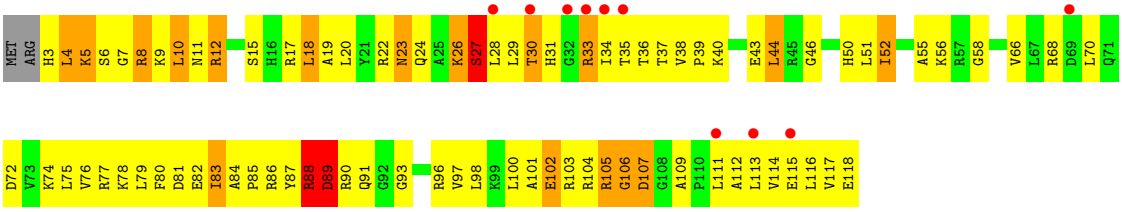


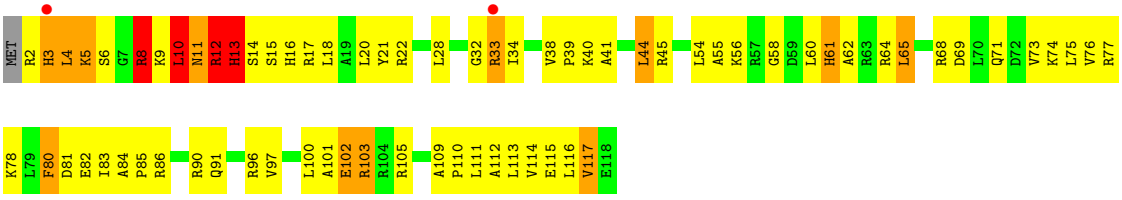


• Molecule 50: 50S ribosomal protein L17

Chain BR:





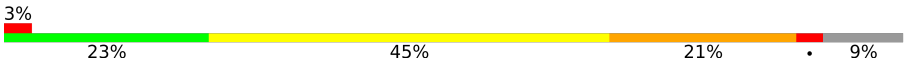


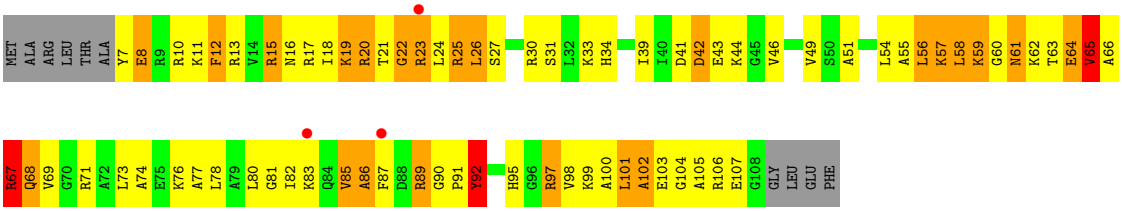
• Molecule 50: 50S ribosomal protein L17

Chain DR:

• Molecule 51: 50S ribosomal protein L18

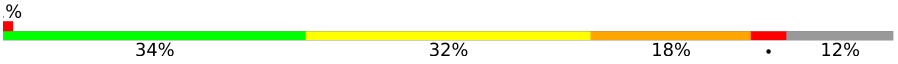
Chain BS:

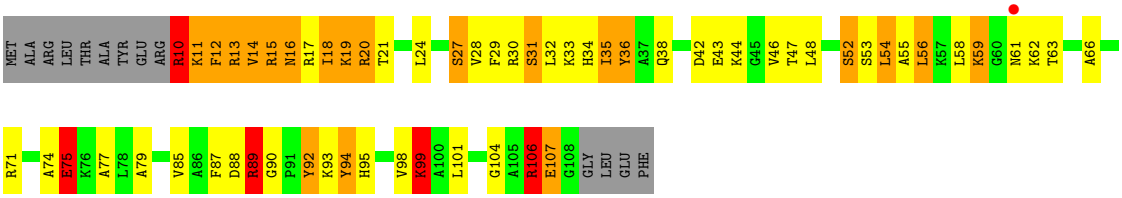




• Molecule 51: 50S ribosomal protein L18

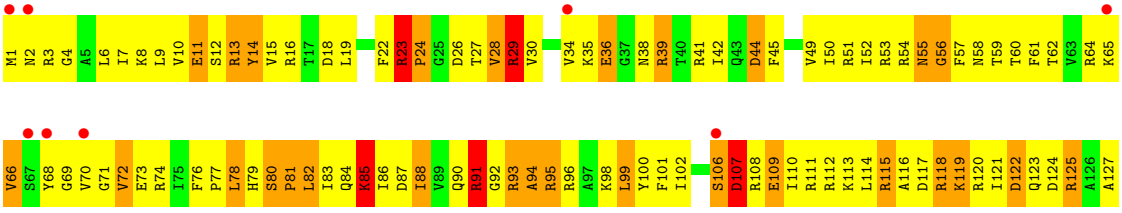
Chain DS:

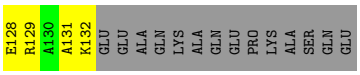




• Molecule 52: 50S ribosomal protein L19

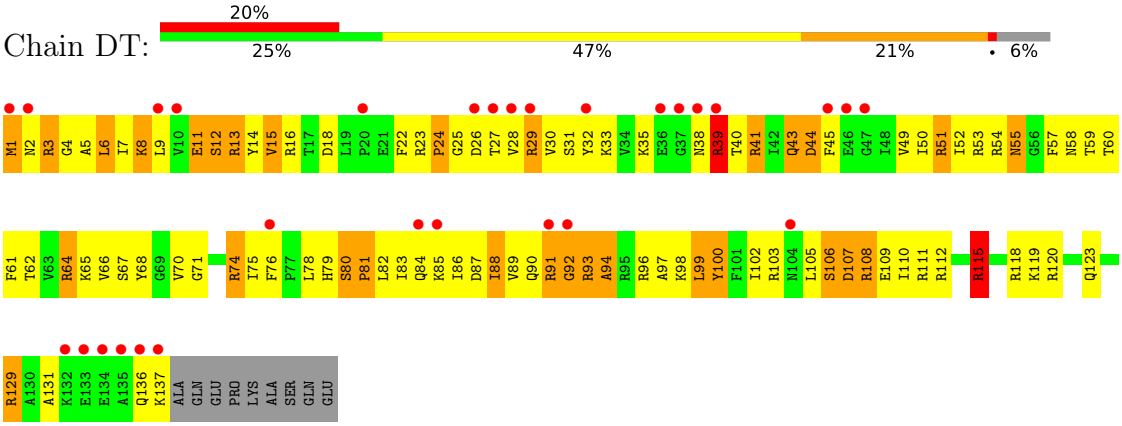
Chain BT:





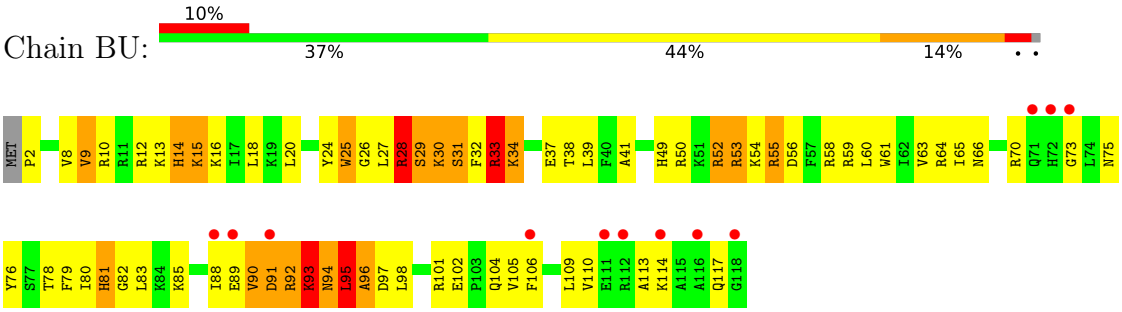
• Molecule 52: 50S ribosomal protein L19

Chain DT:



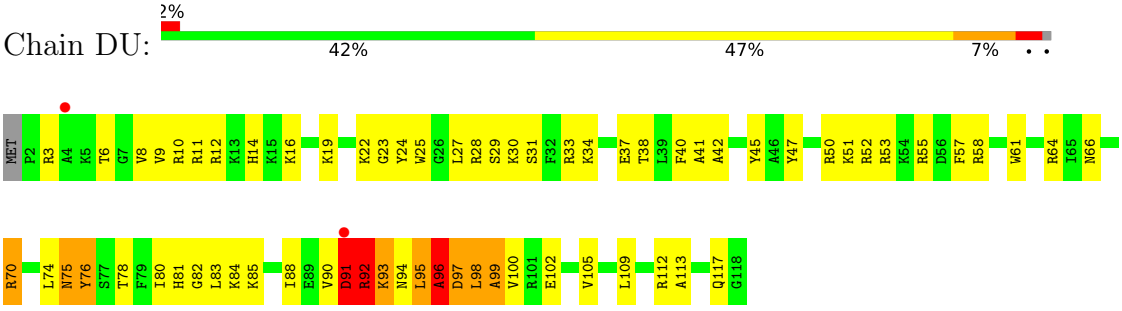
• Molecule 53: 50S ribosomal protein L20

Chain BU:



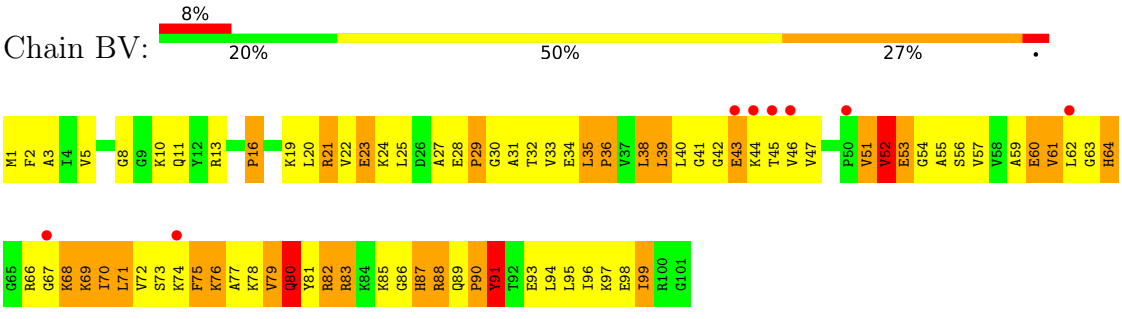
• Molecule 53: 50S ribosomal protein L20

Chain DU:



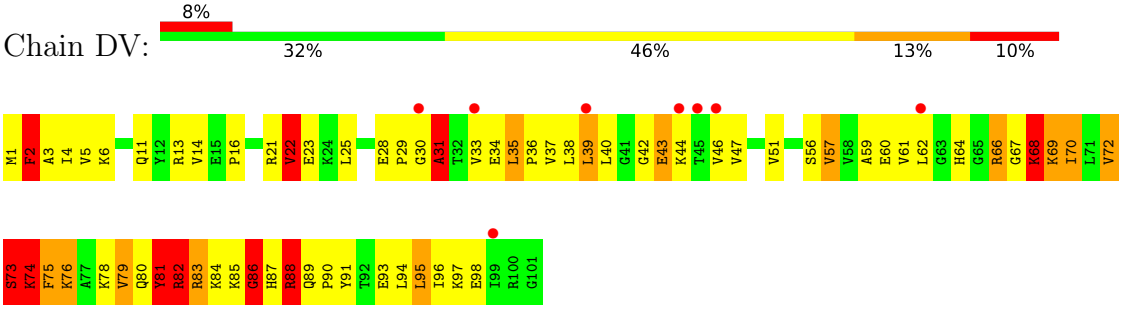
• Molecule 54: 50S ribosomal protein L21

Chain BV:



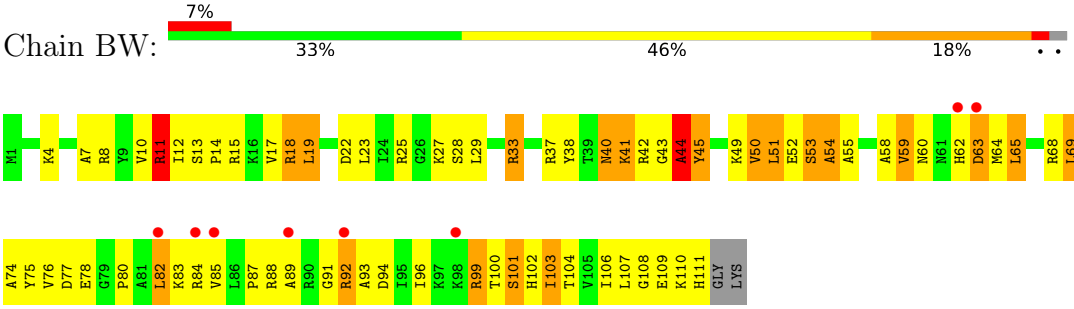
• Molecule 54: 50S ribosomal protein L21

Chain DV:



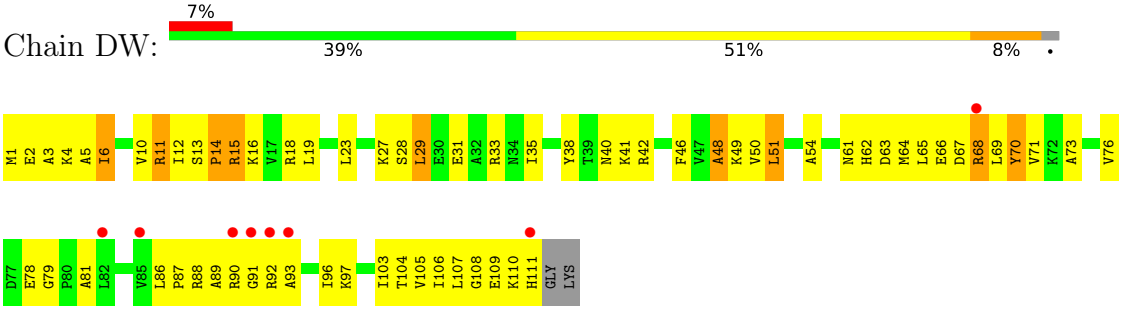
• Molecule 55: 50S ribosomal protein L22

Chain BW:



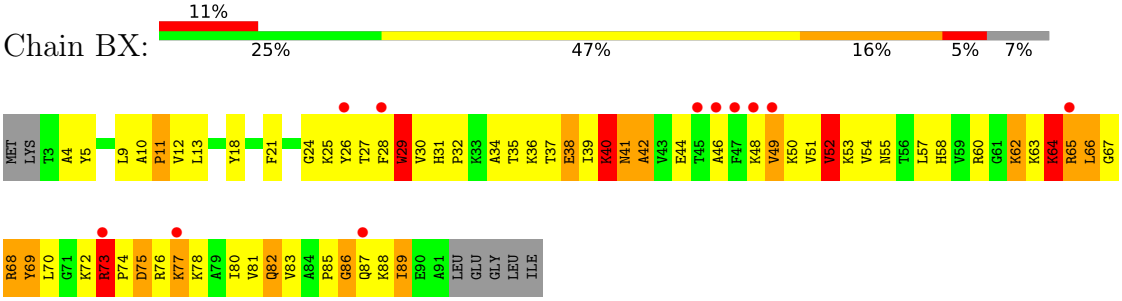
• Molecule 55: 50S ribosomal protein L22

Chain DW:



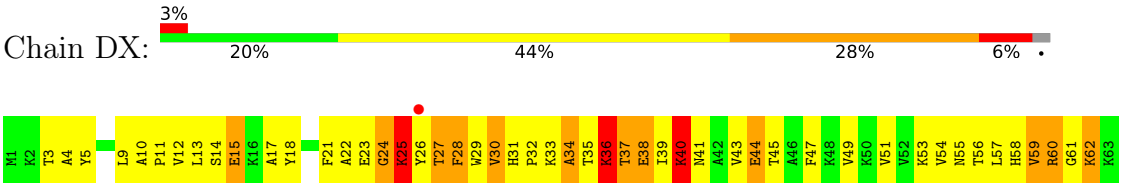
• Molecule 56: 50S ribosomal protein L23

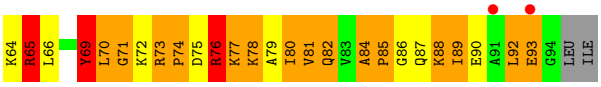
Chain BX:



• Molecule 56: 50S ribosomal protein L23

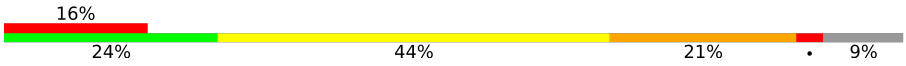
Chain DX:

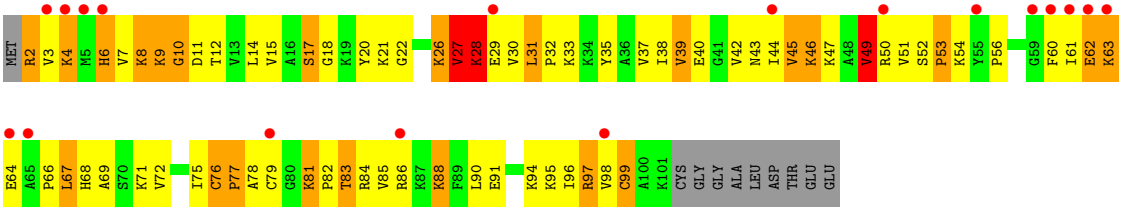




• Molecule 57: 50S ribosomal protein L24

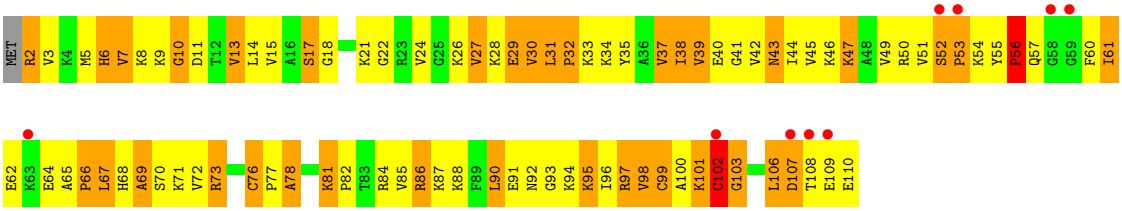
Chain BY:





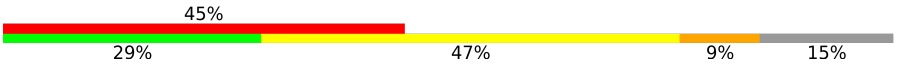
• Molecule 57: 50S ribosomal protein L24

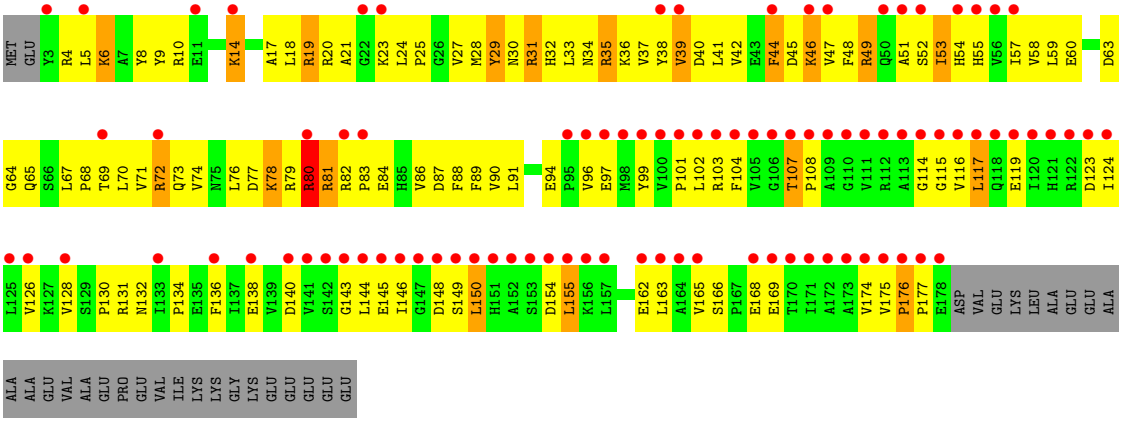
Chain DY:



• Molecule 58: 50S ribosomal protein L25

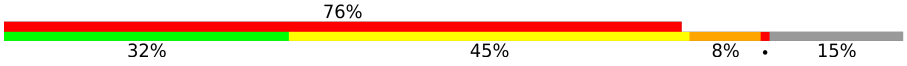
Chain BZ:

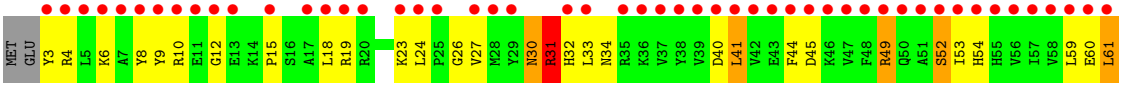


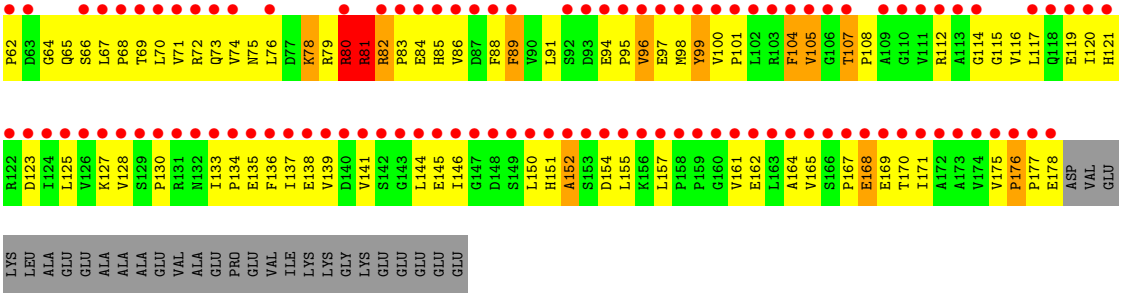


• Molecule 58: 50S ribosomal protein L25

Chain DZ:






P62 D63 G64 Q65 S66 L67 P68 T69 L70 V71 R72 Q73 V74 N75 L76 D77 K78 R79 R80 R81 R82 P83 E84 H85 V86 D87 F88 F89 V90 L91 S92 D93 E94 P95 V96 E97 M98 Y99 V100 P101 L102 R103 F104 V105 G106 T107 P108 A109 G110 V111 R112 A113 G114 G115 V116 L117 Q118 E119 I120 H121
R122 D123 I124 L125 V126 K127 V128 S129 P130 R131 N132 I133 P134 E135 F136 I137 E138 V139 D140 V141 S142 G143 L144 E145 I146 G147 D148 S149 L150 H151 A152 S153 D154 L155 K156 L157 P158 P159 G160 V161 E162 L163 A164 V165 S166 P167 E168 E169 T170 I171 A172 A173 V174 V175 P176 P177 E178 ASP VAL GLU
LYS LEU ALA GLU GLU ALA ALA ALA GLU VAL ALA GLU PRO GLU VAL ILE LYS LYS GLY LYS GLU GLU GLU GLU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.45Å 449.38Å 619.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.06 – 3.27 147.06 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.7 (147.06-3.27) 99.7 (147.06-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.214 , 0.277 0.214 , 0.277	Depositor DCC
R_{free} test set	44294 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	85.1	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 75.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	296449	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EDS, 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	AA	0.93	31/36190 (0.1%)	1.66	836/56486 (1.5%)
1	CA	0.90	14/36193 (0.0%)	1.53	592/56490 (1.0%)
2	AB	0.50	1/1816 (0.1%)	0.90	6/2445 (0.2%)
2	CB	0.45	0/1935	0.66	1/2609 (0.0%)
3	AC	0.43	0/1636	0.68	1/2205 (0.0%)
3	CC	0.50	0/1644	0.68	1/2215 (0.0%)
4	AD	0.61	0/1733	0.82	2/2318 (0.1%)
4	CD	0.53	0/1733	0.74	0/2318
5	AE	0.50	0/1162	0.94	4/1564 (0.3%)
5	CE	0.60	1/1171 (0.1%)	0.79	0/1576
6	AF	0.52	0/856	0.70	0/1154
6	CF	0.56	0/856	0.68	1/1154 (0.1%)
7	AG	0.48	0/1276	0.71	1/1709 (0.1%)
7	CG	0.53	0/1276	0.73	4/1709 (0.2%)
8	AH	1.00	6/1136 (0.5%)	1.06	6/1527 (0.4%)
8	CH	0.54	0/1136	0.73	1/1527 (0.1%)
9	AI	0.45	0/964	0.64	0/1294
9	CI	0.42	0/1029	0.71	2/1379 (0.1%)
10	AJ	0.44	0/807	0.71	0/1085
10	CJ	0.46	0/807	0.76	1/1085 (0.1%)
11	AK	0.54	0/900	0.75	0/1213
11	CK	0.54	0/900	0.72	0/1213
12	AL	0.67	0/972	0.91	1/1301 (0.1%)
12	CL	0.69	0/986	0.96	1/1320 (0.1%)
13	AM	0.44	0/932	0.71	1/1249 (0.1%)
13	CM	0.51	0/956	0.68	0/1281
14	AN	0.55	0/500	0.83	0/664
14	CN	0.58	0/501	0.84	0/664
15	AO	0.48	0/745	0.78	1/992 (0.1%)
15	CO	0.53	0/745	0.67	0/992
16	AP	0.63	0/716	0.88	2/963 (0.2%)
16	CP	0.54	0/716	0.85	2/963 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.57	0/836	0.77	1/1117 (0.1%)
17	CQ	0.56	0/836	0.83	0/1117
18	AR	0.51	0/579	0.78	1/768 (0.1%)
18	CR	0.54	0/579	0.82	0/768
19	AS	0.45	0/642	0.76	0/865
19	CS	0.55	0/642	0.76	0/865
20	AT	0.47	0/765	0.72	1/1007 (0.1%)
20	CT	0.47	0/765	0.77	0/1007
21	AU	0.47	0/212	0.74	0/277
21	CU	0.62	0/221	0.74	0/288
22	AV	0.84	1/1812 (0.1%)	1.59	39/2823 (1.4%)
22	CV	0.96	1/1835 (0.1%)	1.70	38/2857 (1.3%)
23	AW	0.71	1/1813 (0.1%)	1.52	37/2823 (1.3%)
23	AY	1.24	3/459 (0.7%)	1.96	18/714 (2.5%)
23	CW	0.73	1/1813 (0.1%)	1.45	25/2823 (0.9%)
23	CY	0.93	3/507 (0.6%)	1.56	7/789 (0.9%)
24	AX	0.90	0/285	1.66	6/441 (1.4%)
24	CX	1.11	0/285	1.87	13/441 (2.9%)
25	B0	0.64	0/615	0.92	1/819 (0.1%)
25	D0	0.80	1/653 (0.2%)	1.04	1/869 (0.1%)
26	B1	1.05	1/699 (0.1%)	1.30	8/929 (0.9%)
26	D1	1.07	2/699 (0.3%)	1.39	6/929 (0.6%)
27	B2	0.70	0/422	1.04	1/558 (0.2%)
27	D2	1.02	0/448	1.59	7/593 (1.2%)
28	B3	0.59	0/464	0.74	0/623
28	D3	0.65	0/481	0.90	1/646 (0.2%)
29	B4	0.46	0/221	0.72	0/306
29	D4	0.36	0/240	0.76	0/332
30	B5	0.79	0/432	1.00	2/585 (0.3%)
30	D5	0.82	1/481 (0.2%)	1.02	1/649 (0.2%)
31	B6	1.00	1/405 (0.2%)	1.18	3/540 (0.6%)
31	D6	1.10	5/415 (1.2%)	1.24	2/554 (0.4%)
32	B7	0.89	1/426 (0.2%)	1.11	5/561 (0.9%)
32	D7	0.79	1/426 (0.2%)	0.97	2/561 (0.4%)
33	B8	1.06	3/515 (0.6%)	1.47	6/679 (0.9%)
33	D8	0.98	0/502	1.37	6/661 (0.9%)
34	B9	0.56	0/310	0.89	1/407 (0.2%)
34	D9	0.62	0/310	0.95	1/407 (0.2%)
35	BA	1.16	199/68122 (0.3%)	1.89	2611/106350 (2.5%)
35	DA	1.31	367/68122 (0.5%)	2.03	3452/106350 (3.2%)
36	BB	0.81	0/2881	1.58	52/4494 (1.2%)
36	DB	1.00	4/2853 (0.1%)	1.80	95/4451 (2.1%)
37	BC	0.32	0/1144	0.62	0/1554

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	DC	0.31	0/1144	0.57	0/1554
38	BD	0.79	0/2176	1.01	9/2933 (0.3%)
38	DD	0.82	1/2194 (0.0%)	1.05	10/2955 (0.3%)
39	BE	0.70	0/1596	0.98	4/2153 (0.2%)
39	DE	0.80	1/1596 (0.1%)	1.01	3/2153 (0.1%)
40	BF	0.72	2/1650 (0.1%)	0.87	1/2234 (0.0%)
40	DF	0.78	1/1662 (0.1%)	0.98	5/2249 (0.2%)
41	BG	0.47	0/1473	0.78	2/1983 (0.1%)
41	DG	0.52	0/1499	0.81	3/2016 (0.1%)
42	BH	0.45	0/1245	0.69	0/1682
42	DH	0.69	1/1295 (0.1%)	0.89	4/1753 (0.2%)
43	BI	0.52	0/1146	0.76	0/1551
43	DI	0.55	0/1139	0.87	3/1541 (0.2%)
46	BN	0.68	0/1123	0.90	1/1515 (0.1%)
46	DN	0.87	3/1147 (0.3%)	0.96	2/1547 (0.1%)
47	BO	0.71	0/943	0.93	3/1269 (0.2%)
47	DO	0.78	0/943	0.88	0/1269
48	BP	0.90	3/1116 (0.3%)	1.35	14/1485 (0.9%)
48	DP	1.12	7/1131 (0.6%)	1.56	22/1504 (1.5%)
49	BQ	0.70	0/1095	1.00	7/1464 (0.5%)
49	DQ	0.90	0/1104	1.21	5/1476 (0.3%)
50	BR	0.74	0/963	1.09	5/1288 (0.4%)
50	DR	0.74	0/974	1.08	6/1302 (0.5%)
51	BS	0.75	3/822 (0.4%)	1.05	4/1094 (0.4%)
51	DS	0.71	0/789	1.10	2/1050 (0.2%)
52	BT	0.72	0/1114	0.98	4/1488 (0.3%)
52	DT	0.84	2/1155 (0.2%)	1.12	5/1542 (0.3%)
53	BU	0.77	0/982	0.87	4/1306 (0.3%)
53	DU	0.83	1/982 (0.1%)	0.99	2/1306 (0.2%)
54	BV	0.70	0/790	1.48	4/1057 (0.4%)
54	DV	0.92	1/790 (0.1%)	1.32	11/1057 (1.0%)
55	BW	0.82	0/897	1.16	8/1204 (0.7%)
55	DW	0.70	0/897	0.97	5/1204 (0.4%)
56	BX	0.83	2/718 (0.3%)	1.08	2/965 (0.2%)
56	DX	1.06	2/756 (0.3%)	1.39	10/1014 (1.0%)
57	BY	0.66	1/788 (0.1%)	0.86	0/1051
57	DY	0.82	1/848 (0.1%)	1.10	3/1132 (0.3%)
58	BZ	0.46	1/1435 (0.1%)	0.69	0/1949
58	DZ	0.53	0/1435	0.82	2/1949 (0.1%)
All	All	1.01	682/317649 (0.2%)	1.64	8092/475105 (1.7%)

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
2	AB	0	1
2	CB	0	1
3	AC	0	1
3	CC	0	1
4	AD	0	2
4	CD	0	2
7	CG	0	1
8	AH	0	2
9	CI	0	1
10	AJ	0	3
10	CJ	0	2
12	AL	0	3
12	CL	0	4
14	CN	0	2
16	AP	0	2
16	CP	0	1
17	AQ	0	1
17	CQ	0	2
18	AR	0	1
18	CR	0	1
19	CS	0	1
20	AT	0	1
20	CT	0	2
26	B1	0	5
26	D1	0	4
27	B2	0	3
27	D2	0	5
29	D4	0	2
30	B5	0	2
31	B6	0	4
31	D6	0	4
32	B7	0	4
32	D7	0	1
33	B8	0	2
33	D8	0	1
37	DC	0	1
38	BD	0	4
38	DD	0	6
39	BE	0	3
39	DE	0	4
40	BF	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
40	DF	0	1
41	BG	0	4
41	DG	0	1
42	BH	0	1
42	DH	0	2
43	BI	0	2
43	DI	0	3
46	BN	0	3
46	DN	0	5
47	BO	0	3
47	DO	0	1
48	BP	0	10
48	DP	0	12
49	BQ	0	6
49	DQ	0	5
50	BR	0	3
50	DR	0	1
51	BS	0	3
51	DS	0	5
52	BT	0	4
52	DT	0	6
53	BU	0	3
53	DU	0	3
54	BV	0	5
54	DV	0	5
55	BW	0	2
56	BX	0	4
56	DX	0	5
57	BY	0	2
57	DY	0	3
58	DZ	0	1
All	All	0	209

The worst 5 of 682 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	AH	104	ARG	CG-CD	17.27	1.95	1.51
35	BA	783	A	N9-C4	-13.33	1.29	1.37
8	AH	138	TRP	CE3-CZ3	-12.54	1.17	1.38
48	DP	16	ARG	CZ-NH1	-11.74	1.17	1.33
35	DA	528	A	N9-C4	-11.44	1.30	1.37

The worst 5 of 8092 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	BV	38	LEU	CB-CG-CD2	-27.88	63.60	111.00
35	BA	1899	G	N3-C4-N9	-23.15	112.11	126.00
35	BA	2818	G	N1-C6-O6	22.38	133.33	119.90
35	BA	2818	G	C5-C6-O6	-22.14	115.32	128.60
35	DA	1779	U	C5-C6-N1	-21.39	112.01	122.70

There are no chirality outliers.

5 of 209 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	109	SER	Peptide
3	AC	161	GLU	Peptide
4	AD	31	CYS	Peptide
4	AD	32	ALA	Peptide
8	AH	7	ALA	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1281	0
1	CA	32332	0	16317	1094	0
2	AB	1784	0	1833	164	0
2	CB	1900	0	1951	148	0
3	AC	1612	0	1677	106	0
3	CC	1620	0	1689	122	0
4	AD	1703	0	1763	150	0
4	CD	1703	0	1763	120	0
5	AE	1146	0	1207	77	0
5	CE	1155	0	1213	84	0
6	AF	843	0	857	45	0
6	CF	843	0	857	43	0
7	AG	1257	0	1296	98	0
7	CG	1257	0	1296	76	0
8	AH	1116	0	1177	114	0
8	CH	1116	0	1177	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AI	947	0	979	93	0
9	CI	1010	0	1037	86	0
10	AJ	794	0	840	88	0
10	CJ	794	0	840	73	0
11	AK	885	0	904	46	0
11	CK	885	0	904	50	0
12	AL	956	0	1046	89	0
12	CL	970	0	1057	59	0
13	AM	922	0	979	95	0
13	CM	946	0	1008	81	0
14	AN	491	0	529	71	0
14	CN	492	0	530	57	0
15	AO	734	0	771	59	0
15	CO	734	0	771	42	0
16	AP	700	0	720	40	0
16	CP	700	0	720	53	0
17	AQ	823	0	891	53	0
17	CQ	823	0	889	66	0
18	AR	574	0	642	37	0
18	CR	574	0	644	56	0
19	AS	629	0	652	79	0
19	CS	629	0	652	62	0
20	AT	763	0	861	52	0
20	CT	763	0	861	63	0
21	AU	208	0	221	14	0
21	CU	217	0	234	19	0
22	AV	1622	0	825	36	0
22	CV	1643	0	836	49	0
23	AW	1623	0	820	46	0
23	AY	410	0	207	18	0
23	CW	1623	0	821	65	0
23	CY	453	0	229	10	0
24	AX	255	0	129	6	0
24	CX	255	0	129	10	0
25	B0	607	0	628	51	0
25	D0	645	0	673	44	0
26	B1	692	0	764	108	0
26	D1	692	0	764	100	0
27	B2	420	0	461	70	0
27	D2	446	0	486	88	0
28	B3	459	0	512	25	0
28	D3	476	0	529	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	B4	222	0	91	4	0
29	D4	241	0	103	7	0
30	B5	418	0	432	43	0
30	D5	467	0	492	48	0
31	B6	398	0	417	60	0
31	D6	408	0	426	53	0
32	B7	418	0	467	38	0
32	D7	418	0	467	30	0
33	B8	507	0	576	93	0
33	D8	495	0	567	93	0
34	B9	307	0	336	31	0
34	D9	307	0	335	17	0
35	BA	60821	0	30654	2020	0
35	DA	60821	0	30655	1774	0
36	BB	2576	0	1305	111	0
36	DB	2551	0	1295	90	0
37	BC	1141	0	865	41	0
37	DC	1141	0	865	57	0
38	BD	2126	0	2208	194	0
38	DD	2144	0	2234	185	0
39	BE	1563	0	1629	144	0
39	DE	1563	0	1629	133	0
40	BF	1615	0	1665	165	0
40	DF	1627	0	1679	125	0
41	BG	1449	0	1503	110	0
41	DG	1474	0	1535	115	0
42	BH	1222	0	1282	88	0
42	DH	1270	0	1339	95	0
43	BI	1131	0	1218	97	0
43	DI	1124	0	1209	72	0
44	BJ	651	0	171	9	0
44	DJ	651	0	163	4	0
45	BK	700	0	166	0	0
45	DK	700	0	179	5	0
46	BN	1096	0	1168	101	0
46	DN	1120	0	1195	111	0
47	BO	933	0	996	72	0
47	DO	933	0	996	57	0
48	BP	1099	0	1176	221	0
48	DP	1114	0	1187	201	0
49	BQ	1074	0	1129	114	0
49	DQ	1083	0	1135	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	BR	949	0	1008	113	0
50	DR	960	0	1021	90	0
51	BS	813	0	873	115	0
51	DS	781	0	845	87	0
52	BT	1100	0	1164	127	0
52	DT	1141	0	1202	125	0
53	BU	964	0	1022	113	0
53	DU	964	0	1022	108	0
54	BV	779	0	852	122	0
54	DV	779	0	852	108	0
55	BW	886	0	948	89	0
55	DW	886	0	948	53	0
56	BX	704	0	758	103	0
56	DX	742	0	801	126	0
57	BY	775	0	870	91	0
57	DY	835	0	920	127	0
58	BZ	1403	0	1432	118	0
58	DZ	1403	0	1432	91	0
59	AA	209	0	0	0	0
59	AC	1	0	0	0	0
59	AD	1	0	0	0	0
59	AE	1	0	0	0	0
59	AL	1	0	0	0	0
59	AT	1	0	0	0	0
59	AV	7	0	0	0	0
59	AW	20	0	0	0	0
59	AX	3	0	0	0	0
59	B0	1	0	0	0	0
59	B1	2	0	0	0	0
59	B2	1	0	0	0	0
59	B5	1	0	0	0	0
59	B7	1	0	0	0	0
59	B8	2	0	0	0	0
59	BA	457	0	0	0	0
59	BB	17	0	0	0	0
59	BC	2	0	0	0	0
59	BE	2	0	0	0	0
59	BF	3	0	0	0	0
59	BQ	1	0	0	0	0
59	BS	1	0	0	0	0
59	BU	5	0	0	0	0
59	BV	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	BX	2	0	0	0	0
59	CA	195	0	0	0	0
59	CE	1	0	0	0	0
59	CF	1	0	0	0	0
59	CG	1	0	0	0	0
59	CI	1	0	0	0	0
59	CU	1	0	0	0	0
59	CV	4	0	0	0	0
59	CW	13	0	0	0	0
59	CX	2	0	0	0	0
59	D2	2	0	0	0	0
59	D5	1	0	0	0	0
59	DA	392	0	0	0	0
59	DB	12	0	0	0	0
59	DE	1	0	0	0	0
59	DF	2	0	0	0	0
59	DN	1	0	0	0	0
59	DO	2	0	0	0	0
59	DV	1	0	0	0	0
60	AA	41	0	0	2	0
60	CA	41	0	0	1	0
61	AD	1	0	0	0	0
61	AN	1	0	0	0	0
61	B9	1	0	0	0	0
61	CD	1	0	0	0	0
61	CN	1	0	0	0	0
61	D9	1	0	0	0	0
62	AA	2	0	0	1	0
All	All	296449	0	198495	13485	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

The worst 5 of 13485 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:142:LEU:CD2	2:AB:142:LEU:CG	1.77	1.58
4:AD:122:ARG:HH12	4:AD:136:PRO:CD	1.22	1.50
4:AD:122:ARG:NH1	4:AD:136:PRO:HD3	1.27	1.48
8:AH:104:ARG:CD	8:AH:104:ARG:CG	1.95	1.43
58:DZ:61:LEU:HD12	58:DZ:62:PRO:CD	1.52	1.35

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	216/256 (84%)	148 (68%)	42 (19%)	26 (12%)	0 2
2	CB	232/256 (91%)	148 (64%)	59 (25%)	25 (11%)	0 3
3	AC	204/239 (85%)	145 (71%)	41 (20%)	18 (9%)	1 5
3	CC	205/239 (86%)	153 (75%)	37 (18%)	15 (7%)	1 7
4	AD	206/209 (99%)	148 (72%)	35 (17%)	23 (11%)	0 2
4	CD	206/209 (99%)	150 (73%)	41 (20%)	15 (7%)	1 7
5	AE	148/162 (91%)	113 (76%)	24 (16%)	11 (7%)	1 7
5	CE	149/162 (92%)	114 (76%)	27 (18%)	8 (5%)	2 12
6	AF	99/101 (98%)	80 (81%)	12 (12%)	7 (7%)	1 8
6	CF	99/101 (98%)	84 (85%)	12 (12%)	3 (3%)	4 25
7	AG	153/156 (98%)	103 (67%)	33 (22%)	17 (11%)	0 2
7	CG	153/156 (98%)	112 (73%)	30 (20%)	11 (7%)	1 8
8	AH	136/138 (99%)	98 (72%)	25 (18%)	13 (10%)	0 4
8	CH	136/138 (99%)	100 (74%)	26 (19%)	10 (7%)	1 7
9	AI	119/128 (93%)	80 (67%)	20 (17%)	19 (16%)	0 1
9	CI	125/128 (98%)	87 (70%)	23 (18%)	15 (12%)	0 2
10	AJ	96/105 (91%)	61 (64%)	23 (24%)	12 (12%)	0 2
10	CJ	96/105 (91%)	66 (69%)	20 (21%)	10 (10%)	0 3
11	AK	117/129 (91%)	89 (76%)	19 (16%)	9 (8%)	1 6
11	CK	117/129 (91%)	86 (74%)	23 (20%)	8 (7%)	1 8
12	AL	120/132 (91%)	81 (68%)	23 (19%)	16 (13%)	0 1
12	CL	122/132 (92%)	86 (70%)	21 (17%)	15 (12%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	AM	114/126 (90%)	78 (68%)	22 (19%)	14 (12%)	0 2
13	CM	117/126 (93%)	88 (75%)	16 (14%)	13 (11%)	0 2
14	AN	58/61 (95%)	35 (60%)	16 (28%)	7 (12%)	0 2
14	CN	58/61 (95%)	36 (62%)	13 (22%)	9 (16%)	0 1
15	AO	86/89 (97%)	67 (78%)	14 (16%)	5 (6%)	1 11
15	CO	86/89 (97%)	61 (71%)	19 (22%)	6 (7%)	1 8
16	AP	81/88 (92%)	58 (72%)	17 (21%)	6 (7%)	1 7
16	CP	81/88 (92%)	53 (65%)	22 (27%)	6 (7%)	1 7
17	AQ	97/105 (92%)	81 (84%)	13 (13%)	3 (3%)	4 24
17	CQ	97/105 (92%)	74 (76%)	13 (13%)	10 (10%)	0 3
18	AR	68/88 (77%)	55 (81%)	8 (12%)	5 (7%)	1 7
18	CR	68/88 (77%)	48 (71%)	12 (18%)	8 (12%)	0 2
19	AS	76/93 (82%)	33 (43%)	30 (40%)	13 (17%)	0 1
19	CS	76/93 (82%)	46 (60%)	15 (20%)	15 (20%)	0 0
20	AT	97/106 (92%)	64 (66%)	23 (24%)	10 (10%)	0 3
20	CT	97/106 (92%)	67 (69%)	18 (19%)	12 (12%)	0 2
21	AU	22/27 (82%)	15 (68%)	3 (14%)	4 (18%)	0 1
21	CU	23/27 (85%)	19 (83%)	1 (4%)	3 (13%)	0 1
25	B0	74/85 (87%)	56 (76%)	13 (18%)	5 (7%)	1 8
25	D0	80/85 (94%)	59 (74%)	13 (16%)	8 (10%)	0 3
26	B1	86/98 (88%)	45 (52%)	21 (24%)	20 (23%)	0 0
26	D1	86/98 (88%)	60 (70%)	12 (14%)	14 (16%)	0 1
27	B2	48/72 (67%)	14 (29%)	20 (42%)	14 (29%)	0 0
27	D2	51/72 (71%)	22 (43%)	16 (31%)	13 (26%)	0 0
28	B3	56/60 (93%)	47 (84%)	7 (12%)	2 (4%)	3 21
28	D3	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	1 5
29	B4	43/71 (61%)	10 (23%)	13 (30%)	20 (46%)	0 0
29	D4	47/71 (66%)	11 (23%)	17 (36%)	19 (40%)	0 0
30	B5	52/60 (87%)	34 (65%)	9 (17%)	9 (17%)	0 1
30	D5	58/60 (97%)	40 (69%)	14 (24%)	4 (7%)	1 8
31	B6	44/54 (82%)	19 (43%)	8 (18%)	17 (39%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
31	D6	45/54 (83%)	19 (42%)	14 (31%)	12 (27%)	0 0
32	B7	46/49 (94%)	36 (78%)	6 (13%)	4 (9%)	1 5
32	D7	46/49 (94%)	42 (91%)	4 (9%)	0	100 100
33	B8	61/65 (94%)	37 (61%)	15 (25%)	9 (15%)	0 1
33	D8	60/65 (92%)	35 (58%)	13 (22%)	12 (20%)	0 0
34	B9	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1 11
34	D9	35/37 (95%)	25 (71%)	7 (20%)	3 (9%)	1 5
37	BC	182/229 (80%)	82 (45%)	54 (30%)	46 (25%)	0 0
37	DC	182/229 (80%)	78 (43%)	63 (35%)	41 (22%)	0 0
38	BD	271/276 (98%)	203 (75%)	45 (17%)	23 (8%)	1 5
38	DD	273/276 (99%)	212 (78%)	43 (16%)	18 (7%)	1 9
39	BE	202/206 (98%)	147 (73%)	35 (17%)	20 (10%)	0 3
39	DE	202/206 (98%)	137 (68%)	36 (18%)	29 (14%)	0 1
40	BF	204/210 (97%)	130 (64%)	39 (19%)	35 (17%)	0 1
40	DF	206/210 (98%)	152 (74%)	35 (17%)	19 (9%)	1 4
41	BG	176/182 (97%)	117 (66%)	42 (24%)	17 (10%)	0 4
41	DG	179/182 (98%)	132 (74%)	32 (18%)	15 (8%)	1 5
42	BH	157/180 (87%)	92 (59%)	43 (27%)	22 (14%)	0 1
42	DH	163/180 (91%)	104 (64%)	33 (20%)	26 (16%)	0 1
43	BI	143/148 (97%)	88 (62%)	35 (24%)	20 (14%)	0 1
43	DI	142/148 (96%)	91 (64%)	30 (21%)	21 (15%)	0 1
46	BN	135/140 (96%)	91 (67%)	20 (15%)	24 (18%)	0 1
46	DN	138/140 (99%)	90 (65%)	22 (16%)	26 (19%)	0 1
47	BO	120/122 (98%)	89 (74%)	21 (18%)	10 (8%)	1 6
47	DO	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	19 52
48	BP	142/150 (95%)	64 (45%)	38 (27%)	40 (28%)	0 0
48	DP	144/150 (96%)	63 (44%)	35 (24%)	46 (32%)	0 0
49	BQ	133/141 (94%)	76 (57%)	34 (26%)	23 (17%)	0 1
49	DQ	134/141 (95%)	91 (68%)	27 (20%)	16 (12%)	0 2
50	BR	114/118 (97%)	83 (73%)	19 (17%)	12 (10%)	0 3
50	DR	115/118 (98%)	92 (80%)	12 (10%)	11 (10%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	BS	100/112 (89%)	58 (58%)	21 (21%)	21 (21%)	0	0
51	DS	97/112 (87%)	59 (61%)	22 (23%)	16 (16%)	0	1
52	BT	130/146 (89%)	70 (54%)	34 (26%)	26 (20%)	0	0
52	DT	135/146 (92%)	96 (71%)	25 (18%)	14 (10%)	0	3
53	BU	115/118 (98%)	86 (75%)	17 (15%)	12 (10%)	0	3
53	DU	115/118 (98%)	96 (84%)	11 (10%)	8 (7%)	1	8
54	BV	99/101 (98%)	50 (50%)	21 (21%)	28 (28%)	0	0
54	DV	99/101 (98%)	62 (63%)	22 (22%)	15 (15%)	0	1
55	BW	109/113 (96%)	84 (77%)	16 (15%)	9 (8%)	1	6
55	DW	109/113 (96%)	95 (87%)	5 (5%)	9 (8%)	1	6
56	BX	87/96 (91%)	46 (53%)	25 (29%)	16 (18%)	0	1
56	DX	92/96 (96%)	63 (68%)	9 (10%)	20 (22%)	0	0
57	BY	98/110 (89%)	45 (46%)	27 (28%)	26 (26%)	0	0
57	DY	107/110 (97%)	53 (50%)	26 (24%)	28 (26%)	0	0
58	BZ	174/206 (84%)	113 (65%)	43 (25%)	18 (10%)	0	3
58	DZ	174/206 (84%)	120 (69%)	33 (19%)	21 (12%)	0	2
All	All	11584/12586 (92%)	7801 (67%)	2288 (20%)	1495 (13%)	0	1

5 of 1495 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	22	LYS
2	AB	48	MET
2	AB	124	SER
2	AB	132	LYS
2	AB	150	SER

5.3.2 Protein sidechains (i)

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	AB	189/220 (86%)	167 (88%)	22 (12%)	5 22
2	CB	202/220 (92%)	186 (92%)	16 (8%)	12 37
3	AC	160/188 (85%)	148 (92%)	12 (8%)	13 39
3	CC	161/188 (86%)	150 (93%)	11 (7%)	16 44
4	AD	180/181 (99%)	164 (91%)	16 (9%)	9 32
4	CD	180/181 (99%)	164 (91%)	16 (9%)	9 32
5	AE	115/123 (94%)	105 (91%)	10 (9%)	10 34
5	CE	116/123 (94%)	104 (90%)	12 (10%)	7 26
6	AF	90/90 (100%)	83 (92%)	7 (8%)	12 38
6	CF	90/90 (100%)	89 (99%)	1 (1%)	73 85
7	AG	126/127 (99%)	114 (90%)	12 (10%)	8 29
7	CG	126/127 (99%)	117 (93%)	9 (7%)	14 42
8	AH	119/119 (100%)	110 (92%)	9 (8%)	13 39
8	CH	119/119 (100%)	107 (90%)	12 (10%)	7 27
9	AI	92/99 (93%)	82 (89%)	10 (11%)	6 24
9	CI	98/99 (99%)	85 (87%)	13 (13%)	4 17
10	AJ	88/92 (96%)	75 (85%)	13 (15%)	3 14
10	CJ	88/92 (96%)	83 (94%)	5 (6%)	20 51
11	AK	90/99 (91%)	80 (89%)	10 (11%)	6 24
11	CK	90/99 (91%)	84 (93%)	6 (7%)	16 45
12	AL	103/109 (94%)	96 (93%)	7 (7%)	16 44
12	CL	104/109 (95%)	90 (86%)	14 (14%)	4 17
13	AM	93/101 (92%)	82 (88%)	11 (12%)	5 21
13	CM	95/101 (94%)	84 (88%)	11 (12%)	5 22
14	AN	49/50 (98%)	41 (84%)	8 (16%)	2 10
14	CN	49/50 (98%)	44 (90%)	5 (10%)	7 27
15	AO	79/80 (99%)	72 (91%)	7 (9%)	9 32
15	CO	79/80 (99%)	77 (98%)	2 (2%)	47 72
16	AP	72/74 (97%)	68 (94%)	4 (6%)	21 51
16	CP	72/74 (97%)	68 (94%)	4 (6%)	21 51
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	17 47
17	CQ	94/97 (97%)	88 (94%)	6 (6%)	17 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	AR	61/77 (79%)	60 (98%)	1 (2%)	62 79
18	CR	61/77 (79%)	54 (88%)	7 (12%)	5 22
19	AS	69/80 (86%)	63 (91%)	6 (9%)	10 34
19	CS	69/80 (86%)	58 (84%)	11 (16%)	2 11
20	AT	76/82 (93%)	76 (100%)	0	100 100
20	CT	76/82 (93%)	69 (91%)	7 (9%)	9 31
21	AU	19/22 (86%)	15 (79%)	4 (21%)	1 4
21	CU	20/22 (91%)	16 (80%)	4 (20%)	1 5
25	B0	61/67 (91%)	59 (97%)	2 (3%)	38 66
25	D0	64/67 (96%)	62 (97%)	2 (3%)	40 67
26	B1	73/83 (88%)	65 (89%)	8 (11%)	6 24
26	D1	73/83 (88%)	66 (90%)	7 (10%)	8 29
27	B2	46/67 (69%)	38 (83%)	8 (17%)	2 8
27	D2	49/67 (73%)	45 (92%)	4 (8%)	11 36
28	B3	50/52 (96%)	49 (98%)	1 (2%)	55 76
28	D3	52/52 (100%)	50 (96%)	2 (4%)	33 62
30	B5	46/52 (88%)	41 (89%)	5 (11%)	6 24
30	D5	52/52 (100%)	47 (90%)	5 (10%)	8 29
31	B6	45/52 (86%)	36 (80%)	9 (20%)	1 5
31	D6	46/52 (88%)	38 (83%)	8 (17%)	2 8
32	B7	41/42 (98%)	36 (88%)	5 (12%)	5 20
32	D7	41/42 (98%)	38 (93%)	3 (7%)	14 40
33	B8	53/55 (96%)	47 (89%)	6 (11%)	6 23
33	D8	52/55 (94%)	49 (94%)	3 (6%)	20 50
34	B9	34/34 (100%)	31 (91%)	3 (9%)	10 33
34	D9	34/34 (100%)	31 (91%)	3 (9%)	10 33
37	BC	61/181 (34%)	58 (95%)	3 (5%)	25 56
37	DC	61/181 (34%)	57 (93%)	4 (7%)	16 46
38	BD	215/218 (99%)	198 (92%)	17 (8%)	12 37
38	DD	217/218 (100%)	198 (91%)	19 (9%)	10 33
39	BE	165/166 (99%)	151 (92%)	14 (8%)	10 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	DE	165/166 (99%)	153 (93%)	12 (7%)	14 40
40	BF	164/166 (99%)	150 (92%)	14 (8%)	10 35
40	DF	165/166 (99%)	157 (95%)	8 (5%)	25 56
41	BG	152/156 (97%)	145 (95%)	7 (5%)	27 58
41	DG	155/156 (99%)	145 (94%)	10 (6%)	17 46
42	BH	132/148 (89%)	125 (95%)	7 (5%)	22 53
42	DH	138/148 (93%)	129 (94%)	9 (6%)	17 46
43	BI	122/124 (98%)	110 (90%)	12 (10%)	8 29
43	DI	121/124 (98%)	111 (92%)	10 (8%)	11 35
46	BN	116/119 (98%)	106 (91%)	10 (9%)	10 34
46	DN	119/119 (100%)	110 (92%)	9 (8%)	13 39
47	BO	100/100 (100%)	90 (90%)	10 (10%)	7 28
47	DO	100/100 (100%)	92 (92%)	8 (8%)	12 37
48	BP	111/116 (96%)	98 (88%)	13 (12%)	5 22
48	DP	112/116 (97%)	89 (80%)	23 (20%)	1 4
49	BQ	106/111 (96%)	91 (86%)	15 (14%)	3 16
49	DQ	107/111 (96%)	95 (89%)	12 (11%)	6 23
50	BR	99/101 (98%)	90 (91%)	9 (9%)	9 31
50	DR	100/101 (99%)	89 (89%)	11 (11%)	6 24
51	BS	81/88 (92%)	71 (88%)	10 (12%)	4 20
51	DS	78/88 (89%)	65 (83%)	13 (17%)	2 10
52	BT	116/127 (91%)	99 (85%)	17 (15%)	3 14
52	DT	120/127 (94%)	101 (84%)	19 (16%)	2 11
53	BU	93/94 (99%)	81 (87%)	12 (13%)	4 18
53	DU	93/94 (99%)	89 (96%)	4 (4%)	29 59
54	BV	82/82 (100%)	75 (92%)	7 (8%)	10 35
54	DV	82/82 (100%)	74 (90%)	8 (10%)	8 29
55	BW	91/92 (99%)	79 (87%)	12 (13%)	4 17
55	DW	91/92 (99%)	85 (93%)	6 (7%)	16 46
56	BX	72/78 (92%)	63 (88%)	9 (12%)	4 19
56	DX	76/78 (97%)	64 (84%)	12 (16%)	2 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
57	BY	84/91 (92%)	75 (89%)	9 (11%)	6 25
57	DY	90/91 (99%)	78 (87%)	12 (13%)	4 17
58	BZ	155/179 (87%)	138 (89%)	17 (11%)	6 24
58	DZ	155/179 (87%)	141 (91%)	14 (9%)	9 32
All	All	9527/10302 (92%)	8649 (91%)	878 (9%)	9 31

5 of 878 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CC	20	SER
14	CN	24	CYS
58	DZ	145	GLU
51	DS	71	ARG
4	CD	59	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
2	CB	104	ASN
17	CQ	45	HIS
3	CC	63	ASN
10	CJ	84	GLN
31	D6	26	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1520 (98%)	533 (35%)	67 (4%)
1	CA	1503/1520 (98%)	451 (30%)	39 (2%)
22	AV	75/77 (97%)	27 (36%)	1 (1%)
22	CV	76/77 (98%)	30 (39%)	0
23	AW	75/76 (98%)	63 (84%)	8 (10%)
23	AY	18/76 (23%)	8 (44%)	0
23	CW	75/76 (98%)	50 (66%)	4 (5%)
23	CY	20/76 (26%)	6 (30%)	0
24	AX	11/24 (45%)	4 (36%)	1 (9%)
24	CX	11/24 (45%)	4 (36%)	1 (9%)
35	BA	2823/2839 (99%)	984 (34%)	91 (3%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	DA	2823/2839 (99%)	882 (31%)	74 (2%)
36	BB	119/122 (97%)	39 (32%)	2 (1%)
36	DB	118/122 (96%)	37 (31%)	5 (4%)
All	All	9250/9468 (97%)	3118 (33%)	293 (3%)

5 of 3118 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	10	A
1	AA	14	U
1	AA	22	G
1	AA	31	G

5 of 293 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	DA	574	C
35	DA	2859	G
35	DA	859	G
35	DA	1740	G
35	BA	405	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1384 ligands modelled in this entry, 1382 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	EDS	AA	1805	-	38,43,43	1.75	9 (23%)	38,61,61	1.54	7 (18%)
60	EDS	CA	1787	-	38,43,43	1.80	6 (15%)	38,61,61	1.96	14 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	EDS	AA	1805	-	-	4/23/79/79	0/3/3/3
60	EDS	CA	1787	-	-	4/23/79/79	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	AA	1805	EDS	CBE-NAK	5.54	1.46	1.34
60	CA	1787	EDS	OAC-CBA	5.00	1.50	1.43
60	CA	1787	EDS	CBE-NAK	4.87	1.44	1.34
60	AA	1805	EDS	OAJ-CBO	-4.21	1.20	1.42
60	CA	1787	EDS	OAF-CAZ	-4.13	1.37	1.44

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	AA	1805	EDS	CAT-CAS-CAQ	4.66	118.62	108.96
60	CA	1787	EDS	CBL-NAO-CBN	-3.68	107.50	113.33
60	CA	1787	EDS	CAV-CAR-NAK	-3.58	105.32	110.86
60	CA	1787	EDS	CBA-OAC-CAW	3.58	117.29	111.53
60	CA	1787	EDS	OAJ-CBO-CBN	3.55	124.58	111.59

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	CA	1787	EDS	CAY-CAX-NAM-CBH
60	AA	1805	EDS	CBO-CBN-NAO-CBL
60	CA	1787	EDS	OAG-CBB-OAB-CAT
60	AA	1805	EDS	CBI-CBL-NAO-CBN

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Mol	Chain	Res	Type	Atoms
60	AA	1805	EDS	CBG-CBK-CBM-NAP

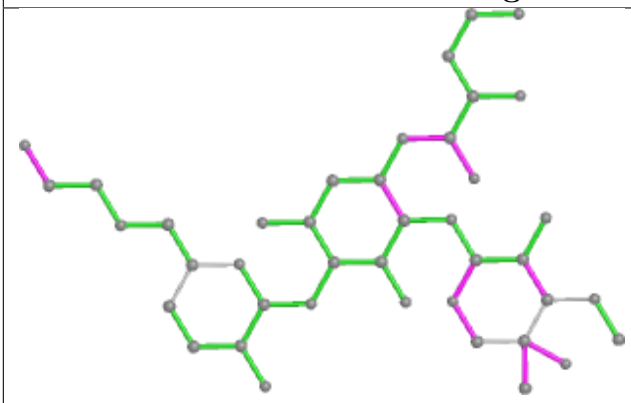
There are no ring outliers.

2 monomers are involved in 3 short contacts:

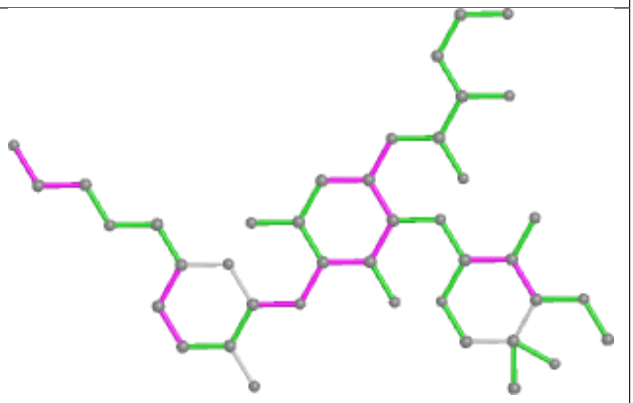
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	AA	1805	EDS	2	0
60	CA	1787	EDS	1	0

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

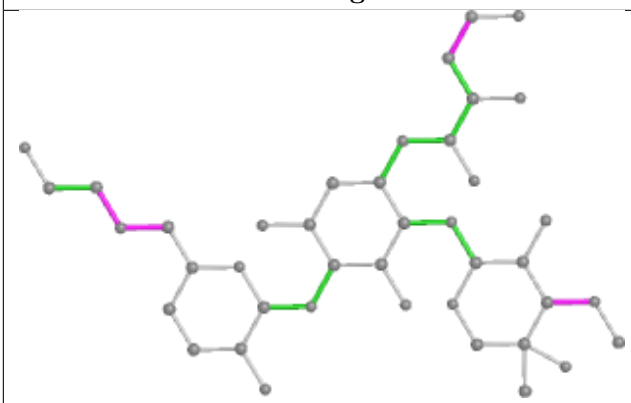
Ligand EDS AA 1805



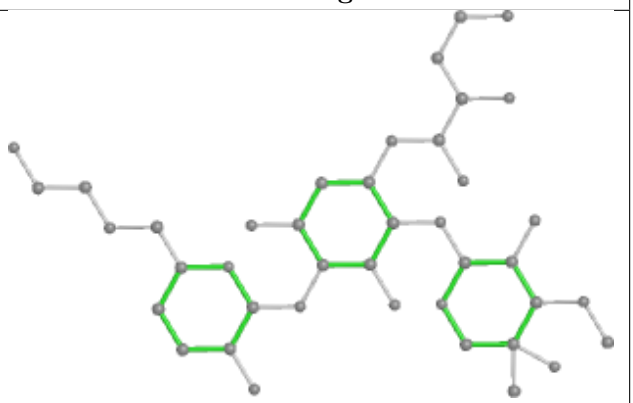
Bond lengths



Bond angles

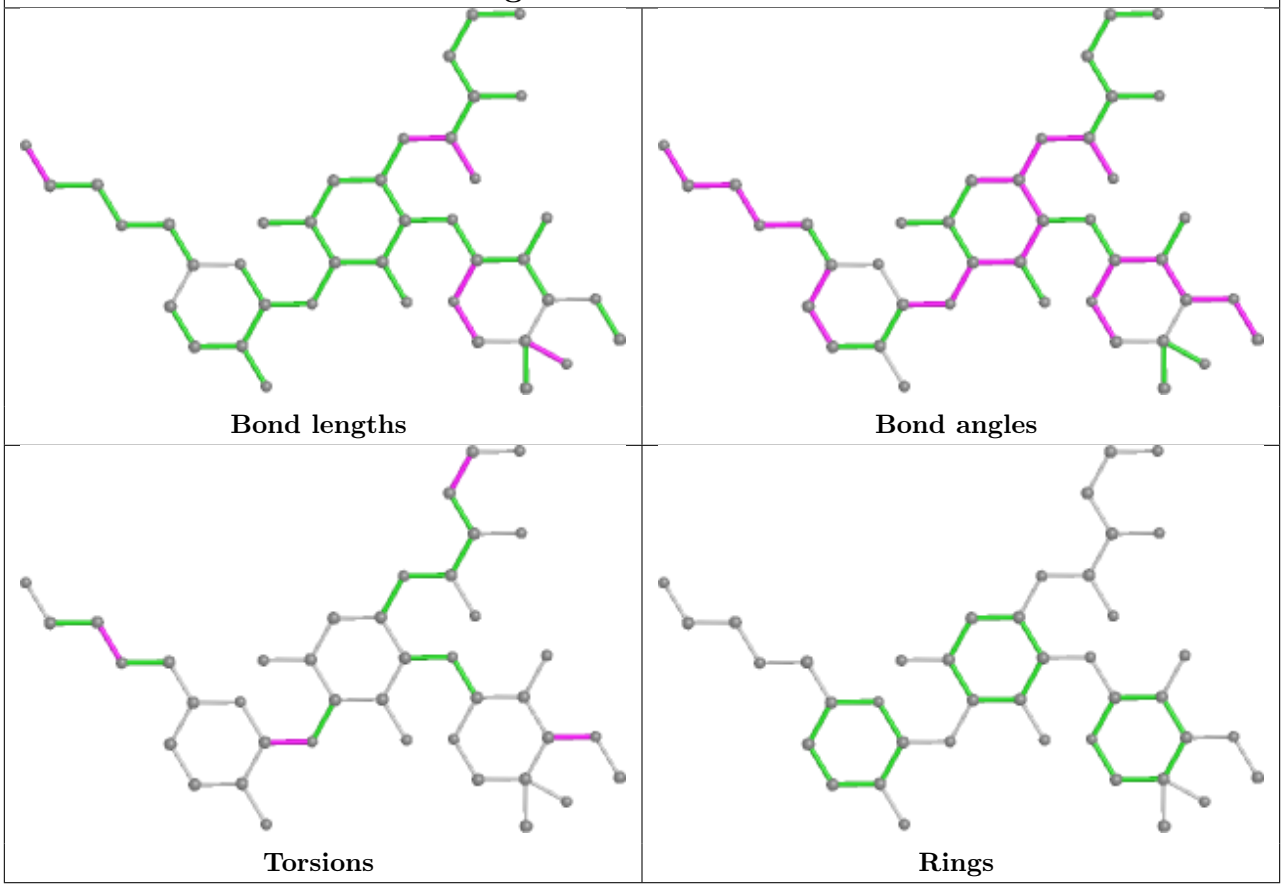


Torsions



Rings

Ligand EDS CA 1787



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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^{th} 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^2)	Q<0.9
1	AA	1504/1520 (98%)	-0.39	25 (1%) 70 67	45, 87, 160, 209	0
1	CA	1504/1520 (98%)	-0.40	13 (0%) 84 84	41, 84, 187, 269	0
2	AB	218/256 (85%)	1.43	67 (30%) 0 0	101, 144, 193, 209	0
2	CB	234/256 (91%)	-0.17	5 (2%) 63 61	92, 134, 190, 208	0
3	AC	206/239 (86%)	2.09	97 (47%) 0 0	89, 116, 150, 163	0
3	CC	207/239 (86%)	1.55	72 (34%) 0 0	77, 109, 151, 174	0
4	AD	208/209 (99%)	0.04	3 (1%) 75 74	65, 80, 100, 111	0
4	CD	208/209 (99%)	0.34	18 (8%) 10 10	73, 93, 118, 130	0
5	AE	150/162 (92%)	0.88	31 (20%) 1 1	70, 91, 117, 132	0
5	CE	151/162 (93%)	-0.13	2 (1%) 77 76	63, 83, 110, 144	0
6	AF	101/101 (100%)	-0.52	0 100 100	69, 87, 102, 133	0
6	CF	101/101 (100%)	0.49	11 (10%) 5 5	68, 89, 110, 129	0
7	AG	155/156 (99%)	1.04	31 (20%) 1 1	90, 114, 148, 163	0
7	CG	155/156 (99%)	1.35	21 (13%) 3 3	90, 109, 144, 150	0
8	AH	138/138 (100%)	-0.15	2 (1%) 75 74	69, 95, 112, 129	0
8	CH	138/138 (100%)	-0.25	0 100 100	70, 87, 103, 110	0
9	AI	121/128 (94%)	0.05	5 (4%) 37 35	90, 141, 171, 181	0
9	CI	127/128 (99%)	0.29	11 (8%) 10 10	77, 134, 175, 186	0
10	AJ	98/105 (93%)	0.49	9 (9%) 9 9	87, 150, 182, 186	0
10	CJ	98/105 (93%)	2.33	49 (50%) 0 0	75, 151, 194, 200	0
11	AK	119/129 (92%)	0.24	5 (4%) 36 34	72, 89, 120, 186	0
11	CK	119/129 (92%)	1.85	48 (40%) 0 0	54, 90, 135, 188	0
12	AL	122/132 (92%)	1.02	24 (19%) 1 1	56, 70, 94, 129	0
12	CL	124/132 (93%)	0.45	5 (4%) 38 36	49, 64, 106, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	116/126 (92%)	0.38	12 (10%) 6 6	84, 121, 142, 155	0
13	CM	119/126 (94%)	0.26	14 (11%) 4 4	68, 110, 127, 143	0
14	AN	60/61 (98%)	1.17	16 (26%) 0 0	92, 111, 123, 129	0
14	CN	60/61 (98%)	1.30	16 (26%) 0 0	75, 96, 112, 123	0
15	AO	88/89 (98%)	-0.40	0 100 100	68, 89, 116, 119	0
15	CO	88/89 (98%)	-0.30	3 (3%) 45 43	64, 86, 110, 123	0
16	AP	83/88 (94%)	-0.71	0 100 100	65, 77, 100, 140	0
16	CP	83/88 (94%)	0.31	5 (6%) 21 21	75, 88, 119, 176	0
17	AQ	99/105 (94%)	0.84	11 (11%) 5 5	65, 81, 105, 117	0
17	CQ	99/105 (94%)	1.65	40 (40%) 0 0	76, 88, 106, 117	0
18	AR	70/88 (79%)	-0.28	1 (1%) 75 74	70, 90, 121, 132	0
18	CR	70/88 (79%)	1.24	17 (24%) 0 0	67, 86, 131, 149	0
19	AS	78/93 (83%)	1.25	19 (24%) 0 0	106, 141, 172, 180	0
19	CS	78/93 (83%)	0.65	10 (12%) 3 3	85, 113, 165, 167	0
20	AT	99/106 (93%)	0.36	6 (6%) 21 20	71, 89, 135, 151	0
20	CT	99/106 (93%)	0.98	15 (15%) 2 2	78, 104, 140, 145	0
21	AU	24/27 (88%)	-0.24	0 100 100	90, 114, 134, 139	0
21	CU	25/27 (92%)	-0.30	1 (4%) 38 36	86, 96, 126, 130	0
22	AV	76/77 (98%)	-0.24	0 100 100	56, 97, 125, 154	0
22	CV	77/77 (100%)	-0.17	2 (2%) 56 52	43, 88, 118, 155	0
23	AW	76/76 (100%)	0.46	3 (3%) 39 37	51, 193, 217, 221	0
23	AY	19/76 (25%)	-0.17	0 100 100	75, 101, 161, 166	0
23	CW	76/76 (100%)	0.82	12 (15%) 2 2	48, 194, 225, 230	0
23	CY	21/76 (27%)	-0.12	0 100 100	63, 99, 162, 202	0
24	AX	12/24 (50%)	-0.20	0 100 100	64, 74, 143, 145	0
24	CX	12/24 (50%)	0.01	0 100 100	53, 60, 121, 127	0
25	B0	76/85 (89%)	0.65	7 (9%) 9 9	49, 69, 93, 149	0
25	D0	82/85 (96%)	0.46	7 (8%) 10 11	42, 57, 88, 102	0
26	B1	88/98 (89%)	1.18	19 (21%) 0 1	46, 65, 124, 140	0
26	D1	88/98 (89%)	1.35	20 (22%) 0 1	38, 60, 110, 120	0
27	B2	50/72 (69%)	0.38	6 (12%) 4 4	92, 120, 151, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
27	D2	53/72 (73%)	0.12	1 (1%) 66 64	54, 69, 107, 120	0
28	B3	58/60 (96%)	1.09	12 (20%) 1 1	60, 74, 106, 109	0
28	D3	60/60 (100%)	0.45	6 (10%) 7 7	43, 57, 101, 113	0
29	B4	45/71 (63%)	0.79	8 (17%) 1 1	91, 152, 167, 176	0
29	D4	49/71 (69%)	-0.71	0 100 100	81, 130, 153, 160	0
30	B5	54/60 (90%)	0.82	7 (12%) 3 3	38, 65, 120, 134	0
30	D5	60/60 (100%)	0.50	7 (11%) 4 4	28, 64, 147, 159	0
31	B6	46/54 (85%)	-0.06	2 (4%) 35 33	68, 89, 104, 117	0
31	D6	47/54 (87%)	1.26	7 (14%) 2 2	67, 82, 116, 132	0
32	B7	48/49 (97%)	1.15	9 (18%) 1 1	38, 49, 78, 83	0
32	D7	48/49 (97%)	0.20	2 (4%) 36 34	29, 34, 68, 88	0
33	B8	63/65 (96%)	0.77	8 (12%) 3 3	49, 70, 86, 122	0
33	D8	62/65 (95%)	0.98	7 (11%) 5 5	41, 53, 71, 82	0
34	B9	37/37 (100%)	0.47	3 (8%) 12 11	77, 92, 106, 114	0
34	D9	37/37 (100%)	0.30	3 (8%) 12 11	59, 77, 98, 101	0
35	BA	2824/2839 (99%)	-0.25	23 (0%) 86 86	36, 63, 194, 265	0
35	DA	2824/2839 (99%)	-0.19	47 (1%) 70 67	27, 50, 193, 262	0
36	BB	120/122 (98%)	-0.57	0 100 100	76, 99, 132, 148	0
36	DB	119/122 (97%)	-0.52	0 100 100	53, 78, 113, 159	0
37	BC	190/229 (82%)	1.29	56 (29%) 0 0	161, 211, 232, 239	0
37	DC	190/229 (82%)	1.85	73 (38%) 0 0	166, 210, 231, 235	0
38	BD	273/276 (98%)	0.39	13 (4%) 30 29	34, 55, 77, 89	0
38	DD	275/276 (99%)	0.16	6 (2%) 62 59	28, 47, 73, 112	0
39	BE	204/206 (99%)	0.57	18 (8%) 10 10	41, 68, 120, 139	0
39	DE	204/206 (99%)	0.18	7 (3%) 45 43	27, 55, 101, 125	0
40	BF	206/210 (98%)	0.57	21 (10%) 6 6	34, 76, 149, 186	0
40	DF	208/210 (99%)	0.23	10 (4%) 30 29	29, 56, 138, 190	0
41	BG	178/182 (97%)	0.68	20 (11%) 5 5	84, 108, 143, 182	0
41	DG	181/182 (99%)	0.54	13 (7%) 15 15	67, 91, 134, 186	0
42	BH	159/180 (88%)	1.73	61 (38%) 0 0	117, 156, 198, 206	0
42	DH	165/180 (91%)	0.01	4 (2%) 59 55	57, 80, 107, 168	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
43	BI	145/148 (97%)	0.44	14 (9%) 7 8	61, 99, 133, 152	0
43	DI	144/148 (97%)	0.39	8 (5%) 24 23	55, 140, 180, 195	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BK	0/147	-	-	-	-
45	DK	0/147	-	-	-	-
46	BN	137/140 (97%)	1.12	39 (28%) 0 0	50, 81, 126, 143	0
46	DN	140/140 (100%)	-0.04	6 (4%) 35 33	42, 60, 102, 120	0
47	BO	122/122 (100%)	1.34	37 (30%) 0 0	46, 66, 87, 98	0
47	DO	122/122 (100%)	0.25	4 (3%) 46 44	38, 53, 77, 90	0
48	BP	144/150 (96%)	0.60	11 (7%) 13 13	44, 90, 126, 143	0
48	DP	146/150 (97%)	0.67	11 (7%) 14 13	32, 69, 100, 190	0
49	BQ	135/141 (95%)	1.33	34 (25%) 0 0	54, 85, 119, 154	0
49	DQ	136/141 (96%)	1.94	53 (38%) 0 0	45, 66, 106, 139	0
50	BR	116/118 (98%)	0.61	10 (8%) 10 10	46, 64, 103, 117	0
50	DR	117/118 (99%)	0.03	2 (1%) 70 67	37, 53, 73, 90	0
51	BS	102/112 (91%)	-0.18	3 (2%) 51 50	71, 102, 120, 127	0
51	DS	99/112 (88%)	-0.19	1 (1%) 82 82	62, 82, 104, 107	0
52	BT	132/146 (90%)	0.38	8 (6%) 21 20	54, 77, 131, 169	0
52	DT	137/146 (93%)	1.19	29 (21%) 0 1	48, 68, 157, 221	0
53	BU	117/118 (99%)	0.33	12 (10%) 6 6	44, 72, 113, 127	0
53	DU	117/118 (99%)	-0.07	2 (1%) 70 67	33, 53, 80, 106	0
54	BV	101/101 (100%)	0.38	8 (7%) 12 12	48, 110, 134, 183	0
54	DV	101/101 (100%)	0.51	8 (7%) 12 12	37, 81, 121, 153	0
55	BW	111/113 (98%)	0.53	8 (7%) 15 15	47, 61, 106, 123	0
55	DW	111/113 (98%)	0.30	8 (7%) 15 15	37, 46, 80, 135	0
56	BX	89/96 (92%)	0.65	11 (12%) 4 4	61, 82, 138, 159	0
56	DX	94/96 (97%)	0.22	3 (3%) 47 46	40, 55, 97, 140	0
57	BY	100/110 (90%)	0.95	18 (18%) 1 1	63, 105, 143, 160	0
57	DY	109/110 (99%)	0.26	9 (8%) 11 11	49, 76, 174, 200	0
58	BZ	176/206 (85%)	3.69	92 (52%) 0 0	92, 153, 201, 217	0
58	DZ	176/206 (85%)	5.18	156 (88%) 0 0	68, 128, 208, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	21060/22694 (92%)	0.29	1875 (8%)	9	10	27, 80, 183, 269	0

The worst 5 of 1875 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	CG	84	ASN	29.5
58	DZ	106	GLY	20.4
58	BZ	154	ASP	19.6
7	CG	83	ALA	19.2
7	CG	85	TYR	17.8

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3397	1/1	-0.22	0.29	190,190,190,190	0
59	MG	AA	1713	1/1	-0.04	0.33	137,137,137,137	0
59	MG	BC	302	1/1	-0.04	0.28	171,171,171,171	0
59	MG	BA	3323	1/1	-0.01	0.34	159,159,159,159	0
59	MG	AW	105	1/1	0.01	0.72	170,170,170,170	0
59	MG	BA	3344	1/1	0.07	0.65	81,81,81,81	0
59	MG	CW	109	1/1	0.07	1.10	125,125,125,125	0
59	MG	CW	112	1/1	0.08	0.45	191,191,191,191	0
59	MG	CA	1675	1/1	0.10	0.91	77,77,77,77	0
59	MG	BA	3293	1/1	0.14	0.21	108,108,108,108	0
59	MG	AA	1756	1/1	0.16	0.86	107,107,107,107	0
59	MG	AA	1804	1/1	0.18	0.95	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3285	1/1	0.18	1.01	103,103,103,103	0
59	MG	BA	3437	1/1	0.20	0.16	126,126,126,126	0
59	MG	AW	114	1/1	0.25	0.48	193,193,193,193	0
59	MG	DA	3315	1/1	0.28	0.95	71,71,71,71	0
59	MG	DA	3203	1/1	0.30	0.89	57,57,57,57	0
59	MG	BA	3431	1/1	0.30	0.37	94,94,94,94	0
59	MG	CW	108	1/1	0.31	0.79	130,130,130,130	0
59	MG	CA	1668	1/1	0.32	0.34	75,75,75,75	0
59	MG	BA	3324	1/1	0.36	0.24	194,194,194,194	0
59	MG	BA	3351	1/1	0.39	0.27	116,116,116,116	0
59	MG	BA	3302	1/1	0.41	0.48	75,75,75,75	0
59	MG	CW	102	1/1	0.43	0.38	165,165,165,165	0
59	MG	AW	107	1/1	0.44	0.25	115,115,115,115	0
59	MG	DA	3007	1/1	0.44	0.68	77,77,77,77	0
59	MG	DO	202	1/1	0.45	1.27	86,86,86,86	0
59	MG	BA	3257	1/1	0.46	0.97	77,77,77,77	0
59	MG	AA	1611	1/1	0.46	0.34	87,87,87,87	0
59	MG	BA	3433	1/1	0.46	0.32	94,94,94,94	0
59	MG	BA	3222	1/1	0.47	0.35	78,78,78,78	0
59	MG	AA	1775	1/1	0.47	0.14	75,75,75,75	0
59	MG	DB	206	1/1	0.48	0.24	91,91,91,91	0
59	MG	AW	118	1/1	0.48	0.22	188,188,188,188	0
59	MG	DA	3326	1/1	0.49	0.23	68,68,68,68	0
59	MG	BA	3322	1/1	0.49	0.21	130,130,130,130	0
59	MG	BB	216	1/1	0.49	0.35	92,92,92,92	0
59	MG	BA	3301	1/1	0.50	0.25	115,115,115,115	0
59	MG	CA	1725	1/1	0.50	0.51	80,80,80,80	0
59	MG	CA	1620	1/1	0.51	0.54	105,105,105,105	0
59	MG	AW	104	1/1	0.51	1.21	171,171,171,171	0
59	MG	BA	3408	1/1	0.53	0.18	93,93,93,93	0
59	MG	CA	1627	1/1	0.54	0.62	49,49,49,49	0
59	MG	AA	1738	1/1	0.54	0.28	57,57,57,57	0
59	MG	DA	3374	1/1	0.55	0.35	65,65,65,65	0
59	MG	DB	202	1/1	0.55	0.26	83,83,83,83	0
59	MG	BA	3213	1/1	0.55	0.36	72,72,72,72	0
59	MG	DA	3230	1/1	0.55	0.80	98,98,98,98	0
59	MG	CA	1652	1/1	0.56	0.66	85,85,85,85	0
59	MG	AA	1650	1/1	0.56	0.30	80,80,80,80	0
59	MG	BA	3434	1/1	0.56	0.62	90,90,90,90	0
59	MG	CA	1683	1/1	0.56	0.23	74,74,74,74	0
59	MG	AA	1772	1/1	0.56	0.24	86,86,86,86	0
59	MG	DB	211	1/1	0.56	0.42	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3438	1/1	0.56	0.20	104,104,104,104	0
59	MG	BB	207	1/1	0.57	0.31	115,115,115,115	0
59	MG	DB	207	1/1	0.57	0.73	73,73,73,73	0
59	MG	AA	1808	1/1	0.58	0.43	65,65,65,65	0
59	MG	DA	3316	1/1	0.58	0.56	63,63,63,63	0
59	MG	AA	1677	1/1	0.58	0.26	72,72,72,72	0
59	MG	BB	217	1/1	0.59	0.29	98,98,98,98	0
59	MG	BA	3325	1/1	0.59	0.22	164,164,164,164	0
59	MG	CA	1700	1/1	0.59	0.35	87,87,87,87	0
59	MG	AA	1724	1/1	0.59	0.22	77,77,77,77	0
59	MG	DA	3143	1/1	0.60	0.28	67,67,67,67	0
59	MG	AA	1740	1/1	0.61	0.07	114,114,114,114	0
59	MG	CA	1643	1/1	0.61	0.19	100,100,100,100	0
59	MG	CA	1792	1/1	0.61	0.36	76,76,76,76	0
59	MG	BA	3218	1/1	0.61	0.22	77,77,77,77	0
59	MG	AA	1697	1/1	0.62	0.50	76,76,76,76	0
59	MG	BA	3442	1/1	0.62	0.38	57,57,57,57	0
59	MG	AA	1759	1/1	0.62	0.18	93,93,93,93	0
59	MG	DA	3348	1/1	0.62	1.02	72,72,72,72	0
59	MG	AW	117	1/1	0.62	0.60	125,125,125,125	0
59	MG	AA	1760	1/1	0.63	0.70	105,105,105,105	0
59	MG	DA	3337	1/1	0.63	0.34	67,67,67,67	0
59	MG	BS	201	1/1	0.63	0.27	97,97,97,97	0
59	MG	BA	3007	1/1	0.64	0.19	69,69,69,69	0
59	MG	BA	3456	1/1	0.64	0.55	73,73,73,73	0
59	MG	CA	1690	1/1	0.64	0.65	84,84,84,84	0
59	MG	CW	104	1/1	0.64	0.27	174,174,174,174	0
59	MG	AA	1674	1/1	0.64	0.49	61,61,61,61	0
59	MG	DA	3210	1/1	0.64	0.36	71,71,71,71	0
59	MG	BA	3157	1/1	0.65	0.26	63,63,63,63	0
59	MG	BA	3364	1/1	0.65	0.48	62,62,62,62	0
59	MG	BA	3224	1/1	0.65	0.41	62,62,62,62	0
59	MG	CE	201	1/1	0.66	0.91	84,84,84,84	0
59	MG	AA	1707	1/1	0.66	0.17	87,87,87,87	0
59	MG	CW	103	1/1	0.66	0.36	178,178,178,178	0
59	MG	AW	110	1/1	0.66	0.58	134,134,134,134	0
59	MG	DA	3163	1/1	0.66	0.88	79,79,79,79	0
59	MG	BA	3405	1/1	0.66	0.77	80,80,80,80	0
59	MG	DA	3342	1/1	0.66	0.50	59,59,59,59	0
59	MG	BB	208	1/1	0.67	0.15	83,83,83,83	0
59	MG	BA	3142	1/1	0.67	0.70	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3206	1/1	0.67	0.43	82,82,82,82	0
59	MG	CA	1640	1/1	0.67	0.25	91,91,91,91	0
59	MG	BA	3398	1/1	0.67	0.25	104,104,104,104	0
59	MG	BA	3003	1/1	0.67	0.33	84,84,84,84	0
59	MG	AA	1763	1/1	0.67	0.14	66,66,66,66	0
59	MG	DA	3320	1/1	0.67	0.45	67,67,67,67	0
59	MG	CA	1602	1/1	0.67	0.54	72,72,72,72	0
59	MG	BA	3080	1/1	0.68	0.35	43,43,43,43	0
59	MG	BA	3132	1/1	0.68	0.44	72,72,72,72	0
59	MG	BA	3331	1/1	0.68	0.22	88,88,88,88	0
59	MG	AA	1645	1/1	0.68	0.43	79,79,79,79	0
59	MG	DA	3356	1/1	0.68	0.63	68,68,68,68	0
59	MG	BA	3011	1/1	0.68	1.51	65,65,65,65	0
59	MG	BA	3353	1/1	0.68	1.11	75,75,75,75	0
59	MG	DA	3244	1/1	0.68	0.15	147,147,147,147	0
59	MG	CA	1695	1/1	0.68	0.43	59,59,59,59	0
59	MG	CA	1636	1/1	0.68	0.26	69,69,69,69	0
59	MG	BA	3059	1/1	0.68	0.35	65,65,65,65	0
59	MG	CW	106	1/1	0.69	0.48	133,133,133,133	0
59	MG	DA	3318	1/1	0.69	0.28	67,67,67,67	0
59	MG	AA	1801	1/1	0.69	0.36	69,69,69,69	0
59	MG	BA	3389	1/1	0.69	0.47	74,74,74,74	0
59	MG	AW	115	1/1	0.69	0.39	193,193,193,193	0
59	MG	AV	103	1/1	0.69	0.36	93,93,93,93	0
59	MG	CA	1733	1/1	0.69	0.11	81,81,81,81	0
59	MG	CA	1742	1/1	0.69	0.66	59,59,59,59	0
59	MG	CA	1766	1/1	0.69	0.15	69,69,69,69	0
59	MG	CA	1646	1/1	0.69	0.80	72,72,72,72	0
59	MG	BA	3306	1/1	0.69	0.72	56,56,56,56	0
59	MG	BA	3187	1/1	0.69	0.38	93,93,93,93	0
59	MG	CA	1619	1/1	0.69	0.40	66,66,66,66	0
59	MG	BA	3108	1/1	0.69	0.45	69,69,69,69	0
59	MG	BX	101	1/1	0.70	0.23	48,48,48,48	0
59	MG	AA	1681	1/1	0.70	0.55	76,76,76,76	0
59	MG	BA	3145	1/1	0.70	0.60	62,62,62,62	0
59	MG	AT	201	1/1	0.70	0.54	75,75,75,75	0
59	MG	BA	3303	1/1	0.70	0.34	73,73,73,73	0
59	MG	BA	3427	1/1	0.70	0.44	84,84,84,84	0
59	MG	CA	1706	1/1	0.70	0.25	61,61,61,61	0
59	MG	BA	3305	1/1	0.70	0.37	77,77,77,77	0
59	MG	CA	1642	1/1	0.70	0.17	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3367	1/1	0.70	0.27	61,61,61,61	0
59	MG	BA	3168	1/1	0.70	0.23	89,89,89,89	0
59	MG	AA	1770	1/1	0.70	0.41	74,74,74,74	0
59	MG	CA	1648	1/1	0.70	0.18	96,96,96,96	0
59	MG	DA	3224	1/1	0.70	0.49	40,40,40,40	0
59	MG	CA	1649	1/1	0.70	0.74	76,76,76,76	0
59	MG	BA	3198	1/1	0.70	0.14	54,54,54,54	0
59	MG	AA	1777	1/1	0.71	0.90	81,81,81,81	0
59	MG	BA	3366	1/1	0.71	0.12	89,89,89,89	0
59	MG	CW	107	1/1	0.71	0.27	145,145,145,145	0
59	MG	DA	3353	1/1	0.71	0.32	51,51,51,51	0
59	MG	BA	3254	1/1	0.71	0.43	89,89,89,89	0
59	MG	CA	1650	1/1	0.71	0.34	78,78,78,78	0
59	MG	BA	3271	1/1	0.72	0.60	61,61,61,61	0
59	MG	CA	1677	1/1	0.72	0.41	68,68,68,68	0
59	MG	DA	3382	1/1	0.72	0.47	80,80,80,80	0
59	MG	BA	3014	1/1	0.72	0.68	55,55,55,55	0
59	MG	BA	3025	1/1	0.72	0.20	61,61,61,61	0
59	MG	CA	1762	1/1	0.72	0.28	57,57,57,57	0
59	MG	CA	1660	1/1	0.72	0.21	65,65,65,65	0
59	MG	AA	1706	1/1	0.72	0.24	86,86,86,86	0
59	MG	DA	3331	1/1	0.73	0.18	99,99,99,99	0
59	MG	CA	1703	1/1	0.73	0.12	47,47,47,47	0
59	MG	AA	1670	1/1	0.73	0.40	68,68,68,68	0
59	MG	CA	1714	1/1	0.73	0.18	67,67,67,67	0
59	MG	BA	3051	1/1	0.73	0.20	66,66,66,66	0
59	MG	AL	201	1/1	0.73	0.94	61,61,61,61	0
59	MG	CA	1678	1/1	0.73	0.39	78,78,78,78	0
59	MG	DA	3246	1/1	0.73	0.45	58,58,58,58	0
59	MG	DA	3307	1/1	0.73	0.94	64,64,64,64	0
59	MG	CA	1761	1/1	0.73	0.26	66,66,66,66	0
59	MG	AA	1700	1/1	0.73	0.34	78,78,78,78	0
59	MG	AW	113	1/1	0.73	0.42	96,96,96,96	0
59	MG	AA	1660	1/1	0.73	1.08	84,84,84,84	0
59	MG	AA	1727	1/1	0.73	0.21	63,63,63,63	0
59	MG	CW	101	1/1	0.74	0.34	101,101,101,101	0
59	MG	BF	302	1/1	0.74	0.34	61,61,61,61	0
59	MG	DA	3322	1/1	0.74	0.20	56,56,56,56	0
59	MG	DA	3182	1/1	0.74	0.29	56,56,56,56	0
59	MG	DA	3194	1/1	0.74	0.20	62,62,62,62	0
59	MG	DA	3258	1/1	0.74	0.44	65,65,65,65	0
59	MG	AA	1675	1/1	0.74	0.27	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3192	1/1	0.74	0.25	80,80,80,80	0
59	MG	AD	301	1/1	0.74	0.44	69,69,69,69	0
59	MG	CA	1758	1/1	0.75	0.20	67,67,67,67	0
59	MG	BA	3400	1/1	0.75	0.44	59,59,59,59	0
59	MG	DA	3280	1/1	0.75	0.44	46,46,46,46	0
59	MG	DA	3152	1/1	0.75	0.44	61,61,61,61	0
59	MG	DA	3213	1/1	0.75	0.30	71,71,71,71	0
59	MG	AA	1683	1/1	0.75	0.31	74,74,74,74	0
59	MG	CA	1686	1/1	0.75	0.19	77,77,77,77	0
59	MG	AW	119	1/1	0.75	0.63	194,194,194,194	0
59	MG	AA	1686	1/1	0.76	0.13	86,86,86,86	0
59	MG	CA	1735	1/1	0.76	0.36	63,63,63,63	0
59	MG	BA	3365	1/1	0.76	0.33	54,54,54,54	0
59	MG	CA	1749	1/1	0.76	0.24	60,60,60,60	0
59	MG	BA	3024	1/1	0.76	0.33	82,82,82,82	0
59	MG	DA	3232	1/1	0.76	0.13	93,93,93,93	0
59	MG	BA	3093	1/1	0.76	0.34	75,75,75,75	0
59	MG	BA	3162	1/1	0.76	0.32	55,55,55,55	0
59	MG	DA	3008	1/1	0.76	0.52	76,76,76,76	0
59	MG	AA	1619	1/1	0.76	1.15	83,83,83,83	0
59	MG	DA	3299	1/1	0.76	0.39	63,63,63,63	0
59	MG	CA	1637	1/1	0.76	0.84	71,71,71,71	0
59	MG	CA	1665	1/1	0.76	0.30	72,72,72,72	0
59	MG	AA	1765	1/1	0.76	0.19	84,84,84,84	0
59	MG	CA	1674	1/1	0.76	0.49	69,69,69,69	0
59	MG	BA	3356	1/1	0.76	0.19	69,69,69,69	0
59	MG	BA	3457	1/1	0.77	0.52	82,82,82,82	0
59	MG	AA	1718	1/1	0.77	0.24	89,89,89,89	0
59	MG	DA	3004	1/1	0.77	0.28	89,89,89,89	0
59	MG	DA	3005	1/1	0.77	0.72	56,56,56,56	0
59	MG	BA	3180	1/1	0.77	0.14	79,79,79,79	0
59	MG	CA	1743	1/1	0.77	0.18	67,67,67,67	0
59	MG	DA	3383	1/1	0.77	0.37	92,92,92,92	0
59	MG	BB	211	1/1	0.77	0.26	74,74,74,74	0
59	MG	BA	3186	1/1	0.77	0.41	65,65,65,65	0
59	MG	AW	112	1/1	0.77	0.38	112,112,112,112	0
59	MG	AA	1712	1/1	0.77	0.07	67,67,67,67	0
59	MG	BA	3230	1/1	0.77	0.32	89,89,89,89	0
59	MG	BA	3313	1/1	0.78	0.64	68,68,68,68	0
59	MG	DA	3321	1/1	0.78	0.23	63,63,63,63	0
59	MG	CA	1750	1/1	0.78	0.31	70,70,70,70	0
59	MG	CA	1751	1/1	0.78	0.16	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AV	102	1/1	0.78	0.60	74,74,74,74	0
59	MG	DA	3211	1/1	0.78	0.32	55,55,55,55	0
59	MG	BA	3350	1/1	0.78	0.45	91,91,91,91	0
59	MG	CA	1721	1/1	0.78	0.20	81,81,81,81	0
59	MG	DA	3350	1/1	0.78	0.37	58,58,58,58	0
59	MG	BQ	201	1/1	0.78	0.23	51,51,51,51	0
59	MG	CA	1783	1/1	0.78	0.23	64,64,64,64	0
59	MG	DA	3357	1/1	0.78	0.22	63,63,63,63	0
59	MG	CA	1732	1/1	0.78	0.24	85,85,85,85	0
59	MG	BA	3126	1/1	0.78	0.45	61,61,61,61	0
59	MG	DA	3105	1/1	0.78	0.47	40,40,40,40	0
59	MG	DA	3136	1/1	0.78	0.49	46,46,46,46	0
59	MG	CI	201	1/1	0.78	0.29	86,86,86,86	0
59	MG	AA	1743	1/1	0.78	0.74	80,80,80,80	0
59	MG	DA	3160	1/1	0.78	0.18	73,73,73,73	0
59	MG	AW	101	1/1	0.78	0.81	154,154,154,154	0
59	MG	BA	3327	1/1	0.78	0.36	109,109,109,109	0
59	MG	DV	201	1/1	0.78	1.76	100,100,100,100	0
59	MG	BA	3171	1/1	0.79	0.26	76,76,76,76	0
59	MG	BA	3172	1/1	0.79	0.13	62,62,62,62	0
59	MG	DA	3086	1/1	0.79	0.47	50,50,50,50	0
59	MG	CV	103	1/1	0.79	0.30	80,80,80,80	0
59	MG	AA	1676	1/1	0.79	0.90	88,88,88,88	0
59	MG	BA	3216	1/1	0.79	0.20	88,88,88,88	0
59	MG	CA	1671	1/1	0.79	0.10	106,106,106,106	0
59	MG	AA	1604	1/1	0.79	0.27	64,64,64,64	0
59	MG	B1	101	1/1	0.79	0.34	52,52,52,52	0
59	MG	DA	3166	1/1	0.79	0.40	63,63,63,63	0
59	MG	CA	1605	1/1	0.79	0.24	69,69,69,69	0
59	MG	CA	1608	1/1	0.79	0.23	75,75,75,75	0
59	MG	CA	1775	1/1	0.79	0.39	76,76,76,76	0
59	MG	BA	3399	1/1	0.79	0.54	89,89,89,89	0
59	MG	DA	3002	1/1	0.79	0.35	58,58,58,58	0
59	MG	BA	3357	1/1	0.79	0.50	63,63,63,63	0
59	MG	CA	1794	1/1	0.79	0.39	66,66,66,66	0
59	MG	CA	1793	1/1	0.80	0.43	75,75,75,75	0
59	MG	CA	1689	1/1	0.80	0.40	66,66,66,66	0
59	MG	BA	3340	1/1	0.80	0.30	62,62,62,62	0
59	MG	CA	1664	1/1	0.80	0.48	75,75,75,75	0
59	MG	BA	3317	1/1	0.80	0.29	99,99,99,99	0
59	MG	BA	3385	1/1	0.80	0.71	84,84,84,84	0
59	MG	DA	3373	1/1	0.80	0.55	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3167	1/1	0.80	0.28	77,77,77,77	0
59	MG	AA	1754	1/1	0.80	0.20	77,77,77,77	0
59	MG	AA	1776	1/1	0.80	0.51	72,72,72,72	0
59	MG	DA	3387	1/1	0.80	1.10	102,102,102,102	0
59	MG	AA	1634	1/1	0.80	0.43	69,69,69,69	0
59	MG	BA	3286	1/1	0.80	0.42	69,69,69,69	0
59	MG	BA	3086	1/1	0.80	0.57	61,61,61,61	0
59	MG	DA	3332	1/1	0.80	0.24	68,68,68,68	0
59	MG	CA	1656	1/1	0.80	0.17	74,74,74,74	0
59	MG	DA	3256	1/1	0.80	0.67	59,59,59,59	0
59	MG	BA	3420	1/1	0.81	0.23	77,77,77,77	0
59	MG	CW	110	1/1	0.81	0.30	197,197,197,197	0
59	MG	AA	1745	1/1	0.81	0.46	77,77,77,77	0
59	MG	CA	1767	1/1	0.81	0.36	67,67,67,67	0
59	MG	BA	3233	1/1	0.81	0.17	69,69,69,69	0
59	MG	CA	1720	1/1	0.81	0.32	67,67,67,67	0
59	MG	BC	301	1/1	0.81	0.19	166,166,166,166	0
59	MG	CA	1673	1/1	0.81	0.13	92,92,92,92	0
59	MG	DA	3014	1/1	0.81	0.43	55,55,55,55	0
59	MG	CA	1729	1/1	0.81	0.23	77,77,77,77	0
59	MG	AA	1764	1/1	0.81	0.46	79,79,79,79	0
59	MG	BA	3256	1/1	0.81	0.67	79,79,79,79	0
59	MG	BA	3152	1/1	0.81	0.39	46,46,46,46	0
59	MG	AW	106	1/1	0.81	0.39	149,149,149,149	0
59	MG	BA	3182	1/1	0.81	0.13	69,69,69,69	0
59	MG	BX	102	1/1	0.81	0.20	47,47,47,47	0
59	MG	AA	1789	1/1	0.81	0.23	126,126,126,126	0
59	MG	AX	102	1/1	0.81	0.25	79,79,79,79	0
59	MG	DA	3190	1/1	0.81	0.66	61,61,61,61	0
59	MG	BA	3229	1/1	0.81	0.38	54,54,54,54	0
59	MG	BA	3413	1/1	0.81	0.62	59,59,59,59	0
59	MG	B1	102	1/1	0.82	0.38	67,67,67,67	0
59	MG	BA	3002	1/1	0.82	0.31	60,60,60,60	0
59	MG	AA	1757	1/1	0.82	0.58	60,60,60,60	0
59	MG	AA	1602	1/1	0.82	0.37	56,56,56,56	0
59	MG	BA	3439	1/1	0.82	0.28	69,69,69,69	0
59	MG	CA	1765	1/1	0.82	0.57	60,60,60,60	0
59	MG	CA	1623	1/1	0.82	0.19	66,66,66,66	0
59	MG	DA	3116	1/1	0.82	0.39	41,41,41,41	0
59	MG	BA	3227	1/1	0.82	0.36	78,78,78,78	0
59	MG	AA	1679	1/1	0.82	0.36	59,59,59,59	0
59	MG	BA	3113	1/1	0.82	0.32	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	1692	1/1	0.82	0.13	96,96,96,96	0
59	MG	DA	3333	1/1	0.82	0.16	57,57,57,57	0
59	MG	BA	3388	1/1	0.82	0.38	59,59,59,59	0
59	MG	AA	1654	1/1	0.82	0.61	79,79,79,79	0
59	MG	DA	3176	1/1	0.82	0.47	70,70,70,70	0
59	MG	BA	3022	1/1	0.82	0.49	61,61,61,61	0
59	MG	BB	215	1/1	0.82	0.36	76,76,76,76	0
59	MG	DA	3355	1/1	0.82	0.20	39,39,39,39	0
59	MG	CA	1647	1/1	0.82	0.44	67,67,67,67	0
59	MG	CA	1716	1/1	0.82	0.30	80,80,80,80	0
59	MG	BA	3133	1/1	0.82	0.78	94,94,94,94	0
59	MG	DA	3208	1/1	0.82	0.38	63,63,63,63	0
59	MG	AA	1752	1/1	0.82	0.34	64,64,64,64	0
59	MG	DA	3380	1/1	0.82	0.27	59,59,59,59	0
59	MG	BA	3143	1/1	0.82	0.29	58,58,58,58	0
59	MG	BA	3339	1/1	0.82	0.22	58,58,58,58	0
59	MG	AA	1647	1/1	0.82	0.67	95,95,95,95	0
59	MG	BF	303	1/1	0.82	0.22	42,42,42,42	0
59	MG	BA	3199	1/1	0.82	0.18	60,60,60,60	0
59	MG	BA	3203	1/1	0.82	0.50	58,58,58,58	0
59	MG	AA	1666	1/1	0.82	0.29	58,58,58,58	0
59	MG	BA	3352	1/1	0.82	0.40	66,66,66,66	0
59	MG	DA	3003	1/1	0.82	0.43	63,63,63,63	0
59	MG	CA	1741	1/1	0.83	0.46	57,57,57,57	0
59	MG	AA	1794	1/1	0.83	1.00	103,103,103,103	0
59	MG	AA	1656	1/1	0.83	0.35	102,102,102,102	0
59	MG	BA	3424	1/1	0.83	0.32	52,52,52,52	0
59	MG	CA	1644	1/1	0.83	0.27	75,75,75,75	0
59	MG	DA	3344	1/1	0.83	0.28	43,43,43,43	0
59	MG	BA	3263	1/1	0.83	0.48	60,60,60,60	0
59	MG	DA	3064	1/1	0.83	0.50	32,32,32,32	0
59	MG	CA	1753	1/1	0.83	0.31	82,82,82,82	0
59	MG	CA	1754	1/1	0.83	0.47	53,53,53,53	0
59	MG	DA	3111	1/1	0.83	0.38	28,28,28,28	0
59	MG	AA	1710	1/1	0.83	0.21	53,53,53,53	0
59	MG	DA	3124	1/1	0.83	0.44	61,61,61,61	0
59	MG	BA	3276	1/1	0.83	0.42	70,70,70,70	0
59	MG	DA	3274	1/1	0.83	0.24	45,45,45,45	0
59	MG	BA	3096	1/1	0.83	0.28	47,47,47,47	0
59	MG	AA	1761	1/1	0.83	0.48	52,52,52,52	0
59	MG	AA	1726	1/1	0.83	0.39	72,72,72,72	0
59	MG	BA	3219	1/1	0.83	0.08	181,181,181,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	1772	1/1	0.83	0.52	49,49,49,49	0
59	MG	BA	3255	1/1	0.83	0.58	85,85,85,85	0
59	MG	DA	3181	1/1	0.83	0.10	56,56,56,56	0
59	MG	D2	102	1/1	0.83	0.30	35,35,35,35	0
59	MG	DA	3001	1/1	0.83	0.70	71,71,71,71	0
59	MG	BA	3329	1/1	0.83	0.32	50,50,50,50	0
59	MG	CA	1614	1/1	0.84	0.16	65,65,65,65	0
59	MG	BA	3409	1/1	0.84	0.41	61,61,61,61	0
59	MG	BA	3231	1/1	0.84	0.40	55,55,55,55	0
59	MG	BA	3418	1/1	0.84	0.37	61,61,61,61	0
59	MG	BA	3232	1/1	0.84	0.41	74,74,74,74	0
59	MG	AA	1617	1/1	0.84	0.37	81,81,81,81	0
59	MG	AA	1672	1/1	0.84	0.31	58,58,58,58	0
59	MG	BA	3338	1/1	0.84	0.52	89,89,89,89	0
59	MG	BA	3019	1/1	0.84	0.27	68,68,68,68	0
59	MG	BA	3221	1/1	0.84	0.28	87,87,87,87	0
59	MG	CA	1681	1/1	0.84	0.65	69,69,69,69	0
59	MG	BA	3392	1/1	0.84	0.68	83,83,83,83	0
59	MG	AA	1705	1/1	0.84	0.17	83,83,83,83	0
59	MG	BU	205	1/1	0.84	0.42	57,57,57,57	0
59	MG	DA	3233	1/1	0.84	0.33	53,53,53,53	0
59	MG	BA	3116	1/1	0.84	0.49	69,69,69,69	0
59	MG	BA	3125	1/1	0.84	0.20	65,65,65,65	0
59	MG	DA	3366	1/1	0.84	0.58	67,67,67,67	0
59	MG	BA	3206	1/1	0.84	0.32	50,50,50,50	0
59	MG	DA	3140	1/1	0.84	0.52	43,43,43,43	0
59	MG	DA	3264	1/1	0.84	0.48	64,64,64,64	0
59	MG	DA	3271	1/1	0.84	0.15	61,61,61,61	0
59	MG	CA	1756	1/1	0.84	0.27	72,72,72,72	0
59	MG	BA	3280	1/1	0.84	0.13	107,107,107,107	0
59	MG	CA	1655	1/1	0.84	0.55	57,57,57,57	0
59	MG	DA	3304	1/1	0.84	0.20	70,70,70,70	0
59	MG	DA	3162	1/1	0.84	0.21	53,53,53,53	0
59	MG	DA	3311	1/1	0.84	0.32	70,70,70,70	0
59	MG	AA	1696	1/1	0.84	0.19	81,81,81,81	0
59	MG	CW	111	1/1	0.84	1.21	75,75,75,75	0
59	MG	DA	3317	1/1	0.84	0.31	52,52,52,52	0
59	MG	CA	1791	1/1	0.85	0.39	78,78,78,78	0
59	MG	BA	3015	1/1	0.85	0.36	37,37,37,37	0
59	MG	AA	1783	1/1	0.85	0.84	74,74,74,74	0
59	MG	AA	1788	1/1	0.85	0.45	94,94,94,94	0
59	MG	CA	1796	1/1	0.85	0.52	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3225	1/1	0.85	0.46	37,37,37,37	0
59	MG	CA	1682	1/1	0.85	0.22	67,67,67,67	0
59	MG	DA	3108	1/1	0.85	0.27	48,48,48,48	0
59	MG	BA	3156	1/1	0.85	0.25	78,78,78,78	0
59	MG	CA	1747	1/1	0.85	0.36	40,40,40,40	0
59	MG	AE	201	1/1	0.85	0.17	86,86,86,86	0
59	MG	BB	201	1/1	0.85	0.32	87,87,87,87	0
59	MG	BA	3412	1/1	0.85	0.27	64,64,64,64	0
59	MG	DA	3261	1/1	0.85	0.57	50,50,50,50	0
59	MG	AA	1721	1/1	0.85	0.19	63,63,63,63	0
59	MG	CA	1609	1/1	0.85	0.17	69,69,69,69	0
59	MG	BB	209	1/1	0.85	0.32	109,109,109,109	0
59	MG	AA	1601	1/1	0.85	0.70	73,73,73,73	0
59	MG	AA	1742	1/1	0.85	0.10	72,72,72,72	0
59	MG	CA	1707	1/1	0.85	0.38	53,53,53,53	0
59	MG	DA	3169	1/1	0.85	0.26	37,37,37,37	0
59	MG	BA	3332	1/1	0.85	0.40	75,75,75,75	0
59	MG	DA	3391	1/1	0.85	0.21	61,61,61,61	0
59	MG	BA	3079	1/1	0.85	0.41	65,65,65,65	0
59	MG	CA	1669	1/1	0.85	0.52	78,78,78,78	0
59	MG	BA	3013	1/1	0.85	0.42	62,62,62,62	0
59	MG	BA	3177	1/1	0.85	0.08	58,58,58,58	0
59	MG	DA	3195	1/1	0.85	0.36	52,52,52,52	0
59	MG	AA	1733	1/1	0.85	0.41	67,67,67,67	0
59	MG	BA	3071	1/1	0.86	0.53	51,51,51,51	0
59	MG	BA	3287	1/1	0.86	0.20	51,51,51,51	0
59	MG	DA	3301	1/1	0.86	0.26	136,136,136,136	0
59	MG	CA	1708	1/1	0.86	0.38	55,55,55,55	0
59	MG	DA	3141	1/1	0.86	0.23	40,40,40,40	0
59	MG	BA	3012	1/1	0.86	0.30	66,66,66,66	0
59	MG	DA	3145	1/1	0.86	0.28	64,64,64,64	0
59	MG	DA	3148	1/1	0.86	0.33	44,44,44,44	0
59	MG	AV	106	1/1	0.86	0.30	96,96,96,96	0
59	MG	AX	101	1/1	0.86	0.52	71,71,71,71	0
59	MG	AA	1797	1/1	0.86	0.28	73,73,73,73	0
59	MG	AA	1747	1/1	0.86	0.25	68,68,68,68	0
59	MG	CA	1661	1/1	0.86	0.36	56,56,56,56	0
59	MG	BA	3248	1/1	0.86	0.41	54,54,54,54	0
59	MG	DA	3328	1/1	0.86	0.14	155,155,155,155	0
59	MG	BA	3107	1/1	0.86	0.42	53,53,53,53	0
59	MG	CA	1667	1/1	0.86	0.47	62,62,62,62	0
59	MG	CA	1740	1/1	0.86	0.40	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3163	1/1	0.86	0.16	81,81,81,81	0
59	MG	AA	1694	1/1	0.86	0.26	77,77,77,77	0
59	MG	BA	3367	1/1	0.86	0.20	85,85,85,85	0
59	MG	BA	3371	1/1	0.86	0.47	68,68,68,68	0
59	MG	CA	1615	1/1	0.86	0.26	56,56,56,56	0
59	MG	BA	3381	1/1	0.86	0.30	53,53,53,53	0
59	MG	BA	3383	1/1	0.86	0.25	35,35,35,35	0
59	MG	AA	1648	1/1	0.86	0.12	81,81,81,81	0
59	MG	BA	3258	1/1	0.86	0.68	69,69,69,69	0
59	MG	DA	3363	1/1	0.86	0.30	48,48,48,48	0
59	MG	AW	116	1/1	0.86	0.86	76,76,76,76	0
59	MG	BA	3028	1/1	0.86	0.42	23,23,23,23	0
59	MG	DA	3372	1/1	0.86	0.21	68,68,68,68	0
59	MG	DA	3231	1/1	0.86	0.20	71,71,71,71	0
59	MG	CA	1638	1/1	0.86	0.23	75,75,75,75	0
59	MG	BA	3328	1/1	0.86	0.93	80,80,80,80	0
59	MG	DA	3234	1/1	0.86	0.64	72,72,72,72	0
59	MG	BA	3275	1/1	0.86	0.38	45,45,45,45	0
59	MG	AA	1603	1/1	0.86	0.09	65,65,65,65	0
59	MG	DA	3249	1/1	0.86	0.27	68,68,68,68	0
59	MG	BA	3278	1/1	0.86	0.38	86,86,86,86	0
59	MG	DA	3103	1/1	0.86	0.92	59,59,59,59	0
59	MG	CA	1699	1/1	0.86	0.15	66,66,66,66	0
59	MG	AW	109	1/1	0.86	0.26	154,154,154,154	0
59	MG	BA	3063	1/1	0.86	0.35	46,46,46,46	0
59	MG	CA	1705	1/1	0.86	0.48	46,46,46,46	0
59	MG	AW	111	1/1	0.87	0.93	139,139,139,139	0
59	MG	CA	1633	1/1	0.87	0.29	61,61,61,61	0
59	MG	CA	1672	1/1	0.87	0.14	94,94,94,94	0
59	MG	BA	3292	1/1	0.87	0.30	48,48,48,48	0
59	MG	AA	1644	1/1	0.87	0.46	50,50,50,50	0
59	MG	AA	1748	1/1	0.87	0.39	98,98,98,98	0
59	MG	AA	1774	1/1	0.87	0.35	61,61,61,61	0
59	MG	BA	3169	1/1	0.87	0.34	49,49,49,49	0
59	MG	AA	1658	1/1	0.87	0.32	63,63,63,63	0
59	MG	CU	101	1/1	0.87	0.17	84,84,84,84	0
59	MG	DA	3228	1/1	0.87	0.62	43,43,43,43	0
59	MG	BA	3435	1/1	0.87	0.19	73,73,73,73	0
59	MG	BA	3345	1/1	0.87	0.31	74,74,74,74	0
59	MG	BU	203	1/1	0.87	0.35	82,82,82,82	0
59	MG	BA	3112	1/1	0.87	0.72	42,42,42,42	0
59	MG	AA	1701	1/1	0.87	0.39	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3243	1/1	0.87	0.52	42,42,42,42	0
59	MG	BA	3441	1/1	0.87	0.50	50,50,50,50	0
59	MG	AA	1627	1/1	0.87	0.33	56,56,56,56	0
59	MG	DA	3147	1/1	0.87	0.27	31,31,31,31	0
59	MG	DA	3254	1/1	0.87	0.37	66,66,66,66	0
59	MG	DA	3255	1/1	0.87	0.28	55,55,55,55	0
59	MG	CA	1654	1/1	0.87	0.48	45,45,45,45	0
59	MG	BA	3454	1/1	0.87	0.27	61,61,61,61	0
59	MG	DA	3368	1/1	0.87	0.93	50,50,50,50	0
59	MG	BA	3217	1/1	0.87	0.42	72,72,72,72	0
59	MG	CA	1759	1/1	0.87	0.29	61,61,61,61	0
59	MG	DA	3269	1/1	0.87	0.29	32,32,32,32	0
59	MG	DA	3379	1/1	0.87	0.14	53,53,53,53	0
59	MG	AA	1615	1/1	0.87	0.63	32,32,32,32	0
59	MG	BA	3236	1/1	0.87	0.47	48,48,48,48	0
59	MG	DA	3275	1/1	0.87	0.30	53,53,53,53	0
59	MG	DA	3279	1/1	0.87	0.73	52,52,52,52	0
59	MG	DA	3167	1/1	0.87	0.30	76,76,76,76	0
59	MG	DA	3290	1/1	0.87	0.18	68,68,68,68	0
59	MG	BA	3284	1/1	0.87	0.32	62,62,62,62	0
59	MG	BA	3411	1/1	0.87	0.33	52,52,52,52	0
59	MG	BA	3242	1/1	0.87	0.38	49,49,49,49	0
59	MG	BA	3244	1/1	0.87	0.74	85,85,85,85	0
59	MG	DA	3186	1/1	0.87	1.18	43,43,43,43	0
59	MG	CA	1625	1/1	0.88	0.32	71,71,71,71	0
59	MG	AA	1649	1/1	0.88	0.20	54,54,54,54	0
59	MG	DA	3134	1/1	0.88	0.51	49,49,49,49	0
59	MG	DA	3135	1/1	0.88	0.23	56,56,56,56	0
59	MG	BA	3127	1/1	0.88	0.24	77,77,77,77	0
59	MG	DA	3139	1/1	0.88	0.49	57,57,57,57	0
59	MG	AA	1780	1/1	0.88	0.22	72,72,72,72	0
59	MG	BA	3259	1/1	0.88	0.25	55,55,55,55	0
59	MG	BA	3260	1/1	0.88	0.34	59,59,59,59	0
59	MG	CA	1776	1/1	0.88	0.26	53,53,53,53	0
59	MG	CA	1697	1/1	0.88	0.21	77,77,77,77	0
59	MG	AA	1730	1/1	0.88	0.35	59,59,59,59	0
59	MG	BB	204	1/1	0.88	0.35	98,98,98,98	0
59	MG	DA	3156	1/1	0.88	0.65	67,67,67,67	0
59	MG	DA	3314	1/1	0.88	0.12	64,64,64,64	0
59	MG	DA	3159	1/1	0.88	0.41	41,41,41,41	0
59	MG	BA	3266	1/1	0.88	0.35	64,64,64,64	0
59	MG	BA	3269	1/1	0.88	0.21	166,166,166,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3394	1/1	0.88	0.40	61,61,61,61	0
59	MG	BA	3396	1/1	0.88	0.39	63,63,63,63	0
59	MG	BB	214	1/1	0.88	0.27	84,84,84,84	0
59	MG	CA	1710	1/1	0.88	0.14	120,120,120,120	0
59	MG	CV	102	1/1	0.88	0.38	62,62,62,62	0
59	MG	AA	1762	1/1	0.88	0.29	100,100,100,100	0
59	MG	AA	1623	1/1	0.88	0.35	79,79,79,79	0
59	MG	CA	1717	1/1	0.88	0.35	48,48,48,48	0
59	MG	DA	3187	1/1	0.88	0.46	53,53,53,53	0
59	MG	BA	3330	1/1	0.88	0.10	104,104,104,104	0
59	MG	BA	3228	1/1	0.88	0.27	68,68,68,68	0
59	MG	AA	1735	1/1	0.88	0.44	56,56,56,56	0
59	MG	DA	3202	1/1	0.88	0.21	54,54,54,54	0
59	MG	CA	1728	1/1	0.88	0.18	73,73,73,73	0
59	MG	AW	102	1/1	0.88	0.50	79,79,79,79	0
59	MG	CA	1657	1/1	0.88	0.10	88,88,88,88	0
59	MG	BA	3282	1/1	0.88	0.27	76,76,76,76	0
59	MG	AA	1749	1/1	0.88	0.14	105,105,105,105	0
59	MG	CA	1736	1/1	0.88	0.41	63,63,63,63	0
59	MG	DA	3215	1/1	0.88	0.76	46,46,46,46	0
59	MG	CA	1739	1/1	0.88	0.23	131,131,131,131	0
59	MG	BA	3342	1/1	0.88	0.38	64,64,64,64	0
59	MG	DA	3229	1/1	0.88	0.25	52,52,52,52	0
59	MG	AA	1737	1/1	0.88	0.32	78,78,78,78	0
59	MG	BA	3416	1/1	0.88	0.24	50,50,50,50	0
59	MG	AW	120	1/1	0.88	0.30	104,104,104,104	0
59	MG	AA	1691	1/1	0.88	0.62	45,45,45,45	0
59	MG	BA	3207	1/1	0.88	0.24	46,46,46,46	0
59	MG	BA	3164	1/1	0.88	0.18	78,78,78,78	0
59	MG	BA	3300	1/1	0.88	0.45	62,62,62,62	0
59	MG	BA	3246	1/1	0.88	0.29	54,54,54,54	0
59	MG	AA	1635	1/1	0.88	0.45	53,53,53,53	0
59	MG	DB	203	1/1	0.88	0.17	59,59,59,59	0
59	MG	DA	3253	1/1	0.88	0.16	80,80,80,80	0
59	MG	BA	3362	1/1	0.88	0.63	83,83,83,83	0
59	MG	AA	1741	1/1	0.88	0.11	69,69,69,69	0
59	MG	BA	3304	1/1	0.88	0.20	71,71,71,71	0
59	MG	AA	1703	1/1	0.88	0.54	72,72,72,72	0
59	MG	DA	3293	1/1	0.89	0.30	16,16,16,16	0
59	MG	CA	1694	1/1	0.89	0.16	80,80,80,80	0
59	MG	BU	202	1/1	0.89	0.23	52,52,52,52	0
59	MG	AA	1636	1/1	0.89	0.42	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3017	1/1	0.89	0.25	43,43,43,43	0
59	MG	BA	3136	1/1	0.89	0.30	51,51,51,51	0
59	MG	DA	3188	1/1	0.89	0.44	30,30,30,30	0
59	MG	BA	3440	1/1	0.89	0.43	54,54,54,54	0
59	MG	BA	3214	1/1	0.89	0.39	59,59,59,59	0
59	MG	CA	1760	1/1	0.89	0.11	92,92,92,92	0
59	MG	DA	3197	1/1	0.89	0.47	49,49,49,49	0
59	MG	BA	3270	1/1	0.89	0.20	73,73,73,73	0
59	MG	BA	3234	1/1	0.89	0.51	83,83,83,83	0
59	MG	DA	3019	1/1	0.89	0.47	52,52,52,52	0
59	MG	DA	3325	1/1	0.89	0.23	56,56,56,56	0
59	MG	BA	3308	1/1	0.89	0.32	53,53,53,53	0
59	MG	DA	3074	1/1	0.89	0.22	40,40,40,40	0
59	MG	CA	1709	1/1	0.89	0.46	49,49,49,49	0
59	MG	DA	3100	1/1	0.89	0.36	29,29,29,29	0
59	MG	AA	1714	1/1	0.89	0.12	88,88,88,88	0
59	MG	BA	3315	1/1	0.89	0.32	64,64,64,64	0
59	MG	BA	3173	1/1	0.89	0.20	62,62,62,62	0
59	MG	BA	3001	1/1	0.89	0.63	56,56,56,56	0
59	MG	AA	1717	1/1	0.89	0.14	67,67,67,67	0
59	MG	DA	3349	1/1	0.89	0.99	39,39,39,39	1
59	MG	AA	1729	1/1	0.89	0.19	61,61,61,61	0
59	MG	DA	3132	1/1	0.89	0.39	44,44,44,44	0
59	MG	CA	1722	1/1	0.89	0.17	67,67,67,67	0
59	MG	CA	1723	1/1	0.89	0.09	132,132,132,132	0
59	MG	DA	3235	1/1	0.89	0.94	73,73,73,73	0
59	MG	BA	3253	1/1	0.89	0.27	97,97,97,97	0
59	MG	BB	213	1/1	0.89	0.32	50,50,50,50	0
59	MG	CA	1634	1/1	0.89	0.22	68,68,68,68	0
59	MG	CA	1730	1/1	0.89	0.18	93,93,93,93	0
59	MG	AA	1685	1/1	0.89	0.05	104,104,104,104	0
59	MG	BA	3008	1/1	0.89	0.36	49,49,49,49	0
59	MG	CA	1734	1/1	0.89	0.53	75,75,75,75	0
59	MG	AA	1781	1/1	0.89	0.26	70,70,70,70	0
59	MG	BA	3423	1/1	0.89	0.61	61,61,61,61	0
59	MG	DA	3154	1/1	0.89	0.12	54,54,54,54	0
59	MG	BA	3376	1/1	0.89	0.49	81,81,81,81	0
59	MG	BA	3380	1/1	0.89	0.20	60,60,60,60	0
59	MG	AV	107	1/1	0.89	0.26	63,63,63,63	0
59	MG	AA	1655	1/1	0.89	0.65	73,73,73,73	0
59	MG	BA	3299	1/1	0.89	0.20	63,63,63,63	0
59	MG	DB	204	1/1	0.89	0.29	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3278	1/1	0.89	0.66	52,52,52,52	0
59	MG	CA	1745	1/1	0.89	0.20	51,51,51,51	0
59	MG	CA	1691	1/1	0.89	0.14	65,65,65,65	0
59	MG	DA	3282	1/1	0.89	0.63	52,52,52,52	0
59	MG	AA	1787	1/1	0.89	0.08	84,84,84,84	0
59	MG	DA	3313	1/1	0.90	0.36	47,47,47,47	0
59	MG	CA	1610	1/1	0.90	0.26	76,76,76,76	0
59	MG	CA	1613	1/1	0.90	0.13	63,63,63,63	0
59	MG	BA	3226	1/1	0.90	0.20	57,57,57,57	0
59	MG	CA	1789	1/1	0.90	0.13	89,89,89,89	0
59	MG	BA	3160	1/1	0.90	0.18	57,57,57,57	0
59	MG	CA	1727	1/1	0.90	0.09	99,99,99,99	0
59	MG	CA	1618	1/1	0.90	0.28	65,65,65,65	0
59	MG	BA	3055	1/1	0.90	0.31	23,23,23,23	0
59	MG	BA	3122	1/1	0.90	0.22	27,27,27,27	0
59	MG	BB	203	1/1	0.90	0.33	99,99,99,99	0
59	MG	BA	3200	1/1	0.90	0.32	68,68,68,68	0
59	MG	CA	1626	1/1	0.90	0.37	94,94,94,94	0
59	MG	AA	1616	1/1	0.90	0.17	63,63,63,63	0
59	MG	BA	3166	1/1	0.90	0.11	105,105,105,105	0
59	MG	DA	3144	1/1	0.90	0.20	45,45,45,45	0
59	MG	CA	1737	1/1	0.90	0.41	82,82,82,82	0
59	MG	CA	1738	1/1	0.90	0.28	95,95,95,95	0
59	MG	BA	3311	1/1	0.90	0.35	63,63,63,63	0
59	MG	DA	3248	1/1	0.90	0.61	44,44,44,44	0
59	MG	AA	1690	1/1	0.90	0.30	69,69,69,69	0
59	MG	DA	3250	1/1	0.90	0.33	48,48,48,48	0
59	MG	BA	3210	1/1	0.90	0.17	56,56,56,56	0
59	MG	AA	1767	1/1	0.90	0.25	47,47,47,47	0
59	MG	BA	3417	1/1	0.90	0.38	43,43,43,43	0
59	MG	DA	3358	1/1	0.90	0.16	72,72,72,72	0
59	MG	BA	3237	1/1	0.90	0.42	37,37,37,37	0
59	MG	BA	3279	1/1	0.90	0.28	66,66,66,66	0
59	MG	BA	3421	1/1	0.90	0.55	50,50,50,50	0
59	MG	BA	3422	1/1	0.90	0.11	48,48,48,48	0
59	MG	AA	1746	1/1	0.90	0.10	87,87,87,87	0
59	MG	CA	1752	1/1	0.90	0.32	41,41,41,41	0
59	MG	BA	3369	1/1	0.90	0.36	60,60,60,60	0
59	MG	AA	1758	1/1	0.90	0.54	42,42,42,42	0
59	MG	BA	3326	1/1	0.90	0.31	130,130,130,130	0
59	MG	DA	3381	1/1	0.90	0.21	57,57,57,57	0
59	MG	BA	3245	1/1	0.90	0.41	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	AA	1699	1/1	0.90	0.05	105,105,105,105	0
59	MG	AA	1633	1/1	0.90	0.23	64,64,64,64	0
59	MG	DA	3286	1/1	0.90	0.28	35,35,35,35	0
59	MG	DB	201	1/1	0.90	0.12	65,65,65,65	0
59	MG	AA	1798	1/1	0.90	0.37	75,75,75,75	0
59	MG	DA	3192	1/1	0.90	0.22	53,53,53,53	0
59	MG	DA	3296	1/1	0.90	0.29	46,46,46,46	0
59	MG	AA	1618	1/1	0.90	0.20	65,65,65,65	0
59	MG	AA	1750	1/1	0.90	0.31	68,68,68,68	0
59	MG	BA	3295	1/1	0.90	0.34	51,51,51,51	0
59	MG	DO	201	1/1	0.90	0.27	64,64,64,64	0
59	MG	AW	103	1/1	0.90	0.75	105,105,105,105	0
59	MG	AA	1711	1/1	0.90	0.09	60,60,60,60	0
59	MG	BA	3057	1/1	0.91	0.59	52,52,52,52	0
59	MG	CA	1611	1/1	0.91	0.31	71,71,71,71	0
59	MG	BA	3134	1/1	0.91	0.30	30,30,30,30	0
59	MG	AV	104	1/1	0.91	0.73	102,102,102,102	0
59	MG	AV	105	1/1	0.91	0.58	62,62,62,62	0
59	MG	AA	1625	1/1	0.91	0.14	66,66,66,66	0
59	MG	AA	1613	1/1	0.91	0.17	89,89,89,89	0
59	MG	BA	3208	1/1	0.91	0.15	36,36,36,36	0
59	MG	CA	1744	1/1	0.91	0.33	94,94,94,94	0
59	MG	CA	1685	1/1	0.91	0.18	56,56,56,56	0
59	MG	BA	3147	1/1	0.91	0.26	58,58,58,58	0
59	MG	BA	3316	1/1	0.91	0.80	59,59,59,59	0
59	MG	BA	3151	1/1	0.91	0.40	78,78,78,78	0
59	MG	BA	3384	1/1	0.91	0.83	63,63,63,63	0
59	MG	BA	3320	1/1	0.91	0.35	173,173,173,173	0
59	MG	BA	3386	1/1	0.91	0.26	83,83,83,83	0
59	MG	AA	1779	1/1	0.91	0.58	58,58,58,58	0
59	MG	BA	3082	1/1	0.91	0.34	42,42,42,42	0
59	MG	AA	1736	1/1	0.91	0.44	56,56,56,56	0
59	MG	BA	3089	1/1	0.91	0.26	42,42,42,42	0
59	MG	BA	3090	1/1	0.91	0.27	73,73,73,73	0
59	MG	AA	1766	1/1	0.91	0.10	54,54,54,54	0
59	MG	AA	1809	1/1	0.91	0.66	57,57,57,57	0
59	MG	BA	3098	1/1	0.91	0.41	55,55,55,55	0
59	MG	AA	1629	1/1	0.91	0.27	61,61,61,61	0
59	MG	AA	1631	1/1	0.91	0.31	62,62,62,62	0
59	MG	CA	1770	1/1	0.91	0.32	80,80,80,80	0
59	MG	BA	3109	1/1	0.91	0.32	32,32,32,32	0
59	MG	CA	1713	1/1	0.91	0.12	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3170	1/1	0.91	0.35	66,66,66,66	0
59	MG	CA	1777	1/1	0.91	0.22	60,60,60,60	0
59	MG	DA	3360	1/1	0.91	0.14	55,55,55,55	0
59	MG	AA	1640	1/1	0.91	0.36	42,42,42,42	0
59	MG	B0	101	1/1	0.91	0.27	44,44,44,44	0
59	MG	CA	1718	1/1	0.91	0.35	81,81,81,81	0
59	MG	AA	1642	1/1	0.91	0.24	57,57,57,57	0
59	MG	BA	3415	1/1	0.91	0.53	71,71,71,71	0
59	MG	AA	1790	1/1	0.91	0.17	120,120,120,120	0
59	MG	BA	3178	1/1	0.91	0.12	53,53,53,53	0
59	MG	B5	101	1/1	0.91	0.27	30,30,30,30	0
59	MG	CF	201	1/1	0.91	0.35	69,69,69,69	0
59	MG	DA	3153	1/1	0.91	0.25	49,49,49,49	0
59	MG	DA	3268	1/1	0.91	0.33	53,53,53,53	0
59	MG	CA	1662	1/1	0.91	0.16	60,60,60,60	0
59	MG	DA	3385	1/1	0.91	0.11	226,226,226,226	0
59	MG	DA	3386	1/1	0.91	0.76	181,181,181,181	0
59	MG	BA	3036	1/1	0.91	0.32	56,56,56,56	0
59	MG	DA	3390	1/1	0.91	0.43	49,49,49,49	0
59	MG	DA	3157	1/1	0.91	0.26	42,42,42,42	0
59	MG	BA	3298	1/1	0.91	0.23	65,65,65,65	0
59	MG	BA	3184	1/1	0.91	0.36	59,59,59,59	0
59	MG	CV	104	1/1	0.91	0.25	55,55,55,55	0
59	MG	B8	101	1/1	0.91	0.38	79,79,79,79	0
59	MG	DA	3164	1/1	0.91	0.17	57,57,57,57	0
59	MG	BA	3131	1/1	0.91	0.36	55,55,55,55	0
59	MG	AA	1731	1/1	0.91	0.35	56,56,56,56	0
59	MG	BA	3363	1/1	0.91	0.34	43,43,43,43	0
59	MG	DA	3172	1/1	0.91	0.26	48,48,48,48	0
59	MG	DA	3297	1/1	0.91	0.41	50,50,50,50	0
59	MG	BA	3188	1/1	0.92	0.33	66,66,66,66	0
59	MG	BA	3058	1/1	0.92	0.15	47,47,47,47	0
59	MG	BA	3358	1/1	0.92	0.11	73,73,73,73	0
59	MG	AA	1791	1/1	0.92	0.24	91,91,91,91	0
59	MG	DA	3114	1/1	0.92	0.07	32,32,32,32	0
59	MG	BA	3161	1/1	0.92	0.44	35,35,35,35	0
59	MG	DA	3319	1/1	0.92	0.53	81,81,81,81	0
59	MG	BA	3062	1/1	0.92	0.34	30,30,30,30	0
59	MG	DA	3216	1/1	0.92	0.41	26,26,26,26	0
59	MG	DA	3220	1/1	0.92	0.30	47,47,47,47	0
59	MG	AA	1792	1/1	0.92	0.10	99,99,99,99	0
59	MG	DA	3227	1/1	0.92	0.25	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CG	201	1/1	0.92	0.42	72,72,72,72	0
59	MG	DA	3330	1/1	0.92	0.34	55,55,55,55	0
59	MG	BA	3067	1/1	0.92	0.58	36,36,36,36	0
59	MG	BA	3165	1/1	0.92	0.33	44,44,44,44	0
59	MG	AA	1626	1/1	0.92	0.29	60,60,60,60	0
59	MG	DA	3336	1/1	0.92	0.56	62,62,62,62	0
59	MG	BA	3209	1/1	0.92	0.20	45,45,45,45	0
59	MG	BA	3372	1/1	0.92	0.32	70,70,70,70	0
59	MG	CA	1696	1/1	0.92	0.39	44,44,44,44	0
59	MG	AA	1673	1/1	0.92	0.13	55,55,55,55	0
59	MG	AA	1695	1/1	0.92	0.26	51,51,51,51	0
59	MG	B2	101	1/1	0.92	0.49	49,49,49,49	0
59	MG	CW	105	1/1	0.92	0.43	107,107,107,107	0
59	MG	DA	3247	1/1	0.92	0.27	41,41,41,41	0
59	MG	DA	3150	1/1	0.92	0.16	54,54,54,54	0
59	MG	BA	3021	1/1	0.92	0.24	61,61,61,61	0
59	MG	CA	1653	1/1	0.92	0.41	38,38,38,38	0
59	MG	AA	1663	1/1	0.92	0.45	61,61,61,61	0
59	MG	BA	3436	1/1	0.92	0.18	65,65,65,65	0
59	MG	BA	3297	1/1	0.92	0.08	66,66,66,66	0
59	MG	AA	1802	1/1	0.92	0.28	85,85,85,85	0
59	MG	AA	1723	1/1	0.92	0.18	64,64,64,64	0
59	MG	DA	3370	1/1	0.92	0.43	37,37,37,37	0
59	MG	AA	1785	1/1	0.92	0.41	52,52,52,52	0
59	MG	AA	1657	1/1	0.92	0.21	92,92,92,92	0
59	MG	DA	3267	1/1	0.92	0.42	53,53,53,53	0
59	MG	CA	1663	1/1	0.92	0.36	71,71,71,71	0
59	MG	AA	1668	1/1	0.92	0.11	47,47,47,47	0
59	MG	BA	3444	1/1	0.92	0.47	58,58,58,58	0
59	MG	AA	1688	1/1	0.92	0.37	50,50,50,50	0
59	MG	BA	3261	1/1	0.92	0.29	59,59,59,59	0
59	MG	DA	3276	1/1	0.92	0.33	38,38,38,38	0
59	MG	BA	3346	1/1	0.92	0.51	128,128,128,128	0
59	MG	DA	3180	1/1	0.92	0.14	26,26,26,26	0
59	MG	AA	1628	1/1	0.92	0.24	52,52,52,52	0
59	MG	DA	3018	1/1	0.92	0.30	73,73,73,73	0
59	MG	BA	3153	1/1	0.92	0.23	42,42,42,42	0
59	MG	DA	3040	1/1	0.92	0.24	22,22,22,22	0
59	MG	DA	3049	1/1	0.92	0.52	38,38,38,38	0
59	MG	DA	3050	1/1	0.92	0.26	44,44,44,44	0
59	MG	BA	3307	1/1	0.92	0.47	39,39,39,39	0
59	MG	CA	1624	1/1	0.92	0.30	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3076	1/1	0.92	0.17	29,29,29,29	0
59	MG	BA	3111	1/1	0.92	0.21	52,52,52,52	0
59	MG	DA	3201	1/1	0.92	0.11	45,45,45,45	0
59	MG	BA	3354	1/1	0.92	0.35	38,38,38,38	0
59	MG	AA	1641	1/1	0.93	0.17	78,78,78,78	0
59	MG	BA	3174	1/1	0.93	0.23	48,48,48,48	0
59	MG	AA	1784	1/1	0.93	0.41	70,70,70,70	0
59	MG	DA	3221	1/1	0.93	0.24	51,51,51,51	0
59	MG	DA	3222	1/1	0.93	0.62	38,38,38,38	0
59	MG	BA	3144	1/1	0.93	0.37	54,54,54,54	0
59	MG	BA	3099	1/1	0.93	0.23	40,40,40,40	0
59	MG	BA	3390	1/1	0.93	0.37	30,30,30,30	0
59	MG	AA	1607	1/1	0.93	0.19	53,53,53,53	0
59	MG	BA	3009	1/1	0.93	0.14	48,48,48,48	0
59	MG	BA	3349	1/1	0.93	0.41	73,73,73,73	0
59	MG	DA	3327	1/1	0.93	0.48	89,89,89,89	0
59	MG	BA	3185	1/1	0.93	0.17	63,63,63,63	0
59	MG	CA	1659	1/1	0.93	0.43	50,50,50,50	0
59	MG	BA	3010	1/1	0.93	0.26	48,48,48,48	0
59	MG	DA	3151	1/1	0.93	0.31	40,40,40,40	0
59	MG	BA	3449	1/1	0.93	0.58	46,46,46,46	0
59	MG	CA	1712	1/1	0.93	0.13	86,86,86,86	0
59	MG	AA	1768	1/1	0.93	0.21	63,63,63,63	0
59	MG	BA	3312	1/1	0.93	0.21	65,65,65,65	0
59	MG	DA	3343	1/1	0.93	0.40	26,26,26,26	0
59	MG	AA	1716	1/1	0.93	0.09	99,99,99,99	0
59	MG	AA	1620	1/1	0.93	0.42	38,38,38,38	0
59	MG	AA	1698	1/1	0.93	0.14	54,54,54,54	0
59	MG	DA	3252	1/1	0.93	0.23	68,68,68,68	0
59	MG	AA	1732	1/1	0.93	0.61	56,56,56,56	0
59	MG	CA	1621	1/1	0.93	0.19	67,67,67,67	0
59	MG	BB	205	1/1	0.93	0.14	65,65,65,65	0
59	MG	CA	1774	1/1	0.93	0.62	49,49,49,49	0
59	MG	BA	3076	1/1	0.93	0.23	65,65,65,65	0
59	MG	DA	3259	1/1	0.93	0.47	34,34,34,34	0
59	MG	DA	3260	1/1	0.93	0.41	43,43,43,43	0
59	MG	DA	3168	1/1	0.93	0.52	60,60,60,60	0
59	MG	BA	3321	1/1	0.93	0.08	175,175,175,175	0
59	MG	AA	1719	1/1	0.93	0.31	112,112,112,112	0
59	MG	BA	3204	1/1	0.93	0.40	40,40,40,40	0
59	MG	CA	1784	1/1	0.93	0.09	66,66,66,66	0
59	MG	DA	3051	1/1	0.93	0.25	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3272	1/1	0.93	0.24	57,57,57,57	0
59	MG	DA	3375	1/1	0.93	0.20	84,84,84,84	0
59	MG	AA	1630	1/1	0.93	0.12	67,67,67,67	0
59	MG	DA	3065	1/1	0.93	0.32	23,23,23,23	0
59	MG	DA	3070	1/1	0.93	0.42	41,41,41,41	0
59	MG	BA	3129	1/1	0.93	0.66	61,61,61,61	0
59	MG	CA	1680	1/1	0.93	0.09	84,84,84,84	0
59	MG	DA	3084	1/1	0.93	0.39	41,41,41,41	0
59	MG	AA	1722	1/1	0.93	0.14	75,75,75,75	0
59	MG	AA	1653	1/1	0.93	0.30	45,45,45,45	0
59	MG	DA	3289	1/1	0.93	0.33	50,50,50,50	0
59	MG	CA	1795	1/1	0.93	0.18	62,62,62,62	0
59	MG	B8	102	1/1	0.93	0.27	58,58,58,58	0
59	MG	CA	1639	1/1	0.93	0.36	48,48,48,48	0
59	MG	AA	1646	1/1	0.93	0.44	67,67,67,67	0
59	MG	AA	1782	1/1	0.93	0.16	116,116,116,116	0
59	MG	BA	3139	1/1	0.93	0.41	37,37,37,37	0
59	MG	DA	3121	1/1	0.93	0.23	41,41,41,41	0
59	MG	DA	3306	1/1	0.93	0.13	39,39,39,39	0
59	MG	DB	212	1/1	0.93	0.20	99,99,99,99	0
59	MG	DF	301	1/1	0.93	0.44	66,66,66,66	0
59	MG	DN	201	1/1	0.93	0.33	98,98,98,98	0
59	MG	BA	3140	1/1	0.93	0.26	36,36,36,36	0
59	MG	BA	3432	1/1	0.93	0.22	48,48,48,48	0
59	MG	DA	3214	1/1	0.93	0.60	31,31,31,31	0
59	MG	DA	3251	1/1	0.94	0.18	53,53,53,53	0
59	MG	DA	3081	1/1	0.94	0.58	39,39,39,39	0
59	MG	BA	3430	1/1	0.94	0.13	69,69,69,69	0
59	MG	AA	1806	1/1	0.94	0.46	30,30,30,30	0
59	MG	DA	3091	1/1	0.94	0.38	37,37,37,37	0
59	MG	DA	3094	1/1	0.94	0.34	38,38,38,38	0
59	MG	CA	1679	1/1	0.94	0.18	63,63,63,63	0
59	MG	CA	1755	1/1	0.94	0.38	47,47,47,47	0
59	MG	DA	3104	1/1	0.94	0.22	23,23,23,23	0
59	MG	BA	3041	1/1	0.94	0.62	46,46,46,46	0
59	MG	DA	3263	1/1	0.94	0.57	38,38,38,38	0
59	MG	DA	3106	1/1	0.94	0.16	32,32,32,32	0
59	MG	BA	3264	1/1	0.94	0.46	55,55,55,55	0
59	MG	BA	3368	1/1	0.94	0.15	57,57,57,57	0
59	MG	DA	3113	1/1	0.94	0.19	23,23,23,23	0
59	MG	CA	1612	1/1	0.94	0.62	37,37,37,37	0
59	MG	BA	3118	1/1	0.94	0.46	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3267	1/1	0.94	0.34	51,51,51,51	0
59	MG	CA	1687	1/1	0.94	0.32	56,56,56,56	0
59	MG	DA	3130	1/1	0.94	0.21	41,41,41,41	0
59	MG	CA	1688	1/1	0.94	0.28	81,81,81,81	0
59	MG	BA	3155	1/1	0.94	0.15	61,61,61,61	0
59	MG	BA	3042	1/1	0.94	0.49	52,52,52,52	0
59	MG	BA	3084	1/1	0.94	0.19	58,58,58,58	0
59	MG	DA	3285	1/1	0.94	0.29	44,44,44,44	0
59	MG	BA	3043	1/1	0.94	0.23	52,52,52,52	0
59	MG	BA	3087	1/1	0.94	0.16	53,53,53,53	0
59	MG	CA	1622	1/1	0.94	0.28	50,50,50,50	0
59	MG	BA	3197	1/1	0.94	1.09	68,68,68,68	0
59	MG	CA	1778	1/1	0.94	0.38	77,77,77,77	0
59	MG	BA	3004	1/1	0.94	0.53	48,48,48,48	0
59	MG	DA	3298	1/1	0.94	0.20	50,50,50,50	0
59	MG	BA	3446	1/1	0.94	0.45	53,53,53,53	0
59	MG	CA	1785	1/1	0.94	0.30	46,46,46,46	0
59	MG	DA	3303	1/1	0.94	0.13	48,48,48,48	0
59	MG	DA	3149	1/1	0.94	0.47	40,40,40,40	0
59	MG	BA	3447	1/1	0.94	0.21	35,35,35,35	0
59	MG	CA	1701	1/1	0.94	0.36	53,53,53,53	0
59	MG	CA	1702	1/1	0.94	0.14	75,75,75,75	0
59	MG	BA	3448	1/1	0.94	0.55	44,44,44,44	0
59	MG	CA	1704	1/1	0.94	0.23	66,66,66,66	0
59	MG	CA	1629	1/1	0.94	0.32	45,45,45,45	0
59	MG	BA	3005	1/1	0.94	0.27	53,53,53,53	0
59	MG	DA	3158	1/1	0.94	0.30	51,51,51,51	0
59	MG	BA	3450	1/1	0.94	0.11	57,57,57,57	0
59	MG	BA	3451	1/1	0.94	0.34	45,45,45,45	0
59	MG	BA	3453	1/1	0.94	2.01	172,172,172,172	0
59	MG	BA	3281	1/1	0.94	0.47	68,68,68,68	0
59	MG	BA	3092	1/1	0.94	0.28	57,57,57,57	0
59	MG	BA	3202	1/1	0.94	0.52	65,65,65,65	0
59	MG	CA	1641	1/1	0.94	0.36	71,71,71,71	0
59	MG	BA	3016	1/1	0.94	0.65	27,27,27,27	0
59	MG	BA	3393	1/1	0.94	0.43	34,34,34,34	0
59	MG	BA	3006	1/1	0.94	0.47	49,49,49,49	0
59	MG	BA	3241	1/1	0.94	0.64	41,41,41,41	0
59	MG	BA	3289	1/1	0.94	0.28	49,49,49,49	0
59	MG	BA	3290	1/1	0.94	0.69	47,47,47,47	0
59	MG	DA	3335	1/1	0.94	0.42	51,51,51,51	0
59	MG	BA	3135	1/1	0.94	0.18	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3184	1/1	0.94	0.07	49,49,49,49	0
59	MG	DA	3338	1/1	0.94	0.58	37,37,37,37	0
59	MG	DA	3185	1/1	0.94	0.32	31,31,31,31	0
59	MG	BB	210	1/1	0.94	0.29	93,93,93,93	0
59	MG	CA	1726	1/1	0.94	0.30	64,64,64,64	0
59	MG	AA	1755	1/1	0.94	0.40	70,70,70,70	0
59	MG	DA	3189	1/1	0.94	0.34	47,47,47,47	0
59	MG	BA	3138	1/1	0.94	0.15	34,34,34,34	0
59	MG	BA	3296	1/1	0.94	0.44	59,59,59,59	0
59	MG	AA	1704	1/1	0.94	0.65	61,61,61,61	0
59	MG	CW	113	1/1	0.94	0.21	123,123,123,123	0
59	MG	D2	101	1/1	0.94	0.13	59,59,59,59	0
59	MG	CA	1731	1/1	0.94	0.37	51,51,51,51	0
59	MG	BA	3348	1/1	0.94	0.30	63,63,63,63	0
59	MG	BA	3100	1/1	0.94	0.29	32,32,32,32	0
59	MG	DA	3364	1/1	0.94	0.23	46,46,46,46	0
59	MG	DA	3365	1/1	0.94	0.14	38,38,38,38	0
59	MG	BA	3249	1/1	0.94	0.27	49,49,49,49	0
59	MG	DA	3207	1/1	0.94	0.73	83,83,83,83	0
59	MG	BA	3414	1/1	0.94	0.28	48,48,48,48	0
59	MG	BA	3250	1/1	0.94	0.49	30,30,30,30	0
59	MG	BA	3212	1/1	0.94	0.28	64,64,64,64	0
59	MG	AA	1810	1/1	0.94	0.14	88,88,88,88	0
59	MG	DA	3010	1/1	0.94	0.19	40,40,40,40	0
59	MG	DA	3011	1/1	0.94	0.40	27,27,27,27	0
59	MG	DA	3378	1/1	0.94	0.13	35,35,35,35	0
59	MG	BA	3065	1/1	0.94	0.30	35,35,35,35	0
59	MG	AW	108	1/1	0.94	0.15	154,154,154,154	0
59	MG	AC	301	1/1	0.94	0.32	66,66,66,66	0
59	MG	DA	3020	1/1	0.94	0.41	29,29,29,29	0
59	MG	DA	3026	1/1	0.94	0.42	28,28,28,28	0
59	MG	DA	3038	1/1	0.94	0.17	41,41,41,41	0
59	MG	DA	3039	1/1	0.94	0.43	27,27,27,27	0
59	MG	BU	204	1/1	0.94	0.15	64,64,64,64	0
59	MG	AA	1662	1/1	0.94	0.76	43,43,43,43	0
59	MG	BA	3179	1/1	0.94	0.16	66,66,66,66	0
59	MG	BA	3220	1/1	0.94	0.16	59,59,59,59	0
59	MG	DA	3060	1/1	0.94	0.65	24,24,24,24	0
59	MG	DA	3062	1/1	0.94	0.57	26,26,26,26	0
59	MG	CA	1601	1/1	0.94	0.44	53,53,53,53	0
59	MG	DA	3241	1/1	0.94	0.38	33,33,33,33	0
59	MG	CA	1748	1/1	0.94	0.39	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DB	208	1/1	0.94	0.30	55,55,55,55	0
59	MG	DA	3067	1/1	0.94	0.37	26,26,26,26	0
59	MG	DA	3245	1/1	0.94	0.27	47,47,47,47	0
59	MG	DA	3069	1/1	0.94	0.19	48,48,48,48	0
59	MG	BA	3310	1/1	0.94	0.45	44,44,44,44	0
59	MG	CA	1603	1/1	0.94	0.66	55,55,55,55	0
59	MG	DA	3075	1/1	0.94	0.18	29,29,29,29	0
59	MG	CA	1676	1/1	0.94	0.39	49,49,49,49	0
59	MG	DA	3073	1/1	0.95	0.29	38,38,38,38	0
59	MG	CA	1788	1/1	0.95	0.19	124,124,124,124	0
59	MG	BA	3314	1/1	0.95	0.71	66,66,66,66	0
59	MG	BA	3273	1/1	0.95	0.30	42,42,42,42	0
59	MG	DA	3080	1/1	0.95	0.25	51,51,51,51	0
59	MG	BA	3191	1/1	0.95	0.32	51,51,51,51	0
59	MG	BA	3110	1/1	0.95	0.47	35,35,35,35	0
59	MG	DA	3204	1/1	0.95	0.35	26,26,26,26	0
59	MG	DA	3085	1/1	0.95	0.31	42,42,42,42	0
59	MG	CA	1724	1/1	0.95	0.22	120,120,120,120	0
59	MG	BA	3319	1/1	0.95	0.23	133,133,133,133	0
59	MG	DA	3209	1/1	0.95	0.14	80,80,80,80	0
59	MG	BA	3277	1/1	0.95	0.27	56,56,56,56	0
59	MG	AA	1715	1/1	0.95	0.28	52,52,52,52	0
59	MG	AA	1667	1/1	0.95	0.36	64,64,64,64	0
59	MG	CA	1670	1/1	0.95	0.29	68,68,68,68	0
59	MG	AA	1744	1/1	0.95	0.23	70,70,70,70	0
59	MG	BA	3382	1/1	0.95	0.29	43,43,43,43	0
59	MG	AA	1680	1/1	0.95	0.19	51,51,51,51	0
59	MG	AA	1689	1/1	0.95	0.26	53,53,53,53	0
59	MG	AA	1708	1/1	0.95	0.34	61,61,61,61	0
59	MG	AA	1709	1/1	0.95	0.16	59,59,59,59	0
59	MG	DA	3226	1/1	0.95	0.25	51,51,51,51	0
59	MG	CA	1616	1/1	0.95	0.52	32,32,32,32	0
59	MG	DA	3117	1/1	0.95	0.22	57,57,57,57	0
59	MG	BA	3205	1/1	0.95	0.24	48,48,48,48	0
59	MG	BA	3081	1/1	0.95	0.38	37,37,37,37	0
59	MG	DA	3127	1/1	0.95	0.29	31,31,31,31	0
59	MG	AV	101	1/1	0.95	0.36	61,61,61,61	0
59	MG	DA	3339	1/1	0.95	0.45	47,47,47,47	0
59	MG	BA	3083	1/1	0.95	0.28	28,28,28,28	0
59	MG	BA	3291	1/1	0.95	0.46	63,63,63,63	0
59	MG	BA	3333	1/1	0.95	0.39	51,51,51,51	0
59	MG	DA	3347	1/1	0.95	0.14	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3238	1/1	0.95	0.48	26,26,26,26	0
59	MG	AA	1796	1/1	0.95	0.24	47,47,47,47	0
59	MG	DA	3137	1/1	0.95	0.72	25,25,25,25	0
59	MG	BA	3029	1/1	0.95	0.36	50,50,50,50	0
59	MG	BA	3294	1/1	0.95	0.35	35,35,35,35	0
59	MG	CA	1746	1/1	0.95	0.12	79,79,79,79	0
59	MG	DA	3142	1/1	0.95	0.36	30,30,30,30	0
59	MG	BA	3341	1/1	0.95	0.23	57,57,57,57	0
59	MG	CX	102	1/1	0.95	0.36	49,49,49,49	0
59	MG	DA	3362	1/1	0.95	0.30	56,56,56,56	0
59	MG	BA	3251	1/1	0.95	0.36	46,46,46,46	0
59	MG	BA	3343	1/1	0.95	0.27	70,70,70,70	0
59	MG	BA	3030	1/1	0.95	0.27	52,52,52,52	0
59	MG	BA	3034	1/1	0.95	0.34	27,27,27,27	0
59	MG	BA	3410	1/1	0.95	0.14	206,206,206,206	0
59	MG	AA	1637	1/1	0.95	0.25	71,71,71,71	0
59	MG	BA	3347	1/1	0.95	0.26	47,47,47,47	0
59	MG	DA	3371	1/1	0.95	0.54	46,46,46,46	0
59	MG	DA	3006	1/1	0.95	0.63	63,63,63,63	0
59	MG	AA	1652	1/1	0.95	0.21	92,92,92,92	0
59	MG	AA	1799	1/1	0.95	0.37	41,41,41,41	0
59	MG	BA	3095	1/1	0.95	0.59	30,30,30,30	0
59	MG	AA	1800	1/1	0.95	0.19	74,74,74,74	0
59	MG	AA	1751	1/1	0.95	0.57	52,52,52,52	0
59	MG	DA	3265	1/1	0.95	0.30	38,38,38,38	0
59	MG	DA	3015	1/1	0.95	0.22	29,29,29,29	0
59	MG	CA	1645	1/1	0.95	0.39	50,50,50,50	0
59	MG	AA	1692	1/1	0.95	0.43	48,48,48,48	0
59	MG	BA	3262	1/1	0.95	0.43	31,31,31,31	0
59	MG	BF	301	1/1	0.95	0.18	45,45,45,45	0
59	MG	AA	1684	1/1	0.95	0.42	44,44,44,44	0
59	MG	DA	3388	1/1	0.95	0.21	46,46,46,46	0
59	MG	BA	3105	1/1	0.95	0.24	43,43,43,43	0
59	MG	CA	1771	1/1	0.95	0.13	62,62,62,62	0
59	MG	DA	3392	1/1	0.95	0.29	28,28,28,28	0
59	MG	BA	3146	1/1	0.95	0.35	43,43,43,43	0
59	MG	CA	1773	1/1	0.95	0.51	44,44,44,44	0
59	MG	AA	1678	1/1	0.95	0.29	82,82,82,82	0
59	MG	BU	201	1/1	0.95	0.23	74,74,74,74	0
59	MG	DA	3284	1/1	0.95	0.14	35,35,35,35	0
59	MG	BA	3149	1/1	0.95	0.50	38,38,38,38	0
59	MG	BA	3429	1/1	0.95	0.45	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3288	1/1	0.95	0.28	22,22,22,22	0
59	MG	CA	1715	1/1	0.95	0.09	104,104,104,104	0
59	MG	AA	1807	1/1	0.95	0.30	66,66,66,66	0
59	MG	DF	302	1/1	0.95	0.20	42,42,42,42	0
59	MG	DA	3068	1/1	0.95	0.35	16,16,16,16	0
59	MG	AA	1786	1/1	0.95	0.28	56,56,56,56	0
59	MG	BV	201	1/1	0.95	0.29	33,33,33,33	0
59	MG	DA	3071	1/1	0.95	0.24	53,53,53,53	0
60	EDS	AA	1805	41/41	0.95	0.20	47,55,60,66	0
59	MG	DA	3300	1/1	0.96	0.35	33,33,33,33	0
59	MG	DA	3093	1/1	0.96	0.12	22,22,22,22	0
59	MG	DA	3199	1/1	0.96	0.21	52,52,52,52	0
59	MG	DA	3200	1/1	0.96	0.38	45,45,45,45	0
59	MG	DA	3305	1/1	0.96	0.07	62,62,62,62	0
59	MG	BA	3334	1/1	0.96	0.24	54,54,54,54	0
59	MG	CA	1711	1/1	0.96	0.64	72,72,72,72	0
59	MG	DA	3308	1/1	0.96	0.26	47,47,47,47	0
59	MG	DA	3102	1/1	0.96	0.34	27,27,27,27	0
59	MG	CA	1666	1/1	0.96	0.35	60,60,60,60	0
59	MG	BA	3379	1/1	0.96	0.12	74,74,74,74	0
59	MG	BA	3335	1/1	0.96	0.13	81,81,81,81	0
59	MG	CX	101	1/1	0.96	0.46	44,44,44,44	0
59	MG	BB	212	1/1	0.96	0.27	48,48,48,48	0
59	MG	CA	1763	1/1	0.96	0.14	50,50,50,50	0
59	MG	BA	3425	1/1	0.96	0.23	67,67,67,67	0
59	MG	BA	3336	1/1	0.96	0.21	73,73,73,73	0
59	MG	BA	3428	1/1	0.96	0.40	71,71,71,71	0
59	MG	CA	1768	1/1	0.96	0.54	58,58,58,58	0
59	MG	DA	3118	1/1	0.96	0.81	51,51,51,51	0
59	MG	DA	3218	1/1	0.96	0.47	29,29,29,29	0
59	MG	DA	3120	1/1	0.96	0.56	37,37,37,37	0
59	MG	BA	3176	1/1	0.96	0.77	66,66,66,66	0
59	MG	AA	1624	1/1	0.96	0.22	63,63,63,63	0
59	MG	BA	3272	1/1	0.96	0.41	44,44,44,44	0
59	MG	DA	3225	1/1	0.96	0.42	42,42,42,42	0
59	MG	CA	1631	1/1	0.96	0.33	31,31,31,31	0
59	MG	AA	1795	1/1	0.96	0.71	47,47,47,47	0
59	MG	DA	3133	1/1	0.96	0.46	22,22,22,22	0
59	MG	DA	3009	1/1	0.96	0.20	29,29,29,29	0
59	MG	AA	1693	1/1	0.96	0.30	56,56,56,56	0
59	MG	BA	3158	1/1	0.96	0.10	71,71,71,71	0
59	MG	BA	3159	1/1	0.96	0.13	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3183	1/1	0.96	0.67	68,68,68,68	0
59	MG	CA	1779	1/1	0.96	0.54	46,46,46,46	0
59	MG	DA	3345	1/1	0.96	0.48	53,53,53,53	0
59	MG	DA	3346	1/1	0.96	0.32	13,13,13,13	0
59	MG	CA	1782	1/1	0.96	0.15	58,58,58,58	0
59	MG	DA	3236	1/1	0.96	0.69	35,35,35,35	0
59	MG	DA	3237	1/1	0.96	0.23	34,34,34,34	0
59	MG	BA	3247	1/1	0.96	0.12	34,34,34,34	0
59	MG	DA	3351	1/1	0.96	0.14	40,40,40,40	0
59	MG	DA	3240	1/1	0.96	0.16	27,27,27,27	0
59	MG	BA	3035	1/1	0.96	0.37	30,30,30,30	0
59	MG	DA	3032	1/1	0.96	0.45	28,28,28,28	0
59	MG	DA	3033	1/1	0.96	0.17	26,26,26,26	0
59	MG	DA	3146	1/1	0.96	0.35	46,46,46,46	0
59	MG	DA	3359	1/1	0.96	0.11	57,57,57,57	0
59	MG	DA	3035	1/1	0.96	0.79	44,44,44,44	0
59	MG	DA	3036	1/1	0.96	0.24	62,62,62,62	0
59	MG	DA	3037	1/1	0.96	0.47	31,31,31,31	0
59	MG	AA	1669	1/1	0.96	0.20	57,57,57,57	0
59	MG	BA	3066	1/1	0.96	0.22	47,47,47,47	0
59	MG	AA	1665	1/1	0.96	0.14	86,86,86,86	0
59	MG	DA	3044	1/1	0.96	0.23	23,23,23,23	0
59	MG	DA	3045	1/1	0.96	0.42	38,38,38,38	0
59	MG	DA	3155	1/1	0.96	0.23	56,56,56,56	0
59	MG	DA	3046	1/1	0.96	0.42	35,35,35,35	0
59	MG	BA	3252	1/1	0.96	0.64	50,50,50,50	0
59	MG	BA	3068	1/1	0.96	0.41	36,36,36,36	0
59	MG	BA	3189	1/1	0.96	0.28	42,42,42,42	0
59	MG	DA	3052	1/1	0.96	0.34	20,20,20,20	0
59	MG	DA	3053	1/1	0.96	0.32	29,29,29,29	0
59	MG	BA	3402	1/1	0.96	0.22	54,54,54,54	0
59	MG	BA	3288	1/1	0.96	0.17	78,78,78,78	0
59	MG	CA	1693	1/1	0.96	0.23	87,87,87,87	0
59	MG	BA	3190	1/1	0.96	0.30	38,38,38,38	0
59	MG	AA	1682	1/1	0.96	0.15	117,117,117,117	0
59	MG	DA	3384	1/1	0.96	0.20	188,188,188,188	0
59	MG	BA	3124	1/1	0.96	0.36	49,49,49,49	0
59	MG	DA	3270	1/1	0.96	0.31	45,45,45,45	0
59	MG	DA	3170	1/1	0.96	0.11	87,87,87,87	0
59	MG	DA	3171	1/1	0.96	0.26	46,46,46,46	0
59	MG	CA	1606	1/1	0.96	0.35	41,41,41,41	0
59	MG	DA	3173	1/1	0.96	0.21	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	1698	1/1	0.96	0.07	74,74,74,74	0
59	MG	BA	3194	1/1	0.96	0.23	54,54,54,54	0
59	MG	DA	3072	1/1	0.96	0.52	22,22,22,22	0
59	MG	BA	3073	1/1	0.96	0.34	37,37,37,37	0
59	MG	AA	1661	1/1	0.96	0.51	40,40,40,40	0
59	MG	DB	205	1/1	0.96	0.20	66,66,66,66	0
59	MG	DA	3283	1/1	0.96	0.26	33,33,33,33	0
59	MG	BA	3048	1/1	0.96	0.26	69,69,69,69	0
59	MG	CA	1658	1/1	0.96	0.48	55,55,55,55	0
59	MG	DB	209	1/1	0.96	0.30	46,46,46,46	0
59	MG	AA	1606	1/1	0.96	0.22	65,65,65,65	0
59	MG	BA	3201	1/1	0.96	0.55	49,49,49,49	0
59	MG	DE	301	1/1	0.96	0.39	25,25,25,25	0
59	MG	DA	3082	1/1	0.96	0.35	32,32,32,32	0
59	MG	BA	3130	1/1	0.96	0.27	54,54,54,54	0
59	MG	DA	3191	1/1	0.96	0.21	32,32,32,32	0
59	MG	AA	1739	1/1	0.96	0.29	44,44,44,44	0
59	MG	DA	3193	1/1	0.96	0.37	50,50,50,50	0
59	MG	AA	1803	1/1	0.96	0.11	70,70,70,70	0
59	MG	BA	3154	1/1	0.96	0.54	50,50,50,50	0
60	EDS	CA	1787	41/41	0.96	0.20	39,46,57,70	0
59	MG	AA	1771	1/1	0.97	0.27	48,48,48,48	0
59	MG	BA	3039	1/1	0.97	0.26	45,45,45,45	0
59	MG	AA	1702	1/1	0.97	0.12	93,93,93,93	0
59	MG	CA	1780	1/1	0.97	0.16	71,71,71,71	0
59	MG	DA	3287	1/1	0.97	0.14	30,30,30,30	0
59	MG	AA	1773	1/1	0.97	0.32	52,52,52,52	0
59	MG	DA	3054	1/1	0.97	0.27	18,18,18,18	0
59	MG	DA	3056	1/1	0.97	0.15	32,32,32,32	0
59	MG	AA	1664	1/1	0.97	0.12	89,89,89,89	0
59	MG	DA	3294	1/1	0.97	0.61	34,34,34,34	0
59	MG	DA	3295	1/1	0.97	0.31	66,66,66,66	0
59	MG	DA	3061	1/1	0.97	0.39	21,21,21,21	0
59	MG	DA	3178	1/1	0.97	0.16	40,40,40,40	0
59	MG	BA	3128	1/1	0.97	0.54	41,41,41,41	0
59	MG	DA	3063	1/1	0.97	0.54	19,19,19,19	0
59	MG	BA	3211	1/1	0.97	0.21	44,44,44,44	0
59	MG	DA	3183	1/1	0.97	0.28	49,49,49,49	0
59	MG	DA	3302	1/1	0.97	0.31	48,48,48,48	0
59	MG	BA	3085	1/1	0.97	0.26	30,30,30,30	0
59	MG	AA	1725	1/1	0.97	0.66	54,54,54,54	0
59	MG	CA	1790	1/1	0.97	0.22	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	CA	1651	1/1	0.97	0.34	60,60,60,60	0
59	MG	BA	3050	1/1	0.97	0.25	25,25,25,25	0
59	MG	CA	1719	1/1	0.97	0.14	57,57,57,57	0
59	MG	BE	301	1/1	0.97	0.30	35,35,35,35	0
59	MG	BE	302	1/1	0.97	0.20	23,23,23,23	0
59	MG	BA	3309	1/1	0.97	0.56	31,31,31,31	0
59	MG	BA	3419	1/1	0.97	0.48	49,49,49,49	0
59	MG	BA	3088	1/1	0.97	0.25	42,42,42,42	0
59	MG	AA	1643	1/1	0.97	0.17	58,58,58,58	0
59	MG	DA	3196	1/1	0.97	0.23	26,26,26,26	0
59	MG	BA	3360	1/1	0.97	0.33	51,51,51,51	0
59	MG	DA	3198	1/1	0.97	0.45	52,52,52,52	0
59	MG	BA	3054	1/1	0.97	0.30	16,16,16,16	0
59	MG	DA	3083	1/1	0.97	0.33	33,33,33,33	0
59	MG	DA	3323	1/1	0.97	0.30	43,43,43,43	0
59	MG	CV	101	1/1	0.97	0.38	31,31,31,31	0
59	MG	BA	3018	1/1	0.97	0.39	36,36,36,36	0
59	MG	AA	1638	1/1	0.97	0.35	43,43,43,43	0
59	MG	DA	3087	1/1	0.97	0.23	17,17,17,17	0
59	MG	DA	3329	1/1	0.97	0.06	94,94,94,94	0
59	MG	DA	3205	1/1	0.97	0.59	35,35,35,35	0
59	MG	DA	3088	1/1	0.97	0.54	24,24,24,24	0
59	MG	DA	3089	1/1	0.97	0.40	46,46,46,46	0
59	MG	BA	3137	1/1	0.97	0.24	33,33,33,33	0
59	MG	DA	3334	1/1	0.97	0.28	21,21,21,21	0
59	MG	DA	3092	1/1	0.97	0.23	26,26,26,26	0
59	MG	BA	3094	1/1	0.97	0.26	30,30,30,30	0
59	MG	BA	3223	1/1	0.97	0.24	52,52,52,52	0
59	MG	DA	3098	1/1	0.97	0.37	29,29,29,29	0
59	MG	AA	1793	1/1	0.97	0.19	85,85,85,85	0
59	MG	DA	3341	1/1	0.97	0.28	45,45,45,45	0
59	MG	DA	3101	1/1	0.97	0.55	37,37,37,37	0
59	MG	BA	3181	1/1	0.97	0.35	44,44,44,44	0
59	MG	BA	3370	1/1	0.97	0.17	47,47,47,47	0
59	MG	AA	1651	1/1	0.97	0.14	78,78,78,78	0
59	MG	BA	3060	1/1	0.97	0.35	26,26,26,26	0
59	MG	CA	1604	1/1	0.97	0.23	42,42,42,42	0
59	MG	DA	3107	1/1	0.97	0.22	31,31,31,31	0
59	MG	AA	1659	1/1	0.97	0.34	74,74,74,74	0
59	MG	DA	3109	1/1	0.97	0.35	17,17,17,17	0
59	MG	DA	3110	1/1	0.97	0.29	20,20,20,20	0
59	MG	DA	3352	1/1	0.97	0.21	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3377	1/1	0.97	0.15	30,30,30,30	0
59	MG	DA	3354	1/1	0.97	0.33	36,36,36,36	0
59	MG	AA	1639	1/1	0.97	0.17	49,49,49,49	0
59	MG	BA	3101	1/1	0.97	0.37	49,49,49,49	0
59	MG	BA	3102	1/1	0.97	0.45	31,31,31,31	0
59	MG	BA	3104	1/1	0.97	0.54	38,38,38,38	0
59	MG	BA	3026	1/1	0.97	0.40	19,19,19,19	0
59	MG	AA	1614	1/1	0.97	0.11	85,85,85,85	0
59	MG	DA	3361	1/1	0.97	0.19	42,42,42,42	0
59	MG	BA	3443	1/1	0.97	0.40	37,37,37,37	0
59	MG	DA	3122	1/1	0.97	0.32	47,47,47,47	0
59	MG	BA	3235	1/1	0.97	0.44	29,29,29,29	0
59	MG	BA	3445	1/1	0.97	0.39	36,36,36,36	0
59	MG	DA	3129	1/1	0.97	0.26	34,34,34,34	0
59	MG	CA	1617	1/1	0.97	0.34	51,51,51,51	0
59	MG	DA	3242	1/1	0.97	0.38	36,36,36,36	0
59	MG	DA	3369	1/1	0.97	0.16	58,58,58,58	0
59	MG	DA	3131	1/1	0.97	0.47	26,26,26,26	0
59	MG	AA	1605	1/1	0.97	0.46	37,37,37,37	0
59	MG	BA	3387	1/1	0.97	0.14	42,42,42,42	0
59	MG	AX	103	1/1	0.97	0.27	52,52,52,52	0
59	MG	BA	3031	1/1	0.97	0.31	25,25,25,25	0
59	MG	BA	3196	1/1	0.97	0.13	56,56,56,56	0
59	MG	BA	3243	1/1	0.97	0.20	52,52,52,52	0
59	MG	DA	3138	1/1	0.97	0.59	34,34,34,34	0
59	MG	CA	1757	1/1	0.97	0.64	60,60,60,60	0
59	MG	BA	3032	1/1	0.97	0.52	45,45,45,45	0
59	MG	DA	3012	1/1	0.97	0.35	45,45,45,45	0
59	MG	BA	3337	1/1	0.97	0.21	80,80,80,80	0
59	MG	BA	3455	1/1	0.97	0.19	59,59,59,59	0
59	MG	DA	3016	1/1	0.97	0.30	18,18,18,18	0
59	MG	DA	3257	1/1	0.97	0.30	21,21,21,21	0
59	MG	BA	3395	1/1	0.97	0.16	37,37,37,37	0
59	MG	BA	3075	1/1	0.97	0.28	21,21,21,21	0
59	MG	DA	3389	1/1	0.97	0.25	24,24,24,24	0
59	MG	CA	1630	1/1	0.97	0.19	120,120,120,120	0
59	MG	CA	1764	1/1	0.97	0.55	29,29,29,29	0
59	MG	DA	3262	1/1	0.97	0.42	51,51,51,51	0
59	MG	DA	3027	1/1	0.97	0.26	32,32,32,32	0
59	MG	AA	1769	1/1	0.97	0.26	71,71,71,71	0
59	MG	CA	1632	1/1	0.97	0.18	54,54,54,54	0
59	MG	DA	3266	1/1	0.97	0.49	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BB	202	1/1	0.97	0.17	98,98,98,98	0
59	MG	BA	3115	1/1	0.97	0.22	48,48,48,48	0
59	MG	CA	1635	1/1	0.97	0.45	35,35,35,35	0
59	MG	BA	3078	1/1	0.97	0.61	35,35,35,35	0
59	MG	BA	3117	1/1	0.97	0.39	26,26,26,26	0
59	MG	BB	206	1/1	0.97	0.35	94,94,94,94	0
59	MG	DA	3273	1/1	0.97	0.33	54,54,54,54	0
59	MG	DA	3041	1/1	0.97	0.32	24,24,24,24	0
59	MG	DA	3042	1/1	0.97	0.32	52,52,52,52	0
59	MG	BA	3401	1/1	0.97	0.42	42,42,42,42	0
59	MG	DA	3277	1/1	0.97	0.17	49,49,49,49	0
59	MG	AA	1610	1/1	0.97	0.17	95,95,95,95	0
59	MG	BA	3121	1/1	0.97	0.31	47,47,47,47	0
59	MG	DA	3048	1/1	0.97	0.44	14,14,14,14	0
59	MG	DA	3281	1/1	0.97	0.39	38,38,38,38	0
59	MG	DA	3165	1/1	0.97	0.25	34,34,34,34	0
61	ZN	AN	101	1/1	0.97	0.06	100,100,100,100	0
59	MG	AA	1671	1/1	0.98	0.21	85,85,85,85	0
59	MG	AA	1621	1/1	0.98	0.22	58,58,58,58	0
59	MG	DA	3324	1/1	0.98	0.23	46,46,46,46	0
59	MG	BA	3193	1/1	0.98	0.48	37,37,37,37	0
59	MG	BA	3265	1/1	0.98	0.19	55,55,55,55	0
59	MG	BA	3077	1/1	0.98	0.39	52,52,52,52	0
59	MG	DA	3066	1/1	0.98	0.38	23,23,23,23	0
59	MG	BA	3195	1/1	0.98	0.48	42,42,42,42	0
59	MG	BA	3268	1/1	0.98	0.22	48,48,48,48	0
59	MG	BA	3052	1/1	0.98	0.35	58,58,58,58	0
59	MG	DA	3239	1/1	0.98	0.21	35,35,35,35	0
59	MG	CA	1607	1/1	0.98	0.26	59,59,59,59	0
59	MG	BA	3053	1/1	0.98	0.22	47,47,47,47	0
59	MG	BA	3106	1/1	0.98	0.16	62,62,62,62	0
59	MG	AA	1720	1/1	0.98	0.26	59,59,59,59	0
59	MG	BA	3452	1/1	0.98	0.39	51,51,51,51	0
59	MG	D5	101	1/1	0.98	0.14	44,44,44,44	0
59	MG	BA	3033	1/1	0.98	0.23	37,37,37,37	0
59	MG	DA	3340	1/1	0.98	0.12	84,84,84,84	0
59	MG	DA	3077	1/1	0.98	0.36	21,21,21,21	0
59	MG	DA	3078	1/1	0.98	0.41	33,33,33,33	0
59	MG	DA	3161	1/1	0.98	0.34	37,37,37,37	0
59	MG	AA	1753	1/1	0.98	0.52	22,22,22,22	0
59	MG	CA	1769	1/1	0.98	0.42	35,35,35,35	0
59	MG	BA	3403	1/1	0.98	0.44	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3355	1/1	0.98	0.21	60,60,60,60	0
59	MG	BA	3406	1/1	0.98	0.12	72,72,72,72	0
59	MG	BA	3023	1/1	0.98	0.28	41,41,41,41	0
59	MG	AA	1608	1/1	0.98	0.35	45,45,45,45	0
59	MG	BA	3238	1/1	0.98	0.37	42,42,42,42	0
59	MG	BA	3359	1/1	0.98	0.23	78,78,78,78	0
59	MG	BA	3318	1/1	0.98	0.16	46,46,46,46	0
59	MG	BA	3239	1/1	0.98	0.38	35,35,35,35	0
59	MG	DA	3013	1/1	0.98	0.32	26,26,26,26	0
59	MG	DA	3174	1/1	0.98	0.28	37,37,37,37	0
59	MG	DA	3175	1/1	0.98	0.22	38,38,38,38	0
59	MG	BA	3141	1/1	0.98	0.31	32,32,32,32	0
59	MG	DA	3177	1/1	0.98	0.47	25,25,25,25	0
59	MG	AA	1612	1/1	0.98	0.35	50,50,50,50	0
59	MG	DA	3179	1/1	0.98	0.23	37,37,37,37	0
59	MG	DA	3096	1/1	0.98	0.23	31,31,31,31	0
59	MG	DA	3097	1/1	0.98	0.41	19,19,19,19	0
59	MG	CA	1781	1/1	0.98	0.23	40,40,40,40	0
59	MG	BA	3061	1/1	0.98	0.23	42,42,42,42	0
59	MG	BA	3283	1/1	0.98	0.23	29,29,29,29	0
59	MG	BA	3040	1/1	0.98	0.30	54,54,54,54	0
59	MG	DA	3021	1/1	0.98	0.42	25,25,25,25	0
59	MG	DA	3023	1/1	0.98	0.56	31,31,31,31	0
59	MG	DA	3025	1/1	0.98	0.40	22,22,22,22	0
59	MG	CA	1628	1/1	0.98	0.25	33,33,33,33	0
59	MG	CA	1786	1/1	0.98	0.71	35,35,35,35	0
59	MG	DA	3028	1/1	0.98	0.55	23,23,23,23	0
59	MG	DA	3029	1/1	0.98	0.30	28,28,28,28	0
59	MG	DA	3031	1/1	0.98	0.45	32,32,32,32	0
59	MG	DA	3376	1/1	0.98	0.14	56,56,56,56	0
59	MG	DA	3377	1/1	0.98	0.40	23,23,23,23	0
59	MG	BA	3175	1/1	0.98	0.33	52,52,52,52	0
59	MG	DA	3112	1/1	0.98	0.35	22,22,22,22	0
59	MG	AA	1687	1/1	0.98	0.16	84,84,84,84	0
59	MG	BA	3027	1/1	0.98	0.23	29,29,29,29	0
59	MG	DA	3115	1/1	0.98	0.43	27,27,27,27	0
59	MG	B7	101	1/1	0.98	0.17	39,39,39,39	0
59	MG	CA	1684	1/1	0.98	0.13	79,79,79,79	0
59	MG	BA	3148	1/1	0.98	0.80	24,24,24,24	0
59	MG	DA	3119	1/1	0.98	0.38	44,44,44,44	0
59	MG	BA	3373	1/1	0.98	0.15	73,73,73,73	0
59	MG	BA	3374	1/1	0.98	0.26	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	BA	3375	1/1	0.98	0.19	47,47,47,47	0
59	MG	DA	3123	1/1	0.98	0.23	49,49,49,49	0
59	MG	BA	3120	1/1	0.98	0.20	38,38,38,38	0
59	MG	DA	3125	1/1	0.98	0.22	43,43,43,43	0
59	MG	DA	3126	1/1	0.98	0.42	25,25,25,25	0
59	MG	DA	3043	1/1	0.98	0.18	26,26,26,26	0
59	MG	DA	3128	1/1	0.98	0.22	28,28,28,28	0
59	MG	DA	3212	1/1	0.98	0.33	45,45,45,45	0
59	MG	BA	3150	1/1	0.98	0.69	37,37,37,37	0
59	MG	BA	3378	1/1	0.98	0.18	68,68,68,68	0
59	MG	BA	3215	1/1	0.98	0.34	47,47,47,47	0
59	MG	BA	3091	1/1	0.98	0.25	38,38,38,38	0
59	MG	DA	3217	1/1	0.98	0.11	40,40,40,40	0
59	MG	DB	210	1/1	0.98	0.07	88,88,88,88	0
59	MG	BA	3044	1/1	0.98	0.42	70,70,70,70	0
59	MG	DA	3310	1/1	0.98	0.51	27,27,27,27	0
59	MG	BA	3123	1/1	0.98	0.26	34,34,34,34	0
59	MG	BA	3046	1/1	0.98	0.27	39,39,39,39	0
59	MG	BA	3069	1/1	0.98	0.48	29,29,29,29	0
59	MG	DA	3223	1/1	0.98	0.47	19,19,19,19	0
59	MG	BA	3070	1/1	0.98	0.40	21,21,21,21	0
59	MG	BA	3047	1/1	0.98	0.30	37,37,37,37	0
59	MG	AA	1778	1/1	0.98	0.50	71,71,71,71	0
59	MG	DA	3057	1/1	0.98	0.36	28,28,28,28	0
59	MG	DA	3059	1/1	0.98	0.34	38,38,38,38	0
59	MG	BA	3074	1/1	0.98	0.22	30,30,30,30	0
61	ZN	B9	101	1/1	0.98	0.07	91,91,91,91	0
59	MG	DA	3219	1/1	0.99	0.32	26,26,26,26	0
59	MG	BA	3119	1/1	0.99	0.18	41,41,41,41	0
59	MG	BA	3103	1/1	0.99	0.27	42,42,42,42	0
59	MG	BA	3240	1/1	0.99	0.24	28,28,28,28	0
59	MG	DA	3017	1/1	0.99	0.34	29,29,29,29	0
59	MG	DA	3079	1/1	0.99	0.34	30,30,30,30	0
59	MG	DA	3047	1/1	0.99	0.26	16,16,16,16	0
59	MG	AA	1632	1/1	0.99	0.23	77,77,77,77	0
59	MG	BA	3064	1/1	0.99	0.20	37,37,37,37	0
59	MG	AA	1734	1/1	0.99	0.19	75,75,75,75	0
59	MG	AA	1622	1/1	0.99	0.08	61,61,61,61	0
59	MG	DA	3022	1/1	0.99	0.43	17,17,17,17	0
59	MG	BA	3045	1/1	0.99	0.38	38,38,38,38	0
59	MG	DA	3024	1/1	0.99	0.30	19,19,19,19	0
59	MG	DA	3309	1/1	0.99	0.08	67,67,67,67	0

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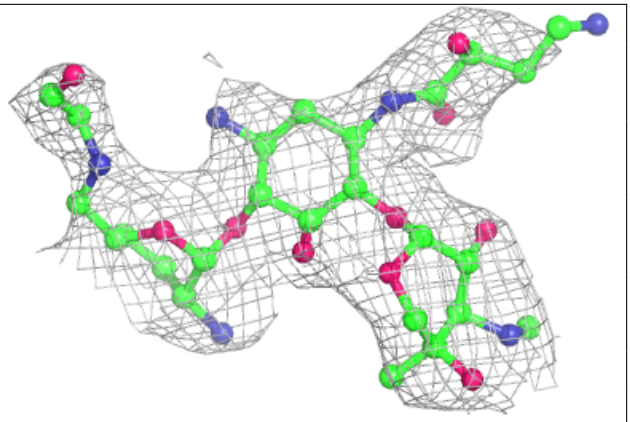
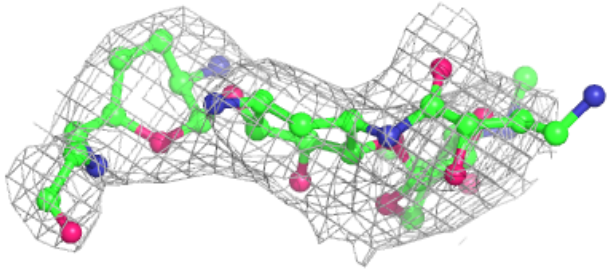
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	MG	DA	3055	1/1	0.99	0.22	54,54,54,54	0
59	MG	BA	3056	1/1	0.99	0.37	31,31,31,31	0
59	MG	DA	3090	1/1	0.99	0.30	31,31,31,31	0
59	MG	BA	3037	1/1	0.99	0.51	28,28,28,28	0
59	MG	DA	3058	1/1	0.99	0.29	29,29,29,29	0
59	MG	BA	3361	1/1	0.99	0.11	42,42,42,42	0
59	MG	BA	3426	1/1	0.99	0.26	67,67,67,67	0
59	MG	DA	3095	1/1	0.99	0.59	24,24,24,24	0
59	MG	BA	3038	1/1	0.99	0.48	32,32,32,32	0
59	MG	DA	3030	1/1	0.99	0.35	28,28,28,28	0
59	MG	BA	3404	1/1	0.99	0.38	46,46,46,46	0
59	MG	DA	3099	1/1	0.99	0.41	33,33,33,33	0
59	MG	BA	3097	1/1	0.99	0.30	46,46,46,46	0
59	MG	AA	1609	1/1	0.99	0.21	80,80,80,80	0
59	MG	DA	3034	1/1	0.99	0.28	36,36,36,36	0
59	MG	BA	3407	1/1	0.99	0.14	54,54,54,54	0
59	MG	BA	3114	1/1	0.99	0.13	49,49,49,49	0
59	MG	BA	3072	1/1	0.99	0.23	31,31,31,31	0
59	MG	BA	3049	1/1	0.99	0.26	35,35,35,35	0
59	MG	BA	3020	1/1	0.99	0.20	49,49,49,49	0
59	MG	AA	1728	1/1	0.99	0.29	88,88,88,88	0
59	MG	DA	3291	1/1	0.99	0.26	44,44,44,44	0
59	MG	DA	3292	1/1	0.99	0.18	21,21,21,21	0
61	ZN	AD	302	1/1	0.99	0.26	64,64,64,64	0
59	MG	BA	3274	1/1	0.99	0.15	58,58,58,58	0
59	MG	BA	3391	1/1	0.99	0.30	44,44,44,44	0
61	ZN	CD	301	1/1	0.99	0.31	68,68,68,68	0
61	ZN	CN	101	1/1	0.99	0.09	77,77,77,77	0
61	ZN	D9	101	1/1	0.99	0.05	75,75,75,75	0
59	MG	DA	3312	1/1	1.00	0.10	46,46,46,46	0

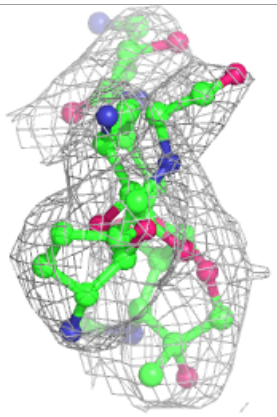
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around EDS AA 1805:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

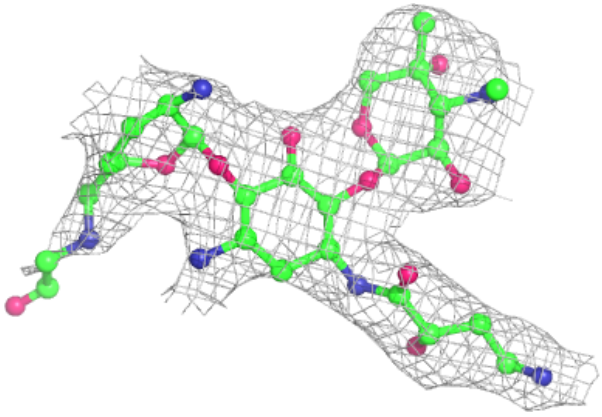


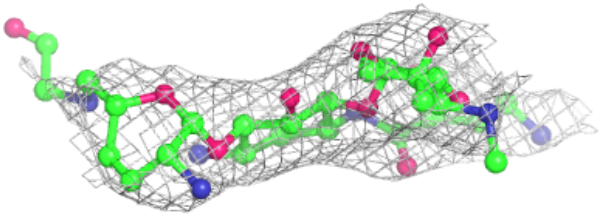


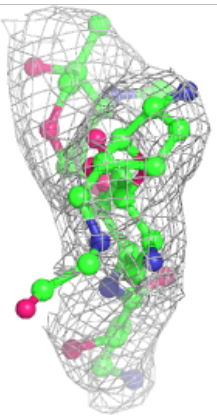


Electron density around EDS CA 1787:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.