



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:13 PM UTC

PDB ID : 4V6A / pdb_00004v6a
Title : Structure of EF-P bound to the 70S ribosome.
Authors : Stanley, R.E.; Blaha, G.
Deposited on : 2009-06-15
Resolution : 3.10 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

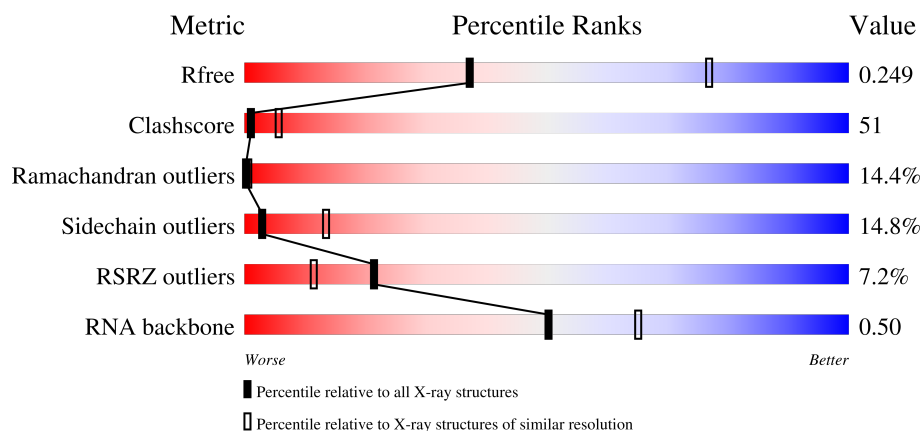
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1509	6% 17% 67% 13% ••
1	CA	1509	5% 21% 65% 12% •
2	AB	256	5% 12% 55% 21% 8% •
2	CB	256	5% 12% 53% 25% 8% •

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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	184	
22	CV	184	
23	AW	77	
23	CW	77	
24	AX	5	
24	CX	5	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	
27	BC	229	
27	DC	229	

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Mol	Chain	Length	Quality of chain
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	
39	DS	112	
40	BT	146	

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Mol	Chain	Length	Quality of chain
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	71	
51	D4	71	
52	B5	60	
52	D5	60	

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Mol	Chain	Length	Quality of chain
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	
56	B9	37	
56	D9	37	

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
57	MG	BA	3021	-	-	-	X
57	MG	BA	3022	-	-	-	X
57	MG	BA	3038	-	-	-	X
57	MG	BA	3053	-	-	-	X
57	MG	BA	3086	-	-	-	X
57	MG	BA	3118	-	-	-	X
57	MG	BA	3139	-	-	-	X
57	MG	BA	3300	-	-	-	X
57	MG	BA	3323	-	-	-	X
57	MG	BA	3333	-	-	-	X
57	MG	BA	3381	-	-	-	X
57	MG	BA	3442	-	-	-	X
57	MG	BA	3444	-	-	-	X
57	MG	BP	201	-	-	-	X
57	MG	CA	1691	-	-	-	X
57	MG	CA	1708	-	-	-	X
57	MG	CW	102	-	-	-	X
57	MG	DA	3033	-	-	-	X
57	MG	DA	3073	-	-	-	X
57	MG	DA	3195	-	-	-	X
57	MG	DA	3199	-	-	-	X
57	MG	DA	3267	-	-	-	X
58	ZN	AD	301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
58	ZN	D9	101	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 290405 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	1495	Total	C	N	O	P	0	0	0
			32144	14306	5964	10379	1495			
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	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- 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	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	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	127	Total	C	N	O		0	0	0
			1004	635	195	174				
9	CI	127	Total	C	N	O		0	0	0
			1004	635	195	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	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	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	120	Total	C	N	O	S	0	0	1
			947	585	196	164	2			
13	CM	120	Total	C	N	O	S	0	0	1
			947	585	196	164	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	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	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	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	80	Total	C	N	O	S	0	0	1
			613	392	110	109	2			
19	CS	78	Total	C	N	O	S	0	0	1
			619	397	111	109	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	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a protein called Elongation factor P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	176	Total	C	N	O	S	0	0	0
			1367	870	223	267	7			
22	CV	176	Total	C	N	O	S	0	0	0
			1367	870	223	267	7			

- Molecule 23 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
23	CW	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 24 is a RNA chain called RNA (5'-R(P*AP*AP*AP*UP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	5	Total	C	N	O	P	0	0	0
			110	49	22	34	5			
24	CX	5	Total	C	N	O	P	0	0	0
			110	49	22	34	5			

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2767	Total	C	N	O	P	0	0	0
			59596	26524	11148	19158	2766			
25	DA	2777	Total	C	N	O	P	0	0	0
			59809	26619	11186	19228	2776			

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 27 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BC	224	Total	C	N	O	S	2	0	0
			1702	1075	309	315	3			
27	DC	220	Total	C	N	O	S	1	0	0
			1640	1033	297	307	3			

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	274	Total	C	N	O	S	0	0	1
			2127	1341	425	358	3			
28	DD	274	Total	C	N	O	S	0	0	1
			2115	1335	419	358	3			

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
29	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
30	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
31	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	168	Total	C	N	O	S	0	0	1
			1231	780	228	222	1			
32	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	146	Total	C	N	O	S	0	0	1
			1043	661	185	196	1			
33	DI	146	Total	C	N	O	S	0	0	1
			871	543	162	165	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
34	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

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

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
36	DP	146	Total	C	N	O	S	0	0	0
			1079	672	216	189	2			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	139	Total	C	N	O	S	0	0	1
			1099	702	209	181	7			
37	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	116	Total	C	N	O		0	0	0
			923	575	191	157				
38	DR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BS	101	Total	C	N	O		0	0	1
			777	489	156	132				
39	DS	99	Total	C	N	O		0	0	1
			771	486	155	130				

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
40	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
41	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 42 is a protein called 50S ribosomal protein L21.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
43	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BX	94	Total	C	N	O	S	0	0	1
			735	477	134	124				
44	DX	93	Total	C	N	O	S	0	0	1
			726	471	132	123				

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	101	Total	C	N	O	S	0	0	1
			757	486	144	123	4			
45	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	182	Total	C	N	O	S	0	0	1
			1438	917	258	261	2			
46	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B0	77	Total	C	N	O	S	0	0	0
			613	379	129	104	1			
47	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	96	Total	C	N	O	S	0	0	0
			757	478	149	129	1			
48	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
49	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	59	Total	C	N	O	S	0	0	1
			460	293	90	77				
50	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 51 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
51	D4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	57	Total	C	N	O	S	0	0	1
			435	272	88	70	5			
52	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	49	Total	C	N	O	S	0	0	1
			401	247	82	68	4			
53	D6	48	Total	C	N	O	S	0	0	0
			322	199	62	57	4			

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
54	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	63	Total	C	N	O	S	0	0	1
			496	317	101	76	2			
55	D8	62	Total	C	N	O	S	0	0	1
			467	299	95	71	2			

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B9	36	Total	C	N	O	S	0	0	0
			294	179	66	46	3			
56	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	117	Total	Mg	0	0
			117	117		
57	AL	1	Total	Mg	0	0
			1	1		
57	AT	1	Total	Mg	0	0
			1	1		
57	AW	2	Total	Mg	0	0
			2	2		
57	BA	459	Total	Mg	0	0
			459	459		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BB	9	Total 9	Mg 9	0	0
57	BD	1	Total 1	Mg 1	0	0
57	BE	1	Total 1	Mg 1	0	0
57	BF	1	Total 1	Mg 1	0	0
57	BH	1	Total 1	Mg 1	0	0
57	BP	3	Total 3	Mg 3	0	0
57	BQ	3	Total 3	Mg 3	0	0
57	BR	1	Total 1	Mg 1	0	0
57	BT	1	Total 1	Mg 1	0	0
57	BU	1	Total 1	Mg 1	0	0
57	BX	1	Total 1	Mg 1	0	0
57	B0	2	Total 2	Mg 2	0	0
57	B1	1	Total 1	Mg 1	0	0
57	B5	4	Total 4	Mg 4	0	0
57	B7	1	Total 1	Mg 1	0	0
57	CA	109	Total 109	Mg 109	0	0
57	CE	1	Total 1	Mg 1	0	0
57	CW	5	Total 5	Mg 5	0	0
57	CX	1	Total 1	Mg 1	0	0
57	DA	305	Total 305	Mg 305	0	0
57	DB	10	Total 10	Mg 10	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DD	1	Total 1	Mg 1	0	0
57	DF	1	Total 1	Mg 1	0	0
57	DP	1	Total 1	Mg 1	0	0
57	DR	1	Total 1	Mg 1	0	0
57	D5	2	Total 2	Mg 2	0	0
57	D6	2	Total 2	Mg 2	0	0

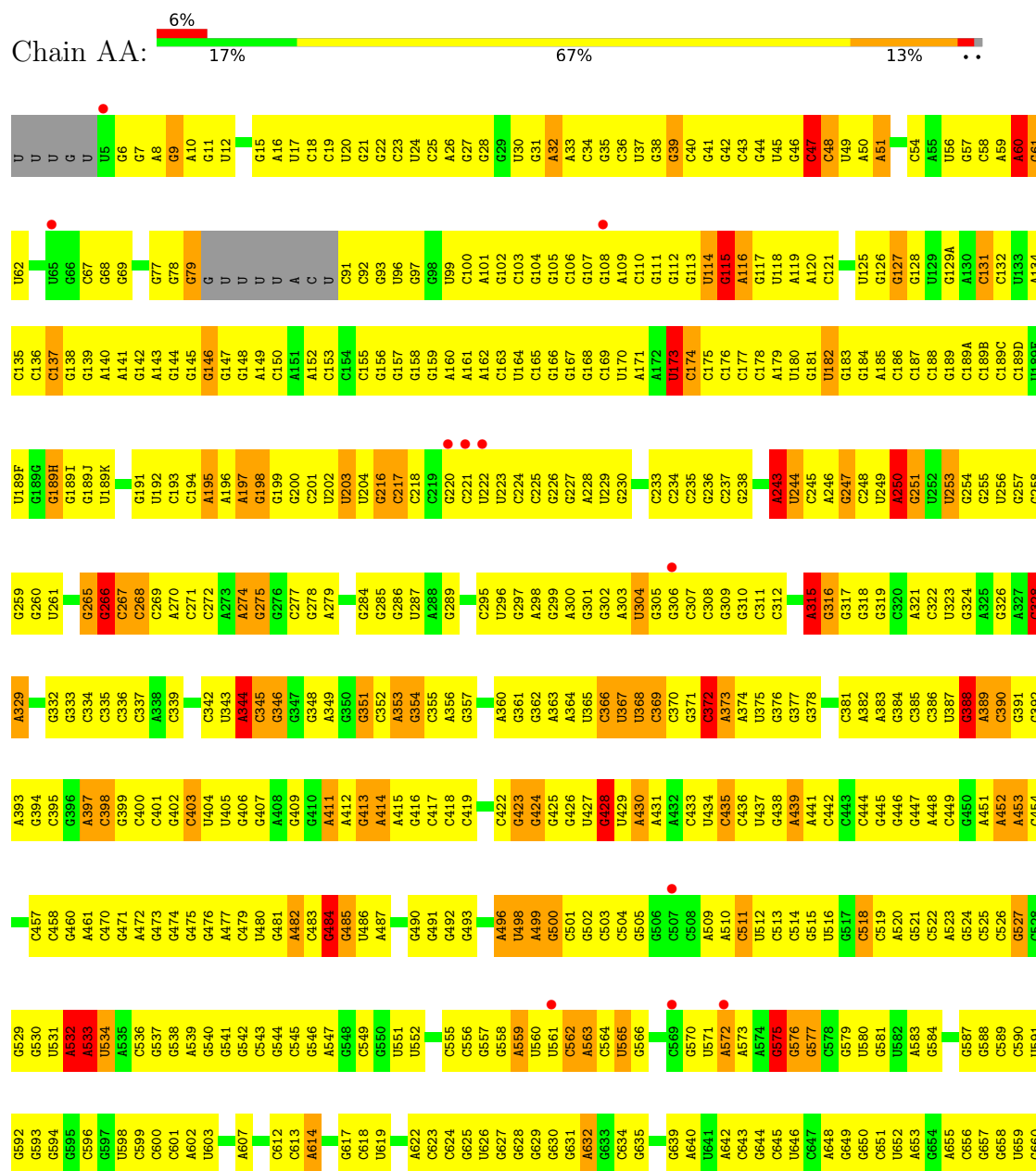
- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

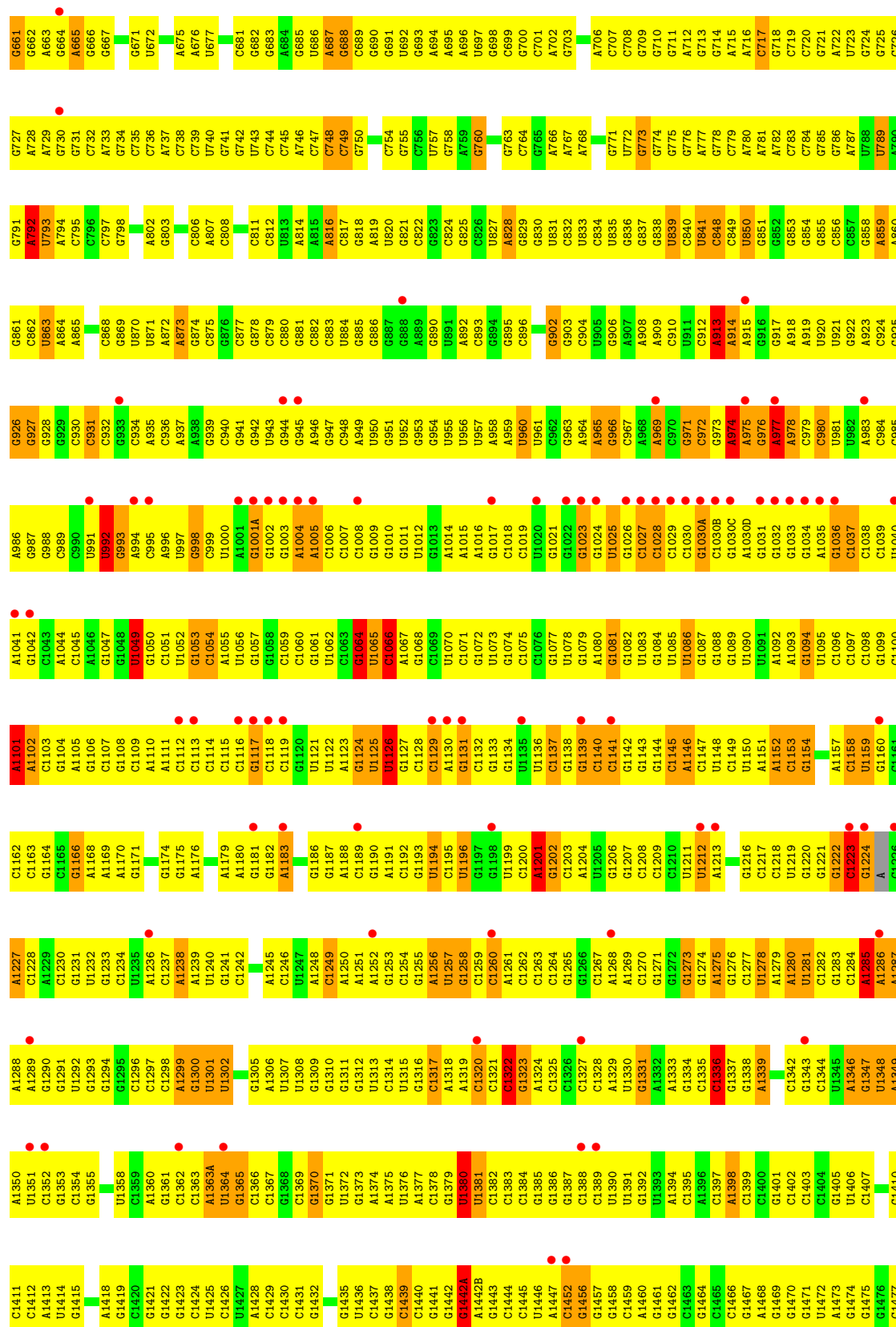
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AD	1	Total 1	Zn 1	0	0
58	B5	1	Total 1	Zn 1	0	0
58	B9	1	Total 1	Zn 1	0	0
58	CD	1	Total 1	Zn 1	0	0
58	D5	1	Total 1	Zn 1	0	0
58	D9	1	Total 1	Zn 1	0	0

3 Residue-property plots

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

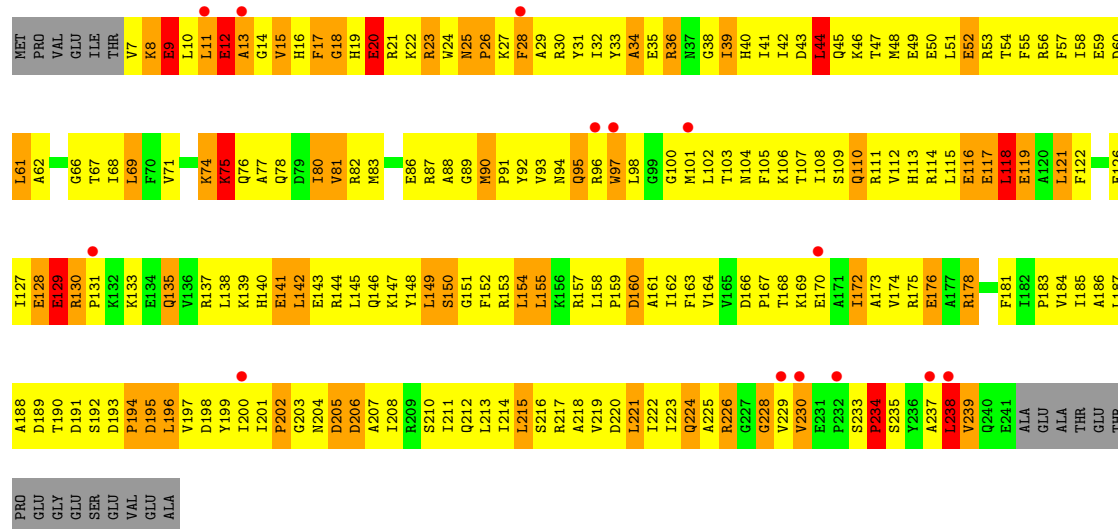
- Molecule 1: 16S ribosomal RNA



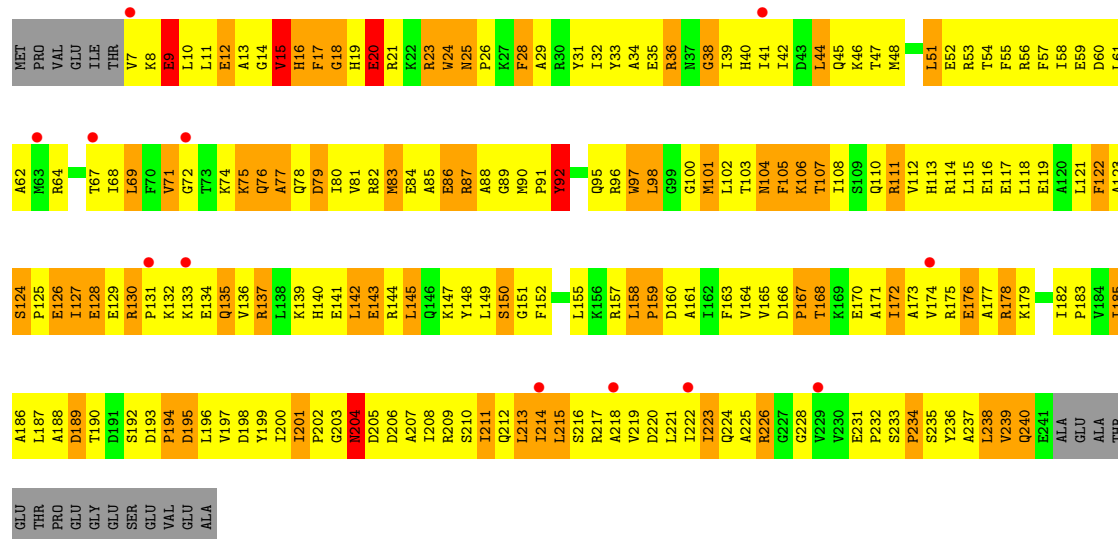
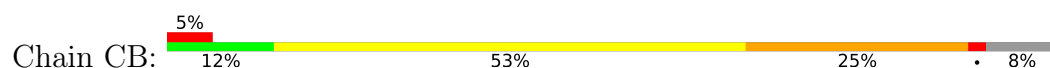


Chain CA:

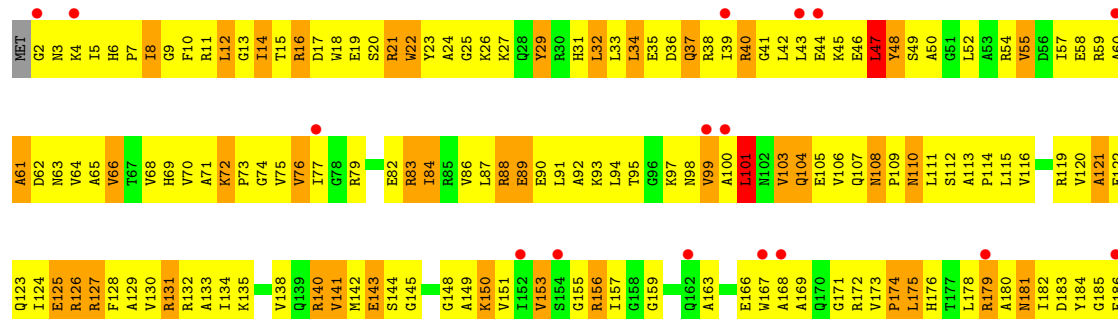
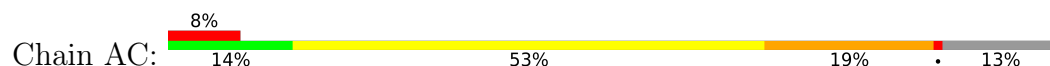


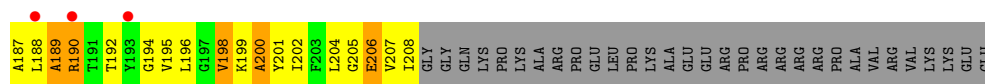


• Molecule 2: 30S ribosomal protein S2

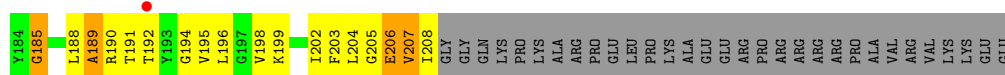
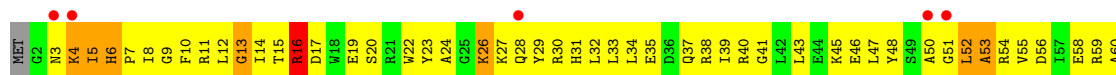
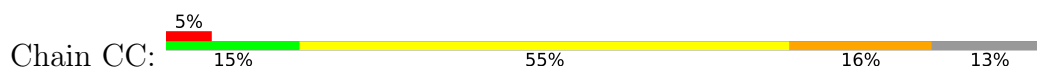


• Molecule 3: 30S ribosomal protein S3

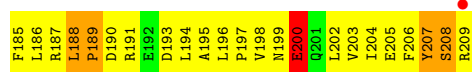
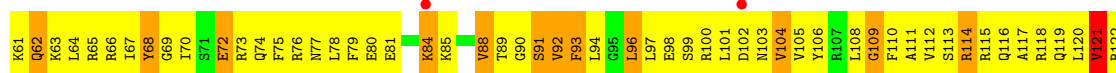
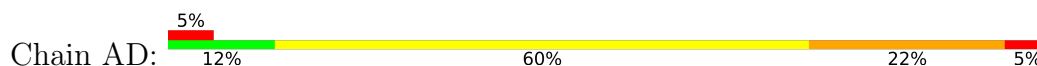




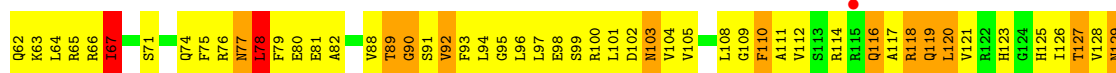
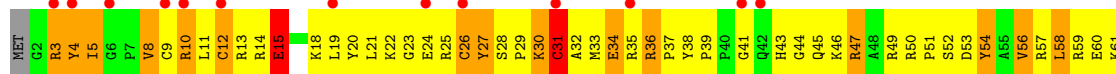
• Molecule 3: 30S ribosomal protein S3

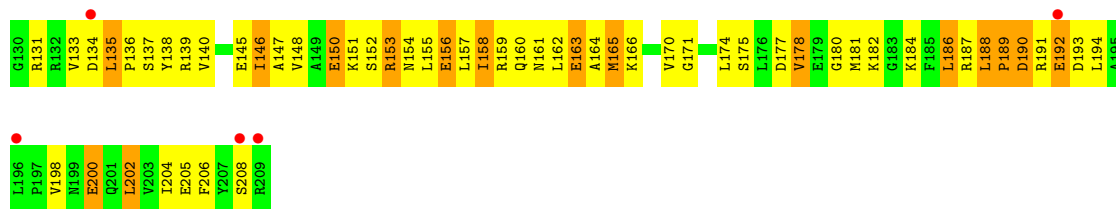


• Molecule 4: 30S ribosomal protein S4

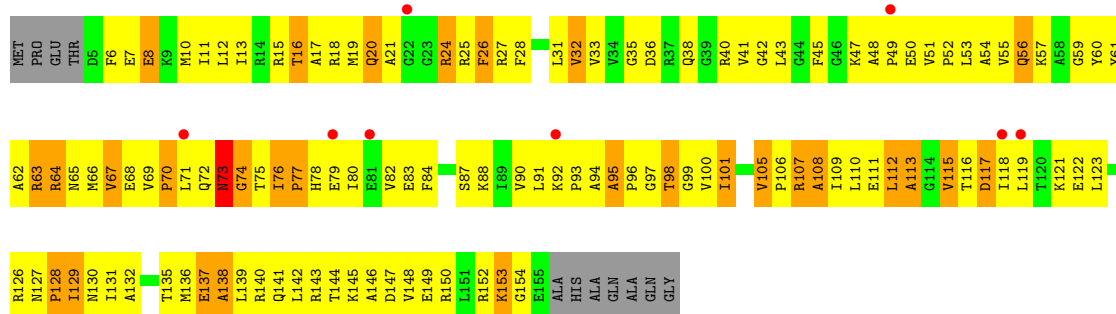
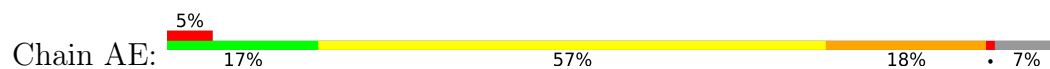


• Molecule 4: 30S ribosomal protein S4

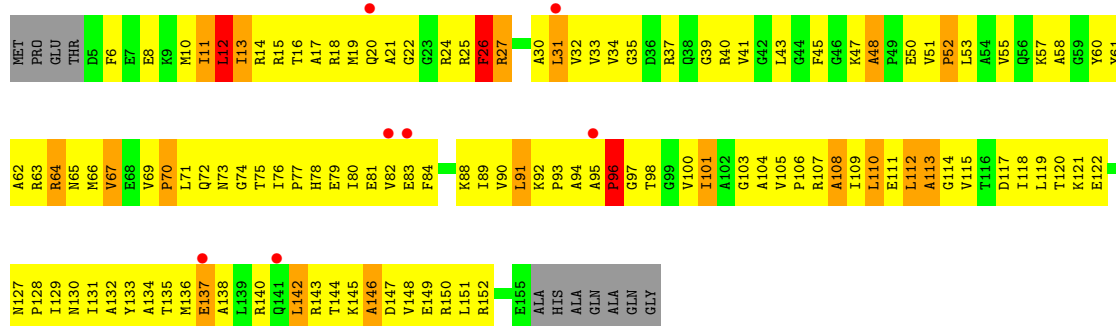




• Molecule 5: 30S ribosomal protein S5



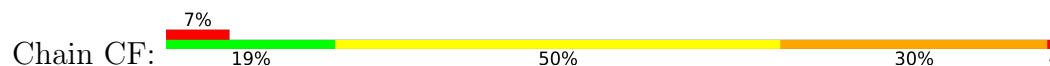
• Molecule 5: 30S ribosomal protein S5

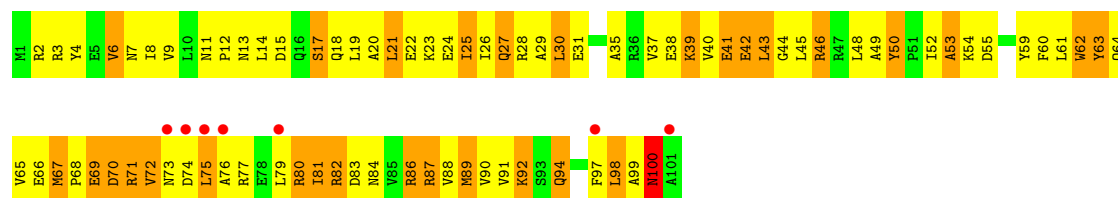


• Molecule 6: 30S ribosomal protein S6

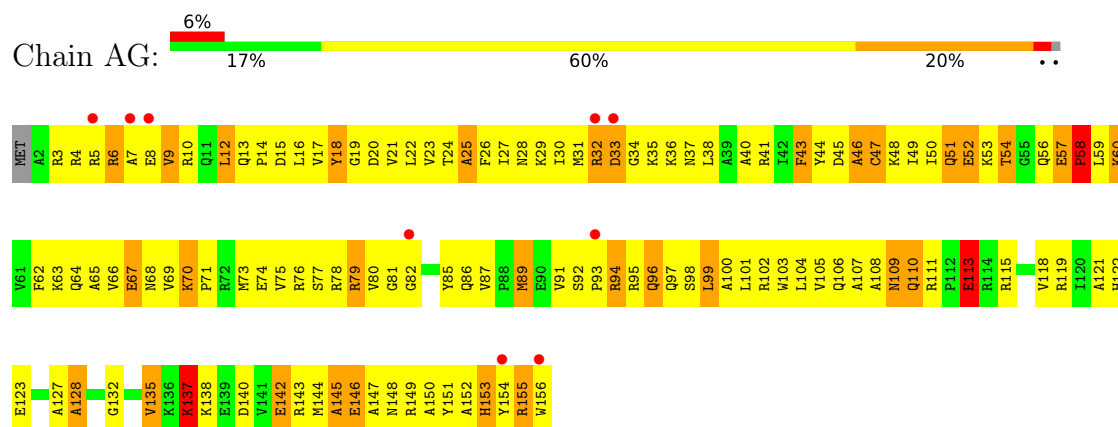


• Molecule 6: 30S ribosomal protein S6

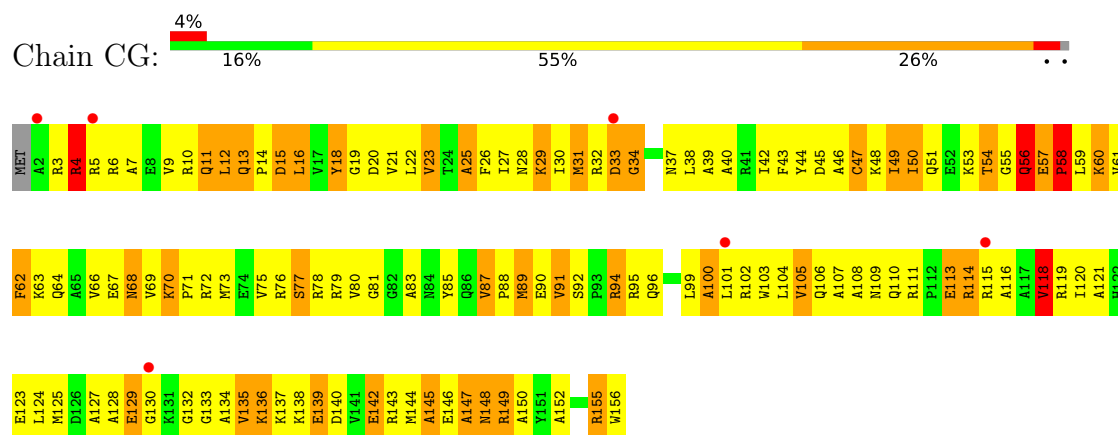




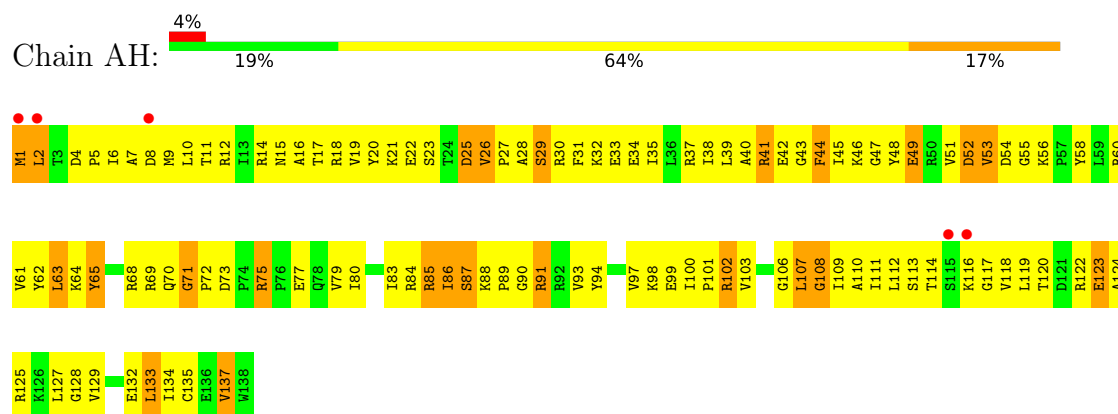
• Molecule 7: 30S ribosomal protein S7



• Molecule 7: 30S ribosomal protein S7



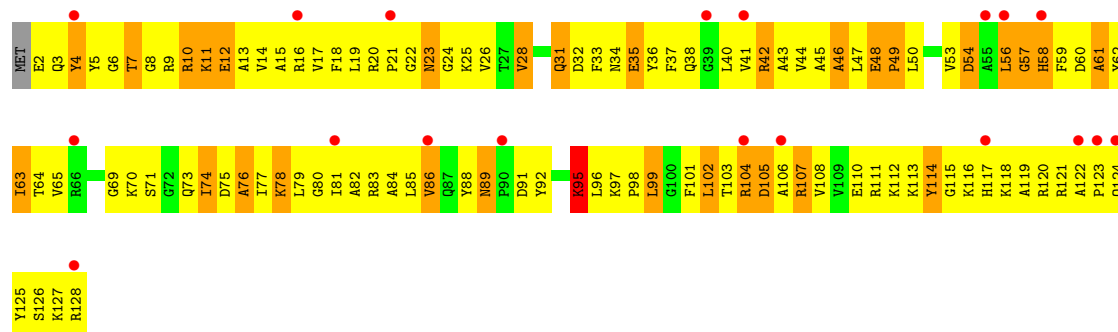
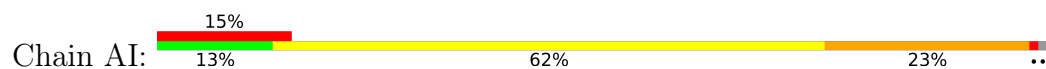
• Molecule 8: 30S ribosomal protein S8



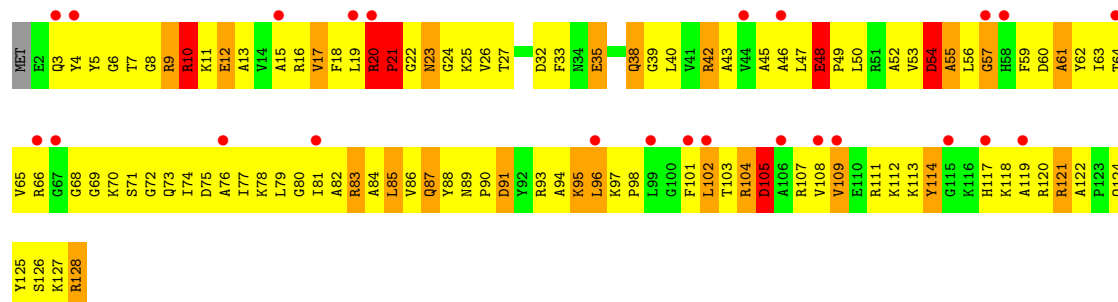
• Molecule 8: 30S ribosomal protein S8



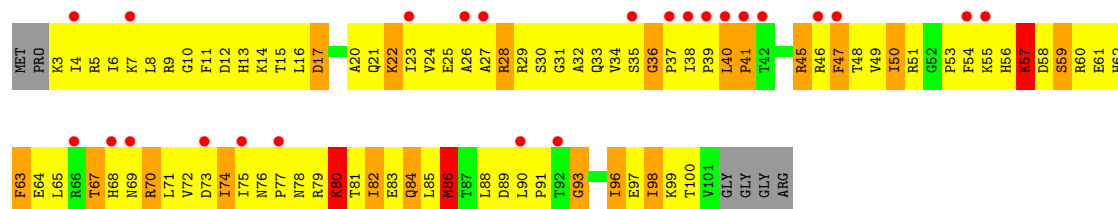
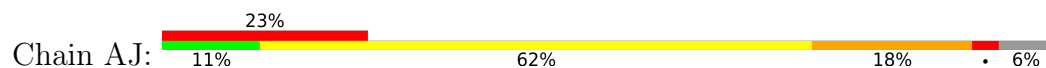
• Molecule 9: 30S ribosomal protein S9



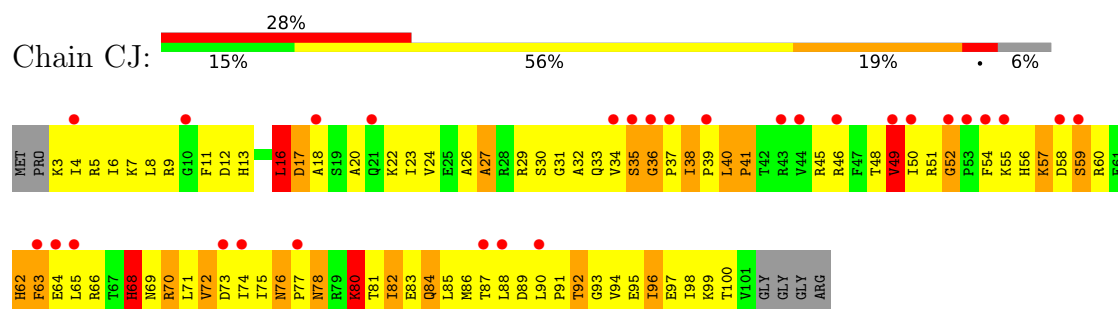
• Molecule 9: 30S ribosomal protein S9



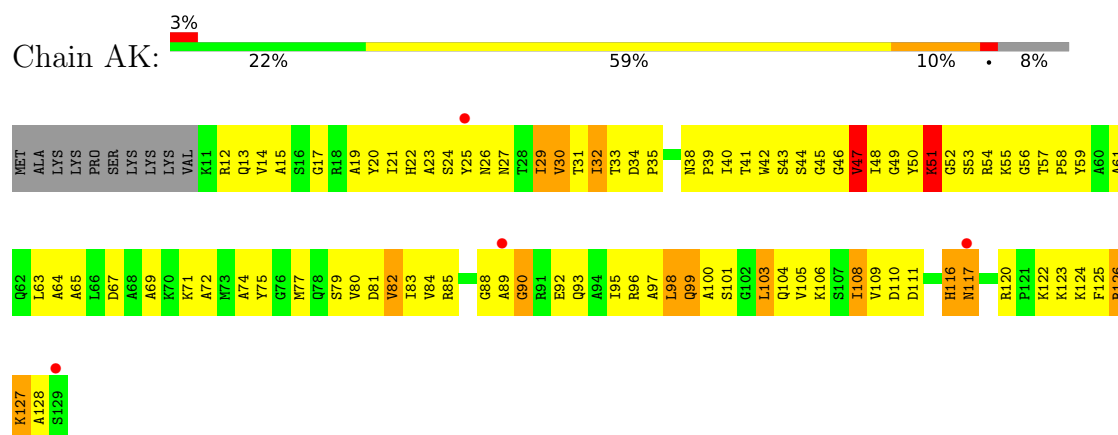
• Molecule 10: 30S ribosomal protein S10



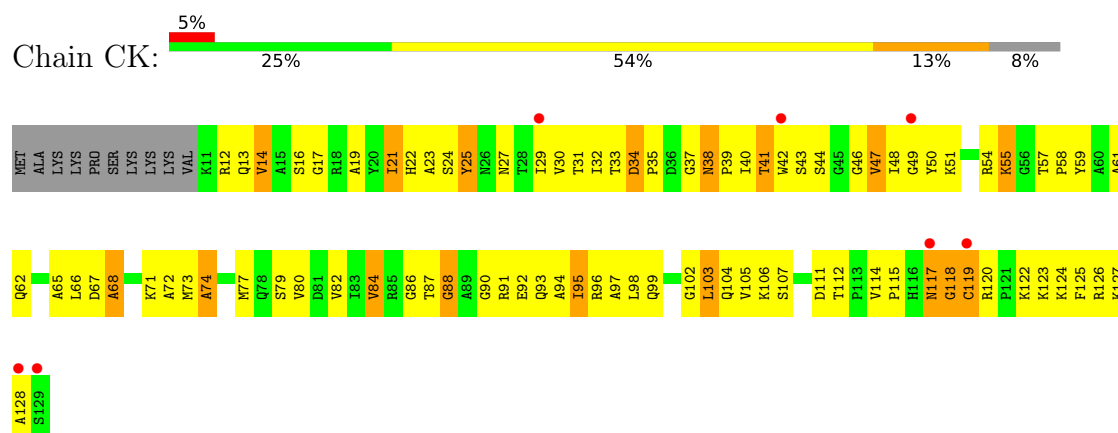
- Molecule 10: 30S ribosomal protein S10



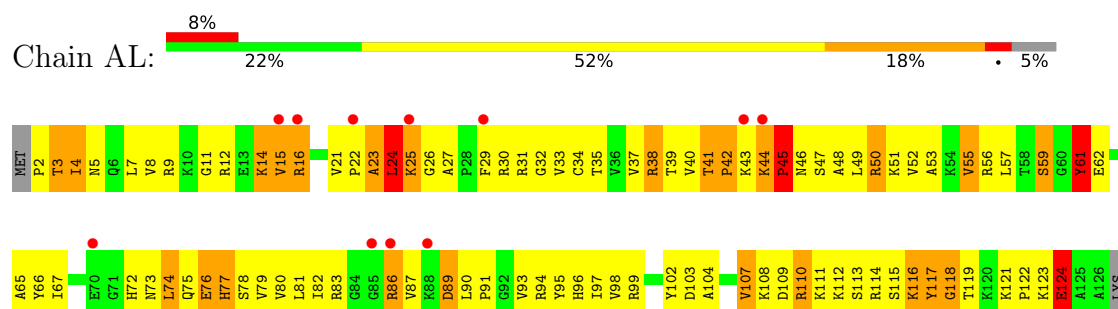
- Molecule 11: 30S ribosomal protein S11



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



THR
ALA
ALA
LYS
LYS

• Molecule 12: 30S ribosomal protein S12

Chain CL: 5% 24% 52% 16% 5%

MET P2 P3 I4 N5 Q6 L7 V8 R9 K10 G11 K12 K13 V15 R16 K17 K18 S19 K20 K21 P22 A23 K24 K25 G26 A27 P28 F29 R30 R31 R32 G33 V33 C34 V35 V36 V37 R38 R39 T39 V40 T41 P42 K43 K44 K45 N46 S47 A48 L49 R50 K51 V52 A53 K54 V55 R56 L57 T58 S59 G60 Y61

E62 V63 T64 A65 Y66 L67 P68 S69 E70 H71 G72 H73 K74 L74 K75 E76 H77 S78 V79 V80 L81 L82 R83 R84 G85 K86 V87 R88 D89 R90 P91 Y95 H96 V98 R99 G100 G101 Y101 Y102 D103 A104 K108 D109 R110 K111 K112 S113 R114 S115 K116 Y117 G118 T119 K120 K121 P122 E123 E124 A125

A126
LYS
THR
ALA
ALA
LYS
LYS

• Molecule 13: 30S ribosomal protein S13

Chain AM: 10% 13% 52% 25% 5% 5%

MET A2 I4 A5 G6 V7 E8 R9 P10 P11 R12 K13 K14 R15 V16 D16 K17 V17 A18 A19 T20 Y21 Y22 Y23 G24 G25 G26 K27 K28 A29 R30 R31 K32 E33 A34 L34 I39 N40 P41 A42 T43 R44 V45 K46 D47 L48 T49 E50 A51 E52 V53 V54 V55 L56 R57 E58 V60 T63 W64

K65 L66 E67 G68 L69 L70 R71 A72 A73 E74 V75 A76 A77 I78 K79 R80 R81 L82 D83 I84 G85 G86 R87 Y87 R88 G89 L90 R91 R92 A93 R94 G95 L96 P97 V98 Q101 R102 T103 R104 T105 N106 A107 R108 T109 R110 K111 G112 P113 R114 R115 T116 V117 A118 G119 K120 K121 LYS ALA PRO ARG

LYS

• Molecule 13: 30S ribosomal protein S13

Chain CM: 7% 15% 45% 29% 6% 5%

MET A2 I4 A5 G6 V7 E8 R9 P10 P11 R12 K13 K14 R15 V16 D16 K17 V17 A18 A19 T20 Y21 Y22 Y23 G24 G25 G26 K27 K28 A29 R30 R31 K32 E33 A34 L34 I39 N40 P41 A42 T43 R44 V45 K46 D47 L48 T49 E50 A51 E52 V53 V54 V55 L56 R57 E58 V60

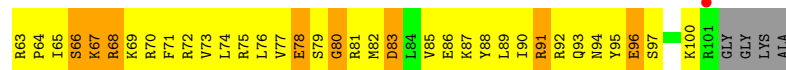
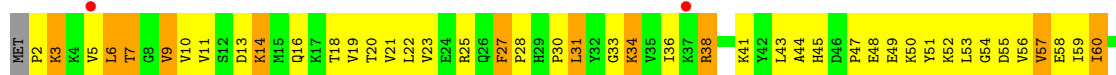
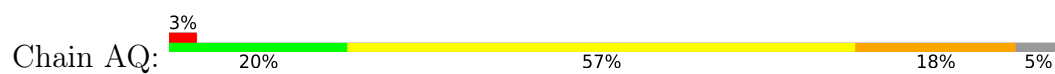
E61 M62 T63 W64 K65 L66 E67 G68 E69 L70 R71 R72 N77 I78 K79 R80 R81 L82 D83 I84 G85 G86 R87 Y87 R88 G89 L90 R91 R92 A93 R94 G95 L96 P97 V98 Q101 R102 T103 N106 A107 R108 T109 R110 K111 G112 P113 R114 R115 T116 V117 A118 G119 K120 K121 LYS ALA PRO ARG

LYS

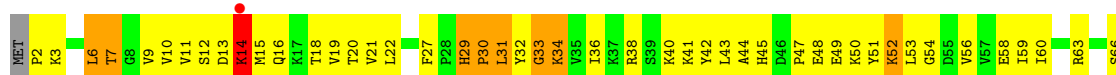
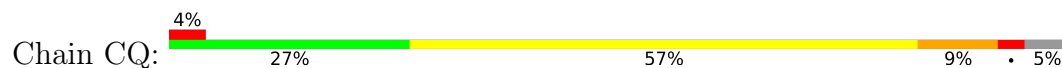
• Molecule 14: 30S ribosomal protein S14

Chain AN: 15% 13% 54% 30% 1%

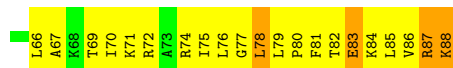
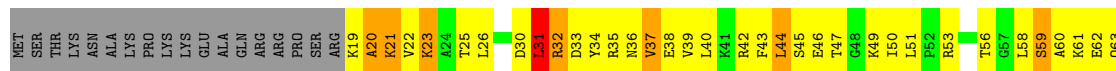
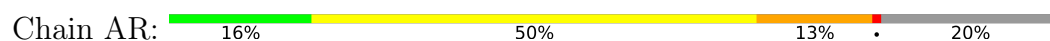
MET A2 K3 K4 A5 L6 I7 E8 K9 A10 K11 K12 T13 P14 K15 F16 K17 V18 Y21 Y22 R23 C24 V25 R26 C27 G28 R29 A30 R31 S32 S33 V34 Y34 F36 F37 G38 L39 C40 R41 I42 C43 L44 R45 E46 L47 A48 H49 K50 G51 Q52 L53 P54 G55 V56 V57 K58 A59 S60 W61



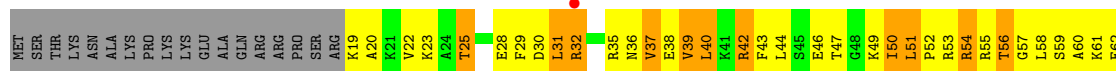
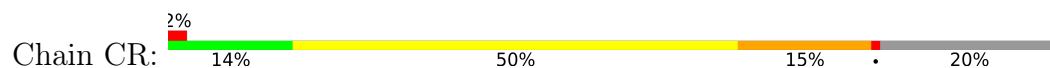
• Molecule 17: 30S ribosomal protein S17



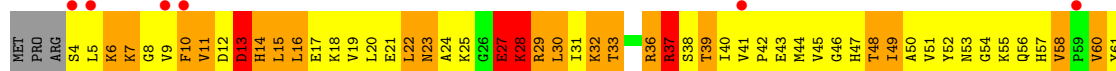
• Molecule 18: 30S ribosomal protein S18

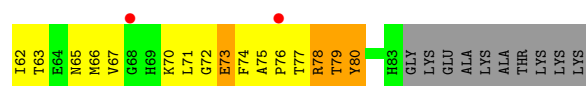


• Molecule 18: 30S ribosomal protein S18

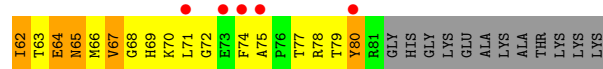
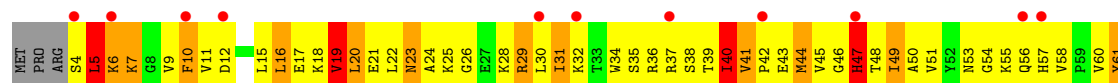
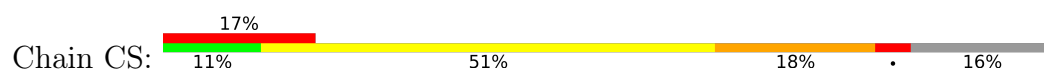


• Molecule 19: 30S ribosomal protein S19

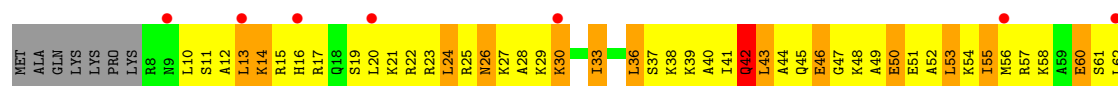
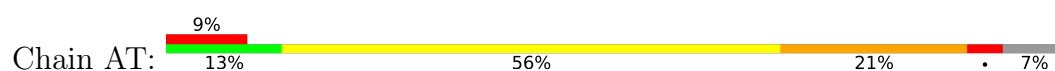




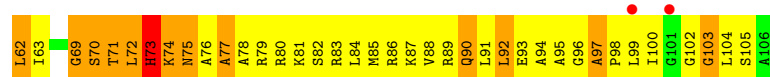
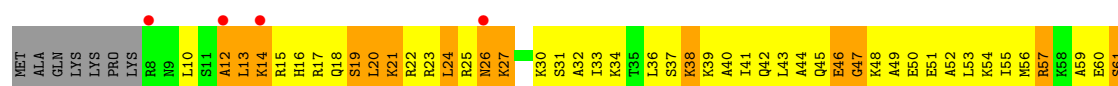
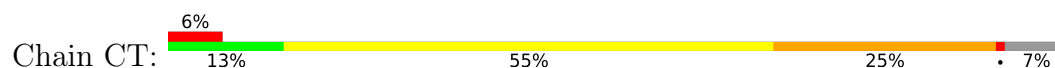
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



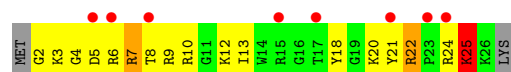
• Molecule 20: 30S ribosomal protein S20



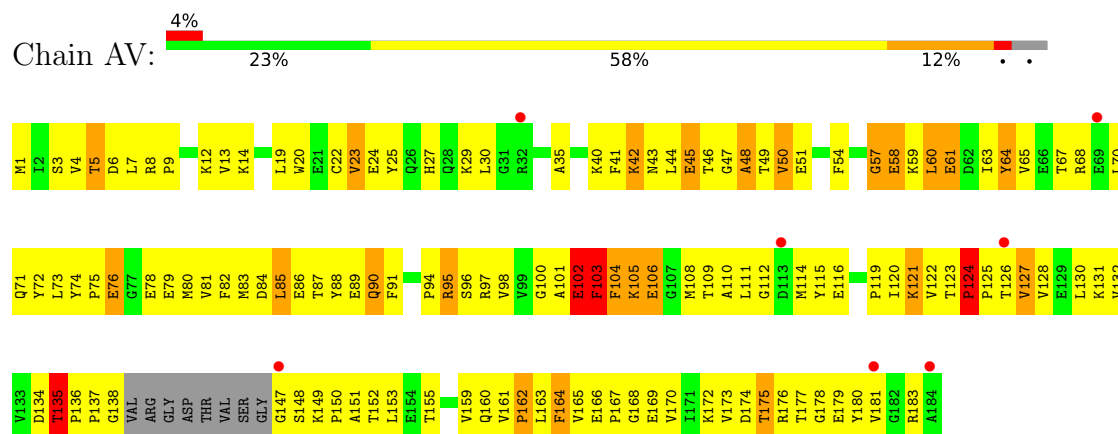
• Molecule 21: 30S ribosomal protein Thx



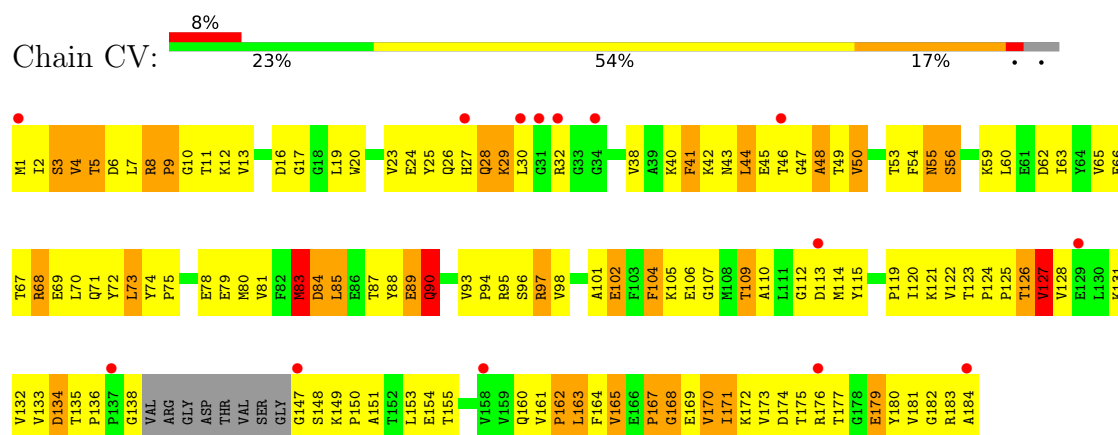
• Molecule 21: 30S ribosomal protein Thx



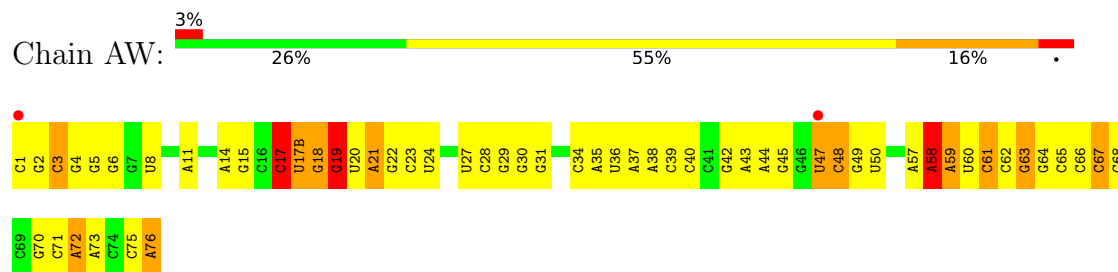
- Molecule 22: Elongation factor P



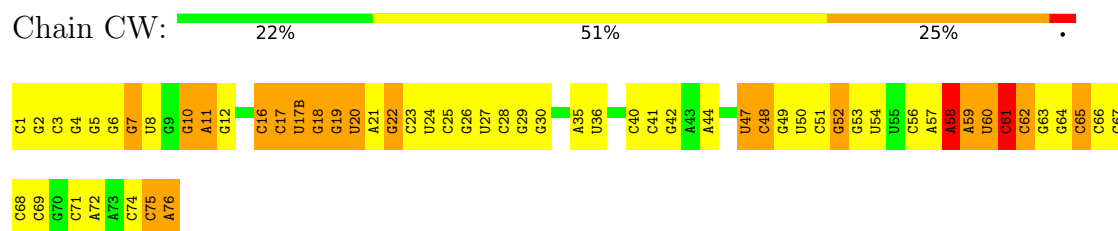
- Molecule 22: Elongation factor P



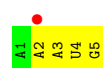
- Molecule 23: tRNA-Met



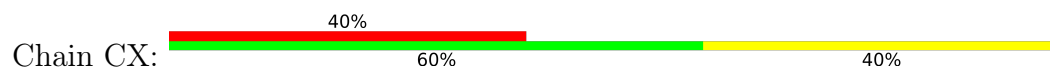
- Molecule 23: tRNA-Met



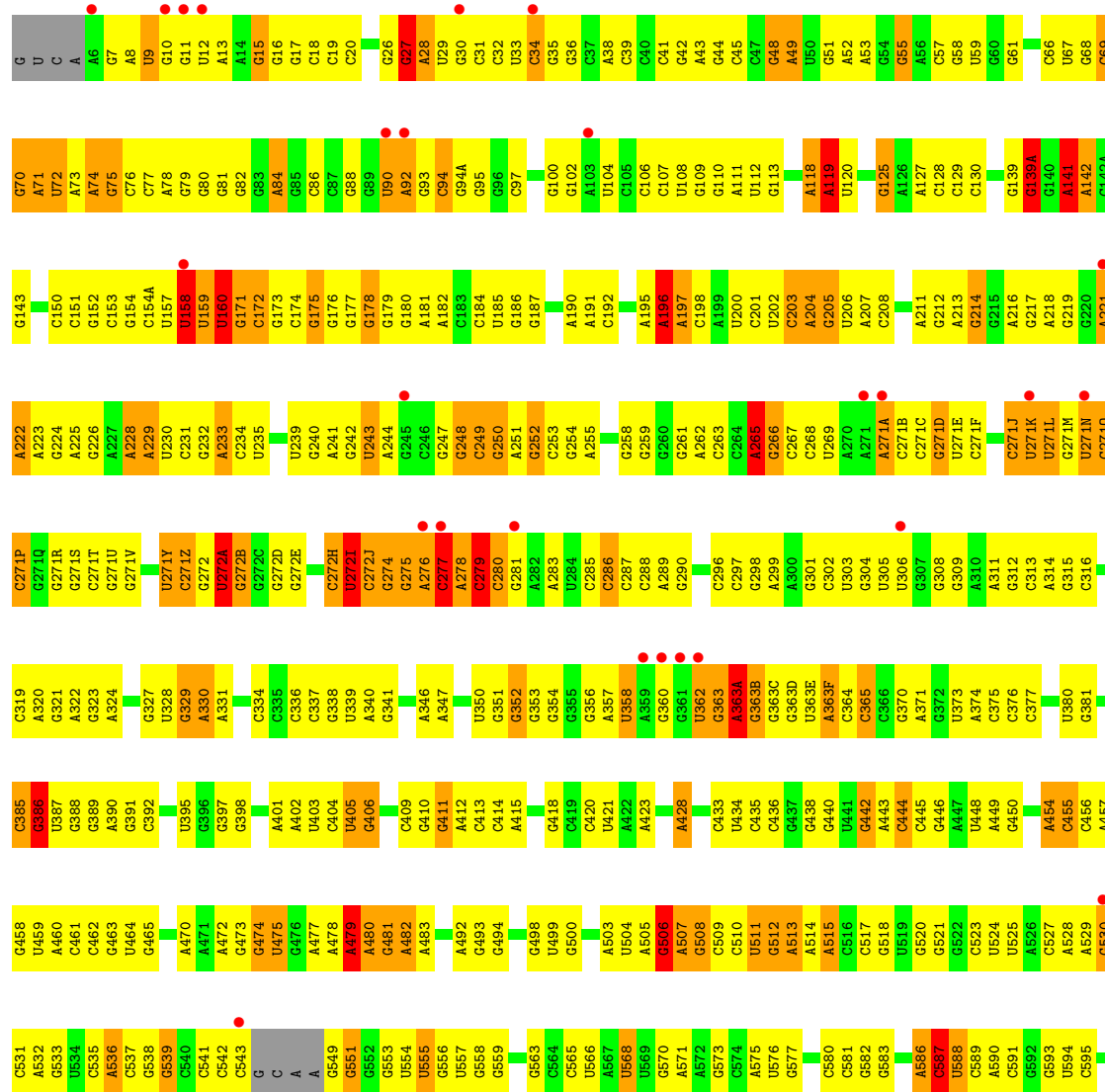
- Molecule 24: RNA (5'-R(P*AP*AP*AP*UP*G)-3')

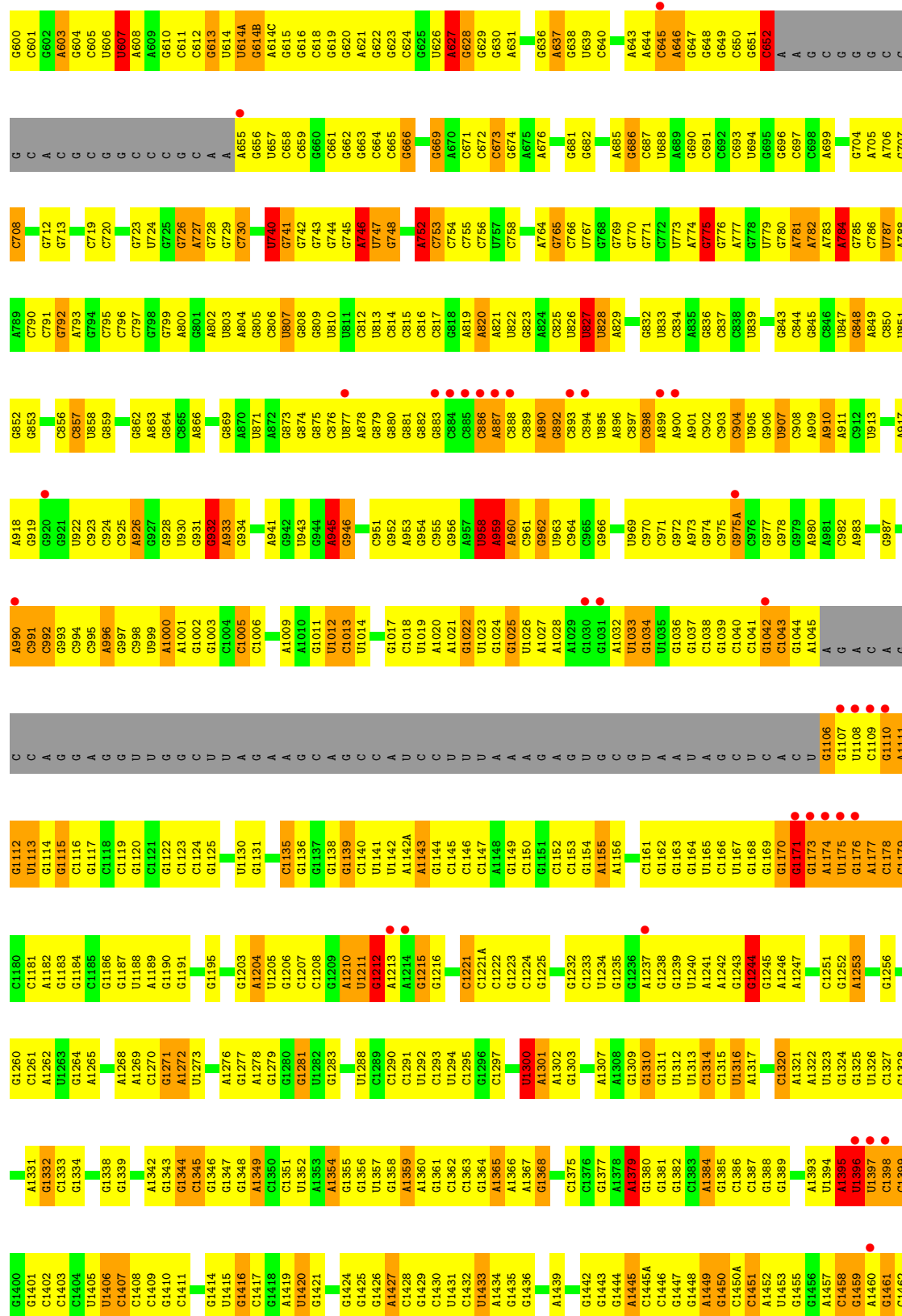


- Molecule 24: RNA (5'-R(P*AP*AP*AP*UP*G)-3')



- Molecule 25: 23S ribosomal RNA





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G2300	C2231	G2161	G2101	G2029	U1963	C1893	G1747	G1747A	G1667	C1598	C1530	C1467
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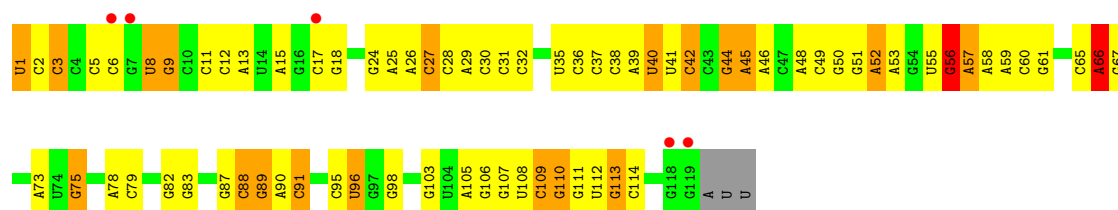
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A	C995	A933	C867	U807	C738	C671	A632	A572	A446	C364	G307	G271D
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C	G1011	G948	G882	A821	C756	C687	G648	U588	C462	G389	G323	G271S
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G	U1013	G950	C885	A824	C758	A689	G650	A590	A394	G325	G325	G271U
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C	U1015	A952	A887	U826	G760	C691	A652	G592	U405	G327	G328	G271W
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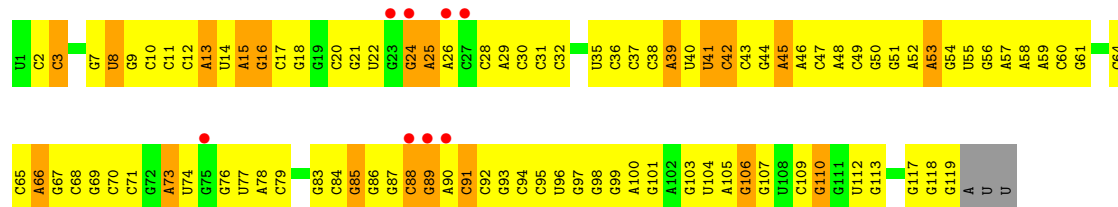
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A2850	U2786	U2726	A2662	C2527	C2528	C2467	G2397	A2333	G2264	G	G2123	A2058
G2851	C2787	G2727	G2663	U2528	G2529	C2468	U2398	G2334	A2268	G	G2124	A2059
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G2853	G2789	G2729	A2665	G2532	G2532	G2470	G2400	A2336	G2270	G	A2126	G2061
G2854	U2790	C2730	C2666	G2533	G2533	C2471	U2401	G2336	G2271	G	G2127	A2062
G2855	G2791	G2731	G2667	A2534	A2534	G2472	C2402	G2339	G2272	G	C2128	C2063
G2856	G2792	G2732	G2668	G2535	G2535	U2473	C2403	G2340	U2273	C	U	C2064
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C2858	G2794	U2734	A2670	U2537	U2537	C2475	G2405	C2342	C2275	U	U	C2066
G2859	G2795	G2735	A2671	G2538	C2538	A2476	U2406	C2343	G2276	G	G	U2068
G2860	U2796	G2736	G2672	U2539	C2539	G2477	G2407	G2344	G2277	G	A	G2069
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G2863	A2801	U2739	A2675	A2542	A2542	C2480	G2410	A2346	G2280	G	C	U2074
G2864	G2802	A2740	G2679	A2543	G2543	G2481	G2411	C2347	G2281	G	C	C2078
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G2867	G2805	G2743	G2682	U2547	U2547	C2484	G2414	G2350	A2199	G	C	C2081
G2868	C2806	C2744	U2682	G2548	G2548	G2485	G2415	C2351	C2284	G	C	U2079
G2869	U2807	G2745	C2683	U2552	U2552	G2486	A2352	G2352	A2286	G	C	U2079
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A2809	A2810	U2747	G2685	U2554	U2554	G2488	C2416	G2354	G2288	G	C	C2081
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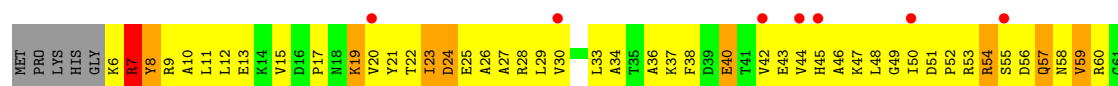
• Molecule 26: 5S ribosomal RNA



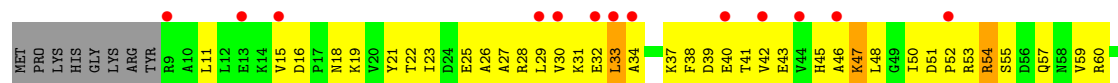
• Molecule 26: 5S ribosomal RNA

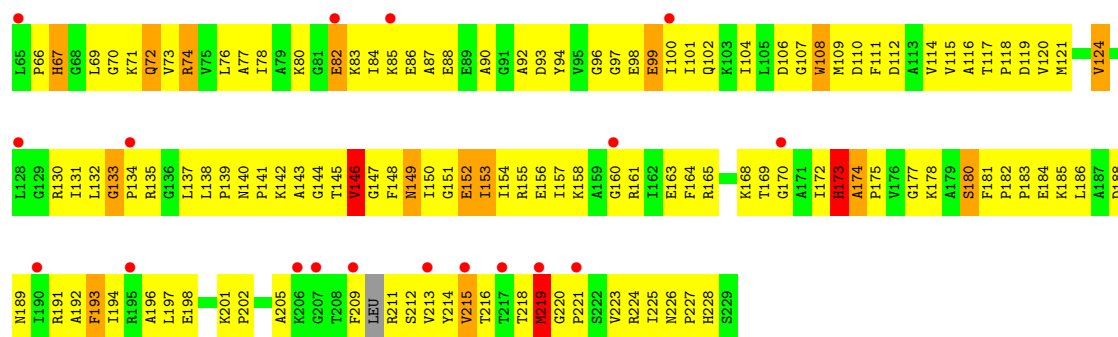


• Molecule 27: 50S ribosomal protein L1

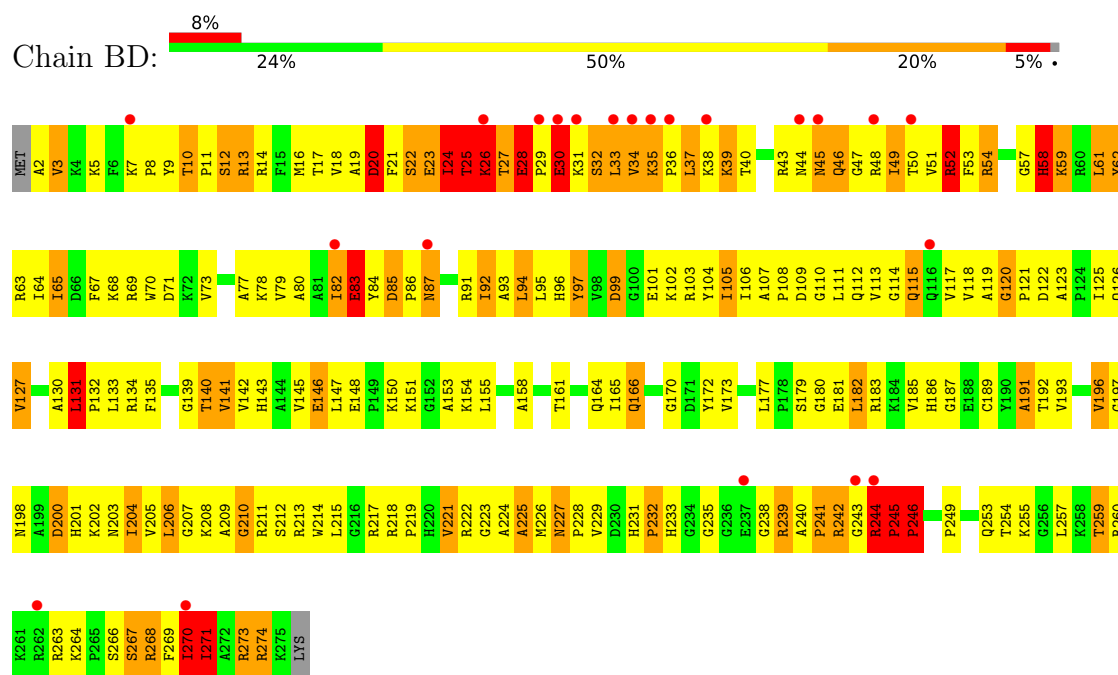


• Molecule 27: 50S ribosomal protein L1

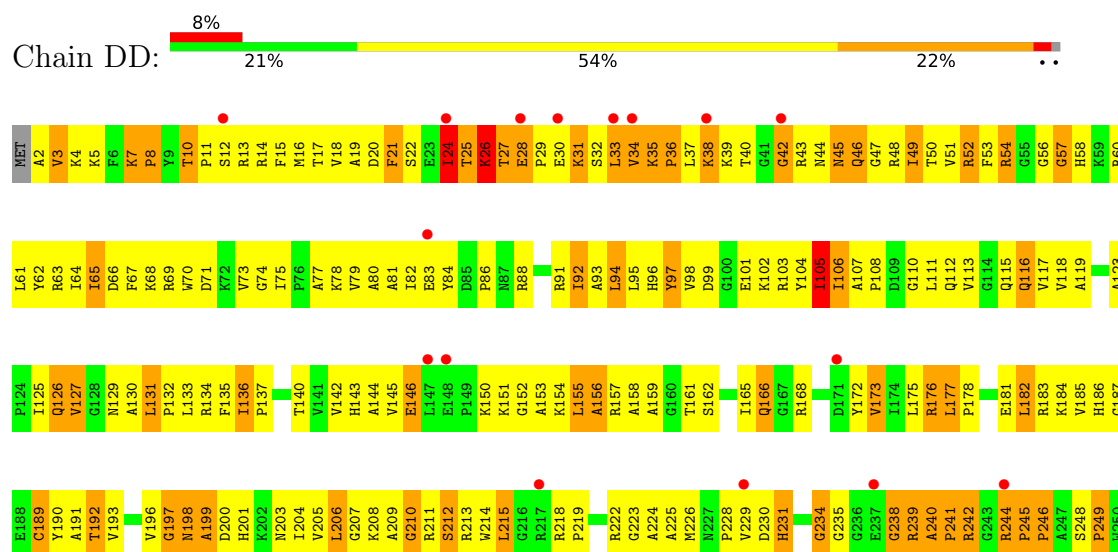


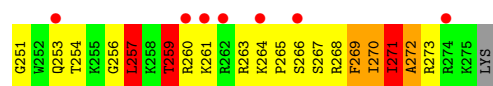


• Molecule 28: 50S ribosomal protein L2

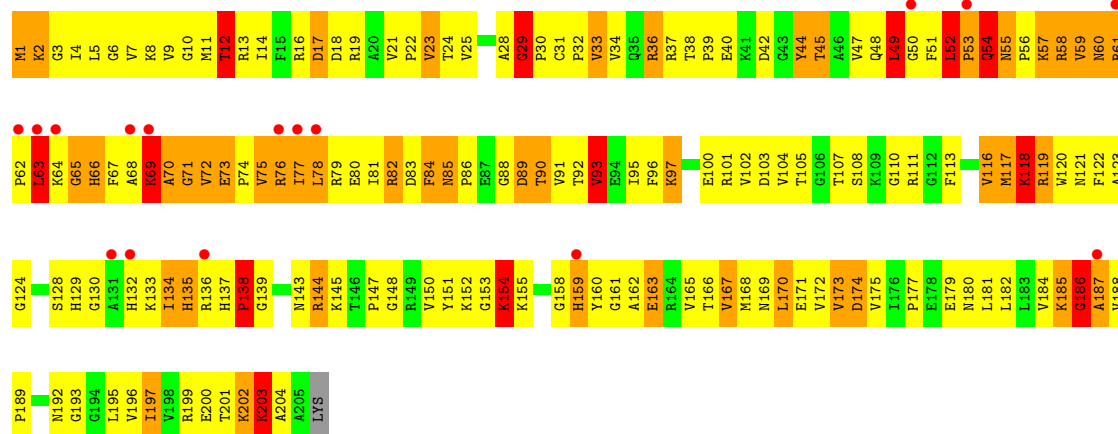
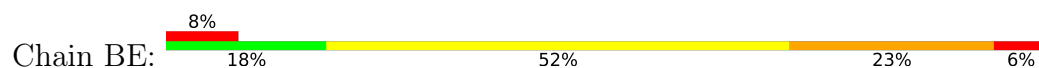


• Molecule 28: 50S ribosomal protein L2

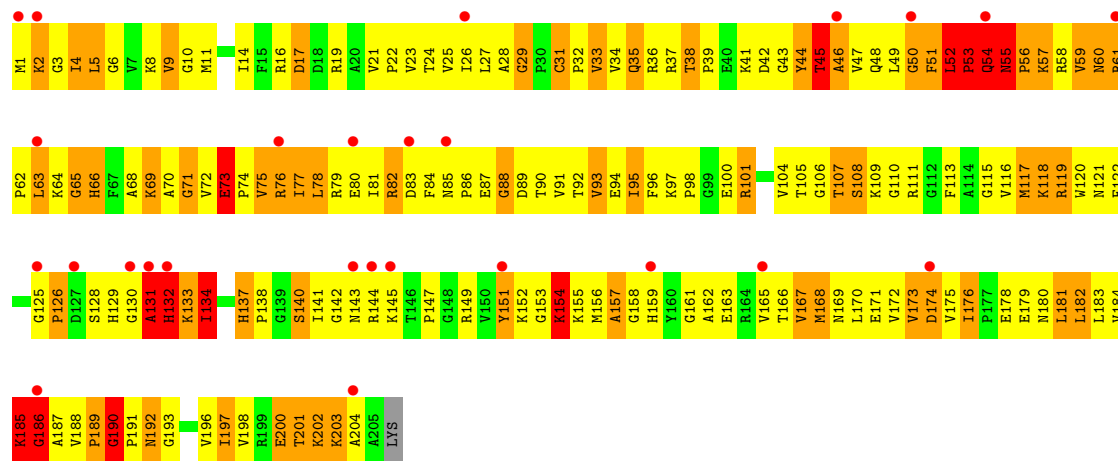




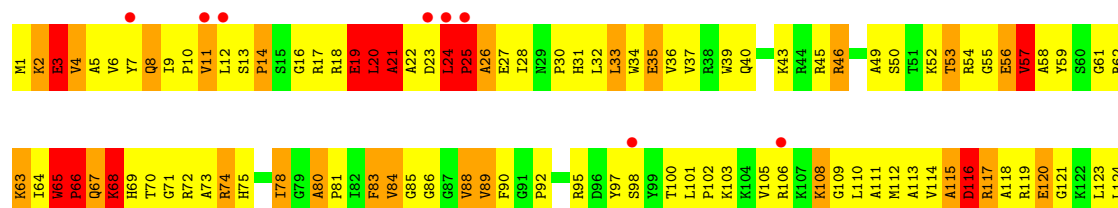
• Molecule 29: 50S ribosomal protein L3

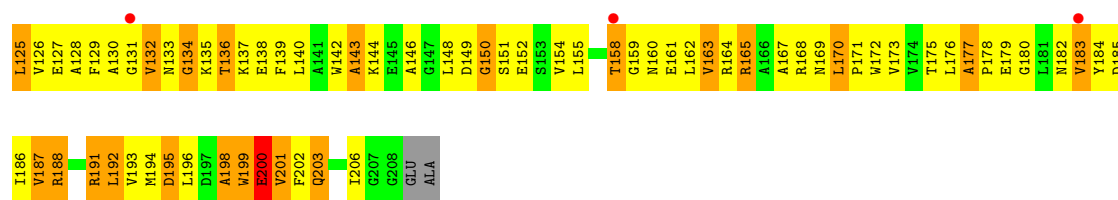


• Molecule 29: 50S ribosomal protein L3

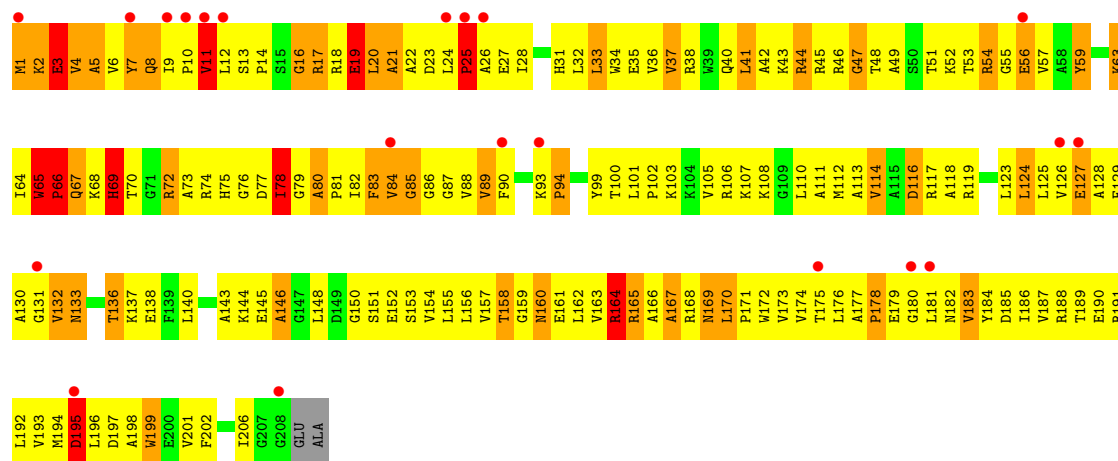
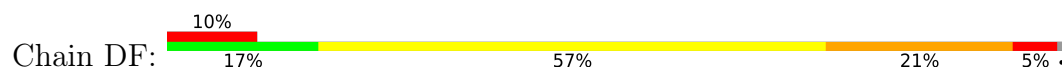


• Molecule 30: 50S ribosomal protein L4

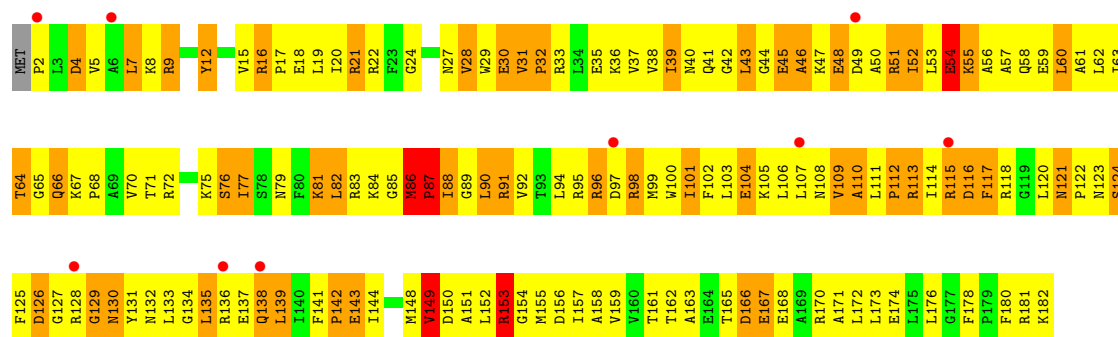
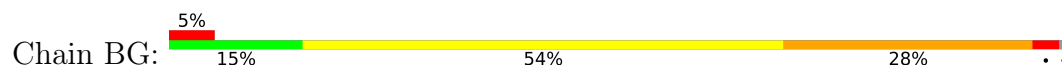




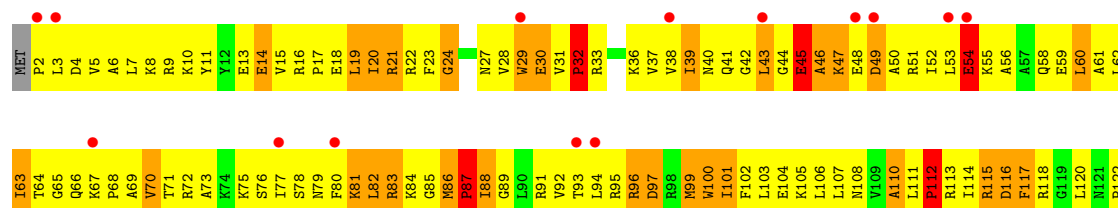
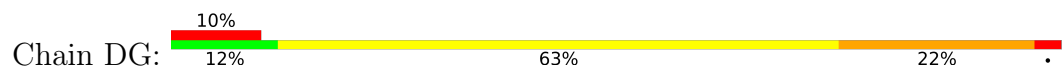
• Molecule 30: 50S ribosomal protein L4



• Molecule 31: 50S ribosomal protein L5

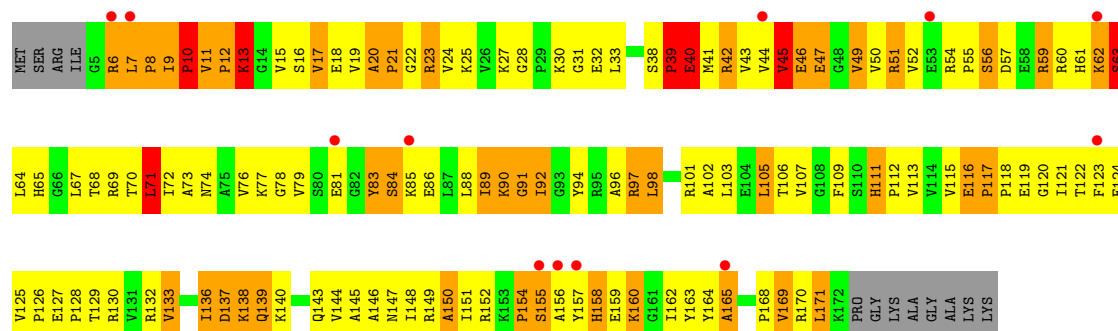
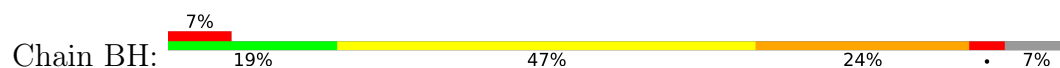


• Molecule 31: 50S ribosomal protein L5

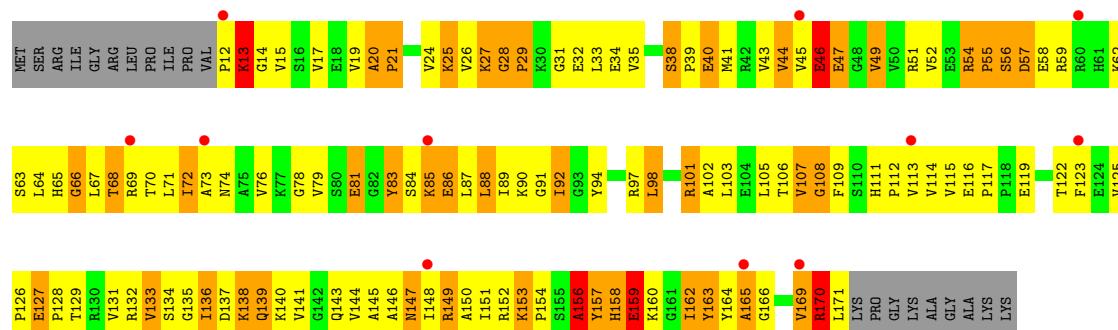
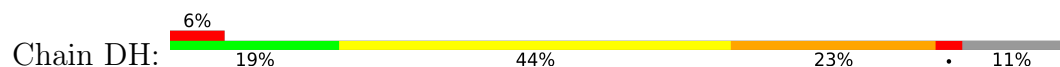




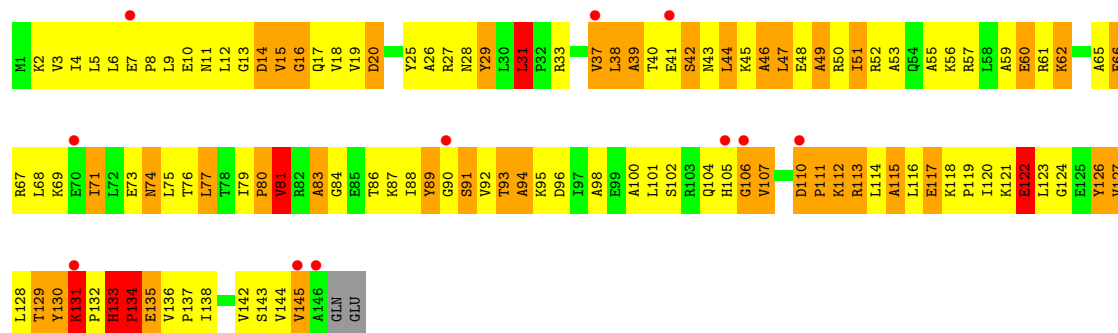
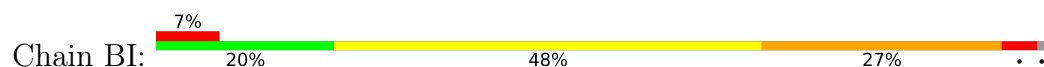
• Molecule 32: 50S ribosomal protein L6



• Molecule 32: 50S ribosomal protein L6

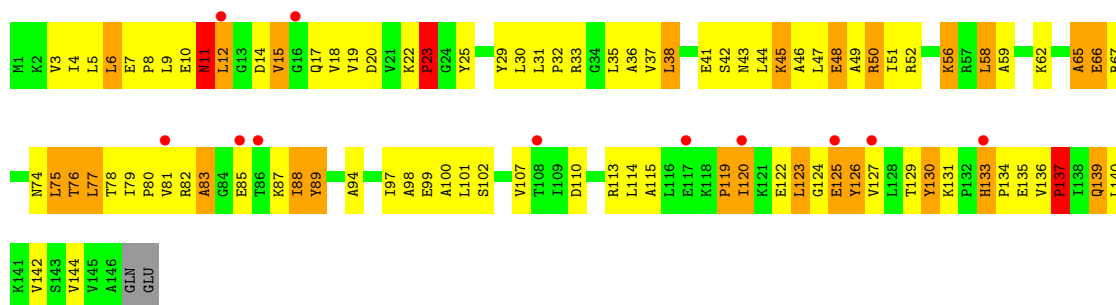


• Molecule 33: 50S ribosomal protein L9

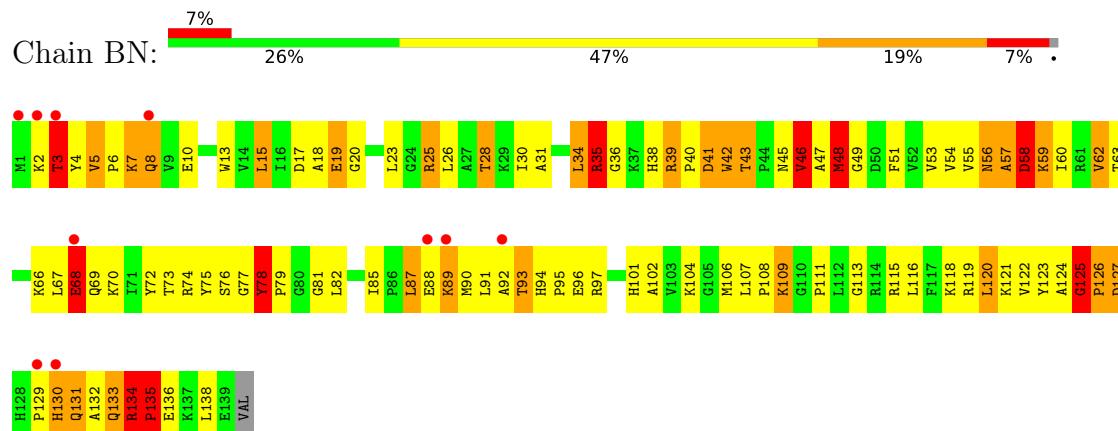


• Molecule 33: 50S ribosomal protein L9

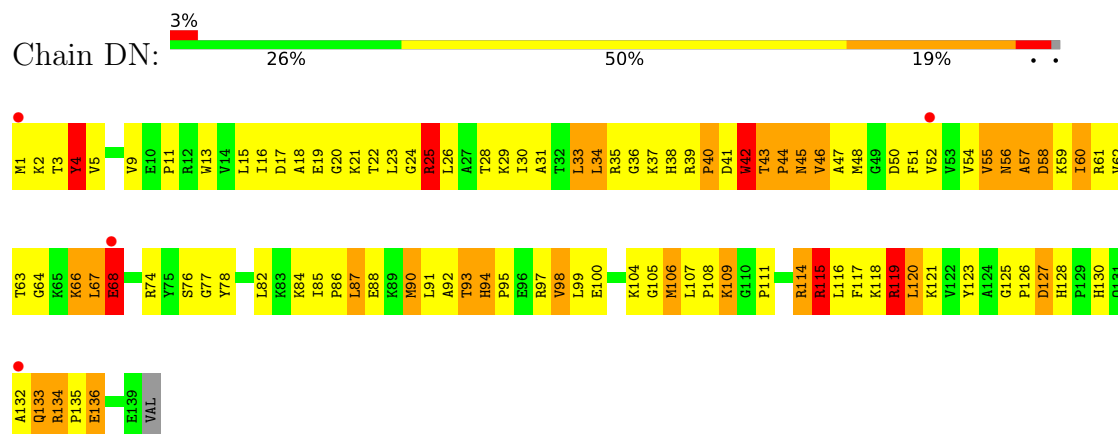




• Molecule 34: 50S ribosomal protein L13



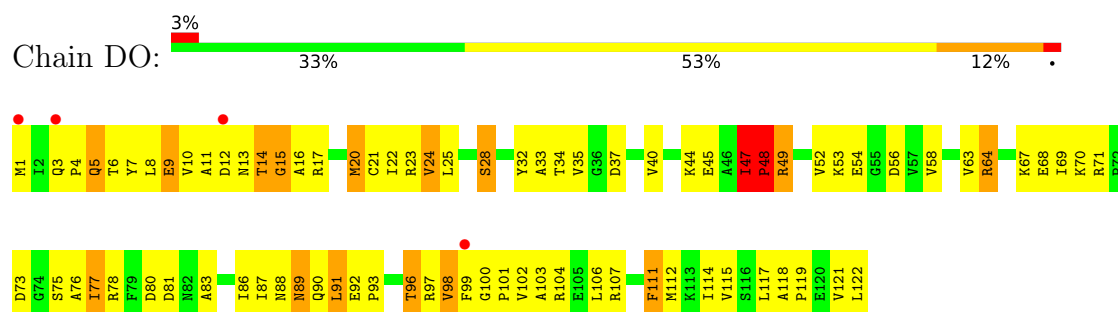
• Molecule 34: 50S ribosomal protein L13



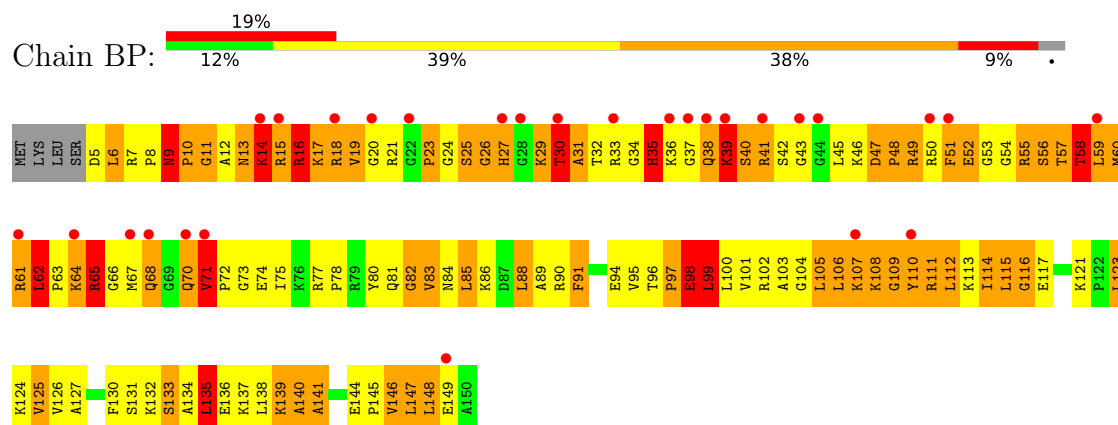
• Molecule 35: 50S ribosomal protein L14



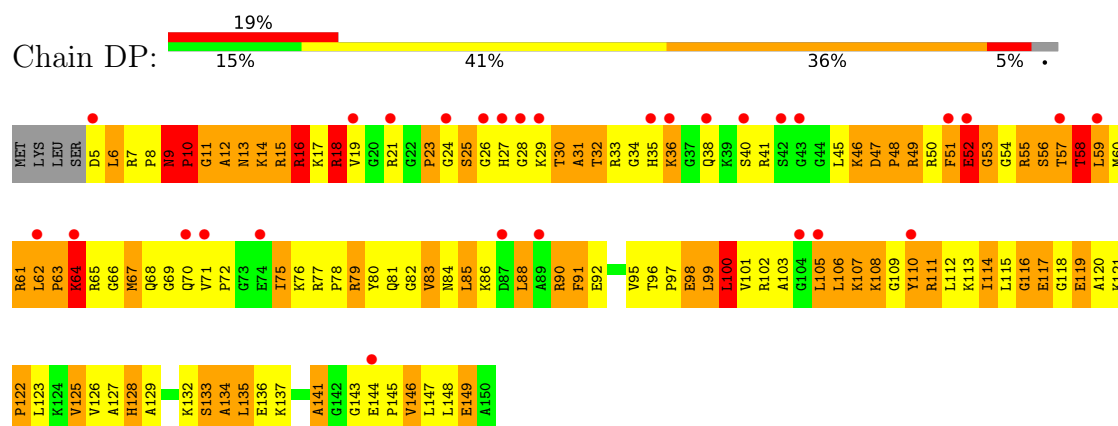
• Molecule 35: 50S ribosomal protein L14



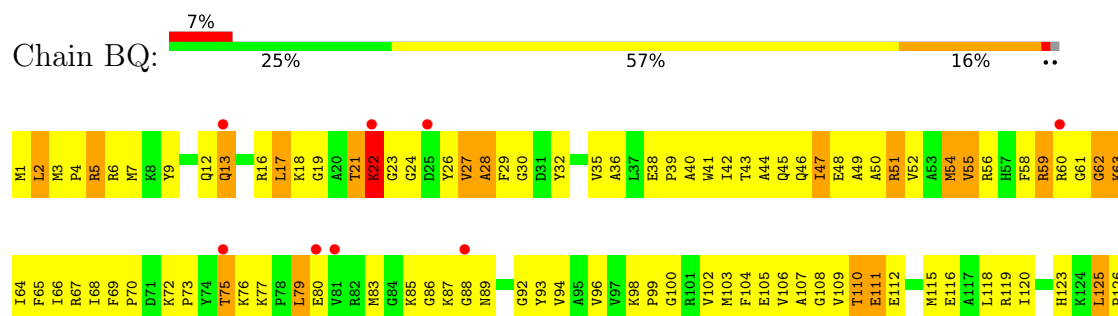
• Molecule 36: 50S ribosomal protein L15

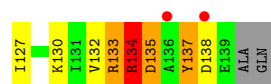


• Molecule 36: 50S ribosomal protein L15

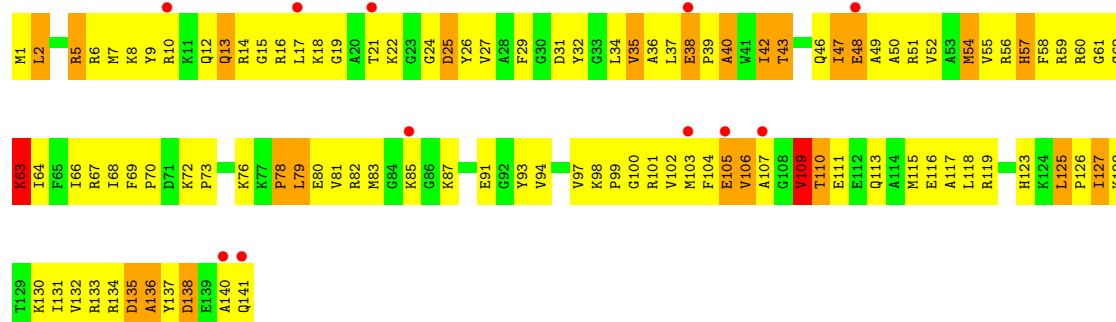


• Molecule 37: 50S ribosomal protein L16

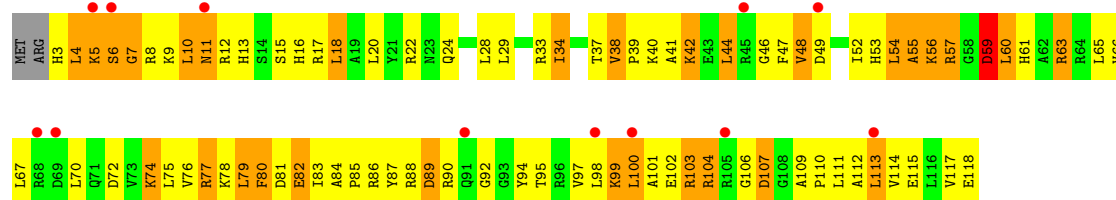




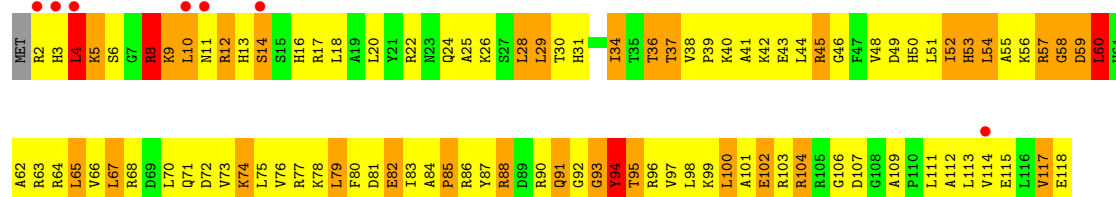
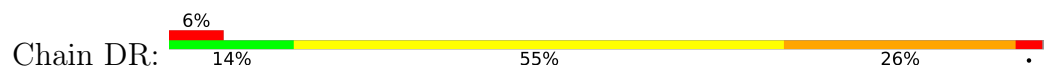
• Molecule 37: 50S ribosomal protein L16



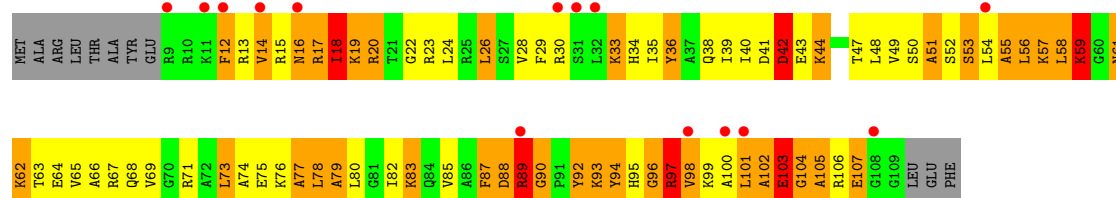
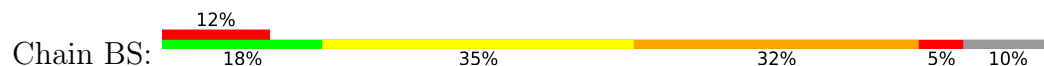
• Molecule 38: 50S ribosomal protein L17



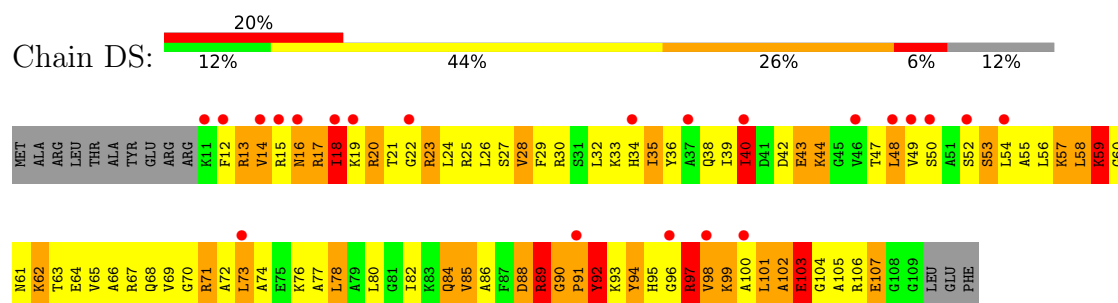
• Molecule 38: 50S ribosomal protein L17



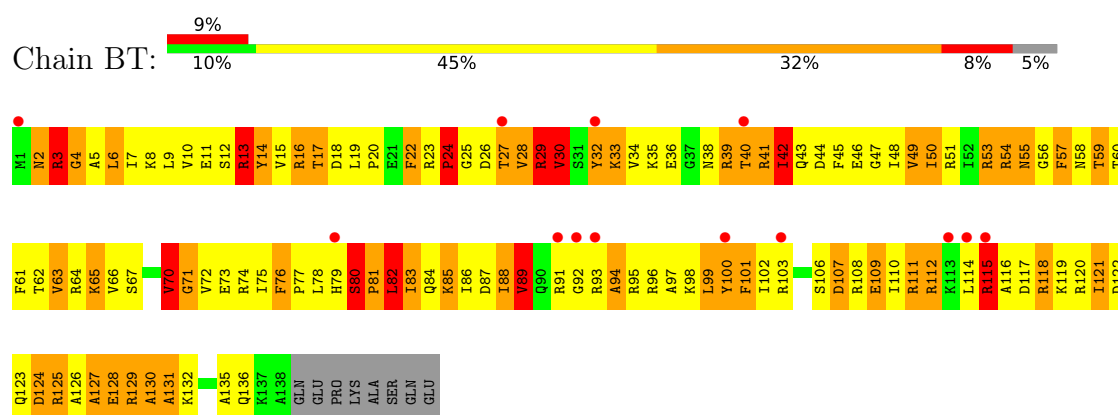
• Molecule 39: 50S ribosomal protein L18



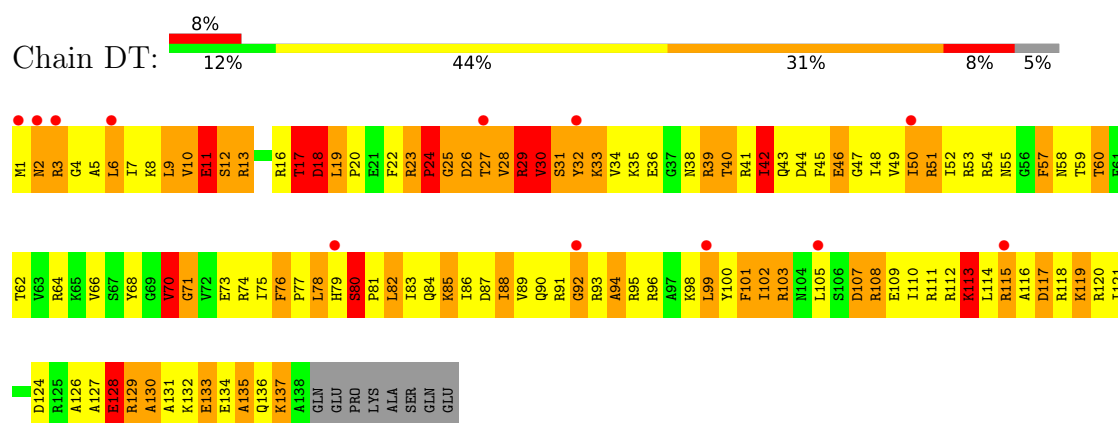
- Molecule 39: 50S ribosomal protein L18



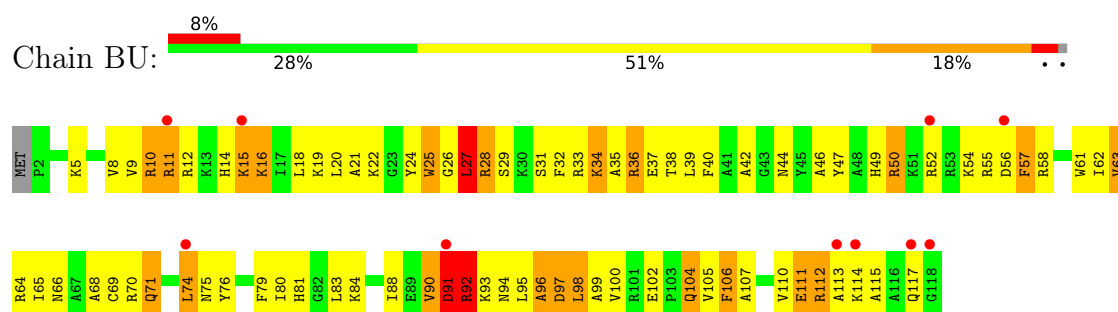
- Molecule 40: 50S ribosomal protein L19



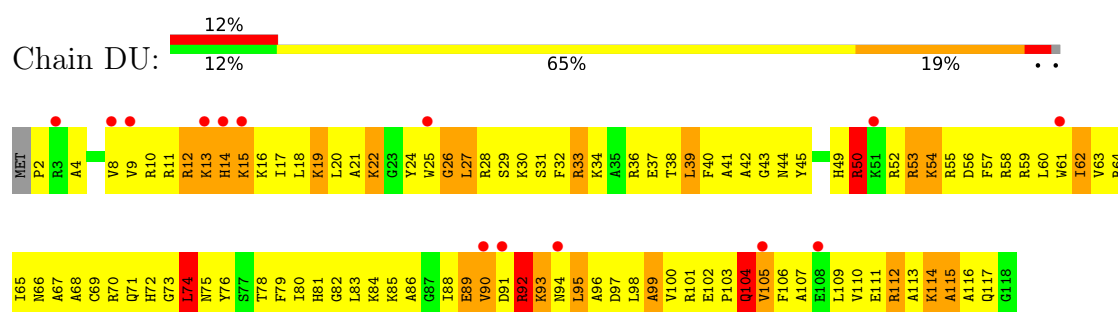
- Molecule 40: 50S ribosomal protein L19



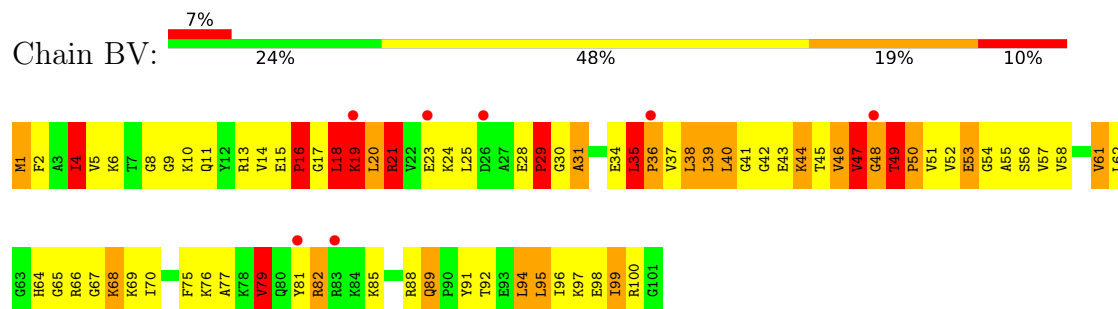
- Molecule 41: 50S ribosomal protein L20



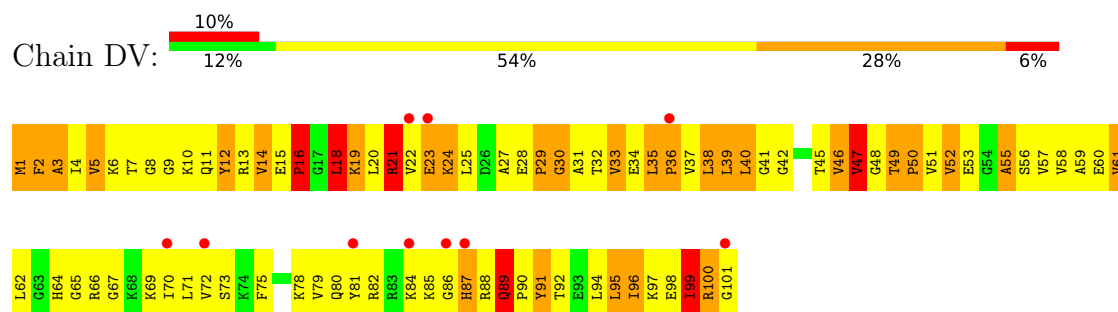
- Molecule 41: 50S ribosomal protein L20



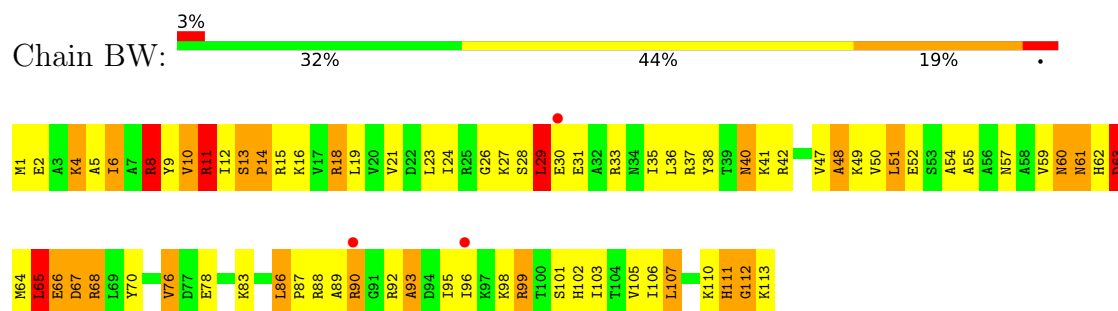
- Molecule 42: 50S ribosomal protein L21



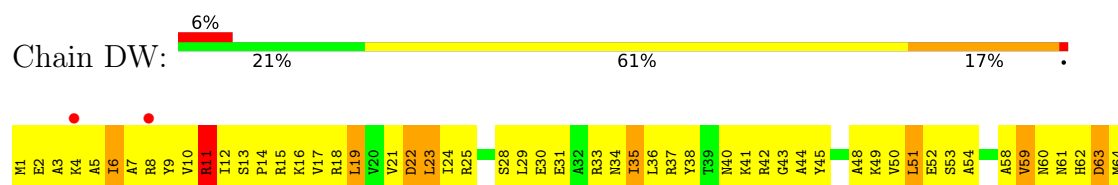
- Molecule 42: 50S ribosomal protein L21



- Molecule 43: 50S ribosomal protein L22

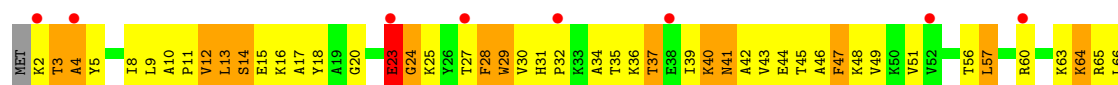


- Molecule 43: 50S ribosomal protein L22

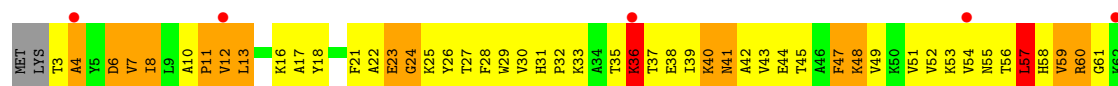




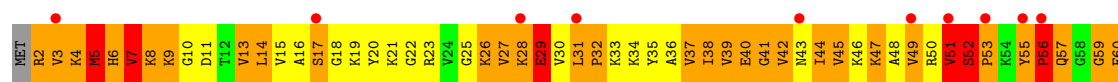
• Molecule 44: 50S ribosomal protein L23



• Molecule 44: 50S ribosomal protein L23



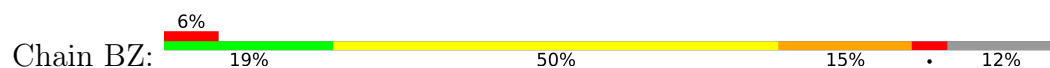
• Molecule 45: 50S ribosomal protein L24

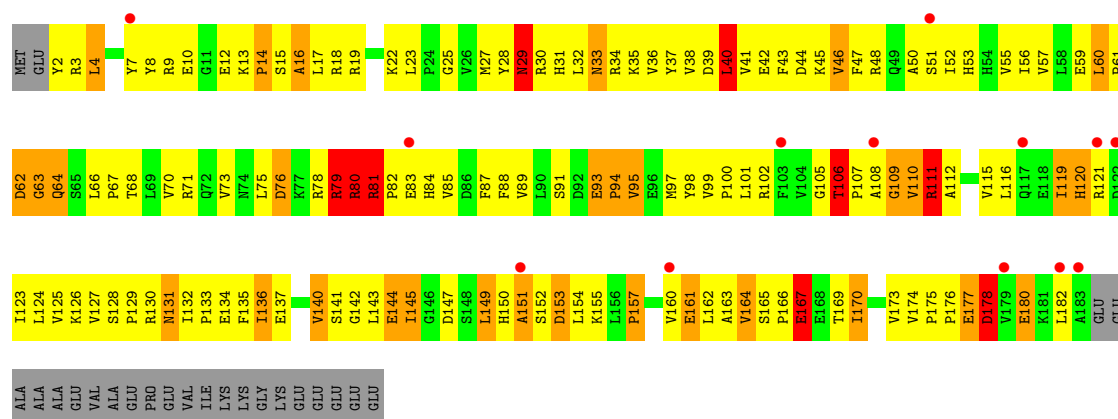


• Molecule 45: 50S ribosomal protein L24

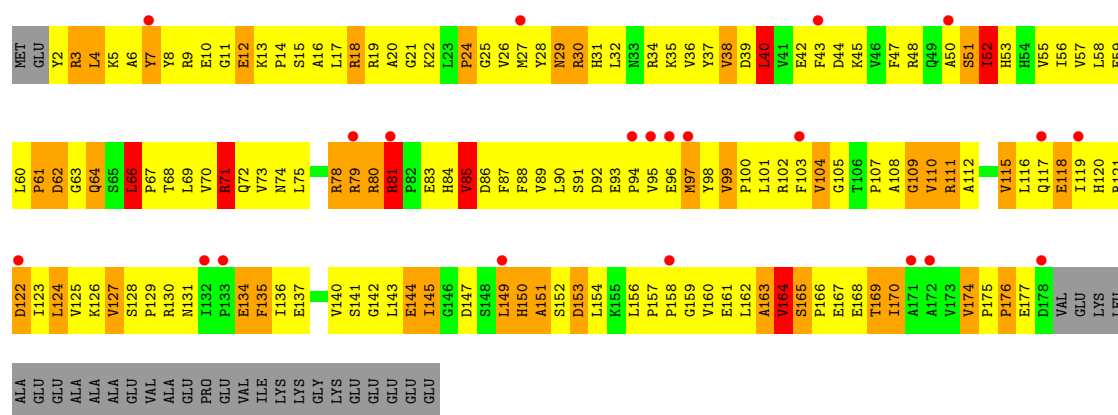
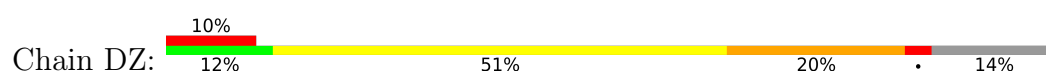


• Molecule 46: 50S ribosomal protein L25

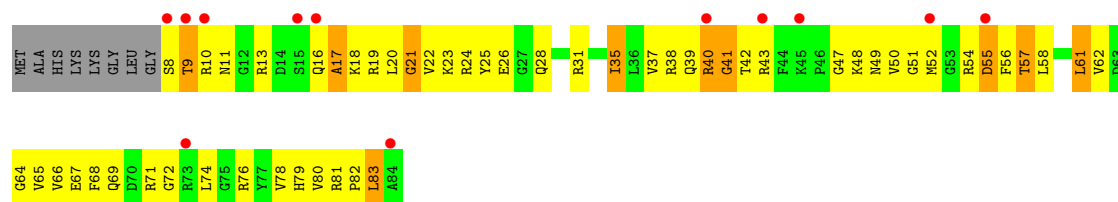




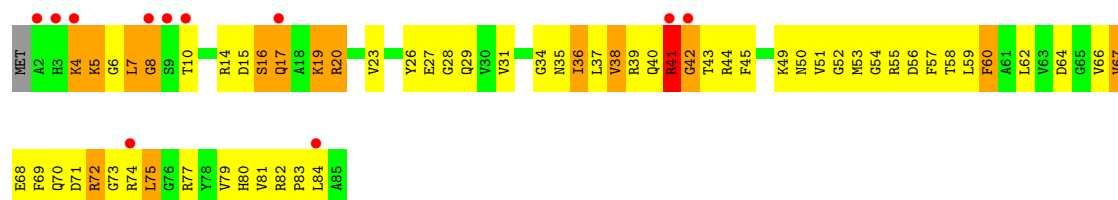
• Molecule 46: 50S ribosomal protein L25



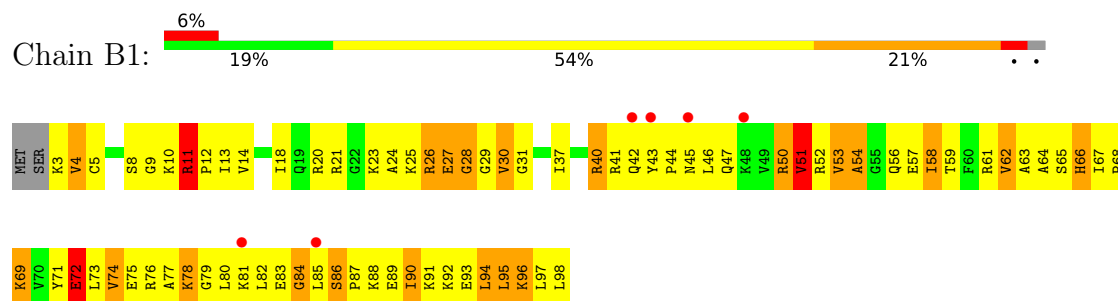
• Molecule 47: 50S ribosomal protein L27



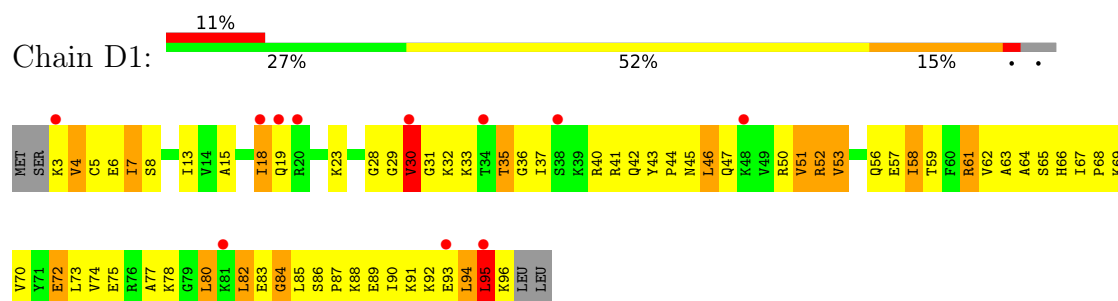
• Molecule 47: 50S ribosomal protein L27



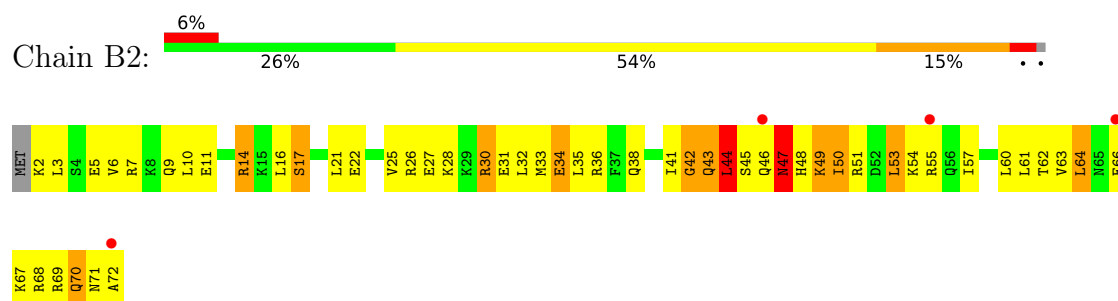
• Molecule 48: 50S ribosomal protein L28



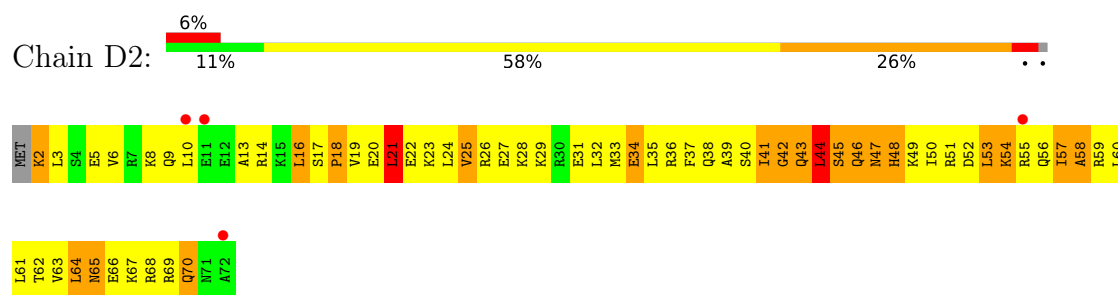
• Molecule 48: 50S ribosomal protein L28



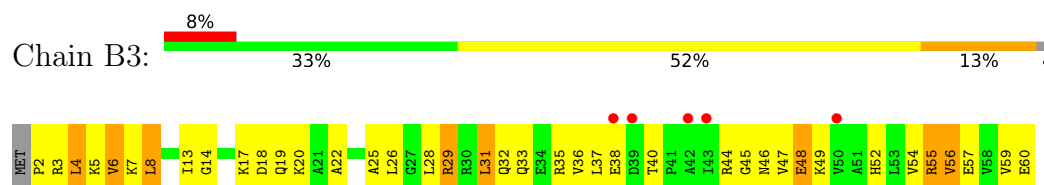
• Molecule 49: 50S ribosomal protein L29



• Molecule 49: 50S ribosomal protein L29

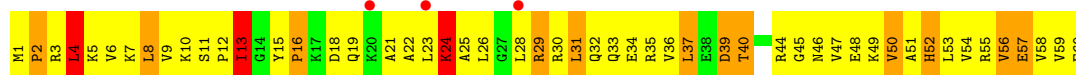


• Molecule 50: 50S ribosomal protein L30



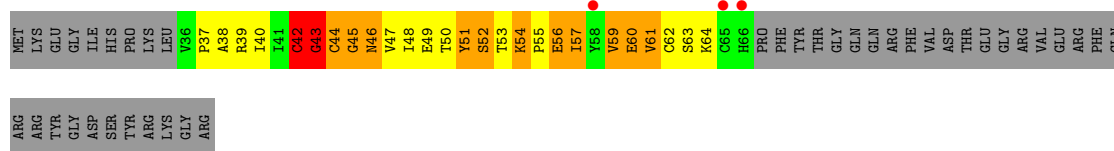
- Molecule 50: 50S ribosomal protein L30

Chain D3: 



- Molecule 51: 50S ribosomal protein L31

Chain B4: 



- Molecule 51: 50S ribosomal protein L31

Chain D4: 

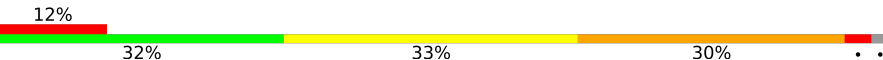


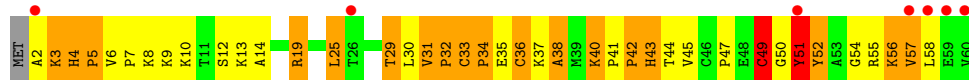
- Molecule 52: 50S ribosomal protein L32

Chain B5: 



- Molecule 52: 50S ribosomal protein L32

Chain D5: 

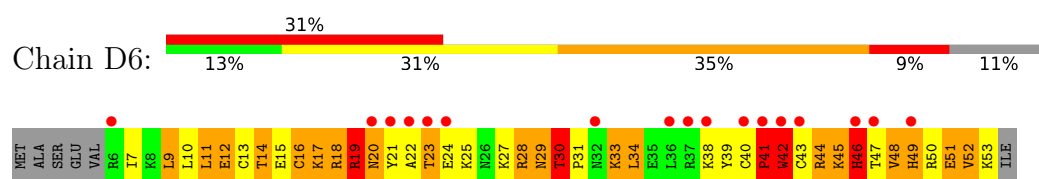


- Molecule 53: 50S ribosomal protein L33

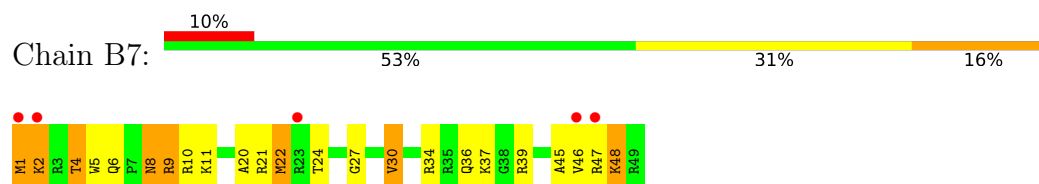
Chain B6: 



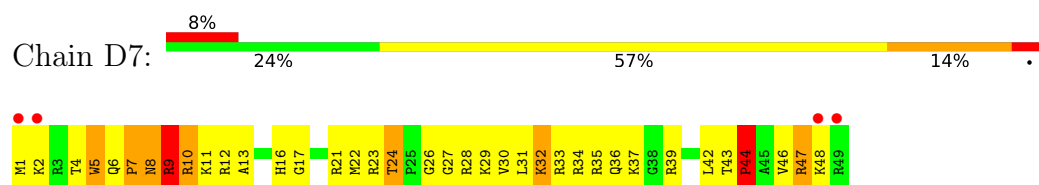
- Molecule 53: 50S ribosomal protein L33



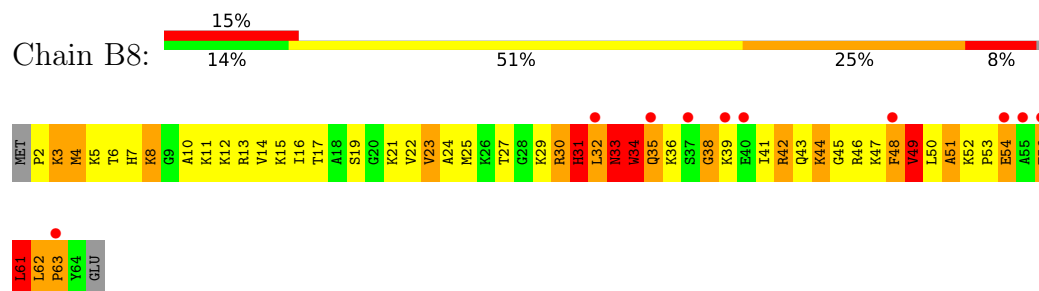
- Molecule 54: 50S ribosomal protein L34



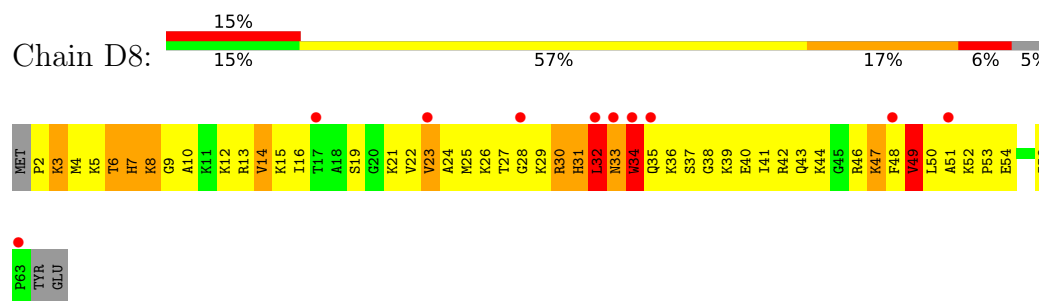
- Molecule 54: 50S ribosomal protein L34



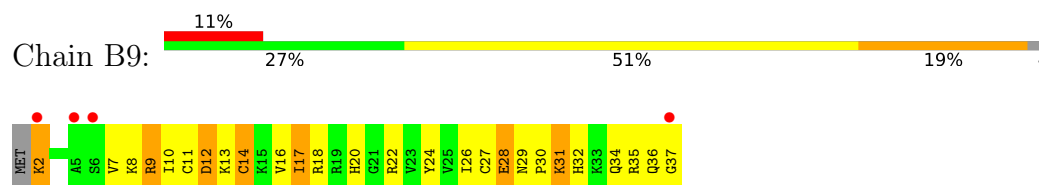
- Molecule 55: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.53Å 447.03Å 622.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.10 200.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.10) 94.7 (200.00-3.10)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.302 0.252 , 0.249	Depositor DCC
R_{free} test set	49631 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	290405	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.52	6/35982 (0.0%)	0.70	47/56156 (0.1%)
1	CA	0.36	0/36193	0.66	27/56490 (0.0%)
2	AB	0.46	0/1936	1.07	16/2611 (0.6%)
2	CB	0.48	0/1936	1.15	20/2611 (0.8%)
3	AC	0.47	0/1637	1.04	9/2207 (0.4%)
3	CC	0.48	0/1637	1.06	10/2207 (0.5%)
4	AD	0.47	0/1733	1.09	19/2318 (0.8%)
4	CD	0.50	0/1733	1.13	14/2318 (0.6%)
5	AE	0.51	0/1163	1.07	9/1566 (0.6%)
5	CE	0.51	0/1163	1.01	4/1566 (0.3%)
6	AF	0.54	0/856	1.02	3/1154 (0.3%)
6	CF	0.47	0/856	1.00	4/1154 (0.3%)
7	AG	0.48	0/1276	1.10	16/1709 (0.9%)
7	CG	0.48	0/1276	1.12	16/1709 (0.9%)
8	AH	0.50	0/1136	1.11	8/1527 (0.5%)
8	CH	0.47	0/1136	1.06	5/1527 (0.3%)
9	AI	0.49	0/1022	1.08	8/1369 (0.6%)
9	CI	0.47	0/1022	1.07	7/1369 (0.5%)
10	AJ	0.52	0/808	1.09	4/1087 (0.4%)
10	CJ	0.55	0/808	1.18	10/1087 (0.9%)
11	AK	0.48	0/900	1.13	8/1213 (0.7%)
11	CK	0.45	0/900	1.07	9/1213 (0.7%)
12	AL	0.48	0/987	1.20	11/1322 (0.8%)
12	CL	0.53	0/987	1.11	7/1322 (0.5%)
13	AM	0.51	0/957	1.19	7/1283 (0.5%)
13	CM	0.51	0/957	1.19	11/1283 (0.9%)
14	AN	0.48	0/501	1.12	5/664 (0.8%)
14	CN	0.51	0/501	0.92	0/664
15	AO	0.53	0/745	1.01	4/992 (0.4%)
15	CO	0.48	0/745	1.03	6/992 (0.6%)
16	AP	0.49	0/717	1.07	5/965 (0.5%)
16	CP	0.52	0/717	1.09	7/965 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.49	0/837	1.00	6/1119 (0.5%)
17	CQ	0.47	0/837	1.07	4/1119 (0.4%)
18	AR	0.47	0/579	1.01	1/768 (0.1%)
18	CR	0.50	0/579	1.09	4/768 (0.5%)
19	AS	0.48	0/625	1.12	6/844 (0.7%)
19	CS	0.54	0/632	1.24	7/853 (0.8%)
20	AT	0.44	0/765	1.19	9/1007 (0.9%)
20	CT	0.48	0/765	1.16	8/1007 (0.8%)
21	AU	0.53	0/213	0.83	0/279
21	CU	0.52	0/213	0.86	0/279
22	AV	0.53	0/1393	1.00	5/1883 (0.3%)
22	CV	0.51	0/1393	0.98	6/1883 (0.3%)
23	AW	0.41	1/1836 (0.1%)	0.71	2/2859 (0.1%)
23	CW	0.37	0/1836	0.70	3/2859 (0.1%)
24	AX	0.56	0/123	0.67	0/188
24	CX	0.55	0/123	0.63	0/188
25	BA	0.46	1/66745 (0.0%)	0.76	88/104189 (0.1%)
25	DA	0.40	1/66983 (0.0%)	0.72	83/104560 (0.1%)
26	BB	0.38	0/2853	0.78	10/4451 (0.2%)
26	DB	0.37	0/2853	0.70	0/4451
27	BC	0.48	0/1732	1.11	11/2335 (0.5%)
27	DC	0.73	1/1668 (0.1%)	1.04	5/2251 (0.2%)
28	BD	0.74	1/2177 (0.0%)	1.28	28/2935 (1.0%)
28	DD	0.62	0/2165	1.25	24/2921 (0.8%)
29	BE	0.68	0/1597	1.28	21/2155 (1.0%)
29	DE	0.64	0/1597	1.27	23/2155 (1.1%)
30	BF	0.70	0/1659	1.31	29/2246 (1.3%)
30	DF	0.53	0/1659	1.13	17/2246 (0.8%)
31	BG	0.51	0/1499	1.10	13/2016 (0.6%)
31	DG	0.50	0/1499	1.18	10/2016 (0.5%)
32	BH	0.67	1/1254 (0.1%)	1.32	17/1703 (1.0%)
32	DH	0.51	0/1246	1.14	11/1684 (0.7%)
33	BI	0.56	0/1056	1.23	12/1443 (0.8%)
33	DI	0.55	0/881	1.15	7/1219 (0.6%)
34	BN	0.69	0/1132	1.21	14/1527 (0.9%)
34	DN	0.49	0/1132	1.07	5/1527 (0.3%)
35	BO	0.66	0/943	1.19	10/1269 (0.8%)
35	DO	0.58	0/943	1.13	7/1269 (0.6%)
36	BP	0.67	0/1131	1.56	29/1504 (1.9%)
36	DP	0.58	0/1095	1.36	13/1460 (0.9%)
37	BQ	0.59	0/1120	1.07	5/1498 (0.3%)
37	DQ	0.55	0/1143	1.07	8/1527 (0.5%)
38	BR	0.67	0/936	1.19	11/1256 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.57	0/974	1.14	9/1302 (0.7%)
39	BS	0.56	0/785	1.24	6/1048 (0.6%)
39	DS	0.55	0/779	1.25	9/1038 (0.9%)
40	BT	0.63	1/1156 (0.1%)	1.34	24/1544 (1.6%)
40	DT	0.57	0/1156	1.34	21/1544 (1.4%)
41	BU	0.69	0/975	1.18	10/1297 (0.8%)
41	DU	0.51	0/975	1.10	9/1297 (0.7%)
42	BV	0.71	0/790	1.27	7/1057 (0.7%)
42	DV	0.51	0/790	1.07	7/1057 (0.7%)
43	BW	0.74	0/907	1.11	9/1216 (0.7%)
43	DW	0.56	0/907	1.01	3/1216 (0.2%)
44	BX	0.69	0/749	1.12	4/1006 (0.4%)
44	DX	0.56	0/740	1.09	7/995 (0.7%)
45	BY	0.74	0/770	1.39	14/1031 (1.4%)
45	DY	0.59	0/789	1.30	9/1053 (0.9%)
46	BZ	0.53	0/1470	1.07	11/1998 (0.6%)
46	DZ	0.48	0/1436	1.04	11/1951 (0.6%)
47	B0	0.61	0/621	1.03	2/827 (0.2%)
47	D0	0.51	0/671	0.98	2/892 (0.2%)
48	B1	0.66	0/764	1.12	5/1014 (0.5%)
48	D1	0.50	0/739	1.01	2/983 (0.2%)
49	B2	0.59	0/600	1.10	4/793 (0.5%)
49	D2	0.46	0/600	1.02	1/793 (0.1%)
50	B3	0.62	0/465	1.06	1/625 (0.2%)
50	D3	0.49	0/473	1.08	6/636 (0.9%)
51	B4	0.59	0/229	1.25	4/311 (1.3%)
51	D4	0.53	0/229	1.10	3/311 (1.0%)
52	B5	0.79	0/449	1.34	9/608 (1.5%)
52	D5	0.68	0/473	1.13	3/639 (0.5%)
53	B6	0.80	1/408 (0.2%)	1.24	5/548 (0.9%)
53	D6	0.61	0/328	1.52	7/450 (1.6%)
54	B7	0.81	0/427	1.23	8/563 (1.4%)
54	D7	0.66	0/427	1.06	1/563 (0.2%)
55	B8	0.72	0/503	1.37	8/663 (1.2%)
55	D8	0.61	0/473	1.17	6/626 (1.0%)
56	B9	0.62	0/297	1.02	1/391 (0.3%)
56	D9	0.47	0/302	1.19	2/397 (0.5%)
All	All	0.48	14/313996 (0.0%)	0.86	1158/468619 (0.2%)

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
1	AA	0	38
1	CA	0	17
23	AW	0	2
23	CW	0	2
25	BA	3	106
25	DA	1	76
26	BB	0	2
26	DB	0	1
28	BD	0	1
52	B5	0	1
52	D5	0	1
All	All	4	247

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1223	C	C4'-C3'	47.48	2.47	1.52
1	AA	1223	C	C3'-C2'	37.99	2.29	1.53
1	AA	1223	C	C3'-O3'	-28.78	0.84	1.42
27	DC	180	SER	CB-OG	20.37	1.82	1.42
1	AA	1222	G	O3'-P	12.49	1.79	1.61

The worst 5 of 1158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1223	C	P-O3'-C3'	-24.58	83.33	120.20
25	BA	1992	G	C2'-C3'-O3'	16.42	134.13	109.50
31	DG	54	GLU	N-CA-C	-15.69	94.09	113.38
25	DA	1992	G	C2'-C3'-O3'	15.62	132.93	109.50
39	BS	16	ASN	N-CA-C	-15.09	93.22	112.23

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	BA	454	A	C3'
25	BA	775	G	C3'
25	BA	1992	G	C3'
25	DA	1992	G	C3'

5 of 247 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	114	U	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	127	G	Sidechain
1	AA	250	A	Sidechain
1	AA	253	U	Sidechain
1	AA	47	C	Sidechain

5.2 Too-close contacts

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	32144	0	16225	1845	0
1	CA	32332	0	16317	1684	0
2	AB	1901	0	1951	381	0
2	CB	1901	0	1951	382	0
3	AC	1613	0	1677	343	0
3	CC	1613	0	1677	287	0
4	AD	1703	0	1763	345	0
4	CD	1703	0	1763	225	0
5	AE	1147	0	1207	175	0
5	CE	1147	0	1207	191	0
6	AF	843	0	857	120	0
6	CF	843	0	857	146	0
7	AG	1257	0	1296	200	0
7	CG	1257	0	1296	225	0
8	AH	1116	0	1177	188	0
8	CH	1116	0	1177	178	0
9	AI	1004	0	1031	196	0
9	CI	1004	0	1031	208	0
10	AJ	795	0	840	224	0
10	CJ	795	0	840	194	0
11	AK	885	0	904	135	0
11	CK	885	0	904	117	0
12	AL	971	0	1057	172	0
12	CL	971	0	1057	139	0
13	AM	947	0	1008	201	0
13	CM	947	0	1008	144	0
14	AN	492	0	533	116	0
14	CN	492	0	533	99	0
15	AO	734	0	771	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	734	0	771	117	0
16	AP	701	0	720	131	0
16	CP	701	0	720	109	0
17	AQ	824	0	891	114	0
17	CQ	824	0	891	92	0
18	AR	574	0	644	111	0
18	CR	574	0	644	107	0
19	AS	613	0	621	137	0
19	CS	619	0	639	122	0
20	AT	763	0	861	154	0
20	CT	763	0	861	150	0
21	AU	209	0	221	16	0
21	CU	209	0	221	32	0
22	AV	1367	0	1364	194	0
22	CV	1367	0	1364	206	0
23	AW	1644	0	834	67	0
23	CW	1644	0	836	74	0
24	AX	110	0	55	4	0
24	CX	110	0	55	3	0
25	BA	59596	0	30049	2584	0
25	DA	59809	0	30157	2947	0
26	BB	2551	0	1295	93	0
26	DB	2551	0	1295	143	0
27	BC	1702	0	1747	288	0
27	DC	1640	0	1651	251	0
28	BD	2127	0	2208	347	0
28	DD	2115	0	2186	352	0
29	BE	1564	0	1629	265	0
29	DE	1564	0	1629	289	0
30	BF	1624	0	1677	291	0
30	DF	1624	0	1677	313	0
31	BG	1474	0	1535	299	0
31	DG	1474	0	1535	286	0
32	BH	1231	0	1260	207	0
32	DH	1223	0	1282	241	0
33	BI	1043	0	1019	186	0
33	DI	871	0	680	107	0
34	BN	1105	0	1180	135	0
34	DN	1105	0	1180	181	0
35	BO	933	0	996	161	0
35	DO	933	0	996	118	0
36	BP	1114	0	1187	342	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DP	1079	0	1117	275	0
37	BQ	1099	0	1160	151	0
37	DQ	1122	0	1179	194	0
38	BR	923	0	949	108	0
38	DR	960	0	1021	165	0
39	BS	777	0	825	185	0
39	DS	771	0	832	166	0
40	BT	1142	0	1202	285	0
40	DT	1142	0	1202	242	0
41	BU	958	0	1015	162	0
41	DU	958	0	1015	240	0
42	BV	779	0	852	171	0
42	DV	779	0	852	215	0
43	BW	896	0	953	99	0
43	DW	896	0	953	128	0
44	BX	735	0	791	87	0
44	DX	726	0	778	127	0
45	BY	757	0	821	205	0
45	DY	776	0	870	206	0
46	BZ	1438	0	1455	207	0
46	DZ	1404	0	1432	311	0
47	B0	613	0	633	91	0
47	D0	662	0	688	115	0
48	B1	757	0	843	114	0
48	D1	732	0	808	100	0
49	B2	598	0	653	61	0
49	D2	598	0	653	115	0
50	B3	460	0	512	46	0
50	D3	468	0	523	94	0
51	B4	226	0	229	48	0
51	D4	226	0	229	40	0
52	B5	435	0	452	62	0
52	D5	459	0	477	66	0
53	B6	401	0	399	123	0
53	D6	322	0	250	87	0
54	B7	419	0	467	29	0
54	D7	419	0	467	53	0
55	B8	496	0	567	117	0
55	D8	467	0	519	119	0
56	B9	294	0	311	43	0
56	D9	299	0	325	32	0
57	AA	117	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AL	1	0	0	0	0
57	AT	1	0	0	0	0
57	AW	2	0	0	0	0
57	B0	2	0	0	0	0
57	B1	1	0	0	0	0
57	B5	4	0	0	0	0
57	B7	1	0	0	0	0
57	BA	459	0	0	1	0
57	BB	9	0	0	0	0
57	BD	1	0	0	0	0
57	BE	1	0	0	0	0
57	BF	1	0	0	0	0
57	BH	1	0	0	0	0
57	BP	3	0	0	0	0
57	BQ	3	0	0	0	0
57	BR	1	0	0	0	0
57	BT	1	0	0	0	0
57	BU	1	0	0	0	0
57	BX	1	0	0	0	0
57	CA	109	0	0	0	0
57	CE	1	0	0	0	0
57	CW	5	0	0	0	0
57	CX	1	0	0	0	0
57	D5	2	0	0	0	0
57	D6	2	0	0	0	0
57	DA	305	0	0	0	0
57	DB	10	0	0	0	0
57	DD	1	0	0	0	0
57	DF	1	0	0	0	0
57	DP	1	0	0	0	0
57	DR	1	0	0	0	0
58	AD	1	0	0	0	0
58	B5	1	0	0	0	0
58	B9	1	0	0	0	0
58	CD	1	0	0	0	0
58	D5	1	0	0	1	0
58	D9	1	0	0	2	0
All	All	290405	0	198457	24570	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 51.

The worst 5 of 24570 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)
52:D5:49:CYS:SG	58:D5:103:ZN:ZN	0.84	1.63
56:D9:14:CYS:SG	58:D9:101:ZN:ZN	1.23	1.27
27:DC:180:SER:CB	27:DC:180:SER:OG	1.82	1.25
36:BP:59:LEU:HA	36:BP:61:ARG:NH1	1.53	1.21
39:BS:97:ARG:NH2	39:BS:98:VAL:HA	1.55	1.20

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	128 (55%)	72 (31%)	33 (14%)	0	1
2	CB	233/256 (91%)	138 (59%)	54 (23%)	41 (18%)	0	0
3	AC	205/239 (86%)	106 (52%)	68 (33%)	31 (15%)	0	0
3	CC	205/239 (86%)	134 (65%)	45 (22%)	26 (13%)	0	1
4	AD	206/209 (99%)	124 (60%)	52 (25%)	30 (15%)	0	0
4	CD	206/209 (99%)	132 (64%)	46 (22%)	28 (14%)	0	1
5	AE	149/162 (92%)	107 (72%)	26 (17%)	16 (11%)	0	2
5	CE	149/162 (92%)	98 (66%)	37 (25%)	14 (9%)	0	3
6	AF	99/101 (98%)	63 (64%)	27 (27%)	9 (9%)	0	3
6	CF	99/101 (98%)	61 (62%)	19 (19%)	19 (19%)	0	0
7	AG	153/156 (98%)	98 (64%)	39 (26%)	16 (10%)	0	2
7	CG	153/156 (98%)	95 (62%)	34 (22%)	24 (16%)	0	0
8	AH	136/138 (99%)	96 (71%)	28 (21%)	12 (9%)	0	3
8	CH	136/138 (99%)	93 (68%)	26 (19%)	17 (12%)	0	1
9	AI	125/128 (98%)	82 (66%)	27 (22%)	16 (13%)	0	1
9	CI	125/128 (98%)	80 (64%)	32 (26%)	13 (10%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	97/105 (92%)	58 (60%)	29 (30%)	10 (10%)	0	2
10	CJ	97/105 (92%)	59 (61%)	26 (27%)	12 (12%)	0	1
11	AK	117/129 (91%)	88 (75%)	23 (20%)	6 (5%)	1	10
11	CK	117/129 (91%)	86 (74%)	25 (21%)	6 (5%)	1	10
12	AL	123/132 (93%)	84 (68%)	23 (19%)	16 (13%)	0	1
12	CL	123/132 (93%)	86 (70%)	21 (17%)	16 (13%)	0	1
13	AM	118/126 (94%)	72 (61%)	24 (20%)	22 (19%)	0	0
13	CM	118/126 (94%)	72 (61%)	22 (19%)	24 (20%)	0	0
14	AN	58/61 (95%)	34 (59%)	14 (24%)	10 (17%)	0	0
14	CN	58/61 (95%)	33 (57%)	15 (26%)	10 (17%)	0	0
15	AO	86/89 (97%)	58 (67%)	20 (23%)	8 (9%)	0	3
15	CO	86/89 (97%)	55 (64%)	19 (22%)	12 (14%)	0	1
16	AP	82/88 (93%)	46 (56%)	26 (32%)	10 (12%)	0	1
16	CP	82/88 (93%)	46 (56%)	26 (32%)	10 (12%)	0	1
17	AQ	98/105 (93%)	73 (74%)	14 (14%)	11 (11%)	0	2
17	CQ	98/105 (93%)	71 (72%)	19 (19%)	8 (8%)	0	4
18	AR	68/88 (77%)	39 (57%)	17 (25%)	12 (18%)	0	0
18	CR	68/88 (77%)	37 (54%)	26 (38%)	5 (7%)	1	5
19	AS	78/93 (84%)	47 (60%)	16 (20%)	15 (19%)	0	0
19	CS	76/93 (82%)	50 (66%)	16 (21%)	10 (13%)	0	1
20	AT	97/106 (92%)	66 (68%)	18 (19%)	13 (13%)	0	1
20	CT	97/106 (92%)	57 (59%)	27 (28%)	13 (13%)	0	1
21	AU	23/27 (85%)	12 (52%)	7 (30%)	4 (17%)	0	0
21	CU	23/27 (85%)	13 (56%)	7 (30%)	3 (13%)	0	1
22	AV	172/184 (94%)	124 (72%)	31 (18%)	17 (10%)	0	3
22	CV	172/184 (94%)	126 (73%)	28 (16%)	18 (10%)	0	2
27	BC	222/229 (97%)	165 (74%)	33 (15%)	24 (11%)	0	2
27	DC	216/229 (94%)	141 (65%)	62 (29%)	13 (6%)	1	7
28	BD	272/276 (99%)	194 (71%)	47 (17%)	31 (11%)	0	1
28	DD	272/276 (99%)	187 (69%)	47 (17%)	38 (14%)	0	1
29	BE	203/206 (98%)	130 (64%)	37 (18%)	36 (18%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	DE	203/206 (98%)	122 (60%)	35 (17%)	46 (23%)	0	0
30	BF	206/210 (98%)	136 (66%)	46 (22%)	24 (12%)	0	1
30	DF	206/210 (98%)	123 (60%)	48 (23%)	35 (17%)	0	0
31	BG	179/182 (98%)	118 (66%)	43 (24%)	18 (10%)	0	3
31	DG	179/182 (98%)	109 (61%)	44 (25%)	26 (14%)	0	0
32	BH	166/180 (92%)	98 (59%)	33 (20%)	35 (21%)	0	0
32	DH	158/180 (88%)	80 (51%)	49 (31%)	29 (18%)	0	0
33	BI	144/148 (97%)	84 (58%)	32 (22%)	28 (19%)	0	0
33	DI	144/148 (97%)	74 (51%)	41 (28%)	29 (20%)	0	0
34	BN	137/140 (98%)	104 (76%)	14 (10%)	19 (14%)	0	1
34	DN	137/140 (98%)	79 (58%)	38 (28%)	20 (15%)	0	0
35	BO	120/122 (98%)	91 (76%)	17 (14%)	12 (10%)	0	3
35	DO	120/122 (98%)	100 (83%)	15 (12%)	5 (4%)	2	13
36	BP	144/150 (96%)	71 (49%)	34 (24%)	39 (27%)	0	0
36	DP	144/150 (96%)	69 (48%)	34 (24%)	41 (28%)	0	0
37	BQ	137/141 (97%)	102 (74%)	23 (17%)	12 (9%)	0	3
37	DQ	139/141 (99%)	91 (66%)	35 (25%)	13 (9%)	0	3
38	BR	114/118 (97%)	82 (72%)	21 (18%)	11 (10%)	0	3
38	DR	115/118 (98%)	81 (70%)	17 (15%)	17 (15%)	0	0
39	BS	99/112 (88%)	44 (44%)	25 (25%)	30 (30%)	0	0
39	DS	97/112 (87%)	48 (50%)	25 (26%)	24 (25%)	0	0
40	BT	136/146 (93%)	86 (63%)	21 (15%)	29 (21%)	0	0
40	DT	136/146 (93%)	72 (53%)	33 (24%)	31 (23%)	0	0
41	BU	115/118 (98%)	74 (64%)	31 (27%)	10 (9%)	0	4
41	DU	115/118 (98%)	75 (65%)	25 (22%)	15 (13%)	0	1
42	BV	99/101 (98%)	68 (69%)	13 (13%)	18 (18%)	0	0
42	DV	99/101 (98%)	57 (58%)	20 (20%)	22 (22%)	0	0
43	BW	111/113 (98%)	75 (68%)	24 (22%)	12 (11%)	0	2
43	DW	111/113 (98%)	82 (74%)	18 (16%)	11 (10%)	0	3
44	BX	92/96 (96%)	64 (70%)	21 (23%)	7 (8%)	1	4
44	DX	91/96 (95%)	64 (70%)	16 (18%)	11 (12%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BY	99/110 (90%)	38 (38%)	23 (23%)	38 (38%)	0	0
45	DY	99/110 (90%)	39 (39%)	26 (26%)	34 (34%)	0	0
46	BZ	180/206 (87%)	114 (63%)	41 (23%)	25 (14%)	0	1
46	DZ	175/206 (85%)	103 (59%)	46 (26%)	26 (15%)	0	0
47	B0	75/85 (88%)	60 (80%)	13 (17%)	2 (3%)	4	20
47	D0	82/85 (96%)	60 (73%)	15 (18%)	7 (8%)	0	4
48	B1	94/98 (96%)	65 (69%)	15 (16%)	14 (15%)	0	0
48	D1	92/98 (94%)	65 (71%)	17 (18%)	10 (11%)	0	2
49	B2	69/72 (96%)	53 (77%)	9 (13%)	7 (10%)	0	3
49	D2	69/72 (96%)	41 (59%)	17 (25%)	11 (16%)	0	0
50	B3	57/60 (95%)	51 (90%)	5 (9%)	1 (2%)	6	28
50	D3	58/60 (97%)	38 (66%)	13 (22%)	7 (12%)	0	1
51	B4	29/71 (41%)	13 (45%)	9 (31%)	7 (24%)	0	0
51	D4	29/71 (41%)	13 (45%)	9 (31%)	7 (24%)	0	0
52	B5	55/60 (92%)	31 (56%)	10 (18%)	14 (26%)	0	0
52	D5	57/60 (95%)	35 (61%)	11 (19%)	11 (19%)	0	0
53	B6	47/54 (87%)	19 (40%)	13 (28%)	15 (32%)	0	0
53	D6	46/54 (85%)	19 (41%)	11 (24%)	16 (35%)	0	0
54	B7	47/49 (96%)	40 (85%)	7 (15%)	0	100	100
54	D7	47/49 (96%)	37 (79%)	6 (13%)	4 (8%)	0	4
55	B8	61/65 (94%)	36 (59%)	16 (26%)	9 (15%)	0	0
55	D8	60/65 (92%)	37 (62%)	14 (23%)	9 (15%)	0	0
56	B9	34/37 (92%)	24 (71%)	9 (26%)	1 (3%)	3	19
56	D9	34/37 (92%)	31 (91%)	3 (9%)	0	100	100
All	All	12117/12954 (94%)	7729 (64%)	2646 (22%)	1742 (14%)	0	0

5 of 1742 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	23	ARG
2	AB	26	PRO
2	AB	75	LYS
2	AB	128	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	173 (86%)	29 (14%)	3	14
2	CB	202/220 (92%)	180 (89%)	22 (11%)	6	24
3	AC	160/188 (85%)	142 (89%)	18 (11%)	5	23
3	CC	160/188 (85%)	146 (91%)	14 (9%)	9	33
4	AD	180/181 (99%)	154 (86%)	26 (14%)	3	14
4	CD	180/181 (99%)	161 (89%)	19 (11%)	6	26
5	AE	115/123 (94%)	99 (86%)	16 (14%)	3	15
5	CE	115/123 (94%)	103 (90%)	12 (10%)	7	27
6	AF	90/90 (100%)	76 (84%)	14 (16%)	2	12
6	CF	90/90 (100%)	78 (87%)	12 (13%)	4	17
7	AG	126/127 (99%)	115 (91%)	11 (9%)	9	34
7	CG	126/127 (99%)	111 (88%)	15 (12%)	5	21
8	AH	119/119 (100%)	108 (91%)	11 (9%)	8	31
8	CH	119/119 (100%)	109 (92%)	10 (8%)	10	35
9	AI	97/99 (98%)	83 (86%)	14 (14%)	3	14
9	CI	97/99 (98%)	79 (81%)	18 (19%)	1	8
10	AJ	88/92 (96%)	76 (86%)	12 (14%)	3	16
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	4	19
11	AK	90/99 (91%)	80 (89%)	10 (11%)	6	24
11	CK	90/99 (91%)	84 (93%)	6 (7%)	15	43
12	AL	104/109 (95%)	94 (90%)	10 (10%)	8	30
12	CL	104/109 (95%)	93 (89%)	11 (11%)	6	26
13	AM	95/101 (94%)	74 (78%)	21 (22%)	1	4
13	CM	95/101 (94%)	75 (79%)	20 (21%)	1	5
14	AN	49/50 (98%)	40 (82%)	9 (18%)	1	8
14	CN	49/50 (98%)	46 (94%)	3 (6%)	17	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	79/80 (99%)	74 (94%)	5 (6%)	16	45
15	CO	79/80 (99%)	74 (94%)	5 (6%)	16	45
16	AP	72/74 (97%)	62 (86%)	10 (14%)	3	15
16	CP	72/74 (97%)	67 (93%)	5 (7%)	14	41
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	20	51
17	CQ	94/97 (97%)	85 (90%)	9 (10%)	8	30
18	AR	61/77 (79%)	58 (95%)	3 (5%)	22	53
18	CR	61/77 (79%)	54 (88%)	7 (12%)	5	23
19	AS	65/80 (81%)	53 (82%)	12 (18%)	1	8
19	CS	68/80 (85%)	56 (82%)	12 (18%)	2	9
20	AT	76/82 (93%)	65 (86%)	11 (14%)	3	14
20	CT	76/82 (93%)	66 (87%)	10 (13%)	4	17
21	AU	19/22 (86%)	16 (84%)	3 (16%)	2	12
21	CU	19/22 (86%)	18 (95%)	1 (5%)	20	51
22	AV	148/154 (96%)	135 (91%)	13 (9%)	9	33
22	CV	148/154 (96%)	127 (86%)	21 (14%)	3	14
27	BC	175/181 (97%)	144 (82%)	31 (18%)	2	9
27	DC	165/181 (91%)	150 (91%)	15 (9%)	9	32
28	BD	215/218 (99%)	177 (82%)	38 (18%)	2	9
28	DD	213/218 (98%)	181 (85%)	32 (15%)	3	13
29	BE	165/166 (99%)	136 (82%)	29 (18%)	2	9
29	DE	165/166 (99%)	138 (84%)	27 (16%)	2	11
30	BF	165/166 (99%)	135 (82%)	30 (18%)	2	8
30	DF	165/166 (99%)	145 (88%)	20 (12%)	5	20
31	BG	155/156 (99%)	123 (79%)	32 (21%)	1	5
31	DG	155/156 (99%)	133 (86%)	22 (14%)	3	14
32	BH	127/148 (86%)	108 (85%)	19 (15%)	3	13
32	DH	132/148 (89%)	112 (85%)	20 (15%)	3	13
33	BI	97/124 (78%)	77 (79%)	20 (21%)	1	5
33	DI	49/124 (40%)	40 (82%)	9 (18%)	1	8
34	BN	117/119 (98%)	94 (80%)	23 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DN	117/119 (98%)	97 (83%)	20 (17%)	2	10
35	BO	100/100 (100%)	89 (89%)	11 (11%)	6	24
35	DO	100/100 (100%)	87 (87%)	13 (13%)	4	18
36	BP	112/116 (97%)	86 (77%)	26 (23%)	1	4
36	DP	103/116 (89%)	80 (78%)	23 (22%)	1	4
37	BQ	109/111 (98%)	92 (84%)	17 (16%)	2	12
37	DQ	111/111 (100%)	99 (89%)	12 (11%)	6	25
38	BR	92/101 (91%)	74 (80%)	18 (20%)	1	6
38	DR	100/101 (99%)	80 (80%)	20 (20%)	1	6
39	BS	76/88 (86%)	61 (80%)	15 (20%)	1	6
39	DS	77/88 (88%)	64 (83%)	13 (17%)	2	10
40	BT	120/127 (94%)	92 (77%)	28 (23%)	1	4
40	DT	120/127 (94%)	98 (82%)	22 (18%)	2	8
41	BU	92/94 (98%)	77 (84%)	15 (16%)	2	11
41	DU	92/94 (98%)	82 (89%)	10 (11%)	6	24
42	BV	82/82 (100%)	62 (76%)	20 (24%)	1	3
42	DV	82/82 (100%)	64 (78%)	18 (22%)	1	4
43	BW	91/92 (99%)	74 (81%)	17 (19%)	1	7
43	DW	91/92 (99%)	82 (90%)	9 (10%)	7	29
44	BX	75/78 (96%)	62 (83%)	13 (17%)	2	9
44	DX	74/78 (95%)	64 (86%)	10 (14%)	4	16
45	BY	79/91 (87%)	61 (77%)	18 (23%)	1	4
45	DY	84/91 (92%)	67 (80%)	17 (20%)	1	5
46	BZ	158/179 (88%)	134 (85%)	24 (15%)	3	13
46	DZ	155/179 (87%)	129 (83%)	26 (17%)	2	10
47	B0	62/67 (92%)	55 (89%)	7 (11%)	5	23
47	D0	66/67 (98%)	54 (82%)	12 (18%)	2	8
48	B1	81/83 (98%)	68 (84%)	13 (16%)	2	12
48	D1	78/83 (94%)	67 (86%)	11 (14%)	3	15
49	B2	66/67 (98%)	57 (86%)	9 (14%)	3	16
49	D2	66/67 (98%)	55 (83%)	11 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B3	50/52 (96%)	39 (78%)	11 (22%)	1	4
50	D3	51/52 (98%)	43 (84%)	8 (16%)	2	12
51	B4	27/63 (43%)	23 (85%)	4 (15%)	3	13
51	D4	27/63 (43%)	24 (89%)	3 (11%)	6	24
52	B5	48/52 (92%)	36 (75%)	12 (25%)	0	2
52	D5	51/52 (98%)	43 (84%)	8 (16%)	2	12
53	B6	43/52 (83%)	32 (74%)	11 (26%)	0	2
53	D6	24/52 (46%)	14 (58%)	10 (42%)	0	0
54	B7	41/42 (98%)	37 (90%)	4 (10%)	7	29
54	D7	41/42 (98%)	32 (78%)	9 (22%)	1	4
55	B8	52/55 (94%)	42 (81%)	10 (19%)	1	7
55	D8	46/55 (84%)	37 (80%)	9 (20%)	1	6
56	B9	32/34 (94%)	25 (78%)	7 (22%)	1	4
56	D9	33/34 (97%)	29 (88%)	4 (12%)	5	20
All	All	9998/10736 (93%)	8517 (85%)	1481 (15%)	3	13

5 of 1481 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	CJ	92	THR
31	DG	116	ASP
13	CM	69	GLU
10	CJ	80	LYS
27	DC	47	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 371 such sidechains are listed below:

Mol	Chain	Res	Type
10	CJ	56	HIS
29	DE	135	HIS
12	CL	6	GLN
20	CT	26	ASN
32	DH	147	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1492/1509 (98%)	236 (15%)	40 (2%)
1	CA	1503/1509 (99%)	227 (15%)	33 (2%)
23	AW	76/77 (98%)	18 (23%)	2 (2%)
23	CW	76/77 (98%)	20 (26%)	6 (7%)
24	AX	4/5 (80%)	0	0
24	CX	4/5 (80%)	0	0
25	BA	2761/2915 (94%)	513 (18%)	77 (2%)
25	DA	2771/2915 (95%)	551 (19%)	84 (3%)
26	BB	118/122 (96%)	19 (16%)	2 (1%)
26	DB	118/122 (96%)	20 (16%)	2 (1%)
All	All	8923/9256 (96%)	1604 (17%)	246 (2%)

5 of 1604 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 246 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2756	U
25	DA	2225	A
1	CA	968	A
25	DA	2171	A
25	DA	2611	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1056 ligands modelled in this entry, 1056 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	1222:G	O3'	1223:C	P	1.79

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, 95th 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	1495/1509 (99%)	0.63	97 (6%)	25	13	43, 73, 89, 96	1 (0%)
1	CA	1504/1509 (99%)	0.52	75 (4%)	34	18	47, 71, 88, 97	1 (0%)
2	AB	235/256 (91%)	0.65	14 (5%)	27	15	65, 75, 82, 88	0
2	CB	235/256 (91%)	0.72	12 (5%)	33	18	66, 76, 82, 85	0
3	AC	207/239 (86%)	0.76	19 (9%)	14	8	67, 75, 82, 86	0
3	CC	207/239 (86%)	0.74	12 (5%)	29	16	67, 75, 81, 84	0
4	AD	208/209 (99%)	0.69	11 (5%)	32	17	61, 72, 79, 85	0
4	CD	208/209 (99%)	0.64	19 (9%)	15	8	55, 68, 75, 83	0
5	AE	151/162 (93%)	0.52	8 (5%)	32	17	60, 69, 76, 83	0
5	CE	151/162 (93%)	0.42	7 (4%)	37	20	60, 69, 77, 90	0
6	AF	101/101 (100%)	0.32	2 (1%)	65	44	56, 67, 76, 81	0
6	CF	101/101 (100%)	0.37	7 (6%)	23	12	61, 70, 78, 83	0
7	AG	155/156 (99%)	0.68	9 (5%)	29	16	63, 74, 80, 83	0
7	CG	155/156 (99%)	0.62	6 (3%)	43	24	67, 74, 81, 84	0
8	AH	138/138 (100%)	0.57	5 (3%)	46	26	56, 69, 74, 79	0
8	CH	138/138 (100%)	0.53	4 (2%)	53	32	57, 70, 76, 82	0
9	AI	127/128 (99%)	1.18	19 (14%)	5	3	66, 77, 83, 87	0
9	CI	127/128 (99%)	1.25	24 (18%)	3	1	70, 77, 83, 86	0
10	AJ	99/105 (94%)	1.49	24 (24%)	2	1	66, 79, 84, 88	0
10	CJ	99/105 (94%)	1.47	29 (29%)	1	1	66, 79, 84, 87	0
11	AK	119/129 (92%)	0.32	4 (3%)	48	28	58, 68, 78, 82	0
11	CK	119/129 (92%)	0.72	7 (5%)	28	15	64, 72, 78, 84	0
12	AL	125/132 (94%)	0.58	11 (8%)	15	9	53, 67, 76, 85	0
12	CL	125/132 (94%)	0.71	7 (5%)	30	16	56, 65, 74, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	120/126 (95%)	0.99	13 (10%) 11 6	66, 75, 81, 83	0
13	CM	120/126 (95%)	0.67	9 (7%) 20 11	65, 75, 81, 84	0
14	AN	60/61 (98%)	1.14	9 (15%) 5 3	65, 74, 80, 82	0
14	CN	60/61 (98%)	1.11	3 (5%) 34 18	62, 74, 78, 82	0
15	AO	88/89 (98%)	0.51	2 (2%) 61 39	52, 66, 74, 79	0
15	CO	88/89 (98%)	0.41	2 (2%) 61 39	59, 68, 76, 78	0
16	AP	84/88 (95%)	0.74	7 (8%) 17 9	62, 69, 77, 80	0
16	CP	84/88 (95%)	0.63	5 (5%) 27 15	59, 66, 75, 83	0
17	AQ	100/105 (95%)	0.50	3 (3%) 52 31	59, 68, 75, 76	0
17	CQ	100/105 (95%)	0.53	4 (4%) 42 23	58, 68, 76, 78	0
18	AR	70/88 (79%)	0.40	0 100 100	58, 69, 78, 85	0
18	CR	70/88 (79%)	0.40	2 (2%) 53 32	63, 69, 77, 82	0
19	AS	80/93 (86%)	1.03	8 (10%) 12 6	66, 76, 83, 86	0
19	CS	78/93 (83%)	1.13	16 (20%) 2 1	70, 76, 82, 84	0
20	AT	99/106 (93%)	0.83	10 (10%) 12 6	62, 71, 79, 83	0
20	CT	99/106 (93%)	0.72	6 (6%) 27 15	63, 69, 77, 83	0
21	AU	25/27 (92%)	1.64	6 (24%) 2 1	67, 74, 81, 83	0
21	CU	25/27 (92%)	1.56	8 (32%) 1 0	68, 77, 83, 85	0
22	AV	176/184 (95%)	0.61	7 (3%) 42 23	51, 71, 79, 83	0
22	CV	176/184 (95%)	0.62	14 (7%) 18 10	58, 72, 80, 84	0
23	AW	77/77 (100%)	0.24	2 (2%) 57 36	45, 69, 81, 92	0
23	CW	77/77 (100%)	0.29	0 100 100	58, 72, 83, 87	0
24	AX	5/5 (100%)	1.05	1 (20%) 3 1	65, 65, 83, 85	0
24	CX	5/5 (100%)	1.16	2 (40%) 1 0	68, 70, 82, 85	0
25	BA	2767/2915 (94%)	0.30	123 (4%) 39 21	25, 53, 82, 97	0
25	DA	2777/2915 (95%)	0.45	129 (4%) 37 20	38, 65, 85, 97	0
26	BB	119/122 (97%)	0.49	5 (4%) 40 22	53, 67, 77, 86	0
26	DB	119/122 (97%)	0.67	8 (6%) 24 13	68, 77, 83, 92	0
27	BC	224/229 (97%)	0.73	14 (6%) 26 14	46, 76, 81, 86	1 (0%)
27	DC	220/229 (96%)	0.88	31 (14%) 6 3	47, 76, 82, 87	1 (0%)
28	BD	274/276 (99%)	0.72	22 (8%) 18 10	38, 53, 65, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DD	274/276 (99%)	0.69	23 (8%) 17 9	42, 59, 70, 77	0
29	BE	205/206 (99%)	0.63	16 (7%) 19 10	38, 58, 73, 77	0
29	DE	205/206 (99%)	0.93	26 (12%) 8 4	46, 65, 78, 82	0
30	BF	208/210 (99%)	0.58	11 (5%) 32 17	35, 58, 78, 88	0
30	DF	208/210 (99%)	0.72	21 (10%) 12 6	52, 69, 78, 90	0
31	BG	181/182 (99%)	0.56	9 (4%) 34 18	60, 71, 79, 86	0
31	DG	181/182 (99%)	0.77	18 (9%) 13 7	65, 73, 81, 85	0
32	BH	168/180 (93%)	0.59	12 (7%) 22 12	25, 66, 75, 82	0
32	DH	160/180 (88%)	0.79	11 (6%) 23 12	66, 76, 82, 87	0
33	BI	146/148 (98%)	0.54	11 (7%) 20 11	55, 71, 77, 84	0
33	DI	146/148 (98%)	0.66	11 (7%) 20 11	60, 73, 80, 83	0
34	BN	139/140 (99%)	0.68	10 (7%) 21 11	46, 59, 72, 77	0
34	DN	139/140 (99%)	0.59	4 (2%) 53 32	60, 70, 77, 82	0
35	BO	122/122 (100%)	0.60	7 (5%) 29 16	44, 59, 70, 73	0
35	DO	122/122 (100%)	0.39	4 (3%) 49 29	50, 63, 71, 75	0
36	BP	146/150 (97%)	1.14	28 (19%) 3 1	40, 65, 76, 81	0
36	DP	146/150 (97%)	1.20	29 (19%) 3 1	52, 70, 78, 82	0
37	BQ	139/141 (98%)	0.78	10 (7%) 21 11	45, 61, 71, 80	0
37	DQ	141/141 (100%)	0.83	11 (7%) 19 10	54, 69, 77, 83	0
38	BR	116/118 (98%)	0.66	12 (10%) 12 6	39, 57, 69, 74	0
38	DR	117/118 (99%)	0.72	7 (5%) 27 15	50, 63, 73, 78	0
39	BS	101/112 (90%)	0.96	14 (13%) 6 4	49, 69, 74, 80	0
39	DS	99/112 (88%)	1.32	22 (22%) 2 1	63, 72, 79, 86	0
40	BT	138/146 (94%)	0.79	13 (9%) 14 8	52, 65, 79, 83	0
40	DT	138/146 (94%)	0.63	12 (8%) 16 9	56, 67, 81, 84	0
41	BU	117/118 (99%)	0.66	10 (8%) 16 9	41, 54, 68, 78	0
41	DU	117/118 (99%)	0.85	14 (11%) 9 5	55, 67, 76, 81	0
42	BV	101/101 (100%)	0.58	7 (6%) 23 12	41, 60, 71, 75	0
42	DV	101/101 (100%)	0.77	10 (9%) 13 7	58, 74, 79, 85	0
43	BW	113/113 (100%)	0.49	3 (2%) 56 35	44, 53, 70, 86	0
43	DW	113/113 (100%)	0.51	7 (6%) 26 14	56, 64, 78, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	94/96 (97%)	0.73	8 (8%) 16 9	42, 57, 69, 79	0
44	DX	93/96 (96%)	0.89	8 (8%) 16 9	53, 67, 73, 81	0
45	BY	101/110 (91%)	1.11	18 (17%) 4 2	51, 64, 77, 81	0
45	DY	101/110 (91%)	1.56	26 (25%) 1 1	63, 74, 82, 85	0
46	BZ	182/206 (88%)	0.76	13 (7%) 22 12	56, 70, 78, 83	0
46	DZ	177/206 (85%)	1.03	21 (11%) 9 5	68, 76, 83, 87	0
47	B0	77/85 (90%)	0.91	12 (15%) 5 2	49, 59, 72, 81	0
47	D0	84/85 (98%)	0.85	11 (13%) 7 4	59, 68, 78, 84	0
48	B1	96/98 (97%)	0.59	6 (6%) 26 14	42, 60, 72, 77	0
48	D1	94/98 (95%)	0.73	11 (11%) 9 5	50, 64, 75, 78	0
49	B2	71/72 (98%)	0.49	4 (5%) 30 16	50, 61, 75, 80	0
49	D2	71/72 (98%)	0.59	4 (5%) 30 16	60, 71, 79, 87	0
50	B3	59/60 (98%)	0.67	5 (8%) 16 9	45, 59, 71, 74	0
50	D3	60/60 (100%)	0.86	3 (5%) 34 18	62, 72, 82, 85	0
51	B4	31/71 (43%)	0.98	3 (9%) 13 7	69, 75, 80, 86	0
51	D4	31/71 (43%)	0.69	1 (3%) 50 30	67, 74, 81, 84	0
52	B5	57/60 (95%)	0.70	5 (8%) 15 9	40, 55, 71, 73	0
52	D5	59/60 (98%)	0.92	7 (11%) 9 5	55, 68, 78, 86	0
53	B6	49/54 (90%)	1.26	13 (26%) 1 1	39, 65, 75, 75	0
53	D6	48/54 (88%)	1.56	17 (35%) 1 0	54, 66, 73, 78	0
54	B7	49/49 (100%)	0.64	5 (10%) 12 6	35, 46, 69, 76	0
54	D7	49/49 (100%)	0.79	4 (8%) 17 10	47, 58, 77, 83	0
55	B8	63/65 (96%)	0.91	10 (15%) 5 2	43, 56, 69, 75	0
55	D8	62/65 (95%)	1.19	10 (16%) 4 2	54, 62, 68, 76	0
56	B9	36/37 (97%)	0.95	4 (11%) 10 5	52, 59, 69, 71	0
56	D9	36/37 (97%)	1.35	6 (16%) 4 2	60, 69, 76, 82	0
All	All	21272/22210 (95%)	0.62	1541 (7%) 21 11	25, 68, 82, 97	4 (0%)

The worst 5 of 1541 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	D8	35	GLN	8.6
1	AA	1224	G	8.5

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Mol	Chain	Res	Type	RSRZ
14	CN	2	ALA	8.0
37	DQ	140	ALA	7.6
25	BA	2802	G	7.3

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 oligosaccharides 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
57	MG	BA	3022	1/1	0.12	1.06	205,205,205,205	0
57	MG	BA	3118	1/1	0.14	1.10	205,205,205,205	0
57	MG	BA	3323	1/1	0.19	0.93	205,205,205,205	0
57	MG	BA	3021	1/1	0.20	0.96	180,180,180,180	0
57	MG	BA	3442	1/1	0.31	1.04	205,205,205,205	0
57	MG	BA	3038	1/1	0.39	0.89	163,163,163,163	0
57	MG	BP	201	1/1	0.43	0.74	205,205,205,205	0
57	MG	BA	3188	1/1	0.44	0.39	87,87,87,87	0
57	MG	BA	3086	1/1	0.57	1.09	130,130,130,130	0
57	MG	CA	1708	1/1	0.60	0.51	76,76,76,76	0
57	MG	BA	3459	1/1	0.61	0.17	35,35,35,35	0
57	MG	BA	3444	1/1	0.62	0.90	101,101,101,101	0
57	MG	BA	3139	1/1	0.63	0.59	72,72,72,72	0
57	MG	BA	3448	1/1	0.68	0.20	54,54,54,54	0
57	MG	DA	3033	1/1	0.68	0.42	59,59,59,59	0
58	ZN	AD	301	1/1	0.68	0.46	192,192,192,192	0
57	MG	AA	1613	1/1	0.69	0.33	75,75,75,75	0
57	MG	AA	1664	1/1	0.69	0.39	77,77,77,77	0
57	MG	DB	208	1/1	0.70	0.28	48,48,48,48	0
57	MG	BA	3053	1/1	0.70	0.58	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3199	1/1	0.71	0.43	67,67,67,67	0
57	MG	AA	1704	1/1	0.73	0.12	64,64,64,64	0
57	MG	AA	1602	1/1	0.73	0.33	77,77,77,77	0
57	MG	DA	3073	1/1	0.74	0.43	49,49,49,49	0
57	MG	CA	1706	1/1	0.74	0.33	59,59,59,59	0
57	MG	BA	3175	1/1	0.74	0.27	71,71,71,71	0
57	MG	BA	3300	1/1	0.74	0.56	67,67,67,67	0
57	MG	BA	3386	1/1	0.75	0.39	68,68,68,68	0
57	MG	DA	3282	1/1	0.75	0.19	65,65,65,65	0
57	MG	BA	3381	1/1	0.76	0.56	66,66,66,66	0
57	MG	CW	102	1/1	0.76	0.55	93,93,93,93	0
57	MG	BA	3333	1/1	0.77	0.58	77,77,77,77	0
57	MG	AA	1669	1/1	0.77	0.33	70,70,70,70	0
57	MG	D6	101	1/1	0.77	0.17	57,57,57,57	0
57	MG	CA	1691	1/1	0.77	0.40	67,67,67,67	0
57	MG	BA	3332	1/1	0.78	0.25	61,61,61,61	0
57	MG	DA	3095	1/1	0.78	0.32	62,62,62,62	0
57	MG	AA	1712	1/1	0.78	0.17	56,56,56,56	0
57	MG	DA	3267	1/1	0.78	0.45	73,73,73,73	0
57	MG	BA	3194	1/1	0.78	0.15	72,72,72,72	0
57	MG	BU	201	1/1	0.78	0.17	21,21,21,21	0
57	MG	CA	1612	1/1	0.78	0.36	55,55,55,55	0
57	MG	DA	3044	1/1	0.78	0.37	69,69,69,69	0
57	MG	BA	3095	1/1	0.79	0.08	45,45,45,45	0
57	MG	AA	1661	1/1	0.79	0.31	67,67,67,67	0
57	MG	AA	1621	1/1	0.79	0.23	48,48,48,48	0
57	MG	DA	3298	1/1	0.79	0.08	33,33,33,33	0
57	MG	AA	1711	1/1	0.79	0.27	58,58,58,58	0
57	MG	CA	1696	1/1	0.79	0.34	54,54,54,54	0
57	MG	BB	201	1/1	0.79	0.26	59,59,59,59	0
57	MG	DA	3195	1/1	0.80	0.42	73,73,73,73	0
57	MG	BA	3084	1/1	0.80	0.61	61,61,61,61	0
57	MG	CA	1605	1/1	0.80	0.31	62,62,62,62	0
57	MG	AA	1619	1/1	0.80	0.25	66,66,66,66	0
57	MG	BA	3432	1/1	0.80	0.63	70,70,70,70	0
57	MG	BA	3433	1/1	0.80	0.34	52,52,52,52	0
57	MG	D5	102	1/1	0.80	0.31	44,44,44,44	0
57	MG	AA	1642	1/1	0.80	0.46	67,67,67,67	0
57	MG	DA	3154	1/1	0.80	0.18	61,61,61,61	0
57	MG	AA	1611	1/1	0.81	0.28	58,58,58,58	0
57	MG	AA	1665	1/1	0.81	0.42	63,63,63,63	0
57	MG	DA	3111	1/1	0.81	0.35	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3417	1/1	0.81	0.34	62,62,62,62	0
57	MG	DA	3290	1/1	0.81	0.34	50,50,50,50	0
57	MG	AA	1608	1/1	0.82	0.18	65,65,65,65	0
57	MG	AA	1645	1/1	0.82	0.21	52,52,52,52	0
57	MG	DA	3215	1/1	0.82	0.27	37,37,37,37	0
57	MG	BA	3213	1/1	0.82	0.27	43,43,43,43	0
57	MG	DA	3276	1/1	0.82	0.13	51,51,51,51	0
57	MG	AA	1615	1/1	0.82	0.22	46,46,46,46	0
57	MG	DA	3067	1/1	0.82	0.25	56,56,56,56	0
57	MG	AA	1675	1/1	0.82	0.18	50,50,50,50	0
57	MG	AA	1681	1/1	0.82	0.26	63,63,63,63	0
57	MG	AA	1689	1/1	0.82	0.12	55,55,55,55	0
57	MG	DA	3153	1/1	0.82	0.17	41,41,41,41	0
57	MG	BA	3047	1/1	0.82	0.41	62,62,62,62	0
57	MG	BA	3190	1/1	0.83	0.27	34,34,34,34	0
57	MG	CW	105	1/1	0.83	0.32	61,61,61,61	0
57	MG	BA	3458	1/1	0.83	0.22	47,47,47,47	0
57	MG	DA	3217	1/1	0.83	0.32	54,54,54,54	0
57	MG	DA	3245	1/1	0.83	0.25	52,52,52,52	0
57	MG	CA	1647	1/1	0.83	0.24	61,61,61,61	0
57	MG	CA	1684	1/1	0.83	0.27	42,42,42,42	0
57	MG	AA	1646	1/1	0.83	0.15	49,49,49,49	0
57	MG	BA	3074	1/1	0.83	0.25	31,31,31,31	0
57	MG	DA	3098	1/1	0.83	0.35	32,32,32,32	0
57	MG	BA	3270	1/1	0.83	0.28	43,43,43,43	0
57	MG	CA	1707	1/1	0.83	0.29	62,62,62,62	0
57	MG	AA	1715	1/1	0.83	0.26	62,62,62,62	0
57	MG	DA	3177	1/1	0.83	0.23	52,52,52,52	0
57	MG	CA	1649	1/1	0.84	0.26	65,65,65,65	0
57	MG	AA	1618	1/1	0.84	0.31	64,64,64,64	0
57	MG	BA	3207	1/1	0.84	0.33	74,74,74,74	0
57	MG	DA	3205	1/1	0.84	0.29	55,55,55,55	0
57	MG	DA	3209	1/1	0.84	0.28	33,33,33,33	0
57	MG	DB	202	1/1	0.84	0.09	61,61,61,61	0
57	MG	DB	205	1/1	0.84	0.37	42,42,42,42	0
57	MG	BA	3407	1/1	0.84	0.27	66,66,66,66	0
57	MG	CA	1613	1/1	0.84	0.22	42,42,42,42	0
57	MG	BA	3449	1/1	0.84	0.23	53,53,53,53	0
57	MG	DA	3256	1/1	0.84	0.21	62,62,62,62	0
57	MG	DA	3243	1/1	0.85	0.22	44,44,44,44	0
57	MG	DA	3145	1/1	0.85	0.43	57,57,57,57	0
57	MG	DA	3246	1/1	0.85	0.28	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1703	1/1	0.85	0.07	51,51,51,51	0
57	MG	DA	3266	1/1	0.85	0.16	46,46,46,46	0
57	MG	BA	3030	1/1	0.85	0.57	37,37,37,37	0
57	MG	DA	3155	1/1	0.85	0.16	60,60,60,60	0
57	MG	DA	3169	1/1	0.85	0.09	18,18,18,18	0
57	MG	BA	3399	1/1	0.85	0.11	38,38,38,38	0
57	MG	DA	3184	1/1	0.85	0.29	54,54,54,54	0
57	MG	BA	3013	1/1	0.85	0.30	56,56,56,56	0
57	MG	BA	3174	1/1	0.85	0.18	53,53,53,53	0
57	MG	AA	1607	1/1	0.85	0.25	51,51,51,51	0
57	MG	CE	201	1/1	0.85	0.20	42,42,42,42	0
57	MG	BA	3367	1/1	0.85	0.22	33,33,33,33	0
57	MG	DA	3131	1/1	0.85	0.16	39,39,39,39	0
57	MG	DA	3164	1/1	0.86	0.19	83,83,83,83	0
57	MG	CA	1676	1/1	0.86	0.27	48,48,48,48	0
57	MG	BA	3418	1/1	0.86	0.09	31,31,31,31	0
57	MG	BA	3424	1/1	0.86	0.16	26,26,26,26	0
57	MG	DA	3192	1/1	0.86	0.14	43,43,43,43	0
57	MG	BA	3125	1/1	0.86	0.28	60,60,60,60	0
57	MG	DA	3198	1/1	0.86	0.23	31,31,31,31	0
57	MG	AA	1631	1/1	0.86	0.17	29,29,29,29	0
57	MG	DA	3200	1/1	0.86	0.34	66,66,66,66	0
57	MG	BA	3306	1/1	0.86	0.20	47,47,47,47	0
57	MG	BA	3318	1/1	0.86	0.21	41,41,41,41	0
57	MG	BA	3064	1/1	0.86	0.21	44,44,44,44	0
57	MG	AA	1706	1/1	0.86	0.13	47,47,47,47	0
57	MG	DA	3220	1/1	0.86	0.20	31,31,31,31	0
57	MG	AA	1709	1/1	0.86	0.41	66,66,66,66	0
57	MG	BA	3351	1/1	0.86	0.26	56,56,56,56	0
57	MG	AA	1632	1/1	0.86	0.33	57,57,57,57	0
57	MG	BA	3369	1/1	0.86	0.24	63,63,63,63	0
57	MG	AA	1701	1/1	0.86	0.27	33,33,33,33	0
57	MG	DA	3085	1/1	0.86	0.17	49,49,49,49	0
57	MG	B5	101	1/1	0.86	0.40	78,78,78,78	0
57	MG	DA	3277	1/1	0.86	0.22	57,57,57,57	0
57	MG	BA	3195	1/1	0.86	0.34	47,47,47,47	0
57	MG	BA	3097	1/1	0.86	0.23	34,34,34,34	0
57	MG	DA	3122	1/1	0.86	0.19	48,48,48,48	0
57	MG	BA	3404	1/1	0.86	0.23	53,53,53,53	0
57	MG	CA	1615	1/1	0.86	0.33	63,63,63,63	0
57	MG	AA	1676	1/1	0.86	0.24	30,30,30,30	0
57	MG	BA	3231	1/1	0.86	0.24	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1657	1/1	0.86	0.15	37,37,37,37	0
57	MG	DA	3160	1/1	0.86	0.24	38,38,38,38	0
57	MG	AA	1667	1/1	0.87	0.20	62,62,62,62	0
57	MG	DA	3248	1/1	0.87	0.21	36,36,36,36	0
57	MG	AA	1692	1/1	0.87	0.09	51,51,51,51	0
57	MG	BA	3151	1/1	0.87	0.20	24,24,24,24	0
57	MG	AA	1649	1/1	0.87	0.31	50,50,50,50	0
57	MG	AA	1604	1/1	0.87	0.25	38,38,38,38	0
57	MG	BA	3425	1/1	0.87	0.14	55,55,55,55	0
57	MG	DA	3279	1/1	0.87	0.24	43,43,43,43	0
57	MG	DA	3281	1/1	0.87	0.09	49,49,49,49	0
57	MG	AA	1609	1/1	0.87	0.26	48,48,48,48	0
57	MG	DA	3283	1/1	0.87	0.21	62,62,62,62	0
57	MG	DA	3286	1/1	0.87	0.12	52,52,52,52	0
57	MG	BA	3100	1/1	0.87	0.34	28,28,28,28	0
57	MG	BA	3434	1/1	0.87	0.10	28,28,28,28	0
57	MG	DA	3152	1/1	0.87	0.40	61,61,61,61	0
57	MG	DB	203	1/1	0.87	0.29	66,66,66,66	0
57	MG	BA	3385	1/1	0.87	0.23	54,54,54,54	0
57	MG	BA	3310	1/1	0.87	0.22	30,30,30,30	0
57	MG	CA	1633	1/1	0.87	0.16	45,45,45,45	0
57	MG	CA	1638	1/1	0.87	0.28	35,35,35,35	0
57	MG	AA	1635	1/1	0.87	0.19	31,31,31,31	0
57	MG	DA	3005	1/1	0.88	0.36	45,45,45,45	0
57	MG	AA	1637	1/1	0.88	0.23	45,45,45,45	0
57	MG	BA	3077	1/1	0.88	0.54	63,63,63,63	0
57	MG	BA	3249	1/1	0.88	0.24	46,46,46,46	0
57	MG	BA	3354	1/1	0.88	0.17	25,25,25,25	0
57	MG	BA	3048	1/1	0.88	0.30	27,27,27,27	0
57	MG	DA	3190	1/1	0.88	0.21	44,44,44,44	0
57	MG	DA	3088	1/1	0.88	0.07	20,20,20,20	0
57	MG	BA	3293	1/1	0.88	0.23	23,23,23,23	0
57	MG	AA	1674	1/1	0.88	0.14	49,49,49,49	0
57	MG	DA	3108	1/1	0.88	0.32	47,47,47,47	0
57	MG	CA	1700	1/1	0.88	0.31	56,56,56,56	0
57	MG	DA	3121	1/1	0.88	0.36	57,57,57,57	0
57	MG	AA	1714	1/1	0.88	0.23	42,42,42,42	0
57	MG	DA	3211	1/1	0.88	0.43	55,55,55,55	0
57	MG	BA	3440	1/1	0.88	0.36	64,64,64,64	0
57	MG	BA	3148	1/1	0.88	0.20	64,64,64,64	0
57	MG	BA	3096	1/1	0.88	0.28	24,24,24,24	0
57	MG	DA	3221	1/1	0.88	0.22	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3445	1/1	0.88	0.25	36,36,36,36	0
57	MG	BA	3211	1/1	0.88	0.19	38,38,38,38	0
57	MG	CA	1709	1/1	0.89	0.17	28,28,28,28	0
57	MG	DA	3194	1/1	0.89	0.24	61,61,61,61	0
57	MG	BB	209	1/1	0.89	0.08	37,37,37,37	0
57	MG	BA	3111	1/1	0.89	0.09	20,20,20,20	0
57	MG	AA	1713	1/1	0.89	0.11	43,43,43,43	0
57	MG	BA	3193	1/1	0.89	0.21	47,47,47,47	0
57	MG	DA	3028	1/1	0.89	0.12	34,34,34,34	0
57	MG	CA	1602	1/1	0.89	0.07	35,35,35,35	0
57	MG	BA	3122	1/1	0.89	0.14	41,41,41,41	0
57	MG	DA	3045	1/1	0.89	0.25	59,59,59,59	0
57	MG	DA	3063	1/1	0.89	0.07	29,29,29,29	0
57	MG	AA	1606	1/1	0.89	0.20	42,42,42,42	0
57	MG	DA	3072	1/1	0.89	0.24	72,72,72,72	0
57	MG	DA	3223	1/1	0.89	0.18	32,32,32,32	0
57	MG	BA	3427	1/1	0.89	0.11	40,40,40,40	0
57	MG	BA	3430	1/1	0.89	0.24	58,58,58,58	0
57	MG	CA	1618	1/1	0.89	0.09	39,39,39,39	0
57	MG	DA	3092	1/1	0.89	0.19	25,25,25,25	0
57	MG	CA	1626	1/1	0.89	0.32	67,67,67,67	0
57	MG	BA	3092	1/1	0.89	0.12	36,36,36,36	0
57	MG	BA	3141	1/1	0.89	0.21	45,45,45,45	0
57	MG	DA	3269	1/1	0.89	0.23	47,47,47,47	0
57	MG	CA	1642	1/1	0.89	0.08	37,37,37,37	0
57	MG	AA	1705	1/1	0.89	0.36	66,66,66,66	0
57	MG	BA	3438	1/1	0.89	0.19	67,67,67,67	0
57	MG	AA	1693	1/1	0.89	0.21	45,45,45,45	0
57	MG	CA	1674	1/1	0.89	0.21	41,41,41,41	0
57	MG	BA	3241	1/1	0.89	0.30	50,50,50,50	0
57	MG	CA	1681	1/1	0.89	0.17	44,44,44,44	0
57	MG	BA	3076	1/1	0.89	0.32	24,24,24,24	0
57	MG	DA	3297	1/1	0.89	0.21	48,48,48,48	0
57	MG	BA	3374	1/1	0.89	0.14	51,51,51,51	0
57	MG	DA	3156	1/1	0.89	0.60	58,58,58,58	0
57	MG	CA	1692	1/1	0.89	0.22	48,48,48,48	0
57	MG	BA	3265	1/1	0.89	0.31	67,67,67,67	0
57	MG	BA	3268	1/1	0.89	0.43	46,46,46,46	0
57	MG	BA	3016	1/1	0.89	0.28	20,20,20,20	0
57	MG	BA	3288	1/1	0.89	0.18	18,18,18,18	0
57	MG	BA	3180	1/1	0.89	0.20	21,21,21,21	0
57	MG	BA	3408	1/1	0.90	0.29	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3187	1/1	0.90	0.29	48,48,48,48	0
57	MG	DA	3189	1/1	0.90	0.12	34,34,34,34	0
57	MG	BA	3127	1/1	0.90	0.20	30,30,30,30	0
57	MG	BA	3254	1/1	0.90	0.09	37,37,37,37	0
57	MG	CA	1603	1/1	0.90	0.11	49,49,49,49	0
57	MG	BA	3421	1/1	0.90	0.14	32,32,32,32	0
57	MG	DA	3014	1/1	0.90	0.16	44,44,44,44	0
57	MG	DA	3015	1/1	0.90	0.17	36,36,36,36	0
57	MG	DA	3021	1/1	0.90	0.14	34,34,34,34	0
57	MG	DA	3203	1/1	0.90	0.11	52,52,52,52	0
57	MG	AA	1616	1/1	0.90	0.23	30,30,30,30	0
57	MG	BA	3339	1/1	0.90	0.17	29,29,29,29	0
57	MG	DA	3034	1/1	0.90	0.18	57,57,57,57	0
57	MG	DA	3040	1/1	0.90	0.28	26,26,26,26	0
57	MG	AA	1614	1/1	0.90	0.33	29,29,29,29	0
57	MG	BA	3099	1/1	0.90	0.36	29,29,29,29	0
57	MG	DA	3050	1/1	0.90	0.32	46,46,46,46	0
57	MG	BA	3431	1/1	0.90	0.31	53,53,53,53	0
57	MG	BA	3359	1/1	0.90	0.26	44,44,44,44	0
57	MG	BA	3362	1/1	0.90	0.14	30,30,30,30	0
57	MG	CA	1640	1/1	0.90	0.34	61,61,61,61	0
57	MG	DA	3079	1/1	0.90	0.11	45,45,45,45	0
57	MG	DA	3255	1/1	0.90	0.17	46,46,46,46	0
57	MG	BA	3275	1/1	0.90	0.19	27,27,27,27	0
57	MG	CA	1643	1/1	0.90	0.08	44,44,44,44	0
57	MG	BA	3280	1/1	0.90	0.10	19,19,19,19	0
57	MG	BA	3372	1/1	0.90	0.19	59,59,59,59	0
57	MG	DA	3274	1/1	0.90	0.09	36,36,36,36	0
57	MG	CA	1652	1/1	0.90	0.45	59,59,59,59	0
57	MG	BA	3043	1/1	0.90	0.25	25,25,25,25	0
57	MG	CA	1664	1/1	0.90	0.18	42,42,42,42	0
57	MG	BA	3443	1/1	0.90	0.25	24,24,24,24	0
57	MG	AA	1653	1/1	0.90	0.17	28,28,28,28	0
57	MG	BA	3383	1/1	0.90	0.18	48,48,48,48	0
57	MG	BA	3212	1/1	0.90	0.33	30,30,30,30	0
57	MG	CA	1686	1/1	0.90	0.23	44,44,44,44	0
57	MG	AA	1657	1/1	0.90	0.22	54,54,54,54	0
57	MG	BA	3391	1/1	0.90	0.21	44,44,44,44	0
57	MG	DA	3305	1/1	0.90	0.24	35,35,35,35	0
57	MG	CA	1694	1/1	0.90	0.27	51,51,51,51	0
57	MG	AA	1679	1/1	0.90	0.35	56,56,56,56	0
57	MG	BA	3403	1/1	0.90	0.19	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3161	1/1	0.90	0.11	50,50,50,50	0
57	MG	BB	208	1/1	0.90	0.21	36,36,36,36	0
57	MG	BA	3314	1/1	0.90	0.10	22,22,22,22	0
57	MG	AA	1668	1/1	0.90	0.08	40,40,40,40	0
57	MG	BA	3184	1/1	0.91	0.33	53,53,53,53	0
57	MG	DA	3175	1/1	0.91	0.24	56,56,56,56	0
57	MG	BA	3102	1/1	0.91	0.32	33,33,33,33	0
57	MG	BA	3033	1/1	0.91	0.23	34,34,34,34	0
57	MG	BQ	202	1/1	0.91	0.12	30,30,30,30	0
57	MG	BA	3398	1/1	0.91	0.14	34,34,34,34	0
57	MG	AA	1699	1/1	0.91	0.17	29,29,29,29	0
57	MG	DA	3010	1/1	0.91	0.41	66,66,66,66	0
57	MG	B5	104	1/1	0.91	0.10	33,33,33,33	0
57	MG	BA	3080	1/1	0.91	0.16	32,32,32,32	0
57	MG	BA	3124	1/1	0.91	0.08	41,41,41,41	0
57	MG	CA	1604	1/1	0.91	0.14	38,38,38,38	0
57	MG	BA	3198	1/1	0.91	0.08	34,34,34,34	0
57	MG	BA	3082	1/1	0.91	0.24	24,24,24,24	0
57	MG	BA	3412	1/1	0.91	0.19	35,35,35,35	0
57	MG	BA	3321	1/1	0.91	0.23	22,22,22,22	0
57	MG	AA	1700	1/1	0.91	0.13	44,44,44,44	0
57	MG	BA	3044	1/1	0.91	0.21	22,22,22,22	0
57	MG	DA	3216	1/1	0.91	0.19	23,23,23,23	0
57	MG	DA	3054	1/1	0.91	0.34	27,27,27,27	0
57	MG	CA	1631	1/1	0.91	0.12	34,34,34,34	0
57	MG	AA	1641	1/1	0.91	0.20	30,30,30,30	0
57	MG	BA	3143	1/1	0.91	0.22	31,31,31,31	0
57	MG	DA	3237	1/1	0.91	0.19	33,33,33,33	0
57	MG	DA	3239	1/1	0.91	0.15	32,32,32,32	0
57	MG	BA	3345	1/1	0.91	0.09	34,34,34,34	0
57	MG	BA	3428	1/1	0.91	0.14	24,24,24,24	0
57	MG	BA	3233	1/1	0.91	0.35	53,53,53,53	0
57	MG	BA	3353	1/1	0.91	0.24	36,36,36,36	0
57	MG	DA	3249	1/1	0.91	0.12	33,33,33,33	0
57	MG	BA	3238	1/1	0.91	0.13	20,20,20,20	0
57	MG	DA	3094	1/1	0.91	0.14	71,71,71,71	0
57	MG	DA	3265	1/1	0.91	0.34	54,54,54,54	0
57	MG	BA	3357	1/1	0.91	0.20	38,38,38,38	0
57	MG	BA	3358	1/1	0.91	0.20	38,38,38,38	0
57	MG	BA	3239	1/1	0.91	0.20	46,46,46,46	0
57	MG	DA	3270	1/1	0.91	0.24	47,47,47,47	0
57	MG	BA	3147	1/1	0.91	0.24	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	1659	1/1	0.91	0.11	58,58,58,58	0
57	MG	BA	3049	1/1	0.91	0.31	24,24,24,24	0
57	MG	DA	3125	1/1	0.91	0.23	26,26,26,26	0
57	MG	BA	3370	1/1	0.91	0.18	48,48,48,48	0
57	MG	DA	3139	1/1	0.91	0.31	58,58,58,58	0
57	MG	DA	3142	1/1	0.91	0.13	51,51,51,51	0
57	MG	DA	3144	1/1	0.91	0.09	44,44,44,44	0
57	MG	BA	3166	1/1	0.91	0.37	38,38,38,38	0
57	MG	BA	3447	1/1	0.91	0.26	27,27,27,27	0
57	MG	AA	1651	1/1	0.91	0.28	49,49,49,49	0
57	MG	BA	3378	1/1	0.91	0.12	55,55,55,55	0
57	MG	CA	1695	1/1	0.91	0.18	38,38,38,38	0
57	MG	BA	3450	1/1	0.91	0.29	44,44,44,44	0
57	MG	DB	204	1/1	0.91	0.07	43,43,43,43	0
57	MG	DA	3158	1/1	0.91	0.28	44,44,44,44	0
57	MG	BA	3379	1/1	0.91	0.23	40,40,40,40	0
57	MG	BA	3029	1/1	0.91	0.17	40,40,40,40	0
57	MG	AA	1605	1/1	0.91	0.23	51,51,51,51	0
57	MG	DA	3168	1/1	0.91	0.20	35,35,35,35	0
57	MG	BA	3126	1/1	0.92	0.22	66,66,66,66	0
57	MG	BA	3052	1/1	0.92	0.27	30,30,30,30	0
57	MG	BA	3130	1/1	0.92	0.20	35,35,35,35	0
57	MG	BR	201	1/1	0.92	0.23	35,35,35,35	0
57	MG	AA	1644	1/1	0.92	0.12	40,40,40,40	0
57	MG	B1	101	1/1	0.92	0.17	63,63,63,63	0
57	MG	CX	101	1/1	0.92	0.17	22,22,22,22	0
57	MG	DA	3001	1/1	0.92	0.17	61,61,61,61	0
57	MG	BA	3406	1/1	0.92	0.17	50,50,50,50	0
57	MG	B5	102	1/1	0.92	0.25	40,40,40,40	0
57	MG	BA	3094	1/1	0.92	0.22	34,34,34,34	0
57	MG	BA	3057	1/1	0.92	0.32	39,39,39,39	0
57	MG	BA	3062	1/1	0.92	0.07	19,19,19,19	0
57	MG	BA	3331	1/1	0.92	0.16	28,28,28,28	0
57	MG	BA	3221	1/1	0.92	0.07	22,22,22,22	0
57	MG	CA	1606	1/1	0.92	0.28	50,50,50,50	0
57	MG	DA	3038	1/1	0.92	0.23	49,49,49,49	0
57	MG	BA	3223	1/1	0.92	0.17	49,49,49,49	0
57	MG	DA	3043	1/1	0.92	0.12	39,39,39,39	0
57	MG	BA	3334	1/1	0.92	0.11	24,24,24,24	0
57	MG	BA	3224	1/1	0.92	0.20	31,31,31,31	0
57	MG	DA	3049	1/1	0.92	0.16	15,15,15,15	0
57	MG	BA	3001	1/1	0.92	0.13	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3218	1/1	0.92	0.15	35,35,35,35	0
57	MG	CA	1623	1/1	0.92	0.37	59,59,59,59	0
57	MG	BA	3069	1/1	0.92	0.18	30,30,30,30	0
57	MG	BA	3163	1/1	0.92	0.12	21,21,21,21	0
57	MG	DA	3231	1/1	0.92	0.26	45,45,45,45	0
57	MG	DA	3071	1/1	0.92	0.20	20,20,20,20	0
57	MG	BA	3071	1/1	0.92	0.21	25,25,25,25	0
57	MG	BA	3171	1/1	0.92	0.31	41,41,41,41	0
57	MG	DA	3075	1/1	0.92	0.20	27,27,27,27	0
57	MG	BA	3242	1/1	0.92	0.13	24,24,24,24	0
57	MG	BA	3244	1/1	0.92	0.32	47,47,47,47	0
57	MG	BA	3436	1/1	0.92	0.30	48,48,48,48	0
57	MG	DA	3254	1/1	0.92	0.26	60,60,60,60	0
57	MG	CA	1644	1/1	0.92	0.12	30,30,30,30	0
57	MG	CA	1646	1/1	0.92	0.15	59,59,59,59	0
57	MG	DA	3263	1/1	0.92	0.07	28,28,28,28	0
57	MG	AA	1686	1/1	0.92	0.14	42,42,42,42	0
57	MG	AA	1601	1/1	0.92	0.25	47,47,47,47	0
57	MG	BA	3255	1/1	0.92	0.29	31,31,31,31	0
57	MG	BA	3258	1/1	0.92	0.09	39,39,39,39	0
57	MG	DA	3114	1/1	0.92	0.25	30,30,30,30	0
57	MG	DA	3272	1/1	0.92	0.21	40,40,40,40	0
57	MG	DA	3117	1/1	0.92	0.25	42,42,42,42	0
57	MG	DA	3275	1/1	0.92	0.21	48,48,48,48	0
57	MG	BA	3264	1/1	0.92	0.07	34,34,34,34	0
57	MG	CA	1668	1/1	0.92	0.17	27,27,27,27	0
57	MG	DA	3278	1/1	0.92	0.08	59,59,59,59	0
57	MG	BA	3176	1/1	0.92	0.17	44,44,44,44	0
57	MG	AA	1690	1/1	0.92	0.07	26,26,26,26	0
57	MG	DA	3133	1/1	0.92	0.09	31,31,31,31	0
57	MG	BA	3119	1/1	0.92	0.30	23,23,23,23	0
57	MG	DA	3141	1/1	0.92	0.13	25,25,25,25	0
57	MG	AA	1677	1/1	0.92	0.17	48,48,48,48	0
57	MG	DA	3296	1/1	0.92	0.20	40,40,40,40	0
57	MG	BA	3023	1/1	0.92	0.32	45,45,45,45	0
57	MG	CA	1689	1/1	0.92	0.20	39,39,39,39	0
57	MG	DA	3151	1/1	0.92	0.16	43,43,43,43	0
57	MG	BA	3451	1/1	0.92	0.07	23,23,23,23	0
57	MG	BA	3456	1/1	0.92	0.23	43,43,43,43	0
57	MG	BA	3192	1/1	0.92	0.26	27,27,27,27	0
57	MG	AA	1640	1/1	0.92	0.24	19,19,19,19	0
57	MG	BA	3387	1/1	0.92	0.18	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BB	203	1/1	0.92	0.19	21,21,21,21	0
57	MG	DA	3159	1/1	0.92	0.36	38,38,38,38	0
57	MG	BA	3294	1/1	0.92	0.19	29,29,29,29	0
57	MG	CA	1693	1/1	0.93	0.23	36,36,36,36	0
57	MG	AA	1688	1/1	0.93	0.17	56,56,56,56	0
57	MG	BA	3271	1/1	0.93	0.23	40,40,40,40	0
57	MG	BA	3273	1/1	0.93	0.21	40,40,40,40	0
57	MG	BB	204	1/1	0.93	0.31	54,54,54,54	0
57	MG	CA	1702	1/1	0.93	0.11	29,29,29,29	0
57	MG	BA	3136	1/1	0.93	0.17	76,76,76,76	0
57	MG	BA	3137	1/1	0.93	0.36	46,46,46,46	0
57	MG	DA	3167	1/1	0.93	0.23	38,38,38,38	0
57	MG	BE	301	1/1	0.93	0.26	43,43,43,43	0
57	MG	BF	301	1/1	0.93	0.16	62,62,62,62	0
57	MG	BH	201	1/1	0.93	0.14	21,21,21,21	0
57	MG	BA	3384	1/1	0.93	0.21	42,42,42,42	0
57	MG	DA	3180	1/1	0.93	0.16	49,49,49,49	0
57	MG	DA	3181	1/1	0.93	0.20	36,36,36,36	0
57	MG	DA	3182	1/1	0.93	0.06	37,37,37,37	0
57	MG	CW	104	1/1	0.93	0.38	52,52,52,52	0
57	MG	BQ	201	1/1	0.93	0.16	24,24,24,24	0
57	MG	AA	1647	1/1	0.93	0.23	45,45,45,45	0
57	MG	BA	3290	1/1	0.93	0.18	22,22,22,22	0
57	MG	DA	3003	1/1	0.93	0.06	30,30,30,30	0
57	MG	BA	3291	1/1	0.93	0.15	24,24,24,24	0
57	MG	DA	3007	1/1	0.93	0.21	54,54,54,54	0
57	MG	BA	3140	1/1	0.93	0.19	33,33,33,33	0
57	MG	BA	3201	1/1	0.93	0.06	24,24,24,24	0
57	MG	BA	3296	1/1	0.93	0.25	25,25,25,25	0
57	MG	DA	3016	1/1	0.93	0.20	24,24,24,24	0
57	MG	DA	3204	1/1	0.93	0.24	41,41,41,41	0
57	MG	DA	3019	1/1	0.93	0.22	35,35,35,35	0
57	MG	BA	3098	1/1	0.93	0.26	25,25,25,25	0
57	MG	DA	3210	1/1	0.93	0.23	41,41,41,41	0
57	MG	DA	3022	1/1	0.93	0.18	21,21,21,21	0
57	MG	CA	1601	1/1	0.93	0.11	39,39,39,39	0
57	MG	BA	3303	1/1	0.93	0.21	26,26,26,26	0
57	MG	BA	3305	1/1	0.93	0.17	41,41,41,41	0
57	MG	BA	3209	1/1	0.93	0.20	23,23,23,23	0
57	MG	AA	1626	1/1	0.93	0.14	35,35,35,35	0
57	MG	BA	3145	1/1	0.93	0.21	29,29,29,29	0
57	MG	CA	1608	1/1	0.93	0.43	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3227	1/1	0.93	0.28	37,37,37,37	0
57	MG	BA	3414	1/1	0.93	0.17	36,36,36,36	0
57	MG	BA	3146	1/1	0.93	0.25	22,22,22,22	0
57	MG	AA	1691	1/1	0.93	0.17	39,39,39,39	0
57	MG	DA	3052	1/1	0.93	0.14	21,21,21,21	0
57	MG	BA	3004	1/1	0.93	0.61	61,61,61,61	0
57	MG	DA	3061	1/1	0.93	0.14	22,22,22,22	0
57	MG	DA	3062	1/1	0.93	0.13	33,33,33,33	0
57	MG	CA	1621	1/1	0.93	0.17	22,22,22,22	0
57	MG	BA	3327	1/1	0.93	0.18	28,28,28,28	0
57	MG	BA	3328	1/1	0.93	0.18	32,32,32,32	0
57	MG	BA	3104	1/1	0.93	0.16	37,37,37,37	0
57	MG	BA	3154	1/1	0.93	0.19	38,38,38,38	0
57	MG	BA	3159	1/1	0.93	0.24	29,29,29,29	0
57	MG	CA	1639	1/1	0.93	0.05	22,22,22,22	0
57	MG	BA	3235	1/1	0.93	0.16	51,51,51,51	0
57	MG	BA	3335	1/1	0.93	0.24	47,47,47,47	0
57	MG	BA	3107	1/1	0.93	0.10	40,40,40,40	0
57	MG	DA	3271	1/1	0.93	0.21	42,42,42,42	0
57	MG	BA	3344	1/1	0.93	0.14	24,24,24,24	0
57	MG	AA	1650	1/1	0.93	0.14	28,28,28,28	0
57	MG	BA	3169	1/1	0.93	0.05	21,21,21,21	0
57	MG	DA	3107	1/1	0.93	0.15	64,64,64,64	0
57	MG	BA	3112	1/1	0.93	0.14	23,23,23,23	0
57	MG	BA	3243	1/1	0.93	0.33	51,51,51,51	0
57	MG	DA	3113	1/1	0.93	0.24	26,26,26,26	0
57	MG	CA	1653	1/1	0.93	0.23	36,36,36,36	0
57	MG	CA	1656	1/1	0.93	0.29	43,43,43,43	0
57	MG	BA	3355	1/1	0.93	0.24	31,31,31,31	0
57	MG	BA	3015	1/1	0.93	0.20	21,21,21,21	0
57	MG	DA	3123	1/1	0.93	0.19	25,25,25,25	0
57	MG	DA	3294	1/1	0.93	0.23	19,19,19,19	0
57	MG	AA	1708	1/1	0.93	0.13	46,46,46,46	0
57	MG	AA	1633	1/1	0.93	0.12	36,36,36,36	0
57	MG	AA	1684	1/1	0.93	0.14	31,31,31,31	0
57	MG	BA	3366	1/1	0.93	0.37	49,49,49,49	0
57	MG	DB	201	1/1	0.93	0.14	53,53,53,53	0
57	MG	CA	1682	1/1	0.93	0.26	40,40,40,40	0
57	MG	AA	1638	1/1	0.93	0.20	55,55,55,55	0
57	MG	BA	3025	1/1	0.93	0.34	31,31,31,31	0
57	MG	BA	3027	1/1	0.93	0.11	26,26,26,26	0
57	MG	DA	3149	1/1	0.93	0.35	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DF	301	1/1	0.93	0.10	49,49,49,49	0
57	MG	CA	1690	1/1	0.93	0.18	44,44,44,44	0
57	MG	BA	3457	1/1	0.93	0.15	35,35,35,35	0
57	MG	BA	3191	1/1	0.93	0.06	40,40,40,40	0
57	MG	CA	1678	1/1	0.94	0.13	25,25,25,25	0
57	MG	BA	3103	1/1	0.94	0.19	21,21,21,21	0
57	MG	BA	3061	1/1	0.94	0.27	25,25,25,25	0
57	MG	BA	3228	1/1	0.94	0.26	36,36,36,36	0
57	MG	DA	3148	1/1	0.94	0.10	24,24,24,24	0
57	MG	BA	3336	1/1	0.94	0.12	29,29,29,29	0
57	MG	CA	1687	1/1	0.94	0.12	37,37,37,37	0
57	MG	BA	3230	1/1	0.94	0.27	34,34,34,34	0
57	MG	BA	3155	1/1	0.94	0.27	37,37,37,37	0
57	MG	BA	3232	1/1	0.94	0.28	38,38,38,38	0
57	MG	BA	3346	1/1	0.94	0.36	50,50,50,50	0
57	MG	BA	3348	1/1	0.94	0.38	55,55,55,55	0
57	MG	BA	3158	1/1	0.94	0.08	37,37,37,37	0
57	MG	AA	1683	1/1	0.94	0.18	31,31,31,31	0
57	MG	BA	3236	1/1	0.94	0.12	62,62,62,62	0
57	MG	CA	1698	1/1	0.94	0.19	33,33,33,33	0
57	MG	DA	3163	1/1	0.94	0.17	32,32,32,32	0
57	MG	BA	3109	1/1	0.94	0.24	21,21,21,21	0
57	MG	DA	3165	1/1	0.94	0.07	43,43,43,43	0
57	MG	BA	3165	1/1	0.94	0.20	25,25,25,25	0
57	MG	BB	202	1/1	0.94	0.17	21,21,21,21	0
57	MG	BA	3240	1/1	0.94	0.19	23,23,23,23	0
57	MG	AA	1697	1/1	0.94	0.20	27,27,27,27	0
57	MG	BA	3168	1/1	0.94	0.20	33,33,33,33	0
57	MG	DA	3179	1/1	0.94	0.15	30,30,30,30	0
57	MG	AA	1698	1/1	0.94	0.15	37,37,37,37	0
57	MG	BD	301	1/1	0.94	0.23	34,34,34,34	0
57	MG	BA	3115	1/1	0.94	0.22	19,19,19,19	0
57	MG	BA	3173	1/1	0.94	0.18	40,40,40,40	0
57	MG	DA	3186	1/1	0.94	0.13	29,29,29,29	0
57	MG	BA	3251	1/1	0.94	0.21	23,23,23,23	0
57	MG	DA	3188	1/1	0.94	0.04	27,27,27,27	0
57	MG	BA	3371	1/1	0.94	0.17	48,48,48,48	0
57	MG	BA	3024	1/1	0.94	0.19	20,20,20,20	0
57	MG	AA	1658	1/1	0.94	0.10	23,23,23,23	0
57	MG	BA	3375	1/1	0.94	0.19	36,36,36,36	0
57	MG	AA	1685	1/1	0.94	0.32	42,42,42,42	0
57	MG	DA	3196	1/1	0.94	0.12	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3012	1/1	0.94	0.26	28,28,28,28	0
57	MG	BX	101	1/1	0.94	0.04	36,36,36,36	0
57	MG	B0	102	1/1	0.94	0.19	33,33,33,33	0
57	MG	BA	3177	1/1	0.94	0.24	21,21,21,21	0
57	MG	BA	3123	1/1	0.94	0.16	43,43,43,43	0
57	MG	BA	3181	1/1	0.94	0.29	19,19,19,19	0
57	MG	DA	3208	1/1	0.94	0.24	59,59,59,59	0
57	MG	AA	1636	1/1	0.94	0.19	62,62,62,62	0
57	MG	BA	3185	1/1	0.94	0.11	17,17,17,17	0
57	MG	DA	3030	1/1	0.94	0.18	46,46,46,46	0
57	MG	DA	3031	1/1	0.94	0.21	24,24,24,24	0
57	MG	BA	3272	1/1	0.94	0.29	23,23,23,23	0
57	MG	BA	3186	1/1	0.94	0.28	24,24,24,24	0
57	MG	BA	3187	1/1	0.94	0.17	45,45,45,45	0
57	MG	BA	3396	1/1	0.94	0.10	26,26,26,26	0
57	MG	DA	3042	1/1	0.94	0.27	28,28,28,28	0
57	MG	AA	1717	1/1	0.94	0.06	25,25,25,25	0
57	MG	DA	3225	1/1	0.94	0.16	44,44,44,44	0
57	MG	BA	3286	1/1	0.94	0.23	24,24,24,24	0
57	MG	DA	3228	1/1	0.94	0.14	25,25,25,25	0
57	MG	BA	3400	1/1	0.94	0.20	32,32,32,32	0
57	MG	DA	3047	1/1	0.94	0.26	26,26,26,26	0
57	MG	BA	3401	1/1	0.94	0.23	46,46,46,46	0
57	MG	DA	3241	1/1	0.94	0.04	26,26,26,26	0
57	MG	DA	3242	1/1	0.94	0.11	32,32,32,32	0
57	MG	BA	3031	1/1	0.94	0.12	21,21,21,21	0
57	MG	CA	1617	1/1	0.94	0.15	35,35,35,35	0
57	MG	DA	3053	1/1	0.94	0.15	21,21,21,21	0
57	MG	BA	3083	1/1	0.94	0.13	22,22,22,22	0
57	MG	CA	1619	1/1	0.94	0.10	34,34,34,34	0
57	MG	DA	3250	1/1	0.94	0.22	26,26,26,26	0
57	MG	AL	201	1/1	0.94	0.19	29,29,29,29	0
57	MG	AA	1617	1/1	0.94	0.24	43,43,43,43	0
57	MG	CA	1625	1/1	0.94	0.18	31,31,31,31	0
57	MG	DA	3260	1/1	0.94	0.06	31,31,31,31	0
57	MG	DA	3261	1/1	0.94	0.14	58,58,58,58	0
57	MG	DA	3262	1/1	0.94	0.13	29,29,29,29	0
57	MG	BA	3002	1/1	0.94	0.16	39,39,39,39	0
57	MG	DA	3264	1/1	0.94	0.08	25,25,25,25	0
57	MG	CA	1629	1/1	0.94	0.22	25,25,25,25	0
57	MG	CA	1630	1/1	0.94	0.06	29,29,29,29	0
57	MG	BA	3410	1/1	0.94	0.15	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3411	1/1	0.94	0.19	53,53,53,53	0
57	MG	CA	1634	1/1	0.94	0.12	37,37,37,37	0
57	MG	AA	1622	1/1	0.94	0.14	36,36,36,36	0
57	MG	BA	3197	1/1	0.94	0.26	20,20,20,20	0
57	MG	DA	3273	1/1	0.94	0.27	55,55,55,55	0
57	MG	DA	3093	1/1	0.94	0.18	19,19,19,19	0
57	MG	BA	3302	1/1	0.94	0.04	37,37,37,37	0
57	MG	BA	3005	1/1	0.94	0.06	23,23,23,23	0
57	MG	BA	3199	1/1	0.94	0.18	23,23,23,23	0
57	MG	DA	3101	1/1	0.94	0.13	35,35,35,35	0
57	MG	DA	3102	1/1	0.94	0.22	32,32,32,32	0
57	MG	BA	3006	1/1	0.94	0.18	27,27,27,27	0
57	MG	BA	3202	1/1	0.94	0.09	19,19,19,19	0
57	MG	AA	1620	1/1	0.94	0.08	27,27,27,27	0
57	MG	DA	3112	1/1	0.94	0.18	27,27,27,27	0
57	MG	BA	3317	1/1	0.94	0.21	27,27,27,27	0
57	MG	BA	3208	1/1	0.94	0.15	56,56,56,56	0
57	MG	DA	3295	1/1	0.94	0.19	40,40,40,40	0
57	MG	DA	3115	1/1	0.94	0.06	36,36,36,36	0
57	MG	AA	1654	1/1	0.94	0.16	29,29,29,29	0
57	MG	DA	3118	1/1	0.94	0.08	33,33,33,33	0
57	MG	DA	3302	1/1	0.94	0.15	36,36,36,36	0
57	MG	DA	3120	1/1	0.94	0.10	25,25,25,25	0
57	MG	BA	3210	1/1	0.94	0.17	24,24,24,24	0
57	MG	BA	3324	1/1	0.94	0.10	25,25,25,25	0
57	MG	CA	1660	1/1	0.94	0.20	22,22,22,22	0
57	MG	AA	1629	1/1	0.94	0.09	56,56,56,56	0
57	MG	DA	3129	1/1	0.94	0.18	47,47,47,47	0
57	MG	BA	3055	1/1	0.94	0.17	24,24,24,24	0
57	MG	BA	3017	1/1	0.94	0.17	20,20,20,20	0
57	MG	D5	101	1/1	0.94	0.14	38,38,38,38	0
57	MG	DA	3135	1/1	0.94	0.17	42,42,42,42	0
57	MG	DA	3136	1/1	0.94	0.09	22,22,22,22	0
57	MG	BA	3149	1/1	0.94	0.16	27,27,27,27	0
57	MG	BA	3361	1/1	0.95	0.17	31,31,31,31	0
57	MG	BA	3257	1/1	0.95	0.09	41,41,41,41	0
57	MG	BA	3364	1/1	0.95	0.20	32,32,32,32	0
57	MG	BA	3365	1/1	0.95	0.13	23,23,23,23	0
57	MG	BA	3134	1/1	0.95	0.14	22,22,22,22	0
57	MG	DA	3162	1/1	0.95	0.10	24,24,24,24	0
57	MG	BA	3263	1/1	0.95	0.18	36,36,36,36	0
57	MG	BA	3018	1/1	0.95	0.28	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3189	1/1	0.95	0.06	14,14,14,14	0
57	MG	DA	3004	1/1	0.95	0.12	21,21,21,21	0
57	MG	BA	3266	1/1	0.95	0.31	26,26,26,26	0
57	MG	BA	3051	1/1	0.95	0.40	51,51,51,51	0
57	MG	DA	3174	1/1	0.95	0.34	23,23,23,23	0
57	MG	BT	201	1/1	0.95	0.14	32,32,32,32	0
57	MG	DA	3176	1/1	0.95	0.23	24,24,24,24	0
57	MG	BA	3373	1/1	0.95	0.06	31,31,31,31	0
57	MG	AA	1672	1/1	0.95	0.18	33,33,33,33	0
57	MG	AA	1716	1/1	0.95	0.18	31,31,31,31	0
57	MG	AA	1624	1/1	0.95	0.26	33,33,33,33	0
57	MG	AA	1630	1/1	0.95	0.30	41,41,41,41	0
57	MG	DA	3183	1/1	0.95	0.17	54,54,54,54	0
57	MG	BA	3380	1/1	0.95	0.18	37,37,37,37	0
57	MG	BA	3059	1/1	0.95	0.20	28,28,28,28	0
57	MG	DA	3023	1/1	0.95	0.17	42,42,42,42	0
57	MG	DA	3024	1/1	0.95	0.09	33,33,33,33	0
57	MG	B7	101	1/1	0.95	0.05	12,12,12,12	0
57	MG	BA	3277	1/1	0.95	0.24	29,29,29,29	0
57	MG	AA	1662	1/1	0.95	0.07	22,22,22,22	0
57	MG	BA	3284	1/1	0.95	0.15	15,15,15,15	0
57	MG	AA	1652	1/1	0.95	0.10	44,44,44,44	0
57	MG	BA	3028	1/1	0.95	0.21	29,29,29,29	0
57	MG	DA	3197	1/1	0.95	0.14	27,27,27,27	0
57	MG	BA	3289	1/1	0.95	0.23	38,38,38,38	0
57	MG	BA	3395	1/1	0.95	0.24	39,39,39,39	0
57	MG	BA	3065	1/1	0.95	0.20	24,24,24,24	0
57	MG	DA	3202	1/1	0.95	0.32	38,38,38,38	0
57	MG	BA	3397	1/1	0.95	0.07	44,44,44,44	0
57	MG	BA	3150	1/1	0.95	0.34	29,29,29,29	0
57	MG	BA	3203	1/1	0.95	0.31	29,29,29,29	0
57	MG	DA	3206	1/1	0.95	0.14	49,49,49,49	0
57	MG	DA	3048	1/1	0.95	0.14	6,6,6,6	0
57	MG	BA	3204	1/1	0.95	0.14	52,52,52,52	0
57	MG	BA	3295	1/1	0.95	0.17	20,20,20,20	0
57	MG	DA	3051	1/1	0.95	0.14	6,6,6,6	0
57	MG	DA	3213	1/1	0.95	0.17	28,28,28,28	0
57	MG	BA	3106	1/1	0.95	0.27	23,23,23,23	0
57	MG	BA	3153	1/1	0.95	0.09	42,42,42,42	0
57	MG	BA	3405	1/1	0.95	0.07	25,25,25,25	0
57	MG	AA	1678	1/1	0.95	0.05	33,33,33,33	0
57	MG	BA	3108	1/1	0.95	0.24	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3304	1/1	0.95	0.23	49,49,49,49	0
57	MG	DA	3065	1/1	0.95	0.18	29,29,29,29	0
57	MG	BA	3409	1/1	0.95	0.07	24,24,24,24	0
57	MG	DA	3068	1/1	0.95	0.16	19,19,19,19	0
57	MG	DA	3069	1/1	0.95	0.32	30,30,30,30	0
57	MG	BA	3157	1/1	0.95	0.10	38,38,38,38	0
57	MG	AA	1625	1/1	0.95	0.12	37,37,37,37	0
57	MG	DA	3238	1/1	0.95	0.13	33,33,33,33	0
57	MG	CA	1636	1/1	0.95	0.13	28,28,28,28	0
57	MG	DA	3074	1/1	0.95	0.20	21,21,21,21	0
57	MG	CA	1637	1/1	0.95	0.07	26,26,26,26	0
57	MG	DA	3078	1/1	0.95	0.14	44,44,44,44	0
57	MG	DA	3244	1/1	0.95	0.18	26,26,26,26	0
57	MG	BA	3308	1/1	0.95	0.15	22,22,22,22	0
57	MG	DA	3080	1/1	0.95	0.20	24,24,24,24	0
57	MG	BA	3110	1/1	0.95	0.19	32,32,32,32	0
57	MG	BA	3416	1/1	0.95	0.25	42,42,42,42	0
57	MG	DA	3090	1/1	0.95	0.14	31,31,31,31	0
57	MG	DA	3091	1/1	0.95	0.07	26,26,26,26	0
57	MG	BA	3311	1/1	0.95	0.18	31,31,31,31	0
57	MG	BA	3217	1/1	0.95	0.16	34,34,34,34	0
57	MG	BA	3419	1/1	0.95	0.23	44,44,44,44	0
57	MG	BA	3219	1/1	0.95	0.13	28,28,28,28	0
57	MG	DA	3097	1/1	0.95	0.21	21,21,21,21	0
57	MG	AA	1680	1/1	0.95	0.27	49,49,49,49	0
57	MG	BA	3320	1/1	0.95	0.15	25,25,25,25	0
57	MG	CA	1650	1/1	0.95	0.06	28,28,28,28	0
57	MG	DA	3105	1/1	0.95	0.19	30,30,30,30	0
57	MG	BA	3008	1/1	0.95	0.25	16,16,16,16	0
57	MG	DA	3268	1/1	0.95	0.28	43,43,43,43	0
57	MG	BA	3322	1/1	0.95	0.23	29,29,29,29	0
57	MG	DA	3109	1/1	0.95	0.17	33,33,33,33	0
57	MG	DA	3110	1/1	0.95	0.19	38,38,38,38	0
57	MG	BA	3113	1/1	0.95	0.11	32,32,32,32	0
57	MG	BA	3226	1/1	0.95	0.25	31,31,31,31	0
57	MG	BA	3036	1/1	0.95	0.20	30,30,30,30	0
57	MG	CA	1663	1/1	0.95	0.09	33,33,33,33	0
57	MG	BA	3079	1/1	0.95	0.20	25,25,25,25	0
57	MG	BA	3170	1/1	0.95	0.09	40,40,40,40	0
57	MG	BA	3011	1/1	0.95	0.17	6,6,6,6	0
57	MG	BA	3437	1/1	0.95	0.06	27,27,27,27	0
57	MG	DA	3280	1/1	0.95	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3172	1/1	0.95	0.27	22,22,22,22	0
57	MG	BA	3081	1/1	0.95	0.31	16,16,16,16	0
57	MG	AA	1695	1/1	0.95	0.22	26,26,26,26	0
57	MG	AA	1612	1/1	0.95	0.25	25,25,25,25	0
57	MG	DA	3288	1/1	0.95	0.24	60,60,60,60	0
57	MG	DA	3128	1/1	0.95	0.16	24,24,24,24	0
57	MG	CA	1685	1/1	0.95	0.05	33,33,33,33	0
57	MG	BA	3338	1/1	0.95	0.05	18,18,18,18	0
57	MG	DA	3132	1/1	0.95	0.21	32,32,32,32	0
57	MG	AA	1628	1/1	0.95	0.27	43,43,43,43	0
57	MG	BA	3446	1/1	0.95	0.43	60,60,60,60	0
57	MG	AA	1634	1/1	0.95	0.17	41,41,41,41	0
57	MG	DA	3303	1/1	0.95	0.17	54,54,54,54	0
57	MG	BA	3178	1/1	0.95	0.23	22,22,22,22	0
57	MG	BA	3087	1/1	0.95	0.18	23,23,23,23	0
57	MG	BA	3129	1/1	0.95	0.11	25,25,25,25	0
57	MG	BA	3349	1/1	0.95	0.17	38,38,38,38	0
57	MG	BA	3182	1/1	0.95	0.21	27,27,27,27	0
57	MG	BA	3352	1/1	0.95	0.18	22,22,22,22	0
57	MG	DB	207	1/1	0.95	0.12	27,27,27,27	0
57	MG	BA	3247	1/1	0.95	0.14	33,33,33,33	0
57	MG	DB	209	1/1	0.95	0.15	41,41,41,41	0
57	MG	BA	3183	1/1	0.95	0.09	22,22,22,22	0
57	MG	BA	3250	1/1	0.95	0.31	22,22,22,22	0
57	MG	BA	3088	1/1	0.95	0.13	24,24,24,24	0
57	MG	BA	3131	1/1	0.95	0.19	26,26,26,26	0
57	MG	BA	3133	1/1	0.95	0.39	60,60,60,60	0
57	MG	CA	1655	1/1	0.96	0.08	34,34,34,34	0
57	MG	DA	3055	1/1	0.96	0.21	24,24,24,24	0
57	MG	DA	3057	1/1	0.96	0.16	22,22,22,22	0
57	MG	DA	3185	1/1	0.96	0.15	37,37,37,37	0
57	MG	BA	3046	1/1	0.96	0.22	32,32,32,32	0
57	MG	BA	3392	1/1	0.96	0.14	52,52,52,52	0
57	MG	BA	3394	1/1	0.96	0.07	28,28,28,28	0
57	MG	BB	207	1/1	0.96	0.04	44,44,44,44	0
57	MG	BA	3007	1/1	0.96	0.20	19,19,19,19	0
57	MG	DA	3191	1/1	0.96	0.10	18,18,18,18	0
57	MG	CA	1665	1/1	0.96	0.15	30,30,30,30	0
57	MG	BA	3072	1/1	0.96	0.30	23,23,23,23	0
57	MG	CA	1670	1/1	0.96	0.28	43,43,43,43	0
57	MG	CA	1671	1/1	0.96	0.20	54,54,54,54	0
57	MG	CA	1672	1/1	0.96	0.13	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3019	1/1	0.96	0.27	25,25,25,25	0
57	MG	BA	3075	1/1	0.96	0.13	24,24,24,24	0
57	MG	CA	1677	1/1	0.96	0.22	27,27,27,27	0
57	MG	AT	201	1/1	0.96	0.05	22,22,22,22	0
57	MG	CA	1680	1/1	0.96	0.13	31,31,31,31	0
57	MG	DA	3082	1/1	0.96	0.18	21,21,21,21	0
57	MG	BA	3337	1/1	0.96	0.21	37,37,37,37	0
57	MG	DA	3086	1/1	0.96	0.26	25,25,25,25	0
57	MG	DA	3207	1/1	0.96	0.17	26,26,26,26	0
57	MG	DA	3087	1/1	0.96	0.23	26,26,26,26	0
57	MG	BA	3285	1/1	0.96	0.09	6,6,6,6	0
57	MG	CA	1683	1/1	0.96	0.21	36,36,36,36	0
57	MG	BP	203	1/1	0.96	0.07	27,27,27,27	0
57	MG	BA	3160	1/1	0.96	0.07	30,30,30,30	0
57	MG	DA	3214	1/1	0.96	0.17	29,29,29,29	0
57	MG	BA	3341	1/1	0.96	0.17	28,28,28,28	0
57	MG	BQ	203	1/1	0.96	0.11	27,27,27,27	0
57	MG	BA	3342	1/1	0.96	0.08	22,22,22,22	0
57	MG	BA	3343	1/1	0.96	0.12	22,22,22,22	0
57	MG	DA	3219	1/1	0.96	0.28	34,34,34,34	0
57	MG	BA	3287	1/1	0.96	0.10	20,20,20,20	0
57	MG	BA	3050	1/1	0.96	0.17	24,24,24,24	0
57	MG	DA	3222	1/1	0.96	0.22	26,26,26,26	0
57	MG	B0	101	1/1	0.96	0.14	30,30,30,30	0
57	MG	BA	3078	1/1	0.96	0.23	29,29,29,29	0
57	MG	DA	3226	1/1	0.96	0.26	32,32,32,32	0
57	MG	AA	1671	1/1	0.96	0.24	42,42,42,42	0
57	MG	BA	3032	1/1	0.96	0.13	6,6,6,6	0
57	MG	CA	1697	1/1	0.96	0.06	39,39,39,39	0
57	MG	BA	3350	1/1	0.96	0.12	37,37,37,37	0
57	MG	BA	3292	1/1	0.96	0.12	24,24,24,24	0
57	MG	BA	3135	1/1	0.96	0.08	23,23,23,23	0
57	MG	DA	3240	1/1	0.96	0.11	35,35,35,35	0
57	MG	CA	1704	1/1	0.96	0.09	26,26,26,26	0
57	MG	CA	1705	1/1	0.96	0.25	48,48,48,48	0
57	MG	AA	1660	1/1	0.96	0.10	31,31,31,31	0
57	MG	DA	3116	1/1	0.96	0.19	33,33,33,33	0
57	MG	BA	3034	1/1	0.96	0.14	19,19,19,19	0
57	MG	BA	3056	1/1	0.96	0.31	26,26,26,26	0
57	MG	BA	3356	1/1	0.96	0.06	21,21,21,21	0
57	MG	BA	3423	1/1	0.96	0.11	25,25,25,25	0
57	MG	BA	3297	1/1	0.96	0.14	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3299	1/1	0.96	0.15	22,22,22,22	0
57	MG	DA	3124	1/1	0.96	0.11	26,26,26,26	0
57	MG	CA	1610	1/1	0.96	0.22	30,30,30,30	0
57	MG	DA	3257	1/1	0.96	0.08	35,35,35,35	0
57	MG	DA	3258	1/1	0.96	0.13	64,64,64,64	0
57	MG	DA	3259	1/1	0.96	0.09	47,47,47,47	0
57	MG	DA	3127	1/1	0.96	0.23	34,34,34,34	0
57	MG	BA	3035	1/1	0.96	0.23	25,25,25,25	0
57	MG	AA	1603	1/1	0.96	0.06	18,18,18,18	0
57	MG	DA	3130	1/1	0.96	0.24	34,34,34,34	0
57	MG	BA	3429	1/1	0.96	0.14	33,33,33,33	0
57	MG	BA	3142	1/1	0.96	0.28	25,25,25,25	0
57	MG	AA	1670	1/1	0.96	0.12	30,30,30,30	0
57	MG	DA	3134	1/1	0.96	0.14	24,24,24,24	0
57	MG	BA	3253	1/1	0.96	0.26	41,41,41,41	0
57	MG	BA	3144	1/1	0.96	0.16	24,24,24,24	0
57	MG	DA	3138	1/1	0.96	0.15	17,17,17,17	0
57	MG	BA	3040	1/1	0.96	0.16	24,24,24,24	0
57	MG	DA	3140	1/1	0.96	0.16	36,36,36,36	0
57	MG	CA	1624	1/1	0.96	0.23	39,39,39,39	0
57	MG	BA	3368	1/1	0.96	0.38	49,49,49,49	0
57	MG	BA	3256	1/1	0.96	0.12	25,25,25,25	0
57	MG	CA	1628	1/1	0.96	0.05	26,26,26,26	0
57	MG	DA	3147	1/1	0.96	0.26	18,18,18,18	0
57	MG	BA	3116	1/1	0.96	0.07	23,23,23,23	0
57	MG	BA	3312	1/1	0.96	0.19	22,22,22,22	0
57	MG	BA	3441	1/1	0.96	0.29	37,37,37,37	0
57	MG	BA	3313	1/1	0.96	0.20	26,26,26,26	0
57	MG	DA	3026	1/1	0.96	0.07	33,33,33,33	0
57	MG	BA	3063	1/1	0.96	0.14	17,17,17,17	0
57	MG	DA	3284	1/1	0.96	0.07	51,51,51,51	0
57	MG	DA	3285	1/1	0.96	0.20	38,38,38,38	0
57	MG	DA	3029	1/1	0.96	0.10	22,22,22,22	0
57	MG	BA	3261	1/1	0.96	0.32	28,28,28,28	0
57	MG	DA	3289	1/1	0.96	0.04	27,27,27,27	0
57	MG	BA	3216	1/1	0.96	0.22	20,20,20,20	0
57	MG	BA	3376	1/1	0.96	0.23	33,33,33,33	0
57	MG	BA	3319	1/1	0.96	0.11	28,28,28,28	0
57	MG	DA	3037	1/1	0.96	0.25	45,45,45,45	0
57	MG	BA	3026	1/1	0.96	0.14	31,31,31,31	0
57	MG	BA	3218	1/1	0.96	0.24	23,23,23,23	0
57	MG	DA	3299	1/1	0.96	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3041	1/1	0.96	0.08	19,19,19,19	0
57	MG	BA	3120	1/1	0.96	0.23	35,35,35,35	0
57	MG	DA	3166	1/1	0.96	0.04	22,22,22,22	0
57	MG	BA	3267	1/1	0.96	0.18	19,19,19,19	0
57	MG	CA	1645	1/1	0.96	0.28	41,41,41,41	0
57	MG	BA	3453	1/1	0.96	0.17	41,41,41,41	0
57	MG	DA	3171	1/1	0.96	0.26	27,27,27,27	0
57	MG	DA	3172	1/1	0.96	0.12	30,30,30,30	0
57	MG	DB	206	1/1	0.96	0.08	19,19,19,19	0
57	MG	DA	3173	1/1	0.96	0.21	33,33,33,33	0
57	MG	BA	3121	1/1	0.96	0.10	20,20,20,20	0
57	MG	CA	1648	1/1	0.96	0.11	28,28,28,28	0
57	MG	DB	210	1/1	0.96	0.08	41,41,41,41	0
57	MG	DD	301	1/1	0.96	0.14	18,18,18,18	0
57	MG	AA	1694	1/1	0.96	0.20	23,23,23,23	0
57	MG	DR	201	1/1	0.96	0.06	22,22,22,22	0
57	MG	BA	3152	1/1	0.96	0.15	23,23,23,23	0
57	MG	BA	3330	1/1	0.96	0.11	21,21,21,21	0
57	MG	BA	3388	1/1	0.96	0.26	37,37,37,37	0
57	MG	CA	1654	1/1	0.96	0.09	17,17,17,17	0
58	ZN	CD	301	1/1	0.96	0.26	81,81,81,81	0
57	MG	BA	3138	1/1	0.97	0.10	39,39,39,39	0
57	MG	BA	3215	1/1	0.97	0.21	35,35,35,35	0
57	MG	CA	1679	1/1	0.97	0.04	29,29,29,29	0
57	MG	BA	3329	1/1	0.97	0.10	26,26,26,26	0
57	MG	AW	102	1/1	0.97	0.07	26,26,26,26	0
57	MG	AA	1648	1/1	0.97	0.19	40,40,40,40	0
57	MG	BA	3269	1/1	0.97	0.25	27,27,27,27	0
57	MG	AA	1623	1/1	0.97	0.12	18,18,18,18	0
57	MG	DA	3081	1/1	0.97	0.19	37,37,37,37	0
57	MG	BA	3179	1/1	0.97	0.27	23,23,23,23	0
57	MG	DA	3083	1/1	0.97	0.08	30,30,30,30	0
57	MG	BA	3003	1/1	0.97	0.10	25,25,25,25	0
57	MG	BA	3222	1/1	0.97	0.20	31,31,31,31	0
57	MG	CA	1688	1/1	0.97	0.07	35,35,35,35	0
57	MG	BA	3274	1/1	0.97	0.22	27,27,27,27	0
57	MG	BA	3054	1/1	0.97	0.29	33,33,33,33	0
57	MG	AA	1639	1/1	0.97	0.26	27,27,27,27	0
57	MG	BA	3340	1/1	0.97	0.18	29,29,29,29	0
57	MG	BA	3278	1/1	0.97	0.17	33,33,33,33	0
57	MG	BA	3279	1/1	0.97	0.15	26,26,26,26	0
57	MG	BA	3020	1/1	0.97	0.21	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3282	1/1	0.97	0.21	22,22,22,22	0
57	MG	BA	3283	1/1	0.97	0.23	20,20,20,20	0
57	MG	DA	3100	1/1	0.97	0.19	21,21,21,21	0
57	MG	BA	3227	1/1	0.97	0.16	21,21,21,21	0
57	MG	CA	1699	1/1	0.97	0.18	32,32,32,32	0
57	MG	BA	3347	1/1	0.97	0.05	28,28,28,28	0
57	MG	BA	3114	1/1	0.97	0.28	24,24,24,24	0
57	MG	CA	1703	1/1	0.97	0.27	34,34,34,34	0
57	MG	BA	3229	1/1	0.97	0.18	6,6,6,6	0
57	MG	CA	1607	1/1	0.97	0.12	37,37,37,37	0
57	MG	BA	3420	1/1	0.97	0.13	45,45,45,45	0
57	MG	DA	3232	1/1	0.97	0.25	40,40,40,40	0
57	MG	DA	3233	1/1	0.97	0.06	17,17,17,17	0
57	MG	DA	3234	1/1	0.97	0.19	33,33,33,33	0
57	MG	DA	3235	1/1	0.97	0.06	24,24,24,24	0
57	MG	CA	1609	1/1	0.97	0.21	27,27,27,27	0
57	MG	AA	1673	1/1	0.97	0.15	40,40,40,40	0
57	MG	BA	3085	1/1	0.97	0.15	17,17,17,17	0
57	MG	BA	3117	1/1	0.97	0.31	42,42,42,42	0
57	MG	CW	101	1/1	0.97	0.12	22,22,22,22	0
57	MG	BA	3037	1/1	0.97	0.11	9,9,9,9	0
57	MG	CW	103	1/1	0.97	0.19	27,27,27,27	0
57	MG	DA	3119	1/1	0.97	0.19	42,42,42,42	0
57	MG	CA	1616	1/1	0.97	0.06	20,20,20,20	0
57	MG	BA	3426	1/1	0.97	0.13	26,26,26,26	0
57	MG	DA	3247	1/1	0.97	0.07	23,23,23,23	0
57	MG	BA	3234	1/1	0.97	0.11	38,38,38,38	0
57	MG	BA	3060	1/1	0.97	0.25	47,47,47,47	0
57	MG	DA	3002	1/1	0.97	0.47	37,37,37,37	0
57	MG	DA	3251	1/1	0.97	0.32	53,53,53,53	0
57	MG	DA	3252	1/1	0.97	0.19	27,27,27,27	0
57	MG	DA	3253	1/1	0.97	0.07	20,20,20,20	0
57	MG	AA	1687	1/1	0.97	0.15	44,44,44,44	0
57	MG	CA	1622	1/1	0.97	0.24	24,24,24,24	0
57	MG	BA	3237	1/1	0.97	0.09	21,21,21,21	0
57	MG	BA	3089	1/1	0.97	0.28	24,24,24,24	0
57	MG	DA	3008	1/1	0.97	0.15	6,6,6,6	0
57	MG	BA	3090	1/1	0.97	0.16	17,17,17,17	0
57	MG	DA	3011	1/1	0.97	0.26	20,20,20,20	0
57	MG	BA	3360	1/1	0.97	0.16	27,27,27,27	0
57	MG	DA	3013	1/1	0.97	0.17	20,20,20,20	0
57	MG	BA	3091	1/1	0.97	0.30	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3435	1/1	0.97	0.05	30,30,30,30	0
57	MG	BA	3298	1/1	0.97	0.10	20,20,20,20	0
57	MG	DA	3017	1/1	0.97	0.23	21,21,21,21	0
57	MG	DA	3018	1/1	0.97	0.22	21,21,21,21	0
57	MG	BA	3039	1/1	0.97	0.42	39,39,39,39	0
57	MG	DA	3020	1/1	0.97	0.22	23,23,23,23	0
57	MG	AA	1656	1/1	0.97	0.12	28,28,28,28	0
57	MG	BA	3439	1/1	0.97	0.05	32,32,32,32	0
57	MG	BA	3301	1/1	0.97	0.19	33,33,33,33	0
57	MG	BA	3041	1/1	0.97	0.25	44,44,44,44	0
57	MG	DA	3025	1/1	0.97	0.17	38,38,38,38	0
57	MG	AA	1707	1/1	0.97	0.08	20,20,20,20	0
57	MG	DA	3027	1/1	0.97	0.17	33,33,33,33	0
57	MG	BA	3245	1/1	0.97	0.16	27,27,27,27	0
57	MG	BA	3128	1/1	0.97	0.29	33,33,33,33	0
57	MG	BA	3248	1/1	0.97	0.18	34,34,34,34	0
57	MG	BA	3200	1/1	0.97	0.20	20,20,20,20	0
57	MG	DA	3157	1/1	0.97	0.14	30,30,30,30	0
57	MG	DA	3032	1/1	0.97	0.14	20,20,20,20	0
57	MG	BA	3309	1/1	0.97	0.03	20,20,20,20	0
57	MG	BA	3164	1/1	0.97	0.05	35,35,35,35	0
57	MG	DA	3035	1/1	0.97	0.24	22,22,22,22	0
57	MG	BA	3068	1/1	0.97	0.12	30,30,30,30	0
57	MG	BA	3009	1/1	0.97	0.12	16,16,16,16	0
57	MG	BA	3070	1/1	0.97	0.09	23,23,23,23	0
57	MG	BA	3206	1/1	0.97	0.11	22,22,22,22	0
57	MG	DA	3291	1/1	0.97	0.16	31,31,31,31	0
57	MG	BA	3455	1/1	0.97	0.16	46,46,46,46	0
57	MG	BA	3315	1/1	0.97	0.04	17,17,17,17	0
57	MG	BA	3316	1/1	0.97	0.19	28,28,28,28	0
57	MG	BA	3382	1/1	0.97	0.17	26,26,26,26	0
57	MG	DA	3046	1/1	0.97	0.21	26,26,26,26	0
57	MG	BA	3132	1/1	0.97	0.19	28,28,28,28	0
57	MG	BA	3045	1/1	0.97	0.15	6,6,6,6	0
57	MG	BA	3010	1/1	0.97	0.17	23,23,23,23	0
57	MG	CA	1658	1/1	0.97	0.11	21,21,21,21	0
57	MG	BA	3259	1/1	0.97	0.10	37,37,37,37	0
57	MG	CA	1662	1/1	0.97	0.28	26,26,26,26	0
57	MG	AA	1627	1/1	0.97	0.14	21,21,21,21	0
57	MG	BB	205	1/1	0.97	0.17	19,19,19,19	0
57	MG	BB	206	1/1	0.97	0.27	31,31,31,31	0
57	MG	DA	3056	1/1	0.97	0.15	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3262	1/1	0.97	0.29	32,32,32,32	0
57	MG	DA	3058	1/1	0.97	0.10	27,27,27,27	0
57	MG	BA	3389	1/1	0.97	0.13	21,21,21,21	0
57	MG	BA	3390	1/1	0.97	0.11	48,48,48,48	0
57	MG	AA	1682	1/1	0.97	0.09	18,18,18,18	0
57	MG	CA	1673	1/1	0.97	0.17	26,26,26,26	0
57	MG	DA	3066	1/1	0.97	0.17	22,22,22,22	0
57	MG	BA	3014	1/1	0.97	0.33	24,24,24,24	0
57	MG	CA	1675	1/1	0.97	0.23	33,33,33,33	0
57	MG	BA	3393	1/1	0.97	0.10	61,61,61,61	0
57	MG	DA	3193	1/1	0.97	0.23	27,27,27,27	0
57	MG	DA	3070	1/1	0.97	0.33	46,46,46,46	0
57	MG	DA	3084	1/1	0.98	0.09	21,21,21,21	0
57	MG	BA	3067	1/1	0.98	0.14	30,30,30,30	0
57	MG	DA	3036	1/1	0.98	0.26	27,27,27,27	0
57	MG	CA	1667	1/1	0.98	0.18	23,23,23,23	0
57	MG	DA	3143	1/1	0.98	0.23	23,23,23,23	0
57	MG	DA	3201	1/1	0.98	0.32	32,32,32,32	0
57	MG	BA	3156	1/1	0.98	0.05	26,26,26,26	0
57	MG	CA	1627	1/1	0.98	0.18	24,24,24,24	0
57	MG	AA	1702	1/1	0.98	0.06	26,26,26,26	0
57	MG	BA	3307	1/1	0.98	0.23	24,24,24,24	0
57	MG	AA	1663	1/1	0.98	0.16	27,27,27,27	0
57	MG	BA	3058	1/1	0.98	0.19	18,18,18,18	0
57	MG	CA	1632	1/1	0.98	0.25	18,18,18,18	0
57	MG	DA	3096	1/1	0.98	0.23	34,34,34,34	0
57	MG	BA	3422	1/1	0.98	0.27	20,20,20,20	0
57	MG	BA	3454	1/1	0.98	0.13	25,25,25,25	0
57	MG	DA	3212	1/1	0.98	0.11	18,18,18,18	0
57	MG	CA	1635	1/1	0.98	0.17	22,22,22,22	0
57	MG	BA	3363	1/1	0.98	0.14	23,23,23,23	0
57	MG	BA	3260	1/1	0.98	0.21	24,24,24,24	0
57	MG	DA	3103	1/1	0.98	0.25	19,19,19,19	0
57	MG	DA	3104	1/1	0.98	0.15	21,21,21,21	0
57	MG	BA	3196	1/1	0.98	0.07	27,27,27,27	0
57	MG	BA	3012	1/1	0.98	0.25	22,22,22,22	0
57	MG	DA	3009	1/1	0.98	0.11	18,18,18,18	0
57	MG	BA	3161	1/1	0.98	0.17	25,25,25,25	0
57	MG	AA	1710	1/1	0.98	0.19	30,30,30,30	0
57	MG	BA	3220	1/1	0.98	0.11	30,30,30,30	0
57	MG	DA	3224	1/1	0.98	0.16	14,14,14,14	0
57	MG	BA	3073	1/1	0.98	0.16	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	3287	1/1	0.98	0.12	48,48,48,48	0
57	MG	AA	1610	1/1	0.98	0.29	21,21,21,21	0
57	MG	DA	3059	1/1	0.98	0.13	26,26,26,26	0
57	MG	DA	3170	1/1	0.98	0.16	22,22,22,22	0
57	MG	DA	3229	1/1	0.98	0.08	19,19,19,19	0
57	MG	DA	3292	1/1	0.98	0.04	17,17,17,17	0
57	MG	DA	3293	1/1	0.98	0.25	39,39,39,39	0
57	MG	DA	3230	1/1	0.98	0.22	23,23,23,23	0
57	MG	AA	1655	1/1	0.98	0.14	6,6,6,6	0
57	MG	AW	101	1/1	0.98	0.07	6,6,6,6	0
57	MG	BA	3225	1/1	0.98	0.14	16,16,16,16	0
57	MG	DA	3064	1/1	0.98	0.11	19,19,19,19	0
57	MG	BA	3105	1/1	0.98	0.07	15,15,15,15	0
57	MG	DA	3300	1/1	0.98	0.12	38,38,38,38	0
57	MG	DA	3301	1/1	0.98	0.09	33,33,33,33	0
57	MG	DA	3236	1/1	0.98	0.04	30,30,30,30	0
57	MG	BA	3205	1/1	0.98	0.09	45,45,45,45	0
57	MG	CA	1651	1/1	0.98	0.09	28,28,28,28	0
57	MG	DA	3178	1/1	0.98	0.07	30,30,30,30	0
57	MG	BA	3377	1/1	0.98	0.08	23,23,23,23	0
57	MG	CA	1614	1/1	0.98	0.06	30,30,30,30	0
57	MG	AA	1643	1/1	0.98	0.08	23,23,23,23	0
57	MG	AA	1696	1/1	0.98	0.18	26,26,26,26	0
57	MG	DA	3126	1/1	0.98	0.11	6,6,6,6	0
57	MG	BA	3326	1/1	0.98	0.12	21,21,21,21	0
57	MG	BA	3252	1/1	0.98	0.07	25,25,25,25	0
57	MG	BP	202	1/1	0.98	0.07	22,22,22,22	0
57	MG	CA	1701	1/1	0.98	0.10	25,25,25,25	0
57	MG	DA	3077	1/1	0.98	0.25	22,22,22,22	0
57	MG	CA	1659	1/1	0.98	0.20	32,32,32,32	0
57	MG	DP	201	1/1	0.98	0.14	38,38,38,38	0
57	MG	BA	3276	1/1	0.98	0.19	21,21,21,21	0
57	MG	CA	1661	1/1	0.98	0.26	26,26,26,26	0
57	MG	BA	3066	1/1	0.98	0.12	14,14,14,14	0
57	MG	BA	3093	1/1	0.98	0.04	23,23,23,23	0
57	MG	D6	102	1/1	0.98	0.21	23,23,23,23	0
57	MG	DA	3137	1/1	0.98	0.16	30,30,30,30	0
58	ZN	B5	105	1/1	0.98	0.06	90,90,90,90	0
57	MG	BA	3415	1/1	0.98	0.16	36,36,36,36	0
57	MG	BA	3413	1/1	0.99	0.10	24,24,24,24	0
57	MG	DA	3006	1/1	0.99	0.24	28,28,28,28	0
57	MG	DA	3089	1/1	0.99	0.07	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1620	1/1	0.99	0.35	29,29,29,29	0
57	MG	CA	1669	1/1	0.99	0.20	21,21,21,21	0
57	MG	DA	3304	1/1	0.99	0.04	35,35,35,35	0
57	MG	BA	3281	1/1	0.99	0.13	29,29,29,29	0
57	MG	BA	3246	1/1	0.99	0.06	11,11,11,11	0
57	MG	BA	3101	1/1	0.99	0.03	21,21,21,21	0
57	MG	BA	3162	1/1	0.99	0.04	21,21,21,21	0
57	MG	DA	3146	1/1	0.99	0.13	60,60,60,60	0
57	MG	BA	3325	1/1	0.99	0.18	22,22,22,22	0
57	MG	CA	1641	1/1	0.99	0.02	18,18,18,18	0
57	MG	CA	1611	1/1	0.99	0.14	25,25,25,25	0
57	MG	DA	3150	1/1	0.99	0.08	21,21,21,21	0
57	MG	DA	3099	1/1	0.99	0.20	23,23,23,23	0
57	MG	DA	3076	1/1	0.99	0.10	19,19,19,19	0
57	MG	B5	103	1/1	0.99	0.14	20,20,20,20	0
57	MG	BA	3452	1/1	0.99	0.06	16,16,16,16	0
57	MG	BA	3167	1/1	0.99	0.12	65,65,65,65	0
57	MG	AA	1666	1/1	0.99	0.11	24,24,24,24	0
57	MG	DA	3039	1/1	0.99	0.10	18,18,18,18	0
57	MG	DA	3106	1/1	0.99	0.34	25,25,25,25	0
57	MG	DA	3060	1/1	0.99	0.18	27,27,27,27	0
57	MG	BA	3214	1/1	0.99	0.06	29,29,29,29	0
57	MG	BA	3042	1/1	0.99	0.13	10,10,10,10	0
57	MG	BA	3402	1/1	0.99	0.04	24,24,24,24	0
58	ZN	B9	101	1/1	0.99	0.06	75,75,75,75	0
57	MG	CA	1666	1/1	0.99	0.16	18,18,18,18	0
58	ZN	D5	103	1/1	0.99	0.24	30,30,30,30	0
58	ZN	D9	101	1/1	1.00	0.25	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.