



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 08:39 pm BST

PDB ID : 4V6A
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

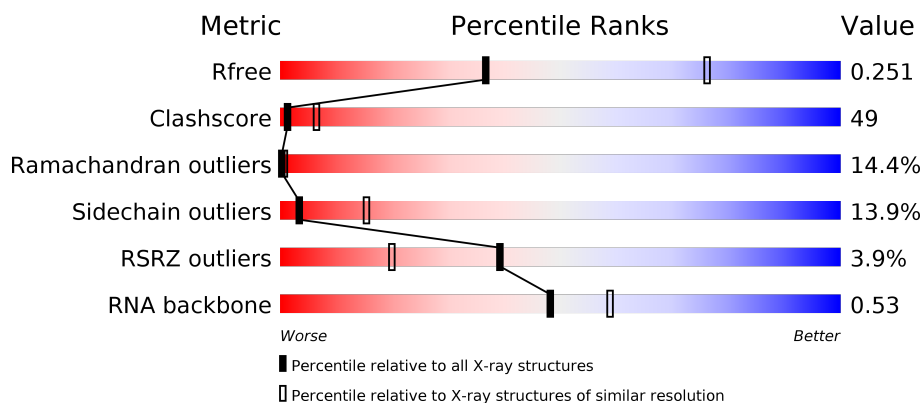
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div>3%</div> <div>17%</div> <div>67%</div> <div>14%</div> <div>..</div> </div>
1	CA	1509	<div> <div>2%</div> <div>21%</div> <div>65%</div> <div>13%</div> <div>.</div> </div>
2	AB	256	<div> <div>7%</div> <div>13%</div> <div>59%</div> <div>19%</div> <div>.</div> <div>8%</div> </div>
2	CB	256	<div> <div>9%</div> <div>15%</div> <div>56%</div> <div>19%</div> <div>.</div> <div>8%</div> </div>

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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	

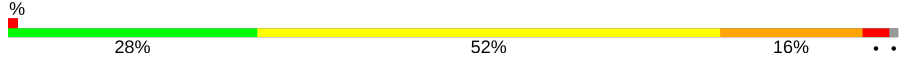
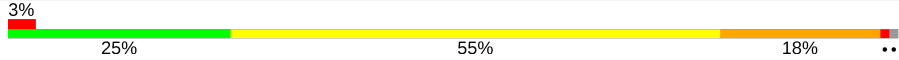
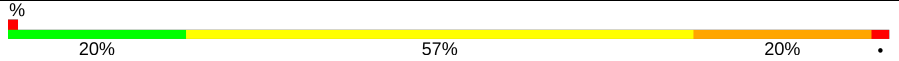
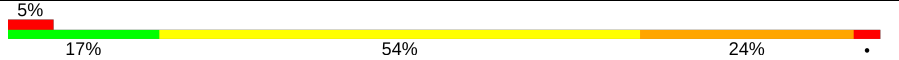
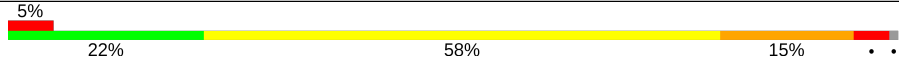
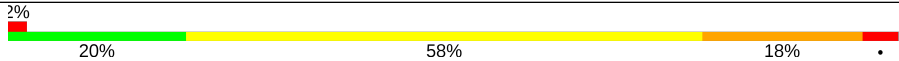
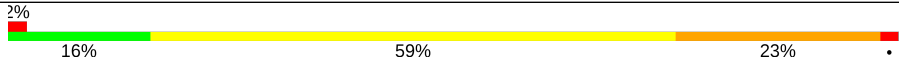
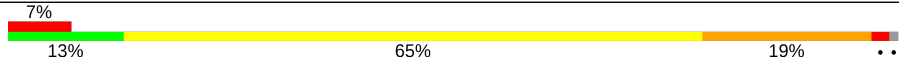
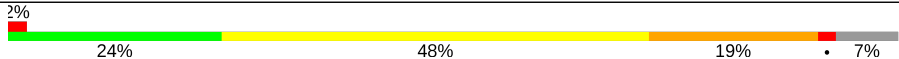
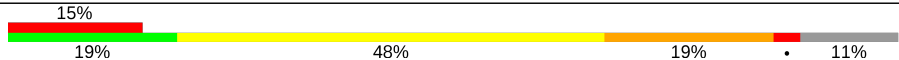
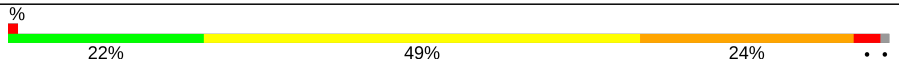
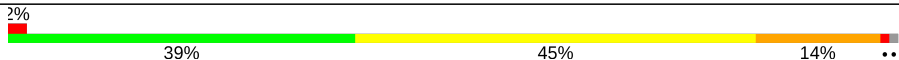
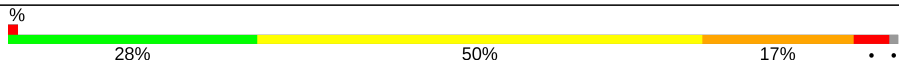
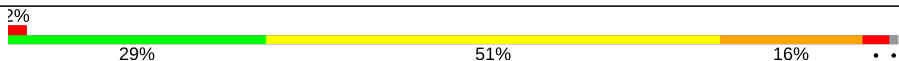
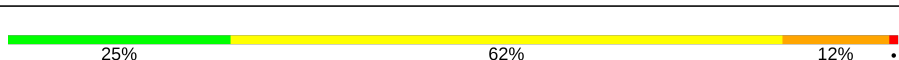
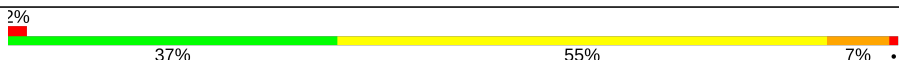
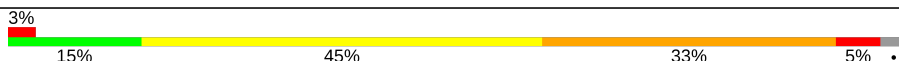
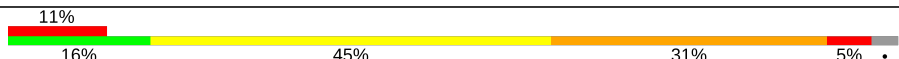
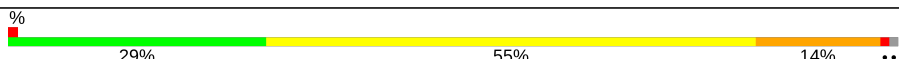
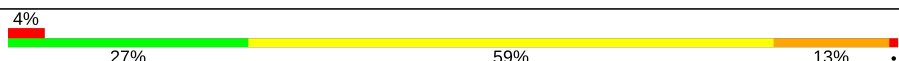
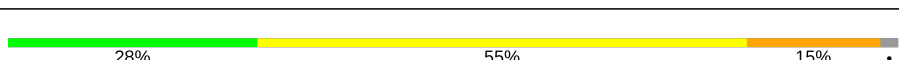
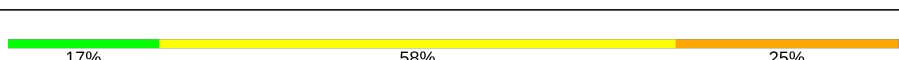
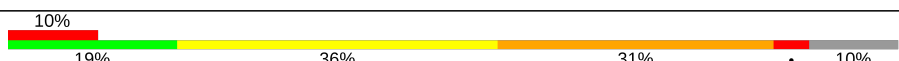
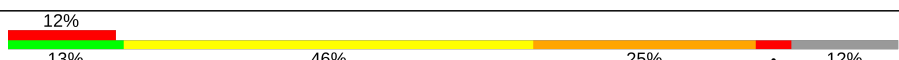
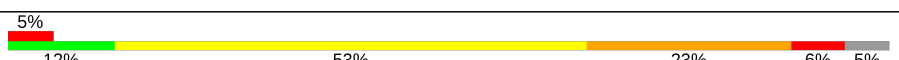
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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	184	
22	CV	184	
23	AW	77	
23	CW	77	
24	AX	5	
24	CX	5	
25	BA	2915	
25	DA	2915	
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	AA	1604	-	-	-	X
57	MG	AA	1611	-	-	-	X
57	MG	AA	1619	-	-	-	X
57	MG	AA	1664	-	-	-	X
57	MG	BA	3022	-	-	-	X
57	MG	BA	3038	-	-	-	X
57	MG	BA	3052	-	-	-	X
57	MG	BA	3086	-	-	-	X
57	MG	BA	3118	-	-	-	X
57	MG	BA	3139	-	-	-	X
57	MG	BA	3188	-	-	-	X
57	MG	BA	3268	-	-	-	X
57	MG	BA	3300	-	-	-	X
57	MG	BA	3323	-	-	-	X
57	MG	BA	3355	-	-	-	X
57	MG	BA	3388	-	-	-	X
57	MG	BA	3432	-	-	-	X
57	MG	BA	3442	-	-	-	X
57	MG	BA	3444	-	-	-	X
57	MG	BA	3448	-	-	-	X
57	MG	BP	201	-	-	-	X
57	MG	CA	1608	-	-	-	X
57	MG	CA	1652	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	CA	1708	-	-	-	X
57	MG	CW	102	-	-	-	X
57	MG	DA	3033	-	-	-	X
57	MG	DA	3072	-	-	-	X
57	MG	DA	3094	-	-	-	X
57	MG	DA	3108	-	-	-	X
57	MG	DA	3111	-	-	-	X
57	MG	DA	3144	-	-	-	X
57	MG	DA	3164	-	-	-	X
57	MG	DA	3175	-	-	-	X
57	MG	DA	3195	-	-	-	X
57	MG	DA	3267	-	-	-	X
57	MG	DB	208	-	-	-	X
58	ZN	AD	301	-	-	-	X
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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BA	459	Total	Mg	0	0
			459	459		
57	CA	109	Total	Mg	0	0
			109	109		
57	DF	1	Total	Mg	0	0
			1	1		
57	BE	1	Total	Mg	0	0
			1	1		
57	AW	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	B1	1	Total 1	Mg 1	0	0
57	BP	3	Total 3	Mg 3	0	0
57	DR	1	Total 1	Mg 1	0	0
57	B5	4	Total 4	Mg 4	0	0
57	BB	9	Total 9	Mg 9	0	0
57	BT	1	Total 1	Mg 1	0	0
57	BF	1	Total 1	Mg 1	0	0
57	BX	1	Total 1	Mg 1	0	0
57	AA	117	Total 117	Mg 117	0	0
57	BQ	3	Total 3	Mg 3	0	0
57	D6	2	Total 2	Mg 2	0	0
57	CX	1	Total 1	Mg 1	0	0
57	BU	1	Total 1	Mg 1	0	0
57	DD	1	Total 1	Mg 1	0	0
57	BR	1	Total 1	Mg 1	0	0
57	DA	305	Total 305	Mg 305	0	0
57	B7	1	Total 1	Mg 1	0	0
57	AL	1	Total 1	Mg 1	0	0
57	DP	1	Total 1	Mg 1	0	0
57	CW	5	Total 5	Mg 5	0	0
57	D5	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BD	1	Total 1	Mg 1	0	0
57	AT	1	Total 1	Mg 1	0	0
57	B0	2	Total 2	Mg 2	0	0
57	CE	1	Total 1	Mg 1	0	0
57	DB	10	Total 10	Mg 10	0	0
57	BH	1	Total 1	Mg 1	0	0

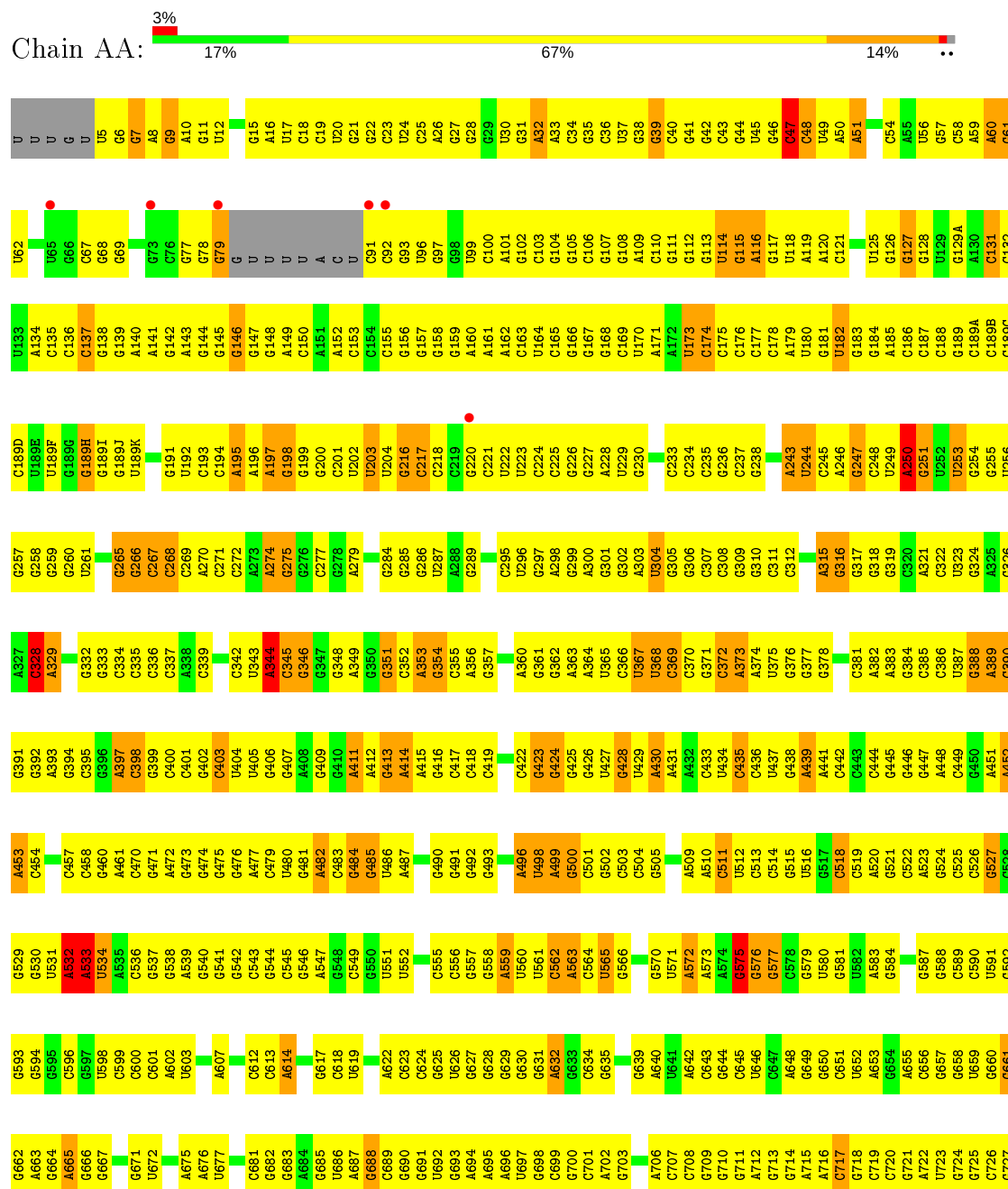
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

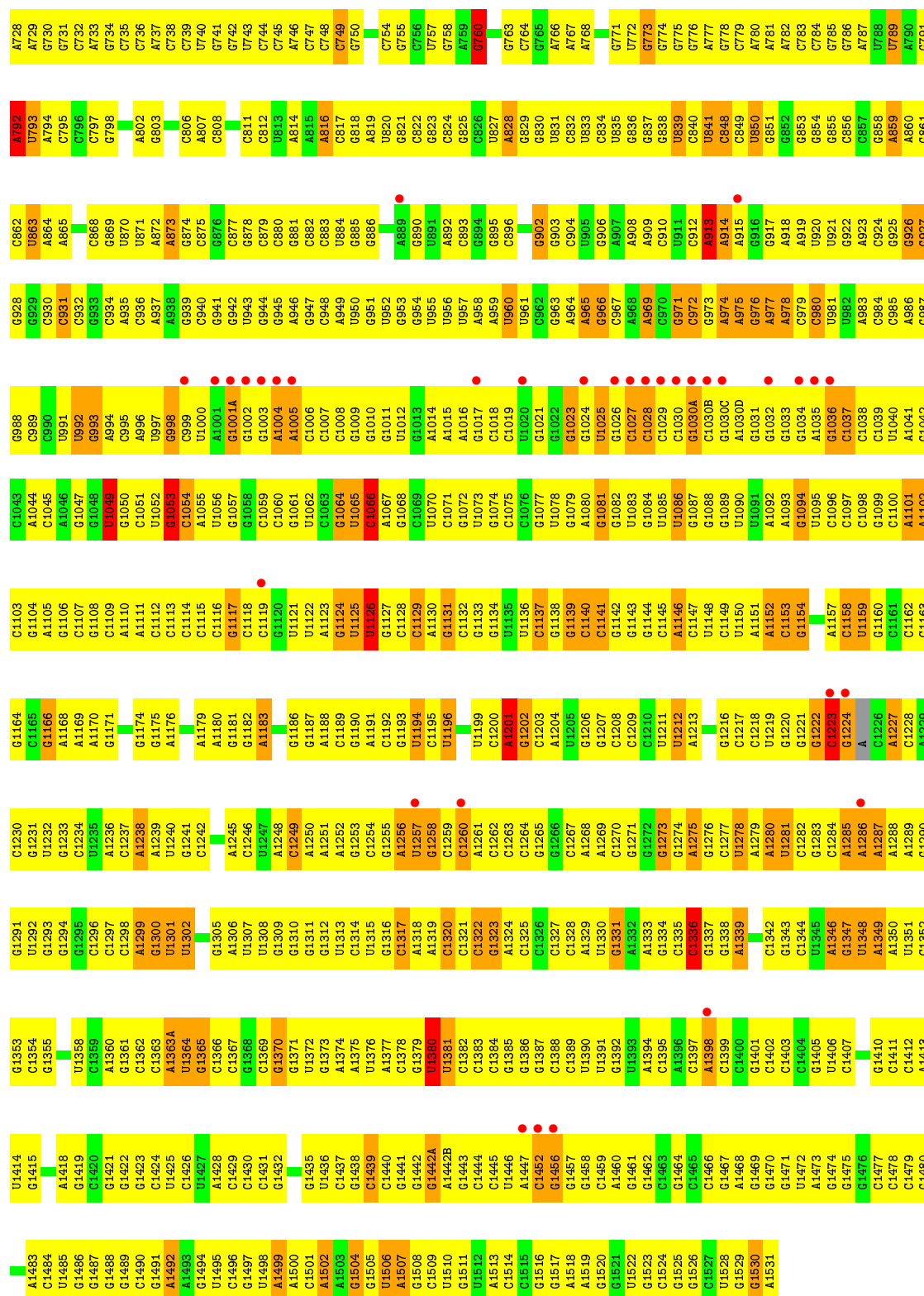
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	B5	1	Total 1	Zn 1	0	0
58	AD	1	Total 1	Zn 1	0	0
58	B9	1	Total 1	Zn 1	0	0
58	D9	1	Total 1	Zn 1	0	0
58	D5	1	Total 1	Zn 1	0	0
58	CD	1	Total 1	Zn 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

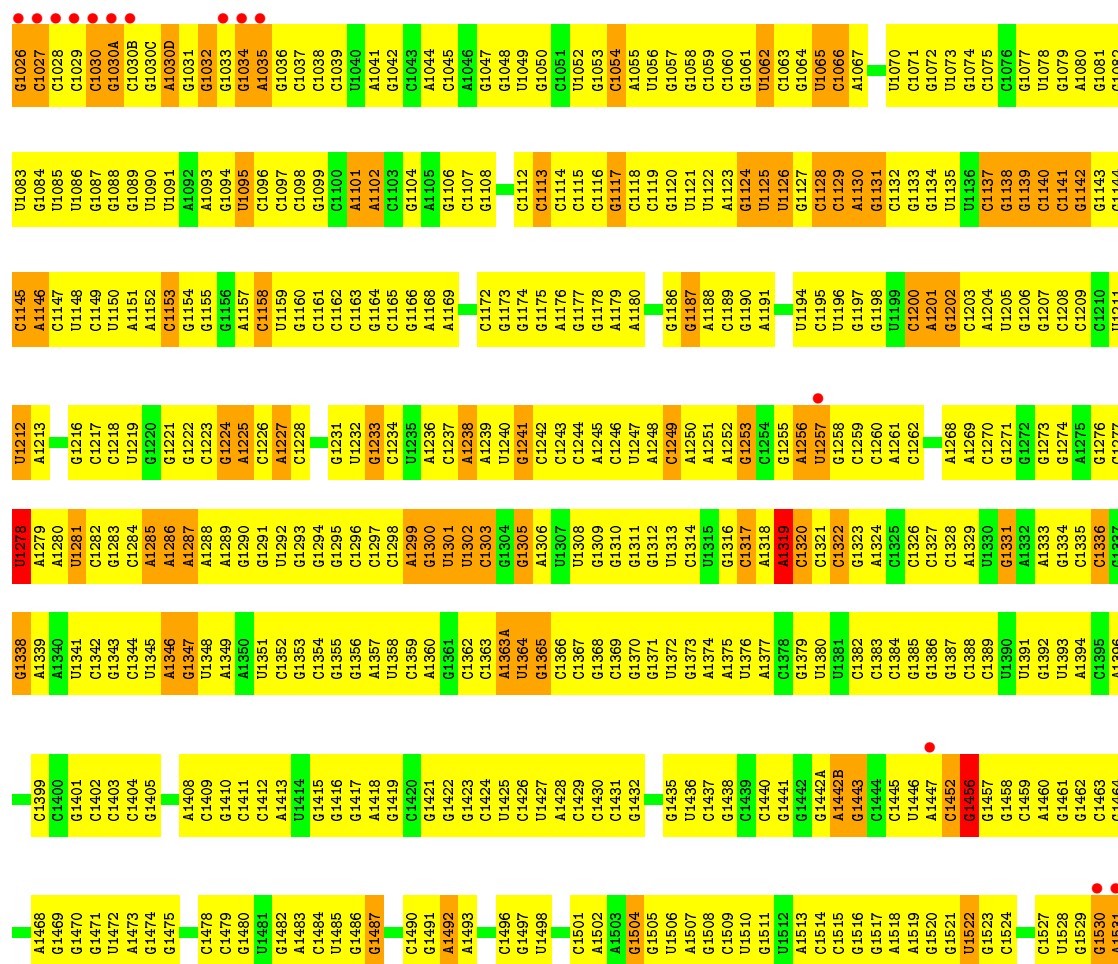
- Molecule 1: 16S ribosomal RNA



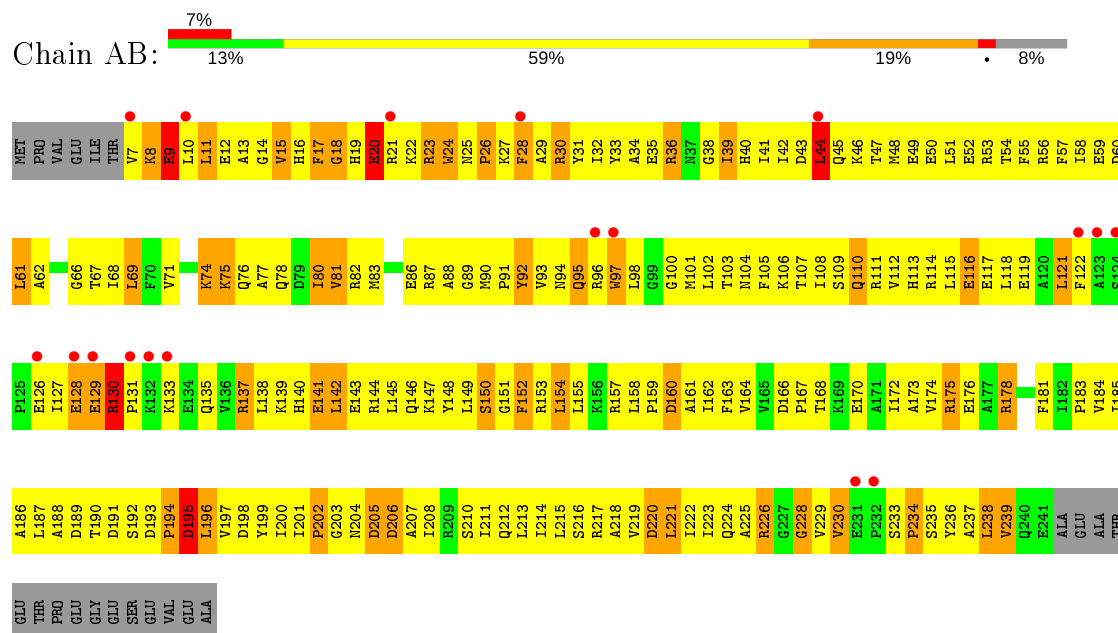


• Molecule 1: 16S ribosomal RNA

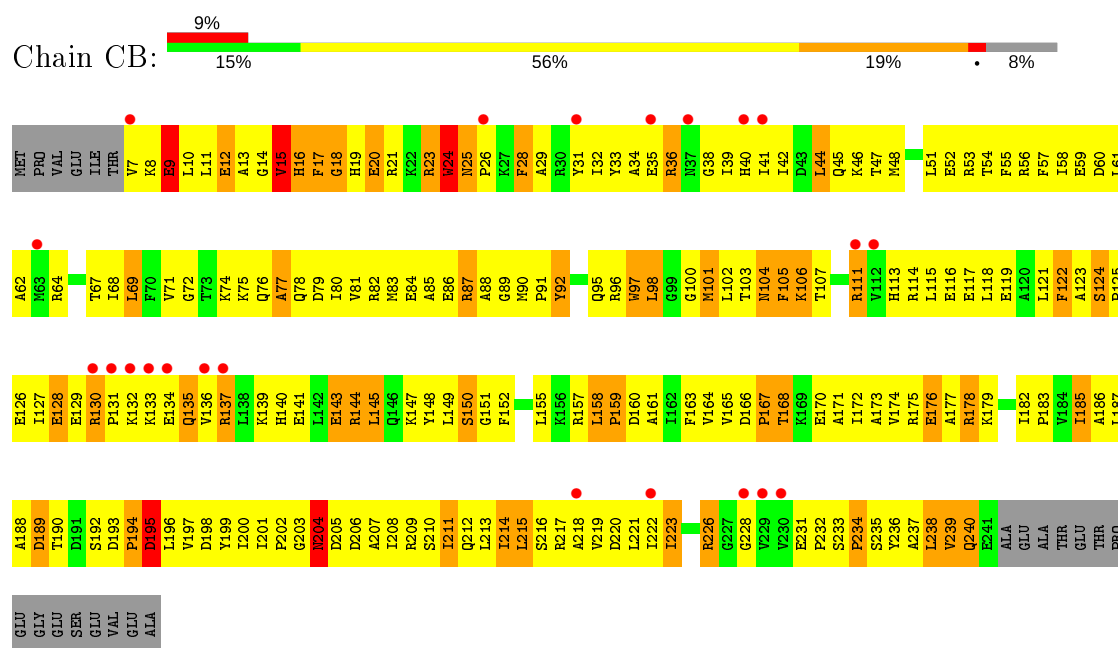




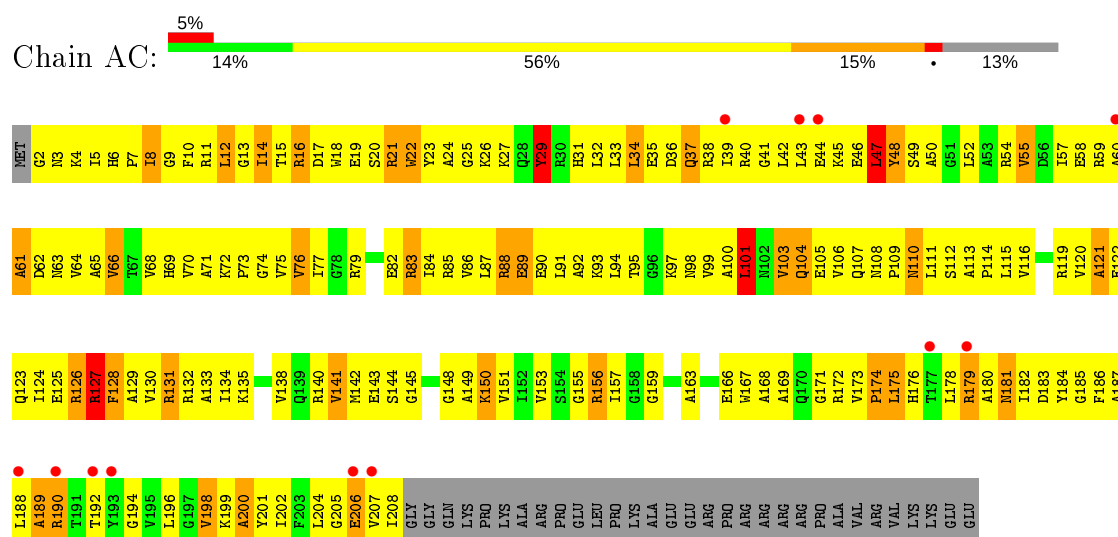
• Molecule 2: 30S ribosomal protein S2



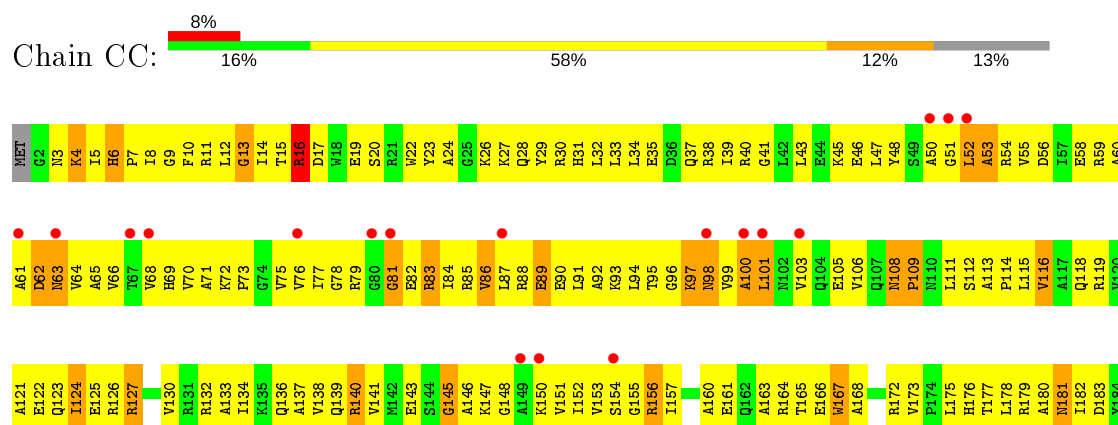
• Molecule 2: 30S ribosomal protein S2

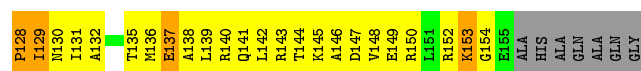


• Molecule 3: 30S ribosomal protein S3

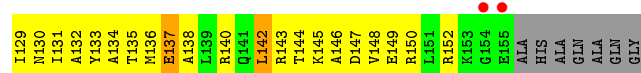
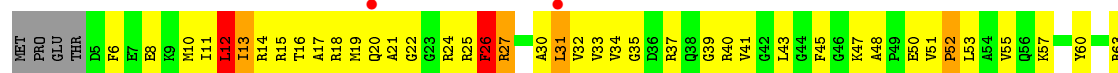


• Molecule 3: 30S ribosomal protein S3

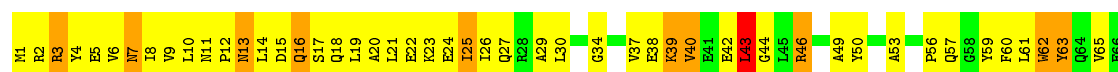




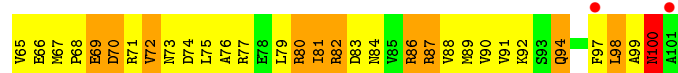
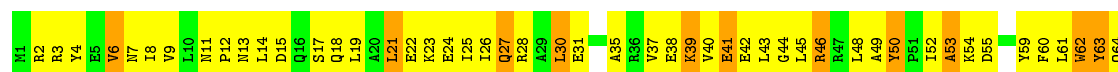
• Molecule 5: 30S ribosomal protein S5



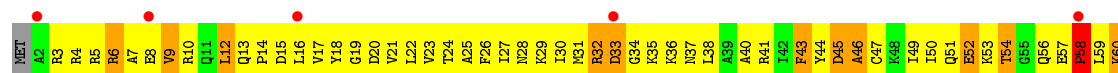
• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6

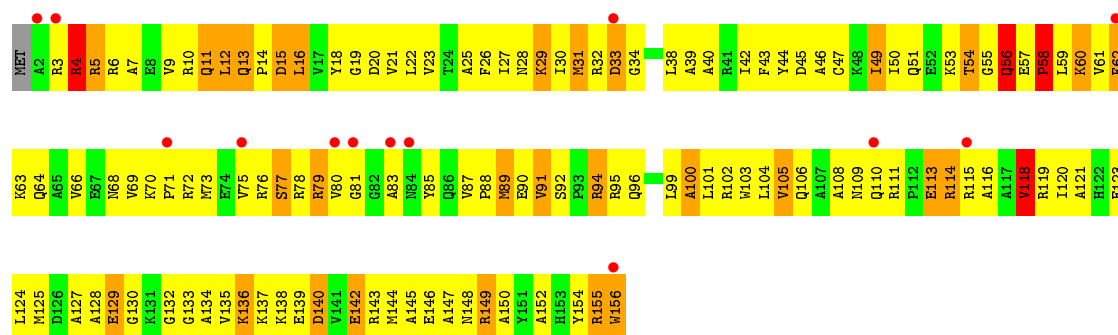


• Molecule 7: 30S ribosomal protein S7

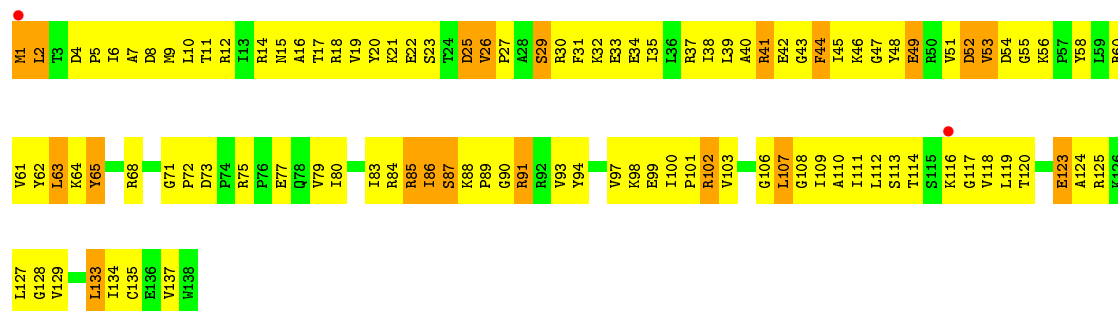




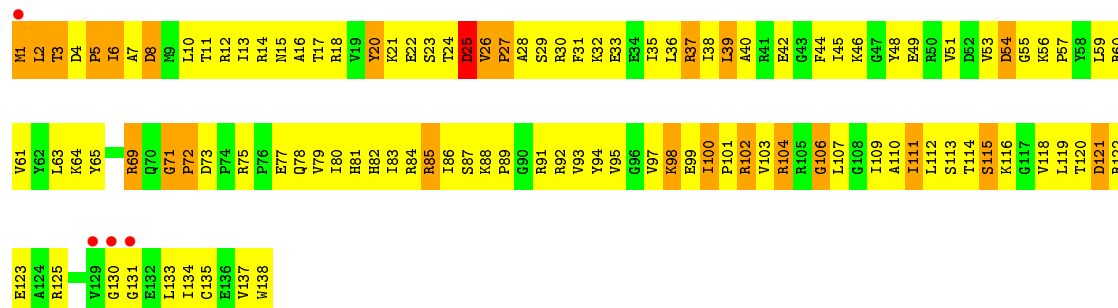
• Molecule 7: 30S ribosomal protein S7



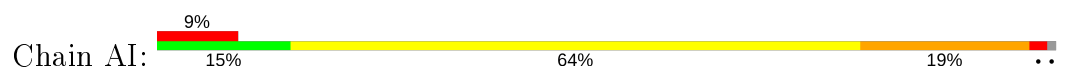
• Molecule 8: 30S ribosomal protein S8

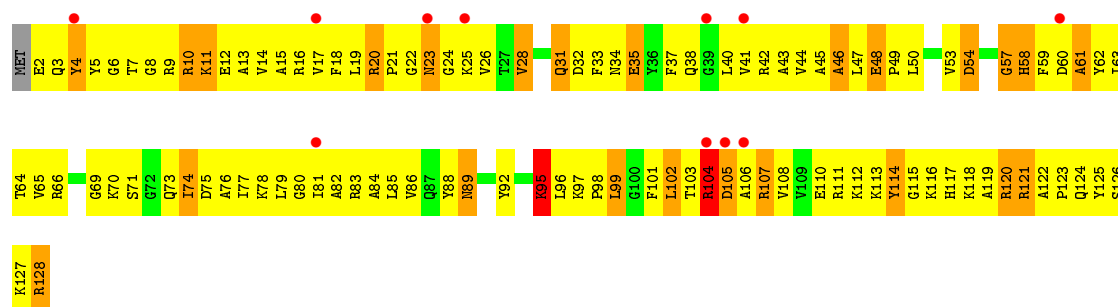


• Molecule 8: 30S ribosomal protein S8

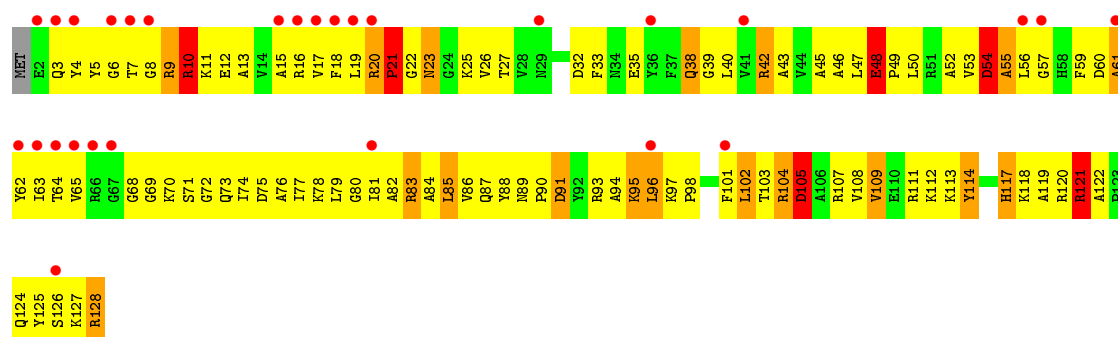


• Molecule 9: 30S ribosomal protein S9

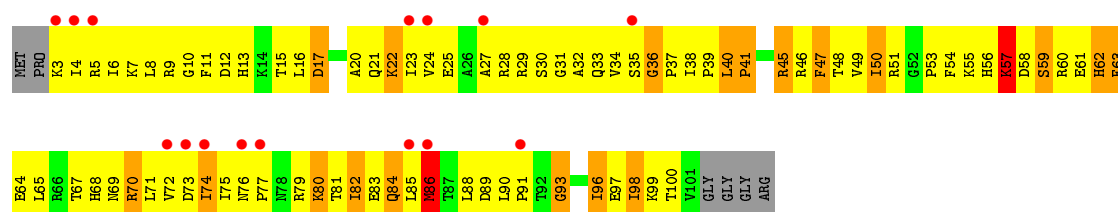
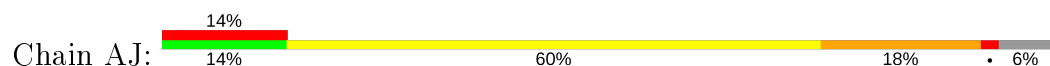




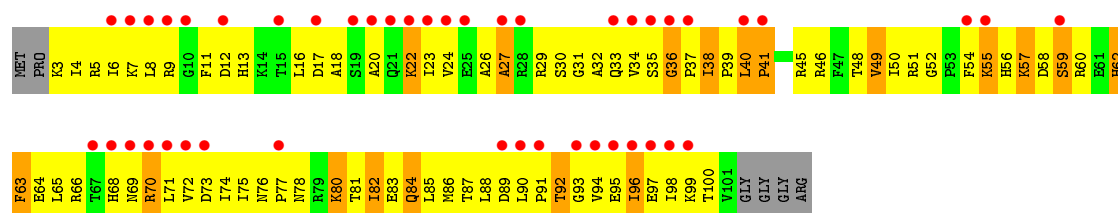
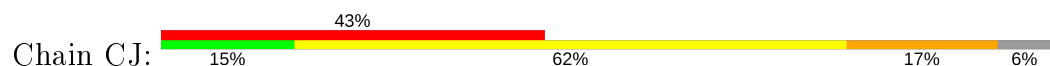
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10

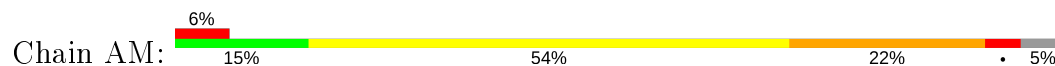


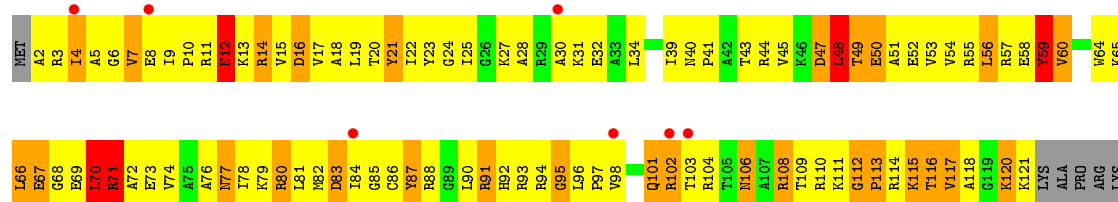
• Molecule 10: 30S ribosomal protein S10



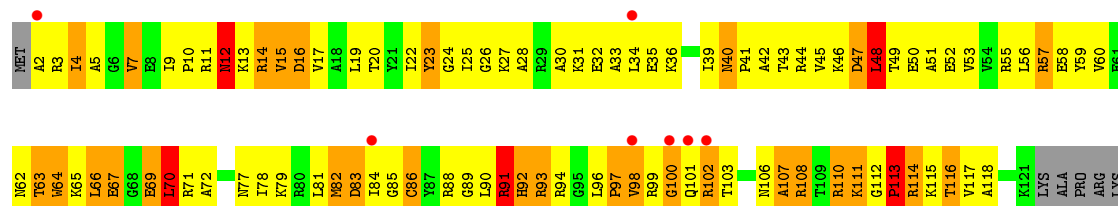
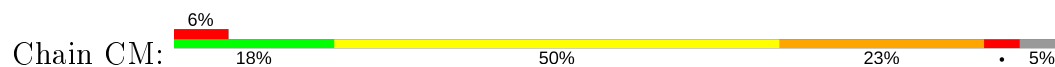
• Molecule 11: 30S ribosomal protein S11



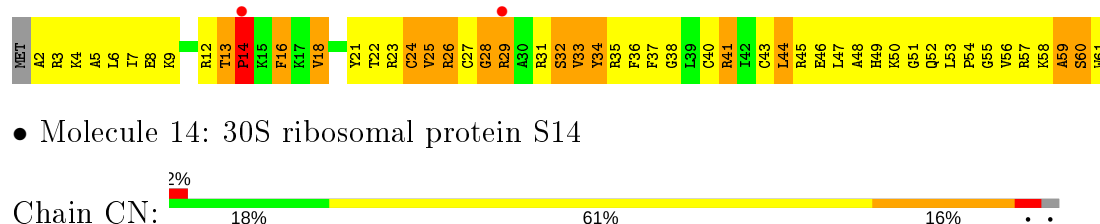
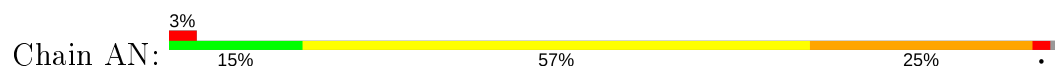




• Molecule 13: 30S ribosomal protein S13



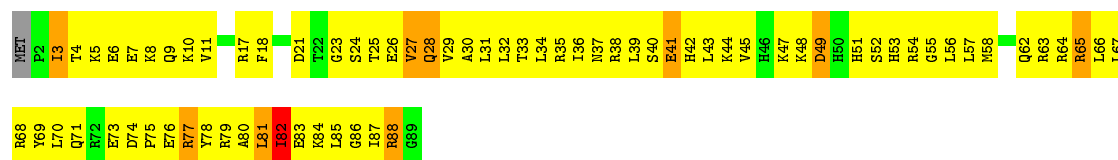
• Molecule 14: 30S ribosomal protein S14



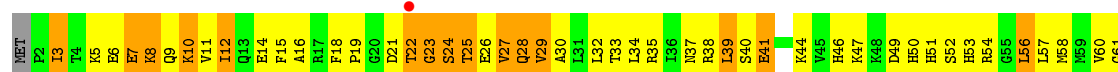
• Molecule 14: 30S ribosomal protein S14

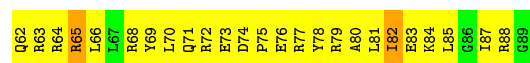


• Molecule 15: 30S ribosomal protein S15

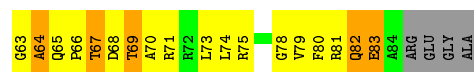
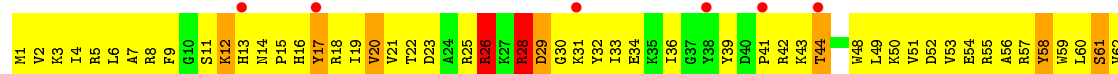


• Molecule 15: 30S ribosomal protein S15

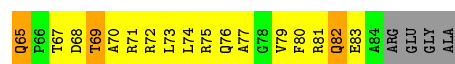




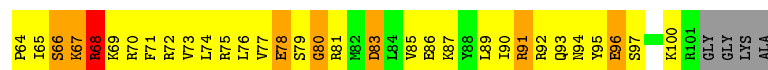
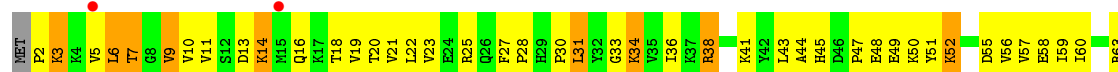
• Molecule 16: 30S ribosomal protein S16



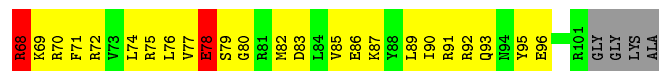
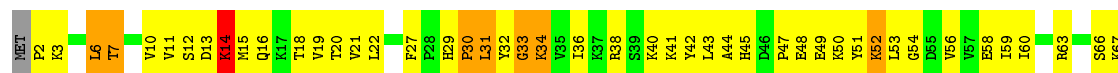
• Molecule 16: 30S ribosomal protein S16



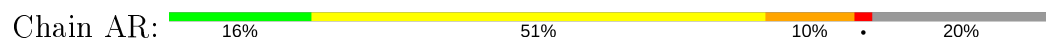
• Molecule 17: 30S ribosomal protein S17



• Molecule 17: 30S ribosomal protein S17

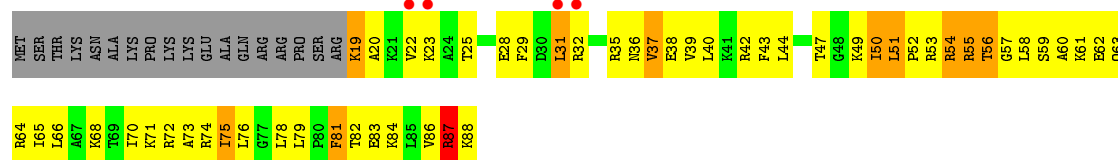
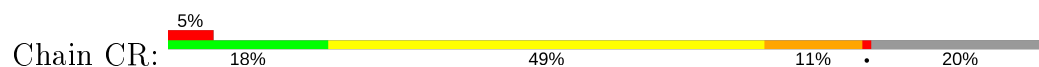


• Molecule 18: 30S ribosomal protein S18

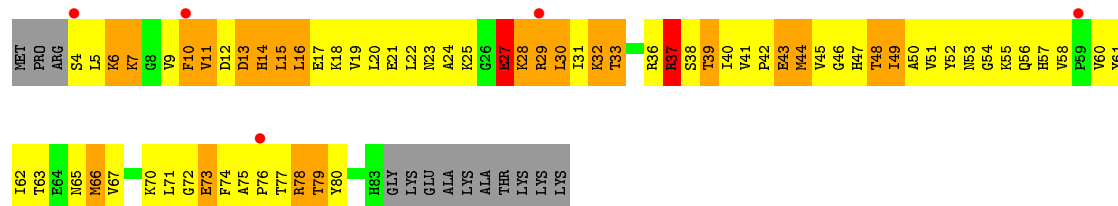
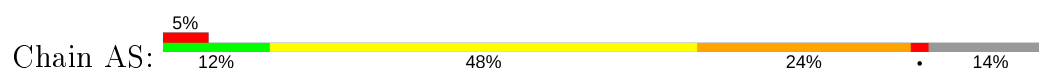




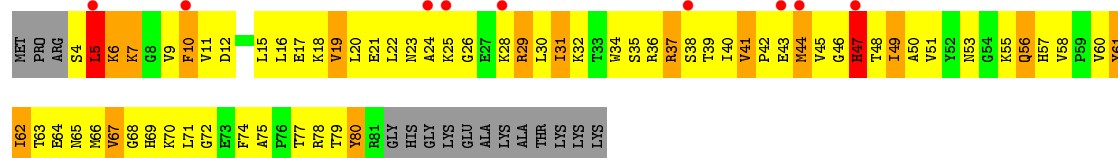
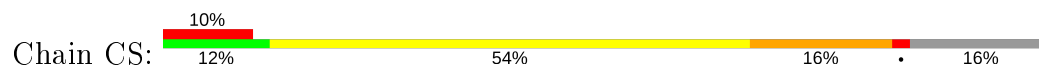
- Molecule 18: 30S ribosomal protein S18



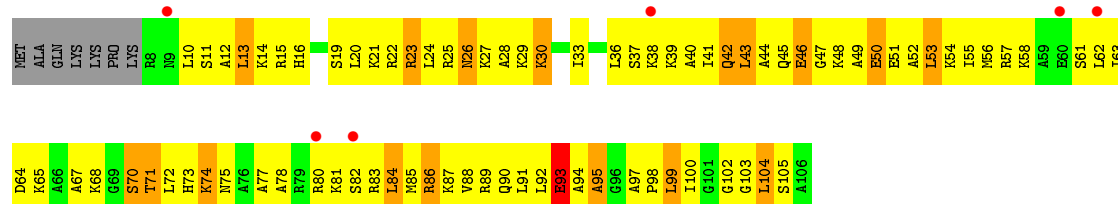
- Molecule 19: 30S ribosomal protein S19



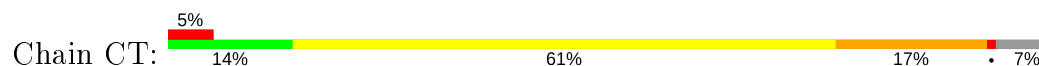
- Molecule 19: 30S ribosomal protein S19

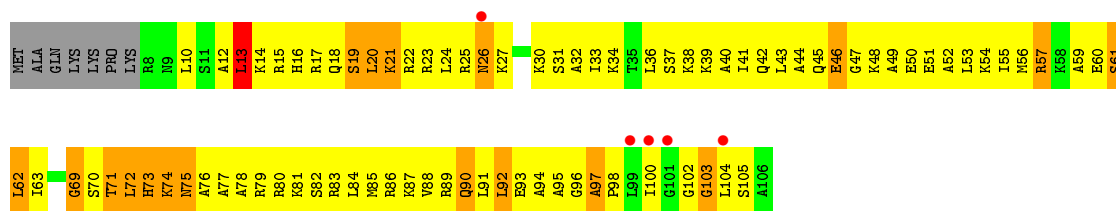


- Molecule 20: 30S ribosomal protein S20

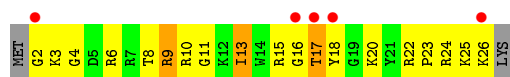


- Molecule 20: 30S ribosomal protein S20

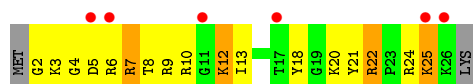




• Molecule 21: 30S ribosomal protein Thx



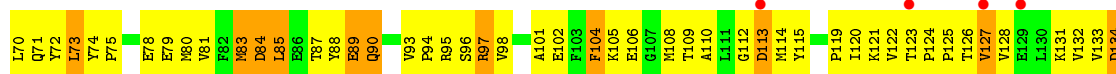
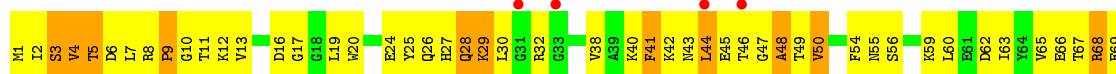
• Molecule 21: 30S ribosomal protein Thx



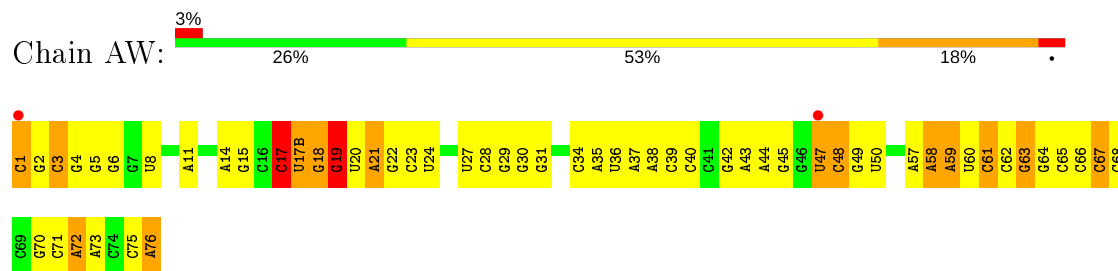
• Molecule 22: Elongation factor P



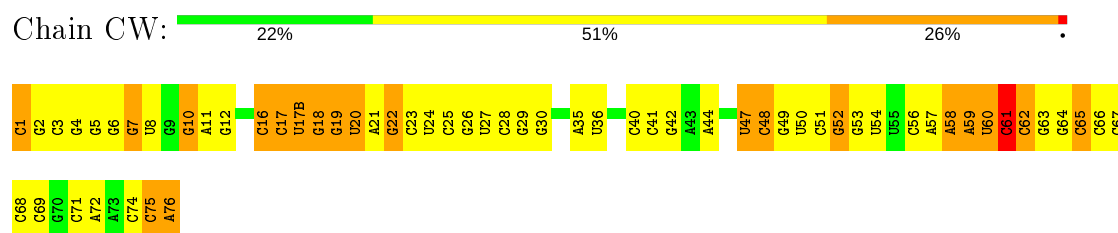
• Molecule 22: Elongation factor P



- Molecule 23: tRNA-Met



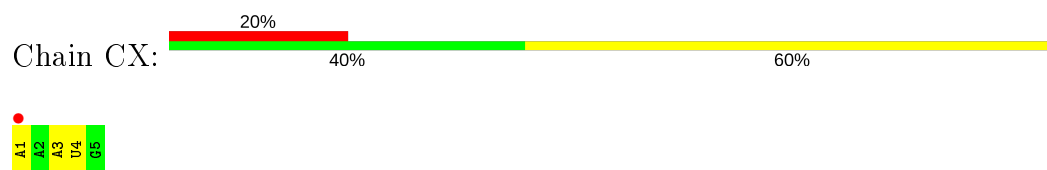
- Molecule 23: tRNA-Met



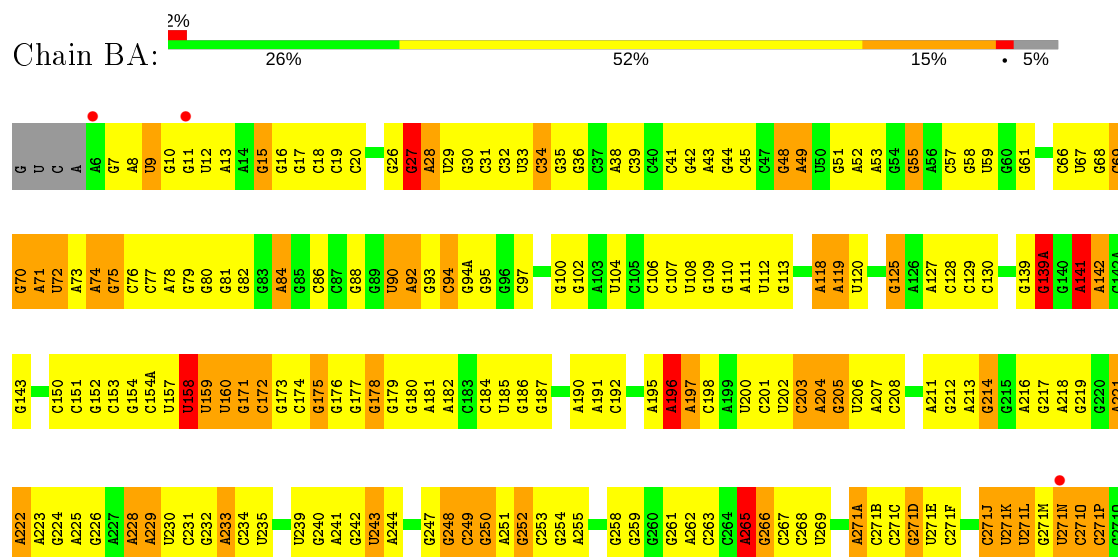
- Molecule 24: RNA (5'-R(P*AP*AP*AP*UP*G)-3')



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

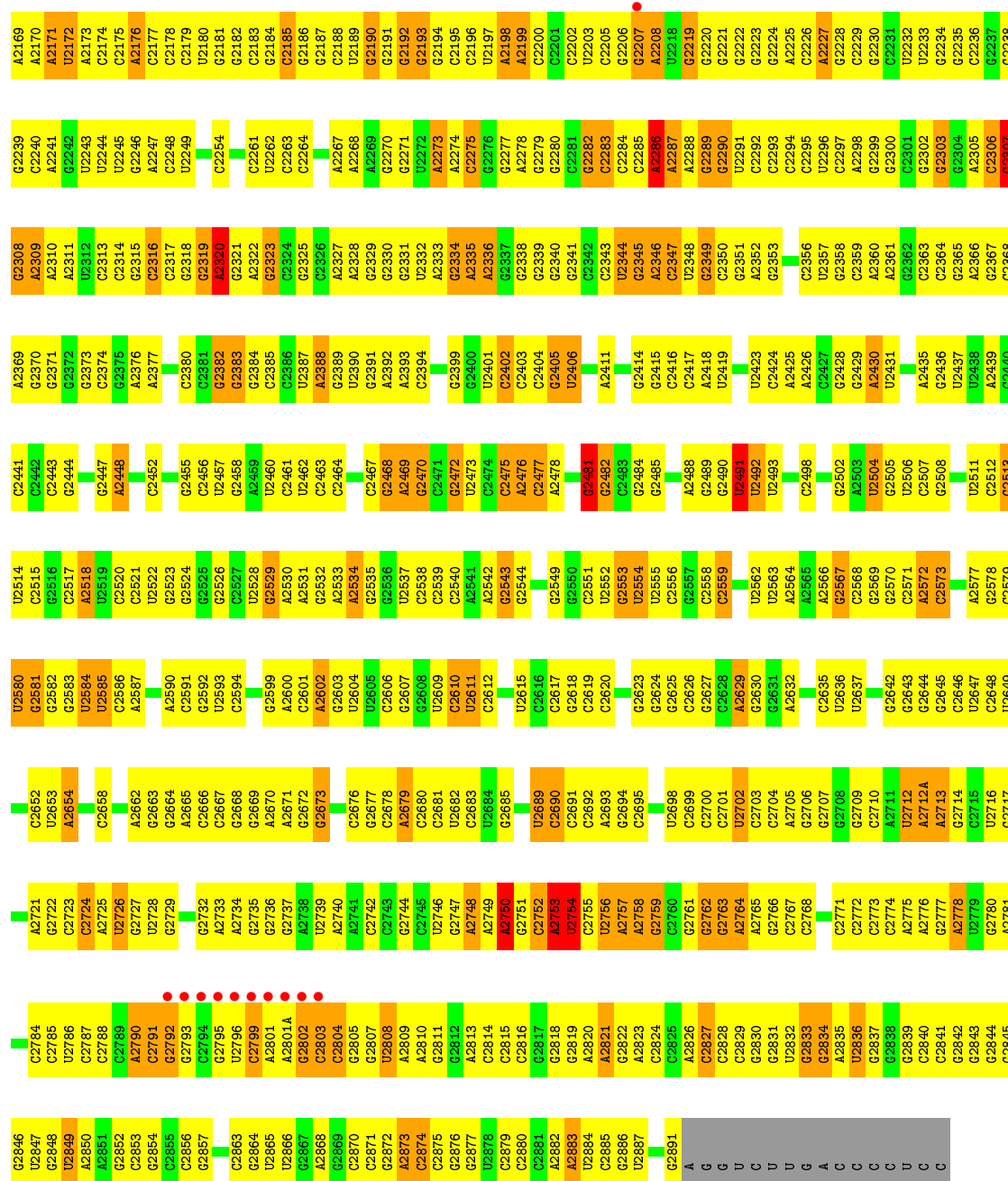


- Molecule 25: 23S ribosomal RNA

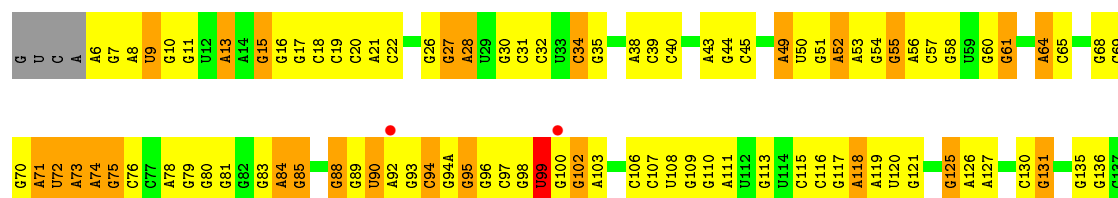




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C2111	C2039	A1972	G1752	G1825	C1902	C1908	A1972	C2039	C2111
G2112	G2040	G1973	G1753	A1826	G1903	G1908	G1973	G2040	G2112
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A2114	A2042		A1755	G1828	G1906	G1907	A2042	A2114	A2114
G2115	C2043	A1981	G1756	U1879	G1907	G1907	A1981	G2115	G2115
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U2118	G2049	G1983	G1759	G1882	G1910	G1910	G1983	U2118	U2118
A2119	C2050	G1984	G1760	G1883	G1911	G1911	G1984	A2119	A2119
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• Molecule 25: 23S ribosomal RNA

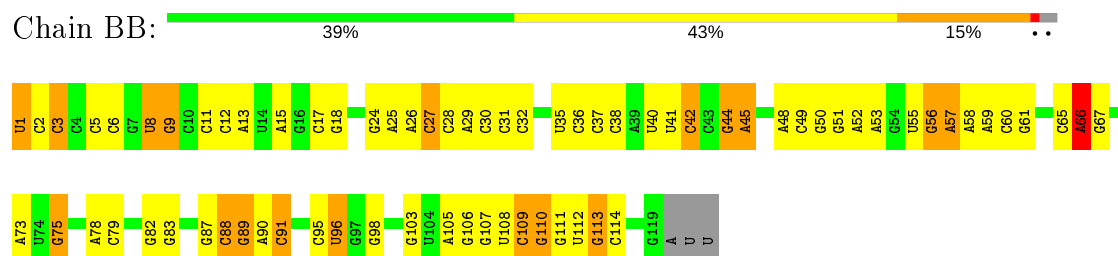




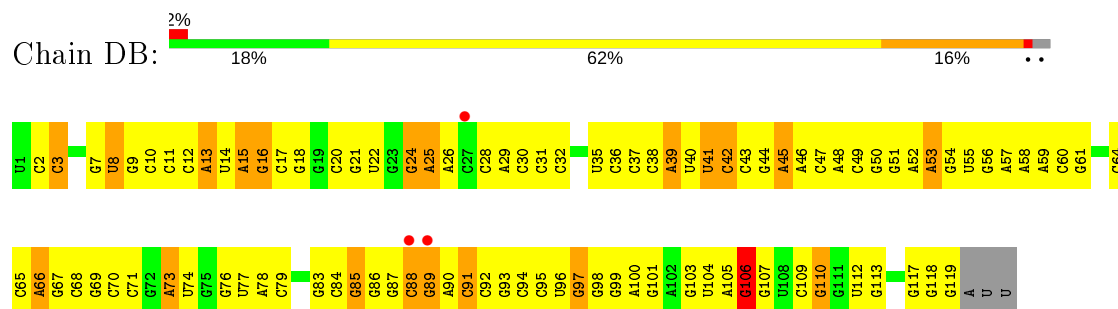
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		A1877	U1796	G1642	C1506	C1506	G1442				U1240	C1179	G1113
G1948	G1948	G1878	C1797	G1642	A1507	A1507	G1443				A1241	C1180	G1114
A2019	G1949	C1879	U1798	G1643	A1507	A1507	G1444				A1242	C1181	G1115
A2020	G1950	C1880	G1799	C1644	A1508	A1508							C1116

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C2910	U2847	A2781	A2721	G2523	G2459	G2389	G2255	G2115	G2048
C2911	G2848	G2782	G2722	G2524	U2462	U2390	G2256	G2116	G2049
C2912	U2849	C2783	C2723	G2525	A2463	A2391	G2257	A2117	C2050
C2913	C2849	C2784	C2724	U2526	C2464	A2392	G2258	A2118	A2051
C2914	A2850	C2785	A2725	G2527	C2465	A2393	U2259	A2119	G2052
C2915	C2851	U2786	U2726	U2528	C2466	C2394	C2261	U2120	C2053
C2916	G2852	C2787	G2727	U2529	C2467	G2395	U2262	G2121	G2054
C2917	C2853	C2788	U2728	G2530	C2468	C2396	C2263	U2122	A2055
C2918	G2854	C2789	G2729	G2531	A2469	G2397	A2264	G2123	G2056
C2919	C2855	A2790	C2730	U2532	G2470	U2398	U2265	G2124	A2057
C2920	G2856	G2791	G2731	A2533	C2471	G2399	A2266	G2125	G2058
C2921	G2857	G2792	G2732	A2534	G2472	U2400	A2267	A2126	A2059
C2922	C2858	C2793	A2733	G2535	U2473	C2401	G2270	G2127	G2060
C2923	G2859	G2794	U2734	G2536	A2735	C2402	G2271	C2128	G2061
C2924	A2860	U2795	G2735	U2537	C2476	C2403	U2272	C	A2062
C2925	G2861	C2796	G2736	C2538	A2477	C2404	A2273	U	C2063
C2926	C2862	U2797	G2737	C2539	C2478	G2405	A2274	G	C2064
C2927	C2863	A2801	G2738	C2540	C2479	U2406	C2275	U	C2065
C2928	G2864	A2801A	U2739	A2541	A2478	G2407	G2276	G	U2068
C2929	U2865	G2802	U2740	U2542	C2480	U2408	G2277	A	G2069
C2930	G2866	C2803	A2741	A2543	C2481	G2409	A2278	A	G2070
C2931	G2867	C2804	C2742	G2544	G2482	G2410	G2279	C	A2071
C2932	A2868	G2805	G2743	U2545	C2483	A2411	G2282	C	U2074
C2933	G2869	C2806	C2744	U2546	C2484	A2412	C2283	C	U2075
C2934	C2870	U2807	G2745	G2547	G2485	G2413	C2284	C	C2076
C2935	G2871	A2808	C2746	G2548	G2486	G2414	C2285	C	U2077
C2936	C2872	C2809	U2747	U2552	G2487	G2415	A2286	G	G2078
C2937	G2873	A2810	G2748	U2553	C2488	C2416	G2287	C	G2079
C2938	C2874	G2811	A2749	U2554	A2489	C2417	A2288	U	A2081
C2939	G2875	C2812	A2750	U2555	G2490	U2418	G2289	C	C2082
C2940	C2876	G2813	G2751	C2556	G2491	U2419	G2290	C	G2083
C2941	G2877	C2814	C2752	C2557	G2492	C2420	U2291	C	C2084
C2942	C2878	U2815	U2753	C2558	U2493	G2421	C2292	G	C2085
C2943	C2879	G2816	G2754	G2559	U2494	A2422	C2293	G	U2086

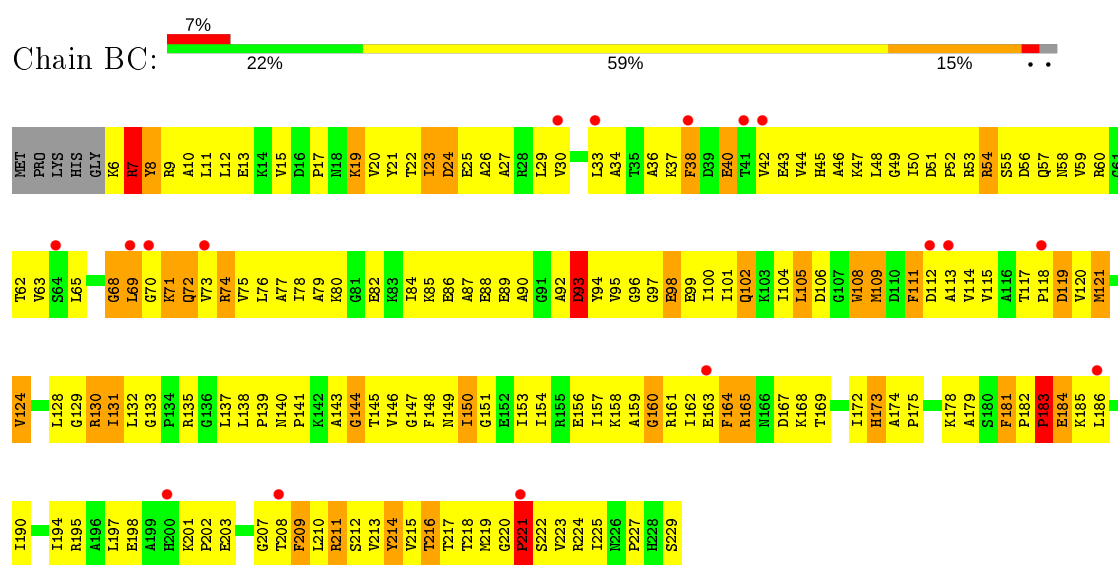
- Molecule 26: 5S ribosomal RNA



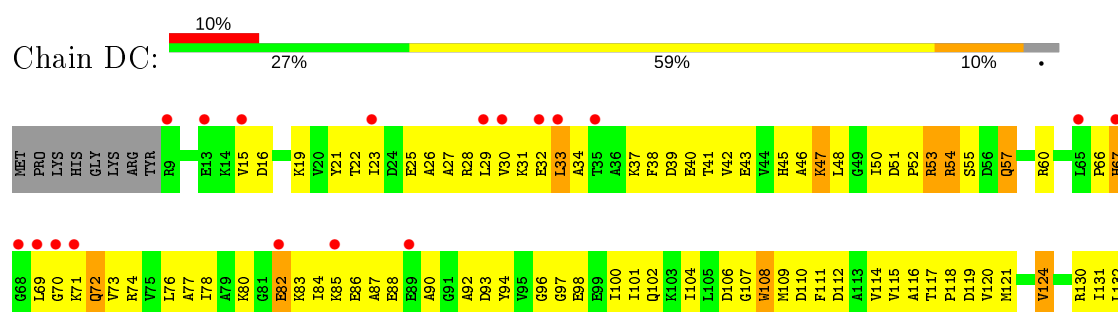
- Molecule 26: 5S ribosomal RNA

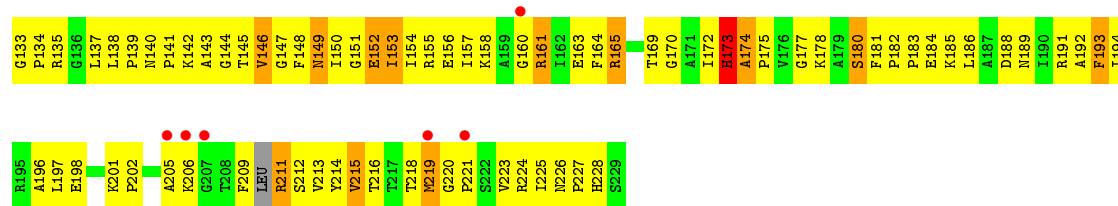


- Molecule 27: 50S ribosomal protein L1

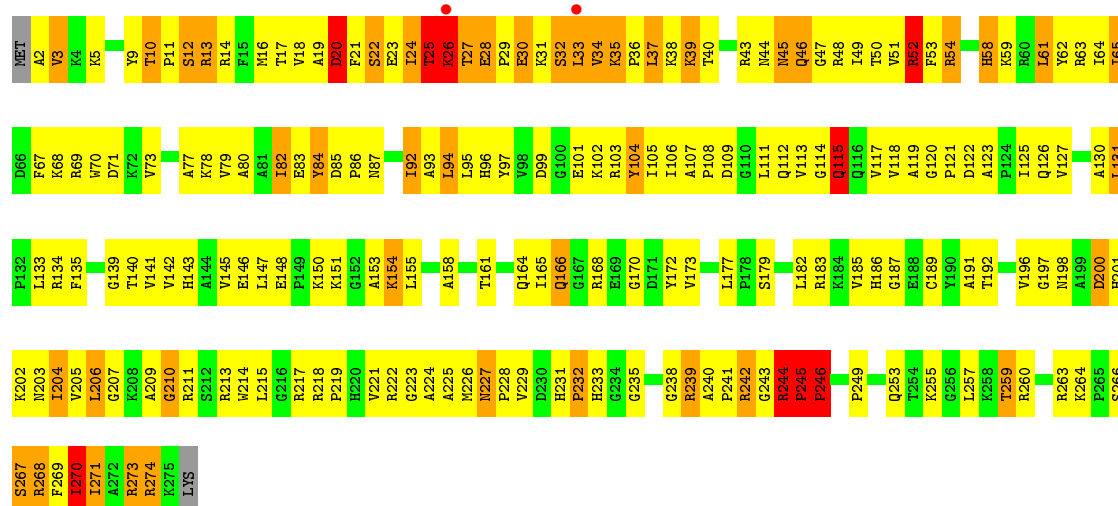


- Molecule 27: 50S ribosomal protein L1

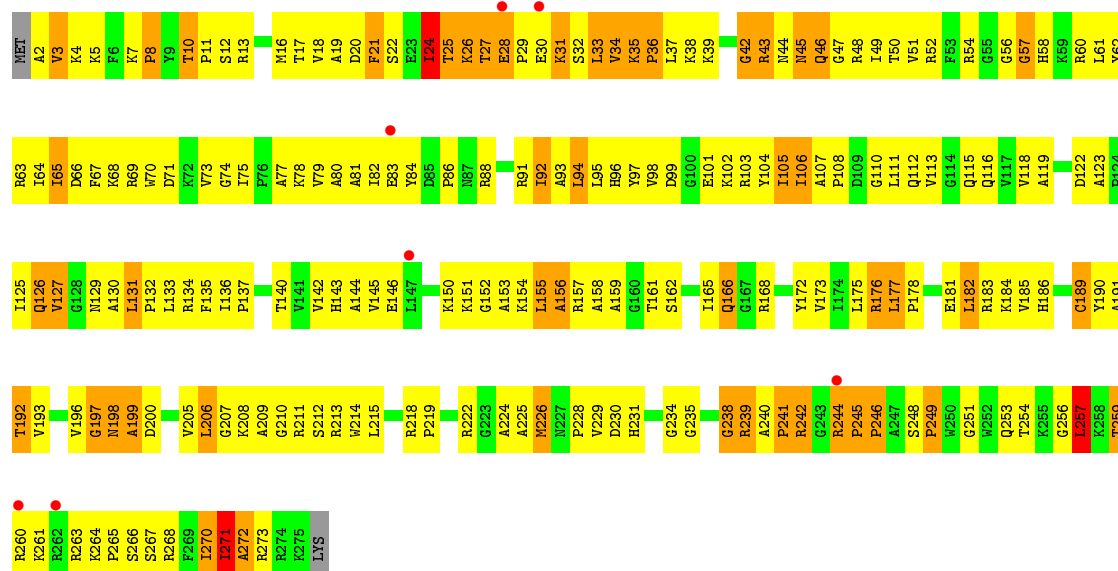




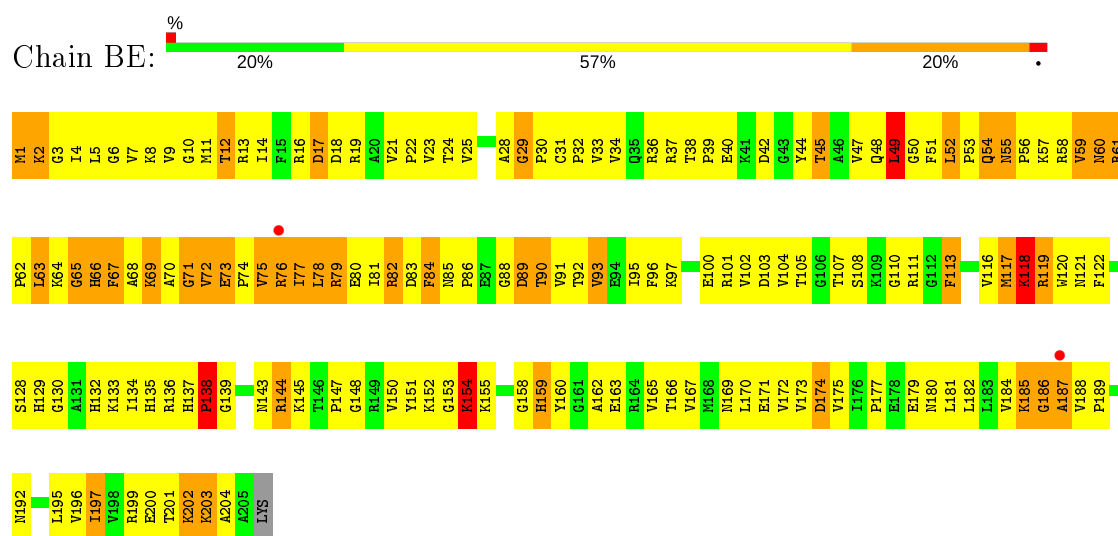
• Molecule 28: 50S ribosomal protein L2



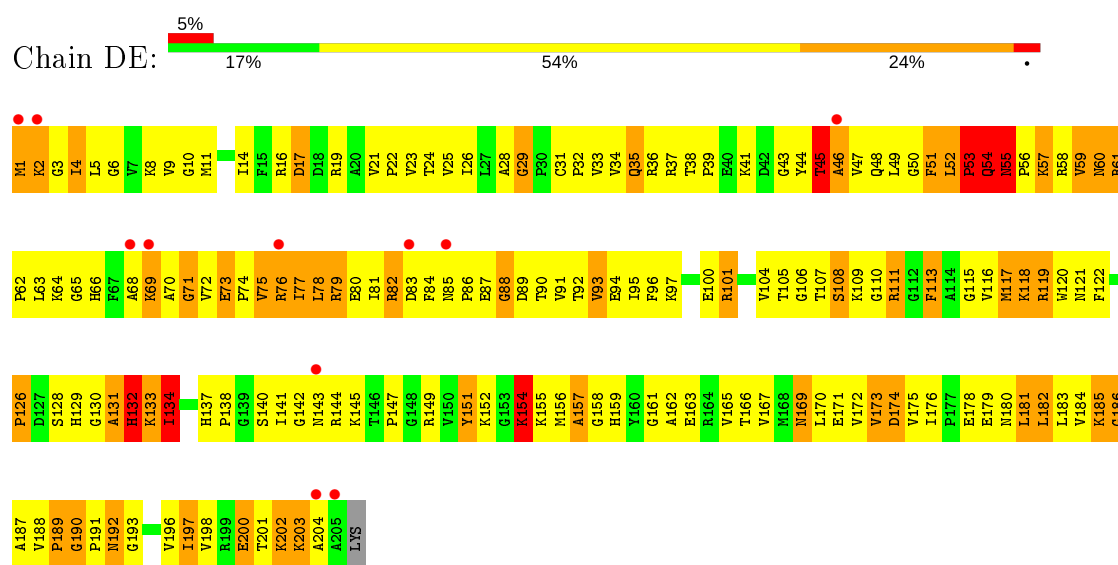
• Molecule 28: 50S ribosomal protein L2



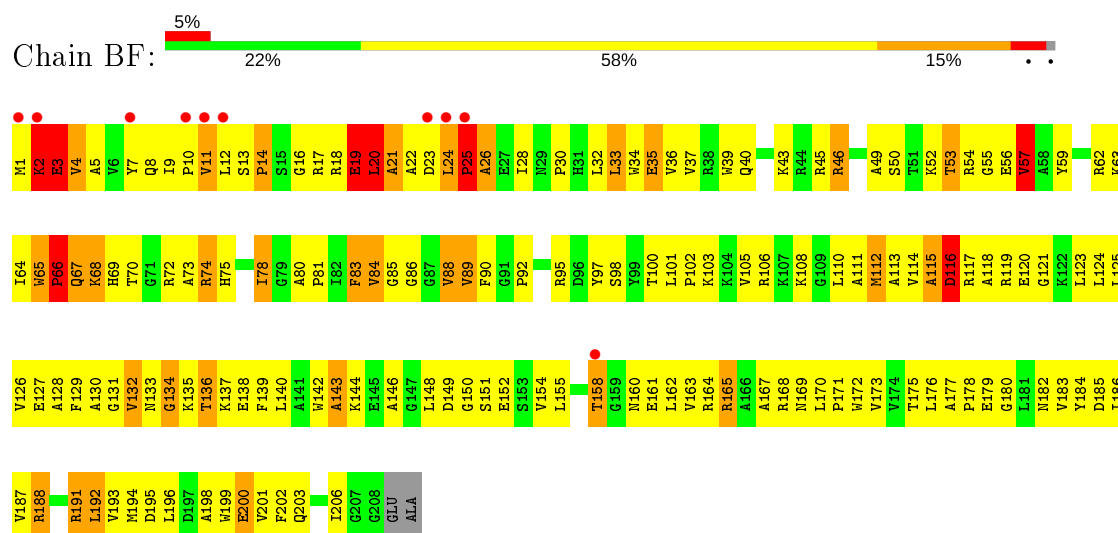
• Molecule 29: 50S ribosomal protein L3



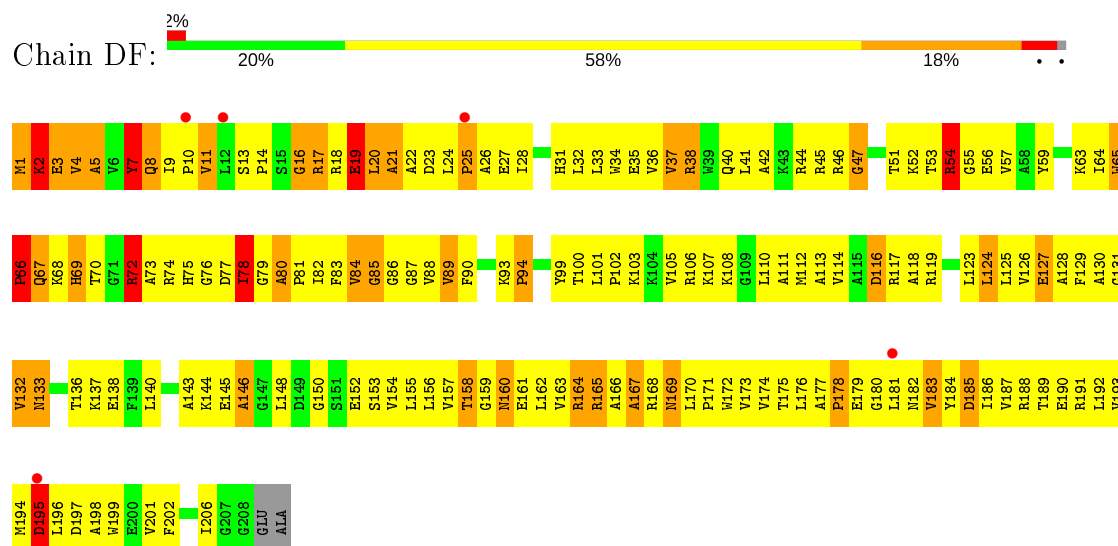
• Molecule 29: 50S ribosomal protein L3



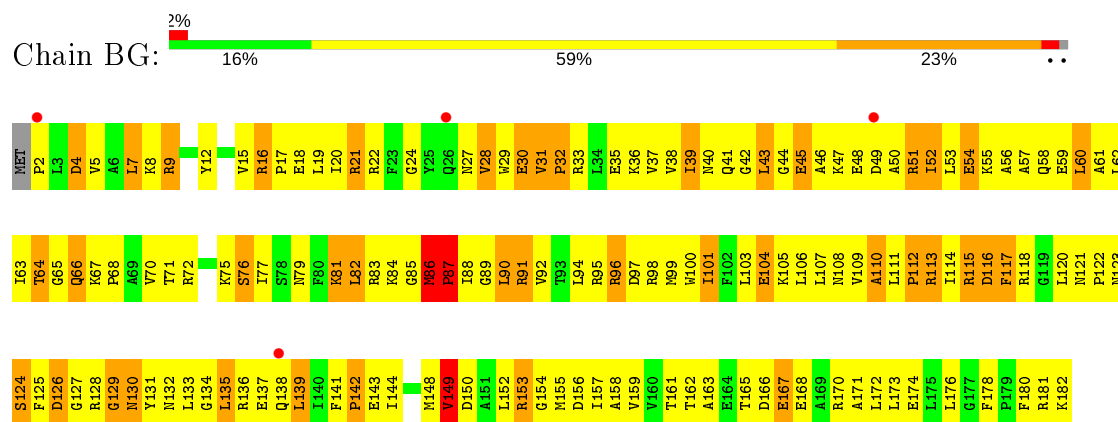
• Molecule 30: 50S ribosomal protein L4



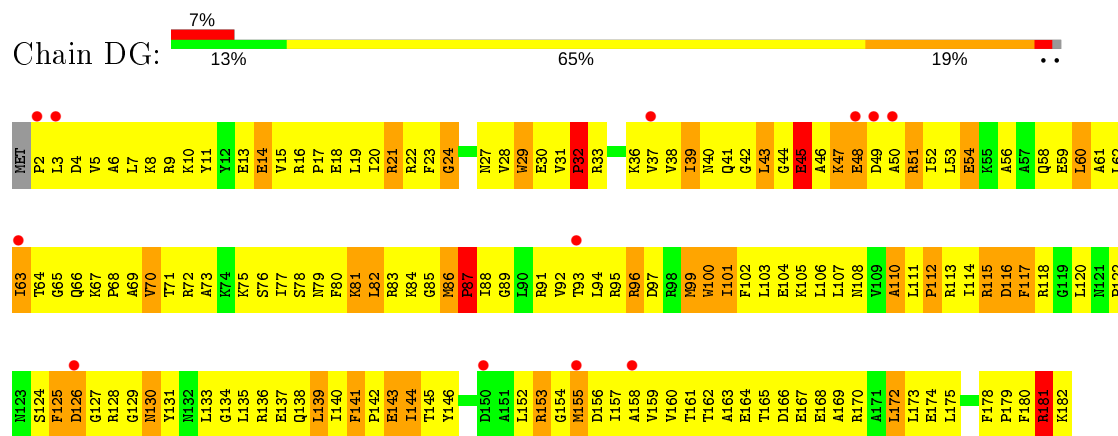
- Molecule 30: 50S ribosomal protein L4



- Molecule 31: 50S ribosomal protein L5

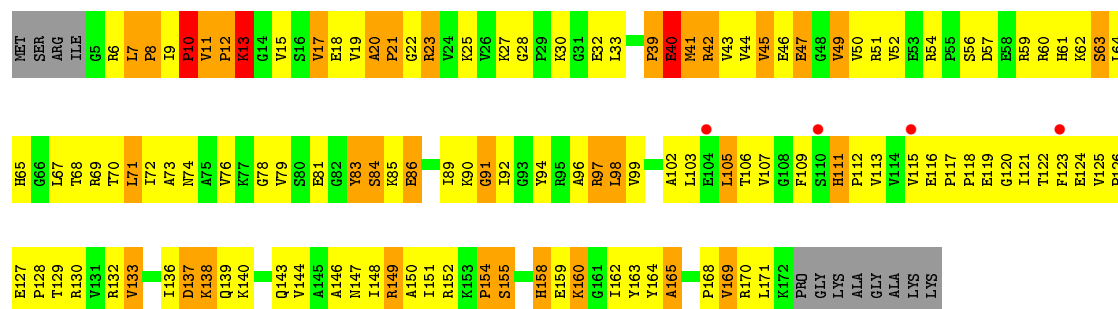


- Molecule 31: 50S ribosomal protein L5

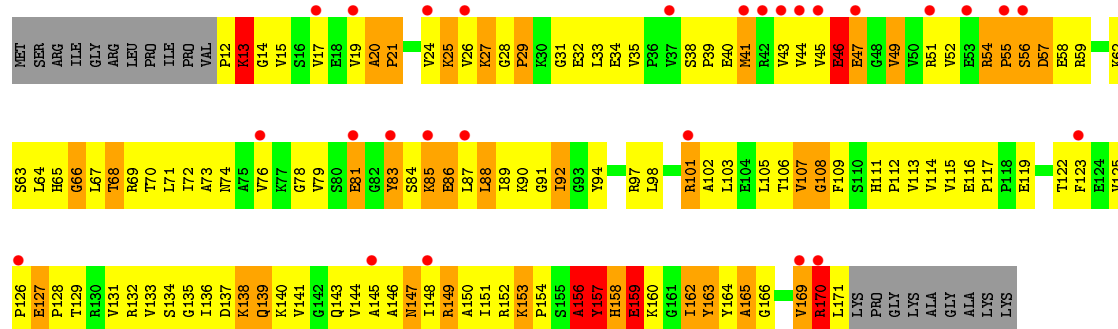
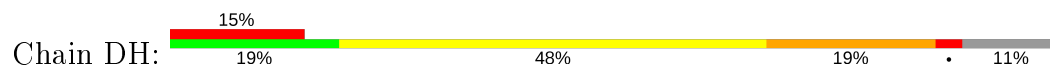


- Molecule 32: 50S ribosomal protein L6

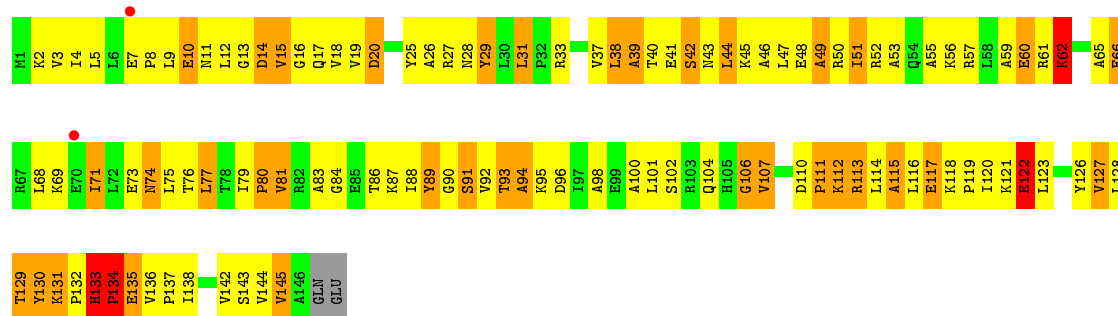




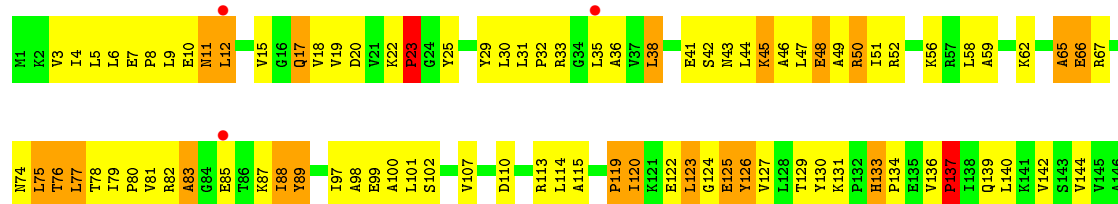
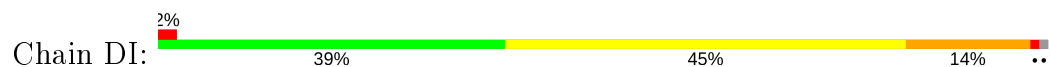
• Molecule 32: 50S ribosomal protein L6



• Molecule 33: 50S ribosomal protein L9

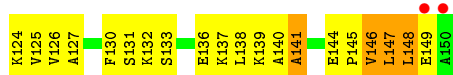
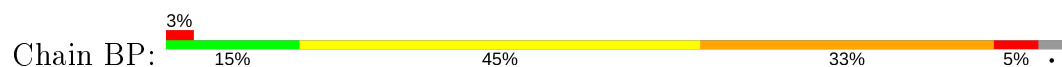


• Molecule 33: 50S ribosomal protein L9

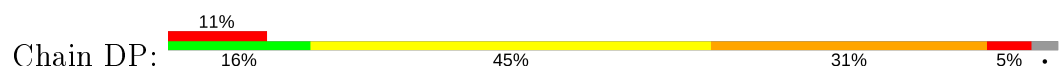




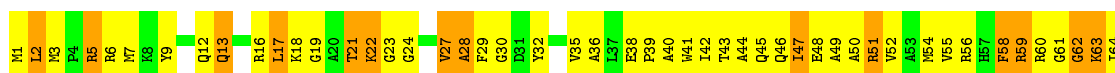
• Molecule 36: 50S ribosomal protein L15



• Molecule 36: 50S ribosomal protein L15

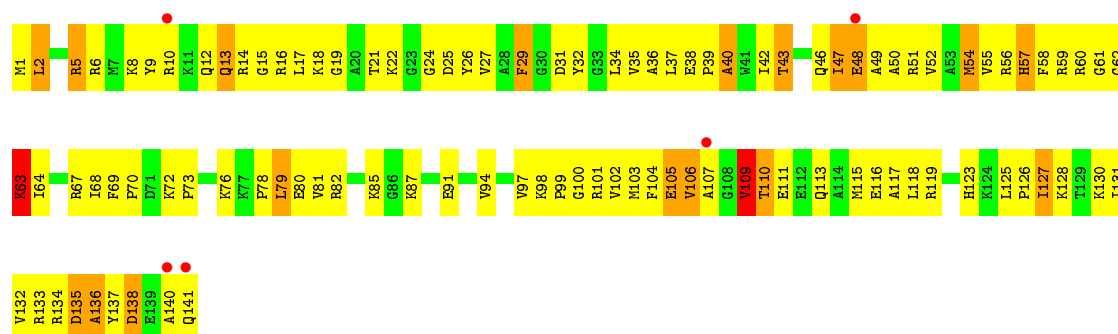


• Molecule 37: 50S ribosomal protein L16



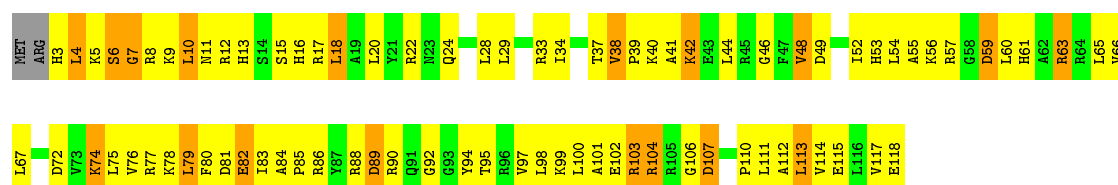
• Molecule 37: 50S ribosomal protein L16





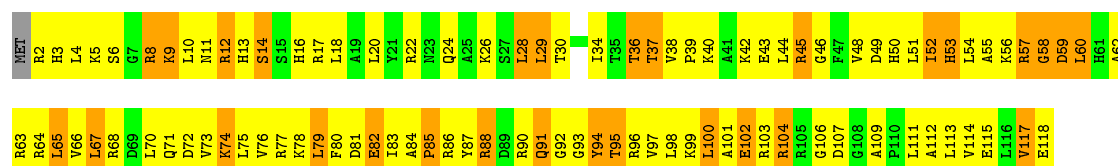
- Molecule 38: 50S ribosomal protein L17

Chain BR: 28% 55% 15%



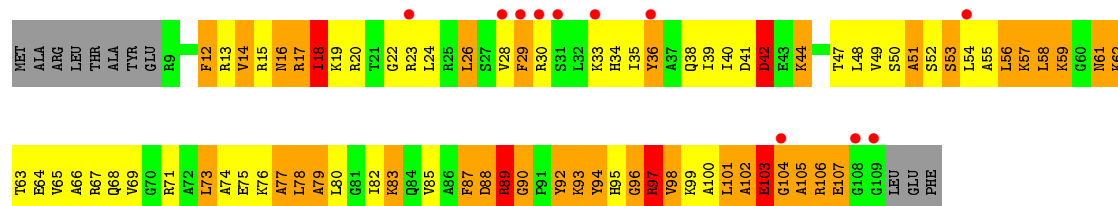
- Molecule 38: 50S ribosomal protein L17

Chain DR: 17% 58% 25%



- Molecule 39: 50S ribosomal protein L18

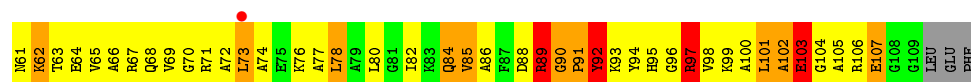
Chain BS: 10% 19% 36% 31% 10%



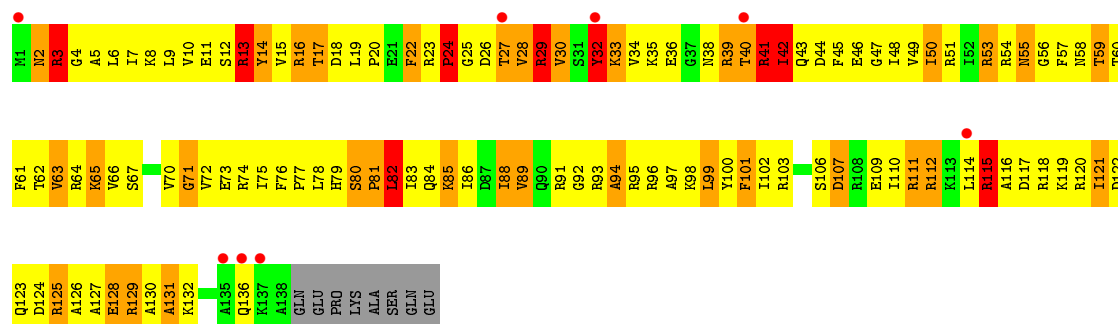
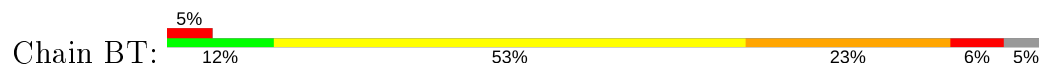
- Molecule 39: 50S ribosomal protein L18

Chain DS: 12% 13% 46% 25% 12%

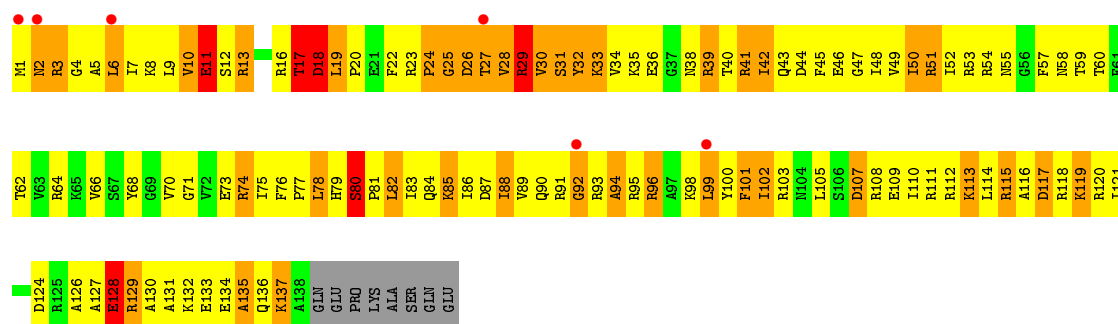
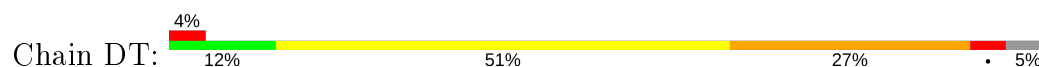




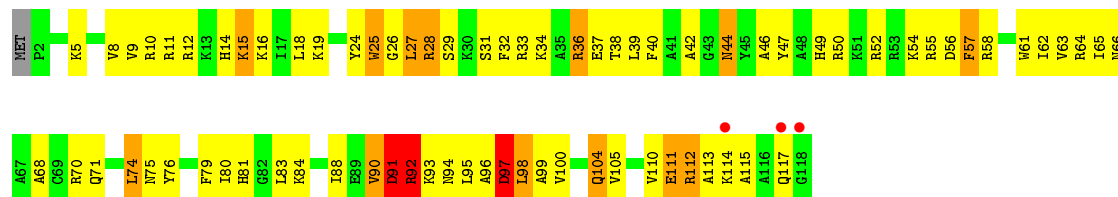
• Molecule 40: 50S ribosomal protein L19



• Molecule 40: 50S ribosomal protein L19

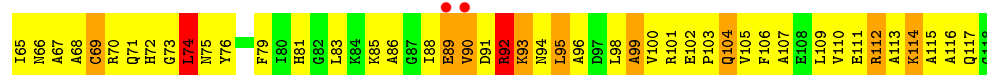


• Molecule 41: 50S ribosomal protein L20

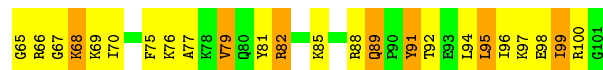
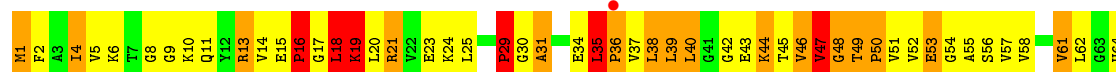


• Molecule 41: 50S ribosomal protein L20

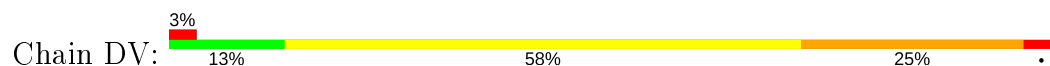




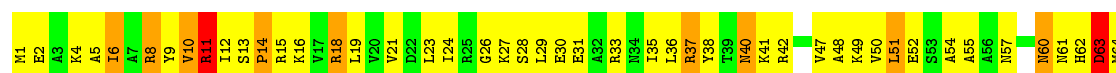
- Molecule 42: 50S ribosomal protein L21



- Molecule 42: 50S ribosomal protein L21



- Molecule 43: 50S ribosomal protein L22

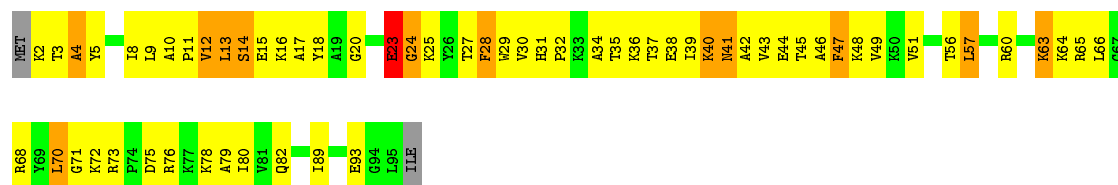


- Molecule 43: 50S ribosomal protein L22

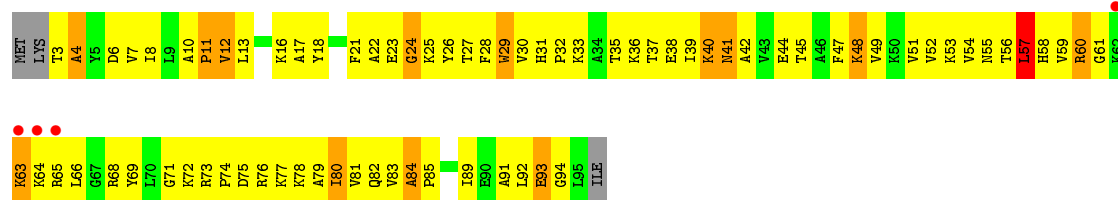


- Molecule 44: 50S ribosomal protein L23

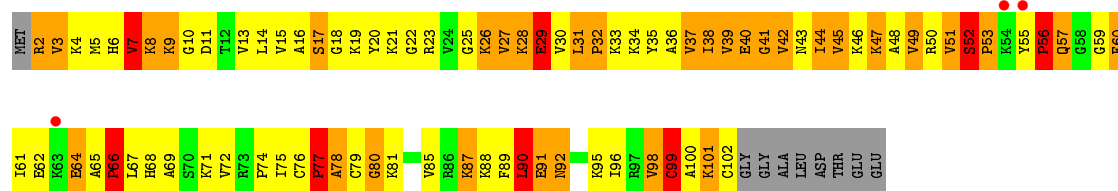




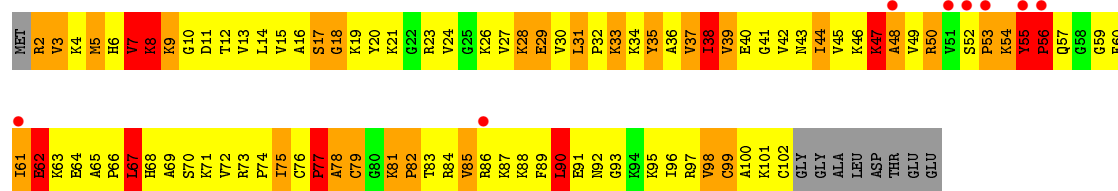
- Molecule 44: 50S ribosomal protein L23



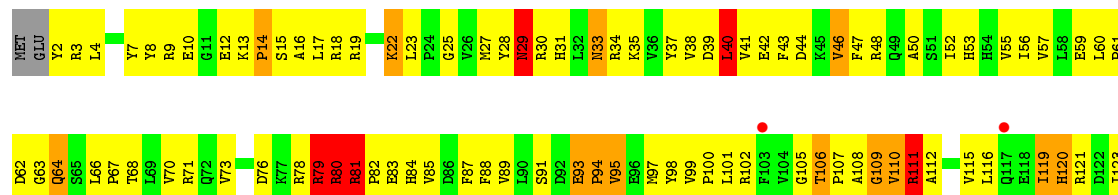
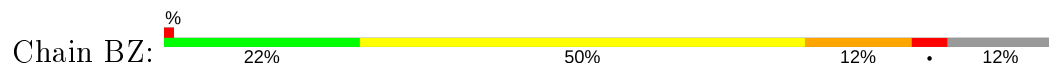
- Molecule 45: 50S ribosomal protein L24

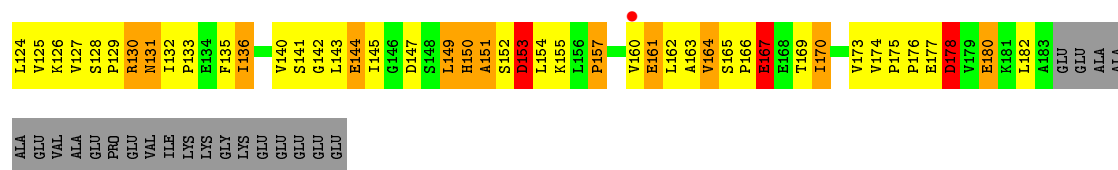


- Molecule 45: 50S ribosomal protein L24

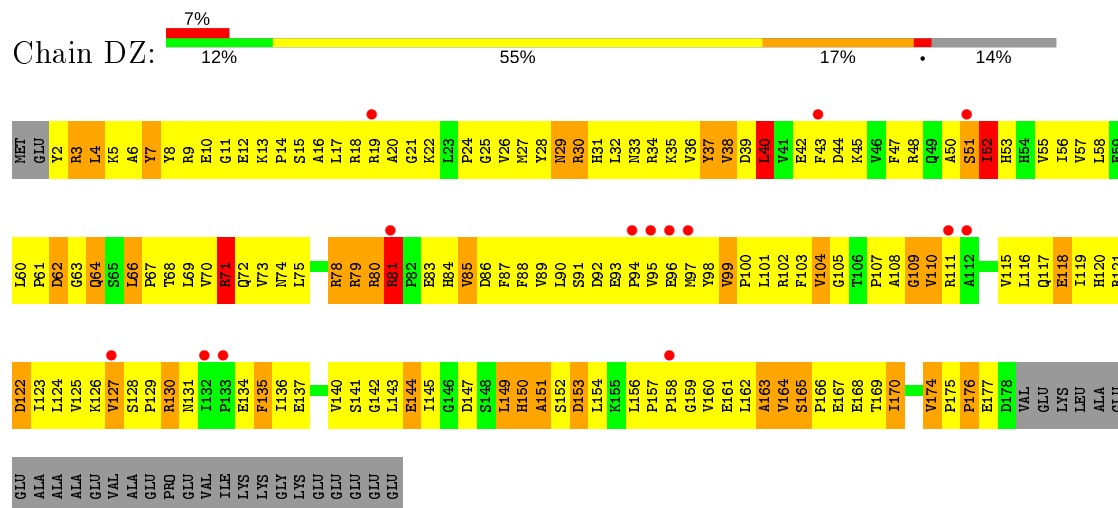


- Molecule 46: 50S ribosomal protein L25

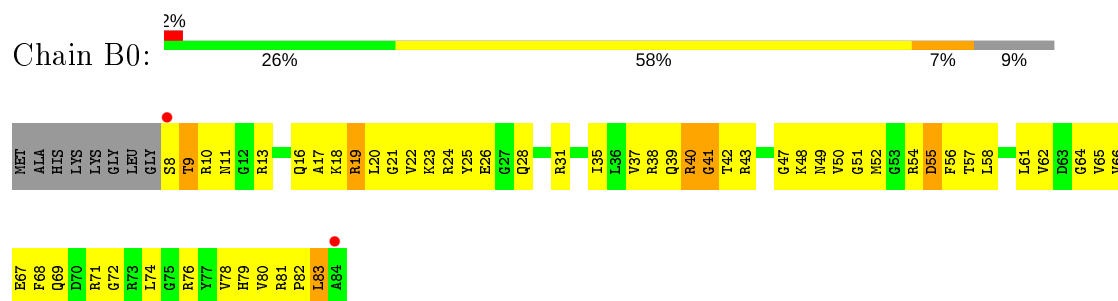




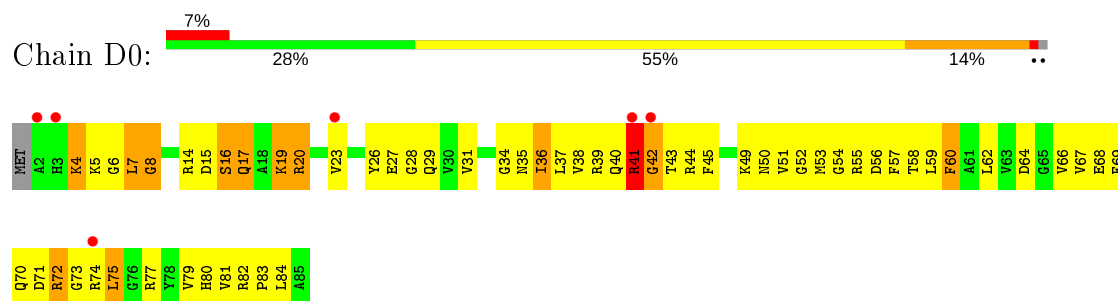
• Molecule 46: 50S ribosomal protein L25



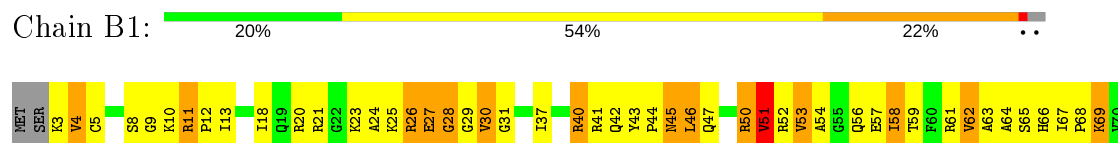
• Molecule 47: 50S ribosomal protein L27



• Molecule 47: 50S ribosomal protein L27



• Molecule 48: 50S ribosomal protein L28

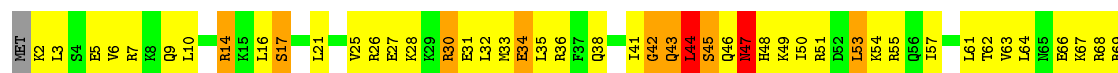




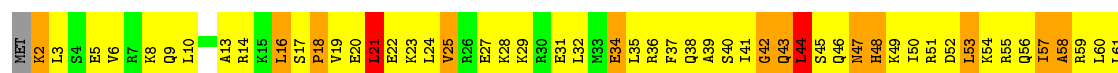
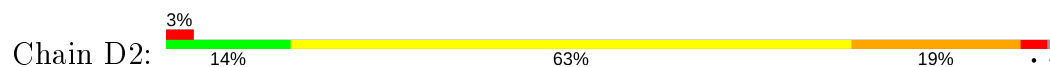
• Molecule 48: 50S ribosomal protein L28



• Molecule 49: 50S ribosomal protein L29



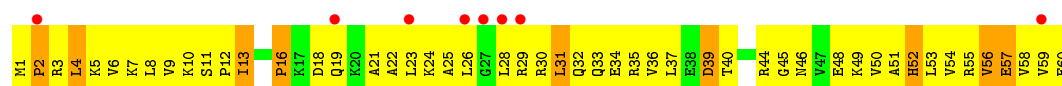
• Molecule 49: 50S ribosomal protein L29



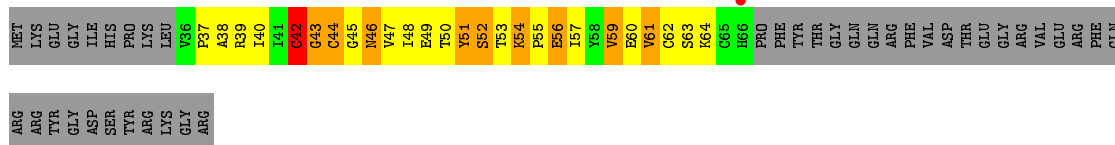
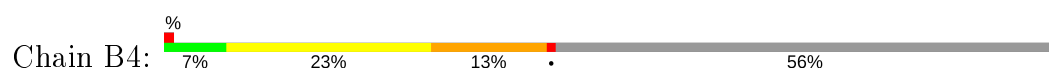
• Molecule 50: 50S ribosomal protein L30



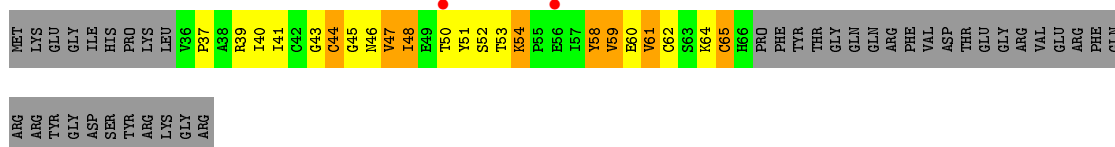
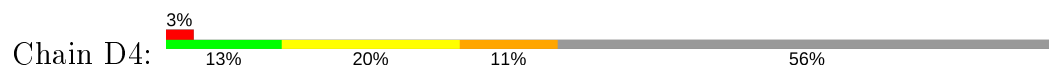
• Molecule 50: 50S ribosomal protein L30



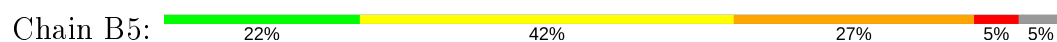
• Molecule 51: 50S ribosomal protein L31



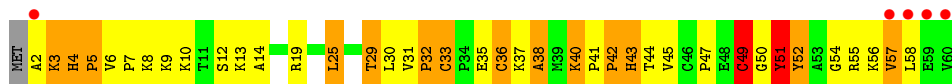
- Molecule 51: 50S ribosomal protein L31



- Molecule 52: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L33

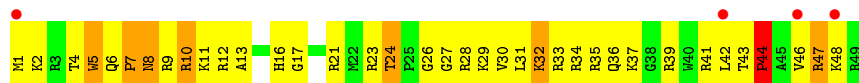


- Molecule 54: 50S ribosomal protein L34

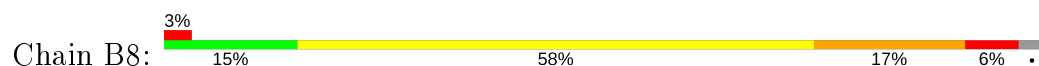




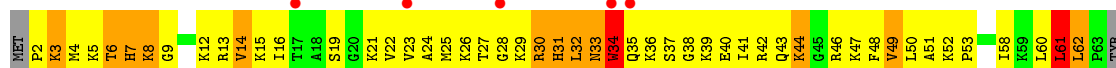
- Molecule 54: 50S ribosomal protein L34



- 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 49.65 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.10) 94.7 (49.65-3.10)	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 0.254 , 0.251	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)	0.25 , 56.8	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	0.88	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	0.82	6/35982 (0.0%)	0.78	24/56156 (0.0%)
1	CA	0.47	0/36193	0.72	9/56490 (0.0%)
2	AB	0.41	0/1936	0.69	0/2611
2	CB	0.43	0/1936	0.73	1/2611 (0.0%)
3	AC	0.41	0/1637	0.66	0/2207
3	CC	0.40	0/1637	0.66	0/2207
4	AD	0.41	0/1733	0.69	0/2318
4	CD	0.42	0/1733	0.72	1/2318 (0.0%)
5	AE	0.42	0/1163	0.68	0/1566
5	CE	0.40	0/1163	0.69	0/1566
6	AF	0.44	0/856	0.71	0/1154
6	CF	0.40	0/856	0.70	0/1154
7	AG	0.42	0/1276	0.67	0/1709
7	CG	0.42	0/1276	0.67	0/1709
8	AH	0.41	0/1136	0.72	0/1527
8	CH	0.39	0/1136	0.67	0/1527
9	AI	0.46	0/1022	0.69	0/1369
9	CI	0.43	0/1022	0.70	0/1369
10	AJ	0.43	0/808	0.71	0/1087
10	CJ	0.45	0/808	0.72	0/1087
11	AK	0.41	0/900	0.72	1/1213 (0.1%)
11	CK	0.39	0/900	0.67	0/1213
12	AL	0.41	0/987	0.78	0/1322
12	CL	0.41	0/987	0.77	1/1322 (0.1%)
13	AM	0.41	0/957	0.78	1/1283 (0.1%)
13	CM	0.39	0/957	0.76	1/1283 (0.1%)
14	AN	0.43	0/501	0.69	0/664
14	CN	0.45	0/501	0.66	0/664
15	AO	0.42	0/745	0.66	0/992
15	CO	0.39	0/745	0.67	1/992 (0.1%)
16	AP	0.42	0/717	0.71	1/965 (0.1%)
16	CP	0.42	0/717	0.73	1/965 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.44	0/837	0.67	0/1119
17	CQ	0.40	0/837	0.70	0/1119
18	AR	0.40	0/579	0.73	0/768
18	CR	0.45	0/579	0.75	0/768
19	AS	0.42	0/625	0.74	0/844
19	CS	0.45	0/632	0.76	0/853
20	AT	0.37	0/765	0.74	0/1007
20	CT	0.38	0/765	0.73	0/1007
21	AU	0.52	0/213	0.58	0/279
21	CU	0.48	0/213	0.61	0/279
22	AV	0.47	0/1393	0.68	0/1883
22	CV	0.46	0/1393	0.67	0/1883
23	AW	0.61	3/1836 (0.2%)	0.90	6/2859 (0.2%)
23	CW	0.50	1/1836 (0.1%)	0.72	1/2859 (0.0%)
24	AX	0.99	1/123 (0.8%)	0.68	0/188
24	CX	0.89	1/123 (0.8%)	0.67	0/188
25	BA	0.68	8/66745 (0.0%)	0.78	54/104189 (0.1%)
25	DA	0.56	10/66983 (0.0%)	0.76	54/104560 (0.1%)
26	BB	0.50	0/2853	0.79	3/4451 (0.1%)
26	DB	0.47	0/2853	0.72	2/4451 (0.0%)
27	BC	0.41	0/1732	0.69	0/2335
27	DC	0.87	1/1668 (0.1%)	0.65	0/2251
28	BD	0.56	0/2177	0.88	4/2935 (0.1%)
28	DD	0.48	0/2165	0.83	0/2921
29	BE	0.52	0/1597	0.84	2/2155 (0.1%)
29	DE	0.49	0/1597	0.84	1/2155 (0.0%)
30	BF	0.54	0/1659	0.82	1/2246 (0.0%)
30	DF	0.44	0/1659	0.74	0/2246
31	BG	0.45	0/1499	0.75	1/2016 (0.0%)
31	DG	0.43	0/1499	0.77	2/2016 (0.1%)
32	BH	0.55	0/1254	0.83	0/1703
32	DH	0.43	0/1246	0.75	2/1684 (0.1%)
33	BI	0.41	0/1056	0.75	0/1443
33	DI	0.37	0/881	0.73	0/1219
34	BN	0.52	0/1132	0.82	2/1527 (0.1%)
34	DN	0.41	0/1132	0.75	0/1527
35	BO	0.52	0/943	0.79	0/1269
35	DO	0.47	0/943	0.72	0/1269
36	BP	0.54	0/1131	1.08	7/1504 (0.5%)
36	DP	0.45	0/1095	0.90	4/1460 (0.3%)
37	BQ	0.46	0/1120	0.70	0/1498
37	DQ	0.45	0/1143	0.71	0/1527
38	BR	0.49	0/936	0.80	1/1256 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DR	0.42	0/974	0.78	0/1302
39	BS	0.47	0/785	0.85	2/1048 (0.2%)
39	DS	0.47	0/779	0.83	1/1038 (0.1%)
40	BT	0.49	0/1156	0.87	3/1544 (0.2%)
40	DT	0.46	0/1156	0.85	1/1544 (0.1%)
41	BU	0.53	0/975	0.79	0/1297
41	DU	0.42	0/975	0.71	0/1297
42	BV	0.54	0/790	0.88	0/1057
42	DV	0.42	0/790	0.77	0/1057
43	BW	0.52	0/907	0.77	0/1216
43	DW	0.42	0/907	0.71	0/1216
44	BX	0.56	0/749	0.81	1/1006 (0.1%)
44	DX	0.47	0/740	0.72	0/995
45	BY	0.58	0/770	0.93	1/1031 (0.1%)
45	DY	0.49	0/789	0.88	1/1053 (0.1%)
46	BZ	0.44	0/1470	0.72	1/1998 (0.1%)
46	DZ	0.42	0/1436	0.70	0/1951
47	B0	0.54	0/621	0.76	0/827
47	D0	0.45	0/671	0.68	0/892
48	B1	0.51	0/764	0.78	0/1014
48	D1	0.41	0/739	0.72	0/983
49	B2	0.45	0/600	0.69	0/793
49	D2	0.42	0/600	0.69	0/793
50	B3	0.47	0/465	0.73	0/625
50	D3	0.36	0/473	0.70	0/636
51	B4	0.57	0/229	0.83	0/311
51	D4	0.46	0/229	0.73	0/311
52	B5	0.58	0/449	0.86	0/608
52	D5	0.51	0/473	0.73	0/639
53	B6	0.68	1/408 (0.2%)	0.95	2/548 (0.4%)
53	D6	0.47	0/328	0.96	1/450 (0.2%)
54	B7	0.59	0/427	0.83	1/563 (0.2%)
54	D7	0.47	0/427	0.74	0/563
55	B8	0.55	0/503	0.94	3/663 (0.5%)
55	D8	0.49	0/473	0.82	0/626
56	B9	0.49	0/297	0.74	0/391
56	D9	0.43	0/302	0.70	0/397
All	All	0.59	32/313996 (0.0%)	0.76	207/468619 (0.0%)

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 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1223	C	C4'-C3'	85.69	2.47	1.53
1	AA	1223	C	C3'-C2'	69.16	2.29	1.52
1	AA	1223	C	C3'-O3'	-41.26	0.84	1.42
27	DC	180	SER	CB-OG	31.26	1.82	1.42
1	AA	1223	C	N3-C4	27.30	1.53	1.33

The worst 5 of 207 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1223	C	C4'-C3'-C2'	-42.89	59.71	102.60
1	AA	1223	C	C3'-C2'-C1'	32.11	127.19	101.50
1	AA	1223	C	P-O3'-C3'	-30.31	83.33	119.70
1	AA	1223	C	O4'-C4'-C3'	20.77	124.77	104.00
1	AA	1223	C	N3-C4-C5	-18.18	114.63	121.90

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	1841	0
1	CA	32332	0	16317	1680	0
2	AB	1901	0	1951	360	0
2	CB	1901	0	1951	361	0
3	AC	1613	0	1677	329	0
3	CC	1613	0	1677	275	0
4	AD	1703	0	1763	325	0
4	CD	1703	0	1763	212	0
5	AE	1147	0	1207	168	0
5	CE	1147	0	1207	177	0
6	AF	843	0	857	111	0
6	CF	843	0	857	137	0
7	AG	1257	0	1296	192	0
7	CG	1257	0	1296	213	0
8	AH	1116	0	1177	183	0
8	CH	1116	0	1177	170	0
9	AI	1004	0	1031	187	0
9	CI	1004	0	1031	200	0
10	AJ	795	0	840	215	0
10	CJ	795	0	840	192	0
11	AK	885	0	904	130	0
11	CK	885	0	904	111	0
12	AL	971	0	1057	168	0
12	CL	971	0	1057	133	0
13	AM	947	0	1008	191	0
13	CM	947	0	1008	135	0
14	AN	492	0	533	111	0
14	CN	492	0	533	95	0
15	AO	734	0	771	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	CO	734	0	771	111	0
16	AP	701	0	720	122	0
16	CP	701	0	720	98	0
17	AQ	824	0	891	108	0
17	CQ	824	0	891	88	0
18	AR	574	0	644	108	0
18	CR	574	0	644	102	0
19	AS	613	0	621	132	0
19	CS	619	0	639	120	0
20	AT	763	0	861	142	0
20	CT	763	0	861	138	0
21	AU	209	0	221	15	0
21	CU	209	0	221	31	0
22	AV	1367	0	1364	182	0
22	CV	1367	0	1364	199	0
23	AW	1644	0	834	67	0
23	CW	1644	0	836	75	0
24	AX	110	0	55	4	0
24	CX	110	0	55	3	0
25	BA	59596	0	30049	2582	0
25	DA	59809	0	30157	2949	0
26	BB	2551	0	1295	92	0
26	DB	2551	0	1295	145	0
27	BC	1702	0	1747	274	0
27	DC	1640	0	1651	242	0
28	BD	2127	0	2208	330	0
28	DD	2115	0	2186	338	0
29	BE	1564	0	1629	252	0
29	DE	1564	0	1629	273	0
30	BF	1624	0	1677	280	0
30	DF	1624	0	1677	300	0
31	BG	1474	0	1535	285	0
31	DG	1474	0	1535	269	0
32	BH	1231	0	1260	198	0
32	DH	1223	0	1282	234	0
33	BI	1043	0	1019	181	0
33	DI	871	0	680	103	0
34	BN	1105	0	1180	132	0
34	DN	1105	0	1180	175	0
35	BO	933	0	996	158	0
35	DO	933	0	996	112	0
36	BP	1114	0	1187	332	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DP	1079	0	1117	265	0
37	BQ	1099	0	1160	144	0
37	DQ	1122	0	1179	190	0
38	BR	923	0	949	105	0
38	DR	960	0	1021	156	0
39	BS	777	0	825	180	0
39	DS	771	0	832	159	0
40	BT	1142	0	1202	274	0
40	DT	1142	0	1202	231	0
41	BU	958	0	1015	150	0
41	DU	958	0	1015	224	0
42	BV	779	0	852	167	0
42	DV	779	0	852	217	0
43	BW	896	0	953	91	0
43	DW	896	0	953	126	0
44	BX	735	0	791	85	0
44	DX	726	0	778	122	0
45	BY	757	0	821	198	0
45	DY	776	0	870	199	0
46	BZ	1438	0	1455	202	0
46	DZ	1404	0	1432	302	0
47	B0	613	0	633	88	0
47	D0	662	0	688	109	0
48	B1	757	0	843	108	0
48	D1	732	0	808	99	0
49	B2	598	0	653	56	0
49	D2	598	0	653	101	0
50	B3	460	0	512	46	0
50	D3	468	0	523	91	0
51	B4	226	0	229	46	0
51	D4	226	0	229	39	0
52	B5	435	0	452	58	0
52	D5	459	0	477	64	0
53	B6	401	0	399	118	0
53	D6	322	0	250	85	0
54	B7	419	0	467	27	0
54	D7	419	0	467	49	0
55	B8	496	0	567	113	0
55	D8	467	0	519	114	0
56	B9	294	0	311	43	0
56	D9	299	0	325	31	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	23826	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 49.

The worst 5 of 23826 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	1
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%)	1	4
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	3
7	CG	153/156 (98%)	95 (62%)	34 (22%)	24 (16%)	0	0
8	AH	136/138 (99%)	96 (71%)	28 (21%)	12 (9%)	1	4
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	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	97/105 (92%)	58 (60%)	29 (30%)	10 (10%)	0	3
10	CJ	97/105 (92%)	59 (61%)	26 (27%)	12 (12%)	0	1
11	AK	117/129 (91%)	88 (75%)	23 (20%)	6 (5%)	2	13
11	CK	117/129 (91%)	86 (74%)	25 (21%)	6 (5%)	2	13
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%)	1	5
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	6
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	3
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	9
28	BD	272/276 (99%)	194 (71%)	47 (17%)	31 (11%)	0	2
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	1
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	1
35	BO	120/122 (98%)	91 (76%)	17 (14%)	12 (10%)	0	3
35	DO	120/122 (98%)	100 (83%)	15 (12%)	5 (4%)	3	16
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%)	1	4
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%)	1	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	5
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%)	5	25
47	D0	82/85 (96%)	60 (73%)	15 (18%)	7 (8%)	1	5
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%)	8	34
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%)	1	5
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%)	4	24
56	D9	34/37 (92%)	31 (91%)	3 (9%)	0	100	100
All	All	12117/12954 (94%)	7729 (64%)	2646 (22%)	1742 (14%)	0	1

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%)	179 (89%)	23 (11%)	5	23
3	AC	160/188 (85%)	142 (89%)	18 (11%)	6	23
3	CC	160/188 (85%)	146 (91%)	14 (9%)	10	36
4	AD	180/181 (99%)	157 (87%)	23 (13%)	4	18
4	CD	180/181 (99%)	158 (88%)	22 (12%)	5	19
5	AE	115/123 (94%)	102 (89%)	13 (11%)	6	23
5	CE	115/123 (94%)	104 (90%)	11 (10%)	8	31
6	AF	90/90 (100%)	77 (86%)	13 (14%)	3	14
6	CF	90/90 (100%)	81 (90%)	9 (10%)	7	28
7	AG	126/127 (99%)	112 (89%)	14 (11%)	6	24
7	CG	126/127 (99%)	110 (87%)	16 (13%)	4	18
8	AH	119/119 (100%)	109 (92%)	10 (8%)	11	38
8	CH	119/119 (100%)	108 (91%)	11 (9%)	9	33
9	AI	97/99 (98%)	80 (82%)	17 (18%)	2	8
9	CI	97/99 (98%)	78 (80%)	19 (20%)	1	6
10	AJ	88/92 (96%)	75 (85%)	13 (15%)	3	13
10	CJ	88/92 (96%)	79 (90%)	9 (10%)	7	27
11	AK	90/99 (91%)	85 (94%)	5 (6%)	21	52
11	CK	90/99 (91%)	81 (90%)	9 (10%)	7	28
12	AL	104/109 (95%)	94 (90%)	10 (10%)	8	31
12	CL	104/109 (95%)	92 (88%)	12 (12%)	5	22
13	AM	95/101 (94%)	74 (78%)	21 (22%)	1	4
13	CM	95/101 (94%)	79 (83%)	16 (17%)	2	9
14	AN	49/50 (98%)	40 (82%)	9 (18%)	1	7
14	CN	49/50 (98%)	44 (90%)	5 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	79/80 (99%)	73 (92%)	6 (8%)	13	41
15	CO	79/80 (99%)	73 (92%)	6 (8%)	13	41
16	AP	72/74 (97%)	64 (89%)	8 (11%)	6	24
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	30
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	10	37
17	CQ	94/97 (97%)	86 (92%)	8 (8%)	10	37
18	AR	61/77 (79%)	57 (93%)	4 (7%)	16	47
18	CR	61/77 (79%)	54 (88%)	7 (12%)	5	22
19	AS	65/80 (81%)	52 (80%)	13 (20%)	1	5
19	CS	68/80 (85%)	56 (82%)	12 (18%)	2	8
20	AT	76/82 (93%)	67 (88%)	9 (12%)	5	21
20	CT	76/82 (93%)	66 (87%)	10 (13%)	4	17
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	26
21	CU	19/22 (86%)	18 (95%)	1 (5%)	22	54
22	AV	148/154 (96%)	136 (92%)	12 (8%)	11	39
22	CV	148/154 (96%)	129 (87%)	19 (13%)	4	18
27	BC	175/181 (97%)	148 (85%)	27 (15%)	2	11
27	DC	165/181 (91%)	146 (88%)	19 (12%)	5	22
28	BD	215/218 (99%)	179 (83%)	36 (17%)	2	9
28	DD	213/218 (98%)	184 (86%)	29 (14%)	3	16
29	BE	165/166 (99%)	144 (87%)	21 (13%)	4	18
29	DE	165/166 (99%)	140 (85%)	25 (15%)	3	12
30	BF	165/166 (99%)	137 (83%)	28 (17%)	2	9
30	DF	165/166 (99%)	143 (87%)	22 (13%)	4	16
31	BG	155/156 (99%)	126 (81%)	29 (19%)	1	7
31	DG	155/156 (99%)	132 (85%)	23 (15%)	3	13
32	BH	127/148 (86%)	115 (91%)	12 (9%)	8	32
32	DH	132/148 (89%)	111 (84%)	21 (16%)	2	11
33	BI	97/124 (78%)	78 (80%)	19 (20%)	1	6
33	DI	49/124 (40%)	41 (84%)	8 (16%)	2	10
34	BN	117/119 (98%)	95 (81%)	22 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DN	117/119 (98%)	100 (86%)	17 (14%)	3	13
35	BO	100/100 (100%)	90 (90%)	10 (10%)	7	28
35	DO	100/100 (100%)	91 (91%)	9 (9%)	9	34
36	BP	112/116 (97%)	88 (79%)	24 (21%)	1	4
36	DP	103/116 (89%)	81 (79%)	22 (21%)	1	4
37	BQ	109/111 (98%)	95 (87%)	14 (13%)	4	18
37	DQ	111/111 (100%)	100 (90%)	11 (10%)	8	29
38	BR	92/101 (91%)	80 (87%)	12 (13%)	4	18
38	DR	100/101 (99%)	83 (83%)	17 (17%)	2	9
39	BS	76/88 (86%)	61 (80%)	15 (20%)	1	6
39	DS	77/88 (88%)	60 (78%)	17 (22%)	1	4
40	BT	120/127 (94%)	94 (78%)	26 (22%)	1	4
40	DT	120/127 (94%)	97 (81%)	23 (19%)	1	6
41	BU	92/94 (98%)	77 (84%)	15 (16%)	2	10
41	DU	92/94 (98%)	82 (89%)	10 (11%)	6	25
42	BV	82/82 (100%)	63 (77%)	19 (23%)	1	3
42	DV	82/82 (100%)	66 (80%)	16 (20%)	1	6
43	BW	91/92 (99%)	77 (85%)	14 (15%)	2	11
43	DW	91/92 (99%)	84 (92%)	7 (8%)	13	41
44	BX	75/78 (96%)	64 (85%)	11 (15%)	3	13
44	DX	74/78 (95%)	66 (89%)	8 (11%)	6	25
45	BY	79/91 (87%)	64 (81%)	15 (19%)	1	6
45	DY	84/91 (92%)	69 (82%)	15 (18%)	2	8
46	BZ	158/179 (88%)	136 (86%)	22 (14%)	3	15
46	DZ	155/179 (87%)	131 (84%)	24 (16%)	2	11
47	B0	62/67 (92%)	56 (90%)	6 (10%)	8	30
47	D0	66/67 (98%)	56 (85%)	10 (15%)	3	12
48	B1	81/83 (98%)	66 (82%)	15 (18%)	1	7
48	D1	78/83 (94%)	69 (88%)	9 (12%)	5	22
49	B2	66/67 (98%)	57 (86%)	9 (14%)	3	16
49	D2	66/67 (98%)	57 (86%)	9 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B3	50/52 (96%)	43 (86%)	7 (14%)	3	15
50	D3	51/52 (98%)	48 (94%)	3 (6%)	19	50
51	B4	27/63 (43%)	23 (85%)	4 (15%)	3	13
51	D4	27/63 (43%)	25 (93%)	2 (7%)	13	42
52	B5	48/52 (92%)	36 (75%)	12 (25%)	0	2
52	D5	51/52 (98%)	44 (86%)	7 (14%)	3	16
53	B6	43/52 (83%)	32 (74%)	11 (26%)	0	1
53	D6	24/52 (46%)	14 (58%)	10 (42%)	0	0
54	B7	41/42 (98%)	38 (93%)	3 (7%)	14	43
54	D7	41/42 (98%)	32 (78%)	9 (22%)	1	4
55	B8	52/55 (94%)	44 (85%)	8 (15%)	2	11
55	D8	46/55 (84%)	36 (78%)	10 (22%)	1	4
56	B9	32/34 (94%)	26 (81%)	6 (19%)	1	6
56	D9	33/34 (97%)	28 (85%)	5 (15%)	3	12
All	All	9998/10736 (93%)	8606 (86%)	1392 (14%)	3	15

5 of 1392 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	BZ	79	ARG
4	CD	127	THR
45	DY	55	TYR
47	B0	9	THR
53	B6	24	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 340 such sidechains are listed below:

Mol	Chain	Res	Type
50	B3	46	ASN
6	CF	64	GLN
46	DZ	64	GLN
54	B7	8	ASN
3	CC	31	HIS

5.3.3 RNA [i](#)

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%)	19 (25%)	6 (7%)
24	AX	4/5 (80%)	0	0
24	CX	4/5 (80%)	0	0
25	BA	2761/2915 (94%)	508 (18%)	77 (2%)
25	DA	2771/2915 (95%)	546 (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%)	1593 (17%)	246 (2%)

5 of 1593 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	2610	C
1	CA	484	G
25	DA	2422	A
25	BA	2750	A
1	CA	79	G

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 carbohydrates 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%)	0.09	40 (2%) 54 31	43, 73, 89, 96	1 (0%)
1	CA	1504/1509 (99%)	0.16	32 (2%) 63 43	47, 71, 88, 97	1 (0%)
2	AB	235/256 (91%)	0.22	18 (7%) 13 5	65, 75, 82, 88	0
2	CB	235/256 (91%)	0.34	22 (9%) 8 3	66, 76, 82, 85	0
3	AC	207/239 (86%)	0.33	12 (5%) 23 10	67, 75, 82, 86	0
3	CC	207/239 (86%)	0.35	19 (9%) 9 3	67, 75, 81, 84	0
4	AD	208/209 (99%)	-0.08	2 (0%) 82 67	61, 72, 79, 85	0
4	CD	208/209 (99%)	-0.05	5 (2%) 59 37	55, 68, 75, 83	0
5	AE	151/162 (93%)	0.22	9 (5%) 21 10	60, 69, 76, 83	0
5	CE	151/162 (93%)	0.21	5 (3%) 46 24	60, 69, 77, 90	0
6	AF	101/101 (100%)	-0.36	1 (0%) 82 67	56, 67, 76, 81	0
6	CF	101/101 (100%)	-0.03	2 (1%) 65 44	61, 70, 78, 83	0
7	AG	155/156 (99%)	0.09	8 (5%) 27 12	63, 74, 80, 83	0
7	CG	155/156 (99%)	0.44	13 (8%) 11 4	67, 74, 81, 84	0
8	AH	138/138 (100%)	-0.04	2 (1%) 75 56	56, 69, 74, 79	0
8	CH	138/138 (100%)	0.02	4 (2%) 51 28	57, 70, 76, 82	0
9	AI	127/128 (99%)	0.55	11 (8%) 10 4	66, 77, 83, 87	0
9	CI	127/128 (99%)	1.02	28 (22%) 0 0	70, 77, 83, 86	0
10	AJ	99/105 (94%)	0.85	15 (15%) 2 1	66, 79, 84, 88	0
10	CJ	99/105 (94%)	1.96	45 (45%) 0 0	66, 79, 84, 87	0
11	AK	119/129 (92%)	0.57	10 (8%) 11 4	58, 68, 78, 82	0
11	CK	119/129 (92%)	0.07	4 (3%) 45 24	64, 72, 78, 84	0
12	AL	125/132 (94%)	-0.10	3 (2%) 59 37	53, 67, 76, 85	0
12	CL	125/132 (94%)	0.29	6 (4%) 30 14	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%)	0.32	7 (5%) 23 10	66, 75, 81, 83	0
13	CM	120/126 (95%)	0.26	7 (5%) 23 10	65, 75, 81, 84	0
14	AN	60/61 (98%)	0.08	2 (3%) 46 24	65, 74, 80, 82	0
14	CN	60/61 (98%)	0.12	1 (1%) 70 49	62, 74, 78, 82	0
15	AO	88/89 (98%)	-0.05	0 100 100	52, 66, 74, 79	0
15	CO	88/89 (98%)	-0.06	1 (1%) 80 64	59, 68, 76, 78	0
16	AP	84/88 (95%)	0.21	6 (7%) 16 6	62, 69, 77, 80	0
16	CP	84/88 (95%)	0.38	2 (2%) 59 37	59, 66, 75, 83	0
17	AQ	100/105 (95%)	0.17	2 (2%) 65 44	59, 68, 75, 76	0
17	CQ	100/105 (95%)	-0.05	0 100 100	58, 68, 76, 78	0
18	AR	70/88 (79%)	0.07	0 100 100	58, 69, 78, 85	0
18	CR	70/88 (79%)	0.50	4 (5%) 23 11	63, 69, 77, 82	0
19	AS	80/93 (86%)	0.40	5 (6%) 20 8	66, 76, 83, 86	0
19	CS	78/93 (83%)	0.60	9 (11%) 4 2	70, 76, 82, 84	0
20	AT	99/106 (93%)	0.28	6 (6%) 21 9	62, 71, 79, 83	0
20	CT	99/106 (93%)	0.25	5 (5%) 28 13	63, 69, 77, 83	0
21	AU	25/27 (92%)	1.11	5 (20%) 1 0	67, 74, 81, 83	0
21	CU	25/27 (92%)	1.48	6 (24%) 0 0	68, 77, 83, 85	0
22	AV	176/184 (95%)	-0.04	3 (1%) 70 49	51, 71, 79, 83	0
22	CV	176/184 (95%)	0.34	13 (7%) 14 5	58, 72, 80, 84	0
23	AW	77/77 (100%)	0.21	2 (2%) 56 33	45, 69, 81, 92	0
23	CW	77/77 (100%)	-0.18	0 100 100	58, 72, 83, 87	0
24	AX	5/5 (100%)	0.66	0 100 100	65, 65, 83, 88	0
24	CX	5/5 (100%)	0.65	1 (20%) 1 0	68, 70, 82, 88	0
25	BA	2767/2915 (94%)	0.07	48 (1%) 70 49	25, 53, 82, 97	0
25	DA	2777/2915 (95%)	0.13	58 (2%) 63 43	38, 65, 85, 97	0
26	BB	119/122 (97%)	-0.17	0 100 100	53, 67, 77, 86	0
26	DB	119/122 (97%)	0.18	3 (2%) 57 34	68, 77, 83, 92	0
27	BC	224/229 (97%)	0.52	17 (7%) 13 5	67, 76, 81, 86	1 (0%)
27	DC	220/229 (96%)	0.55	24 (10%) 5 2	66, 76, 82, 87	1 (0%)
28	BD	274/276 (99%)	-0.06	2 (0%) 87 75	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%)	0.08	7 (2%) 56 33	42, 59, 70, 77	0
29	BE	205/206 (99%)	-0.04	2 (0%) 82 67	38, 58, 73, 77	0
29	DE	205/206 (99%)	0.15	11 (5%) 25 12	46, 65, 78, 82	0
30	BF	208/210 (99%)	0.18	10 (4%) 30 14	35, 58, 78, 88	0
30	DF	208/210 (99%)	0.14	5 (2%) 59 37	52, 69, 78, 90	0
31	BG	181/182 (99%)	0.03	4 (2%) 62 41	60, 71, 79, 86	0
31	DG	181/182 (99%)	0.38	12 (6%) 18 7	65, 73, 81, 85	0
32	BH	168/180 (93%)	0.11	4 (2%) 59 37	25, 66, 75, 82	0
32	DH	160/180 (88%)	0.71	27 (16%) 1 0	66, 76, 82, 87	0
33	BI	146/148 (98%)	-0.14	2 (1%) 75 56	55, 71, 77, 84	0
33	DI	146/148 (98%)	0.03	3 (2%) 63 43	60, 73, 80, 83	0
34	BN	139/140 (99%)	-0.15	2 (1%) 75 56	46, 59, 72, 77	0
34	DN	139/140 (99%)	0.23	3 (2%) 62 41	60, 70, 77, 82	0
35	BO	122/122 (100%)	-0.18	0 100 100	44, 59, 70, 73	0
35	DO	122/122 (100%)	0.14	2 (1%) 72 51	50, 63, 71, 75	0
36	BP	146/150 (97%)	0.33	4 (2%) 54 31	40, 65, 76, 81	0
36	DP	146/150 (97%)	0.66	17 (11%) 4 2	52, 70, 78, 82	0
37	BQ	139/141 (98%)	-0.14	1 (0%) 87 75	45, 61, 71, 80	0
37	DQ	141/141 (100%)	0.15	5 (3%) 44 23	54, 69, 77, 83	0
38	BR	116/118 (98%)	-0.00	0 100 100	39, 57, 69, 74	0
38	DR	117/118 (99%)	0.11	0 100 100	50, 63, 73, 78	0
39	BS	101/112 (90%)	0.60	11 (10%) 5 2	49, 69, 74, 80	0
39	DS	99/112 (88%)	0.57	13 (13%) 3 1	63, 72, 79, 86	0
40	BT	138/146 (94%)	0.14	8 (5%) 23 10	52, 65, 79, 83	0
40	DT	138/146 (94%)	0.15	6 (4%) 35 17	56, 67, 81, 84	0
41	BU	117/118 (99%)	0.07	3 (2%) 56 33	41, 54, 68, 78	0
41	DU	117/118 (99%)	0.10	3 (2%) 56 33	55, 67, 76, 81	0
42	BV	101/101 (100%)	-0.15	1 (0%) 82 67	41, 60, 71, 75	0
42	DV	101/101 (100%)	0.37	3 (2%) 50 27	58, 74, 79, 85	0
43	BW	113/113 (100%)	-0.01	1 (0%) 84 69	44, 53, 70, 86	0
43	DW	113/113 (100%)	-0.02	1 (0%) 84 69	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%)	0.01	0 100 100	42, 57, 69, 79	0
44	DX	93/96 (96%)	0.11	4 (4%) 35 17	53, 67, 73, 81	0
45	BY	101/110 (91%)	0.06	3 (2%) 50 27	51, 64, 77, 81	0
45	DY	101/110 (91%)	0.43	8 (7%) 12 5	63, 74, 82, 85	0
46	BZ	182/206 (88%)	-0.02	3 (1%) 72 51	56, 70, 78, 83	0
46	DZ	177/206 (85%)	0.47	14 (7%) 12 5	68, 76, 83, 87	0
47	B0	77/85 (90%)	0.15	2 (2%) 56 33	49, 59, 72, 81	0
47	D0	84/85 (98%)	0.43	6 (7%) 16 6	59, 68, 78, 84	0
48	B1	96/98 (97%)	-0.09	0 100 100	42, 60, 72, 77	0
48	D1	94/98 (95%)	0.32	6 (6%) 19 8	50, 64, 75, 78	0
49	B2	71/72 (98%)	-0.20	0 100 100	50, 61, 75, 80	0
49	D2	71/72 (98%)	-0.23	2 (2%) 53 30	60, 71, 79, 87	0
50	B3	59/60 (98%)	0.13	5 (8%) 10 4	45, 59, 71, 74	0
50	D3	60/60 (100%)	0.90	8 (13%) 3 1	62, 72, 82, 85	0
51	B4	31/71 (43%)	-0.06	1 (3%) 47 25	69, 75, 80, 86	0
51	D4	31/71 (43%)	0.23	2 (6%) 18 8	67, 74, 81, 84	0
52	B5	57/60 (95%)	-0.22	0 100 100	40, 55, 71, 73	0
52	D5	59/60 (98%)	0.33	5 (8%) 10 4	55, 68, 78, 86	0
53	B6	49/54 (90%)	0.53	8 (16%) 1 1	39, 65, 75, 75	0
53	D6	48/54 (88%)	0.06	3 (6%) 20 8	54, 66, 73, 78	0
54	B7	49/49 (100%)	-0.01	0 100 100	35, 46, 69, 76	0
54	D7	49/49 (100%)	0.76	4 (8%) 11 4	47, 58, 77, 83	0
55	B8	63/65 (96%)	0.11	2 (3%) 47 25	43, 56, 69, 75	0
55	D8	62/65 (95%)	0.33	5 (8%) 12 5	54, 62, 68, 76	0
56	B9	36/37 (97%)	0.45	5 (13%) 2 1	52, 59, 69, 71	0
56	D9	36/37 (97%)	0.30	1 (2%) 53 30	60, 69, 76, 82	0
All	All	21272/22210 (95%)	0.17	823 (3%) 39 20	25, 68, 82, 97	4 (0%)

The worst 5 of 823 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CA	82	U	9.6
1	CA	83	U	8.8

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Mol	Chain	Res	Type	RSRZ
25	DA	2802	G	8.3
45	DY	51	VAL	8.2
1	CA	81	U	7.8

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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	0.18	2.25	205,205,205,205	0
57	MG	BA	3442	1/1	0.39	3.28	205,205,205,205	0
57	MG	BA	3139	1/1	0.43	0.88	72,72,72,72	0
57	MG	CW	102	1/1	0.47	0.48	93,93,93,93	0
57	MG	AA	1611	1/1	0.47	0.91	58,58,58,58	0
57	MG	DA	3072	1/1	0.48	0.53	72,72,72,72	0
57	MG	DA	3164	1/1	0.50	0.65	83,83,83,83	0
57	MG	BA	3332	1/1	0.55	0.17	61,61,61,61	0
57	MG	BA	3448	1/1	0.56	0.42	54,54,54,54	0
57	MG	DA	3277	1/1	0.56	0.27	57,57,57,57	0
57	MG	DA	3255	1/1	0.56	0.31	46,46,46,46	0
57	MG	BA	3323	1/1	0.59	1.30	205,205,205,205	0
57	MG	BA	3207	1/1	0.61	0.26	74,74,74,74	0
57	MG	DA	3151	1/1	0.63	0.30	43,43,43,43	0
57	MG	BA	3118	1/1	0.64	2.55	205,205,205,205	0
57	MG	DA	3211	1/1	0.64	0.35	55,55,55,55	0
57	MG	CA	1618	1/1	0.64	0.25	39,39,39,39	0
57	MG	BP	201	1/1	0.65	1.32	205,205,205,205	0
57	MG	DA	3175	1/1	0.66	0.50	56,56,56,56	0
57	MG	AA	1664	1/1	0.66	0.52	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3188	1/1	0.67	0.85	87,87,87,87	0
57	MG	DA	3184	1/1	0.67	0.36	54,54,54,54	0
57	MG	AA	1604	1/1	0.67	0.41	38,38,38,38	0
57	MG	AA	1642	1/1	0.67	0.35	67,67,67,67	0
57	MG	CE	201	1/1	0.67	0.35	42,42,42,42	0
57	MG	DA	3107	1/1	0.68	0.40	64,64,64,64	0
57	MG	CA	1608	1/1	0.68	0.70	52,52,52,52	0
57	MG	AA	1689	1/1	0.69	0.17	55,55,55,55	0
57	MG	BA	3052	1/1	0.69	0.45	30,30,30,30	0
57	MG	CA	1708	1/1	0.69	0.74	76,76,76,76	0
57	MG	DA	3195	1/1	0.69	0.85	73,73,73,73	0
57	MG	DA	3267	1/1	0.69	0.48	73,73,73,73	0
57	MG	BA	3399	1/1	0.69	0.28	38,38,38,38	0
57	MG	DA	3033	1/1	0.70	0.59	59,59,59,59	0
57	MG	DA	3300	1/1	0.70	0.20	38,38,38,38	0
57	MG	BA	3317	1/1	0.70	0.37	27,27,27,27	0
57	MG	CA	1604	1/1	0.70	0.26	38,38,38,38	0
57	MG	CA	1601	1/1	0.71	0.22	39,39,39,39	0
57	MG	CA	1686	1/1	0.71	0.29	44,44,44,44	0
57	MG	BA	3176	1/1	0.71	0.18	44,44,44,44	0
57	MG	DA	3122	1/1	0.71	0.19	48,48,48,48	0
57	MG	DA	3070	1/1	0.71	0.39	46,46,46,46	0
57	MG	DA	3108	1/1	0.71	0.61	47,47,47,47	0
57	MG	BA	3249	1/1	0.72	0.27	46,46,46,46	0
57	MG	DB	204	1/1	0.72	0.18	43,43,43,43	0
57	MG	DA	3166	1/1	0.73	0.18	22,22,22,22	0
57	MG	BA	3125	1/1	0.73	0.33	60,60,60,60	0
57	MG	AA	1613	1/1	0.73	0.34	75,75,75,75	0
57	MG	DA	3270	1/1	0.73	0.30	47,47,47,47	0
57	MG	BA	3355	1/1	0.74	0.56	31,31,31,31	0
57	MG	DA	3154	1/1	0.74	0.14	61,61,61,61	0
57	MG	DA	3144	1/1	0.74	0.49	44,44,44,44	0
57	MG	BA	3432	1/1	0.74	0.58	70,70,70,70	0
57	MG	DB	202	1/1	0.74	0.12	61,61,61,61	0
57	MG	DB	210	1/1	0.75	0.23	41,41,41,41	0
57	MG	DA	3111	1/1	0.75	0.44	76,76,76,76	0
57	MG	AA	1705	1/1	0.75	0.26	66,66,66,66	0
57	MG	BA	3133	1/1	0.75	0.37	60,60,60,60	0
57	MG	AA	1601	1/1	0.75	0.22	47,47,47,47	0
57	MG	BA	3379	1/1	0.75	0.21	40,40,40,40	0
57	MG	BA	3086	1/1	0.75	1.91	130,130,130,130	0
57	MG	BA	3407	1/1	0.75	0.33	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3246	1/1	0.76	0.33	43,43,43,43	0
57	MG	BA	3388	1/1	0.76	0.40	37,37,37,37	0
57	MG	BA	3424	1/1	0.76	0.16	26,26,26,26	0
57	MG	BA	3449	1/1	0.76	0.21	53,53,53,53	0
57	MG	CA	1652	1/1	0.76	0.47	59,59,59,59	0
57	MG	AA	1622	1/1	0.76	0.22	36,36,36,36	0
57	MG	BA	3344	1/1	0.77	0.22	24,24,24,24	0
57	MG	BA	3431	1/1	0.77	0.38	53,53,53,53	0
57	MG	CA	1655	1/1	0.77	0.19	34,34,34,34	0
57	MG	DA	3266	1/1	0.77	0.36	46,46,46,46	0
57	MG	AA	1709	1/1	0.78	0.21	66,66,66,66	0
58	ZN	AD	301	1/1	0.78	0.59	192,192,192,192	0
57	MG	DA	3123	1/1	0.78	0.24	25,25,25,25	0
57	MG	BA	3268	1/1	0.78	0.61	46,46,46,46	0
57	MG	AA	1621	1/1	0.78	0.19	48,48,48,48	0
57	MG	BA	3258	1/1	0.78	0.27	39,39,39,39	0
57	MG	AA	1637	1/1	0.78	0.36	45,45,45,45	0
57	MG	BA	3038	1/1	0.78	1.44	163,163,163,163	0
57	MG	BA	3029	1/1	0.78	0.14	40,40,40,40	0
57	MG	BA	3175	1/1	0.78	0.23	71,71,71,71	0
57	MG	DB	208	1/1	0.78	0.48	48,48,48,48	0
57	MG	CA	1695	1/1	0.78	0.26	38,38,38,38	0
57	MG	DA	3142	1/1	0.78	0.26	51,51,51,51	0
57	MG	AA	1647	1/1	0.79	0.22	45,45,45,45	0
57	MG	CA	1629	1/1	0.79	0.24	25,25,25,25	0
57	MG	DA	3200	1/1	0.79	0.28	66,66,66,66	0
57	MG	BA	3143	1/1	0.79	0.32	31,31,31,31	0
57	MG	DA	3192	1/1	0.79	0.27	43,43,43,43	0
57	MG	CA	1649	1/1	0.79	0.29	65,65,65,65	0
57	MG	DA	3067	1/1	0.79	0.19	56,56,56,56	0
57	MG	AA	1619	1/1	0.79	0.47	66,66,66,66	0
57	MG	DB	209	1/1	0.79	0.23	41,41,41,41	0
57	MG	DA	3094	1/1	0.79	0.43	71,71,71,71	0
57	MG	DA	3117	1/1	0.80	0.18	42,42,42,42	0
57	MG	DA	3121	1/1	0.80	0.30	57,57,57,57	0
57	MG	BA	3444	1/1	0.80	0.99	101,101,101,101	0
57	MG	BA	3264	1/1	0.80	0.30	34,34,34,34	0
57	MG	BA	3354	1/1	0.80	0.39	25,25,25,25	0
57	MG	BA	3374	1/1	0.80	0.23	51,51,51,51	0
57	MG	DA	3152	1/1	0.80	0.33	61,61,61,61	0
57	MG	CA	1643	1/1	0.80	0.17	44,44,44,44	0
57	MG	AA	1602	1/1	0.80	0.33	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3280	1/1	0.80	0.12	44,44,44,44	0
57	MG	BA	3428	1/1	0.80	0.20	24,24,24,24	0
57	MG	BA	3300	1/1	0.80	0.53	67,67,67,67	0
57	MG	BA	3378	1/1	0.80	0.22	55,55,55,55	0
57	MG	DA	3042	1/1	0.80	0.33	28,28,28,28	0
57	MG	DB	203	1/1	0.81	0.20	66,66,66,66	0
57	MG	BA	3015	1/1	0.81	0.45	21,21,21,21	0
57	MG	AA	1618	1/1	0.81	0.21	64,64,64,64	0
57	MG	CA	1640	1/1	0.81	0.62	61,61,61,61	0
57	MG	AA	1645	1/1	0.81	0.36	52,52,52,52	0
57	MG	CA	1670	1/1	0.81	0.40	43,43,43,43	0
57	MG	BA	3169	1/1	0.81	0.16	21,21,21,21	0
57	MG	BA	3425	1/1	0.81	0.17	55,55,55,55	0
57	MG	AA	1659	1/1	0.81	0.19	58,58,58,58	0
57	MG	AA	1674	1/1	0.81	0.22	49,49,49,49	0
57	MG	DF	301	1/1	0.81	0.54	49,49,49,49	0
57	MG	BA	3254	1/1	0.81	0.27	37,37,37,37	0
57	MG	CA	1646	1/1	0.81	0.20	59,59,59,59	0
57	MG	DA	3204	1/1	0.81	0.12	41,41,41,41	0
57	MG	BA	3153	1/1	0.82	0.14	42,42,42,42	0
57	MG	BA	3194	1/1	0.82	0.08	72,72,72,72	0
57	MG	BA	3349	1/1	0.82	0.24	38,38,38,38	0
57	MG	BA	3434	1/1	0.82	0.29	28,28,28,28	0
57	MG	BA	3239	1/1	0.82	0.24	46,46,46,46	0
57	MG	BA	3361	1/1	0.82	0.24	31,31,31,31	0
57	MG	AA	1603	1/1	0.82	0.11	18,18,18,18	0
57	MG	BA	3383	1/1	0.82	0.20	48,48,48,48	0
57	MG	AA	1704	1/1	0.82	0.15	64,64,64,64	0
57	MG	BA	3236	1/1	0.82	0.27	62,62,62,62	0
57	MG	BA	3095	1/1	0.82	0.27	45,45,45,45	0
57	MG	BA	3223	1/1	0.82	0.24	49,49,49,49	0
57	MG	BA	3385	1/1	0.83	0.14	54,54,54,54	0
57	MG	AA	1711	1/1	0.83	0.24	58,58,58,58	0
57	MG	BA	3191	1/1	0.83	0.13	40,40,40,40	0
57	MG	BA	3459	1/1	0.83	0.18	35,35,35,35	0
57	MG	DA	3045	1/1	0.83	0.26	59,59,59,59	0
57	MG	DA	3269	1/1	0.83	0.27	47,47,47,47	0
57	MG	DA	3256	1/1	0.83	0.27	62,62,62,62	0
57	MG	BA	3238	1/1	0.83	0.43	20,20,20,20	0
57	MG	BA	3226	1/1	0.83	0.38	31,31,31,31	0
57	MG	BA	3180	1/1	0.83	0.31	21,21,21,21	0
57	MG	DA	3254	1/1	0.83	0.41	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3292	1/1	0.83	0.43	24,24,24,24	0
57	MG	DA	3297	1/1	0.83	0.17	48,48,48,48	0
57	MG	DA	3298	1/1	0.83	0.15	33,33,33,33	0
57	MG	DA	3161	1/1	0.83	0.78	50,50,50,50	0
57	MG	AA	1657	1/1	0.83	0.16	54,54,54,54	0
57	MG	DA	3248	1/1	0.83	0.21	36,36,36,36	0
57	MG	DA	3069	1/1	0.84	0.47	30,30,30,30	0
57	MG	DA	3282	1/1	0.84	0.24	65,65,65,65	0
57	MG	BA	3195	1/1	0.84	0.20	47,47,47,47	0
57	MG	DA	3220	1/1	0.84	0.35	31,31,31,31	0
57	MG	DA	3276	1/1	0.84	0.21	51,51,51,51	0
57	MG	DB	201	1/1	0.84	0.23	53,53,53,53	0
57	MG	BA	3190	1/1	0.84	0.21	34,34,34,34	0
57	MG	BA	3001	1/1	0.84	0.17	50,50,50,50	0
57	MG	AA	1687	1/1	0.84	0.29	44,44,44,44	0
57	MG	DA	3149	1/1	0.84	0.49	38,38,38,38	0
57	MG	BA	3211	1/1	0.84	0.27	38,38,38,38	0
57	MG	DA	3198	1/1	0.84	0.23	31,31,31,31	0
57	MG	DA	3129	1/1	0.84	0.23	47,47,47,47	0
57	MG	DA	3169	1/1	0.85	0.40	18,18,18,18	0
57	MG	BA	3446	1/1	0.85	0.69	60,60,60,60	0
57	MG	CA	1681	1/1	0.85	0.18	44,44,44,44	0
57	MG	BA	3408	1/1	0.85	0.43	57,57,57,57	0
57	MG	CW	105	1/1	0.85	0.33	61,61,61,61	0
57	MG	DA	3185	1/1	0.85	0.37	37,37,37,37	0
57	MG	AA	1636	1/1	0.85	0.17	62,62,62,62	0
57	MG	CA	1602	1/1	0.85	0.19	35,35,35,35	0
57	MG	DA	3302	1/1	0.85	0.34	36,36,36,36	0
57	MG	DA	3020	1/1	0.85	0.35	23,23,23,23	0
57	MG	DA	3150	1/1	0.85	0.27	21,21,21,21	0
57	MG	BA	3178	1/1	0.85	0.27	22,22,22,22	0
57	MG	CA	1627	1/1	0.85	0.18	24,24,24,24	0
57	MG	AA	1654	1/1	0.85	0.26	29,29,29,29	0
57	MG	DA	3010	1/1	0.85	0.41	66,66,66,66	0
57	MG	AA	1605	1/1	0.85	0.18	51,51,51,51	0
57	MG	BA	3427	1/1	0.85	0.18	40,40,40,40	0
57	MG	BA	3381	1/1	0.85	0.43	66,66,66,66	0
57	MG	DA	3227	1/1	0.85	0.35	37,37,37,37	0
57	MG	DA	3143	1/1	0.85	0.21	23,23,23,23	0
57	MG	BA	3129	1/1	0.85	0.18	25,25,25,25	0
57	MG	AA	1686	1/1	0.85	0.15	42,42,42,42	0
57	MG	AA	1617	1/1	0.86	0.27	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	1672	1/1	0.86	0.23	29,29,29,29	0
57	MG	AA	1661	1/1	0.86	0.22	67,67,67,67	0
57	MG	BU	201	1/1	0.86	0.35	21,21,21,21	0
57	MG	BA	3251	1/1	0.86	0.27	23,23,23,23	0
57	MG	BA	3458	1/1	0.86	0.47	47,47,47,47	0
57	MG	DA	3025	1/1	0.86	0.18	38,38,38,38	0
57	MG	BA	3346	1/1	0.86	0.50	50,50,50,50	0
57	MG	DA	3028	1/1	0.86	0.14	34,34,34,34	0
57	MG	BA	3372	1/1	0.86	0.25	59,59,59,59	0
57	MG	BA	3257	1/1	0.86	0.24	41,41,41,41	0
57	MG	B0	101	1/1	0.86	0.38	30,30,30,30	0
57	MG	BA	3262	1/1	0.86	0.51	32,32,32,32	0
57	MG	DA	3278	1/1	0.86	0.27	59,59,59,59	0
57	MG	DA	3203	1/1	0.86	0.21	52,52,52,52	0
57	MG	BA	3342	1/1	0.86	0.13	22,22,22,22	0
57	MG	DA	3288	1/1	0.86	0.26	60,60,60,60	0
57	MG	BA	3014	1/1	0.86	0.37	24,24,24,24	0
57	MG	D5	101	1/1	0.86	0.20	38,38,38,38	0
57	MG	AA	1633	1/1	0.86	0.11	36,36,36,36	0
57	MG	DA	3245	1/1	0.86	0.28	52,52,52,52	0
57	MG	CA	1620	1/1	0.86	0.52	29,29,29,29	0
57	MG	BA	3151	1/1	0.86	0.41	24,24,24,24	0
57	MG	DA	3190	1/1	0.86	0.22	44,44,44,44	0
57	MG	BA	3403	1/1	0.86	0.24	48,48,48,48	0
57	MG	DA	3273	1/1	0.87	0.30	55,55,55,55	0
57	MG	DA	3132	1/1	0.87	0.39	32,32,32,32	0
57	MG	BA	3204	1/1	0.87	0.45	52,52,52,52	0
57	MG	DA	3049	1/1	0.87	0.25	15,15,15,15	0
57	MG	BA	3199	1/1	0.87	0.32	23,23,23,23	0
57	MG	BA	3296	1/1	0.87	0.18	25,25,25,25	0
57	MG	DA	3088	1/1	0.87	0.20	20,20,20,20	0
57	MG	BA	3390	1/1	0.87	0.20	48,48,48,48	0
57	MG	AA	1665	1/1	0.87	0.38	63,63,63,63	0
57	MG	AA	1685	1/1	0.87	0.29	42,42,42,42	0
57	MG	BA	3380	1/1	0.87	0.31	37,37,37,37	0
57	MG	DA	3026	1/1	0.87	0.09	33,33,33,33	0
57	MG	BA	3270	1/1	0.87	0.31	43,43,43,43	0
57	MG	DA	3261	1/1	0.87	0.21	58,58,58,58	0
57	MG	BA	3243	1/1	0.87	0.27	51,51,51,51	0
57	MG	CA	1638	1/1	0.87	0.39	35,35,35,35	0
57	MG	DA	3213	1/1	0.87	0.17	28,28,28,28	0
57	MG	BA	3456	1/1	0.87	0.26	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	CA	1635	1/1	0.87	0.25	22,22,22,22	0
57	MG	DA	3021	1/1	0.87	0.26	34,34,34,34	0
57	MG	DA	3158	1/1	0.87	0.36	44,44,44,44	0
57	MG	BA	3412	1/1	0.87	0.27	35,35,35,35	0
57	MG	DA	3073	1/1	0.87	0.45	49,49,49,49	0
57	MG	D6	101	1/1	0.87	0.26	57,57,57,57	0
57	MG	DA	3223	1/1	0.87	0.24	32,32,32,32	0
57	MG	BA	3136	1/1	0.87	0.93	76,76,76,76	0
57	MG	BA	3373	1/1	0.87	0.21	31,31,31,31	0
57	MG	DA	3165	1/1	0.87	0.14	43,43,43,43	0
57	MG	AA	1646	1/1	0.87	0.15	49,49,49,49	0
57	MG	BA	3092	1/1	0.87	0.34	36,36,36,36	0
57	MG	CA	1687	1/1	0.87	0.17	37,37,37,37	0
57	MG	DA	3044	1/1	0.87	0.42	69,69,69,69	0
57	MG	AA	1679	1/1	0.87	0.26	56,56,56,56	0
57	MG	DA	3208	1/1	0.87	0.09	59,59,59,59	0
57	MG	DA	3205	1/1	0.87	0.32	55,55,55,55	0
57	MG	BA	3124	1/1	0.88	0.21	41,41,41,41	0
57	MG	BB	203	1/1	0.88	0.31	21,21,21,21	0
57	MG	BA	3418	1/1	0.88	0.21	31,31,31,31	0
57	MG	BA	3440	1/1	0.88	0.46	64,64,64,64	0
57	MG	BA	3091	1/1	0.88	0.44	21,21,21,21	0
57	MG	DA	3125	1/1	0.88	0.27	26,26,26,26	0
57	MG	CA	1632	1/1	0.88	0.42	18,18,18,18	0
57	MG	BA	3093	1/1	0.88	0.17	23,23,23,23	0
57	MG	BA	3320	1/1	0.88	0.28	25,25,25,25	0
57	MG	DA	3081	1/1	0.88	0.25	37,37,37,37	0
57	MG	BA	3224	1/1	0.88	0.31	31,31,31,31	0
57	MG	DA	3031	1/1	0.88	0.26	24,24,24,24	0
57	MG	BA	3253	1/1	0.88	0.54	41,41,41,41	0
57	MG	DA	3287	1/1	0.88	0.31	48,48,48,48	0
57	MG	BA	3284	1/1	0.88	0.17	15,15,15,15	0
57	MG	BA	3100	1/1	0.88	0.55	28,28,28,28	0
57	MG	BA	3062	1/1	0.88	0.11	19,19,19,19	0
57	MG	BA	3366	1/1	0.88	0.32	49,49,49,49	0
57	MG	DA	3218	1/1	0.88	0.20	35,35,35,35	0
57	MG	DA	3286	1/1	0.88	0.27	52,52,52,52	0
57	MG	DA	3237	1/1	0.88	0.24	33,33,33,33	0
57	MG	AA	1681	1/1	0.88	0.29	63,63,63,63	0
57	MG	DA	3177	1/1	0.88	0.48	52,52,52,52	0
57	MG	AA	1609	1/1	0.88	0.21	48,48,48,48	0
57	MG	BA	3290	1/1	0.88	0.22	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3043	1/1	0.88	0.23	39,39,39,39	0
57	MG	CA	1678	1/1	0.88	0.22	25,25,25,25	0
57	MG	AA	1706	1/1	0.88	0.12	47,47,47,47	0
57	MG	DA	3016	1/1	0.88	0.44	24,24,24,24	0
57	MG	DA	3283	1/1	0.88	0.19	62,62,62,62	0
57	MG	CA	1680	1/1	0.88	0.18	31,31,31,31	0
57	MG	BQ	203	1/1	0.88	0.21	27,27,27,27	0
57	MG	BA	3421	1/1	0.89	0.16	32,32,32,32	0
57	MG	BA	3171	1/1	0.89	0.44	41,41,41,41	0
57	MG	BA	3013	1/1	0.89	0.16	56,56,56,56	0
57	MG	BA	3301	1/1	0.89	0.22	33,33,33,33	0
57	MG	DA	3215	1/1	0.89	0.35	37,37,37,37	0
57	MG	BA	3368	1/1	0.89	0.42	49,49,49,49	0
57	MG	CA	1663	1/1	0.89	0.19	33,33,33,33	0
57	MG	BA	3417	1/1	0.89	0.24	62,62,62,62	0
57	MG	DA	3232	1/1	0.89	0.28	40,40,40,40	0
57	MG	BA	3116	1/1	0.89	0.11	23,23,23,23	0
57	MG	BB	209	1/1	0.89	0.12	37,37,37,37	0
57	MG	BA	3163	1/1	0.89	0.17	21,21,21,21	0
57	MG	BA	3218	1/1	0.89	0.39	23,23,23,23	0
57	MG	DA	3291	1/1	0.89	0.23	31,31,31,31	0
57	MG	BA	3111	1/1	0.89	0.15	20,20,20,20	0
57	MG	DA	3136	1/1	0.89	0.16	22,22,22,22	0
57	MG	CA	1644	1/1	0.89	0.39	30,30,30,30	0
57	MG	DA	3226	1/1	0.89	0.35	32,32,32,32	0
57	MG	BA	3384	1/1	0.89	0.25	42,42,42,42	0
57	MG	DA	3274	1/1	0.89	0.25	36,36,36,36	0
57	MG	AA	1675	1/1	0.89	0.18	50,50,50,50	0
57	MG	BA	3230	1/1	0.89	0.29	34,34,34,34	0
57	MG	CA	1603	1/1	0.89	0.21	49,49,49,49	0
57	MG	CA	1605	1/1	0.89	0.42	62,62,62,62	0
57	MG	B0	102	1/1	0.89	0.23	33,33,33,33	0
57	MG	CA	1665	1/1	0.89	0.25	30,30,30,30	0
57	MG	AA	1703	1/1	0.89	0.15	51,51,51,51	0
57	MG	BA	3248	1/1	0.89	0.31	34,34,34,34	0
57	MG	BA	3198	1/1	0.89	0.16	34,34,34,34	0
57	MG	BA	3311	1/1	0.89	0.18	31,31,31,31	0
57	MG	DA	3038	1/1	0.89	0.47	49,49,49,49	0
57	MG	DA	3014	1/1	0.89	0.24	44,44,44,44	0
57	MG	DA	3222	1/1	0.89	0.31	26,26,26,26	0
57	MG	DA	3001	1/1	0.89	0.32	61,61,61,61	0
57	MG	DA	3251	1/1	0.89	0.31	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3406	1/1	0.89	0.15	50,50,50,50	0
57	MG	AA	1632	1/1	0.89	0.44	57,57,57,57	0
57	MG	BA	3430	1/1	0.89	0.35	58,58,58,58	0
57	MG	DA	3176	1/1	0.89	0.32	24,24,24,24	0
57	MG	BA	3445	1/1	0.89	0.14	36,36,36,36	0
57	MG	DA	3279	1/1	0.89	0.25	43,43,43,43	0
57	MG	BA	3232	1/1	0.89	0.43	38,38,38,38	0
57	MG	BA	3212	1/1	0.89	0.42	30,30,30,30	0
57	MG	CW	103	1/1	0.89	0.34	27,27,27,27	0
57	MG	CA	1660	1/1	0.89	0.41	22,22,22,22	0
57	MG	AA	1715	1/1	0.90	0.14	62,62,62,62	0
57	MG	DA	3194	1/1	0.90	0.21	61,61,61,61	0
57	MG	BR	201	1/1	0.90	0.43	35,35,35,35	0
57	MG	BA	3291	1/1	0.90	0.34	24,24,24,24	0
57	MG	CA	1707	1/1	0.90	0.62	62,62,62,62	0
57	MG	DA	3119	1/1	0.90	0.24	42,42,42,42	0
57	MG	DA	3061	1/1	0.90	0.25	22,22,22,22	0
57	MG	BA	3196	1/1	0.90	0.16	27,27,27,27	0
57	MG	BA	3370	1/1	0.90	0.10	48,48,48,48	0
57	MG	BA	3077	1/1	0.90	0.82	63,63,63,63	0
57	MG	DA	3155	1/1	0.90	0.06	60,60,60,60	0
57	MG	DA	3131	1/1	0.90	0.31	39,39,39,39	0
57	MG	BA	3217	1/1	0.90	0.23	34,34,34,34	0
57	MG	BA	3315	1/1	0.90	0.16	17,17,17,17	0
57	MG	CA	1658	1/1	0.90	0.17	21,21,21,21	0
57	MG	BF	301	1/1	0.90	0.26	62,62,62,62	0
57	MG	CW	104	1/1	0.90	0.39	52,52,52,52	0
57	MG	BA	3205	1/1	0.90	0.10	45,45,45,45	0
57	MG	BA	3233	1/1	0.90	0.69	53,53,53,53	0
57	MG	CA	1623	1/1	0.90	0.33	59,59,59,59	0
57	MG	DA	3137	1/1	0.90	0.20	30,30,30,30	0
57	MG	BA	3318	1/1	0.90	0.39	41,41,41,41	0
57	MG	CA	1613	1/1	0.90	0.43	42,42,42,42	0
57	MG	BA	3141	1/1	0.90	0.30	45,45,45,45	0
57	MG	DA	3050	1/1	0.90	0.40	46,46,46,46	0
57	MG	BA	3347	1/1	0.90	0.15	28,28,28,28	0
57	MG	DA	3299	1/1	0.90	0.15	42,42,42,42	0
57	MG	DA	3065	1/1	0.90	0.35	29,29,29,29	0
57	MG	AA	1713	1/1	0.90	0.14	43,43,43,43	0
57	MG	BA	3157	1/1	0.90	0.15	38,38,38,38	0
57	MG	BA	3097	1/1	0.90	0.40	34,34,34,34	0
57	MG	DA	3293	1/1	0.90	0.23	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3281	1/1	0.90	0.10	49,49,49,49	0
57	MG	DA	3112	1/1	0.90	0.27	27,27,27,27	0
57	MG	BA	3382	1/1	0.90	0.23	26,26,26,26	0
57	MG	CA	1626	1/1	0.90	0.54	67,67,67,67	0
57	MG	CA	1634	1/1	0.90	0.10	37,37,37,37	0
57	MG	DA	3290	1/1	0.90	0.55	50,50,50,50	0
57	MG	DA	3182	1/1	0.90	0.15	37,37,37,37	0
57	MG	DA	3101	1/1	0.90	0.23	35,35,35,35	0
57	MG	BA	3281	1/1	0.90	0.25	29,29,29,29	0
57	MG	CA	1612	1/1	0.90	0.36	55,55,55,55	0
57	MG	DA	3098	1/1	0.90	0.40	32,32,32,32	0
57	MG	AL	201	1/1	0.90	0.38	29,29,29,29	0
57	MG	BA	3166	1/1	0.90	0.56	38,38,38,38	0
57	MG	DA	3238	1/1	0.90	0.23	33,33,33,33	0
57	MG	AA	1701	1/1	0.90	0.32	33,33,33,33	0
57	MG	BA	3422	1/1	0.90	0.45	20,20,20,20	0
57	MG	BA	3074	1/1	0.90	0.38	31,31,31,31	0
57	MG	AA	1717	1/1	0.90	0.27	25,25,25,25	0
57	MG	BA	3028	1/1	0.90	0.22	29,29,29,29	0
57	MG	BA	3294	1/1	0.90	0.33	29,29,29,29	0
57	MG	DA	3201	1/1	0.90	0.45	32,32,32,32	0
57	MG	BA	3329	1/1	0.90	0.07	26,26,26,26	0
57	MG	BB	207	1/1	0.90	0.17	44,44,44,44	0
57	MG	DA	3178	1/1	0.90	0.09	30,30,30,30	0
57	MG	BA	3358	1/1	0.90	0.15	38,38,38,38	0
57	MG	BA	3450	1/1	0.90	0.41	44,44,44,44	0
57	MG	BA	3438	1/1	0.90	0.22	67,67,67,67	0
57	MG	DA	3187	1/1	0.90	0.33	48,48,48,48	0
57	MG	B5	103	1/1	0.90	0.18	20,20,20,20	0
57	MG	BA	3387	1/1	0.90	0.26	46,46,46,46	0
57	MG	BA	3123	1/1	0.90	0.25	43,43,43,43	0
57	MG	DA	3110	1/1	0.90	0.33	38,38,38,38	0
57	MG	DA	3272	1/1	0.90	0.21	40,40,40,40	0
57	MG	CA	1700	1/1	0.90	0.30	56,56,56,56	0
57	MG	BA	3359	1/1	0.90	0.28	44,44,44,44	0
57	MG	CA	1661	1/1	0.90	0.26	26,26,26,26	0
57	MG	BA	3414	1/1	0.91	0.36	36,36,36,36	0
57	MG	BA	3265	1/1	0.91	0.12	67,67,67,67	0
57	MG	BA	3088	1/1	0.91	0.28	24,24,24,24	0
57	MG	BA	3437	1/1	0.91	0.10	27,27,27,27	0
57	MG	DA	3135	1/1	0.91	0.26	42,42,42,42	0
57	MG	BA	3167	1/1	0.91	0.32	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1691	1/1	0.91	0.14	39,39,39,39	0
57	MG	DA	3037	1/1	0.91	0.42	45,45,45,45	0
57	MG	BA	3197	1/1	0.91	0.34	20,20,20,20	0
57	MG	BA	3148	1/1	0.91	0.23	64,64,64,64	0
57	MG	DA	3157	1/1	0.91	0.25	30,30,30,30	0
57	MG	BA	3126	1/1	0.91	0.30	66,66,66,66	0
57	MG	BA	3025	1/1	0.91	0.35	31,31,31,31	0
57	MG	CA	1694	1/1	0.91	0.74	51,51,51,51	0
57	MG	DA	3217	1/1	0.91	0.57	54,54,54,54	0
57	MG	CA	1647	1/1	0.91	0.28	61,61,61,61	0
57	MG	BA	3127	1/1	0.91	0.24	30,30,30,30	0
57	MG	DA	3172	1/1	0.91	0.15	30,30,30,30	0
57	MG	DA	3109	1/1	0.91	0.12	33,33,33,33	0
57	MG	DA	3167	1/1	0.91	0.44	38,38,38,38	0
57	MG	BA	3184	1/1	0.91	0.25	53,53,53,53	0
57	MG	CA	1703	1/1	0.91	0.41	34,34,34,34	0
57	MG	DA	3304	1/1	0.91	0.12	35,35,35,35	0
57	MG	DA	3199	1/1	0.91	0.23	67,67,67,67	0
57	MG	CA	1657	1/1	0.91	0.12	37,37,37,37	0
57	MG	DA	3174	1/1	0.91	0.55	23,23,23,23	0
57	MG	BA	3357	1/1	0.91	0.19	38,38,38,38	0
57	MG	BA	3313	1/1	0.91	0.37	26,26,26,26	0
57	MG	BA	3376	1/1	0.91	0.16	33,33,33,33	0
57	MG	BA	3036	1/1	0.91	0.20	30,30,30,30	0
57	MG	BA	3331	1/1	0.91	0.27	28,28,28,28	0
57	MG	DA	3207	1/1	0.91	0.12	26,26,26,26	0
57	MG	DA	3003	1/1	0.91	0.18	30,30,30,30	0
57	MG	DA	3160	1/1	0.91	0.30	38,38,38,38	0
57	MG	BA	3016	1/1	0.91	0.48	20,20,20,20	0
57	MG	BA	3328	1/1	0.91	0.24	32,32,32,32	0
57	MG	AA	1678	1/1	0.91	0.10	33,33,33,33	0
57	MG	CA	1651	1/1	0.91	0.18	28,28,28,28	0
57	MG	AA	1650	1/1	0.91	0.16	28,28,28,28	0
57	MG	DA	3040	1/1	0.91	0.35	26,26,26,26	0
57	MG	CA	1625	1/1	0.91	0.33	31,31,31,31	0
57	MG	CA	1609	1/1	0.91	0.29	27,27,27,27	0
57	MG	DA	3133	1/1	0.91	0.16	31,31,31,31	0
57	MG	AA	1607	1/1	0.91	0.25	51,51,51,51	0
57	MG	DA	3231	1/1	0.91	0.38	45,45,45,45	0
57	MG	DA	3214	1/1	0.91	0.34	29,29,29,29	0
57	MG	DA	3301	1/1	0.91	0.11	33,33,33,33	0
57	MG	BA	3060	1/1	0.91	0.38	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3064	1/1	0.91	0.40	44,44,44,44	0
57	MG	DA	3171	1/1	0.91	0.47	27,27,27,27	0
57	MG	DA	3249	1/1	0.91	0.14	33,33,33,33	0
57	MG	CA	1698	1/1	0.91	0.18	33,33,33,33	0
57	MG	DA	3241	1/1	0.91	0.10	26,26,26,26	0
57	MG	CA	1645	1/1	0.91	0.28	41,41,41,41	0
57	MG	BA	3322	1/1	0.91	0.34	29,29,29,29	0
57	MG	AA	1669	1/1	0.91	0.21	70,70,70,70	0
57	MG	BA	3053	1/1	0.91	0.47	63,63,63,63	0
57	MG	BA	3242	1/1	0.91	0.26	24,24,24,24	0
57	MG	DA	3024	1/1	0.91	0.13	33,33,33,33	0
57	MG	DA	3030	1/1	0.91	0.14	46,46,46,46	0
57	MG	DP	201	1/1	0.91	0.15	38,38,38,38	0
57	MG	CA	1689	1/1	0.91	0.18	39,39,39,39	0
57	MG	BA	3017	1/1	0.91	0.27	20,20,20,20	0
57	MG	BA	3021	1/1	0.91	1.61	180,180,180,180	0
57	MG	AA	1626	1/1	0.91	0.24	35,35,35,35	0
57	MG	DA	3268	1/1	0.91	0.19	43,43,43,43	0
57	MG	AA	1653	1/1	0.91	0.24	28,28,28,28	0
57	MG	BA	3002	1/1	0.91	0.18	39,39,39,39	0
57	MG	BA	3051	1/1	0.91	0.44	51,51,51,51	0
57	MG	DA	3303	1/1	0.91	0.23	54,54,54,54	0
57	MG	BA	3009	1/1	0.92	0.20	16,16,16,16	0
57	MG	CA	1664	1/1	0.92	0.28	42,42,42,42	0
57	MG	BA	3071	1/1	0.92	0.34	25,25,25,25	0
57	MG	CA	1616	1/1	0.92	0.16	20,20,20,20	0
57	MG	B5	102	1/1	0.92	0.38	40,40,40,40	0
57	MG	BA	3426	1/1	0.92	0.11	26,26,26,26	0
57	MG	BA	3037	1/1	0.92	0.23	9,9,9,9	0
57	MG	DA	3235	1/1	0.92	0.15	24,24,24,24	0
57	MG	AA	1660	1/1	0.92	0.23	31,31,31,31	0
57	MG	DA	3080	1/1	0.92	0.28	24,24,24,24	0
57	MG	CA	1692	1/1	0.92	0.17	48,48,48,48	0
57	MG	DA	3189	1/1	0.92	0.20	34,34,34,34	0
57	MG	BA	3240	1/1	0.92	0.22	23,23,23,23	0
57	MG	BA	3155	1/1	0.92	0.55	37,37,37,37	0
57	MG	BA	3343	1/1	0.92	0.19	22,22,22,22	0
57	MG	DA	3233	1/1	0.92	0.17	17,17,17,17	0
57	MG	AA	1688	1/1	0.92	0.16	56,56,56,56	0
57	MG	BA	3187	1/1	0.92	0.41	45,45,45,45	0
57	MG	BA	3113	1/1	0.92	0.37	32,32,32,32	0
57	MG	DA	3250	1/1	0.92	0.38	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3048	1/1	0.92	0.24	6,6,6,6	0
57	MG	DA	3099	1/1	0.92	0.43	23,23,23,23	0
57	MG	BA	3352	1/1	0.92	0.27	22,22,22,22	0
57	MG	AA	1625	1/1	0.92	0.20	37,37,37,37	0
57	MG	DA	3153	1/1	0.92	0.15	41,41,41,41	0
57	MG	BA	3066	1/1	0.92	0.20	14,14,14,14	0
57	MG	CA	1706	1/1	0.92	0.23	59,59,59,59	0
57	MG	BA	3158	1/1	0.92	0.28	37,37,37,37	0
57	MG	BA	3433	1/1	0.92	0.50	52,52,52,52	0
57	MG	CW	101	1/1	0.92	0.24	22,22,22,22	0
57	MG	BA	3235	1/1	0.92	0.26	51,51,51,51	0
57	MG	BA	3453	1/1	0.92	0.20	41,41,41,41	0
57	MG	DA	3032	1/1	0.92	0.23	20,20,20,20	0
57	MG	BA	3140	1/1	0.92	0.13	33,33,33,33	0
57	MG	BA	3107	1/1	0.92	0.13	40,40,40,40	0
57	MG	CA	1654	1/1	0.92	0.13	17,17,17,17	0
57	MG	BA	3277	1/1	0.92	0.24	29,29,29,29	0
57	MG	BA	3252	1/1	0.92	0.14	25,25,25,25	0
57	MG	BA	3395	1/1	0.92	0.46	39,39,39,39	0
57	MG	DA	3240	1/1	0.92	0.14	35,35,35,35	0
57	MG	CA	1685	1/1	0.92	0.13	33,33,33,33	0
57	MG	CA	1615	1/1	0.92	0.37	63,63,63,63	0
57	MG	DA	3087	1/1	0.92	0.39	26,26,26,26	0
57	MG	AA	1649	1/1	0.92	0.29	50,50,50,50	0
57	MG	AA	1673	1/1	0.92	0.12	40,40,40,40	0
57	MG	AW	101	1/1	0.92	0.19	6,6,6,6	0
57	MG	CA	1702	1/1	0.92	0.32	29,29,29,29	0
57	MG	DA	3023	1/1	0.92	0.23	42,42,42,42	0
57	MG	DA	3228	1/1	0.92	0.22	25,25,25,25	0
57	MG	BA	3350	1/1	0.92	0.19	37,37,37,37	0
57	MG	AA	1616	1/1	0.92	0.27	30,30,30,30	0
57	MG	BA	3162	1/1	0.92	0.10	21,21,21,21	0
57	MG	BA	3439	1/1	0.92	0.17	32,32,32,32	0
57	MG	BA	3345	1/1	0.92	0.29	34,34,34,34	0
57	MG	BA	3069	1/1	0.92	0.27	30,30,30,30	0
57	MG	AA	1702	1/1	0.92	0.11	26,26,26,26	0
57	MG	BA	3297	1/1	0.92	0.23	21,21,21,21	0
57	MG	BA	3193	1/1	0.92	0.12	47,47,47,47	0
57	MG	BA	3394	1/1	0.92	0.12	28,28,28,28	0
57	MG	BA	3369	1/1	0.92	0.13	63,63,63,63	0
57	MG	DA	3239	1/1	0.92	0.23	32,32,32,32	0
57	MG	DA	3196	1/1	0.92	0.31	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3152	1/1	0.92	0.22	23,23,23,23	0
57	MG	BA	3087	1/1	0.92	0.35	23,23,23,23	0
57	MG	BA	3280	1/1	0.92	0.17	19,19,19,19	0
57	MG	BA	3215	1/1	0.92	0.20	35,35,35,35	0
57	MG	BA	3326	1/1	0.92	0.17	21,21,21,21	0
57	MG	DA	3234	1/1	0.92	0.30	33,33,33,33	0
57	MG	BA	3231	1/1	0.92	0.38	54,54,54,54	0
57	MG	BA	3269	1/1	0.92	0.25	27,27,27,27	0
57	MG	BA	3310	1/1	0.92	0.19	30,30,30,30	0
57	MG	CA	1690	1/1	0.92	0.25	44,44,44,44	0
57	MG	BA	3170	1/1	0.92	0.18	40,40,40,40	0
57	MG	BA	3044	1/1	0.92	0.30	22,22,22,22	0
57	MG	CA	1619	1/1	0.92	0.15	34,34,34,34	0
57	MG	BA	3024	1/1	0.92	0.34	20,20,20,20	0
57	MG	BA	3289	1/1	0.92	0.31	38,38,38,38	0
57	MG	BA	3057	1/1	0.92	0.41	39,39,39,39	0
57	MG	BA	3288	1/1	0.92	0.19	18,18,18,18	0
57	MG	AA	1716	1/1	0.92	0.11	31,31,31,31	0
57	MG	DA	3259	1/1	0.92	0.20	47,47,47,47	0
57	MG	BA	3353	1/1	0.92	0.36	36,36,36,36	0
57	MG	DA	3180	1/1	0.92	0.30	49,49,49,49	0
57	MG	DA	3139	1/1	0.92	0.17	58,58,58,58	0
57	MG	AA	1684	1/1	0.92	0.13	31,31,31,31	0
57	MG	DA	3059	1/1	0.92	0.24	26,26,26,26	0
57	MG	BA	3306	1/1	0.92	0.33	47,47,47,47	0
57	MG	BA	3181	1/1	0.93	0.56	19,19,19,19	0
57	MG	CA	1691	1/1	0.93	0.59	67,67,67,67	0
57	MG	CA	1622	1/1	0.93	0.31	24,24,24,24	0
57	MG	CA	1624	1/1	0.93	0.60	39,39,39,39	0
57	MG	AA	1615	1/1	0.93	0.17	46,46,46,46	0
57	MG	CA	1621	1/1	0.93	0.18	22,22,22,22	0
57	MG	DA	3104	1/1	0.93	0.23	21,21,21,21	0
57	MG	CA	1696	1/1	0.93	0.30	54,54,54,54	0
57	MG	AA	1710	1/1	0.93	0.11	30,30,30,30	0
57	MG	BX	101	1/1	0.93	0.14	36,36,36,36	0
57	MG	DA	3262	1/1	0.93	0.27	29,29,29,29	0
57	MG	BA	3079	1/1	0.93	0.34	25,25,25,25	0
57	MG	BA	3006	1/1	0.93	0.24	27,27,27,27	0
57	MG	AA	1648	1/1	0.93	0.14	40,40,40,40	0
57	MG	DA	3183	1/1	0.93	0.23	54,54,54,54	0
57	MG	DA	3225	1/1	0.93	0.31	44,44,44,44	0
57	MG	BA	3005	1/1	0.93	0.20	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3085	1/1	0.93	0.46	49,49,49,49	0
57	MG	CA	1704	1/1	0.93	0.17	26,26,26,26	0
57	MG	BA	3339	1/1	0.93	0.29	29,29,29,29	0
57	MG	BA	3362	1/1	0.93	0.32	30,30,30,30	0
57	MG	BA	3305	1/1	0.93	0.34	41,41,41,41	0
57	MG	CA	1693	1/1	0.93	0.21	36,36,36,36	0
57	MG	DA	3292	1/1	0.93	0.13	17,17,17,17	0
57	MG	BA	3393	1/1	0.93	0.09	61,61,61,61	0
57	MG	BA	3356	1/1	0.93	0.17	21,21,21,21	0
57	MG	DA	3062	1/1	0.93	0.17	33,33,33,33	0
57	MG	BA	3263	1/1	0.93	0.09	36,36,36,36	0
57	MG	BA	3363	1/1	0.93	0.21	23,23,23,23	0
57	MG	DA	3116	1/1	0.93	0.35	33,33,33,33	0
57	MG	B5	104	1/1	0.93	0.23	33,33,33,33	0
57	MG	DA	3017	1/1	0.93	0.39	21,21,21,21	0
57	MG	BA	3105	1/1	0.93	0.16	15,15,15,15	0
57	MG	AA	1631	1/1	0.93	0.16	29,29,29,29	0
57	MG	AA	1635	1/1	0.93	0.42	31,31,31,31	0
57	MG	BA	3319	1/1	0.93	0.07	28,28,28,28	0
57	MG	DA	3046	1/1	0.93	0.40	26,26,26,26	0
57	MG	CA	1662	1/1	0.93	0.43	26,26,26,26	0
57	MG	BA	3075	1/1	0.93	0.21	24,24,24,24	0
57	MG	BA	3404	1/1	0.93	0.06	53,53,53,53	0
57	MG	CA	1637	1/1	0.93	0.15	26,26,26,26	0
57	MG	BA	3447	1/1	0.93	0.42	27,27,27,27	0
57	MG	BA	3182	1/1	0.93	0.45	27,27,27,27	0
57	MG	DA	3141	1/1	0.93	0.19	25,25,25,25	0
57	MG	AA	1644	1/1	0.93	0.27	40,40,40,40	0
57	MG	BA	3174	1/1	0.93	0.18	53,53,53,53	0
57	MG	BA	3030	1/1	0.93	0.42	37,37,37,37	0
57	MG	CA	1684	1/1	0.93	0.21	42,42,42,42	0
57	MG	DA	3209	1/1	0.93	0.26	33,33,33,33	0
57	MG	DA	3140	1/1	0.93	0.24	36,36,36,36	0
57	MG	DA	3147	1/1	0.93	0.50	18,18,18,18	0
57	MG	BA	3365	1/1	0.93	0.34	23,23,23,23	0
57	MG	CA	1671	1/1	0.93	0.10	54,54,54,54	0
57	MG	CA	1675	1/1	0.93	0.47	33,33,33,33	0
57	MG	AA	1629	1/1	0.93	0.15	56,56,56,56	0
57	MG	DA	3305	1/1	0.93	0.38	35,35,35,35	0
57	MG	DA	3252	1/1	0.93	0.52	27,27,27,27	0
57	MG	DA	3206	1/1	0.93	0.17	49,49,49,49	0
57	MG	BA	3117	1/1	0.93	0.60	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	DA	3053	1/1	0.93	0.36	21,21,21,21	0
57	MG	AA	1638	1/1	0.93	0.15	55,55,55,55	0
58	ZN	D5	103	1/1	0.93	0.16	30,30,30,30	0
57	MG	DB	205	1/1	0.93	0.33	42,42,42,42	0
57	MG	CA	1642	1/1	0.93	0.13	37,37,37,37	0
57	MG	AA	1651	1/1	0.93	0.11	49,49,49,49	0
57	MG	BA	3336	1/1	0.93	0.16	29,29,29,29	0
57	MG	BA	3241	1/1	0.93	0.18	50,50,50,50	0
57	MG	CX	101	1/1	0.93	0.20	22,22,22,22	0
57	MG	DA	3130	1/1	0.93	0.37	34,34,34,34	0
57	MG	CA	1648	1/1	0.93	0.10	28,28,28,28	0
57	MG	BA	3156	1/1	0.93	0.09	26,26,26,26	0
57	MG	DA	3090	1/1	0.93	0.23	31,31,31,31	0
57	MG	BA	3227	1/1	0.93	0.29	21,21,21,21	0
57	MG	BA	3027	1/1	0.93	0.19	26,26,26,26	0
57	MG	BA	3308	1/1	0.93	0.31	22,22,22,22	0
57	MG	DA	3271	1/1	0.93	0.20	42,42,42,42	0
57	MG	BT	201	1/1	0.93	0.21	32,32,32,32	0
57	MG	BA	3149	1/1	0.93	0.28	27,27,27,27	0
57	MG	BA	3081	1/1	0.93	0.48	16,16,16,16	0
57	MG	CA	1639	1/1	0.93	0.11	22,22,22,22	0
57	MG	DA	3244	1/1	0.93	0.31	26,26,26,26	0
57	MG	AW	102	1/1	0.93	0.09	26,26,26,26	0
57	MG	DA	3096	1/1	0.93	0.20	34,34,34,34	0
57	MG	DA	3022	1/1	0.94	0.20	21,21,21,21	0
57	MG	BA	3008	1/1	0.94	0.41	16,16,16,16	0
57	MG	CA	1607	1/1	0.94	0.12	37,37,37,37	0
57	MG	AA	1662	1/1	0.94	0.14	22,22,22,22	0
57	MG	DA	3052	1/1	0.94	0.27	21,21,21,21	0
57	MG	BA	3201	1/1	0.94	0.12	24,24,24,24	0
57	MG	BA	3132	1/1	0.94	0.28	28,28,28,28	0
57	MG	BA	3386	1/1	0.94	0.29	68,68,68,68	0
57	MG	BA	3026	1/1	0.94	0.25	31,31,31,31	0
57	MG	BA	3054	1/1	0.94	0.46	33,33,33,33	0
57	MG	DA	3118	1/1	0.94	0.18	33,33,33,33	0
57	MG	BA	3411	1/1	0.94	0.38	53,53,53,53	0
57	MG	BA	3150	1/1	0.94	0.46	29,29,29,29	0
57	MG	DA	3138	1/1	0.94	0.25	17,17,17,17	0
57	MG	BA	3261	1/1	0.94	0.40	28,28,28,28	0
57	MG	DA	3247	1/1	0.94	0.14	23,23,23,23	0
57	MG	AA	1612	1/1	0.94	0.39	25,25,25,25	0
57	MG	AA	1658	1/1	0.94	0.15	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1680	1/1	0.94	0.33	49,49,49,49	0
57	MG	BA	3436	1/1	0.94	0.28	48,48,48,48	0
57	MG	DA	3216	1/1	0.94	0.41	23,23,23,23	0
57	MG	DA	3086	1/1	0.94	0.34	25,25,25,25	0
57	MG	DA	3265	1/1	0.94	0.40	54,54,54,54	0
57	MG	AT	201	1/1	0.94	0.23	22,22,22,22	0
57	MG	BB	205	1/1	0.94	0.25	19,19,19,19	0
57	MG	BA	3200	1/1	0.94	0.33	20,20,20,20	0
57	MG	B1	101	1/1	0.94	0.41	63,63,63,63	0
57	MG	DA	3060	1/1	0.94	0.28	27,27,27,27	0
57	MG	BA	3137	1/1	0.94	0.41	46,46,46,46	0
57	MG	BA	3146	1/1	0.94	0.26	22,22,22,22	0
57	MG	BA	3183	1/1	0.94	0.12	22,22,22,22	0
57	MG	BA	3032	1/1	0.94	0.25	6,6,6,6	0
57	MG	DA	3075	1/1	0.94	0.32	27,27,27,27	0
57	MG	BA	3371	1/1	0.94	0.15	48,48,48,48	0
57	MG	BA	3397	1/1	0.94	0.23	44,44,44,44	0
57	MG	BA	3375	1/1	0.94	0.41	36,36,36,36	0
57	MG	D5	102	1/1	0.94	0.44	44,44,44,44	0
57	MG	AA	1672	1/1	0.94	0.20	33,33,33,33	0
57	MG	AA	1656	1/1	0.94	0.12	28,28,28,28	0
57	MG	BB	201	1/1	0.94	0.30	59,59,59,59	0
57	MG	CA	1653	1/1	0.94	0.19	36,36,36,36	0
57	MG	DA	3114	1/1	0.94	0.30	30,30,30,30	0
57	MG	DA	3029	1/1	0.94	0.14	22,22,22,22	0
57	MG	BA	3405	1/1	0.94	0.09	25,25,25,25	0
57	MG	CA	1677	1/1	0.94	0.36	27,27,27,27	0
57	MG	AA	1690	1/1	0.94	0.09	26,26,26,26	0
57	MG	CA	1659	1/1	0.94	0.36	32,32,32,32	0
57	MG	BA	3192	1/1	0.94	0.26	27,27,27,27	0
57	MG	BA	3225	1/1	0.94	0.16	16,16,16,16	0
57	MG	BA	3161	1/1	0.94	0.21	25,25,25,25	0
57	MG	DA	3008	1/1	0.94	0.27	6,6,6,6	0
57	MG	BA	3172	1/1	0.94	0.52	22,22,22,22	0
57	MG	BA	3042	1/1	0.94	0.31	10,10,10,10	0
57	MG	B7	101	1/1	0.94	0.14	12,12,12,12	0
57	MG	DA	3115	1/1	0.94	0.08	36,36,36,36	0
57	MG	AA	1667	1/1	0.94	0.22	62,62,62,62	0
57	MG	DA	3221	1/1	0.94	0.36	38,38,38,38	0
57	MG	BA	3391	1/1	0.94	0.22	44,44,44,44	0
57	MG	CA	1633	1/1	0.94	0.44	45,45,45,45	0
57	MG	DA	3126	1/1	0.94	0.20	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3410	1/1	0.94	0.14	30,30,30,30	0
57	MG	AA	1640	1/1	0.94	0.24	19,19,19,19	0
57	MG	BA	3050	1/1	0.94	0.30	24,24,24,24	0
57	MG	AA	1697	1/1	0.94	0.16	27,27,27,27	0
57	MG	AA	1712	1/1	0.94	0.19	56,56,56,56	0
57	MG	BA	3451	1/1	0.94	0.20	23,23,23,23	0
57	MG	BA	3260	1/1	0.94	0.22	24,24,24,24	0
57	MG	BA	3209	1/1	0.94	0.25	23,23,23,23	0
57	MG	BB	208	1/1	0.94	0.33	36,36,36,36	0
57	MG	BA	3298	1/1	0.94	0.15	20,20,20,20	0
57	MG	BA	3131	1/1	0.94	0.33	26,26,26,26	0
57	MG	DA	3236	1/1	0.94	0.10	30,30,30,30	0
57	MG	DA	3004	1/1	0.94	0.17	21,21,21,21	0
57	MG	CA	1701	1/1	0.94	0.23	25,25,25,25	0
57	MG	CA	1668	1/1	0.94	0.22	27,27,27,27	0
57	MG	BA	3348	1/1	0.94	0.35	55,55,55,55	0
57	MG	BH	201	1/1	0.94	0.19	21,21,21,21	0
57	MG	BA	3419	1/1	0.94	0.40	44,44,44,44	0
57	MG	DA	3034	1/1	0.94	0.24	57,57,57,57	0
57	MG	DA	3275	1/1	0.94	0.25	48,48,48,48	0
57	MG	DD	301	1/1	0.94	0.19	18,18,18,18	0
57	MG	BA	3309	1/1	0.94	0.07	20,20,20,20	0
57	MG	DA	3264	1/1	0.94	0.11	25,25,25,25	0
57	MG	DA	3210	1/1	0.94	0.24	41,41,41,41	0
57	MG	CA	1631	1/1	0.94	0.29	34,34,34,34	0
57	MG	BA	3173	1/1	0.94	0.13	40,40,40,40	0
57	MG	DA	3055	1/1	0.94	0.26	24,24,24,24	0
57	MG	BA	3271	1/1	0.94	0.22	40,40,40,40	0
57	MG	BA	3061	1/1	0.94	0.39	25,25,25,25	0
57	MG	DA	3260	1/1	0.94	0.13	31,31,31,31	0
57	MG	BA	3082	1/1	0.94	0.32	24,24,24,24	0
57	MG	DA	3296	1/1	0.94	0.35	40,40,40,40	0
57	MG	BA	3220	1/1	0.94	0.23	30,30,30,30	0
57	MG	BA	3402	1/1	0.94	0.13	24,24,24,24	0
57	MG	BA	3256	1/1	0.94	0.19	25,25,25,25	0
57	MG	DA	3162	1/1	0.94	0.20	24,24,24,24	0
57	MG	DA	3124	1/1	0.94	0.17	26,26,26,26	0
57	MG	BA	3121	1/1	0.94	0.19	20,20,20,20	0
57	MG	BA	3333	1/1	0.94	0.59	77,77,77,77	0
57	MG	BA	3189	1/1	0.94	0.09	14,14,14,14	0
57	MG	DA	3191	1/1	0.94	0.21	18,18,18,18	0
57	MG	BA	3046	1/1	0.94	0.31	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3401	1/1	0.94	0.13	46,46,46,46	0
57	MG	DA	3078	1/1	0.94	0.31	44,44,44,44	0
57	MG	AA	1608	1/1	0.94	0.17	65,65,65,65	0
57	MG	BA	3058	1/1	0.94	0.47	18,18,18,18	0
57	MG	BA	3135	1/1	0.95	0.16	23,23,23,23	0
57	MG	BA	3338	1/1	0.95	0.09	18,18,18,18	0
57	MG	BA	3120	1/1	0.95	0.29	35,35,35,35	0
57	MG	BA	3112	1/1	0.95	0.23	23,23,23,23	0
57	MG	BA	3367	1/1	0.95	0.39	33,33,33,33	0
57	MG	AA	1671	1/1	0.95	0.23	42,42,42,42	0
57	MG	BB	206	1/1	0.95	0.32	31,31,31,31	0
57	MG	BA	3279	1/1	0.95	0.07	26,26,26,26	0
57	MG	DA	3102	1/1	0.95	0.41	32,32,32,32	0
57	MG	DA	3103	1/1	0.95	0.53	19,19,19,19	0
57	MG	BA	3259	1/1	0.95	0.19	37,37,37,37	0
57	MG	DA	3285	1/1	0.95	0.23	38,38,38,38	0
57	MG	DA	3063	1/1	0.95	0.17	29,29,29,29	0
57	MG	BA	3282	1/1	0.95	0.40	22,22,22,22	0
57	MG	AA	1698	1/1	0.95	0.35	37,37,37,37	0
57	MG	BA	3316	1/1	0.95	0.18	28,28,28,28	0
57	MG	BA	3330	1/1	0.95	0.17	21,21,21,21	0
57	MG	BA	3104	1/1	0.95	0.17	37,37,37,37	0
57	MG	DA	3105	1/1	0.95	0.37	30,30,30,30	0
57	MG	CA	1683	1/1	0.95	0.15	36,36,36,36	0
57	MG	BA	3377	1/1	0.95	0.11	23,23,23,23	0
57	MG	DA	3212	1/1	0.95	0.20	18,18,18,18	0
57	MG	BA	3415	1/1	0.95	0.22	36,36,36,36	0
57	MG	BA	3033	1/1	0.95	0.22	34,34,34,34	0
57	MG	DA	3071	1/1	0.95	0.31	20,20,20,20	0
57	MG	DA	3295	1/1	0.95	0.25	40,40,40,40	0
57	MG	BA	3295	1/1	0.95	0.26	20,20,20,20	0
57	MG	BA	3334	1/1	0.95	0.18	24,24,24,24	0
57	MG	BQ	202	1/1	0.95	0.27	30,30,30,30	0
57	MG	BA	3114	1/1	0.95	0.38	24,24,24,24	0
57	MG	CA	1709	1/1	0.95	0.33	28,28,28,28	0
57	MG	AA	1624	1/1	0.95	0.33	33,33,33,33	0
57	MG	BA	3210	1/1	0.95	0.30	24,24,24,24	0
57	MG	BA	3041	1/1	0.95	0.47	44,44,44,44	0
57	MG	DA	3095	1/1	0.95	0.30	62,62,62,62	0
57	MG	BQ	201	1/1	0.95	0.20	24,24,24,24	0
57	MG	BA	3083	1/1	0.95	0.14	22,22,22,22	0
57	MG	AA	1700	1/1	0.95	0.19	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3234	1/1	0.95	0.05	38,38,38,38	0
57	MG	BA	3206	1/1	0.95	0.25	22,22,22,22	0
57	MG	BA	3115	1/1	0.95	0.24	19,19,19,19	0
57	MG	BA	3286	1/1	0.95	0.36	24,24,24,24	0
57	MG	DA	3263	1/1	0.95	0.18	28,28,28,28	0
57	MG	CA	1679	1/1	0.95	0.12	29,29,29,29	0
57	MG	BA	3221	1/1	0.95	0.21	22,22,22,22	0
57	MG	BA	3179	1/1	0.95	0.48	23,23,23,23	0
57	MG	CA	1656	1/1	0.95	0.43	43,43,43,43	0
57	MG	BA	3007	1/1	0.95	0.38	19,19,19,19	0
57	MG	DA	3013	1/1	0.95	0.33	20,20,20,20	0
57	MG	DA	3093	1/1	0.95	0.26	19,19,19,19	0
57	MG	AA	1714	1/1	0.95	0.26	42,42,42,42	0
57	MG	BA	3023	1/1	0.95	0.42	45,45,45,45	0
57	MG	CA	1676	1/1	0.95	0.20	48,48,48,48	0
57	MG	B5	101	1/1	0.95	0.40	78,78,78,78	0
57	MG	BA	3321	1/1	0.95	0.37	22,22,22,22	0
57	MG	DA	3224	1/1	0.95	0.41	14,14,14,14	0
57	MG	DA	3243	1/1	0.95	0.12	44,44,44,44	0
57	MG	AA	1614	1/1	0.95	0.38	29,29,29,29	0
57	MG	DA	3179	1/1	0.95	0.33	30,30,30,30	0
57	MG	AA	1666	1/1	0.95	0.14	24,24,24,24	0
57	MG	AA	1683	1/1	0.95	0.31	31,31,31,31	0
57	MG	BA	3084	1/1	0.95	0.69	61,61,61,61	0
57	MG	BA	3138	1/1	0.95	0.13	39,39,39,39	0
57	MG	BA	3165	1/1	0.95	0.19	25,25,25,25	0
57	MG	CA	1697	1/1	0.95	0.08	39,39,39,39	0
57	MG	BA	3454	1/1	0.95	0.14	25,25,25,25	0
57	MG	DA	3077	1/1	0.95	0.39	22,22,22,22	0
57	MG	BA	3080	1/1	0.95	0.29	32,32,32,32	0
57	MG	DA	3188	1/1	0.95	0.11	27,27,27,27	0
57	MG	BA	3011	1/1	0.95	0.22	6,6,6,6	0
57	MG	BA	3145	1/1	0.95	0.35	29,29,29,29	0
57	MG	AA	1693	1/1	0.95	0.11	45,45,45,45	0
57	MG	DA	3106	1/1	0.95	0.50	25,25,25,25	0
57	MG	BA	3103	1/1	0.95	0.32	21,21,21,21	0
57	MG	BA	3055	1/1	0.95	0.26	24,24,24,24	0
57	MG	CA	1674	1/1	0.95	0.27	41,41,41,41	0
57	MG	BP	203	1/1	0.95	0.21	27,27,27,27	0
57	MG	BA	3063	1/1	0.95	0.24	17,17,17,17	0
57	MG	BD	301	1/1	0.96	0.25	34,34,34,34	0
57	MG	AA	1694	1/1	0.96	0.18	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3186	1/1	0.96	0.54	24,24,24,24	0
57	MG	BA	3275	1/1	0.96	0.28	27,27,27,27	0
57	MG	BA	3302	1/1	0.96	0.10	37,37,37,37	0
57	MG	DA	3181	1/1	0.96	0.31	36,36,36,36	0
57	MG	BA	3076	1/1	0.96	0.34	24,24,24,24	0
57	MG	BA	3106	1/1	0.96	0.34	23,23,23,23	0
57	MG	BA	3070	1/1	0.96	0.15	23,23,23,23	0
57	MG	CA	1669	1/1	0.96	0.18	21,21,21,21	0
57	MG	AA	1641	1/1	0.96	0.17	30,30,30,30	0
57	MG	DA	3057	1/1	0.96	0.23	22,22,22,22	0
57	MG	DA	3084	1/1	0.96	0.12	21,21,21,21	0
57	MG	BA	3085	1/1	0.96	0.18	17,17,17,17	0
57	MG	BA	3147	1/1	0.96	0.32	24,24,24,24	0
57	MG	BA	3130	1/1	0.96	0.39	35,35,35,35	0
57	MG	BA	3185	1/1	0.96	0.24	17,17,17,17	0
57	MG	BA	3398	1/1	0.96	0.17	34,34,34,34	0
57	MG	DA	3079	1/1	0.96	0.21	45,45,45,45	0
57	MG	BA	3337	1/1	0.96	0.25	37,37,37,37	0
57	MG	DA	3089	1/1	0.96	0.13	19,19,19,19	0
57	MG	DA	3120	1/1	0.96	0.23	25,25,25,25	0
57	MG	DA	3230	1/1	0.96	0.31	23,23,23,23	0
57	MG	DR	201	1/1	0.96	0.15	22,22,22,22	0
57	MG	AA	1682	1/1	0.96	0.21	18,18,18,18	0
57	MG	AA	1696	1/1	0.96	0.22	26,26,26,26	0
57	MG	BA	3255	1/1	0.96	0.44	31,31,31,31	0
57	MG	BA	3059	1/1	0.96	0.34	28,28,28,28	0
57	MG	BA	3034	1/1	0.96	0.21	19,19,19,19	0
57	MG	DA	3076	1/1	0.96	0.13	19,19,19,19	0
57	MG	BA	3246	1/1	0.96	0.10	11,11,11,11	0
57	MG	DA	3054	1/1	0.96	0.58	27,27,27,27	0
57	MG	DA	3091	1/1	0.96	0.14	26,26,26,26	0
57	MG	AA	1628	1/1	0.96	0.45	43,43,43,43	0
57	MG	BA	3068	1/1	0.96	0.23	30,30,30,30	0
57	MG	BA	3314	1/1	0.96	0.07	22,22,22,22	0
57	MG	DA	3064	1/1	0.96	0.26	19,19,19,19	0
57	MG	DA	3100	1/1	0.96	0.33	21,21,21,21	0
57	MG	BA	3208	1/1	0.96	0.05	56,56,56,56	0
57	MG	CA	1641	1/1	0.96	0.07	18,18,18,18	0
57	MG	BA	3360	1/1	0.96	0.16	27,27,27,27	0
57	MG	DA	3258	1/1	0.96	0.21	64,64,64,64	0
57	MG	CA	1705	1/1	0.96	0.26	48,48,48,48	0
57	MG	AA	1695	1/1	0.96	0.20	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3159	1/1	0.96	0.47	29,29,29,29	0
57	MG	BA	3304	1/1	0.96	0.10	49,49,49,49	0
57	MG	DA	3186	1/1	0.96	0.08	29,29,29,29	0
57	MG	BA	3012	1/1	0.96	0.38	22,22,22,22	0
57	MG	BA	3247	1/1	0.96	0.06	33,33,33,33	0
57	MG	BA	3312	1/1	0.96	0.31	22,22,22,22	0
57	MG	BB	202	1/1	0.96	0.32	21,21,21,21	0
57	MG	AA	1627	1/1	0.96	0.15	21,21,21,21	0
57	MG	DA	3027	1/1	0.96	0.13	33,33,33,33	0
57	MG	BA	3110	1/1	0.96	0.23	32,32,32,32	0
57	MG	BA	3144	1/1	0.96	0.20	24,24,24,24	0
57	MG	DA	3019	1/1	0.96	0.46	35,35,35,35	0
57	MG	BA	3276	1/1	0.96	0.39	21,21,21,21	0
57	MG	DA	3005	1/1	0.96	0.48	45,45,45,45	0
57	MG	BA	3078	1/1	0.96	0.38	29,29,29,29	0
57	MG	BA	3228	1/1	0.96	0.37	36,36,36,36	0
57	MG	DA	3134	1/1	0.96	0.16	24,24,24,24	0
57	MG	AA	1652	1/1	0.96	0.16	44,44,44,44	0
57	MG	BA	3244	1/1	0.96	0.25	47,47,47,47	0
57	MG	BA	3020	1/1	0.96	0.35	19,19,19,19	0
57	MG	DB	206	1/1	0.96	0.16	19,19,19,19	0
57	MG	CA	1606	1/1	0.96	0.38	50,50,50,50	0
57	MG	BA	3122	1/1	0.96	0.38	41,41,41,41	0
57	MG	CA	1628	1/1	0.96	0.12	26,26,26,26	0
57	MG	BA	3273	1/1	0.96	0.21	40,40,40,40	0
57	MG	BA	3203	1/1	0.96	0.35	29,29,29,29	0
57	MG	DA	3229	1/1	0.96	0.17	19,19,19,19	0
57	MG	CA	1688	1/1	0.96	0.12	35,35,35,35	0
57	MG	DA	3092	1/1	0.96	0.36	25,25,25,25	0
57	MG	BA	3222	1/1	0.96	0.30	31,31,31,31	0
57	MG	DA	3202	1/1	0.96	0.58	38,38,38,38	0
57	MG	AA	1643	1/1	0.96	0.15	23,23,23,23	0
57	MG	DA	3015	1/1	0.96	0.22	36,36,36,36	0
57	MG	DA	3242	1/1	0.96	0.09	32,32,32,32	0
57	MG	DA	3113	1/1	0.96	0.42	26,26,26,26	0
57	MG	DA	3068	1/1	0.96	0.22	19,19,19,19	0
57	MG	DA	3007	1/1	0.96	0.43	54,54,54,54	0
57	MG	CA	1611	1/1	0.96	0.10	25,25,25,25	0
57	MG	BA	3278	1/1	0.96	0.17	33,33,33,33	0
57	MG	DA	3173	1/1	0.96	0.19	33,33,33,33	0
57	MG	BA	3457	1/1	0.96	0.16	35,35,35,35	0
57	MG	DA	3128	1/1	0.96	0.26	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3214	1/1	0.96	0.11	29,29,29,29	0
57	MG	AA	1620	1/1	0.96	0.18	27,27,27,27	0
57	MG	AA	1692	1/1	0.96	0.23	51,51,51,51	0
57	MG	AA	1707	1/1	0.96	0.23	20,20,20,20	0
57	MG	DA	3047	1/1	0.96	0.34	26,26,26,26	0
57	MG	BA	3067	1/1	0.96	0.18	30,30,30,30	0
57	MG	AA	1634	1/1	0.96	0.40	41,41,41,41	0
57	MG	BA	3099	1/1	0.96	0.48	29,29,29,29	0
57	MG	DA	3035	1/1	0.96	0.51	22,22,22,22	0
57	MG	BA	3177	1/1	0.96	0.30	21,21,21,21	0
57	MG	BA	3416	1/1	0.96	0.13	42,42,42,42	0
57	MG	DA	3284	1/1	0.96	0.13	51,51,51,51	0
57	MG	DA	3156	1/1	0.96	0.83	58,58,58,58	0
57	MG	BE	301	1/1	0.96	0.29	43,43,43,43	0
57	MG	DA	3168	1/1	0.96	0.24	35,35,35,35	0
57	MG	BA	3400	1/1	0.97	0.08	32,32,32,32	0
57	MG	DA	3041	1/1	0.97	0.16	19,19,19,19	0
57	MG	AA	1610	1/1	0.97	0.45	21,21,21,21	0
57	MG	BA	3335	1/1	0.97	0.10	47,47,47,47	0
57	MG	BA	3119	1/1	0.97	0.42	23,23,23,23	0
57	MG	BA	3164	1/1	0.97	0.16	35,35,35,35	0
57	MG	BA	3441	1/1	0.97	0.41	37,37,37,37	0
57	MG	BA	3031	1/1	0.97	0.20	21,21,21,21	0
57	MG	DA	3056	1/1	0.97	0.22	30,30,30,30	0
57	MG	BA	3134	1/1	0.97	0.17	22,22,22,22	0
57	MG	CA	1630	1/1	0.97	0.11	29,29,29,29	0
57	MG	BA	3272	1/1	0.97	0.48	23,23,23,23	0
57	MG	BA	3299	1/1	0.97	0.21	22,22,22,22	0
57	MG	BA	3098	1/1	0.97	0.24	25,25,25,25	0
57	MG	DA	3294	1/1	0.97	0.41	19,19,19,19	0
58	ZN	B5	105	1/1	0.97	0.17	90,90,90,90	0
57	MG	BA	3396	1/1	0.97	0.11	26,26,26,26	0
57	MG	AA	1708	1/1	0.97	0.11	46,46,46,46	0
57	MG	BA	3423	1/1	0.97	0.08	25,25,25,25	0
57	MG	AA	1677	1/1	0.97	0.13	48,48,48,48	0
57	MG	BA	3089	1/1	0.97	0.37	24,24,24,24	0
57	MG	BA	3160	1/1	0.97	0.15	30,30,30,30	0
57	MG	BB	204	1/1	0.97	0.38	54,54,54,54	0
57	MG	BA	3108	1/1	0.97	0.23	35,35,35,35	0
57	MG	CA	1617	1/1	0.97	0.25	35,35,35,35	0
57	MG	DA	3163	1/1	0.97	0.26	32,32,32,32	0
57	MG	CA	1650	1/1	0.97	0.12	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	AA	1699	1/1	0.97	0.26	29,29,29,29	0
57	MG	DA	3066	1/1	0.97	0.30	22,22,22,22	0
57	MG	DA	3012	1/1	0.97	0.49	28,28,28,28	0
57	MG	BA	3039	1/1	0.97	0.75	39,39,39,39	0
57	MG	BA	3168	1/1	0.97	0.14	33,33,33,33	0
57	MG	DA	3170	1/1	0.97	0.27	22,22,22,22	0
57	MG	BA	3283	1/1	0.97	0.34	20,20,20,20	0
57	MG	DA	3289	1/1	0.97	0.15	27,27,27,27	0
57	MG	AA	1623	1/1	0.97	0.32	18,18,18,18	0
57	MG	DA	3083	1/1	0.97	0.10	30,30,30,30	0
57	MG	DA	3009	1/1	0.97	0.21	18,18,18,18	0
57	MG	BA	3274	1/1	0.97	0.35	27,27,27,27	0
57	MG	BA	3340	1/1	0.97	0.21	29,29,29,29	0
57	MG	DA	3082	1/1	0.97	0.29	21,21,21,21	0
57	MG	CA	1667	1/1	0.97	0.18	23,23,23,23	0
57	MG	DA	3039	1/1	0.97	0.31	18,18,18,18	0
57	MG	BA	3229	1/1	0.97	0.26	6,6,6,6	0
57	MG	BA	3101	1/1	0.97	0.10	21,21,21,21	0
57	MG	DA	3127	1/1	0.97	0.33	34,34,34,34	0
57	MG	BA	3327	1/1	0.97	0.20	28,28,28,28	0
57	MG	AA	1606	1/1	0.97	0.23	42,42,42,42	0
57	MG	BA	3325	1/1	0.97	0.33	22,22,22,22	0
57	MG	BA	3202	1/1	0.97	0.16	19,19,19,19	0
57	MG	BA	3351	1/1	0.97	0.15	56,56,56,56	0
57	MG	DA	3058	1/1	0.97	0.21	27,27,27,27	0
57	MG	BA	3216	1/1	0.97	0.44	20,20,20,20	0
57	MG	CA	1682	1/1	0.97	0.26	40,40,40,40	0
57	MG	DA	3018	1/1	0.97	0.45	21,21,21,21	0
57	MG	BA	3443	1/1	0.97	0.23	24,24,24,24	0
57	MG	BA	3019	1/1	0.97	0.34	25,25,25,25	0
57	MG	BA	3341	1/1	0.97	0.19	28,28,28,28	0
57	MG	DA	3219	1/1	0.97	0.45	34,34,34,34	0
57	MG	BA	3096	1/1	0.97	0.45	24,24,24,24	0
57	MG	BA	3056	1/1	0.97	0.42	26,26,26,26	0
57	MG	DB	207	1/1	0.97	0.18	27,27,27,27	0
57	MG	BA	3109	1/1	0.97	0.29	21,21,21,21	0
57	MG	BA	3142	1/1	0.97	0.30	25,25,25,25	0
57	MG	DA	3197	1/1	0.97	0.27	27,27,27,27	0
57	MG	AA	1630	1/1	0.97	0.29	41,41,41,41	0
57	MG	BA	3307	1/1	0.97	0.46	24,24,24,24	0
57	MG	BA	3413	1/1	0.97	0.29	24,24,24,24	0
57	MG	BA	3213	1/1	0.97	0.29	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BA	3324	1/1	0.97	0.17	25,25,25,25	0
57	MG	AA	1663	1/1	0.97	0.16	27,27,27,27	0
57	MG	BA	3048	1/1	0.97	0.39	27,27,27,27	0
57	MG	AA	1639	1/1	0.97	0.15	27,27,27,27	0
58	ZN	CD	301	1/1	0.97	0.34	81,81,81,81	0
57	MG	D6	102	1/1	0.97	0.18	23,23,23,23	0
57	MG	DA	3145	1/1	0.97	0.73	57,57,57,57	0
57	MG	BA	3003	1/1	0.97	0.12	25,25,25,25	0
57	MG	BA	3072	1/1	0.97	0.43	23,23,23,23	0
57	MG	BA	3045	1/1	0.97	0.22	6,6,6,6	0
57	MG	AA	1676	1/1	0.97	0.30	30,30,30,30	0
57	MG	AA	1670	1/1	0.97	0.24	30,30,30,30	0
57	MG	CA	1673	1/1	0.97	0.17	26,26,26,26	0
57	MG	DA	3002	1/1	0.98	0.64	37,37,37,37	0
57	MG	BA	3293	1/1	0.98	0.24	23,23,23,23	0
57	MG	BA	3049	1/1	0.98	0.43	24,24,24,24	0
57	MG	DA	3146	1/1	0.98	0.25	60,60,60,60	0
57	MG	BA	3267	1/1	0.98	0.16	19,19,19,19	0
57	MG	BA	3237	1/1	0.98	0.13	21,21,21,21	0
57	MG	BA	3128	1/1	0.98	0.40	33,33,33,33	0
57	MG	CA	1636	1/1	0.98	0.16	28,28,28,28	0
57	MG	CA	1610	1/1	0.98	0.34	30,30,30,30	0
57	MG	DA	3193	1/1	0.98	0.31	27,27,27,27	0
57	MG	BA	3245	1/1	0.98	0.18	27,27,27,27	0
57	MG	DA	3097	1/1	0.98	0.26	21,21,21,21	0
57	MG	BA	3285	1/1	0.98	0.14	6,6,6,6	0
57	MG	DA	3051	1/1	0.98	0.18	6,6,6,6	0
57	MG	DA	3253	1/1	0.98	0.21	20,20,20,20	0
57	MG	DA	3074	1/1	0.98	0.26	21,21,21,21	0
57	MG	BA	3409	1/1	0.98	0.11	24,24,24,24	0
57	MG	BA	3364	1/1	0.98	0.17	32,32,32,32	0
57	MG	DA	3148	1/1	0.98	0.33	24,24,24,24	0
57	MG	BA	3435	1/1	0.98	0.05	30,30,30,30	0
57	MG	BA	3010	1/1	0.98	0.24	23,23,23,23	0
57	MG	BA	3094	1/1	0.98	0.30	34,34,34,34	0
57	MG	BA	3455	1/1	0.98	0.21	46,46,46,46	0
57	MG	BA	3303	1/1	0.98	0.34	26,26,26,26	0
57	MG	BA	3392	1/1	0.98	0.14	52,52,52,52	0
57	MG	BA	3429	1/1	0.98	0.05	33,33,33,33	0
57	MG	CA	1666	1/1	0.98	0.41	18,18,18,18	0
57	MG	BA	3035	1/1	0.98	0.41	25,25,25,25	0
57	MG	BA	3047	1/1	0.98	0.39	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	BP	202	1/1	0.98	0.14	22,22,22,22	0
57	MG	BA	3389	1/1	0.98	0.24	21,21,21,21	0
57	MG	BA	3040	1/1	0.98	0.24	24,24,24,24	0
57	MG	AA	1668	1/1	0.98	0.13	40,40,40,40	0
57	MG	BA	3266	1/1	0.98	0.46	26,26,26,26	0
57	MG	DA	3006	1/1	0.98	0.34	28,28,28,28	0
57	MG	BA	3018	1/1	0.98	0.51	21,21,21,21	0
57	MG	BA	3154	1/1	0.98	0.31	38,38,38,38	0
57	MG	BA	3073	1/1	0.98	0.21	23,23,23,23	0
57	MG	DA	3159	1/1	0.98	0.49	38,38,38,38	0
57	MG	BA	3102	1/1	0.98	0.55	33,33,33,33	0
57	MG	BA	3065	1/1	0.98	0.31	24,24,24,24	0
57	MG	BA	3004	1/1	0.98	0.54	61,61,61,61	0
57	MG	BA	3219	1/1	0.98	0.12	28,28,28,28	0
57	MG	CA	1614	1/1	0.98	0.15	30,30,30,30	0
57	MG	CA	1699	1/1	0.98	0.23	32,32,32,32	0
57	MG	DA	3036	1/1	0.98	0.49	27,27,27,27	0
57	MG	BA	3043	1/1	0.98	0.34	25,25,25,25	0
57	MG	BA	3420	1/1	0.98	0.18	45,45,45,45	0
57	MG	DA	3257	1/1	0.98	0.16	35,35,35,35	0
57	MG	BA	3250	1/1	0.99	0.50	22,22,22,22	0
58	ZN	D9	101	1/1	0.99	0.15	30,30,30,30	0
57	MG	DA	3011	1/1	0.99	0.35	20,20,20,20	0
58	ZN	B9	101	1/1	0.99	0.12	75,75,75,75	0
57	MG	AA	1655	1/1	0.99	0.21	6,6,6,6	0
57	MG	BA	3090	1/1	0.99	0.24	17,17,17,17	0
57	MG	BA	3287	1/1	0.99	0.17	20,20,20,20	0
57	MG	BA	3452	1/1	0.99	0.15	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.