



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2017 – 03:03 AM EST

PDB ID : 4V7M
Title : The structures of Capreomycin bound to the 70S ribosome.
Authors : Stanley, R.E.; Blaha, G.
Deposited on : unknown
Resolution : 3.45 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

<http://wwpdb.org/validation/2016/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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

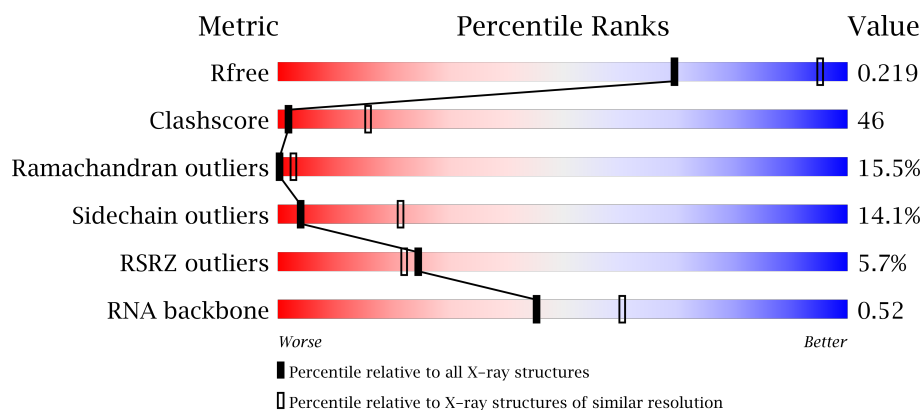
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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.





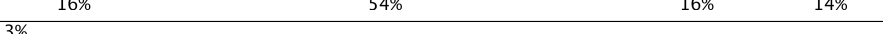
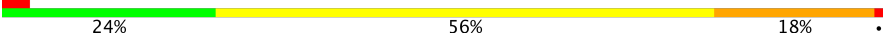
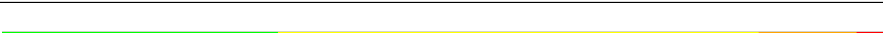
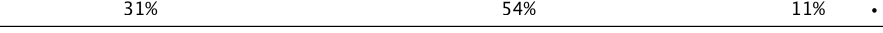
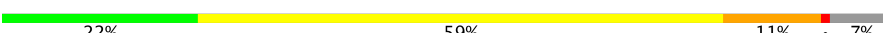
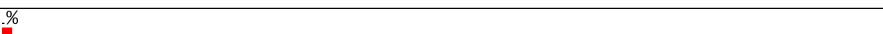
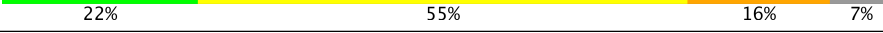
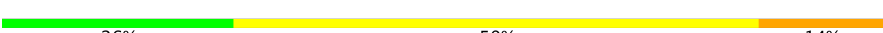
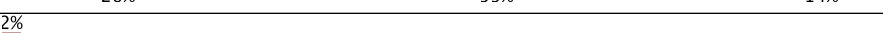
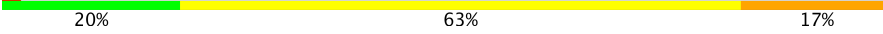

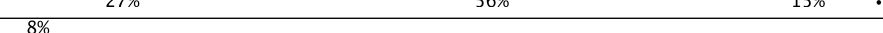
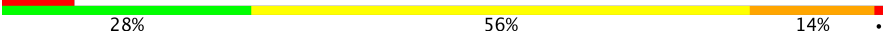

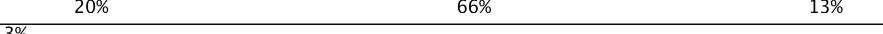


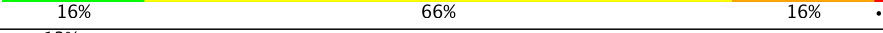
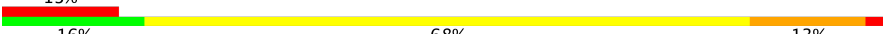



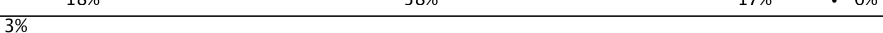
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1135 (3.56-3.36)
Clashscore	112137	1040 (3.52-3.40)
Ramachandran outliers	110173	1009 (3.52-3.40)
Sidechain outliers	110143	1010 (3.52-3.40)
RSRZ outliers	101464	1017 (3.54-3.38)
RNA backbone	2435	1020 (4.02-2.86)

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. 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	1508	<div> <div>2%</div> <div>22% 62% 13%</div> <div>..</div> </div>
1	CA	1508	<div> <div>2%</div> <div>20% 63% 14%</div> <div>..</div> </div>
2	AB	256	<div> <div>4%</div> <div>13% 61% 16% 8%</div> <div>.</div> </div>
2	CB	256	<div> <div>7%</div> <div>17% 58% 14% 8%</div> <div>.</div> </div>


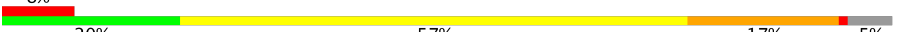

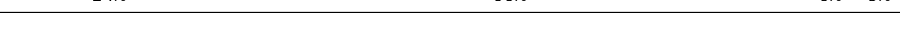
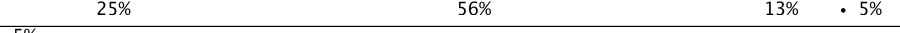
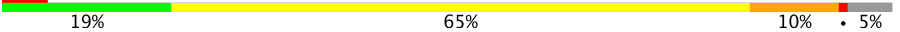
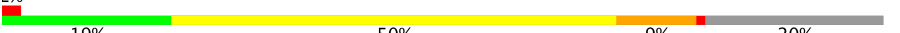

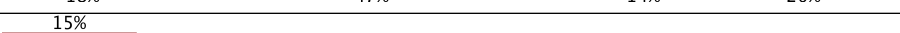
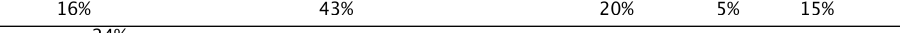
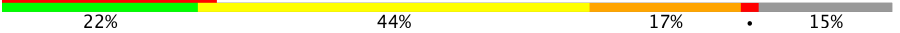
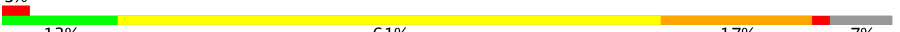

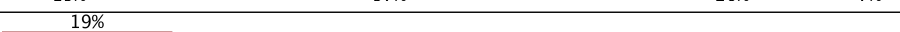
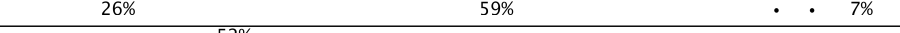




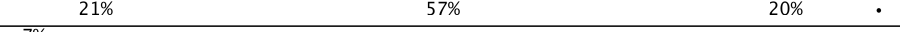
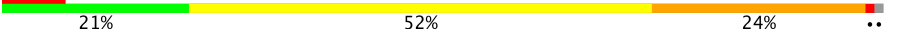
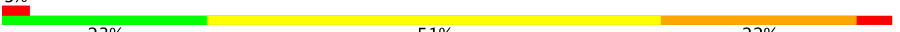

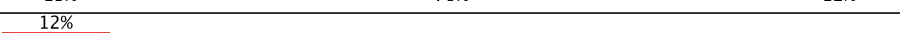

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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	30	
22	CV	30	
23	AW	75	
23	CW	75	
24	AX	77	
25	AY	75	
25	CY	75	
26	AZ	6	
26	CZ	6	
27	BA	2915	
27	DA	2915	
28	BB	122	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	DB	122	
29	BC	229	
29	DC	229	
30	BD	276	
30	DD	276	
31	BE	206	
31	DE	206	
32	BF	210	
32	DF	210	
33	BG	182	
33	DG	182	
34	BH	180	
34	DH	180	
35	BI	148	
35	DI	148	
36	BN	140	
36	DN	140	
37	BO	122	
37	DO	122	
38	BP	150	
38	DP	150	
39	BQ	141	
39	DQ	141	
40	BR	118	
40	DR	118	

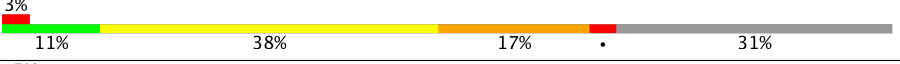
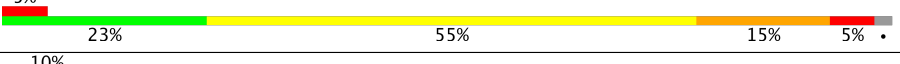
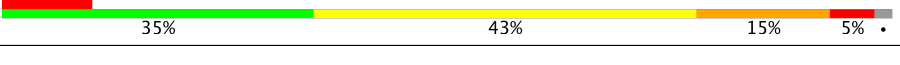

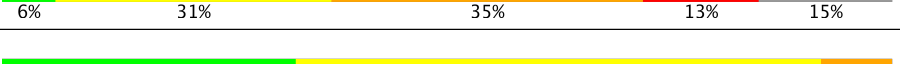
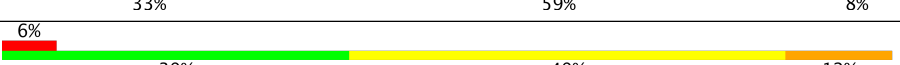
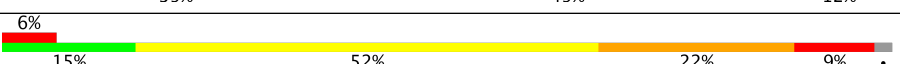
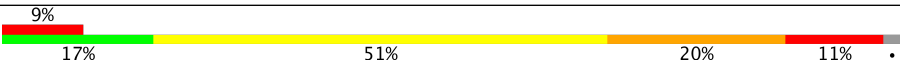

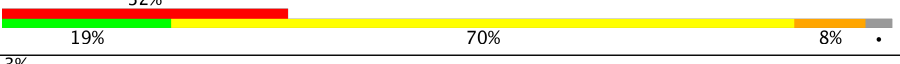
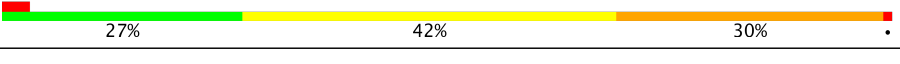

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	BS	112	
41	DS	112	
42	BT	146	
42	DT	146	
43	BU	118	
43	DU	118	
44	BV	101	
44	DV	101	
45	BW	113	
45	DW	113	
46	BX	96	
46	DX	96	
47	BY	110	
47	DY	110	
48	BZ	206	
48	DZ	206	
49	B0	85	
49	D0	85	
50	B1	98	
50	D1	98	
51	B2	72	
51	D2	72	
52	B3	60	
52	D3	60	
53	B4	71	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	D4	71	
54	B5	60	
54	D5	60	
55	B6	54	
55	D6	54	
56	B7	49	
56	D7	49	
57	B8	65	
57	D8	65	
58	B9	37	
58	D9	37	
59	CX	77	

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
26	DPP	AZ	2	-	-	X	-
26	KBE	CZ	1	-	-	X	-
26	DPP	CZ	2	-	-	X	-
60	MG	AA	1615	-	-	-	X
60	MG	AA	1617	-	-	-	X
60	MG	AA	1618	-	-	-	X
60	MG	AA	1621	-	-	-	X
60	MG	AA	1633	-	-	-	X
60	MG	AA	1637	-	-	-	X
60	MG	AA	1640	-	-	-	X
60	MG	AA	1642	-	-	-	X
60	MG	AA	1643	-	-	-	X
60	MG	AA	1646	-	-	-	X
60	MG	AA	1654	-	-	-	X
60	MG	AA	1655	-	-	-	X
60	MG	AA	1675	-	-	-	X
60	MG	BA	3004	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	3005	-	-	-	X
60	MG	BA	3009	-	-	-	X
60	MG	BA	3010	-	-	-	X
60	MG	BA	3013	-	-	-	X
60	MG	BA	3016	-	-	-	X
60	MG	BA	3017	-	-	-	X
60	MG	BA	3018	-	-	-	X
60	MG	BA	3020	-	-	-	X
60	MG	BA	3021	-	-	-	X
60	MG	BA	3027	-	-	-	X
60	MG	BA	3029	-	-	-	X
60	MG	BA	3030	-	-	-	X
60	MG	BA	3031	-	-	-	X
60	MG	BA	3034	-	-	-	X
60	MG	BA	3037	-	-	-	X
60	MG	BA	3042	-	-	-	X
60	MG	BA	3044	-	-	-	X
60	MG	BA	3046	-	-	-	X
60	MG	BA	3049	-	-	-	X
60	MG	BA	3055	-	-	-	X
60	MG	BA	3062	-	-	-	X
60	MG	BA	3070	-	-	-	X
60	MG	BA	3076	-	-	-	X
60	MG	BA	3077	-	-	-	X
60	MG	BA	3078	-	-	-	X
60	MG	BA	3080	-	-	-	X
60	MG	BA	3082	-	-	-	X
60	MG	BA	3083	-	-	-	X
60	MG	BA	3094	-	-	-	X
60	MG	BA	3104	-	-	-	X
60	MG	BA	3108	-	-	-	X
60	MG	BA	3117	-	-	-	X
60	MG	BA	3119	-	-	-	X
60	MG	BA	3121	-	-	-	X
60	MG	BA	3131	-	-	-	X
60	MG	BA	3133	-	-	-	X
60	MG	BA	3134	-	-	-	X
60	MG	BA	3137	-	-	-	X
60	MG	BA	3141	-	-	-	X
60	MG	BA	3142	-	-	-	X
60	MG	BA	3143	-	-	-	X
60	MG	BA	3149	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	3156	-	-	-	X
60	MG	BA	3158	-	-	-	X
60	MG	BA	3162	-	-	-	X
60	MG	BA	3167	-	-	-	X
60	MG	BA	3169	-	-	-	X
60	MG	BA	3177	-	-	-	X
60	MG	BA	3178	-	-	-	X
60	MG	BA	3179	-	-	-	X
60	MG	BA	3227	-	-	-	X
60	MG	BA	3229	-	-	-	X
60	MG	BA	3232	-	-	-	X
60	MG	BA	3234	-	-	-	X
60	MG	BA	3251	-	-	-	X
60	MG	BA	3284	-	-	-	X
60	MG	BA	3293	-	-	-	X
60	MG	BA	3306	-	-	-	X
60	MG	BU	201	-	-	-	X
60	MG	CA	1610	-	-	-	X
60	MG	CA	1612	-	-	-	X
60	MG	CA	1614	-	-	-	X
60	MG	CA	1620	-	-	-	X
60	MG	CA	1622	-	-	-	X
60	MG	CA	1635	-	-	-	X
60	MG	CA	1650	-	-	-	X
60	MG	CA	1657	-	-	-	X
60	MG	CA	1673	-	-	-	X
60	MG	CA	1677	-	-	-	X
60	MG	CA	1682	-	-	-	X
60	MG	CA	1683	-	-	-	X
60	MG	CA	1686	-	-	-	X
60	MG	CA	1692	-	-	-	X
60	MG	DA	3005	-	-	-	X
60	MG	DA	3006	-	-	-	X
60	MG	DA	3008	-	-	-	X
60	MG	DA	3014	-	-	-	X
60	MG	DA	3040	-	-	-	X
60	MG	DA	3042	-	-	-	X
60	MG	DA	3061	-	-	-	X
60	MG	DA	3065	-	-	-	X
60	MG	DA	3073	-	-	-	X
60	MG	DA	3075	-	-	-	X
60	MG	DA	3078	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DA	3084	-	-	-	X
60	MG	DA	3092	-	-	-	X
60	MG	DA	3096	-	-	-	X
60	MG	DA	3102	-	-	-	X
60	MG	DA	3111	-	-	-	X
60	MG	DA	3117	-	-	-	X
60	MG	DA	3118	-	-	-	X
60	MG	DA	3120	-	-	-	X
60	MG	DA	3128	-	-	-	X
60	MG	DA	3139	-	-	-	X
60	MG	DA	3146	-	-	-	X
60	MG	DA	3160	-	-	-	X
60	MG	DA	3167	-	-	-	X
60	MG	DA	3169	-	-	-	X
60	MG	DA	3173	-	-	-	X
60	MG	DA	3174	-	-	-	X
60	MG	DA	3180	-	-	-	X
60	MG	DA	3186	-	-	-	X
60	MG	DA	3193	-	-	-	X
60	MG	DA	3195	-	-	-	X
60	MG	DA	3205	-	-	-	X
60	MG	DA	3206	-	-	-	X
60	MG	DA	3215	-	-	-	X
60	MG	DA	3236	-	-	-	X
60	MG	DA	3237	-	-	-	X
60	MG	DF	301	-	-	-	X
60	MG	DO	201	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 293848 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
			32132	14303	5953	10382	1494			
1	CA	1493	Total	C	N	O	P	0	0	0
			32098	14287	5956	10363	1492			

- 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	206	Total	C	N	O	S	0	0	1
			1604	1011	314	278	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	154	Total	C	N	O	S	0	0	0
			1249	776	251	217	5			

- 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
			1006	637	195	174			
9	CI	127	Total	C	N	O	0	0	0
			1006	637	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			

Continued on next page...

Continued from previous page...

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	116	Total	C	N	O	S	0	0	0
			864	537	164	160	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	122	Total	C	N	O	S	0	0	1
			965	597	200	166	2			
13	CM	118	Total	C	N	O	S	0	0	0
			937	579	193	163	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	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	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 RNA chain called RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0	0
			205	93	40	63	9			
22	CV	10	Total	C	N	O	P	0	0	0
			213	97	42	65	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	0	0	0
			1573	702	279	518	74			
23	CW	74	Total	C	N	O	P	0	0	0
			1573	702	279	518	74			

- Molecule 24 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	77	Total	C	N	O	P	0	0	0
			1639	732	297	534	76			

- Molecule 25 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			
25	CY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	33	G	C	CONFLICT	GB CP001790.1
AY	44	U	A	CONFLICT	GB CP001790.1
CY	33	G	C	CONFLICT	GB CP001790.1
CY	44	U	A	CONFLICT	GB CP001790.1

- Molecule 26 is a protein called capreomycin IA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	AZ	6	Total	C	N	O	0	0	0
			47	25	14	8			
26	CZ	6	Total	C	N	O	0	0	0
			47	25	14	8			

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BA	2789	Total	C	N	O	P	0	0	0
			60072	26734	11238	19312	2788			
27	DA	2775	Total	C	N	O	P	0	0	0
			59767	26598	11176	19219	2774			

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 29 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	BC	191	Total	C	N	O	0	0	1
			1142	691	221	230			
29	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 30 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
30	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 31 is a protein called 50S ribosomal protein L3.

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BF	206	Total	C	N	O	S	0	0	1
			1607	1024	301	280	2			
32	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BH	161	Total	C	N	O	S	0	0	0
			1233	783	227	222	1			
34	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
35	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

Continued on next page...

Continued from previous page...

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

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

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
38	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			
39	DQ	138	Total	C	N	O	S	0	0	0
			1094	697	205	185	7			

- Molecule 40 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
40	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	BS	99	Total	C	N	O	0	0	1
			771	486	155	130			
41	DS	99	Total	C	N	O	0	0	1
			771	486	155	130			

- Molecule 42 is a protein called 50S ribosomal protein L19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
46	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	88	Total	C	N	O	S	0	0	1
			672	432	131	105	4			
47	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 48 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			
48	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
49	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
50	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 51 is a protein called 50S ribosomal protein L29.

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

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B4	49	Total	C	N	O	S	0	0	1
			344	215	60	65	4			
53	D4	49	Total	C	N	O	S	0	0	1
			344	215	60	65	4			

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
54	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B6	48	Total	C	N	O	S	0	0	1
			402	249	83	66	4			
55	D6	46	Total	C	N	O	S	0	0	1
			390	241	80	65	4			

- Molecule 56 is a protein called 50S ribosomal protein L34.

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

- Molecule 57 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
57	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 58 is a protein called 50S ribosomal protein L36.

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

- Molecule 59 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	CX	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CX	46	G	A	CONFLICT	GB CP001637.1

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BA	334	Total	Mg	0	0
			334	334		
60	CA	102	Total	Mg	0	0
			102	102		
60	DF	1	Total	Mg	0	0
			1	1		
60	CV	1	Total	Mg	0	0
			1	1		
60	BE	3	Total	Mg	0	0
			3	3		
60	AW	4	Total	Mg	0	0
			4	4		
60	BP	2	Total	Mg	0	0
			2	2		
60	AX	9	Total	Mg	0	0
			9	9		
60	B5	1	Total	Mg	0	0
			1	1		
60	BB	5	Total	Mg	0	0
			5	5		
60	DO	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BF	1	Total 1	Mg 1	0	0
60	BX	1	Total 1	Mg 1	0	0
60	CK	1	Total 1	Mg 1	0	0
60	D7	1	Total 1	Mg 1	0	0
60	BU	2	Total 2	Mg 2	0	0
60	AA	114	Total 114	Mg 114	0	0
60	DD	2	Total 2	Mg 2	0	0
60	D0	1	Total 1	Mg 1	0	0
60	BG	1	Total 1	Mg 1	0	0
60	BR	1	Total 1	Mg 1	0	0
60	DA	239	Total 239	Mg 239	0	0
60	AG	1	Total 1	Mg 1	0	0
60	DE	1	Total 1	Mg 1	0	0
60	CW	4	Total 4	Mg 4	0	0
60	D5	1	Total 1	Mg 1	0	0
60	BD	1	Total 1	Mg 1	0	0
60	B0	3	Total 3	Mg 3	0	0
60	CE	1	Total 1	Mg 1	0	0
60	DB	3	Total 3	Mg 3	0	0

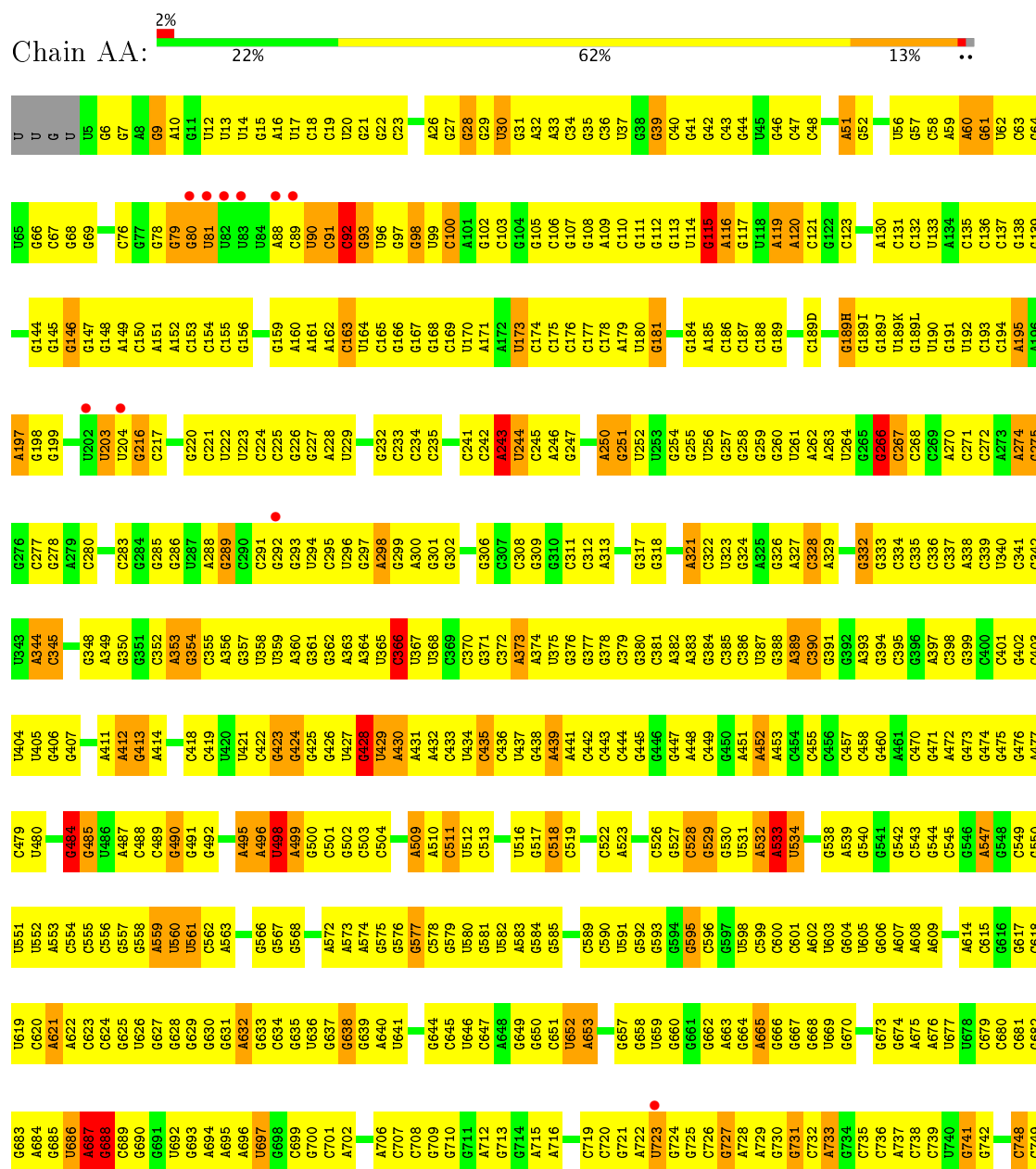
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	B5	1	Total 1	Zn 1	0	0
61	B4	1	Total 1	Zn 1	0	0
61	AD	1	Total 1	Zn 1	0	0
61	B9	1	Total 1	Zn 1	0	0
61	D9	1	Total 1	Zn 1	0	0
61	D5	1	Total 1	Zn 1	0	0
61	D4	1	Total 1	Zn 1	0	0
61	CD	1	Total 1	Zn 1	0	0

3 Residue-property plots

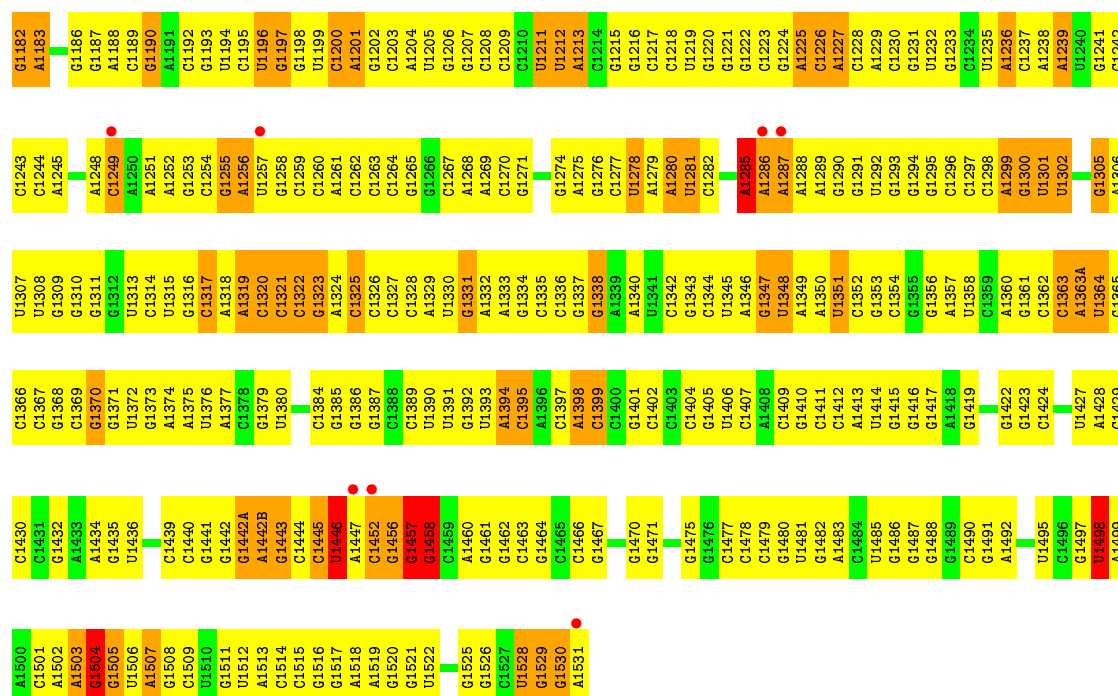
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

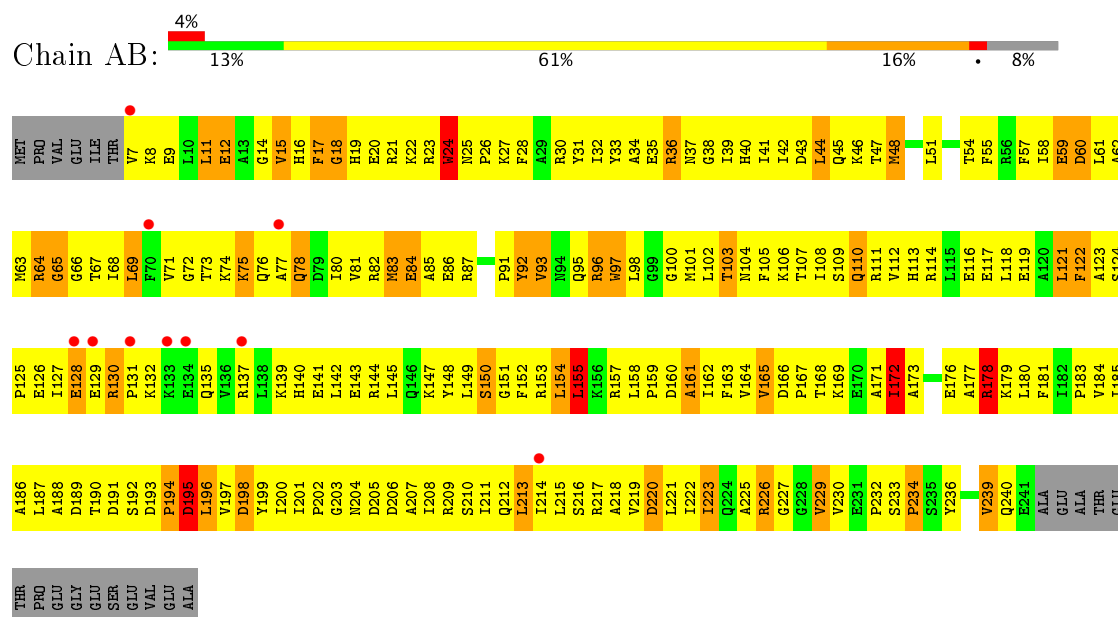




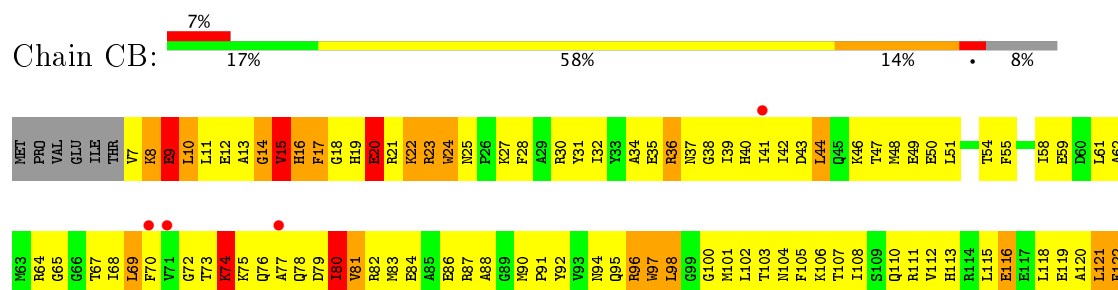


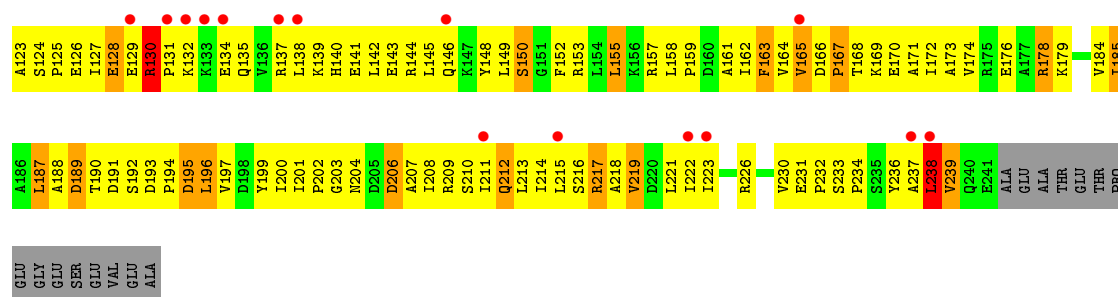


• Molecule 2: 30S ribosomal protein S2



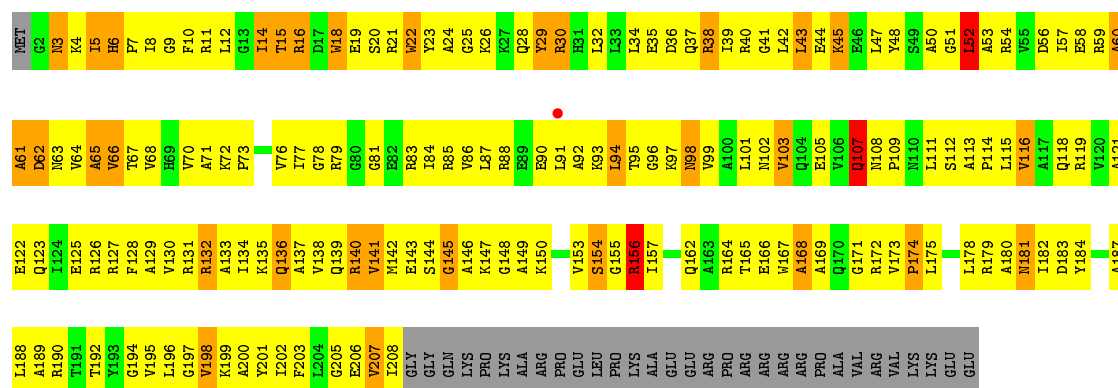
• Molecule 2: 30S ribosomal protein S2





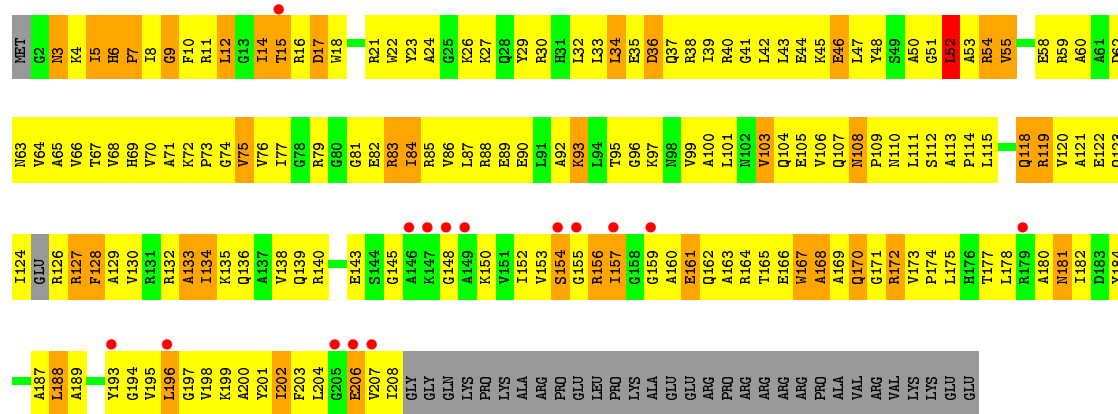
• Molecule 3: 30S ribosomal protein S3

Chain AC: 15% 56% 14% 13%



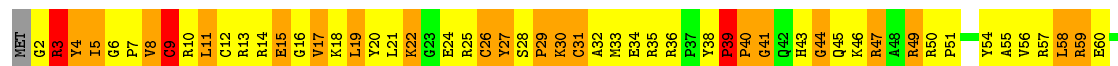
• Molecule 3: 30S ribosomal protein S3

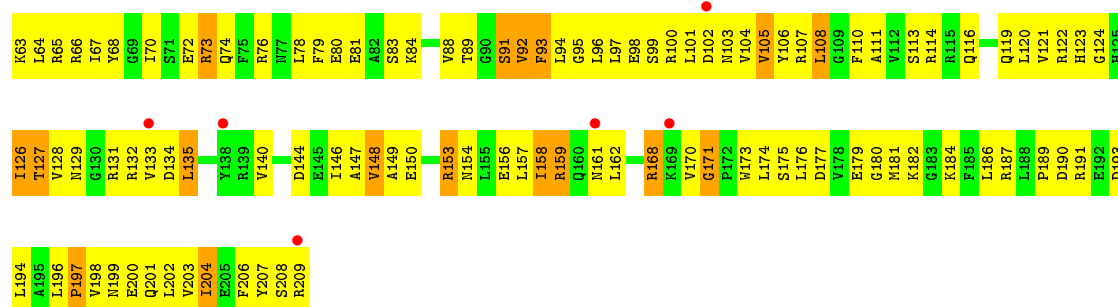
Chain CC: 6% 16% 54% 16% 14%



• Molecule 4: 30S ribosomal protein S4

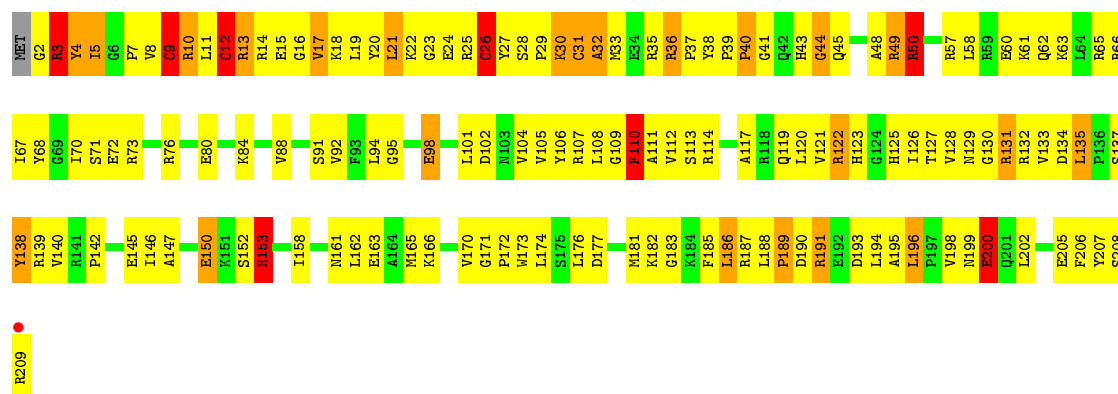
Chain AD: 3% 24% 56% 18%





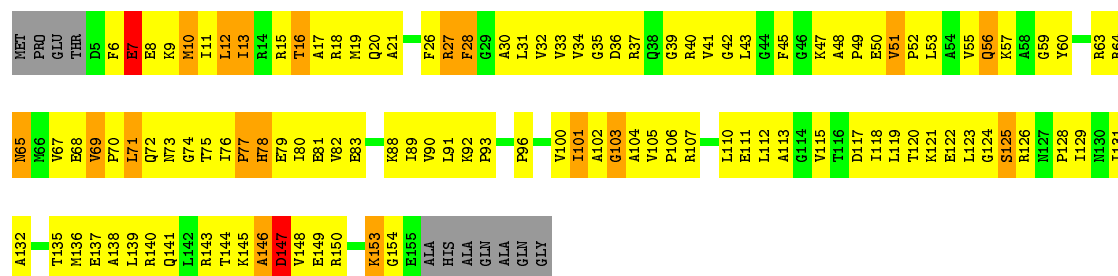
• Molecule 4: 30S ribosomal protein S4

Chain CD: 31% 54% 11% .



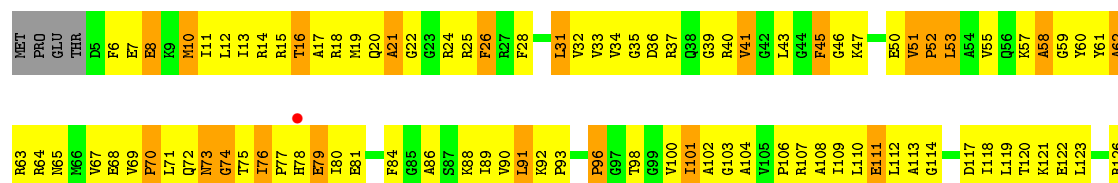
• Molecule 5: 30S ribosomal protein S5

Chain AE: 22% 59% 11% 7% .

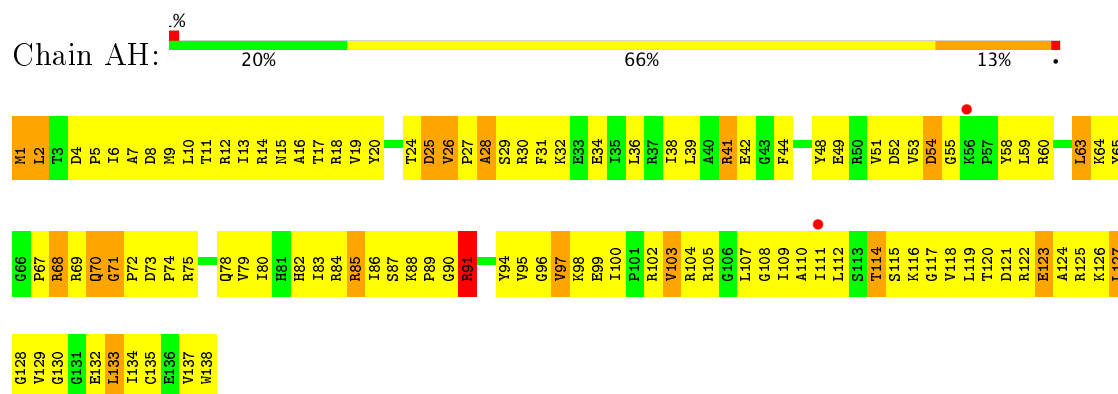


• Molecule 5: 30S ribosomal protein S5

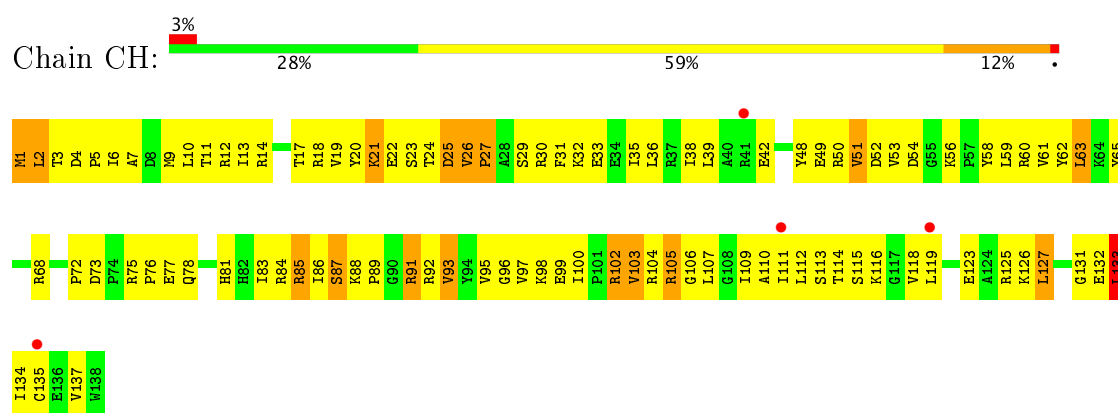
Chain CE: 22% 55% 16% 7% .



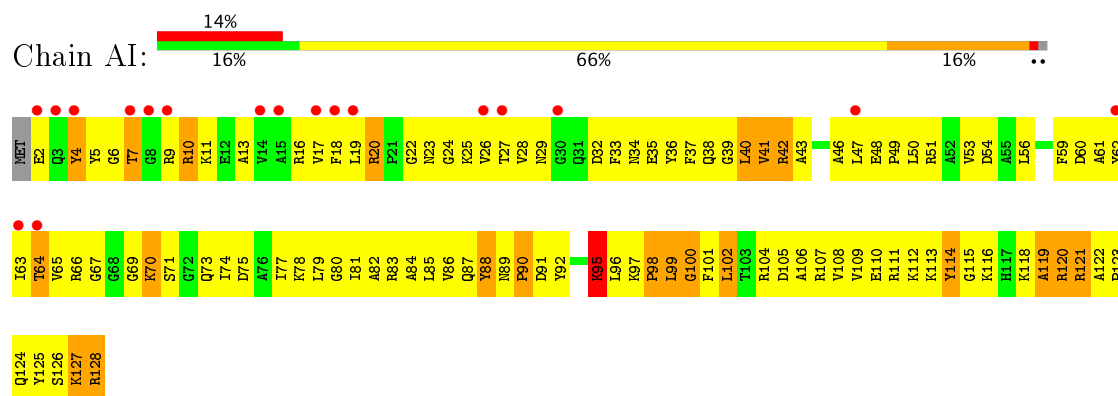
- Molecule 8: 30S ribosomal protein S8



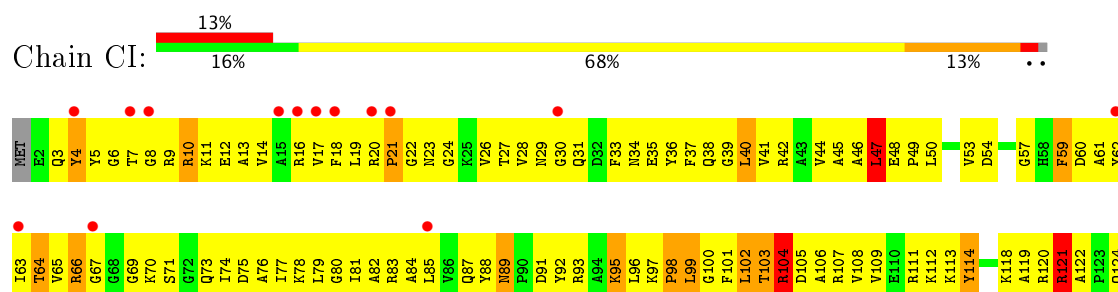
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9

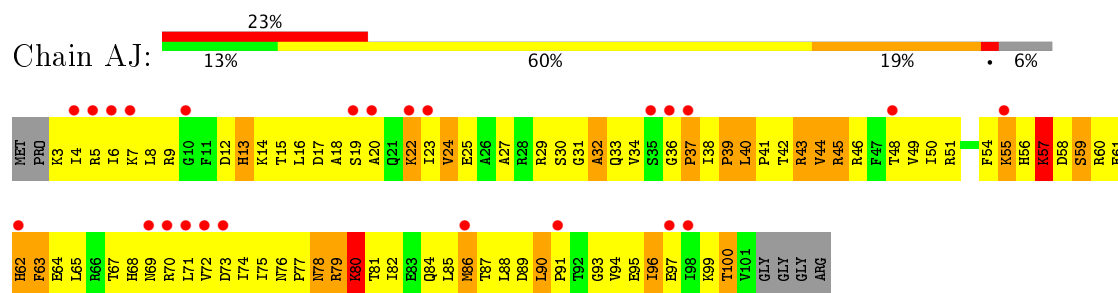


- Molecule 9: 30S ribosomal protein S9

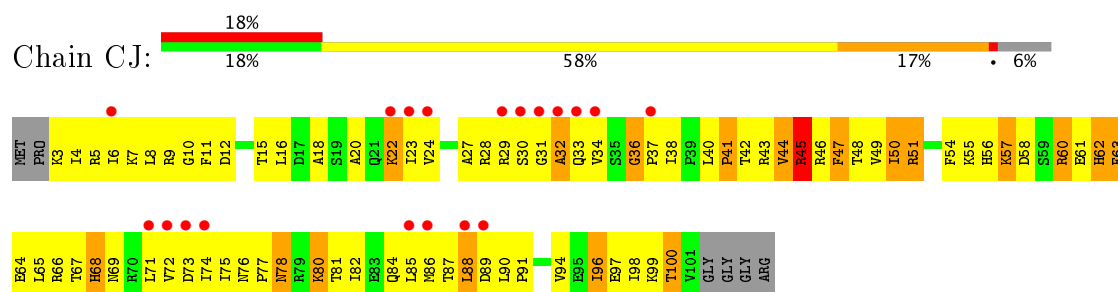




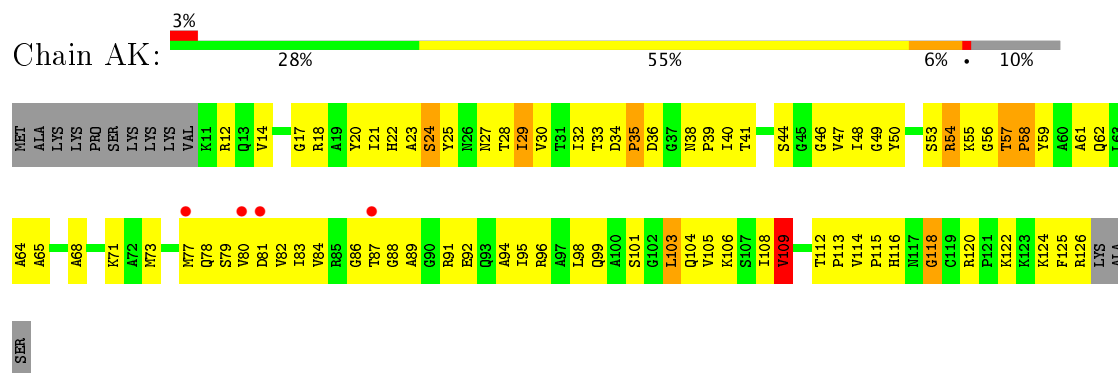
• Molecule 10: 30S ribosomal protein S10



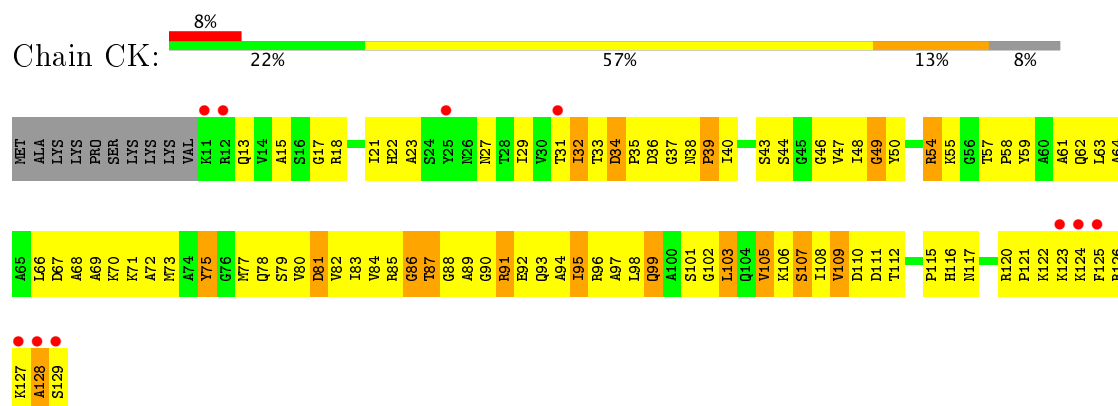
• Molecule 10: 30S ribosomal protein S10



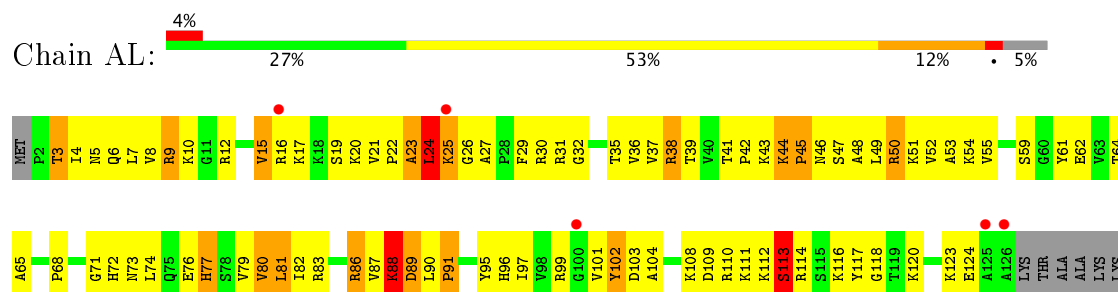
• Molecule 11: 30S ribosomal protein S11



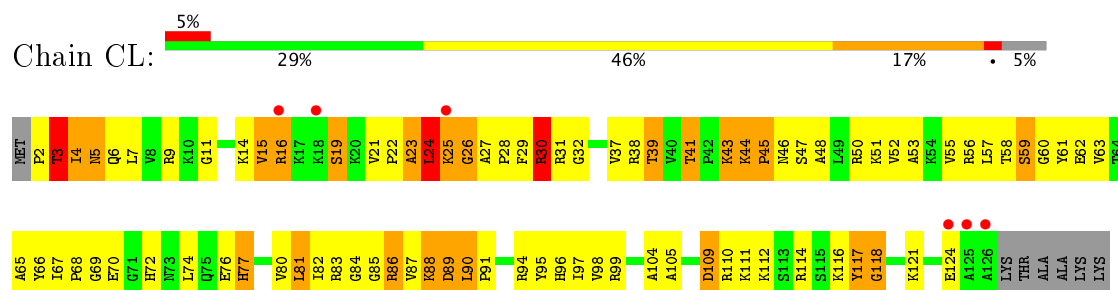
• Molecule 11: 30S ribosomal protein S11



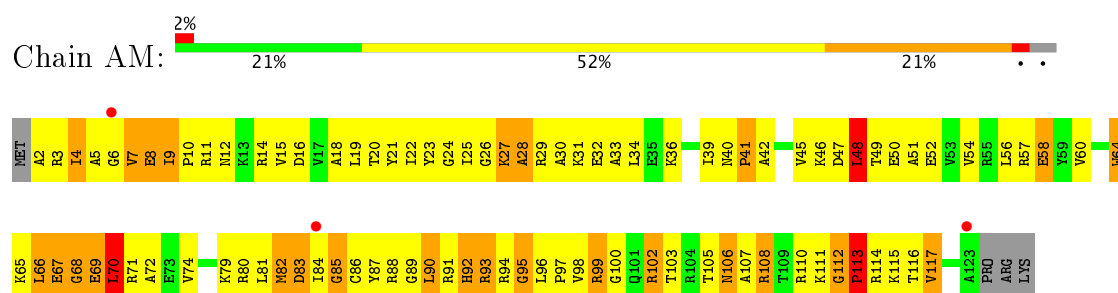
- Molecule 12: 30S ribosomal protein S12



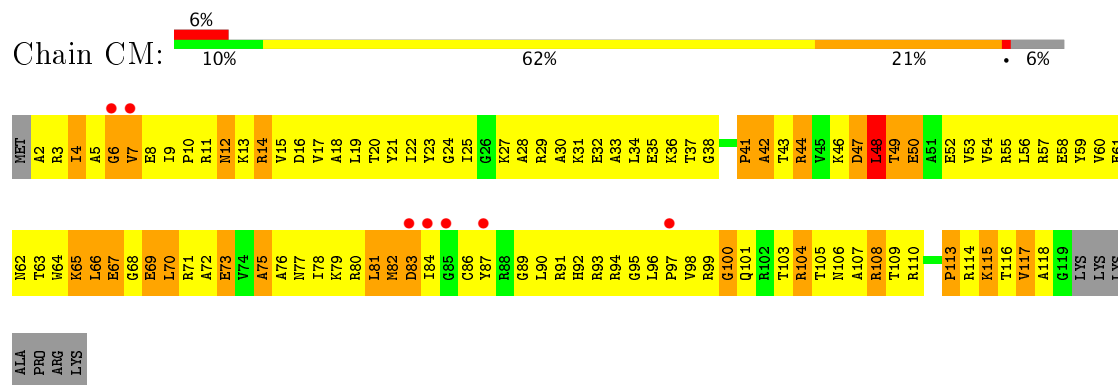
- Molecule 12: 30S ribosomal protein S12



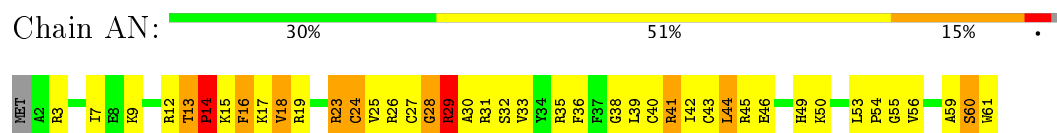
- Molecule 13: 30S ribosomal protein S13



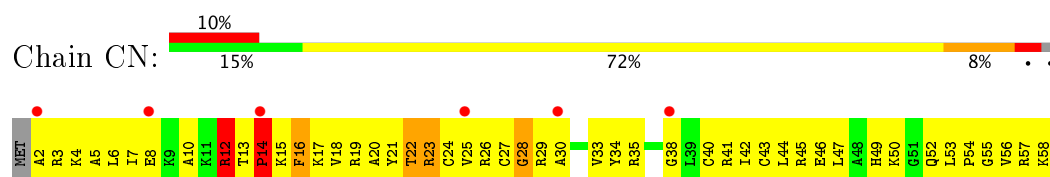
- Molecule 13: 30S ribosomal protein S13



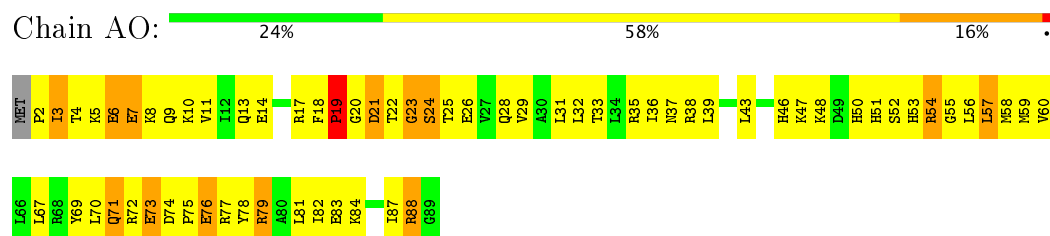
- Molecule 14: 30S ribosomal protein S14



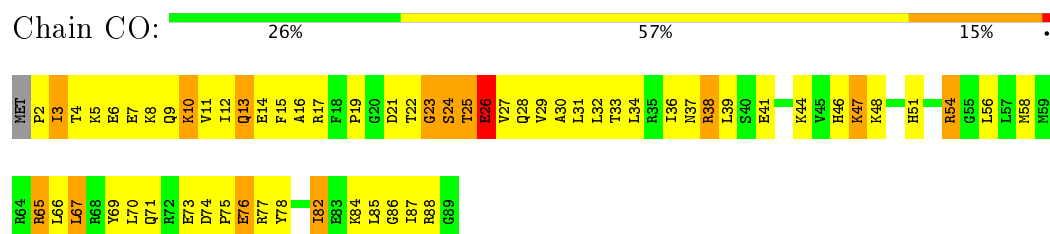
- Molecule 14: 30S ribosomal protein S14



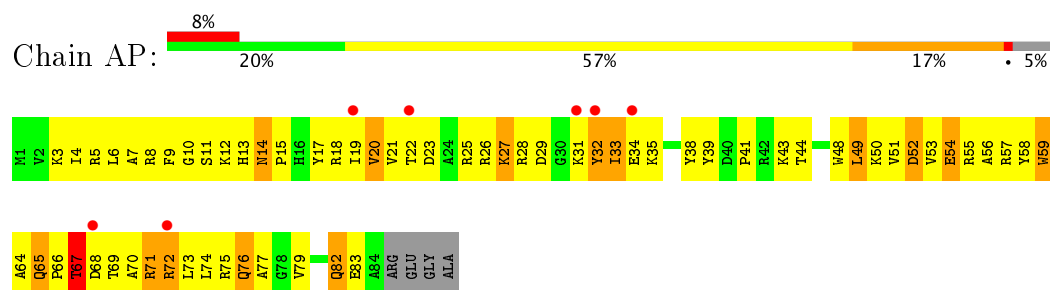
- Molecule 15: 30S ribosomal protein S15



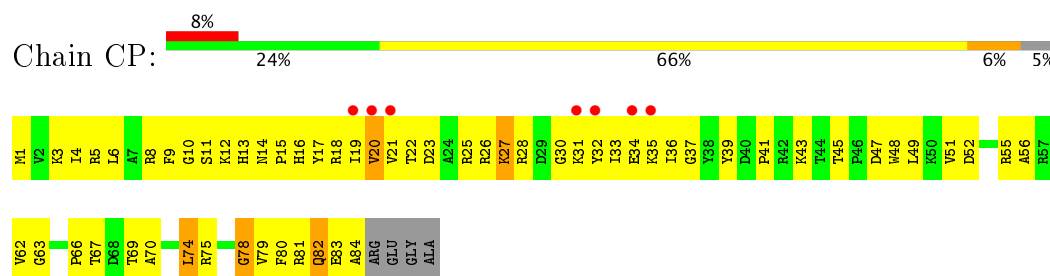
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

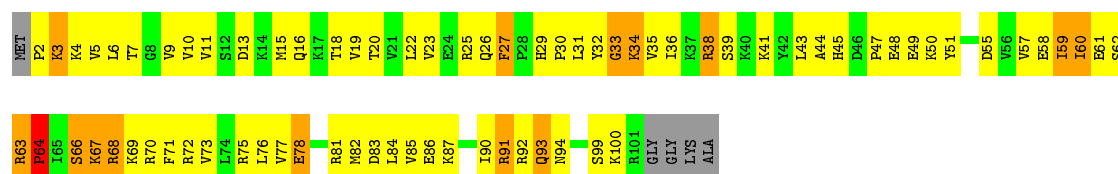


- Molecule 16: 30S ribosomal protein S16

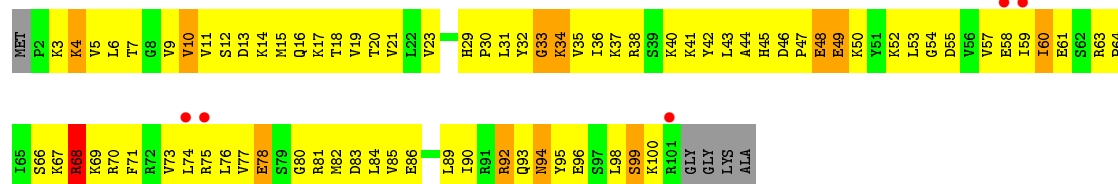


- Molecule 17: 30S ribosomal protein S17

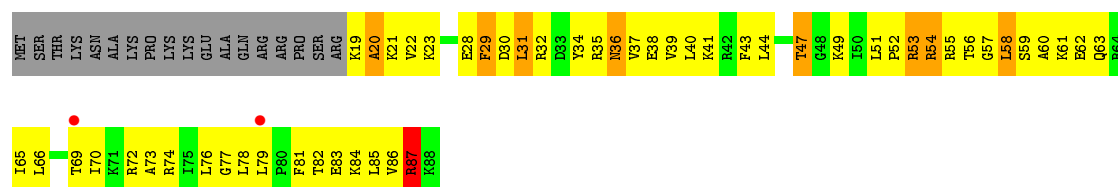
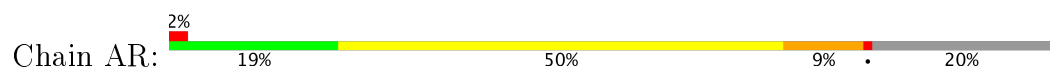




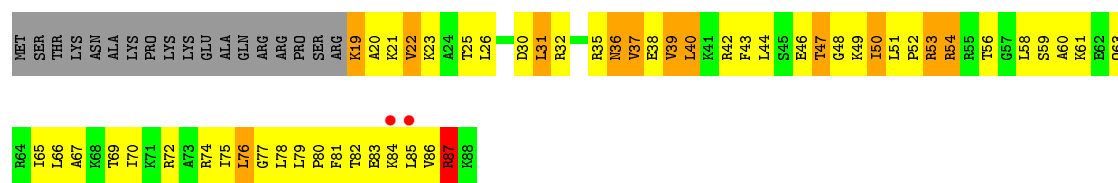
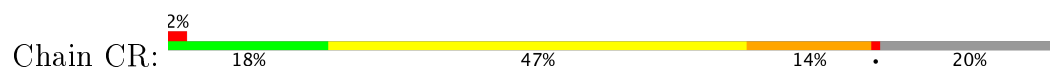
• Molecule 17: 30S ribosomal protein S17



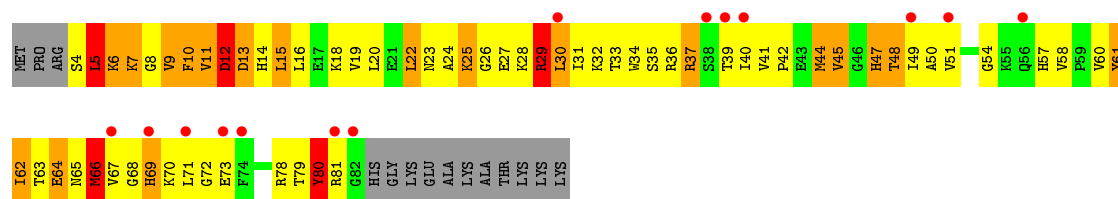
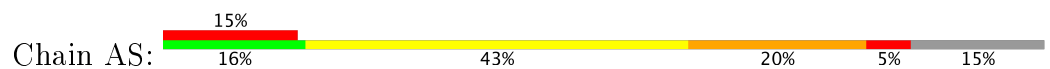
• Molecule 18: 30S ribosomal protein S18



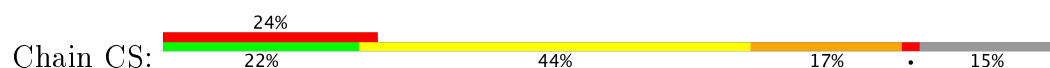
• Molecule 18: 30S ribosomal protein S18

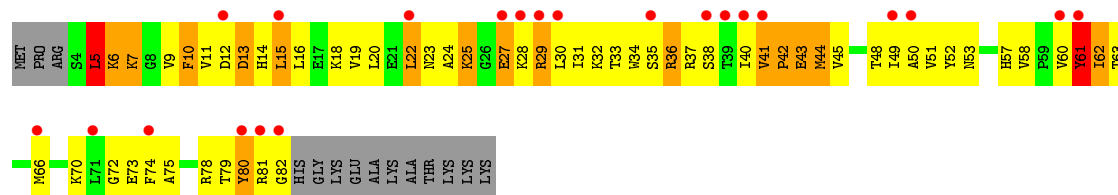


• Molecule 19: 30S ribosomal protein S19

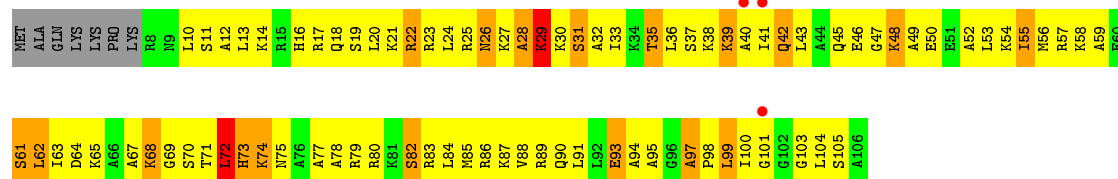
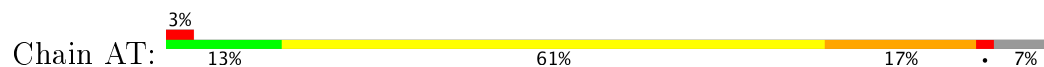


• Molecule 19: 30S ribosomal protein S19

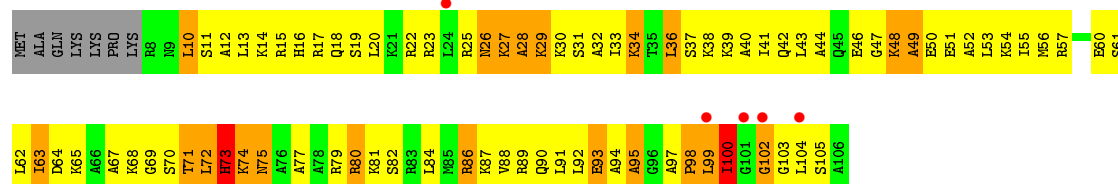
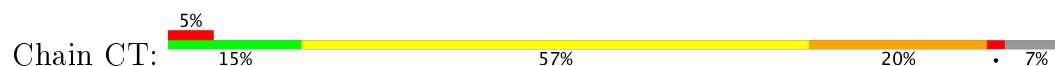




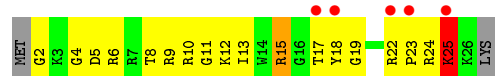
- Molecule 20: 30S ribosomal protein S20



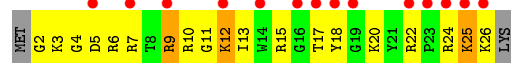
- Molecule 20: 30S ribosomal protein S20



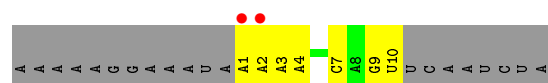
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx

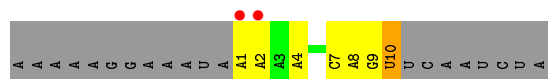


- Molecule 22: RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3')



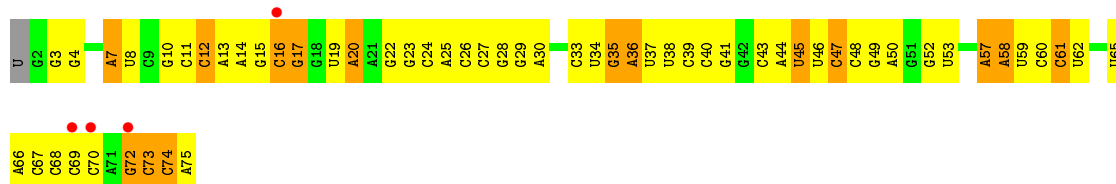
- Molecule 22: RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3')

Chain CV: 7% 10% 20% 67%



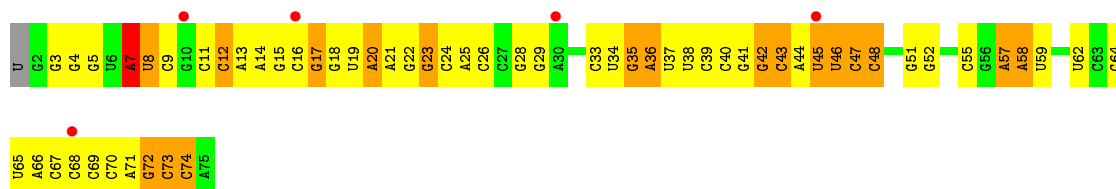
- Molecule 23: tRNA-Gln

Chain AW: 5% 21% 57% 20%



- Molecule 23: tRNA-Gln

Chain CW: 7% 21% 52% 24%



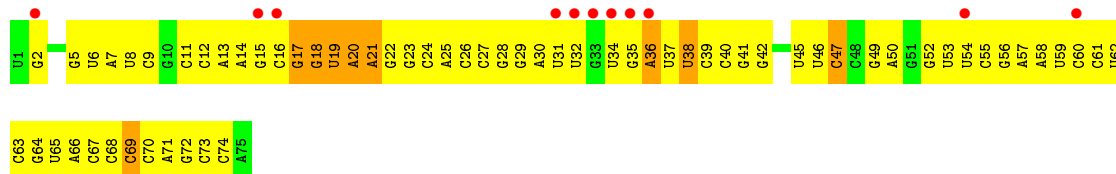
- Molecule 24: tRNA-Met

Chain AX: 3% 23% 51% 22%

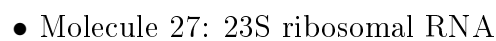
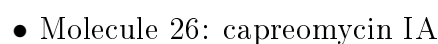
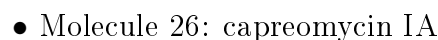


- Molecule 25: tRNA-Gln

Chain AY: 15% 13% 75% 12%

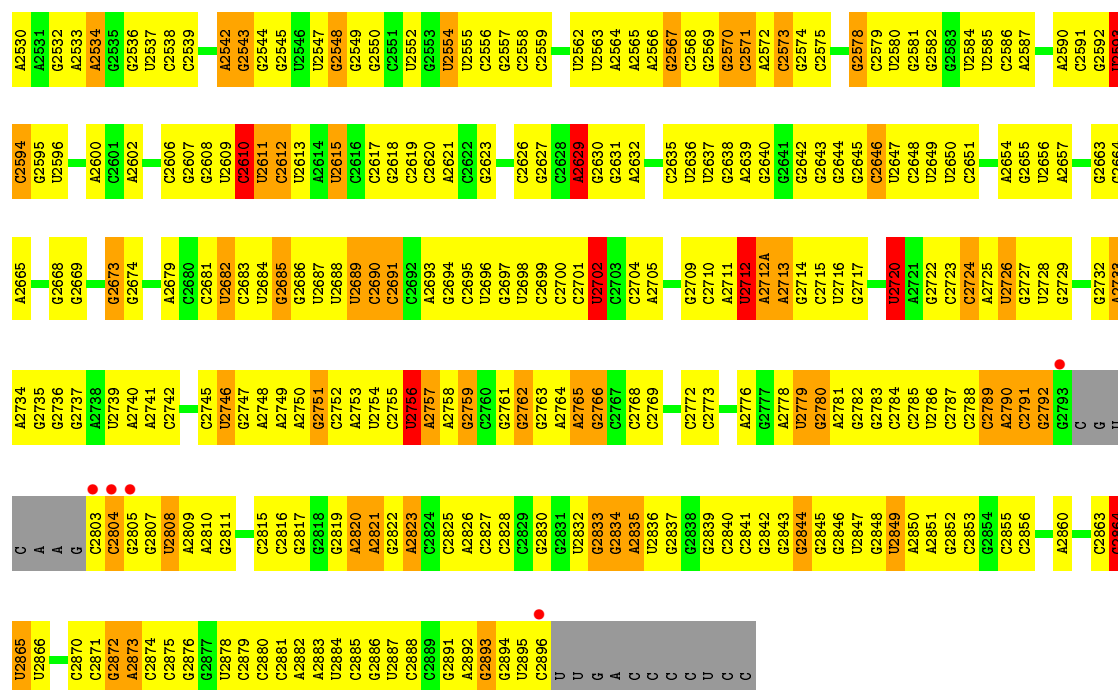


- Molecule 25: tRNA-Gln

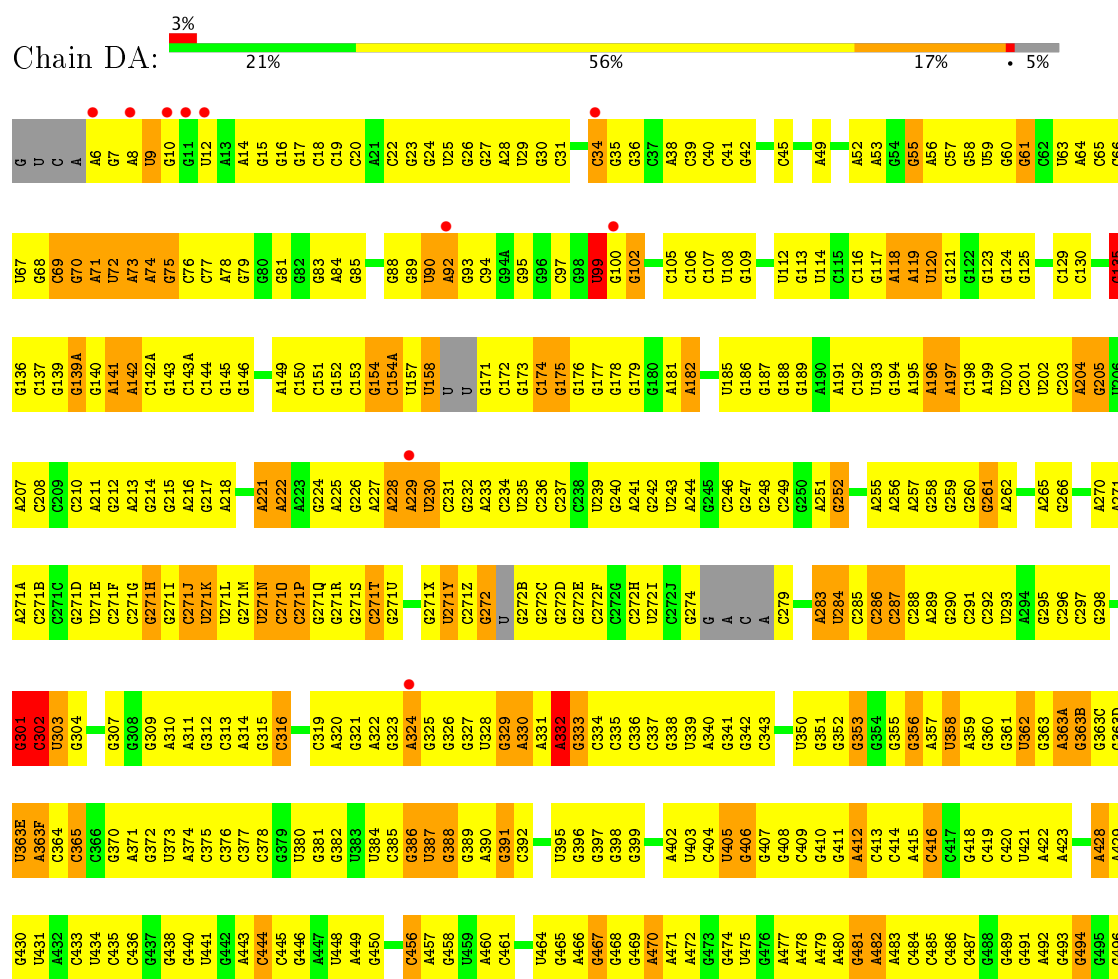


G1437	G1368	U1300	G1221	G1154	G	A1029	U963	A900	G836	C771	G696	A	G592	C523
U1438	G1369	A1301	C1221A	A1155	C	G1030	C964	A901	C837	C772	C697	G	G593	U524
A1439	C1370	A1302	G1222	A1156	U	U1033	C965	C902	C838	U773	C698	C	G594	U525
G1440	G1223	G1303	G1223	G1161	A	U1034	U969	C903	U839	A774	A699	G	U597	
G1441	C1224	C1304	G1224	G1162	A	U1035	C970	C904	C840	G775	G700	G	G598	A528
G1442	G1225	C1305	G1225	G1163	A	G1036	C971	U905	G842	G776		G	G601	A529
G1443		A1306		G1164	U		G972	G906	G843	A777	G704	C	G602	G530
G1444		A1307		U1165	G	G1039	A973	U907	G844	G778	A705	C	G603	C531
A1445	G1376	A1308	G1231	U1166	C	G1040	G974	C908	C944	U779	A706	C	A602	A532
C1446A	A1378	G1309	G1238	U1167	U	C1041	C975	A909	C945	G780	G707	C	A603	G533
C1446	A1379	G1310	G1239	U1168	C	G1042	G976A	A911	C946	A781	C708	C	C604	U534
G1447	G1380	G1311	U1239	G1169	C	C1043	G977	C912	U847	A782	U709	C	C605	G535
G1448	G1381	U1312	U1240	G1170	A	G1044	G978	G913	G848	A783	G710	G	U606	C536
A1449		U1313	A1241	G1171	C	A1045	G978	U914	A849	A784	G711	C	U607	A536
G1450	A1384	C1314	G1245	G	U	A1046	G978	C915	C850	G785	G712	G	G610	C537
C1450A	G1385		G1246	A	G	A1047	A983	C916	C851	C786	G713	G	G611	C541
C1451	C1386	A1247	A1246	U	U1108	A1048	A984	G916	C852	U787	G714	C	C612	C542
A1452	C1387	A1248	A1248	G	C1109	C1049	A985	A917	G853	A788		C	G613	C543
U1453	G1388	G1249		A	G1110	A1050	C986		G854	A789	C719	C	U614	G
U1455	U1389	U1250		C1178	A1111	G1051	C987	U921	G855	C790	C720	G	U614A	C
	U1390	G1251		C1179	U1112	C1052	A988	U922	C856	C791	C721	C	G614B	A
	U1391	G1252		C1180	U1113	C1053	G989	C923	C857	A792	G722	A	A614C	A
		A1253		C1181	G1114	A1054	A990	C925	U858	A793	G723	A	G549	
G1459	U1394	U1326	G1256	G1184	G1115	G1055	C991	A926	G859	G794	U724	A	G616	G551
G1461	C1327	C1327	G1257	G1185	C1116	G	C992	A927	U860	G795	G725		C618	
C1463	U1396	G1328	C1257	G1186	G1117	A	C993	G927	A861	C796	G726	U857	G619	U554
G1464		U1329	C1258	G1187	G1118	G	C994	G928	G862	C797	A727	C858	G620	U555
G1465	C1403	C1330	G1259	G1188	G1119	A	G995	U930	A863	G798	G728	C859	A621	G556
G1466	G1404	A1331	G1260	U1189	G1120	U	A996	G931	G864	G799	G729	C860	G622	U557
G1467	U1405	G1332	C1261	G1190	G1121	U	G997	G932	C865	A800	C730	C861	G623	G558
C1468	U1406	C1333	C1262	G1191	C1122	G	C998	G934	A866	G801		G663	G624	G559
A1469	C1407	U1335	A1263	G1192	G1123	G	U999	G935	G869	A802	G733	C864	G625	C560
G1470	G1408	U1336		G1193	G1124	C	A1000	C936	A870	A803		C865	G626	
A1471	G1409	G1337	C1270	G1194	G1125	U	U937	U937	U871	A804	U740	G666	A627	G563
G1472	C1411	U1338	G1271	A1194	G1126	U	G1002	G938	A872	C806	G742		G628	U566
C1473	A1412		A1272	G1195	A	A		G939	G873	U807	G743	G669	G630	A567
G1474	G1413		U1273	C1196	U1130	G	C1005	G940	G874	G808	G744	A870	A631	U568
G1475		U1342	A1274	G1197	G1131	A	C1006	A941	G875	G809		C671	A632	U569
C1476	G1416	G1343	A1275	U1198	A1132	A	C1007	G942		U810	U747	C672	A633	G570
G1478	C1417	C1344	U1276	U1199	G1133	A		U943	G879	U811	G748	C673	C634	A571
G1479	G1418	G1345	G1277	C1200	U1135	C	A1010	U944	G880	U812	C749	C674	C635	A572
A1480	U1419	G1346	G1278	C1201	G1136	A	G1011	A945	G881	U813		A675	G636	G573
G1481	U1420	G1347	A1278	C1202	G1137	G	U1012	G946	G882	C814	A752	A676	A637	C574
G1482	G1421	G1348	G1279	G1203	G1138	C	C1013	G947	G883	C815	C753	A677	G638	A575
G1484	G1422	C1350	G1280	A1204	G1139	C	U1014	G948	C884	C816	C754	C678	U639	U576
G1485	G1423	U1281	G1281	C1205	C1140	A	G1015	G949	C885	G817	C755	C679	G640	
A1486	G1424	U1282		U1205	U1141	U	G1016	G950	C886	G818	C756	G680	C641	G579
G1487		G1283	A1286	G1208	U1142	C	G1017	C951	A887	A819	U757	G681	G642	C580
G1488	G1425	A1353	A1287	G1209	A1143	C	C1018	G952	C888				A643	C581
U1489	A1427	G1354	U1288	A1210	A1144	U	U1019	A953	C889	C825	A761	G886	A644	G582
A1490	G1428	G1355	C1289	G1211	U1145	U	A1020	A954	A890	U826	U762	C887	G645	G583
G1491	G1429		C1290	G1212	G1146	U	C955	G954	A891	U827	G763	U888	A646	U584
G1492	C1430	A1359	C1291	A1213	G1147	A	G1022	C955	G992	U828	A764	A689	G647	G585
C1493	U1431	U1292	U1292	G1214	C1147	A	A957	G956	C993	U829	G765	G690	G648	A586
A1494	U1432	C1293		G1216	A	A	G1024	U958	C994	A829	C766	C691	G649	C587
A1495	U1433			C1217	G	G	G1025	A959	A896	G831	U767	G692	G650	U588
A1496	G1434		C1297	G1218	U1150	A	U1026	A960	C997	G832		C993	G651	C589
U1497	G1435	A1365	C1298	G1219	G1152	A	A1027	A961	C998	G832	G769	U694	C652	A590
C1498	G1436		G1299	A1220	C1153	U	A1028	G962	A999	A835	G770	G695	A	C591

C2465	C2466	C2467	C2468	A2469	C2470	C2471	C2472	C2473	C2474	C2475	C2476	C2477	C2478	G2481	G2482	G2483	G2484	G2485	G2486	G2487	A2488	U2491	U2492	U2493	G2494	G2495	G2496	G2497	G2498	G2499	U2500	C2501	G2502	G2505	U2506	G2507	G2508	G2512	G2513	U2514	G2515	G2516	G2517	G2518	G2519	G2520	G2521	G2522	G2523	G2524	G2525	G2526	C2527	U2528	G2529											
C2394	C2395	C2396	C2397	G2398	G2399	G2400	U2401	C2402	C2403	C2404	G2405	U2406	G2409	G2410	G2411	G2412	G2413	G2414	G2415	G2416	G2417	G2418	U2419	U2420	G2421	A2422	U2423	G2424	G2425	A2426	G2427	G2428	G2429	A2430	A2434	A2435	G2439	G2440	G2441	G2442	G2443	G2444	U2448	U2449	A2450	A2451	C2452	A2453	U2457	G2458	A2459	G2460	C2461	U2462	C2463	C2464										
A2327	A2328	G2329	G2330	G2331	U2332	A2333	A2334	A2335	A2336	G2337	G2340	G2341	G2342	G2343	U2344	G2345	A2346	G2347	G2348	G2349	G2350	G2351	A2352	G2353	G2354	G2355	G2356	U2357	G2358	G2359	A2360	C2364	G2365	G2369	G2370	G2371	G2372	G2373	G2374	G2375	G2379	G2380	G2381	G2382	G2383	G2384	G2385	G2386	U2387	G2388	G2389	U2390	G2391	A2392	A2393											
C2261	U2262	C2263	A2266	A2267	A2268	A2269	G2270	A2271	A2272	G2273	G2274	C2275	C2276	G2277	A2278	G2279	G2280	G2281	G2282	G2283	G2284	G2285	A2286	A2287	G2288	G2289	G2290	U2291	G2292	C2295	U2296	G2297	A2298	G2299	G2300	C2301	G2302	A2305	G2306	G2307	A2308	U2309	U2310	A2311	G2312	G2313	G2314	G2315	G2316	G2317	G2318	G2319	A2320	G2325	G2326											
U2189	G2190	G2191	G2192	G2193	G2194	G2195	G2196	U2197	A2198	A2199	G2200	G2201	G2202	U2203	G2205	G2206	A2207	U2208	G2209	G2210	G2211	G2212	G2213	G2214	G2215	G2216	G2217	G2218	G2219	G2220	G2223	G2224	A2225	G2226	G2227	G2228	G2229	G2230	G2231	U2232	U2233	G2234	G2235	G2236	G2237	G2238	G2239	G2240	A2241	G2242	G2243	G2244	U2245	G2246	A2247	G2248	U2249	G2250	G2253	G2254	G2255	G2256	U2257	G2258	G2259	G2260
A2126	G2127	C2128	C2129	U2130	G2131	U2132	G2133	G2134	A2135	G2136	G2137	U2138	C2139	C2140	C2141	C2142	U2144	C2145	C2146	G2147	G2148	G2149	U2150	G2151	G2152	G2155	G2156	G2157	A2158	G2159	G2160	C2161	G2162	G2163	G2164	G2165	G2166	U2167	A2171	U2172	A2173	C2174	G2175	A2176	C2177	G2178	C2179	U2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	C2188										
U2058	A2059	A2060	G2061	G2062	C2063	G2064	C2065	G2066	G2067	U2068	G2069	G2070	A2071	G2072	C2073	U2074	U2075	C2078	U2079	G2080	C2081	A2082	G2083	C2084	G2085	U2086	G2087	G2088	U2089	G2090	U2091	G2092	G2093	U2098	U2099	G2100	C2103	G2104	C2108	U2109	C2110	C2111	A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2121	U2122	G2123	G2124	C2125	C2126											
G1987	G1988	G1989	G1990	U1991	G1992	U1993	G1997	G1998	U1999	G2000	A2001	G2002	C2006	G2009	U2010	G2011	G2012	A2013	A2014	A2015	U2016	U2017	C2018	G2019	U2020	A2021	G2022	U2023	G2024	C2025	G2029	A2030	A2031	G2032	A2033	G2036	G2037	G2038	C2039	U2040	A2041	A2042	C2043	C2044	G2048	G2049	C2050	A2051	G2052	C2055	U2056	A2057														
A1912	A1913	G1914	U1915	G1916	U1917	A1918	A1919	G1920	G1921	C1925	U1926	G1929	A1931	A1932	G1933	G1934	A1935	A1936	A1937	U1938	G1939	U1940	U1946	G1947	G1948	U1951	A1952	G1953	U1954	U1955	U1956	C1957	G1958	G1959	U1963	U1964	C1967	G1968	A1969	A1970	A1971	A1972	G1973	G1974	G1975	C1979	G1980	A1981	G1982	U1986	G1987	A1986														
U1833	U1834	G1835	G1836	G1837	G1838	G1839	G1842	G1843	C1844	G1845	G1846	A1847	A1854	G1855	G1856	G1857	G1858	A1859	G1860	G1861	G1862	G1863	U1864	G1865	G1866	G1867	A1876	G1877	G1878	C1879	G1880	C1881	G1882	G1883	U1884	A1885	G1886	G1887	G1888	A1889	A1890	G1891	G1897	U1898	G1899	A1900	A1901	C1902	G1903	G1904	C1905	G1906	G1907	C1908	G1909	G1910	U1911									
C1771	G1772	C1773	C1774	U1775	G1776	U1777	G1778	U1779	A1780	G1781	G1782	A1783	A1784	A1785	G1786	G1787	G1788	A1789	C1790	G1791	G1792	G1793	U1794	G1795	U1796	G1797	U1798	G1799	U1799	G1800	G1801	C1804	U1805	G1806	G1807	U1808	A1809	G1810	G1811	A1812	G1813	G1816	G1817	U1818	A1819	U1820	A1821	G1824	A1825	G1826	C1827	G1828	A1829	C1830	G1831	G1832										
A1690	C1691	U1692	U1693	C1694	G1697	G1698	G1699	A1700	A1701	G1702	G1703	G1704	G1705	U1706	G1707	C1708	U1709	C1710	C1711	C1712	U1713	G1714	G1715	G1716	G1717	G1718	U1719	G1720	G1721	A1722	G1723	U1724	C1745	C1746	G1747	G1747A	G1748	A1749	G1750	C1751	C1752	A1755	G1756	U1757	G1758	A1759	A1762	G1763	G1764	G1765	U1766	C1767	U1768													
G1627	G1628	U1629	G1630	G1631	A1631A	A1632	G1633	A1634	G1635	G1636	A1637	G1638	U1639	C1640	G1641	G1642	G1643	G1644	G1645	C1648	G1649	A1652	G1653	A1654	A1655	G1656	G1657	G1658	U1659	C1660	G1661	C1662	G1663	A1664	A1665	G1666	G1667	A1668	C1670	U1673	G1674	C1675	A1676	A1677	G1678	G1681	C1682	G1683	G1684	G1685	C1686	U1687	A1689													
G1559	C1560	C1561	C1562	U1563	G1568	A1569	A1570	A1571	A1572	G1573	C1574	G1575	U1576	C1577	U1578	A1579	A1580	G1581	C1582	A1583	C1584	A1586	A1587	G1588	G1589	U1590	G1592	G1593	A1594	G1595	A1596	A1597	C1598	C1599	G1600	G1601	U1602	A1603	G1607	A1608	A1609	A1610	C1611	A1544	A1545	G1546	C1547	C1548	C1549	A1618	C1550	C1551	A1554	G1555	C1556	C1557	A1558									

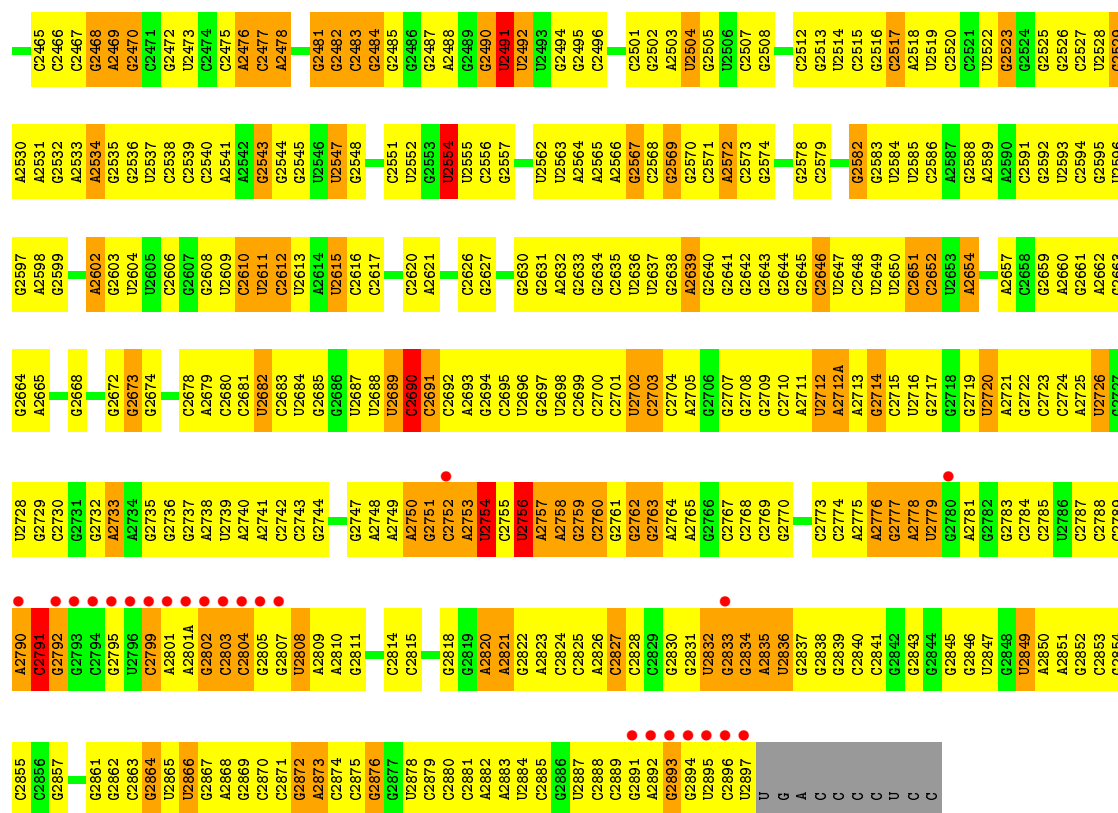


• Molecule 27: 23S ribosomal RNA

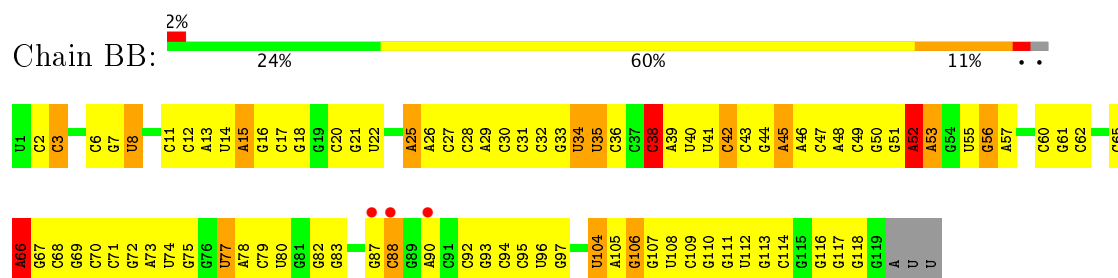




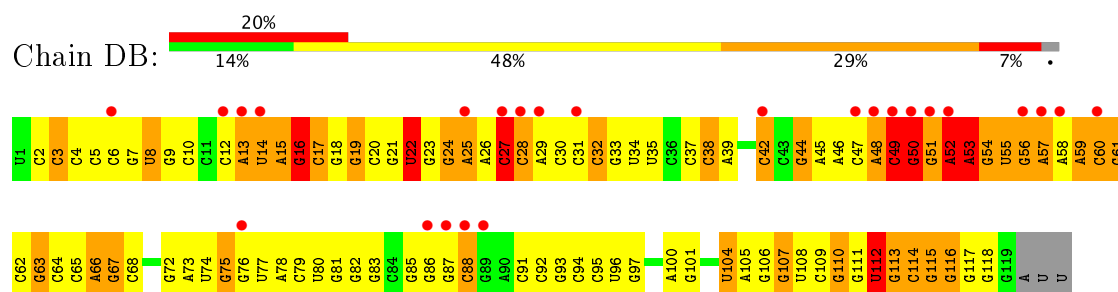
C2395	C2396	C2397	C2398	C2399	C2400	C2401	C2402	C2403	C2404	C2405	C2406	C2407	C2408	C2409	C2410	C2411	C2412	C2413	C2414	C2415	C2416	C2417	C2418	C2419	C2420	C2421	C2422	C2423	C2424	C2425	C2426	C2427	C2428	C2429	C2430	C2435	C2436	C2439	C2440	C2441	C2442	C2443	C2444	C2448	C2449	C2450	C2451	C2452	C2453	C2454	C2457	C2458	C2459	C2460	C2461																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
G2330	G2331	G2332	G2333	G2334	G2335	G2336	G2337	G2338	G2339	G2340	G2341	G2342	G2343	G2344	G2345	G2346	G2347	G2348	G2349	G2350	G2351	G2352	G2353	G2356	G2357	G2358	G2359	G2360	G2361	G2362	G2363	G2364	G2365	G2366	G2367	G2368	G2369	G2370	G2371	A2376	A2377	G2380	G2381	G2382	G2383	G2384	G2385	G2386	G2387	G2388	G2389	G2390	G2391	G2392	G2393	G2394																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
A2267	A2268	A2269	A2270	A2271	A2272	A2273	A2274	A2275	A2276	A2277	A2278	A2279	A2280	A2281	A2282	A2283	A2284	A2285	A2286	A2287	A2288	A2289	A2290	A2291	A2292	A2293	A2294	A2295	A2296	A2297	A2298	A2299	A2300	A2301	A2302	A2303	A2304	A2305	A2306	A2307	A2308	A2309	A2310	A2311	A2312	A2313	A2314	A2315	A2316	A2317	A2318	A2319	A2320	A2325	A2326	A2327	A2328	A2329																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
U2189	U2190	U2191	U2192	U2193	U2197	U2198	U2199	U2200	U2201	U2202	U2203	U2205	U2206	U2207	U2208	U2209	U2210	U2211	U2212	U2213	U2214	U2215	U2216	U2217	U2218	U2219	U2220	U2221	U2222	U2223	U2224	U2225	U2226	U2227	U2228	U2229	U2230	U2231	U2232	U2233	U2234	U2235	U2236	U2237	U2238	U2239	U2240	U2241	U2242	U2243	U2244	U2245	U2246	U2247	U2248	U2249	U2250	U2256	U2257	U2258	U2259	U2260																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G2127	G2128	G2129	G2130	G2131	G2132	G2133	G2134	G2135	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	A2169	A2170	U2171	U2172	U2173	U2174	U2175	A2176	G2177	G2178	G2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	G2191	G2192	G2193	G2194																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
C1996	C1997	C1998	C1999	C2000	A2001	G2004	C2007	C2008	C2009	G2010	G2011	G2012	C2013	A2014	A2015	G2018	A2019	A2020	C2021	U2022	G2023	G2024	C2025	C2026	G2027	U2028	C2029	A2030	U2031	C2032	A2033	U2034	C2035	C2036	C2037	C2038	C2039	C2040	U2041	A2042	C2043	G2046	G2049	C2050	A2051	G2052	C2053	A2054	C2055	C2056	A2057	C2058	C2059	C2060																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
U1926	U1927	U1928	U1929	U1930	U1933	C1934	U1935	U1936	U1937	U1938	U1939	U1940	C1941	U1942	U1943	U1944	U1945	U1946	C1947	U1948	U1951	U1952	U1953	U1954	U1955	U1956	C1957	U1958	U1959	C1962	U1963	U1964	C1967	U1968	U1969	U1970	A1971	A1972	U1980	A1981	U1982	C1983	U1984	U1985	A1986	U1987	C1988	U1989	C1990	U1991	U1992	U1993	U1995	U1996	U1997	U1998	U1999	U2000																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
G1850	G1851	G1852	G1853	G1854	G1855	G1856	G1857	G1858	A1859	G1862	G1863	G1864	G1865	G1866	A1876	A1877	G1878	C1879	U1880	U1881	U1882	G1883	A1884	G1885	U1886	U1887	A1888	U1889	A1890	U1891	C1892	G1897	U1898	A1900	U1901	C1902	U1903	U1904	C1905	C1906	U1907	C1908	U1911	A1912	A1913	C1914	U1915	U1916	U1917	U1918	A1919	U1923	U1924	U1925	U1926	U1927	U1928	U1929	U1930																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
A1786	A1787	A1788	A1789	A1790	A1791	G1792	G1793	U1794	C1795	U1796	C1797	U1798	G1799	C1800	A1801	C1804	U1805	G1806	U1807	U1808	A1809	A1810	G1811	A1812	U1813	G1814	A1815	U1816	A1817	U1818	A1819	A1820	A1821	G1822	U1823	A1824	A1825	U1826	C1827	U1828	A1829	U1833	U1834	A1835	C1836	C1837	G1840	U1841	U1842	U1843	C1844	U1845	U1846	A1847	A1848	A1849	A1850	A1851	A1852	A1853	A1854	A1855	A1856	A1857	A1858	A1859	A1860	A1861	A1862	A1863	A1864	A1865	A1866	A1867	A1868	A1869	A1870	A1871	A1872	A1873	A1874	A1875	A1876	A1877	A1878	A1879	A1880	A1881	A1882	A1883	A1884	A1885	A1886	A1887	A1888	A1889	A1890	A1891	A1892	A1893	A1894	A1895	A1896	A1897	A1898	A1899	A1900	A1901	A1902	A1903	A1904	A1905	A1906	A1907	A1908	A1909	A1910	A1911	A1912	A1913	A1914	A1915	A1916	A1917	A1918	A1919	A1920	A1921	A1922	A1923	A1924	A1925	A1926	A1927	A1928	A1929	A1930	A1931	A1932	A1933	A1934	A1935	A1936	A1937	A1938	A1939	A1940	A1941	A1942	A1943	A1944	A1945	A1946	A1947	A1948	A1949	A1950	A1951	A1952	A1953	A1954	A1955	A1956	A1957	A1958	A1959	A1960	A1961	A1962	A1963	A1964	A1965	A1966	A1967	A1968	A1969	A1970	A1971	A1972	A1973	A1974	A1975	A1976	A1977	A1978	A1979	A1980	A1981	A1982	A1983	A1984	A1985	A1986	A1987	A1988	A1989	A1990	A1991	A1992	A1993	A1994	A1995	A1996	A1997	A1998	A1999	A2000	A2001	A2002	A2003	A2004	A2005	A2006	A2007	A2008	A2009	A2010	A2011	A2012	A2013	A2014	A2015	A2016	A2017	A2018	A2019	A2020	A2021	A2022	A2023	A2024	A2025	A2026	A2027	A2028	A2029	A2030	A2031	A2032	A2033	A2034	A2035	A2036	A2037	A2038	A2039	A2040	A2041	A2042	A2043	A2044	A2045	A2046	A2047	A2048	A2049	A2050	A2051	A2052	A2053	A2054	A2055	A2056	A2057	A2058	A2059	A2060	A2061	A2062	A2063	A2064	A2065	A2066	A2067	A2068	A2069	A2070	A2071	A2072	A2073	A2074	A2075	A2076	A2077	A2078	A2079	A2080	A2081	A2082	A2083	A2084	A2085	A2086	A2087	A2088	A2089	A2090	A2091	A2092	A2093	A2094	A2095	A2096	A2097	A2098	A2099	A2100	A2101	A2102	A2103	A2104	A2105	A2106	A2107	A2108	A2109	A2110	A2111	A2112	A2113	A2114	A2115	A2116	A2117	A2118	A2119	A2120	A2121	A2122	A2123	A2124	A2125	A2126	A2127	A2128	A2129	A2130	A2131	A2132	A2133	A2134	A2135	A2136	A2137	A2138	A2139	A2140	A2141	A2142	A2143	A2144	A2145	A2146	A2147	A2148	A2149	A2150	A2151	A2152	A2153	A2154	A2155	A2156	A2157	A2158	A2159	A2160	A2161	A2162	A2163	A2164	A2165	A2166	A2167	A2168	A2169	A2170	A2171	A2172	A2173	A2174	A2175	A2176	A2177	A2178	A2179	A2180	A2181	A2182	A2183	A2184	A2185	A2186	A2187	A2188	A2189	A2190	A2191	A2192	A2193	A2194	A2195	A2196	A2197	A2198	A2199	A2200	A2201	A2202	A2203	A2204	A2205	A2206	A2207	A2208	A2209	A2210	A2211	A2212	A2213	A2214	A2215	A2216	A2217	A2218	A2219	A2220	A2221	A2222	A2223	A2224	A2225	A2226	A2227	A2228	A2229	A2230	A2231	A2232	A2233	A2234	A2235	A2236	A2237	A2238	A2239	A2240	A2241	A2242	A2243	A2244	A2245	A2246	A2247	A2248	A2249	A2250	A2251	A2252	A2253	A2254	A2255	A2256	A2257	A2258	A2259	A2260	A2261	A2262	A2263	A2264	A2265	A2266	A2267	A2268	A2269	A2270	A2271	A2272	A2273	A2274	A2275	A2276	A2277	A2278	A2279	A2280	A2281	A2282	A2283	A2284	A2285	A2286	A2287	A2288	A2289	A2290	A2291	A2292	A2293	A2294	A2295	A2296	A2297	A2298	A2299	A2300	A2301	A2302	A2303	A2304	A2305	A2306	A2307	A2308	A2309	A2310	A2311	A2312	A2313	A2314	A2315	A2316	A2317	A2318	A2319	A2320	A2321	A2322	A2323	A2324	A2325	A2326	A2327	A2328	A2329	A2330	A2331	A2332	A2333	A2334	A2335	A2336	A2337	A2338	A2339	A2340	A2341	A2342	A2343	A2344	A2345	A2346	A2347	A2348	A2349	A2350	A2351	A2352	A2353	A2354	A2355	A2356	A2357	A2358	A2359	A2360	A2361	A2362	A2363	A2364	A2365	A2366	A2367	A2368	A2369	A2370	A2371	A2372	A2373	A2374	A2375	A2376	A2377	A2378	A2379	A2380	A2381	A2382	A2383	A2384	A2385	A2386	A2387	A2388	A2389	A2390	A2391	A2392	A2393	A2394	A2395	A2396	A2397	A2398	A2399	A2400	A2401	A2402	A2403	A2404	A2405	A2406	A2407	A2408	A2409	A2410	A2411	A2412	A2413	A2414	A2415	A2416	A2417	A2418	A2419	A2420	A2421	A2422	A2423	A2424	A2425	A2426	A2427	A2428	A2429	A2430	A2431	A2432	A2433	A2434	A2435	A2436	A2437	A2438	A2439	A2440	A2441	A2442	A2443	A2444	A2445	A2446	A2447	A2448	A2449	A2450	A2451	A2452	A2453	A2454	A2455	A2456	A2457	A2458	A2459	A2460	A2461	A2462	A2463	A2464	A2465	A2466	A2467	A2468	A2469	A2470	A2471	A2472	A2473	A2474	A2475	A2476	A2477	A2478	A2479	A2480	A2481	A2482	A2483	A2484	A2485	A2486	A2487	A2488	A2489	A2490	A2491	A2492	A2493	A2494	A2495	A2496	A2497	A2498	A2499	A2500	A2501	A2502	A2503	A2504	A2505	A2506	A2507	A2508	A2509	A2510	A2511	A2512	A2513	A2514	A2515	A2516	A2517	A2518	A2519	A2520	A2521	A2522	A2523	A2524	A2525	A2526	A2527	A2528	A2529	A2530	A2531	A2532	A2533	A2534	A2535	A2536	A2537	A2538	A2539	A2540	A2541	A2542	A2543	A2544	A2545	A2546	A2547	A2548	A2549	A2550	A2551	A2552	A2553	A2554	A2555	A2556	A2557	A2558	A2559	A2560	A2561	A2562	A2563	A2564	A2565	A2566	A2567	A2568	A2569	A2570	A2571	A2572	A2573	A2574	A2575	A2576	A2577	A2578	A2579	A2580	A2581	A2582	A2583	A2584	A2585	A2586	A2587	A2588	A2589	A2590	A2591	A2592	A2593	A2594	A2595	A2596	A2597	A2598	A2599	A2600	A2601	A2602	A2603	A2604	A2605	A2606	A2607	A2608	A2609	A2610	A2611	A2612	A2613	A2614	A2615	A2616	A2617	A2618	A2619	A2620	A2621	A2622	A2623	A2624	A2625	A2626	A2627	A2628	A2629	A2630	A2631	A2632	A2633	A2634	A2635	A2636	A2637	A2638	A2639	A2640	A2641	A2642	A2643	A2644	A2645	A2646	A2647	A2648	A2649	A2650	A2651	A2652	A2653	A2654	A2655	A2656	A2657	A2658	A2659	A2660	A2661	A2662	A2663	A2664	A2665	A2666	A2667	A2668	A2669	A2670	A2671



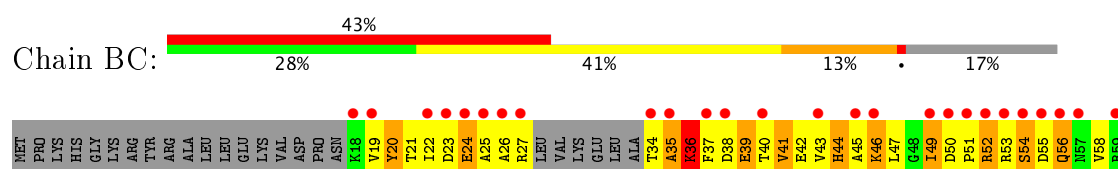
• Molecule 28: 5S ribosomal RNA

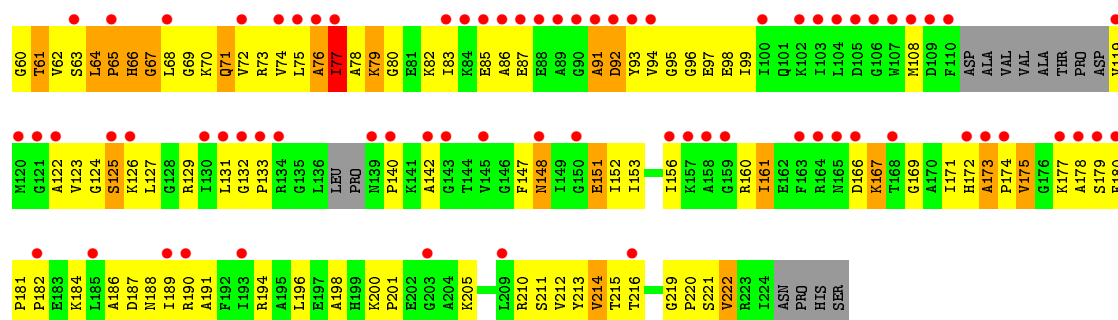


• Molecule 28: 5S ribosomal RNA

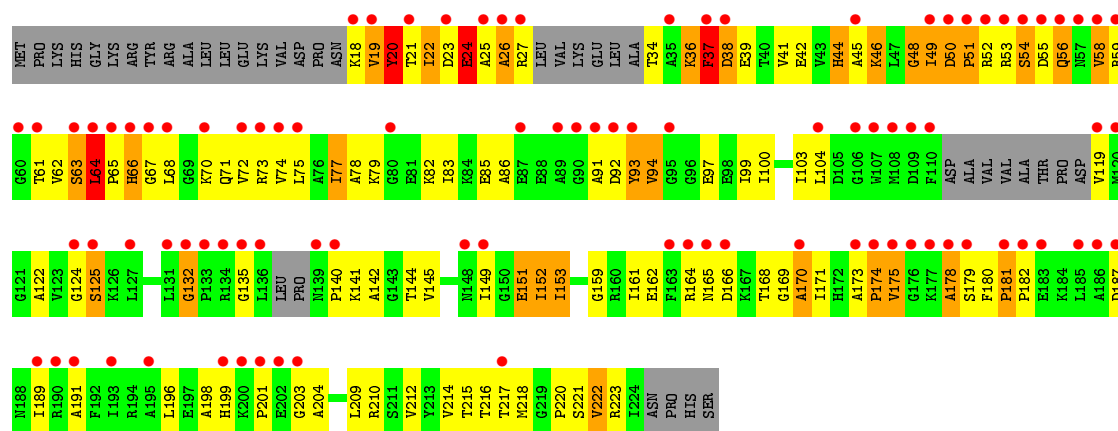


• Molecule 29: 50S ribosomal protein L1

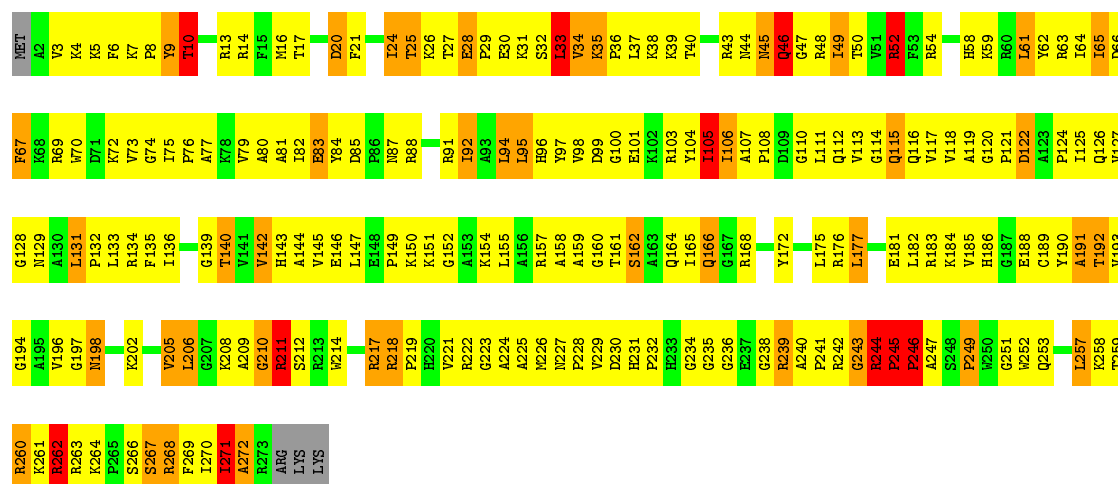




• Molecule 29: 50S ribosomal protein L1

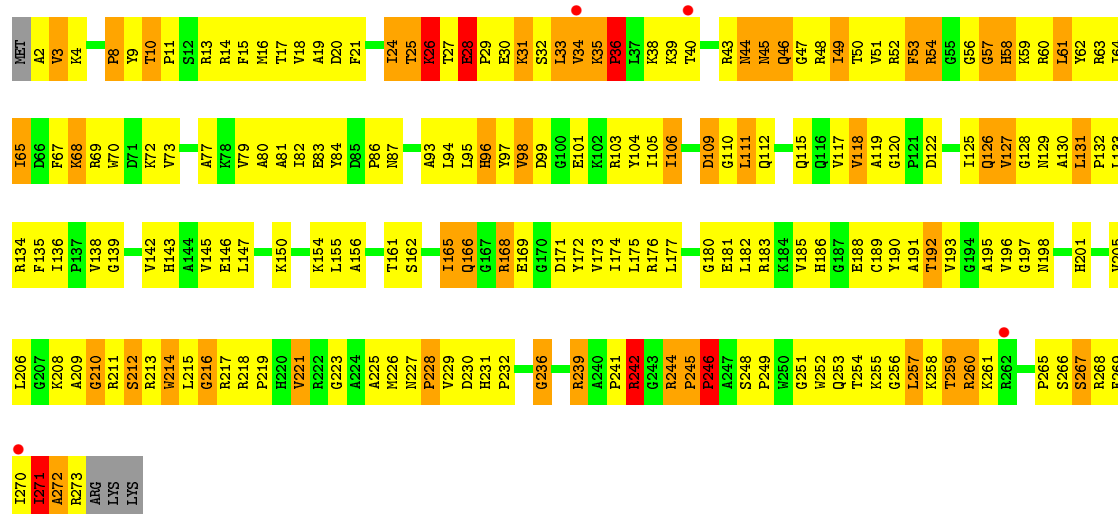


• Molecule 30: 50S ribosomal protein L2

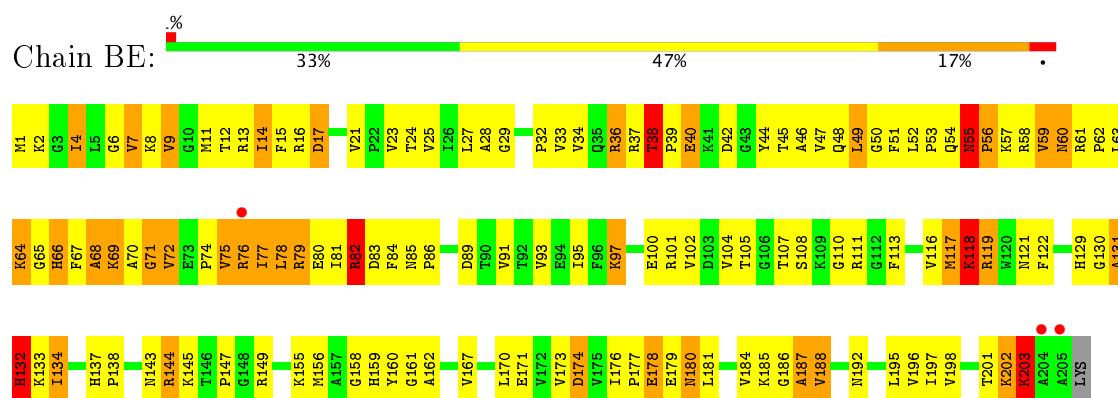


• Molecule 30: 50S ribosomal protein L2

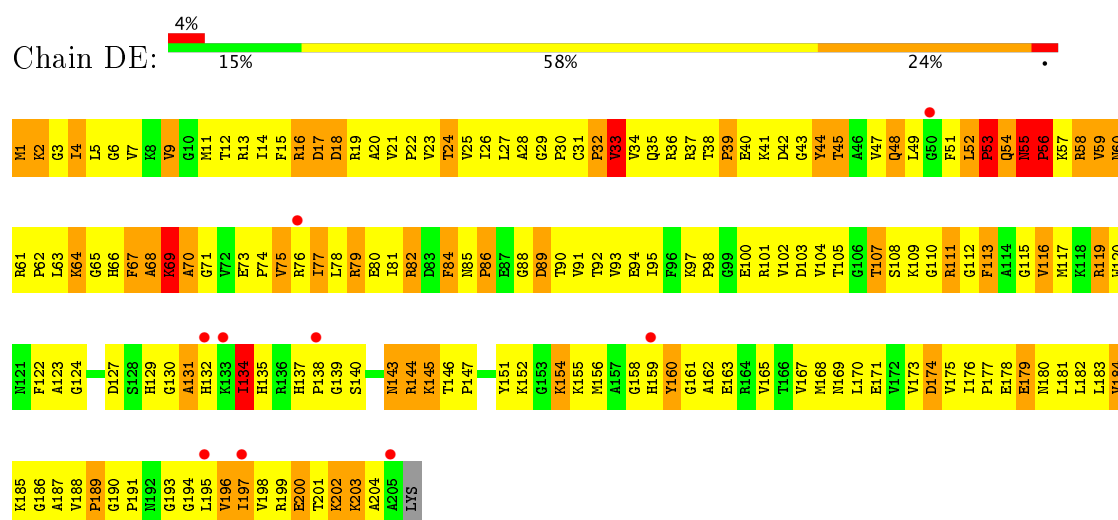




• Molecule 31: 50S ribosomal protein L3

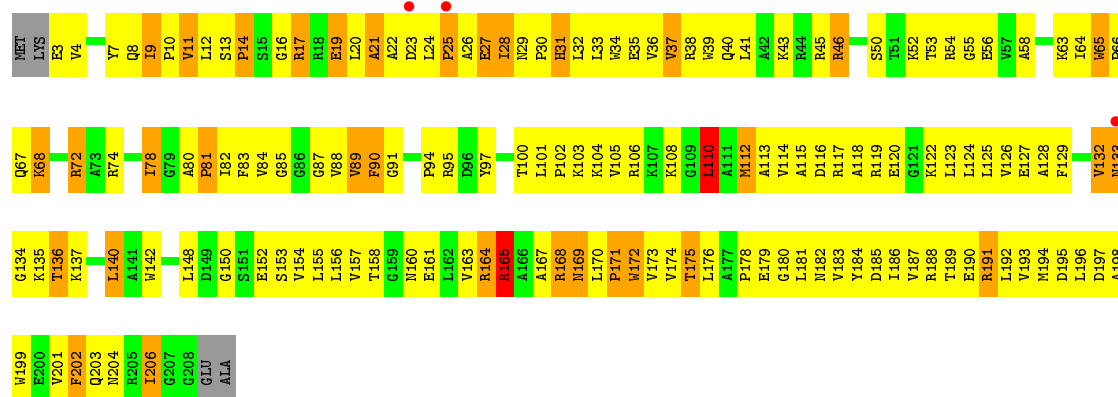


• Molecule 31: 50S ribosomal protein L3

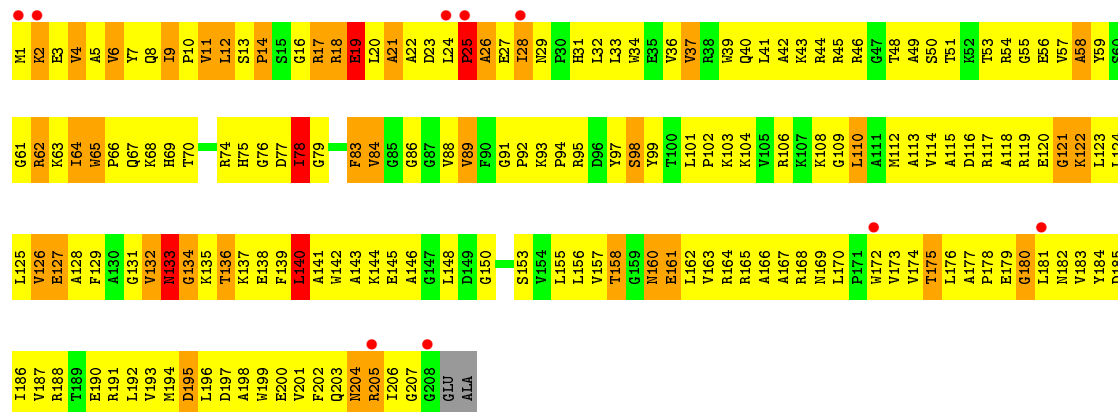


• Molecule 32: 50S ribosomal protein L4

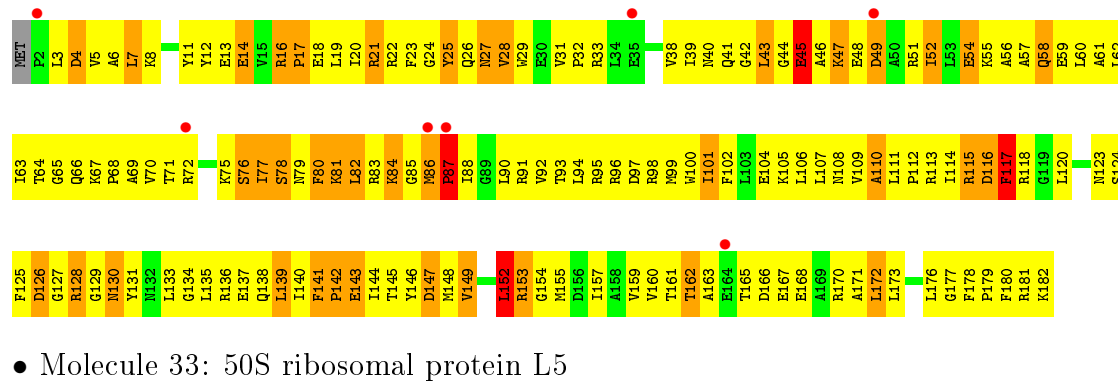




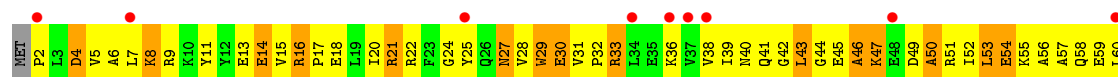
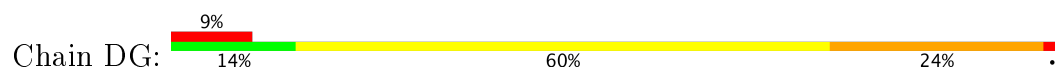
• Molecule 32: 50S ribosomal protein L4

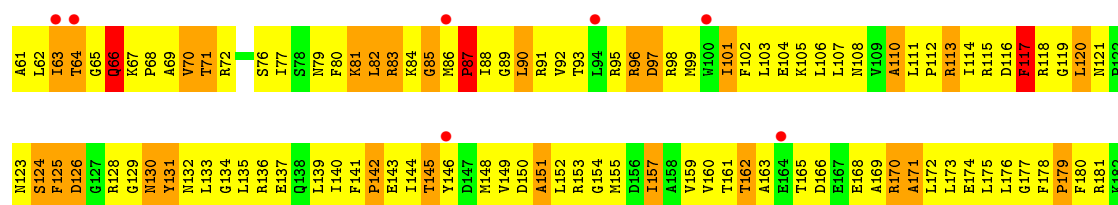


• Molecule 33: 50S ribosomal protein L5

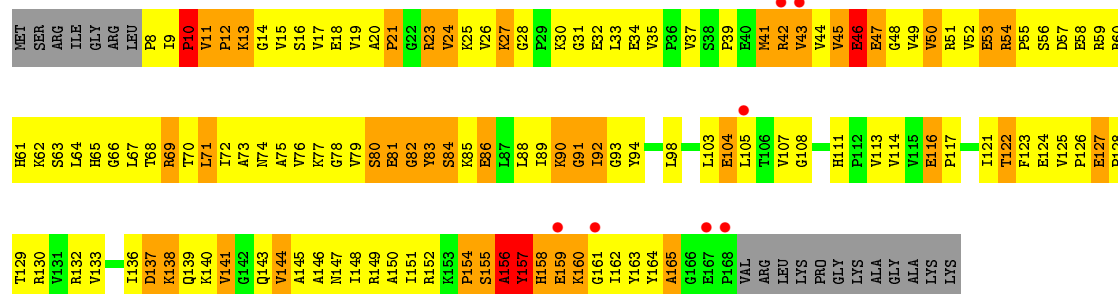
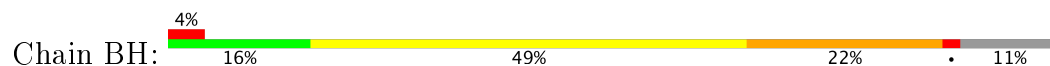


• Molecule 33: 50S ribosomal protein L5

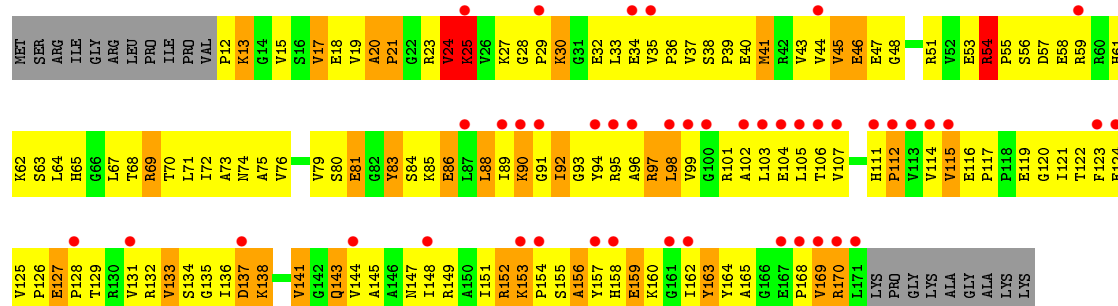
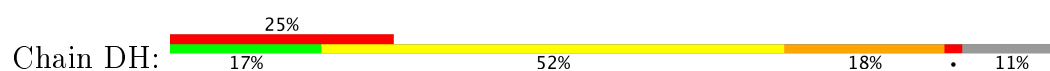




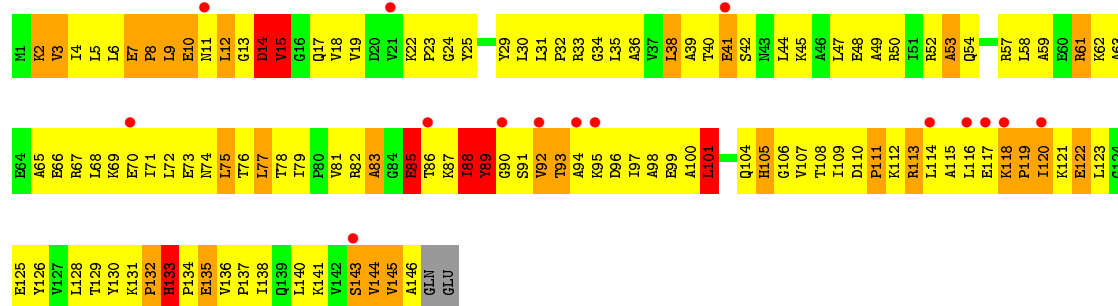
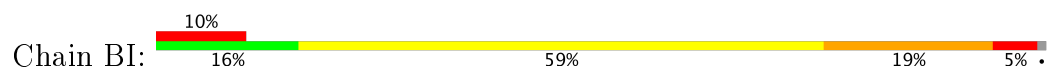
• Molecule 34: 50S ribosomal protein L6



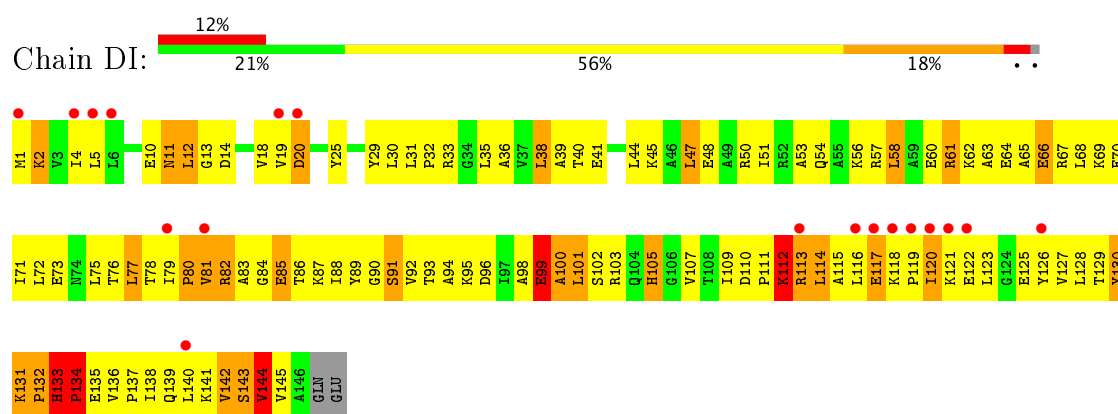
• Molecule 34: 50S ribosomal protein L6



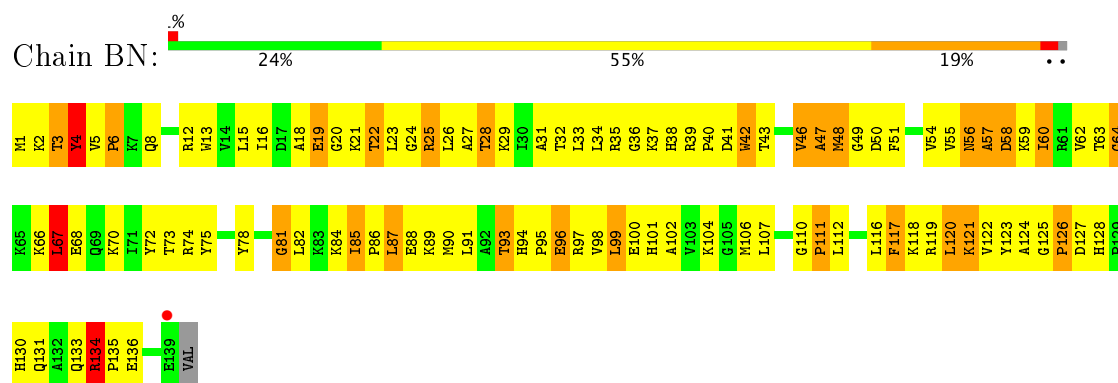
• Molecule 35: 50S ribosomal protein L9



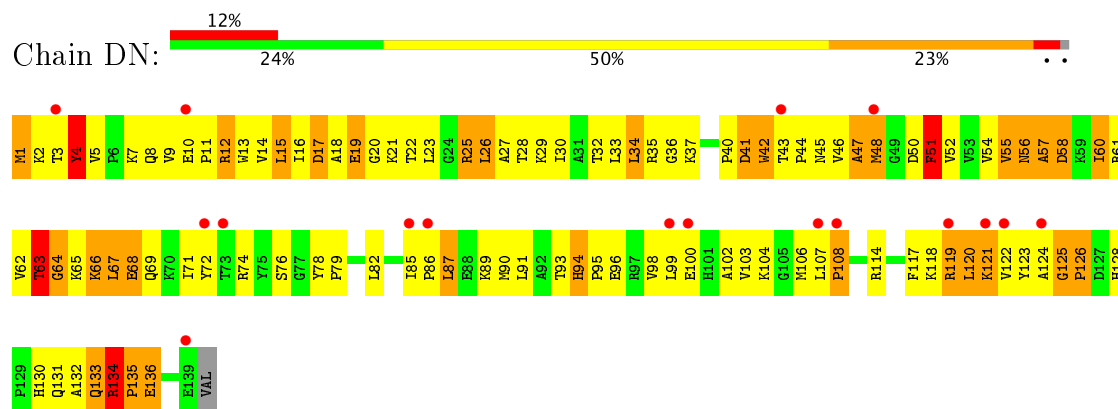
• Molecule 35: 50S ribosomal protein L9



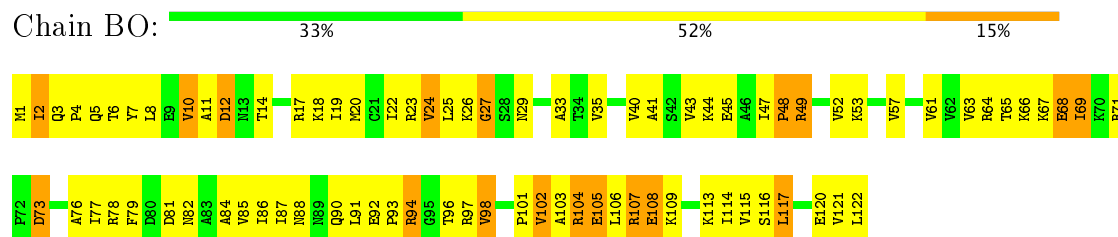
• Molecule 36: 50S ribosomal protein L13



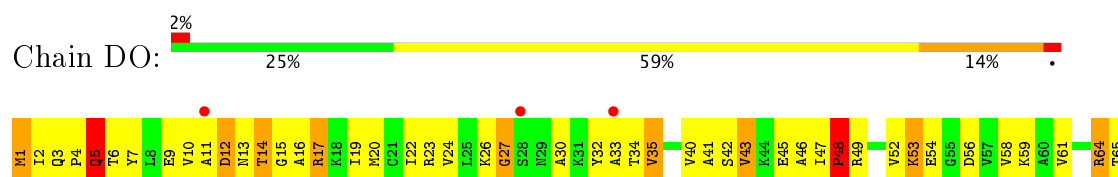
• Molecule 36: 50S ribosomal protein L13



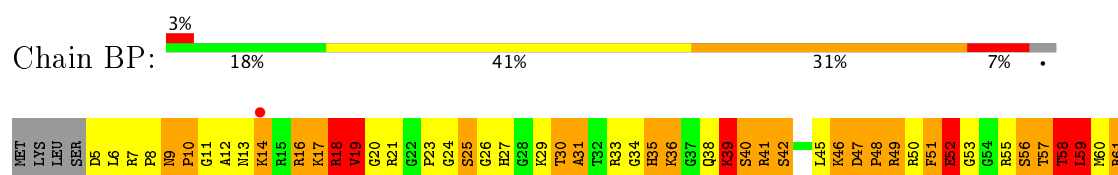
• Molecule 37: 50S ribosomal protein L14



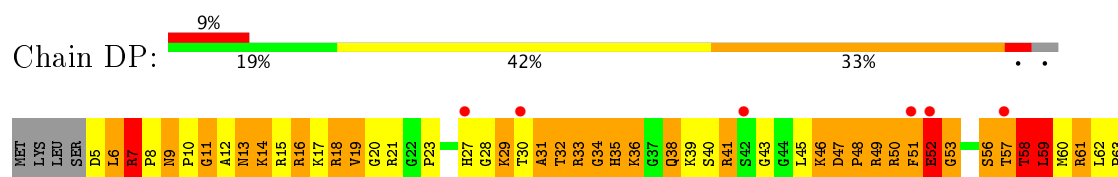
• Molecule 37: 50S ribosomal protein L14



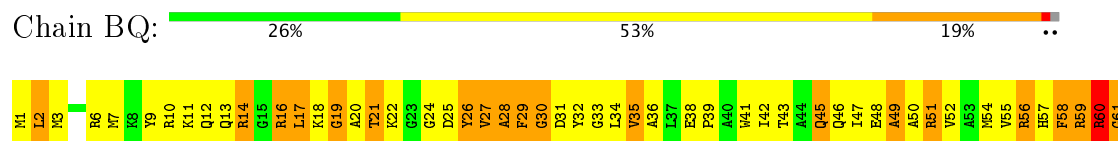
• Molecule 38: 50S ribosomal protein L15



• Molecule 38: 50S ribosomal protein L15

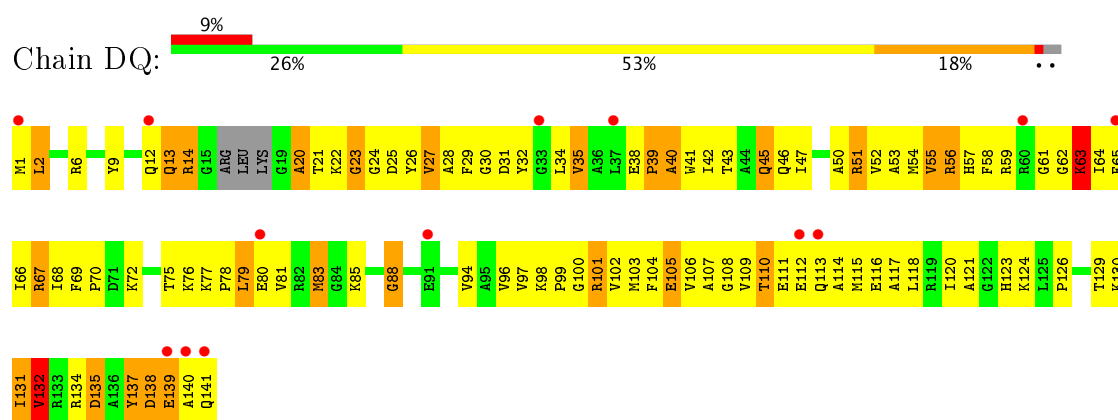


• Molecule 39: 50S ribosomal protein L16

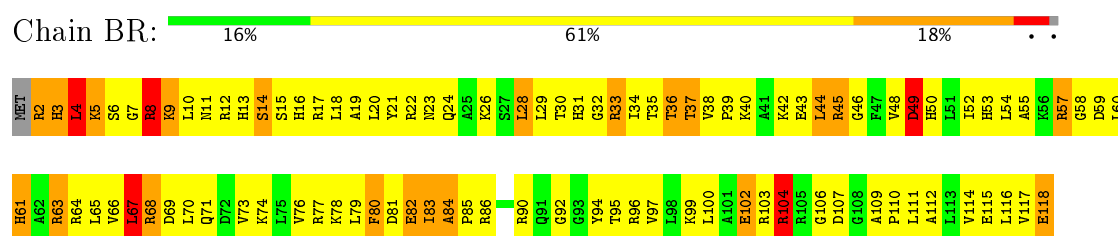


• Molecule 39: 50S ribosomal protein L16

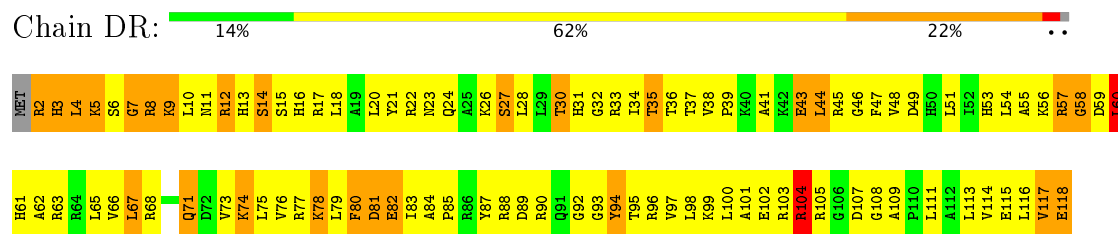




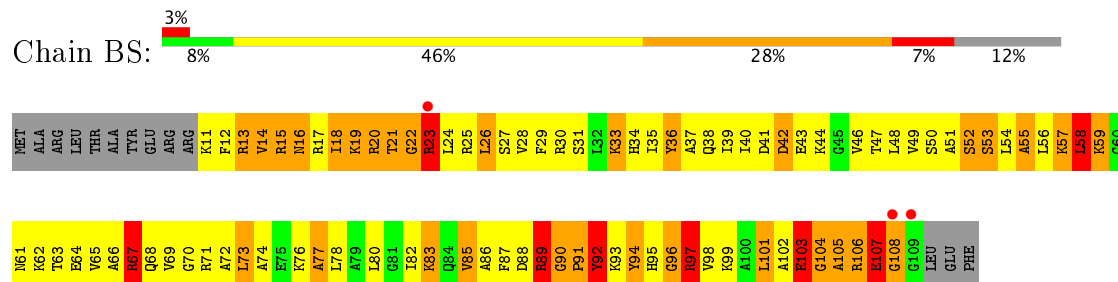
- Molecule 40: 50S ribosomal protein L17



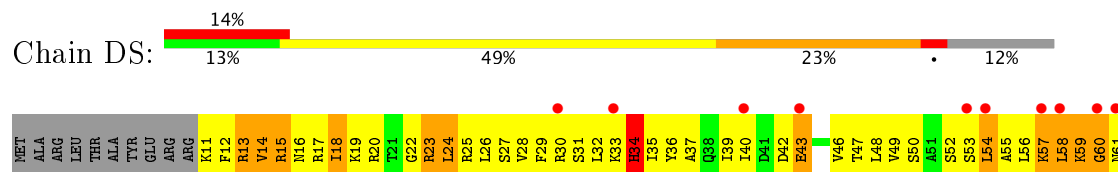
- Molecule 40: 50S ribosomal protein L17



- Molecule 41: 50S ribosomal protein L18

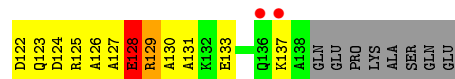
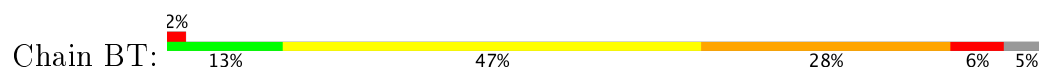


- Molecule 41: 50S ribosomal protein L18

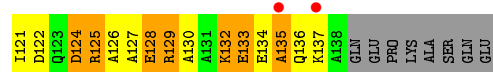




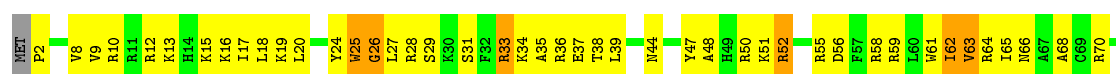
- Molecule 42: 50S ribosomal protein L19



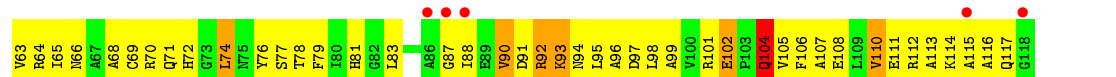
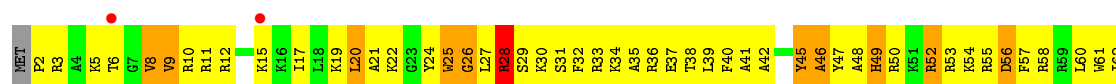
- Molecule 42: 50S ribosomal protein L19



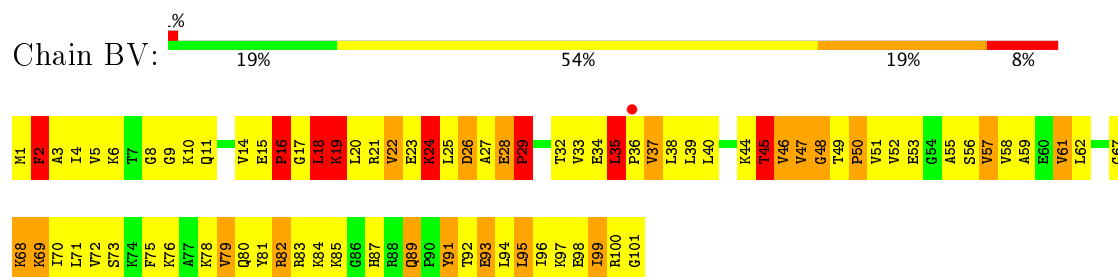
- Molecule 43: 50S ribosomal protein L20



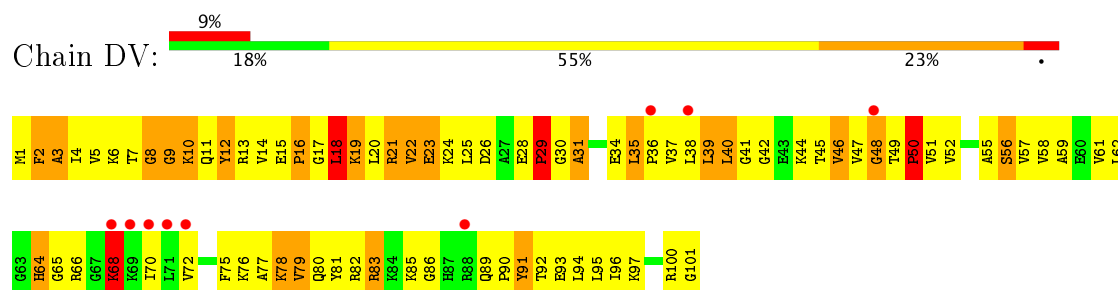
- Molecule 43: 50S ribosomal protein L20



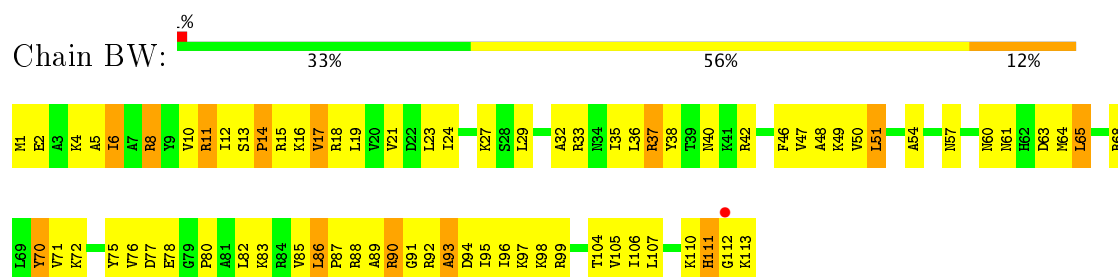
- Molecule 44: 50S ribosomal protein L21



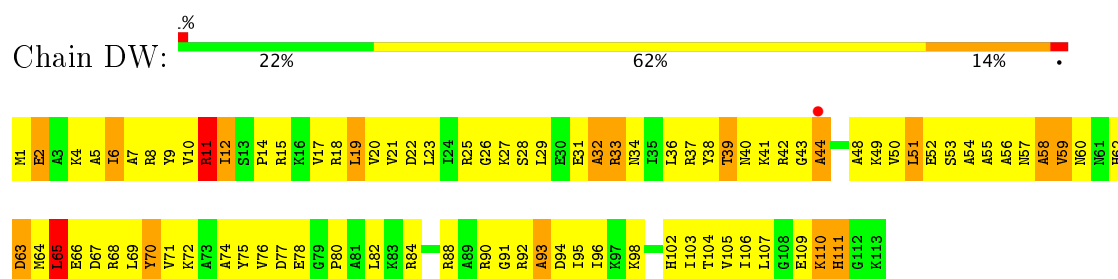
- Molecule 44: 50S ribosomal protein L21



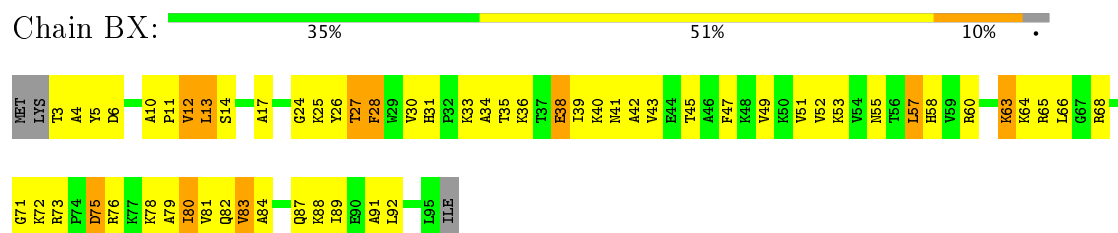
- Molecule 45: 50S ribosomal protein L22



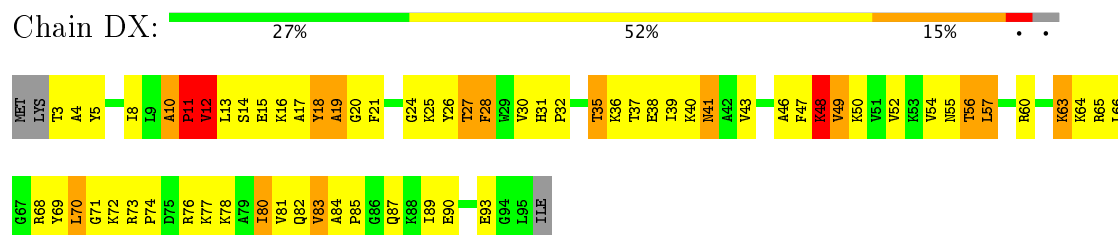
- Molecule 45: 50S ribosomal protein L22



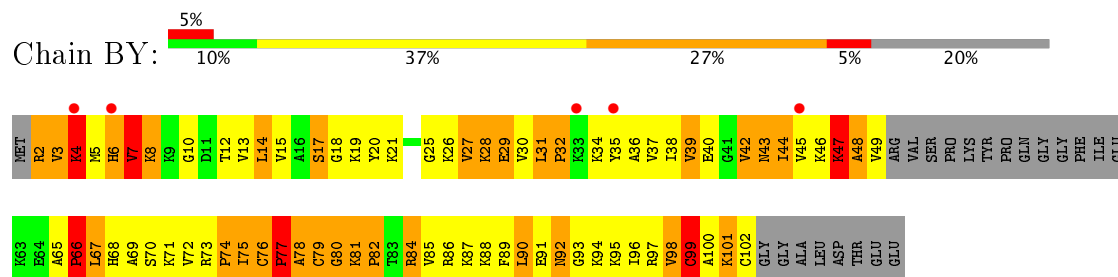
- Molecule 46: 50S ribosomal protein L23



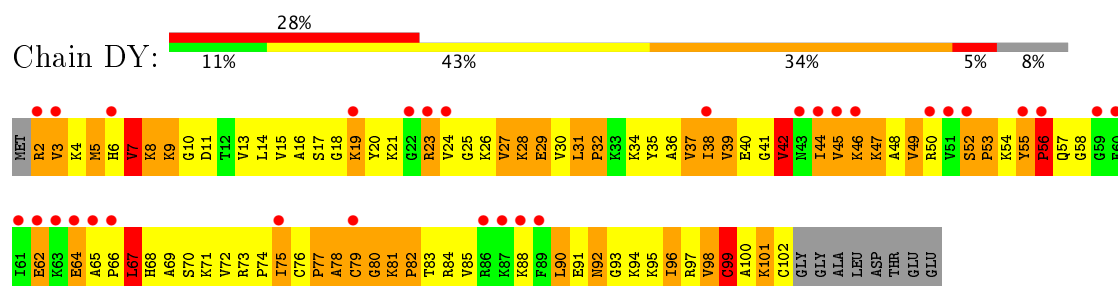
- Molecule 46: 50S ribosomal protein L23



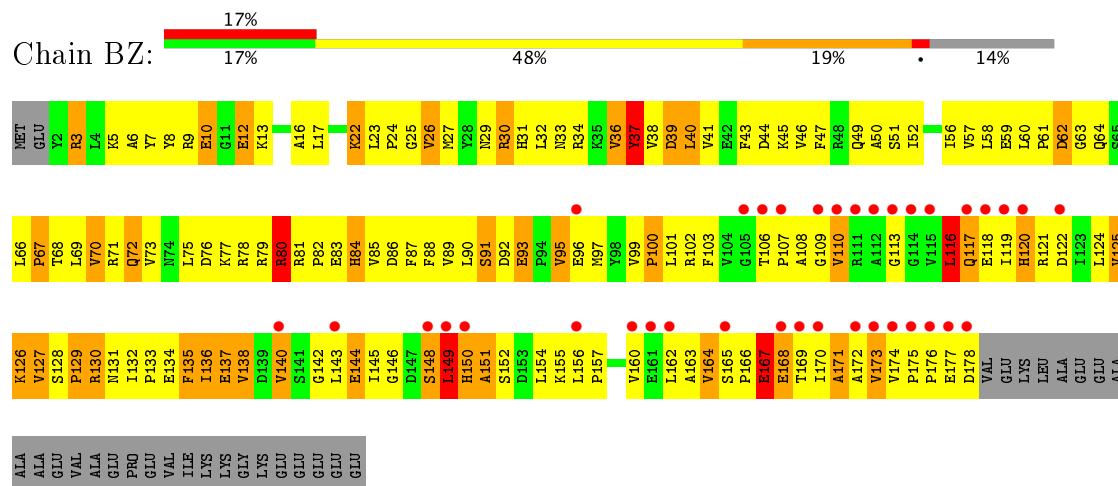
- Molecule 47: 50S ribosomal protein L24



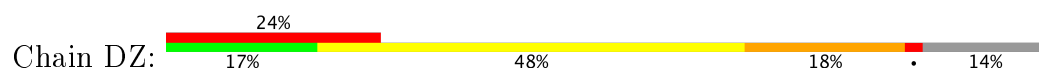
- Molecule 47: 50S ribosomal protein L24

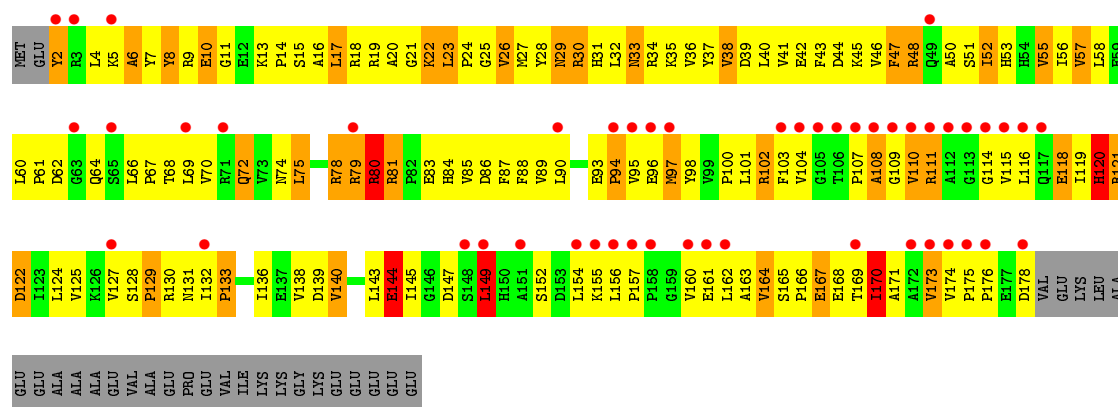


- Molecule 48: 50S ribosomal protein L25

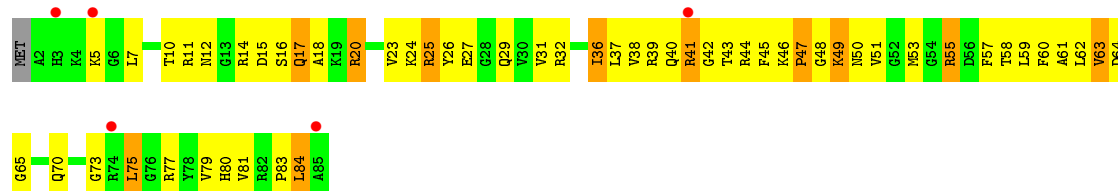


- Molecule 48: 50S ribosomal protein L25

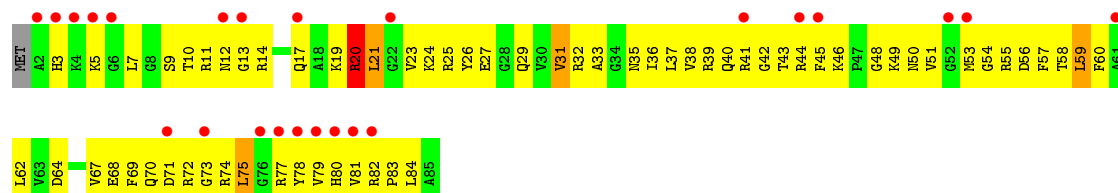




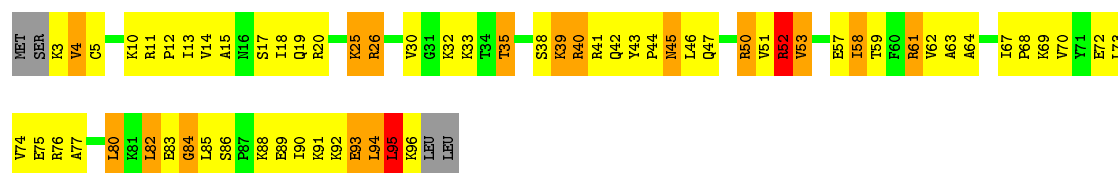
• Molecule 49: 50S ribosomal protein L27



• Molecule 49: 50S ribosomal protein L27



• Molecule 50: 50S ribosomal protein L28

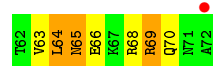
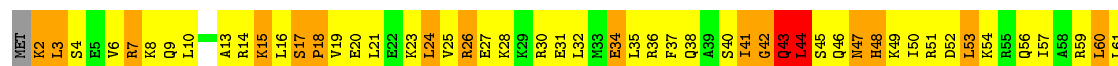
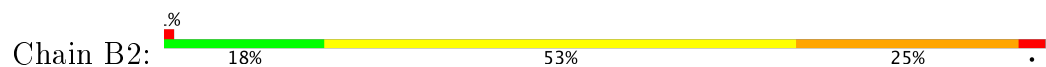


• Molecule 50: 50S ribosomal protein L28

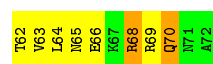
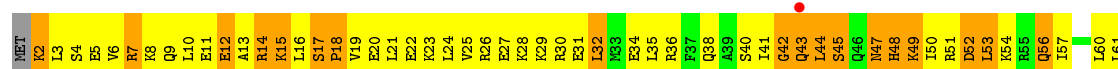
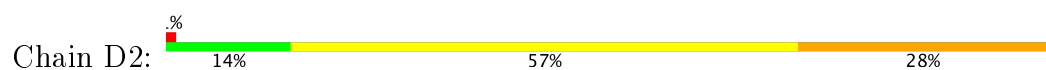




- Molecule 51: 50S ribosomal protein L29



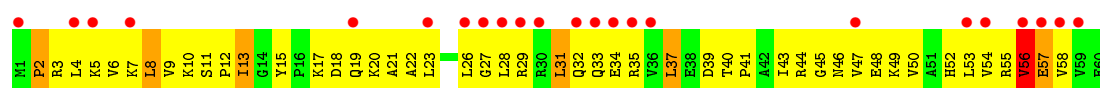
- Molecule 51: 50S ribosomal protein L29



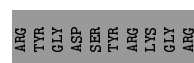
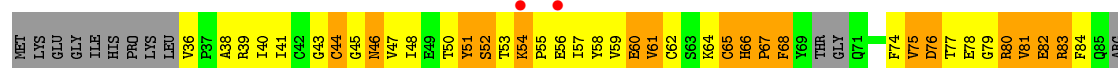
- Molecule 52: 50S ribosomal protein L30



- Molecule 52: 50S ribosomal protein L30

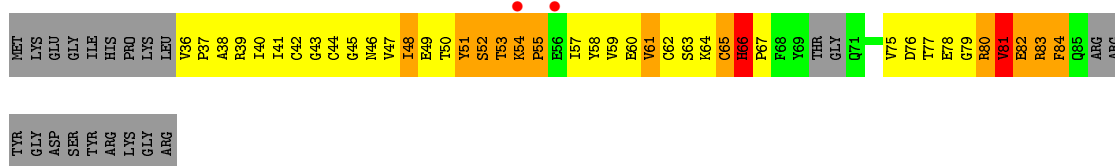


- Molecule 53: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L31





- Molecule 54: 50S ribosomal protein L32



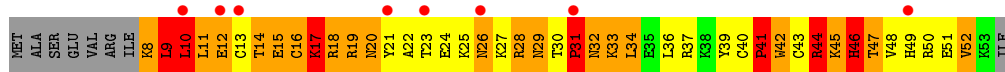
- Molecule 54: 50S ribosomal protein L32



- Molecule 55: 50S ribosomal protein L33



- Molecule 55: 50S ribosomal protein L33



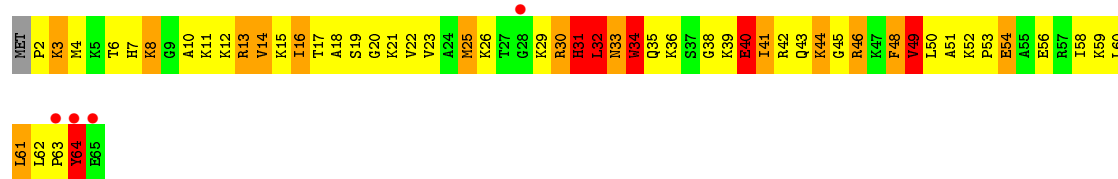
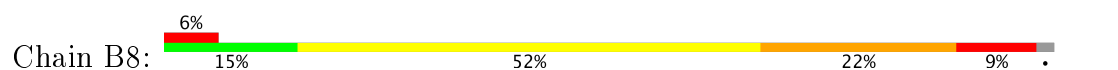
- Molecule 56: 50S ribosomal protein L34



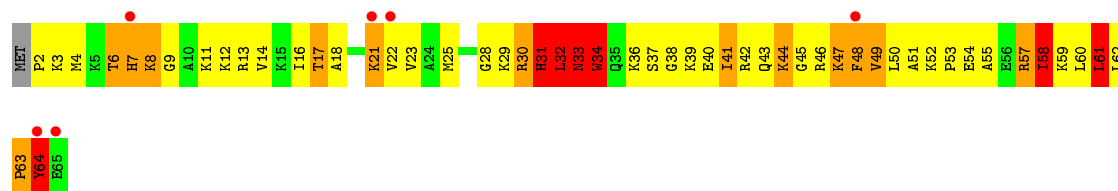
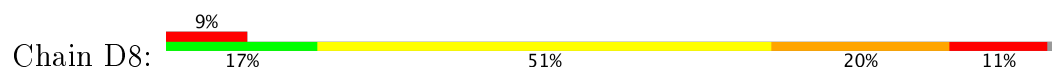
- Molecule 56: 50S ribosomal protein L34



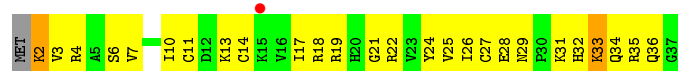
- Molecule 57: 50S ribosomal protein L35



- Molecule 57: 50S ribosomal protein L35



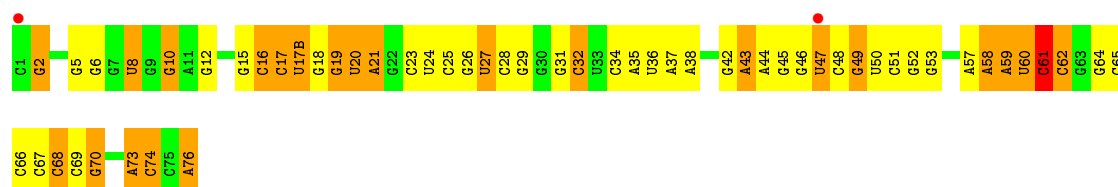
- Molecule 58: 50S ribosomal protein L36



- Molecule 58: 50S ribosomal protein L36



- Molecule 59: RNA (77-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.35Å 448.24Å 631.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.45 49.75 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.45) 82.3 (49.75-3.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.268 0.219 , 0.219	Depositor DCC
R_{free} test set	33187 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	74.9	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	293848	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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, DPP, MG, KBE, UAL, MYN

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	0.48	0/35968	0.74	23/56136 (0.0%)
1	CA	0.50	9/35932 (0.0%)	0.75	27/56082 (0.0%)
2	AB	0.39	0/1936	0.68	0/2611
2	CB	0.37	0/1936	0.66	0/2611
3	AC	0.38	0/1637	0.65	0/2207
3	CC	0.37	0/1627	0.67	0/2192
4	AD	0.42	0/1733	0.71	0/2318
4	CD	0.44	0/1733	0.72	1/2318 (0.0%)
5	AE	0.41	0/1163	0.68	0/1566
5	CE	0.42	0/1163	0.68	0/1566
6	AF	0.44	0/856	0.75	1/1154 (0.1%)
6	CF	0.43	0/856	0.71	0/1154
7	AG	0.38	0/1276	0.61	0/1709
7	CG	0.39	0/1267	0.62	0/1696
8	AH	0.40	0/1136	0.72	0/1527
8	CH	0.38	0/1136	0.70	0/1527
9	AI	0.38	0/1024	0.68	0/1372
9	CI	0.36	0/1024	0.67	0/1372
10	AJ	0.36	0/808	0.66	0/1087
10	CJ	0.36	0/808	0.67	0/1087
11	AK	0.41	0/879	0.75	0/1187
11	CK	0.39	0/900	0.68	0/1213
12	AL	0.44	0/987	0.80	0/1322
12	CL	0.44	0/987	0.74	0/1322
13	AM	0.37	0/975	0.75	2/1305 (0.2%)
13	CM	0.36	0/947	0.72	0/1270
14	AN	0.41	0/501	0.69	0/664
14	CN	0.45	0/501	0.67	0/664
15	AO	0.39	0/745	0.64	0/992
15	CO	0.37	0/745	0.64	0/992
16	AP	0.40	0/717	0.70	0/965
16	CP	0.43	0/717	0.74	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.43	0/837	0.67	0/1119
17	CQ	0.40	0/837	0.68	0/1119
18	AR	0.48	0/579	0.75	0/768
18	CR	0.41	0/579	0.72	0/768
19	AS	0.40	0/643	0.70	1/867 (0.1%)
19	CS	0.37	0/643	0.66	0/867
20	AT	0.38	0/765	0.72	1/1007 (0.1%)
20	CT	0.37	0/765	0.70	0/1007
21	AU	0.42	0/213	0.60	0/279
21	CU	0.34	0/213	0.62	0/279
22	AV	0.48	0/230	0.65	0/357
22	CV	0.45	0/239	0.69	0/371
23	AW	0.47	0/1756	0.78	0/2734
23	CW	0.46	0/1756	0.75	2/2734 (0.1%)
24	AX	0.58	2/1831 (0.1%)	0.87	6/2853 (0.2%)
25	AY	0.37	0/1776	0.71	0/2766
25	CY	0.36	0/1776	0.71	0/2766
26	AZ	0.91	0/5	0.51	0/5
26	CZ	0.51	0/5	0.85	0/5
27	BA	0.61	3/67273 (0.0%)	0.79	62/105005 (0.1%)
27	DA	0.51	1/66930 (0.0%)	0.77	45/104469 (0.0%)
28	BB	0.57	0/2853	0.81	6/4451 (0.1%)
28	DB	0.79	6/2853 (0.2%)	0.95	13/4451 (0.3%)
29	BC	0.31	0/1145	0.60	0/1556
29	DC	0.30	0/1145	0.61	0/1556
30	BD	0.54	0/2155	0.86	3/2907 (0.1%)
30	DD	0.51	0/2155	0.82	2/2907 (0.1%)
31	BE	0.56	0/1597	0.87	2/2155 (0.1%)
31	DE	0.42	0/1597	0.75	0/2155
32	BF	0.50	0/1642	0.82	1/2225 (0.0%)
32	DF	0.42	0/1659	0.75	1/2246 (0.0%)
33	BG	0.44	0/1499	0.78	0/2016
33	DG	0.40	0/1499	0.72	0/2016
34	BH	0.59	0/1258	0.91	2/1703 (0.1%)
34	DH	0.33	0/1246	0.67	0/1684
35	BI	0.39	0/1147	0.74	0/1553
35	DI	0.37	0/1147	0.75	0/1553
36	BN	0.54	0/1132	0.91	2/1527 (0.1%)
36	DN	0.41	0/1132	0.77	1/1527 (0.1%)
37	BO	0.54	0/943	0.80	0/1269
37	DO	0.44	0/943	0.69	0/1269
38	BP	0.59	0/1131	1.16	5/1504 (0.3%)
38	DP	0.48	0/1131	1.00	5/1504 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	BQ	0.53	0/1128	0.77	0/1508
39	DQ	0.42	0/1114	0.68	0/1488
40	BR	0.55	0/974	0.92	2/1302 (0.2%)
40	DR	0.43	0/974	0.81	0/1302
41	BS	0.55	0/779	0.97	2/1038 (0.2%)
41	DS	0.43	0/779	0.75	0/1038
42	BT	0.57	0/1156	0.96	5/1544 (0.3%)
42	DT	0.46	0/1156	0.83	1/1544 (0.1%)
43	BU	0.57	0/975	0.85	0/1297
43	DU	0.38	0/975	0.69	0/1297
44	BV	0.58	0/790	0.95	2/1057 (0.2%)
44	DV	0.41	0/790	0.72	0/1057
45	BW	0.53	0/907	0.77	0/1216
45	DW	0.41	0/907	0.72	0/1216
46	BX	0.51	0/740	0.78	0/995
46	DX	0.48	0/740	0.73	0/995
47	BY	0.61	0/680	0.93	1/904 (0.1%)
47	DY	0.46	0/789	0.82	1/1053 (0.1%)
48	BZ	0.41	0/1436	0.72	0/1951
48	DZ	0.36	0/1436	0.70	0/1951
49	B0	0.47	0/671	0.74	0/892
49	D0	0.41	0/671	0.67	0/892
50	B1	0.49	0/739	0.76	1/983 (0.1%)
50	D1	0.43	0/739	0.76	0/983
51	B2	0.45	0/600	0.74	0/793
51	D2	0.39	0/600	0.67	0/793
52	B3	0.48	0/473	0.76	0/636
52	D3	0.34	0/473	0.63	0/636
53	B4	0.43	0/349	0.71	0/474
53	D4	0.39	0/349	0.64	0/474
54	B5	0.62	0/473	1.04	2/639 (0.3%)
54	D5	0.50	0/473	0.82	0/639
55	B6	0.72	0/409	1.07	0/548
55	D6	0.70	0/397	1.12	4/531 (0.8%)
56	B7	0.55	0/427	0.80	0/563
56	D7	0.48	0/427	0.73	0/563
57	B8	0.63	0/516	1.02	2/681 (0.3%)
57	D8	0.51	0/516	0.87	1/681 (0.1%)
58	B9	0.53	0/302	0.80	0/397
58	D9	0.39	0/302	0.70	0/397
59	CX	0.47	0/1832	0.75	1/2855 (0.0%)
All	All	0.51	21/318243 (0.0%)	0.77	239/475835 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	35
1	CA	1	31
19	AS	0	1
23	AW	0	1
23	CW	0	1
24	AX	0	1
27	BA	4	96
27	DA	0	63
28	BB	0	3
28	DB	0	6
42	BT	0	1
59	CX	0	2
All	All	5	241

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	46	A	C6-N6	-11.79	1.24	1.33
1	CA	101	A	C6-N6	-8.09	1.27	1.33
1	CA	1458	G	C5-C6	-7.73	1.34	1.42
1	CA	70	G	C5-C6	-7.36	1.34	1.42
1	CA	1446	U	N1-C2	-7.30	1.31	1.38

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	46	A	C5-C6-N1	-12.54	111.43	117.70
28	DB	53	A	O5'-P-OP2	11.96	125.06	110.70
24	AX	46	A	C6-N1-C2	10.83	125.10	118.60
24	AX	46	A	N1-C2-N3	-10.72	123.94	129.30
27	BA	1992	G	C2'-C3'-O3'	10.30	132.16	109.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	BA	1378	A	C3'
27	BA	1799	G	C3'
27	BA	1992	G	C3'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
27	BA	2497	A	C3'
1	CA	533	A	C3'

5 of 241 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	181	G	Sidechain
1	AA	298	A	Sidechain
1	AA	37	U	Sidechain
1	AA	388	G	Sidechain
1	AA	490	G	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32132	0	16219	1429	0
1	CA	32098	0	16199	1614	0
2	AB	1901	0	1951	312	0
2	CB	1901	0	1951	269	0
3	AC	1613	0	1677	278	0
3	CC	1604	0	1670	270	0
4	AD	1703	0	1763	264	0
4	CD	1703	0	1763	197	0
5	AE	1147	0	1207	160	0
5	CE	1147	0	1207	172	0
6	AF	843	0	857	91	0
6	CF	843	0	857	99	0
7	AG	1257	0	1296	161	0
7	CG	1249	0	1286	155	0
8	AH	1116	0	1177	165	0
8	CH	1116	0	1177	143	0
9	AI	1006	0	1034	176	0
9	CI	1006	0	1034	201	0
10	AJ	795	0	840	159	0
10	CJ	795	0	840	175	0
11	AK	864	0	881	94	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	CK	885	0	904	117	0
12	AL	971	0	1057	122	0
12	CL	971	0	1057	128	0
13	AM	965	0	1034	166	0
13	CM	937	0	995	162	0
14	AN	492	0	533	77	0
14	CN	492	0	533	108	0
15	AO	734	0	771	94	0
15	CO	734	0	771	99	0
16	AP	701	0	720	107	0
16	CP	701	0	720	96	0
17	AQ	824	0	891	114	0
17	CQ	824	0	891	125	0
18	AR	574	0	644	87	0
18	CR	574	0	644	83	0
19	AS	630	0	652	126	0
19	CS	630	0	652	110	0
20	AT	763	0	861	134	0
20	CT	763	0	861	131	0
21	AU	209	0	221	26	0
21	CU	209	0	221	24	0
22	AV	205	0	106	7	0
22	CV	213	0	110	11	0
23	AW	1573	0	800	86	0
23	CW	1573	0	800	72	0
24	AX	1639	0	835	72	0
25	AY	1591	0	810	72	0
25	CY	1591	0	810	81	0
26	AZ	47	0	40	11	0
26	CZ	47	0	40	14	0
27	BA	60072	0	30294	2481	0
27	DA	59767	0	30140	2934	0
28	BB	2551	0	1295	107	0
28	DB	2551	0	1295	201	0
29	BC	1142	0	865	119	0
29	DC	1142	0	865	116	0
30	BD	2105	0	2182	345	0
30	DD	2105	0	2182	317	0
31	BE	1564	0	1629	250	0
31	DE	1564	0	1629	346	0
32	BF	1607	0	1652	226	0
32	DF	1624	0	1677	293	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	BG	1474	0	1535	250	0
33	DG	1474	0	1535	310	0
34	BH	1233	0	1294	217	0
34	DH	1223	0	1282	184	0
35	BI	1132	0	1218	207	0
35	DI	1132	0	1218	223	0
36	BN	1105	0	1180	153	0
36	DN	1105	0	1180	195	0
37	BO	933	0	996	114	0
37	DO	933	0	996	145	0
38	BP	1114	0	1187	303	0
38	DP	1114	0	1187	329	0
39	BQ	1107	0	1166	179	0
39	DQ	1094	0	1141	150	0
40	BR	960	0	1021	148	0
40	DR	960	0	1021	182	0
41	BS	771	0	832	185	0
41	DS	771	0	832	188	0
42	BT	1142	0	1202	236	0
42	DT	1142	0	1202	303	0
43	BU	958	0	1014	151	0
43	DU	958	0	1015	187	0
44	BV	779	0	852	162	0
44	DV	779	0	852	141	0
45	BW	896	0	953	108	0
45	DW	896	0	953	135	0
46	BX	726	0	778	75	0
46	DX	726	0	778	87	0
47	BY	672	0	766	190	0
47	DY	776	0	870	211	0
48	BZ	1404	0	1432	215	0
48	DZ	1404	0	1432	266	0
49	B0	662	0	688	83	0
49	D0	662	0	688	92	0
50	B1	732	0	808	97	0
50	D1	732	0	808	98	0
51	B2	598	0	653	75	0
51	D2	598	0	653	95	0
52	B3	468	0	523	46	0
52	D3	468	0	523	71	0
53	B4	344	0	305	69	0
53	D4	344	0	305	62	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	B5	459	0	476	80	0
54	D5	459	0	477	62	0
55	B6	402	0	413	109	0
55	D6	390	0	404	135	0
56	B7	419	0	467	46	0
56	D7	419	0	467	41	0
57	B8	508	0	576	130	0
57	D8	508	0	576	138	0
58	B9	299	0	323	34	0
58	D9	299	0	323	57	0
59	CX	1640	0	837	62	0
60	AA	114	0	0	0	0
60	AG	1	0	0	0	0
60	AW	4	0	0	0	0
60	AX	9	0	0	0	0
60	B0	3	0	0	0	0
60	B5	1	0	0	0	0
60	BA	334	0	0	0	0
60	BB	5	0	0	0	0
60	BD	1	0	0	0	0
60	BE	3	0	0	0	0
60	BF	1	0	0	0	0
60	BG	1	0	0	0	0
60	BP	2	0	0	0	0
60	BR	1	0	0	0	0
60	BU	2	0	0	0	0
60	BX	1	0	0	0	0
60	CA	102	0	0	0	0
60	CE	1	0	0	0	0
60	CK	1	0	0	0	0
60	CV	1	0	0	0	0
60	CW	4	0	0	0	0
60	D0	1	0	0	0	0
60	D5	1	0	0	0	0
60	D7	1	0	0	0	0
60	DA	239	0	0	0	0
60	DB	3	0	0	0	0
60	DD	2	0	0	0	0
60	DE	1	0	0	0	0
60	DF	1	0	0	0	0
60	DO	1	0	0	0	0
61	AD	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B4	1	0	0	0	0
61	B5	1	0	0	0	0
61	B9	1	0	0	0	0
61	CD	1	0	0	0	0
61	D4	1	0	0	0	0
61	D5	1	0	0	0	0
61	D9	1	0	0	0	0
All	All	293848	0	198788	22560	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 46.

The worst 5 of 22560 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)
55:B6:15:GLU:CD	55:B6:18:ARG:HE	1.41	1.22
4:AD:19:LEU:HD11	4:AD:67:ILE:HG13	1.24	1.19
1:CA:1321:C:H3'	1:CA:1322:C:H5''	1.21	1.19
13:AM:90:LEU:HD23	13:AM:93:ARG:HG2	1.23	1.18
2:AB:166:ASP:HB3	2:AB:169:LYS:HB2	1.24	1.18

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	147 (63%)	57 (24%)	29 (12%)	0	5
2	CB	233/256 (91%)	144 (62%)	56 (24%)	33 (14%)	0	3
3	AC	205/239 (86%)	122 (60%)	53 (26%)	30 (15%)	0	3
3	CC	202/239 (84%)	116 (57%)	48 (24%)	38 (19%)	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AD	206/209 (99%)	138 (67%)	39 (19%)	29 (14%)	0	3
4	CD	206/209 (99%)	141 (68%)	39 (19%)	26 (13%)	0	5
5	AE	149/162 (92%)	98 (66%)	34 (23%)	17 (11%)	0	6
5	CE	149/162 (92%)	107 (72%)	27 (18%)	15 (10%)	1	8
6	AF	99/101 (98%)	74 (75%)	16 (16%)	9 (9%)	1	9
6	CF	99/101 (98%)	71 (72%)	21 (21%)	7 (7%)	1	14
7	AG	153/156 (98%)	108 (71%)	28 (18%)	17 (11%)	0	7
7	CG	150/156 (96%)	93 (62%)	39 (26%)	18 (12%)	0	6
8	AH	136/138 (99%)	87 (64%)	37 (27%)	12 (9%)	1	10
8	CH	136/138 (99%)	92 (68%)	37 (27%)	7 (5%)	2	22
9	AI	125/128 (98%)	86 (69%)	26 (21%)	13 (10%)	0	7
9	CI	125/128 (98%)	72 (58%)	43 (34%)	10 (8%)	1	12
10	AJ	97/105 (92%)	59 (61%)	27 (28%)	11 (11%)	0	6
10	CJ	97/105 (92%)	52 (54%)	34 (35%)	11 (11%)	0	6
11	AK	114/129 (88%)	82 (72%)	26 (23%)	6 (5%)	2	21
11	CK	117/129 (91%)	81 (69%)	25 (21%)	11 (9%)	1	9
12	AL	123/132 (93%)	78 (63%)	29 (24%)	16 (13%)	0	4
12	CL	123/132 (93%)	82 (67%)	19 (15%)	22 (18%)	0	2
13	AM	120/126 (95%)	69 (58%)	28 (23%)	23 (19%)	0	2
13	CM	116/126 (92%)	66 (57%)	24 (21%)	26 (22%)	0	1
14	AN	58/61 (95%)	33 (57%)	17 (29%)	8 (14%)	0	4
14	CN	58/61 (95%)	40 (69%)	11 (19%)	7 (12%)	0	6
15	AO	86/89 (97%)	61 (71%)	16 (19%)	9 (10%)	0	7
15	CO	86/89 (97%)	62 (72%)	15 (17%)	9 (10%)	0	7
16	AP	82/88 (93%)	54 (66%)	19 (23%)	9 (11%)	0	7
16	CP	82/88 (93%)	56 (68%)	24 (29%)	2 (2%)	7	42
17	AQ	98/105 (93%)	76 (78%)	13 (13%)	9 (9%)	1	9
17	CQ	98/105 (93%)	64 (65%)	23 (24%)	11 (11%)	0	6
18	AR	68/88 (77%)	48 (71%)	14 (21%)	6 (9%)	1	10
18	CR	68/88 (77%)	50 (74%)	11 (16%)	7 (10%)	0	8
19	AS	77/93 (83%)	46 (60%)	13 (17%)	18 (23%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	CS	77/93 (83%)	49 (64%)	18 (23%)	10 (13%)	0	4
20	AT	97/106 (92%)	57 (59%)	25 (26%)	15 (16%)	0	3
20	CT	97/106 (92%)	64 (66%)	18 (19%)	15 (16%)	0	3
21	AU	23/27 (85%)	15 (65%)	7 (30%)	1 (4%)	3	27
21	CU	23/27 (85%)	19 (83%)	1 (4%)	3 (13%)	0	4
29	BC	183/229 (80%)	67 (37%)	66 (36%)	50 (27%)	0	0
29	DC	183/229 (80%)	62 (34%)	69 (38%)	52 (28%)	0	0
30	BD	270/276 (98%)	175 (65%)	54 (20%)	41 (15%)	0	3
30	DD	270/276 (98%)	180 (67%)	51 (19%)	39 (14%)	0	3
31	BE	203/206 (98%)	133 (66%)	38 (19%)	32 (16%)	0	2
31	DE	203/206 (98%)	115 (57%)	49 (24%)	39 (19%)	0	2
32	BF	204/210 (97%)	141 (69%)	40 (20%)	23 (11%)	0	6
32	DF	206/210 (98%)	126 (61%)	44 (21%)	36 (18%)	0	2
33	BG	179/182 (98%)	114 (64%)	31 (17%)	34 (19%)	0	2
33	DG	179/182 (98%)	98 (55%)	53 (30%)	28 (16%)	0	3
34	BH	159/180 (88%)	92 (58%)	31 (20%)	36 (23%)	0	1
34	DH	158/180 (88%)	96 (61%)	30 (19%)	32 (20%)	0	1
35	BI	144/148 (97%)	72 (50%)	37 (26%)	35 (24%)	0	1
35	DI	144/148 (97%)	73 (51%)	48 (33%)	23 (16%)	0	2
36	BN	137/140 (98%)	98 (72%)	23 (17%)	16 (12%)	0	6
36	DN	137/140 (98%)	83 (61%)	30 (22%)	24 (18%)	0	2
37	BO	120/122 (98%)	95 (79%)	19 (16%)	6 (5%)	2	23
37	DO	120/122 (98%)	84 (70%)	23 (19%)	13 (11%)	0	7
38	BP	144/150 (96%)	68 (47%)	33 (23%)	43 (30%)	0	0
38	DP	144/150 (96%)	69 (48%)	38 (26%)	37 (26%)	0	1
39	BQ	137/141 (97%)	99 (72%)	25 (18%)	13 (10%)	1	9
39	DQ	134/141 (95%)	86 (64%)	28 (21%)	20 (15%)	0	3
40	BR	115/118 (98%)	73 (64%)	24 (21%)	18 (16%)	0	2
40	DR	115/118 (98%)	69 (60%)	29 (25%)	17 (15%)	0	3
41	BS	97/112 (87%)	46 (47%)	25 (26%)	26 (27%)	0	1
41	DS	97/112 (87%)	44 (45%)	28 (29%)	25 (26%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BT	136/146 (93%)	81 (60%)	25 (18%)	30 (22%)	0	1
42	DT	136/146 (93%)	71 (52%)	28 (21%)	37 (27%)	0	0
43	BU	115/118 (98%)	79 (69%)	27 (24%)	9 (8%)	1	12
43	DU	115/118 (98%)	63 (55%)	36 (31%)	16 (14%)	0	4
44	BV	99/101 (98%)	59 (60%)	18 (18%)	22 (22%)	0	1
44	DV	99/101 (98%)	56 (57%)	25 (25%)	18 (18%)	0	2
45	BW	111/113 (98%)	86 (78%)	20 (18%)	5 (4%)	3	26
45	DW	111/113 (98%)	74 (67%)	23 (21%)	14 (13%)	0	5
46	BX	91/96 (95%)	71 (78%)	19 (21%)	1 (1%)	17	58
46	DX	91/96 (95%)	63 (69%)	16 (18%)	12 (13%)	0	4
47	BY	84/110 (76%)	30 (36%)	25 (30%)	29 (34%)	0	0
47	DY	99/110 (90%)	36 (36%)	27 (27%)	36 (36%)	0	0
48	BZ	175/206 (85%)	94 (54%)	46 (26%)	35 (20%)	0	2
48	DZ	175/206 (85%)	85 (49%)	52 (30%)	38 (22%)	0	1
49	B0	82/85 (96%)	66 (80%)	11 (13%)	5 (6%)	2	18
49	D0	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	2	23
50	B1	92/98 (94%)	72 (78%)	13 (14%)	7 (8%)	1	12
50	D1	92/98 (94%)	70 (76%)	11 (12%)	11 (12%)	0	6
51	B2	69/72 (96%)	43 (62%)	13 (19%)	13 (19%)	0	2
51	D2	69/72 (96%)	41 (59%)	16 (23%)	12 (17%)	0	2
52	B3	58/60 (97%)	49 (84%)	4 (7%)	5 (9%)	1	11
52	D3	58/60 (97%)	46 (79%)	6 (10%)	6 (10%)	0	8
53	B4	45/71 (63%)	18 (40%)	10 (22%)	17 (38%)	0	0
53	D4	45/71 (63%)	19 (42%)	11 (24%)	15 (33%)	0	0
54	B5	57/60 (95%)	41 (72%)	8 (14%)	8 (14%)	0	4
54	D5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	0	5
55	B6	46/54 (85%)	18 (39%)	9 (20%)	19 (41%)	0	0
55	D6	44/54 (82%)	15 (34%)	12 (27%)	17 (39%)	0	0
56	B7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	17
56	D7	47/49 (96%)	40 (85%)	5 (11%)	2 (4%)	3	27
57	B8	62/65 (95%)	30 (48%)	19 (31%)	13 (21%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	D8	62/65 (95%)	33 (53%)	17 (27%)	12 (19%)	0	2
58	B9	34/37 (92%)	27 (79%)	5 (15%)	2 (6%)	2	19
58	D9	34/37 (92%)	24 (71%)	7 (21%)	3 (9%)	1	10
All	All	11692/12586 (93%)	7260 (62%)	2616 (22%)	1816 (16%)	0	3

5 of 1816 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	24	TRP
2	AB	122	PHE
2	AB	128	GLU
2	AB	154	LEU

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%)	177 (88%)	25 (12%)	5	26
2	CB	202/220 (92%)	177 (88%)	25 (12%)	5	26
3	AC	160/188 (85%)	144 (90%)	16 (10%)	9	36
3	CC	159/188 (85%)	142 (89%)	17 (11%)	8	33
4	AD	180/181 (99%)	159 (88%)	21 (12%)	6	28
4	CD	180/181 (99%)	162 (90%)	18 (10%)	9	36
5	AE	115/123 (94%)	103 (90%)	12 (10%)	8	35
5	CE	115/123 (94%)	99 (86%)	16 (14%)	4	22
6	AF	90/90 (100%)	82 (91%)	8 (9%)	11	42
6	CF	90/90 (100%)	79 (88%)	11 (12%)	6	27
7	AG	126/127 (99%)	109 (86%)	17 (14%)	4	23
7	CG	125/127 (98%)	115 (92%)	10 (8%)	14	48
8	AH	119/119 (100%)	106 (89%)	13 (11%)	7	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	119/119 (100%)	105 (88%)	14 (12%)	6	28
9	AI	97/99 (98%)	85 (88%)	12 (12%)	5	26
9	CI	97/99 (98%)	82 (84%)	15 (16%)	3	17
10	AJ	88/92 (96%)	73 (83%)	15 (17%)	2	13
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	5	26
11	AK	88/99 (89%)	82 (93%)	6 (7%)	18	56
11	CK	90/99 (91%)	83 (92%)	7 (8%)	15	48
12	AL	104/109 (95%)	92 (88%)	12 (12%)	6	29
12	CL	104/109 (95%)	92 (88%)	12 (12%)	6	29
13	AM	97/101 (96%)	84 (87%)	13 (13%)	4	23
13	CM	94/101 (93%)	82 (87%)	12 (13%)	5	25
14	AN	49/50 (98%)	43 (88%)	6 (12%)	6	27
14	CN	49/50 (98%)	47 (96%)	2 (4%)	35	70
15	AO	79/80 (99%)	71 (90%)	8 (10%)	9	36
15	CO	79/80 (99%)	69 (87%)	10 (13%)	5	25
16	AP	72/74 (97%)	62 (86%)	10 (14%)	4	22
16	CP	72/74 (97%)	65 (90%)	7 (10%)	9	37
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	12	44
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	26	62
18	AR	61/77 (79%)	57 (93%)	4 (7%)	19	57
18	CR	61/77 (79%)	53 (87%)	8 (13%)	5	24
19	AS	69/80 (86%)	55 (80%)	14 (20%)	1	7
19	CS	69/80 (86%)	55 (80%)	14 (20%)	1	7
20	AT	76/82 (93%)	63 (83%)	13 (17%)	2	13
20	CT	76/82 (93%)	66 (87%)	10 (13%)	5	24
21	AU	19/22 (86%)	17 (90%)	2 (10%)	8	34
21	CU	19/22 (86%)	17 (90%)	2 (10%)	8	34
26	AZ	1/1 (100%)	1 (100%)	0	100	100
26	CZ	1/1 (100%)	1 (100%)	0	100	100
29	BC	61/181 (34%)	55 (90%)	6 (10%)	9	37
29	DC	61/181 (34%)	52 (85%)	9 (15%)	3	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BD	213/218 (98%)	184 (86%)	29 (14%)	4	23
30	DD	213/218 (98%)	183 (86%)	30 (14%)	4	21
31	BE	165/166 (99%)	142 (86%)	23 (14%)	4	22
31	DE	165/166 (99%)	133 (81%)	32 (19%)	1	8
32	BF	163/166 (98%)	142 (87%)	21 (13%)	5	25
32	DF	165/166 (99%)	143 (87%)	22 (13%)	4	24
33	BG	155/156 (99%)	136 (88%)	19 (12%)	5	27
33	DG	155/156 (99%)	133 (86%)	22 (14%)	4	21
34	BH	134/148 (90%)	116 (87%)	18 (13%)	4	23
34	DH	132/148 (89%)	119 (90%)	13 (10%)	9	37
35	BI	122/124 (98%)	107 (88%)	15 (12%)	5	27
35	DI	122/124 (98%)	104 (85%)	18 (15%)	3	19
36	BN	117/119 (98%)	94 (80%)	23 (20%)	1	7
36	DN	117/119 (98%)	98 (84%)	19 (16%)	3	15
37	BO	100/100 (100%)	84 (84%)	16 (16%)	3	16
37	DO	100/100 (100%)	88 (88%)	12 (12%)	6	27
38	BP	112/116 (97%)	86 (77%)	26 (23%)	1	4
38	DP	112/116 (97%)	90 (80%)	22 (20%)	1	8
39	BQ	110/111 (99%)	89 (81%)	21 (19%)	2	8
39	DQ	108/111 (97%)	96 (89%)	12 (11%)	7	31
40	BR	100/101 (99%)	83 (83%)	17 (17%)	2	13
40	DR	100/101 (99%)	84 (84%)	16 (16%)	3	16
41	BS	77/88 (88%)	53 (69%)	24 (31%)	0	2
41	DS	77/88 (88%)	67 (87%)	10 (13%)	5	24
42	BT	120/127 (94%)	88 (73%)	32 (27%)	0	3
42	DT	120/127 (94%)	87 (72%)	33 (28%)	0	3
43	BU	92/94 (98%)	78 (85%)	14 (15%)	3	18
43	DU	92/94 (98%)	82 (89%)	10 (11%)	7	32
44	BV	82/82 (100%)	64 (78%)	18 (22%)	1	5
44	DV	82/82 (100%)	65 (79%)	17 (21%)	1	6
45	BW	91/92 (99%)	78 (86%)	13 (14%)	4	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DW	91/92 (99%)	84 (92%)	7 (8%)	15	49
46	BX	74/78 (95%)	63 (85%)	11 (15%)	3	19
46	DX	74/78 (95%)	58 (78%)	16 (22%)	1	5
47	BY	73/91 (80%)	59 (81%)	14 (19%)	1	8
47	DY	84/91 (92%)	69 (82%)	15 (18%)	2	11
48	BZ	155/179 (87%)	131 (84%)	24 (16%)	3	17
48	DZ	155/179 (87%)	138 (89%)	17 (11%)	7	32
49	B0	66/67 (98%)	60 (91%)	6 (9%)	11	41
49	D0	66/67 (98%)	58 (88%)	8 (12%)	6	27
50	B1	78/83 (94%)	65 (83%)	13 (17%)	2	14
50	D1	78/83 (94%)	72 (92%)	6 (8%)	15	49
51	B2	66/67 (98%)	52 (79%)	14 (21%)	1	6
51	D2	66/67 (98%)	58 (88%)	8 (12%)	6	27
52	B3	51/52 (98%)	44 (86%)	7 (14%)	4	22
52	D3	51/52 (98%)	46 (90%)	5 (10%)	9	37
53	B4	34/63 (54%)	30 (88%)	4 (12%)	6	28
53	D4	34/63 (54%)	28 (82%)	6 (18%)	2	11
54	B5	51/52 (98%)	42 (82%)	9 (18%)	2	11
54	D5	51/52 (98%)	41 (80%)	10 (20%)	1	8
55	B6	44/52 (85%)	27 (61%)	17 (39%)	0	1
55	D6	44/52 (85%)	30 (68%)	14 (32%)	0	2
56	B7	41/42 (98%)	37 (90%)	4 (10%)	9	37
56	D7	41/42 (98%)	35 (85%)	6 (15%)	3	20
57	B8	53/55 (96%)	40 (76%)	13 (24%)	1	4
57	D8	53/55 (96%)	39 (74%)	14 (26%)	0	3
58	B9	33/34 (97%)	32 (97%)	1 (3%)	46	78
58	D9	33/34 (97%)	31 (94%)	2 (6%)	22	59
All	All	9644/10430 (92%)	8280 (86%)	1364 (14%)	4	21

5 of 1364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BZ	167	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	CD	138	TYR
47	DY	42	VAL
50	B1	80	LEU
56	B7	48	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 345 such sidechains are listed below:

Mol	Chain	Res	Type
50	B1	45	ASN
3	CC	181	ASN
46	DX	41	ASN
51	B2	43	GLN
58	B9	20	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1493/1508 (99%)	234 (15%)	56 (3%)
1	CA	1491/1508 (98%)	248 (16%)	61 (4%)
22	AV	9/30 (30%)	1 (11%)	0
22	CV	9/30 (30%)	2 (22%)	0
23	AW	73/75 (97%)	15 (20%)	3 (4%)
23	CW	73/75 (97%)	20 (27%)	3 (4%)
24	AX	76/77 (98%)	24 (31%)	4 (5%)
25	AY	74/75 (98%)	19 (25%)	0
25	CY	74/75 (98%)	20 (27%)	0
27	BA	2779/2915 (95%)	539 (19%)	96 (3%)
27	DA	2765/2915 (94%)	555 (20%)	114 (4%)
28	BB	118/122 (96%)	16 (13%)	3 (2%)
28	DB	118/122 (96%)	40 (33%)	5 (4%)
59	CX	76/77 (98%)	21 (27%)	2 (2%)
All	All	9228/9604 (96%)	1754 (19%)	347 (3%)

5 of 1754 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	28	G
1	AA	31	G
1	AA	32	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	AA	39	G

5 of 347 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	2778	A
1	CA	968	A
27	DA	2490	G
28	BB	66	A
1	CA	366	C

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
26	KBE	AZ	1	26	8,8,9	1.45	1 (12%)	7,8,10	2.51	2 (28%)
26	DPP	AZ	2	26	4,5,6	1.49	1 (25%)	1,5,7	2.35	1 (100%)
26	UAL	AZ	3	26	8,8,9	2.26	2 (25%)	4,9,11	1.96	1 (25%)
26	MYN	AZ	4	26	10,11,12	1.66	1 (10%)	8,14,16	1.40	1 (12%)
26	DPP	AZ	5	26	4,5,6	1.26	1 (25%)	1,5,7	1.66	0
26	KBE	CZ	1	26	8,8,9	1.18	1 (12%)	7,8,10	2.15	2 (28%)
26	DPP	CZ	2	26	4,5,6	0.98	0	1,5,7	2.13	1 (100%)
26	UAL	CZ	3	26	8,8,9	2.27	2 (25%)	4,9,11	1.51	1 (25%)
26	MYN	CZ	4	26	10,11,12	1.30	1 (10%)	8,14,16	1.45	1 (12%)
26	DPP	CZ	5	26	4,5,6	0.89	0	1,5,7	1.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	KBE	AZ	1	26	-	0/7/7/8	0/0/0/0
26	DPP	AZ	2	26	-	0/2/4/6	0/0/0/0
26	UAL	AZ	3	26	-	0/3/7/9	0/0/0/0
26	MYN	AZ	4	26	-	0/1/16/18	0/1/1/1
26	DPP	AZ	5	26	-	0/2/4/6	0/0/0/0
26	KBE	CZ	1	26	-	0/7/7/8	0/0/0/0
26	DPP	CZ	2	26	-	0/2/4/6	0/0/0/0
26	UAL	CZ	3	26	-	0/3/7/9	0/0/0/0
26	MYN	CZ	4	26	-	0/1/16/18	0/1/1/1
26	DPP	CZ	5	26	-	0/2/4/6	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AZ	3	UAL	C1-N1	-4.08	1.33	1.40
26	CZ	3	UAL	C1-N1	-3.82	1.33	1.40
26	AZ	1	KBE	CA-C	-3.61	1.39	1.49
26	CZ	1	KBE	CA-C	-3.16	1.40	1.49
26	AZ	5	DPP	CA-C	2.35	1.53	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AZ	3	UAL	O-C-CA	-3.72	120.72	125.47
26	CZ	3	UAL	O-C-CA	-2.74	121.97	125.47
26	AZ	1	KBE	O-C-CA	-2.55	117.22	125.48
26	AZ	4	MYN	CA-CB-N1	-2.54	107.30	111.41
26	CZ	4	MYN	CG-CB-CA	-2.48	109.33	112.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	AZ	1	KBE	5	0
26	AZ	2	DPP	4	0
26	AZ	3	UAL	3	0
26	AZ	4	MYN	3	0
26	CZ	1	KBE	10	0
26	CZ	2	DPP	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	CZ	3	UAL	2	0
26	CZ	4	MYN	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 850 ligands modelled in this entry, 850 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](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1495/1508 (99%)	-0.07	28 (1%) 67 61	32, 72, 154, 200	0
1	CA	1493/1508 (99%)	0.16	31 (2%) 64 58	38, 81, 158, 200	0
2	AB	235/256 (91%)	0.19	10 (4%) 36 31	69, 98, 133, 148	0
2	CB	235/256 (91%)	0.30	19 (8%) 13 14	74, 103, 147, 165	0
3	AC	207/239 (86%)	-0.05	1 (0%) 90 87	66, 86, 109, 114	0
3	CC	206/239 (86%)	0.26	15 (7%) 16 16	76, 98, 123, 136	0
4	AD	208/209 (99%)	0.21	6 (2%) 52 45	52, 73, 87, 92	0
4	CD	208/209 (99%)	0.10	1 (0%) 90 87	47, 68, 85, 89	0
5	AE	151/162 (93%)	-0.12	0 100 100	49, 67, 94, 107	0
5	CE	151/162 (93%)	0.09	1 (0%) 87 83	53, 75, 94, 100	0
6	AF	101/101 (100%)	-0.37	0 100 100	54, 69, 84, 98	0
6	CF	101/101 (100%)	-0.01	2 (1%) 65 60	49, 73, 83, 98	0
7	AG	155/156 (99%)	0.42	11 (7%) 17 16	62, 82, 107, 124	0
7	CG	154/156 (98%)	0.15	12 (7%) 14 14	69, 92, 116, 124	0
8	AH	138/138 (100%)	0.33	2 (1%) 75 70	54, 71, 82, 96	0
8	CH	138/138 (100%)	0.29	4 (2%) 52 45	55, 75, 87, 97	0
9	AI	127/128 (99%)	0.73	18 (14%) 3 4	57, 99, 123, 126	0
9	CI	127/128 (99%)	0.81	16 (12%) 4 6	72, 106, 123, 129	0
10	AJ	99/105 (94%)	1.08	24 (24%) 1 1	69, 108, 130, 130	0
10	CJ	99/105 (94%)	1.07	19 (19%) 1 2	79, 115, 136, 143	0
11	AK	116/129 (89%)	0.28	4 (3%) 46 40	53, 67, 89, 107	0
11	CK	119/129 (92%)	0.40	10 (8%) 12 13	56, 76, 99, 114	0
12	AL	125/132 (94%)	0.23	5 (4%) 39 34	49, 63, 80, 103	0
12	CL	125/132 (94%)	0.23	6 (4%) 31 27	51, 71, 83, 99	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	122/126 (96%)	0.07	3 (2%) 58 51	63, 87, 97, 102	0
13	CM	118/126 (93%)	0.25	7 (5%) 23 21	77, 100, 114, 120	0
14	AN	60/61 (98%)	0.17	0 100 100	52, 77, 91, 97	0
14	CN	60/61 (98%)	1.01	6 (10%) 8 9	75, 92, 101, 105	0
15	AO	88/89 (98%)	-0.12	0 100 100	47, 65, 82, 93	0
15	CO	88/89 (98%)	-0.12	0 100 100	50, 70, 87, 92	0
16	AP	84/88 (95%)	0.65	7 (8%) 12 13	50, 68, 95, 109	0
16	CP	84/88 (95%)	0.53	7 (8%) 12 13	55, 66, 85, 109	0
17	AQ	100/105 (95%)	-0.19	0 100 100	53, 69, 84, 88	0
17	CQ	100/105 (95%)	0.24	5 (5%) 30 26	59, 73, 91, 94	0
18	AR	70/88 (79%)	0.45	2 (2%) 52 45	49, 68, 94, 100	0
18	CR	70/88 (79%)	-0.05	2 (2%) 52 45	56, 74, 99, 104	0
19	AS	79/93 (84%)	0.95	14 (17%) 2 2	63, 90, 110, 115	0
19	CS	79/93 (84%)	1.53	22 (27%) 1 1	91, 111, 132, 138	0
20	AT	99/106 (93%)	0.45	3 (3%) 51 44	54, 75, 104, 110	0
20	CT	99/106 (93%)	0.51	5 (5%) 29 25	63, 76, 111, 114	0
21	AU	25/27 (92%)	1.33	5 (20%) 1 1	74, 82, 90, 95	0
21	CU	25/27 (92%)	2.34	14 (56%) 0 0	72, 93, 105, 109	0
22	AV	10/30 (33%)	1.00	2 (20%) 1 1	51, 66, 125, 128	0
22	CV	10/30 (33%)	0.98	2 (20%) 1 1	65, 81, 134, 138	0
23	AW	74/75 (98%)	0.33	4 (5%) 26 24	49, 117, 149, 154	0
23	CW	74/75 (98%)	0.92	5 (6%) 18 18	79, 129, 148, 165	0
24	AX	77/77 (100%)	0.02	2 (2%) 56 49	35, 85, 115, 128	0
25	AY	75/75 (100%)	0.77	11 (14%) 3 4	62, 157, 189, 191	0
25	CY	75/75 (100%)	0.87	9 (12%) 5 7	76, 170, 192, 197	0
26	AZ	1/6 (16%)	-0.54	0 100 100	64, 64, 64, 64	0
26	CZ	1/6 (16%)	-0.04	0 100 100	91, 91, 91, 91	0
27	BA	2789/2915 (95%)	-0.19	54 (1%) 67 61	19, 44, 164, 200	0
27	DA	2775/2915 (95%)	0.48	78 (2%) 53 47	30, 72, 170, 200	0
28	BB	119/122 (97%)	-0.14	3 (2%) 58 51	36, 70, 127, 168	0
28	DB	119/122 (97%)	1.10	25 (21%) 1 1	109, 142, 170, 179	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	BC	191/229 (83%)	2.50	98 (51%) 0 0	103, 169, 180, 186	0
29	DC	191/229 (83%)	2.38	93 (48%) 0 0	125, 170, 183, 186	0
30	BD	272/276 (98%)	-0.28	0 100 100	18, 41, 61, 73	0
30	DD	272/276 (98%)	0.10	4 (1%) 74 68	31, 52, 69, 81	0
31	BE	205/206 (99%)	-0.24	3 (1%) 74 68	16, 42, 76, 94	0
31	DE	205/206 (99%)	0.51	9 (4%) 35 30	44, 80, 112, 119	0
32	BF	206/210 (98%)	-0.22	3 (1%) 74 68	17, 46, 110, 129	0
32	DF	208/210 (99%)	0.52	9 (4%) 36 31	40, 69, 120, 132	0
33	BG	181/182 (99%)	0.30	7 (3%) 40 35	49, 74, 102, 119	0
33	DG	181/182 (99%)	0.63	16 (8%) 11 12	75, 101, 117, 125	0
34	BH	161/180 (89%)	0.17	7 (4%) 36 31	39, 65, 81, 95	0
34	DH	160/180 (88%)	1.36	45 (28%) 1 1	106, 129, 153, 161	0
35	BI	146/148 (98%)	0.69	15 (10%) 7 9	57, 134, 150, 159	0
35	DI	146/148 (98%)	0.72	18 (12%) 5 6	62, 107, 139, 150	0
36	BN	139/140 (99%)	-0.08	1 (0%) 87 83	23, 43, 67, 73	0
36	DN	139/140 (99%)	0.90	17 (12%) 5 6	69, 86, 106, 108	0
37	BO	122/122 (100%)	-0.31	0 100 100	22, 44, 60, 67	0
37	DO	122/122 (100%)	0.32	3 (2%) 58 51	47, 72, 80, 86	0
38	BP	146/150 (97%)	0.16	5 (3%) 46 40	17, 60, 91, 121	0
38	DP	146/150 (97%)	0.98	14 (9%) 9 10	45, 82, 103, 126	0
39	BQ	139/141 (98%)	-0.11	0 100 100	29, 47, 70, 82	0
39	DQ	138/141 (97%)	0.83	13 (9%) 9 10	58, 88, 107, 136	0
40	BR	117/118 (99%)	-0.26	0 100 100	17, 37, 59, 66	0
40	DR	117/118 (99%)	0.34	0 100 100	39, 64, 81, 88	0
41	BS	99/112 (88%)	0.29	3 (3%) 51 44	40, 65, 82, 91	0
41	DS	99/112 (88%)	1.05	16 (16%) 2 3	71, 93, 106, 109	0
42	BT	138/146 (94%)	0.06	3 (2%) 62 55	27, 53, 108, 143	0
42	DT	138/146 (94%)	0.41	10 (7%) 16 16	64, 79, 136, 142	0
43	BU	117/118 (99%)	-0.31	0 100 100	20, 37, 59, 86	0
43	DU	117/118 (99%)	0.49	7 (5%) 23 21	48, 80, 111, 120	0
44	BV	101/101 (100%)	0.08	1 (0%) 82 76	18, 49, 68, 74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	DV	101/101 (100%)	0.53	9 (8%) 10 12	54, 100, 114, 122	0
45	BW	113/113 (100%)	-0.20	1 (0%) 84 78	21, 34, 64, 102	0
45	DW	113/113 (100%)	0.46	1 (0%) 84 78	39, 61, 93, 118	0
46	BX	93/96 (96%)	-0.15	0 100 100	31, 45, 69, 76	0
46	DX	93/96 (96%)	0.45	0 100 100	39, 66, 79, 85	0
47	BY	88/110 (80%)	0.59	5 (5%) 24 22	41, 58, 79, 87	0
47	DY	101/110 (91%)	1.53	31 (30%) 0 1	62, 83, 144, 153	0
48	BZ	177/206 (85%)	1.04	36 (20%) 1 1	52, 85, 159, 164	0
48	DZ	177/206 (85%)	1.72	49 (27%) 1 1	93, 123, 178, 184	0
49	B0	84/85 (98%)	0.35	5 (5%) 23 21	27, 49, 71, 85	0
49	D0	84/85 (98%)	1.30	24 (28%) 1 1	66, 82, 96, 104	0
50	B1	94/98 (95%)	0.07	0 100 100	28, 49, 80, 91	0
50	D1	94/98 (95%)	0.65	6 (6%) 20 19	40, 62, 94, 101	0
51	B2	71/72 (98%)	-0.09	1 (1%) 75 70	37, 62, 93, 106	0
51	D2	71/72 (98%)	0.22	1 (1%) 75 70	59, 78, 98, 117	0
52	B3	60/60 (100%)	0.16	1 (1%) 70 64	27, 44, 69, 103	0
52	D3	60/60 (100%)	1.61	23 (38%) 0 0	70, 88, 111, 119	0
53	B4	49/71 (69%)	-0.24	2 (4%) 38 33	72, 97, 116, 119	0
53	D4	49/71 (69%)	0.11	2 (4%) 38 33	100, 115, 120, 121	0
54	B5	59/60 (98%)	-0.13	3 (5%) 29 25	21, 38, 93, 115	0
54	D5	59/60 (98%)	0.50	6 (10%) 7 9	46, 62, 116, 136	0
55	B6	48/54 (88%)	-0.07	0 100 100	29, 58, 71, 90	0
55	D6	46/54 (85%)	1.01	8 (17%) 2 2	50, 81, 91, 101	0
56	B7	49/49 (100%)	-0.15	0 100 100	20, 32, 77, 90	0
56	D7	49/49 (100%)	0.68	3 (6%) 22 21	36, 47, 84, 92	0
57	B8	64/65 (98%)	0.46	4 (6%) 21 19	26, 44, 62, 99	0
57	D8	64/65 (98%)	1.12	6 (9%) 9 10	51, 66, 85, 109	0
58	B9	36/37 (97%)	0.63	1 (2%) 53 47	15, 45, 57, 59	0
58	D9	36/37 (97%)	1.47	12 (33%) 0 0	79, 94, 99, 102	0
59	CX	77/77 (100%)	0.25	2 (2%) 56 49	63, 100, 127, 140	0
All	All	21180/22202 (95%)	0.30	1204 (5%) 24 22	15, 72, 152, 200	0

The worst 5 of 1204 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	BC	179	SER	15.0
29	DC	57	ASN	13.1
29	DC	179	SER	12.9
48	DZ	110	VAL	12.8
27	DA	2802	G	12.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
26	KBE	CZ	1	9/10	0.81	0.52	-	95,98,100,100	0
26	DPP	CZ	2	6/7	0.88	0.21	-	92,93,95,98	0
26	UAL	AZ	3	9/10	0.87	0.24	-	63,66,70,71	0
26	DPP	CZ	5	6/7	0.85	0.26	-	88,89,89,90	0
26	MYN	AZ	4	11/12	0.90	0.23	-	61,64,65,65	0
26	DPP	AZ	2	6/7	0.93	0.21	-	66,67,69,71	0
26	MYN	CZ	4	11/12	0.86	0.22	-	88,89,91,92	0
26	DPP	AZ	5	6/7	0.93	0.20	-	62,64,65,65	0
26	UAL	CZ	3	9/10	0.81	0.28	-	91,92,93,93	0
26	KBE	AZ	1	9/10	0.83	0.59	-	71,74,78,79	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1646	1/1	0.15	1.02	56.45	71,71,71,71	0
60	MG	CA	1614	1/1	0.92	0.94	49.57	50,50,50,50	0
60	MG	AA	1621	1/1	0.90	0.66	39.83	28,28,28,28	0
60	MG	BA	3080	1/1	0.95	0.45	38.19	15,15,15,15	0
60	MG	BA	3293	1/1	0.88	0.55	28.68	45,45,45,45	0
60	MG	CA	1682	1/1	0.90	0.62	26.64	41,41,41,41	0
60	MG	BA	3021	1/1	0.94	0.39	25.54	1,1,1,1	0
60	MG	BA	3005	1/1	0.97	0.43	24.55	1,1,1,1	0
60	MG	BA	3131	1/1	0.93	0.35	24.42	1,1,1,1	0
60	MG	CA	1650	1/1	0.95	0.46	23.48	1,1,1,1	0
60	MG	AA	1642	1/1	0.91	0.41	20.64	41,41,41,41	0
60	MG	BA	3229	1/1	0.91	0.40	18.72	49,49,49,49	0
60	MG	BA	3121	1/1	0.93	0.50	18.15	23,23,23,23	0
60	MG	BA	3070	1/1	0.98	0.51	17.96	1,1,1,1	0
60	MG	BA	3177	1/1	0.78	0.43	17.68	41,41,41,41	0
60	MG	AA	1618	1/1	0.97	0.40	16.40	22,22,22,22	0
60	MG	CA	1683	1/1	0.86	0.52	16.40	53,53,53,53	0
60	MG	BA	3018	1/1	0.98	0.23	16.31	1,1,1,1	0
60	MG	BA	3142	1/1	0.83	0.36	16.23	30,30,30,30	0
60	MG	BA	3104	1/1	0.82	0.39	15.71	42,42,42,42	0
60	MG	BA	3076	1/1	0.97	0.38	15.62	1,1,1,1	0
60	MG	DA	3075	1/1	0.91	0.50	15.24	1,1,1,1	0
60	MG	BA	3227	1/1	0.91	0.37	14.50	33,33,33,33	0
60	MG	DA	3111	1/1	0.72	0.47	14.02	64,64,64,64	0
60	MG	AA	1643	1/1	0.84	0.31	13.38	29,29,29,29	0
60	MG	BA	3034	1/1	0.82	0.40	13.29	1,1,1,1	0
60	MG	BA	3020	1/1	0.97	0.40	12.97	1,1,1,1	0
60	MG	BA	3078	1/1	0.94	0.33	12.57	1,1,1,1	0
60	MG	BA	3009	1/1	0.98	0.35	12.48	1,1,1,1	0
60	MG	BA	3137	1/1	0.97	0.37	12.44	1,1,1,1	0
60	MG	DA	3120	1/1	0.85	0.38	11.95	3,3,3,3	0
60	MG	BA	3030	1/1	0.98	0.38	11.69	7,7,7,7	0
60	MG	DA	3084	1/1	0.71	0.52	11.52	71,71,71,71	0
60	MG	BA	3232	1/1	0.95	0.29	11.11	1,1,1,1	0
60	MG	DA	3180	1/1	0.96	0.57	10.83	5,5,5,5	0
60	MG	BA	3134	1/1	0.97	0.36	10.54	12,12,12,12	0
60	MG	DA	3042	1/1	0.69	0.41	9.78	46,46,46,46	0
60	MG	BA	3017	1/1	0.97	0.32	9.69	1,1,1,1	0
60	MG	BA	3306	1/1	0.95	0.29	9.55	5,5,5,5	0
60	MG	BA	3251	1/1	0.82	0.32	9.01	1,1,1,1	0
60	MG	DA	3169	1/1	0.91	0.36	8.95	16,16,16,16	0
60	MG	BA	3141	1/1	0.88	0.30	8.88	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3167	1/1	0.96	0.26	8.60	22,22,22,22	0
60	MG	DA	3206	1/1	0.92	0.33	8.57	12,12,12,12	0
60	MG	DA	3173	1/1	0.81	0.48	8.47	10,10,10,10	0
60	MG	BA	3156	1/1	0.96	0.39	8.40	7,7,7,7	0
60	MG	DA	3006	1/1	0.93	0.35	8.39	4,4,4,4	0
60	MG	BA	3108	1/1	0.99	0.41	8.34	2,2,2,2	0
60	MG	BA	3094	1/1	0.83	0.25	8.29	11,11,11,11	0
60	MG	BA	3037	1/1	0.95	0.39	8.24	33,33,33,33	0
60	MG	BA	3133	1/1	0.98	0.35	8.17	1,1,1,1	0
60	MG	DA	3160	1/1	0.91	0.36	8.13	27,27,27,27	0
60	MG	DA	3128	1/1	0.64	0.36	8.03	24,24,24,24	0
60	MG	BA	3049	1/1	0.97	0.32	7.98	1,1,1,1	0
60	MG	BA	3044	1/1	0.96	0.34	7.88	1,1,1,1	0
60	MG	BA	3169	1/1	0.96	0.30	7.74	16,16,16,16	0
60	MG	AA	1637	1/1	0.53	0.30	7.69	44,44,44,44	0
60	MG	BA	3083	1/1	0.97	0.30	7.67	1,1,1,1	0
60	MG	BA	3234	1/1	0.95	0.33	7.31	15,15,15,15	0
60	MG	DA	3096	1/1	0.81	0.40	7.26	16,16,16,16	0
60	MG	CA	1657	1/1	0.93	0.56	7.17	23,23,23,23	0
60	MG	BA	3031	1/1	0.96	0.30	7.05	1,1,1,1	0
60	MG	BA	3016	1/1	0.98	0.30	6.82	1,1,1,1	0
60	MG	DA	3195	1/1	0.89	0.38	6.45	18,18,18,18	0
60	MG	BU	201	1/1	0.97	0.43	6.44	23,23,23,23	0
60	MG	BA	3149	1/1	0.92	0.34	6.40	14,14,14,14	0
60	MG	DA	3005	1/1	0.90	0.31	6.39	28,28,28,28	0
60	MG	DA	3118	1/1	0.81	0.34	6.37	22,22,22,22	0
60	MG	BA	3013	1/1	0.96	0.32	6.19	1,1,1,1	0
60	MG	BA	3077	1/1	0.82	0.24	6.12	1,1,1,1	0
60	MG	AA	1617	1/1	0.93	0.43	6.06	13,13,13,13	0
60	MG	BA	3162	1/1	0.79	0.27	5.96	56,56,56,56	0
60	MG	BA	3027	1/1	0.97	0.28	5.86	1,1,1,1	0
60	MG	DA	3040	1/1	0.80	0.39	5.56	19,19,19,19	0
60	MG	DA	3008	1/1	0.96	0.46	5.42	13,13,13,13	0
60	MG	BA	3082	1/1	0.90	0.24	5.25	44,44,44,44	0
60	MG	BA	3143	1/1	0.97	0.22	5.11	32,32,32,32	0
60	MG	AA	1655	1/1	0.99	0.25	5.07	2,2,2,2	0
60	MG	DA	3193	1/1	0.85	0.28	4.90	29,29,29,29	0
60	MG	CA	1673	1/1	0.78	0.25	4.88	15,15,15,15	0
60	MG	BA	3117	1/1	0.96	0.28	4.79	1,1,1,1	0
60	MG	AA	1640	1/1	0.62	0.25	4.75	70,70,70,70	0
60	MG	BA	3042	1/1	0.85	0.23	4.68	1,1,1,1	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3092	1/1	0.73	0.30	4.62	17,17,17,17	0
60	MG	BA	3062	1/1	0.96	0.23	4.58	1,1,1,1	0
60	MG	DA	3237	1/1	0.85	0.36	4.55	10,10,10,10	0
60	MG	BA	3029	1/1	0.97	0.26	4.48	36,36,36,36	0
60	MG	DA	3174	1/1	0.91	0.32	4.46	6,6,6,6	0
60	MG	BA	3158	1/1	0.93	0.52	4.44	35,35,35,35	0
60	MG	DA	3014	1/1	0.80	0.36	4.40	4,4,4,4	0
60	MG	BA	3010	1/1	0.91	0.25	4.38	2,2,2,2	0
60	MG	DA	3117	1/1	0.68	0.46	4.34	49,49,49,49	0
60	MG	CA	1612	1/1	0.90	0.42	4.31	35,35,35,35	0
60	MG	AA	1633	1/1	0.87	0.24	4.23	8,8,8,8	0
60	MG	CA	1635	1/1	0.96	0.29	4.21	20,20,20,20	0
60	MG	BA	3284	1/1	0.79	0.23	4.20	21,21,21,21	0
60	MG	BA	3004	1/1	0.98	0.23	4.11	8,8,8,8	0
60	MG	BA	3119	1/1	0.95	0.23	4.08	91,91,91,91	0
60	MG	BA	3179	1/1	0.92	0.26	3.98	17,17,17,17	0
60	MG	CA	1677	1/1	0.83	0.38	3.90	51,51,51,51	0
60	MG	BA	3055	1/1	0.97	0.21	3.83	1,1,1,1	0
60	MG	DA	3205	1/1	0.86	0.36	3.82	2,2,2,2	0
60	MG	DF	301	1/1	0.56	0.56	3.77	53,53,53,53	0
60	MG	BA	3046	1/1	0.98	0.24	3.53	10,10,10,10	0
60	MG	DA	3215	1/1	0.84	0.28	3.52	23,23,23,23	0
60	MG	DO	201	1/1	0.60	0.52	3.41	65,65,65,65	0
60	MG	CA	1622	1/1	0.95	0.26	3.24	12,12,12,12	0
60	MG	CA	1610	1/1	0.93	0.26	3.15	48,48,48,48	0
60	MG	DA	3146	1/1	0.93	0.31	2.93	17,17,17,17	0
60	MG	DA	3073	1/1	0.87	0.29	2.84	58,58,58,58	0
60	MG	DA	3061	1/1	0.96	0.33	2.84	21,21,21,21	0
60	MG	DA	3167	1/1	0.88	0.26	2.77	36,36,36,36	0
60	MG	AA	1615	1/1	0.99	0.27	2.68	18,18,18,18	0
60	MG	CA	1692	1/1	0.72	0.27	2.67	32,32,32,32	0
60	MG	DA	3102	1/1	0.84	0.35	2.59	1,1,1,1	0
60	MG	AA	1675	1/1	0.98	0.25	2.48	4,4,4,4	0
60	MG	DA	3186	1/1	0.89	0.23	2.40	53,53,53,53	0
60	MG	DA	3078	1/1	0.76	0.30	2.37	26,26,26,26	0
60	MG	DA	3139	1/1	0.86	0.39	2.35	1,1,1,1	0
60	MG	BA	3178	1/1	0.97	0.22	2.27	1,1,1,1	0
60	MG	AA	1654	1/1	0.96	0.21	2.25	68,68,68,68	0
60	MG	DA	3065	1/1	0.73	0.27	2.22	28,28,28,28	0
60	MG	CA	1620	1/1	0.96	0.20	2.20	32,32,32,32	0
60	MG	CA	1686	1/1	0.49	0.28	2.07	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3236	1/1	0.93	0.28	2.07	39,39,39,39	0
60	MG	AA	1614	1/1	0.88	0.19	1.90	22,22,22,22	0
60	MG	DA	3041	1/1	0.77	0.31	1.90	1,1,1,1	0
60	MG	BA	3231	1/1	0.97	0.19	1.86	2,2,2,2	0
60	MG	DA	3126	1/1	0.85	0.34	1.86	7,7,7,7	0
60	MG	DA	3229	1/1	0.89	0.26	1.85	20,20,20,20	0
60	MG	AA	1604	1/1	0.88	0.27	1.82	14,14,14,14	0
60	MG	DA	3050	1/1	0.90	0.26	1.77	38,38,38,38	0
60	MG	AA	1704	1/1	0.90	0.19	1.77	13,13,13,13	0
60	MG	BD	301	1/1	0.96	0.26	1.73	12,12,12,12	0
60	MG	CA	1629	1/1	0.96	0.25	1.72	16,16,16,16	0
60	MG	BA	3114	1/1	0.82	0.21	1.71	14,14,14,14	0
60	MG	DA	3234	1/1	0.94	0.36	1.67	40,40,40,40	0
60	MG	DA	3035	1/1	0.96	0.24	1.62	1,1,1,1	0
60	MG	CA	1608	1/1	0.96	0.30	1.58	24,24,24,24	0
60	MG	BA	3040	1/1	0.98	0.20	1.47	1,1,1,1	0
60	MG	BA	3048	1/1	0.99	0.19	1.46	1,1,1,1	0
60	MG	DA	3182	1/1	0.93	0.34	1.43	23,23,23,23	0
60	MG	BA	3111	1/1	0.93	0.19	1.38	1,1,1,1	0
60	MG	DA	3016	1/1	0.72	0.28	1.30	12,12,12,12	0
60	MG	BA	3291	1/1	0.93	0.21	1.29	14,14,14,14	0
60	MG	BA	3172	1/1	0.90	0.17	1.29	18,18,18,18	0
60	MG	CA	1654	1/1	0.91	0.20	1.27	44,44,44,44	0
60	MG	DA	3091	1/1	0.84	0.29	1.22	55,55,55,55	0
60	MG	BA	3099	1/1	0.99	0.19	1.18	8,8,8,8	0
60	MG	CA	1601	1/1	0.88	0.24	1.14	1,1,1,1	0
60	MG	AA	1613	1/1	0.94	0.23	1.11	36,36,36,36	0
60	MG	DA	3052	1/1	0.82	0.22	1.02	14,14,14,14	0
60	MG	AA	1711	1/1	0.88	0.17	0.97	15,15,15,15	0
60	MG	DA	3216	1/1	0.81	0.20	0.81	24,24,24,24	0
60	MG	B0	101	1/1	0.90	0.24	0.78	4,4,4,4	0
60	MG	DA	3043	1/1	0.84	0.26	0.70	9,9,9,9	0
60	MG	DA	3210	1/1	0.86	0.28	0.70	2,2,2,2	0
60	MG	BA	3219	1/1	0.92	0.19	0.69	15,15,15,15	0
60	MG	BA	3074	1/1	0.92	0.18	0.66	4,4,4,4	0
60	MG	DA	3059	1/1	0.93	0.27	0.63	6,6,6,6	0
60	MG	DA	3099	1/1	0.98	0.24	0.62	14,14,14,14	0
60	MG	DA	3026	1/1	0.88	0.27	0.59	4,4,4,4	0
60	MG	BA	3145	1/1	0.94	0.29	0.59	31,31,31,31	0
60	MG	DA	3090	1/1	0.93	0.28	0.46	21,21,21,21	0
60	MG	DA	3055	1/1	0.98	0.23	0.45	17,17,17,17	0
60	MG	BA	3066	1/1	0.93	0.19	0.38	1,1,1,1	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3100	1/1	0.95	0.22	0.36	18,18,18,18	0
60	MG	AX	104	1/1	0.77	0.20	0.33	57,57,57,57	0
60	MG	AA	1697	1/1	0.82	0.20	0.23	27,27,27,27	0
60	MG	CA	1604	1/1	0.94	0.21	0.23	1,1,1,1	0
60	MG	AA	1635	1/1	0.93	0.20	0.20	23,23,23,23	0
60	MG	B0	103	1/1	0.92	0.23	0.17	22,22,22,22	0
60	MG	CA	1646	1/1	0.89	0.21	0.16	1,1,1,1	0
60	MG	BA	3022	1/1	0.94	0.15	0.08	19,19,19,19	0
60	MG	DA	3219	1/1	0.89	0.22	0.04	19,19,19,19	0
60	MG	AA	1665	1/1	0.92	0.15	0.02	31,31,31,31	0
60	MG	CA	1672	1/1	0.93	0.18	-0.04	21,21,21,21	0
61	ZN	AD	301	1/1	0.96	0.25	-0.05	46,46,46,46	0
60	MG	CA	1627	1/1	0.88	0.23	-0.10	9,9,9,9	0
60	MG	DA	3089	1/1	0.88	0.21	-0.16	27,27,27,27	0
60	MG	DA	3142	1/1	0.72	0.25	-0.16	37,37,37,37	0
61	ZN	CD	301	1/1	0.95	0.26	-0.27	49,49,49,49	0
60	MG	DA	3033	1/1	0.94	0.20	-0.30	4,4,4,4	0
60	MG	DD	302	1/1	0.90	0.23	-0.36	6,6,6,6	0
60	MG	BA	3267	1/1	0.96	0.15	-0.36	6,6,6,6	0
60	MG	CA	1701	1/1	0.93	0.18	-0.39	53,53,53,53	0
60	MG	BU	202	1/1	0.94	0.20	-0.43	1,1,1,1	0
60	MG	AA	1641	1/1	0.97	0.17	-0.50	13,13,13,13	0
60	MG	CA	1689	1/1	0.93	0.15	-0.54	7,7,7,7	0
60	MG	CA	1631	1/1	0.67	0.18	-0.54	19,19,19,19	0
60	MG	DA	3196	1/1	0.92	0.20	-0.59	1,1,1,1	0
60	MG	DA	3122	1/1	0.73	0.20	-0.65	40,40,40,40	0
60	MG	BE	302	1/1	0.97	0.15	-0.69	1,1,1,1	0
60	MG	AA	1674	1/1	0.99	0.14	-0.74	32,32,32,32	0
60	MG	BA	3324	1/1	0.96	0.15	-0.75	1,1,1,1	0
60	MG	DA	3070	1/1	0.94	0.21	-0.76	14,14,14,14	0
60	MG	BA	3224	1/1	0.90	0.12	-0.82	20,20,20,20	0
60	MG	DA	3037	1/1	0.94	0.20	-0.84	24,24,24,24	0
60	MG	AA	1603	1/1	0.96	0.17	-0.85	32,32,32,32	0
60	MG	BA	3323	1/1	0.97	0.14	-0.88	2,2,2,2	0
60	MG	AA	1689	1/1	0.94	0.16	-0.93	2,2,2,2	0
60	MG	AA	1658	1/1	0.96	0.15	-0.97	1,1,1,1	0
60	MG	DA	3067	1/1	0.95	0.18	-0.99	23,23,23,23	0
60	MG	DA	3153	1/1	0.78	0.18	-1.00	13,13,13,13	0
60	MG	BA	3058	1/1	0.96	0.13	-1.12	1,1,1,1	0
60	MG	BA	3325	1/1	0.90	0.13	-1.17	19,19,19,19	0
60	MG	AA	1713	1/1	0.74	0.13	-1.19	43,43,43,43	0
60	MG	DA	3077	1/1	0.82	0.18	-1.21	13,13,13,13	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3002	1/1	0.92	0.15	-1.23	9,9,9,9	0
60	MG	AA	1693	1/1	0.98	0.14	-1.24	31,31,31,31	0
60	MG	DA	3101	1/1	0.95	0.17	-1.29	20,20,20,20	0
60	MG	DA	3015	1/1	0.90	0.16	-1.34	1,1,1,1	0
60	MG	BF	301	1/1	0.94	0.13	-1.37	14,14,14,14	0
60	MG	B5	101	1/1	0.95	0.11	-1.39	16,16,16,16	0
60	MG	DA	3105	1/1	0.94	0.19	-1.44	59,59,59,59	0
60	MG	DA	3045	1/1	0.97	0.16	-1.44	11,11,11,11	0
60	MG	AA	1659	1/1	0.96	0.15	-1.48	23,23,23,23	0
60	MG	BB	204	1/1	0.96	0.14	-1.50	21,21,21,21	0
61	ZN	B4	101	1/1	0.91	0.05	-1.55	89,89,89,89	0
60	MG	AA	1639	1/1	0.96	0.11	-1.56	29,29,29,29	0
60	MG	AA	1634	1/1	0.97	0.13	-1.57	1,1,1,1	0
60	MG	AA	1668	1/1	0.98	0.13	-1.58	24,24,24,24	0
61	ZN	B5	102	1/1	0.89	0.09	-1.60	51,51,51,51	0
60	MG	BA	3011	1/1	0.98	0.16	-1.63	1,1,1,1	0
60	MG	BA	3332	1/1	0.96	0.13	-1.67	1,1,1,1	0
61	ZN	D9	101	1/1	0.91	0.07	-1.69	93,93,93,93	0
60	MG	BA	3309	1/1	0.80	0.13	-1.71	1,1,1,1	0
60	MG	DA	3076	1/1	0.94	0.12	-1.74	25,25,25,25	0
60	MG	DA	3179	1/1	0.84	0.15	-1.84	19,19,19,19	0
60	MG	BA	3115	1/1	0.95	0.14	-1.95	1,1,1,1	0
60	MG	DA	3133	1/1	0.86	0.18	-2.00	16,16,16,16	0
61	ZN	B9	101	1/1	0.97	0.07	-2.01	44,44,44,44	0
60	MG	BA	3218	1/1	0.94	0.12	-2.06	9,9,9,9	0
60	MG	CA	1663	1/1	0.98	0.12	-2.07	31,31,31,31	0
61	ZN	D5	102	1/1	0.90	0.09	-2.09	75,75,75,75	0
60	MG	BR	201	1/1	0.99	0.06	-2.12	1,1,1,1	0
60	MG	AA	1688	1/1	0.89	0.12	-2.15	49,49,49,49	0
60	MG	AA	1611	1/1	0.97	0.13	-2.25	33,33,33,33	0
60	MG	BA	3147	1/1	0.99	0.12	-2.28	8,8,8,8	0
60	MG	DA	3011	1/1	0.88	0.18	-2.35	4,4,4,4	0
60	MG	BA	3245	1/1	0.94	0.11	-2.37	25,25,25,25	0
60	MG	BA	3233	1/1	0.96	0.12	-2.47	1,1,1,1	0
61	ZN	D4	101	1/1	0.90	0.05	-2.52	113,113,113,113	0
60	MG	DA	3009	1/1	0.93	0.18	-2.55	12,12,12,12	0
60	MG	CA	1630	1/1	0.96	0.14	-2.57	57,57,57,57	0
60	MG	DA	3030	1/1	0.93	0.14	-2.76	8,8,8,8	0
60	MG	BA	3163	1/1	0.91	0.09	-2.79	12,12,12,12	0
60	MG	DB	203	1/1	0.82	0.11	-2.97	54,54,54,54	0
60	MG	CK	201	1/1	0.91	0.09	-3.04	19,19,19,19	0
60	MG	BA	3154	1/1	0.93	0.11	-3.05	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3054	1/1	0.94	0.12	-3.26	6,6,6,6	0
60	MG	CA	1617	1/1	0.96	0.16	-3.32	1,1,1,1	0
60	MG	CA	1699	1/1	0.96	0.08	-3.54	30,30,30,30	0
60	MG	AA	1667	1/1	0.96	0.17	-3.59	15,15,15,15	0
60	MG	DA	3232	1/1	0.84	0.14	-3.60	3,3,3,3	0
60	MG	AA	1678	1/1	0.94	0.13	-3.74	29,29,29,29	0
60	MG	DA	3156	1/1	0.70	0.11	-3.77	47,47,47,47	0
60	MG	BA	3087	1/1	0.97	0.09	-3.78	6,6,6,6	0
60	MG	BA	3112	1/1	0.97	0.13	-3.87	11,11,11,11	0
60	MG	DA	3187	1/1	0.97	0.09	-3.96	27,27,27,27	0
60	MG	AX	107	1/1	0.97	0.11	-4.05	8,8,8,8	0
60	MG	DA	3046	1/1	0.97	0.08	-4.10	28,28,28,28	0
60	MG	DA	3023	1/1	0.90	0.10	-4.12	14,14,14,14	0
60	MG	CA	1628	1/1	0.98	0.10	-4.36	12,12,12,12	0
60	MG	DA	3114	1/1	0.92	0.12	-5.20	34,34,34,34	0
60	MG	BA	3273	1/1	0.94	0.09	-5.51	1,1,1,1	0
60	MG	DA	3208	1/1	0.85	0.15	-6.01	12,12,12,12	0
60	MG	BA	3257	1/1	0.99	0.06	-7.11	22,22,22,22	0
60	MG	AA	1609	1/1	0.98	0.22	-	1,1,1,1	0
60	MG	DA	3027	1/1	0.88	0.92	-	38,38,38,38	0
60	MG	BA	3095	1/1	0.89	0.72	-	47,47,47,47	0
60	MG	BA	3221	1/1	0.96	0.48	-	35,35,35,35	0
60	MG	DA	3131	1/1	0.81	0.86	-	63,63,63,63	0
60	MG	DA	3140	1/1	0.80	0.34	-	24,24,24,24	0
60	MG	BA	3303	1/1	0.75	0.56	-	32,32,32,32	0
60	MG	BA	3209	1/1	0.94	0.37	-	24,24,24,24	0
60	MG	DA	3034	1/1	0.80	0.19	-	1,1,1,1	0
60	MG	BA	3305	1/1	0.94	0.25	-	32,32,32,32	0
60	MG	DA	3138	1/1	0.75	0.17	-	63,63,63,63	0
60	MG	BA	3150	1/1	0.96	0.42	-	9,9,9,9	0
60	MG	DA	3082	1/1	0.92	0.24	-	15,15,15,15	0
60	MG	BA	3191	1/1	0.84	0.33	-	6,6,6,6	0
60	MG	BA	3226	1/1	0.91	0.24	-	39,39,39,39	0
60	MG	BA	3072	1/1	0.96	0.12	-	6,6,6,6	0
60	MG	BA	3283	1/1	0.91	0.60	-	38,38,38,38	0
60	MG	DA	3224	1/1	0.93	0.11	-	18,18,18,18	0
60	MG	BA	3097	1/1	0.91	0.32	-	44,44,44,44	0
60	MG	AA	1652	1/1	0.93	0.38	-	28,28,28,28	0
60	MG	BA	3198	1/1	0.90	0.19	-	5,5,5,5	0
60	MG	DA	3158	1/1	0.91	0.55	-	49,49,49,49	0
60	MG	CA	1680	1/1	0.96	0.07	-	44,44,44,44	0
60	MG	BA	3281	1/1	0.94	0.26	-	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1626	1/1	0.75	0.24	-	51,51,51,51	0
60	MG	DA	3207	1/1	0.93	0.16	-	1,1,1,1	0
60	MG	CA	1659	1/1	0.96	0.62	-	46,46,46,46	0
60	MG	BA	3206	1/1	0.97	0.33	-	6,6,6,6	0
60	MG	BB	203	1/1	0.94	0.25	-	35,35,35,35	0
60	MG	CA	1670	1/1	0.90	0.26	-	26,26,26,26	0
60	MG	CA	1668	1/1	0.88	0.32	-	30,30,30,30	0
60	MG	DA	3147	1/1	0.94	0.20	-	26,26,26,26	0
60	MG	DA	3202	1/1	0.75	0.22	-	18,18,18,18	0
60	MG	CA	1688	1/1	0.97	0.09	-	37,37,37,37	0
60	MG	DA	3060	1/1	0.71	0.35	-	23,23,23,23	0
60	MG	BA	3238	1/1	0.80	0.41	-	29,29,29,29	0
60	MG	BA	3298	1/1	0.89	0.32	-	13,13,13,13	0
60	MG	BA	3067	1/1	0.96	0.10	-	1,1,1,1	0
60	MG	DA	3141	1/1	0.78	0.62	-	36,36,36,36	0
60	MG	DA	3031	1/1	0.85	0.14	-	9,9,9,9	0
60	MG	BA	3246	1/1	0.92	0.26	-	1,1,1,1	0
60	MG	DA	3053	1/1	0.81	0.55	-	32,32,32,32	0
60	MG	AA	1650	1/1	0.98	0.14	-	15,15,15,15	0
60	MG	AA	1632	1/1	0.93	0.42	-	48,48,48,48	0
60	MG	CA	1690	1/1	0.96	0.28	-	31,31,31,31	0
60	MG	DD	301	1/1	0.96	0.08	-	21,21,21,21	0
60	MG	BA	3132	1/1	0.98	0.31	-	1,1,1,1	0
60	MG	CA	1662	1/1	0.95	0.13	-	38,38,38,38	0
60	MG	DA	3004	1/1	0.96	0.29	-	7,7,7,7	0
60	MG	BA	3152	1/1	0.97	0.41	-	6,6,6,6	0
60	MG	BA	3278	1/1	0.98	0.10	-	15,15,15,15	0
60	MG	BA	3159	1/1	0.92	0.21	-	20,20,20,20	0
60	MG	DA	3171	1/1	0.73	0.44	-	52,52,52,52	0
60	MG	AA	1677	1/1	0.90	0.24	-	30,30,30,30	0
60	MG	BA	3122	1/1	0.88	0.33	-	12,12,12,12	0
60	MG	BA	3186	1/1	0.72	0.30	-	60,60,60,60	0
60	MG	DA	3058	1/1	0.89	0.22	-	1,1,1,1	0
60	MG	CA	1700	1/1	0.60	0.40	-	36,36,36,36	0
60	MG	AA	1616	1/1	0.90	0.25	-	32,32,32,32	0
60	MG	CA	1698	1/1	0.81	0.51	-	29,29,29,29	0
60	MG	AW	101	1/1	0.86	0.30	-	48,48,48,48	0
60	MG	DA	3235	1/1	0.84	0.44	-	61,61,61,61	0
60	MG	CA	1693	1/1	0.93	0.23	-	20,20,20,20	0
60	MG	BA	3073	1/1	0.98	0.30	-	1,1,1,1	0
60	MG	CA	1616	1/1	0.76	0.48	-	52,52,52,52	0
60	MG	BA	3318	1/1	0.84	0.24	-	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3330	1/1	0.95	0.20	-	12,12,12,12	0
60	MG	CV	601	1/1	0.73	0.47	-	16,16,16,16	0
60	MG	CA	1694	1/1	0.85	0.71	-	51,51,51,51	0
60	MG	DA	3165	1/1	0.79	0.27	-	14,14,14,14	0
60	MG	BA	3160	1/1	0.88	0.43	-	29,29,29,29	0
60	MG	DA	3098	1/1	0.81	0.35	-	27,27,27,27	0
60	MG	DA	3211	1/1	0.87	0.24	-	23,23,23,23	0
60	MG	DA	3177	1/1	0.89	0.30	-	13,13,13,13	0
60	MG	AX	103	1/1	0.71	0.20	-	51,51,51,51	0
60	MG	BA	3051	1/1	0.82	0.38	-	14,14,14,14	0
60	MG	CA	1636	1/1	0.87	0.24	-	26,26,26,26	0
60	MG	DA	3001	1/1	0.78	0.40	-	51,51,51,51	0
60	MG	BA	3197	1/1	0.90	0.21	-	24,24,24,24	0
60	MG	BA	3205	1/1	0.88	0.36	-	30,30,30,30	0
60	MG	CA	1697	1/1	0.94	0.27	-	27,27,27,27	0
60	MG	CA	1649	1/1	0.69	0.31	-	54,54,54,54	0
60	MG	BA	3173	1/1	0.89	0.19	-	50,50,50,50	0
60	MG	CA	1625	1/1	0.95	0.25	-	3,3,3,3	0
60	MG	BA	3228	1/1	0.93	0.64	-	52,52,52,52	0
60	MG	BA	3090	1/1	0.97	0.05	-	13,13,13,13	0
60	MG	BA	3313	1/1	0.89	0.45	-	45,45,45,45	0
60	MG	DA	3072	1/1	0.93	0.32	-	8,8,8,8	0
60	MG	AA	1666	1/1	0.97	0.09	-	9,9,9,9	0
60	MG	BA	3063	1/1	0.96	0.20	-	1,1,1,1	0
60	MG	BA	3220	1/1	0.98	0.17	-	1,1,1,1	0
60	MG	CA	1684	1/1	0.83	0.18	-	33,33,33,33	0
60	MG	BA	3059	1/1	0.84	0.50	-	25,25,25,25	0
60	MG	DA	3161	1/1	0.65	0.18	-	33,33,33,33	0
60	MG	BA	3155	1/1	0.94	0.35	-	14,14,14,14	0
60	MG	BA	3148	1/1	0.89	0.15	-	1,1,1,1	0
60	MG	AA	1629	1/1	0.82	0.22	-	51,51,51,51	0
60	MG	DA	3143	1/1	0.90	0.62	-	54,54,54,54	0
60	MG	DA	3108	1/1	0.94	0.26	-	18,18,18,18	0
60	MG	BA	3161	1/1	0.93	0.50	-	24,24,24,24	0
60	MG	BA	3001	1/1	0.87	0.26	-	43,43,43,43	0
60	MG	DA	3151	1/1	0.95	0.34	-	26,26,26,26	0
60	MG	BA	3190	1/1	0.86	0.12	-	39,39,39,39	0
60	MG	BA	3035	1/1	0.94	0.19	-	1,1,1,1	0
60	MG	BA	3047	1/1	0.93	0.14	-	1,1,1,1	0
60	MG	DA	3109	1/1	0.69	0.20	-	50,50,50,50	0
60	MG	DA	3223	1/1	0.84	0.33	-	13,13,13,13	0
60	MG	DA	3137	1/1	0.84	0.72	-	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3271	1/1	0.85	0.14	-	28,28,28,28	0
60	MG	BA	3157	1/1	0.96	0.25	-	10,10,10,10	0
60	MG	BA	3212	1/1	0.97	0.28	-	11,11,11,11	0
60	MG	AA	1622	1/1	0.88	0.32	-	12,12,12,12	0
60	MG	AA	1671	1/1	0.59	0.42	-	49,49,49,49	0
60	MG	BA	3255	1/1	0.78	0.33	-	19,19,19,19	0
60	MG	BA	3327	1/1	0.98	0.32	-	17,17,17,17	0
60	MG	AX	105	1/1	0.94	0.08	-	12,12,12,12	0
60	MG	BA	3012	1/1	0.97	0.27	-	1,1,1,1	0
60	MG	AA	1601	1/1	0.85	0.29	-	47,47,47,47	0
60	MG	DA	3021	1/1	0.67	0.28	-	27,27,27,27	0
60	MG	DA	3095	1/1	0.70	0.15	-	61,61,61,61	0
60	MG	BA	3182	1/1	0.95	0.24	-	1,1,1,1	0
60	MG	BA	3107	1/1	0.94	0.46	-	65,65,65,65	0
60	MG	DA	3106	1/1	0.95	0.12	-	23,23,23,23	0
60	MG	BA	3075	1/1	0.95	0.32	-	2,2,2,2	0
60	MG	BA	3280	1/1	0.84	0.18	-	7,7,7,7	0
60	MG	AA	1663	1/1	0.96	0.28	-	14,14,14,14	0
60	MG	DA	3022	1/1	0.94	0.28	-	11,11,11,11	0
60	MG	CW	102	1/1	0.90	0.15	-	40,40,40,40	0
60	MG	DA	3222	1/1	0.89	0.29	-	24,24,24,24	0
60	MG	CA	1613	1/1	0.88	0.47	-	36,36,36,36	0
60	MG	CA	1695	1/1	0.93	0.14	-	40,40,40,40	0
60	MG	AA	1664	1/1	0.88	0.29	-	46,46,46,46	0
60	MG	BA	3038	1/1	0.98	0.25	-	1,1,1,1	0
60	MG	DA	3064	1/1	0.90	0.48	-	12,12,12,12	0
60	MG	BA	3263	1/1	0.93	0.19	-	47,47,47,47	0
60	MG	AA	1610	1/1	0.91	0.16	-	36,36,36,36	0
60	MG	DA	3007	1/1	0.88	0.31	-	1,1,1,1	0
60	MG	BA	3312	1/1	0.85	0.25	-	22,22,22,22	0
60	MG	BA	3213	1/1	0.92	0.48	-	49,49,49,49	0
60	MG	BA	3002	1/1	0.94	0.31	-	17,17,17,17	0
60	MG	CA	1653	1/1	0.86	0.23	-	36,36,36,36	0
60	MG	AA	1712	1/1	0.96	0.48	-	36,36,36,36	0
60	MG	BA	3129	1/1	0.96	0.21	-	1,1,1,1	0
60	MG	CA	1634	1/1	0.90	0.19	-	16,16,16,16	0
60	MG	BA	3210	1/1	0.76	0.29	-	33,33,33,33	0
60	MG	BA	3253	1/1	0.95	0.30	-	39,39,39,39	0
60	MG	BA	3085	1/1	0.64	0.39	-	70,70,70,70	0
60	MG	AW	103	1/1	0.19	0.63	-	72,72,72,72	0
60	MG	BA	3302	1/1	0.86	0.17	-	11,11,11,11	0
60	MG	BA	3170	1/1	0.83	0.38	-	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3051	1/1	0.94	0.51	-	18,18,18,18	0
60	MG	AX	109	1/1	0.96	0.12	-	16,16,16,16	0
60	MG	DA	3010	1/1	0.95	0.46	-	1,1,1,1	0
60	MG	AA	1623	1/1	0.96	0.33	-	10,10,10,10	0
60	MG	BA	3249	1/1	0.94	0.54	-	13,13,13,13	0
60	MG	DA	3157	1/1	0.73	0.24	-	58,58,58,58	0
60	MG	BA	3244	1/1	0.96	0.21	-	34,34,34,34	0
60	MG	DA	3226	1/1	0.86	0.10	-	30,30,30,30	0
60	MG	AA	1692	1/1	0.97	0.29	-	19,19,19,19	0
60	MG	DA	3132	1/1	0.97	0.26	-	6,6,6,6	0
60	MG	BA	3194	1/1	0.90	0.57	-	54,54,54,54	0
60	MG	CA	1602	1/1	0.93	0.31	-	26,26,26,26	0
60	MG	DA	3221	1/1	0.91	0.50	-	52,52,52,52	0
60	MG	BA	3297	1/1	0.95	0.16	-	42,42,42,42	0
60	MG	BA	3333	1/1	0.88	0.35	-	1,1,1,1	0
60	MG	BA	3101	1/1	0.91	0.41	-	31,31,31,31	0
60	MG	BA	3064	1/1	0.87	0.70	-	45,45,45,45	0
60	MG	CA	1651	1/1	0.95	0.15	-	35,35,35,35	0
60	MG	AA	1698	1/1	0.95	0.29	-	23,23,23,23	0
60	MG	DA	3228	1/1	0.68	0.69	-	34,34,34,34	0
60	MG	AA	1708	1/1	0.76	0.26	-	41,41,41,41	0
60	MG	DA	3081	1/1	0.94	0.34	-	3,3,3,3	0
60	MG	BA	3052	1/1	0.97	0.33	-	1,1,1,1	0
60	MG	DA	3107	1/1	0.89	0.41	-	37,37,37,37	0
60	MG	DA	3028	1/1	0.93	0.20	-	1,1,1,1	0
60	MG	CA	1640	1/1	0.74	0.27	-	41,41,41,41	0
60	MG	BA	3320	1/1	0.96	0.10	-	23,23,23,23	0
60	MG	DA	3047	1/1	0.89	0.45	-	29,29,29,29	0
60	MG	CA	1638	1/1	0.68	0.38	-	31,31,31,31	0
60	MG	BA	3174	1/1	0.89	0.09	-	7,7,7,7	0
60	MG	BA	3050	1/1	0.93	0.30	-	1,1,1,1	0
60	MG	BA	3091	1/1	0.98	0.31	-	1,1,1,1	0
60	MG	DA	3213	1/1	0.86	0.21	-	31,31,31,31	0
60	MG	CA	1685	1/1	0.71	0.48	-	59,59,59,59	0
60	MG	CW	104	1/1	0.69	0.17	-	57,57,57,57	0
60	MG	BA	3311	1/1	0.91	0.42	-	40,40,40,40	0
60	MG	BA	3329	1/1	0.68	0.16	-	45,45,45,45	0
60	MG	AA	1706	1/1	0.98	0.14	-	28,28,28,28	0
60	MG	BA	3192	1/1	0.88	0.44	-	31,31,31,31	0
60	MG	CA	1681	1/1	0.96	0.47	-	44,44,44,44	0
60	MG	BA	3256	1/1	0.97	0.15	-	23,23,23,23	0
60	MG	BB	202	1/1	0.94	0.12	-	9,9,9,9	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3144	1/1	0.80	0.30	-	59,59,59,59	0
60	MG	DA	3013	1/1	0.85	0.38	-	30,30,30,30	0
60	MG	BA	3140	1/1	0.80	0.52	-	26,26,26,26	0
60	MG	CA	1609	1/1	0.75	0.51	-	50,50,50,50	0
60	MG	BA	3266	1/1	0.92	0.30	-	12,12,12,12	0
60	MG	DA	3159	1/1	0.69	0.39	-	32,32,32,32	0
60	MG	CA	1702	1/1	0.80	0.43	-	27,27,27,27	0
60	MG	AW	102	1/1	0.91	0.13	-	36,36,36,36	0
60	MG	BA	3033	1/1	0.96	0.42	-	1,1,1,1	0
60	MG	AA	1649	1/1	0.97	0.25	-	25,25,25,25	0
60	MG	BA	3239	1/1	0.98	0.23	-	2,2,2,2	0
60	MG	DA	3238	1/1	0.94	0.69	-	42,42,42,42	0
60	MG	DA	3113	1/1	0.94	0.47	-	2,2,2,2	0
60	MG	BA	3310	1/1	0.85	0.28	-	38,38,38,38	0
60	MG	AX	101	1/1	0.88	0.15	-	41,41,41,41	0
60	MG	BA	3248	1/1	0.96	0.21	-	34,34,34,34	0
60	MG	AA	1682	1/1	0.72	0.13	-	48,48,48,48	0
60	MG	CA	1660	1/1	0.91	0.16	-	21,21,21,21	0
60	MG	BA	3039	1/1	0.98	0.22	-	1,1,1,1	0
60	MG	AA	1691	1/1	0.94	0.39	-	23,23,23,23	0
60	MG	BA	3110	1/1	0.96	0.33	-	6,6,6,6	0
60	MG	DA	3071	1/1	0.94	0.27	-	19,19,19,19	0
60	MG	AA	1636	1/1	0.96	0.41	-	28,28,28,28	0
60	MG	BA	3081	1/1	0.95	0.13	-	19,19,19,19	0
60	MG	CA	1678	1/1	0.90	0.53	-	25,25,25,25	0
60	MG	BA	3041	1/1	0.96	0.29	-	1,1,1,1	0
60	MG	BA	3241	1/1	0.80	1.36	-	80,80,80,80	0
60	MG	AX	102	1/1	0.91	0.16	-	57,57,57,57	0
60	MG	CA	1679	1/1	0.93	0.16	-	43,43,43,43	0
60	MG	CW	103	1/1	0.30	0.34	-	73,73,73,73	0
60	MG	AA	1672	1/1	0.80	0.24	-	53,53,53,53	0
60	MG	BA	3225	1/1	0.94	0.27	-	9,9,9,9	0
60	MG	DA	3184	1/1	0.67	0.86	-	35,35,35,35	0
60	MG	BX	101	1/1	0.83	0.23	-	31,31,31,31	0
60	MG	B0	102	1/1	0.80	0.40	-	40,40,40,40	0
60	MG	BG	201	1/1	0.95	0.20	-	30,30,30,30	0
60	MG	BA	3236	1/1	0.94	0.36	-	11,11,11,11	0
60	MG	CA	1641	1/1	0.46	0.29	-	66,66,66,66	0
60	MG	BA	3057	1/1	0.96	0.11	-	3,3,3,3	0
60	MG	DA	3123	1/1	0.85	0.42	-	40,40,40,40	0
60	MG	BA	3193	1/1	0.96	0.26	-	22,22,22,22	0
60	MG	DA	3087	1/1	0.96	0.47	-	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3128	1/1	0.94	0.19	-	16,16,16,16	0
60	MG	BA	3126	1/1	0.96	0.11	-	5,5,5,5	0
60	MG	DA	3129	1/1	0.82	0.23	-	20,20,20,20	0
60	MG	DA	3130	1/1	0.81	0.43	-	27,27,27,27	0
60	MG	AA	1680	1/1	0.80	0.62	-	70,70,70,70	0
60	MG	BA	3237	1/1	0.97	0.19	-	1,1,1,1	0
60	MG	DA	3134	1/1	0.89	0.25	-	59,59,59,59	0
60	MG	BA	3065	1/1	0.99	0.16	-	2,2,2,2	0
60	MG	DA	3170	1/1	0.78	0.51	-	33,33,33,33	0
60	MG	BA	3102	1/1	0.95	0.17	-	1,1,1,1	0
60	MG	BA	3287	1/1	0.93	0.11	-	7,7,7,7	0
60	MG	CW	101	1/1	0.85	0.12	-	55,55,55,55	0
60	MG	BA	3292	1/1	0.94	0.31	-	27,27,27,27	0
60	MG	CA	1632	1/1	0.89	0.35	-	6,6,6,6	0
60	MG	BA	3250	1/1	0.93	0.32	-	12,12,12,12	0
60	MG	AA	1683	1/1	0.87	0.14	-	16,16,16,16	0
60	MG	AA	1628	1/1	0.98	0.17	-	10,10,10,10	0
60	MG	CA	1615	1/1	0.95	0.46	-	28,28,28,28	0
60	MG	CA	1603	1/1	0.86	0.23	-	38,38,38,38	0
60	MG	AA	1714	1/1	0.98	0.18	-	6,6,6,6	0
60	MG	DA	3199	1/1	0.56	0.44	-	35,35,35,35	0
60	MG	AA	1670	1/1	0.84	0.30	-	54,54,54,54	0
60	MG	DA	3214	1/1	0.87	0.37	-	21,21,21,21	0
60	MG	BA	3184	1/1	0.84	0.62	-	40,40,40,40	0
60	MG	AA	1700	1/1	0.92	0.30	-	74,74,74,74	0
60	MG	CA	1676	1/1	0.78	0.20	-	25,25,25,25	0
60	MG	BA	3300	1/1	0.92	0.18	-	22,22,22,22	0
60	MG	DA	3020	1/1	0.88	0.46	-	40,40,40,40	0
60	MG	DA	3063	1/1	0.92	0.21	-	24,24,24,24	0
60	MG	BA	3208	1/1	0.96	0.27	-	1,1,1,1	0
60	MG	DA	3163	1/1	0.95	0.49	-	32,32,32,32	0
60	MG	DA	3104	1/1	0.77	0.44	-	42,42,42,42	0
60	MG	BA	3285	1/1	0.95	0.12	-	1,1,1,1	0
60	MG	BA	3328	1/1	0.93	0.27	-	34,34,34,34	0
60	MG	DA	3191	1/1	0.94	0.41	-	31,31,31,31	0
60	MG	BA	3014	1/1	0.98	0.49	-	1,1,1,1	0
60	MG	DA	3125	1/1	0.74	0.19	-	49,49,49,49	0
60	MG	BA	3093	1/1	0.96	0.30	-	1,1,1,1	0
60	MG	AA	1651	1/1	0.88	0.51	-	53,53,53,53	0
60	MG	DA	3185	1/1	0.85	0.62	-	10,10,10,10	0
60	MG	BA	3222	1/1	0.86	0.29	-	26,26,26,26	0
60	MG	AA	1648	1/1	0.83	0.45	-	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3136	1/1	0.94	0.27	-	42,42,42,42	0
60	MG	BA	3165	1/1	0.85	0.15	-	48,48,48,48	0
60	MG	DA	3217	1/1	0.70	0.56	-	27,27,27,27	0
60	MG	DA	3115	1/1	0.83	0.29	-	36,36,36,36	0
60	MG	BA	3151	1/1	0.98	0.17	-	22,22,22,22	0
60	MG	DA	3074	1/1	0.81	0.62	-	48,48,48,48	0
60	MG	DA	3150	1/1	0.93	0.23	-	28,28,28,28	0
60	MG	AA	1624	1/1	0.99	0.35	-	1,1,1,1	0
60	MG	DA	3145	1/1	0.81	0.49	-	35,35,35,35	0
60	MG	AA	1657	1/1	0.87	0.45	-	37,37,37,37	0
60	MG	BA	3086	1/1	0.98	0.14	-	4,4,4,4	0
60	MG	BA	3123	1/1	0.97	0.14	-	6,6,6,6	0
60	MG	BA	3211	1/1	0.93	0.33	-	36,36,36,36	0
60	MG	BA	3043	1/1	0.97	0.40	-	1,1,1,1	0
60	MG	BA	3036	1/1	0.93	0.56	-	8,8,8,8	0
60	MG	DA	3239	1/1	0.59	0.34	-	34,34,34,34	0
60	MG	BA	3168	1/1	0.93	0.34	-	60,60,60,60	0
60	MG	BA	3282	1/1	0.90	0.32	-	20,20,20,20	0
60	MG	BE	303	1/1	0.96	0.32	-	58,58,58,58	0
60	MG	BA	3294	1/1	0.76	0.71	-	90,90,90,90	0
60	MG	DA	3038	1/1	0.94	0.57	-	8,8,8,8	0
60	MG	AA	1679	1/1	0.90	0.15	-	36,36,36,36	0
60	MG	DA	3192	1/1	0.85	0.18	-	10,10,10,10	0
60	MG	BA	3272	1/1	0.89	0.23	-	15,15,15,15	0
60	MG	AA	1684	1/1	0.95	0.36	-	69,69,69,69	0
60	MG	AA	1608	1/1	0.88	0.46	-	22,22,22,22	0
60	MG	CA	1626	1/1	0.94	0.42	-	31,31,31,31	0
60	MG	AA	1627	1/1	0.92	0.24	-	22,22,22,22	0
60	MG	BA	3199	1/1	0.99	0.19	-	1,1,1,1	0
60	MG	CA	1652	1/1	0.58	0.28	-	61,61,61,61	0
60	MG	DA	3025	1/1	0.77	0.39	-	1,1,1,1	0
60	MG	DA	3066	1/1	0.78	0.56	-	40,40,40,40	0
60	MG	D7	101	1/1	0.66	0.30	-	36,36,36,36	0
60	MG	BA	3204	1/1	0.83	0.33	-	25,25,25,25	0
60	MG	AA	1656	1/1	0.97	0.25	-	10,10,10,10	0
60	MG	BA	3321	1/1	0.96	0.42	-	1,1,1,1	0
60	MG	BA	3243	1/1	0.86	0.51	-	45,45,45,45	0
60	MG	CA	1674	1/1	0.77	0.45	-	55,55,55,55	0
60	MG	BA	3202	1/1	0.97	0.22	-	1,1,1,1	0
60	MG	BA	3008	1/1	0.95	0.20	-	4,4,4,4	0
60	MG	BA	3331	1/1	0.85	0.69	-	35,35,35,35	0
60	MG	DA	3154	1/1	0.56	0.81	-	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1639	1/1	0.94	0.31	-	16,16,16,16	0
60	MG	BA	3032	1/1	0.95	0.23	-	1,1,1,1	0
60	MG	AA	1607	1/1	0.90	0.72	-	51,51,51,51	0
60	MG	BA	3166	1/1	0.96	0.28	-	8,8,8,8	0
60	MG	BA	3088	1/1	0.96	0.13	-	1,1,1,1	0
60	MG	BA	3028	1/1	0.98	0.13	-	1,1,1,1	0
60	MG	DA	3152	1/1	0.94	0.32	-	8,8,8,8	0
60	MG	BA	3261	1/1	0.92	0.31	-	16,16,16,16	0
60	MG	AA	1606	1/1	0.99	0.29	-	1,1,1,1	0
60	MG	DA	3119	1/1	0.91	0.34	-	5,5,5,5	0
60	MG	DA	3188	1/1	0.15	0.27	-	72,72,72,72	0
60	MG	BA	3214	1/1	0.92	0.17	-	54,54,54,54	0
60	MG	DA	3003	1/1	0.88	0.27	-	17,17,17,17	0
60	MG	DA	3220	1/1	0.85	0.45	-	30,30,30,30	0
60	MG	BA	3295	1/1	0.87	0.29	-	41,41,41,41	0
60	MG	CA	1675	1/1	0.92	0.34	-	31,31,31,31	0
60	MG	AA	1602	1/1	0.98	0.05	-	1,1,1,1	0
60	MG	DA	3083	1/1	0.84	0.57	-	35,35,35,35	0
60	MG	BA	3277	1/1	0.92	0.39	-	1,1,1,1	0
60	MG	BA	3216	1/1	0.95	0.17	-	25,25,25,25	0
60	MG	AA	1699	1/1	0.91	0.19	-	21,21,21,21	0
60	MG	BA	3105	1/1	0.94	0.17	-	8,8,8,8	0
60	MG	BA	3098	1/1	0.94	0.44	-	1,1,1,1	0
60	MG	AA	1612	1/1	0.94	0.25	-	15,15,15,15	0
60	MG	BA	3125	1/1	0.95	0.21	-	1,1,1,1	0
60	MG	BA	3164	1/1	0.96	0.35	-	33,33,33,33	0
60	MG	BA	3270	1/1	0.89	0.24	-	32,32,32,32	0
60	MG	DA	3069	1/1	0.94	0.66	-	6,6,6,6	0
60	MG	DA	3085	1/1	0.84	0.51	-	1,1,1,1	0
60	MG	DA	3200	1/1	0.86	0.51	-	42,42,42,42	0
60	MG	BA	3025	1/1	0.94	0.33	-	31,31,31,31	0
60	MG	CA	1647	1/1	0.89	0.31	-	44,44,44,44	0
60	MG	DA	3019	1/1	0.79	0.29	-	6,6,6,6	0
60	MG	DA	3218	1/1	0.83	0.56	-	50,50,50,50	0
60	MG	CA	1655	1/1	0.94	0.31	-	29,29,29,29	0
60	MG	DA	3017	1/1	0.96	0.26	-	1,1,1,1	0
60	MG	DA	3135	1/1	0.91	0.45	-	11,11,11,11	0
60	MG	DA	3056	1/1	0.92	0.16	-	2,2,2,2	0
60	MG	BA	3118	1/1	0.93	0.83	-	46,46,46,46	0
60	MG	BA	3146	1/1	0.96	0.19	-	13,13,13,13	0
60	MG	DA	3178	1/1	0.84	0.22	-	22,22,22,22	0
60	MG	BA	3153	1/1	0.95	0.51	-	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3149	1/1	0.55	0.37	-	39,39,39,39	0
60	MG	BA	3279	1/1	0.90	0.23	-	29,29,29,29	0
60	MG	DA	3068	1/1	0.79	0.22	-	9,9,9,9	0
60	MG	DA	3230	1/1	0.97	0.05	-	17,17,17,17	0
60	MG	BA	3247	1/1	0.98	0.17	-	35,35,35,35	0
60	MG	DA	3201	1/1	0.67	0.33	-	36,36,36,36	0
60	MG	BA	3258	1/1	0.91	0.23	-	32,32,32,32	0
60	MG	BA	3185	1/1	0.83	0.10	-	3,3,3,3	0
60	MG	CA	1691	1/1	0.91	0.27	-	21,21,21,21	0
60	MG	AA	1681	1/1	0.92	0.24	-	58,58,58,58	0
60	MG	BA	3188	1/1	0.94	0.10	-	30,30,30,30	0
60	MG	CA	1664	1/1	0.96	0.10	-	83,83,83,83	0
60	MG	CA	1661	1/1	0.97	0.21	-	9,9,9,9	0
60	MG	AA	1695	1/1	0.79	0.18	-	30,30,30,30	0
60	MG	BA	3183	1/1	0.95	0.20	-	1,1,1,1	0
60	MG	AA	1653	1/1	0.92	0.21	-	38,38,38,38	0
60	MG	BA	3196	1/1	0.91	0.31	-	21,21,21,21	0
60	MG	AG	201	1/1	0.85	0.21	-	42,42,42,42	0
60	MG	BA	3135	1/1	0.98	0.13	-	20,20,20,20	0
60	MG	AA	1660	1/1	0.89	0.42	-	49,49,49,49	0
60	MG	CA	1658	1/1	0.82	0.27	-	30,30,30,30	0
60	MG	AA	1647	1/1	0.95	0.29	-	39,39,39,39	0
60	MG	BA	3203	1/1	0.86	0.20	-	17,17,17,17	0
60	MG	CA	1687	1/1	0.95	0.25	-	17,17,17,17	0
60	MG	DA	3231	1/1	0.82	0.69	-	49,49,49,49	0
60	MG	BA	3240	1/1	0.89	0.39	-	75,75,75,75	0
60	MG	DA	3227	1/1	0.82	0.26	-	36,36,36,36	0
60	MG	DA	3148	1/1	0.76	0.58	-	42,42,42,42	0
60	MG	AA	1710	1/1	0.96	0.60	-	29,29,29,29	0
60	MG	D0	101	1/1	0.87	0.29	-	12,12,12,12	0
60	MG	BA	3264	1/1	0.92	0.28	-	32,32,32,32	0
60	MG	AA	1707	1/1	0.62	0.39	-	52,52,52,52	0
60	MG	BB	205	1/1	0.97	0.24	-	1,1,1,1	0
60	MG	BA	3019	1/1	0.96	0.34	-	1,1,1,1	0
60	MG	DA	3225	1/1	0.68	0.41	-	39,39,39,39	0
60	MG	BA	3023	1/1	0.98	0.08	-	1,1,1,1	0
60	MG	DA	3144	1/1	0.90	0.29	-	53,53,53,53	0
60	MG	AW	104	1/1	0.92	0.25	-	31,31,31,31	0
60	MG	BA	3296	1/1	0.95	0.28	-	26,26,26,26	0
60	MG	BA	3103	1/1	0.86	0.26	-	1,1,1,1	0
60	MG	CA	1656	1/1	0.73	0.29	-	39,39,39,39	0
60	MG	BA	3084	1/1	0.87	0.22	-	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BE	301	1/1	0.97	0.14	-	1,1,1,1	0
60	MG	DE	301	1/1	0.87	0.23	-	1,1,1,1	0
60	MG	BA	3252	1/1	0.99	0.06	-	4,4,4,4	0
60	MG	DA	3088	1/1	0.91	0.29	-	22,22,22,22	0
60	MG	CA	1633	1/1	0.63	0.46	-	62,62,62,62	0
60	MG	AA	1662	1/1	0.96	0.14	-	21,21,21,21	0
60	MG	BA	3180	1/1	0.94	0.42	-	40,40,40,40	0
60	MG	CA	1644	1/1	0.58	0.64	-	67,67,67,67	0
60	MG	CA	1621	1/1	0.89	0.44	-	30,30,30,30	0
60	MG	DA	3057	1/1	0.87	0.13	-	32,32,32,32	0
60	MG	CA	1643	1/1	0.94	0.28	-	7,7,7,7	0
60	MG	AA	1638	1/1	0.51	0.74	-	76,76,76,76	0
60	MG	DA	3197	1/1	0.92	0.46	-	21,21,21,21	0
60	MG	CA	1667	1/1	0.91	0.25	-	5,5,5,5	0
60	MG	AA	1694	1/1	0.94	0.28	-	5,5,5,5	0
60	MG	BA	3200	1/1	0.96	0.20	-	14,14,14,14	0
60	MG	BA	3045	1/1	0.99	0.24	-	2,2,2,2	0
60	MG	BA	3130	1/1	0.94	0.41	-	1,1,1,1	0
60	MG	BA	3116	1/1	0.98	0.11	-	26,26,26,26	0
60	MG	CA	1606	1/1	0.90	0.64	-	45,45,45,45	0
60	MG	CA	1696	1/1	0.87	0.18	-	91,91,91,91	0
60	MG	DA	3189	1/1	0.66	0.17	-	57,57,57,57	0
60	MG	BA	3113	1/1	0.90	0.22	-	1,1,1,1	0
60	MG	CA	1671	1/1	0.94	0.14	-	24,24,24,24	0
60	MG	BA	3259	1/1	0.97	0.20	-	16,16,16,16	0
60	MG	BA	3289	1/1	0.61	0.37	-	42,42,42,42	0
60	MG	BA	3187	1/1	0.82	0.46	-	17,17,17,17	0
60	MG	DA	3172	1/1	0.86	0.33	-	6,6,6,6	0
60	MG	CA	1618	1/1	0.94	0.16	-	14,14,14,14	0
60	MG	DA	3097	1/1	0.78	0.24	-	51,51,51,51	0
60	MG	AA	1669	1/1	0.97	0.18	-	35,35,35,35	0
60	MG	AX	106	1/1	0.93	0.28	-	25,25,25,25	0
60	MG	AA	1644	1/1	0.85	0.40	-	39,39,39,39	0
60	MG	BA	3262	1/1	0.97	0.17	-	3,3,3,3	0
60	MG	DA	3093	1/1	0.79	0.47	-	31,31,31,31	0
60	MG	DA	3103	1/1	0.91	0.62	-	26,26,26,26	0
60	MG	DA	3190	1/1	0.69	0.25	-	43,43,43,43	0
60	MG	BA	3235	1/1	0.94	0.18	-	1,1,1,1	0
60	MG	DA	3094	1/1	0.84	0.47	-	16,16,16,16	0
60	MG	DA	3116	1/1	0.67	0.39	-	47,47,47,47	0
60	MG	BA	3254	1/1	0.99	0.06	-	72,72,72,72	0
60	MG	BA	3223	1/1	0.92	0.35	-	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3198	1/1	0.57	0.20	-	32,32,32,32	0
60	MG	DA	3049	1/1	0.90	0.26	-	36,36,36,36	0
60	MG	DA	3175	1/1	0.53	0.26	-	72,72,72,72	0
60	MG	BA	3026	1/1	0.91	0.31	-	7,7,7,7	0
60	MG	DA	3162	1/1	0.83	0.43	-	44,44,44,44	0
60	MG	AA	1701	1/1	0.86	0.31	-	11,11,11,11	0
60	MG	BA	3304	1/1	0.93	0.21	-	36,36,36,36	0
60	MG	DA	3039	1/1	0.84	0.18	-	53,53,53,53	0
60	MG	DA	3121	1/1	0.97	0.59	-	34,34,34,34	0
60	MG	DA	3212	1/1	0.83	0.19	-	4,4,4,4	0
60	MG	BA	3175	1/1	0.91	0.20	-	26,26,26,26	0
60	MG	DA	3124	1/1	0.73	0.39	-	36,36,36,36	0
60	MG	DA	3194	1/1	0.83	0.43	-	44,44,44,44	0
60	MG	BA	3106	1/1	0.91	0.30	-	3,3,3,3	0
60	MG	BA	3109	1/1	0.68	0.24	-	58,58,58,58	0
60	MG	BA	3201	1/1	0.89	0.69	-	53,53,53,53	0
60	MG	DA	3036	1/1	0.94	0.27	-	5,5,5,5	0
60	MG	BA	3334	1/1	0.93	0.20	-	1,1,1,1	0
60	MG	BA	3308	1/1	0.96	0.33	-	30,30,30,30	0
60	MG	DA	3176	1/1	0.55	0.45	-	54,54,54,54	0
60	MG	AA	1687	1/1	0.94	0.18	-	20,20,20,20	0
60	MG	AA	1709	1/1	0.86	0.35	-	36,36,36,36	0
60	MG	DA	3209	1/1	0.51	0.36	-	5,5,5,5	0
60	MG	DB	201	1/1	0.88	0.68	-	51,51,51,51	0
60	MG	BA	3061	1/1	0.93	0.20	-	17,17,17,17	0
60	MG	BA	3171	1/1	0.59	0.20	-	36,36,36,36	0
60	MG	DA	3155	1/1	0.76	0.56	-	31,31,31,31	0
60	MG	CA	1607	1/1	0.68	0.51	-	29,29,29,29	0
60	MG	BA	3260	1/1	0.88	0.96	-	65,65,65,65	0
60	MG	BA	3307	1/1	0.92	0.24	-	19,19,19,19	0
60	MG	AA	1620	1/1	0.82	0.42	-	31,31,31,31	0
60	MG	BA	3217	1/1	0.95	0.14	-	1,1,1,1	0
60	MG	DA	3080	1/1	0.84	0.49	-	36,36,36,36	0
60	MG	AA	1690	1/1	0.95	0.43	-	23,23,23,23	0
60	MG	BA	3316	1/1	0.76	0.44	-	35,35,35,35	0
60	MG	CA	1611	1/1	0.90	0.37	-	66,66,66,66	0
60	MG	BA	3181	1/1	0.93	0.36	-	16,16,16,16	0
60	MG	DA	3166	1/1	0.75	0.39	-	36,36,36,36	0
60	MG	CA	1642	1/1	0.88	0.10	-	28,28,28,28	0
60	MG	BA	3092	1/1	0.93	0.41	-	3,3,3,3	0
60	MG	DB	202	1/1	0.56	0.77	-	80,80,80,80	0
60	MG	AA	1630	1/1	0.66	0.68	-	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1624	1/1	0.86	0.58	-	40,40,40,40	0
60	MG	DA	3112	1/1	0.96	0.45	-	7,7,7,7	0
60	MG	DA	3029	1/1	0.94	0.43	-	1,1,1,1	0
60	MG	DA	3164	1/1	0.64	0.21	-	64,64,64,64	0
60	MG	AA	1673	1/1	0.89	0.18	-	39,39,39,39	0
60	MG	BA	3315	1/1	0.95	0.35	-	29,29,29,29	0
60	MG	AA	1703	1/1	0.98	0.24	-	35,35,35,35	0
60	MG	AX	108	1/1	0.87	0.38	-	34,34,34,34	0
60	MG	BA	3096	1/1	0.93	0.39	-	34,34,34,34	0
60	MG	DA	3168	1/1	0.89	0.65	-	55,55,55,55	0
60	MG	BA	3230	1/1	0.90	0.26	-	19,19,19,19	0
60	MG	BA	3100	1/1	0.97	0.11	-	10,10,10,10	0
60	MG	BA	3317	1/1	0.97	0.15	-	22,22,22,22	0
60	MG	DA	3079	1/1	0.91	0.34	-	19,19,19,19	0
60	MG	D5	101	1/1	0.87	0.19	-	10,10,10,10	0
60	MG	DA	3062	1/1	0.78	0.42	-	8,8,8,8	0
60	MG	AA	1625	1/1	0.88	0.25	-	21,21,21,21	0
60	MG	DA	3203	1/1	0.78	0.44	-	38,38,38,38	0
60	MG	BA	3269	1/1	0.93	0.40	-	12,12,12,12	0
60	MG	AA	1686	1/1	0.87	0.29	-	34,34,34,34	0
60	MG	CA	1648	1/1	0.95	0.35	-	24,24,24,24	0
60	MG	CA	1619	1/1	0.95	0.43	-	20,20,20,20	0
60	MG	DA	3024	1/1	0.93	0.35	-	5,5,5,5	0
60	MG	CA	1623	1/1	0.88	0.52	-	33,33,33,33	0
60	MG	AA	1685	1/1	0.89	0.27	-	69,69,69,69	0
60	MG	BA	3060	1/1	0.94	0.27	-	4,4,4,4	0
60	MG	DA	3018	1/1	0.96	0.18	-	15,15,15,15	0
60	MG	BP	202	1/1	0.96	0.28	-	1,1,1,1	0
60	MG	AA	1605	1/1	0.89	0.20	-	35,35,35,35	0
60	MG	BA	3024	1/1	0.96	0.13	-	11,11,11,11	0
60	MG	BA	3007	1/1	0.94	0.28	-	1,1,1,1	0
60	MG	BA	3290	1/1	0.86	0.44	-	24,24,24,24	0
60	MG	BA	3276	1/1	0.92	0.37	-	16,16,16,16	0
60	MG	BA	3299	1/1	0.94	0.18	-	13,13,13,13	0
60	MG	BA	3138	1/1	0.89	0.20	-	1,1,1,1	0
60	MG	DA	3044	1/1	0.96	0.19	-	1,1,1,1	0
60	MG	AA	1645	1/1	0.82	0.41	-	22,22,22,22	0
60	MG	BA	3242	1/1	0.96	0.48	-	49,49,49,49	0
60	MG	BA	3056	1/1	0.89	0.19	-	1,1,1,1	0
60	MG	BA	3015	1/1	0.83	0.14	-	5,5,5,5	0
60	MG	BA	3215	1/1	0.68	0.71	-	60,60,60,60	0
60	MG	BA	3120	1/1	0.90	0.53	-	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3012	1/1	0.91	0.33	-	1,1,1,1	0
60	MG	DA	3032	1/1	0.93	0.14	-	1,1,1,1	0
60	MG	BA	3265	1/1	0.86	0.38	-	13,13,13,13	0
60	MG	DA	3086	1/1	0.58	0.83	-	58,58,58,58	0
60	MG	BA	3068	1/1	0.96	0.07	-	11,11,11,11	0
60	MG	BA	3319	1/1	0.87	0.32	-	31,31,31,31	0
60	MG	BA	3127	1/1	0.95	0.27	-	1,1,1,1	0
60	MG	DA	3054	1/1	0.87	0.33	-	21,21,21,21	0
60	MG	CE	201	1/1	0.95	0.13	-	56,56,56,56	0
60	MG	DA	3048	1/1	0.84	0.31	-	23,23,23,23	0
60	MG	AA	1702	1/1	0.79	0.34	-	41,41,41,41	0
60	MG	CA	1645	1/1	0.94	0.78	-	56,56,56,56	0
60	MG	CA	1669	1/1	0.91	0.12	-	16,16,16,16	0
60	MG	DA	3204	1/1	0.76	0.48	-	67,67,67,67	0
60	MG	BA	3189	1/1	0.74	0.21	-	40,40,40,40	0
60	MG	BA	3139	1/1	0.94	0.25	-	1,1,1,1	0
60	MG	DA	3136	1/1	0.53	0.44	-	31,31,31,31	0
60	MG	AA	1676	1/1	0.96	0.31	-	11,11,11,11	0
60	MG	AA	1631	1/1	0.93	0.39	-	12,12,12,12	0
60	MG	BA	3176	1/1	0.97	0.37	-	1,1,1,1	0
60	MG	BA	3274	1/1	0.87	0.19	-	21,21,21,21	0
60	MG	AA	1661	1/1	0.95	0.25	-	21,21,21,21	0
60	MG	BA	3053	1/1	0.97	0.18	-	1,1,1,1	0
60	MG	BA	3326	1/1	0.98	0.13	-	21,21,21,21	0
60	MG	CA	1665	1/1	0.87	0.30	-	33,33,33,33	0
60	MG	CA	1605	1/1	0.95	0.41	-	6,6,6,6	0
60	MG	AA	1705	1/1	0.95	0.15	-	4,4,4,4	0
60	MG	DA	3110	1/1	0.39	0.52	-	48,48,48,48	0
60	MG	BA	3069	1/1	0.97	0.18	-	1,1,1,1	0
60	MG	BA	3322	1/1	0.98	0.30	-	10,10,10,10	0
60	MG	BA	3079	1/1	0.74	0.31	-	7,7,7,7	0
60	MG	DA	3127	1/1	0.66	0.32	-	20,20,20,20	0
60	MG	BA	3314	1/1	0.91	0.17	-	35,35,35,35	0
60	MG	CA	1666	1/1	0.96	0.20	-	9,9,9,9	0
60	MG	BP	201	1/1	0.96	0.18	-	11,11,11,11	0
60	MG	BA	3195	1/1	0.82	0.61	-	49,49,49,49	0
60	MG	DA	3181	1/1	0.88	0.51	-	50,50,50,50	0
60	MG	BB	201	1/1	0.92	0.24	-	46,46,46,46	0
60	MG	CA	1637	1/1	0.82	0.73	-	57,57,57,57	0
60	MG	BA	3268	1/1	0.98	0.20	-	1,1,1,1	0
60	MG	BA	3288	1/1	0.97	0.24	-	29,29,29,29	0
60	MG	BA	3003	1/1	0.91	0.25	-	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3006	1/1	0.93	0.38	-	37,37,37,37	0
60	MG	BA	3124	1/1	0.96	0.41	-	13,13,13,13	0
60	MG	DA	3233	1/1	0.90	0.21	-	1,1,1,1	0
60	MG	BA	3275	1/1	0.90	0.19	-	7,7,7,7	0
60	MG	BA	3207	1/1	0.90	0.22	-	21,21,21,21	0
60	MG	DA	3183	1/1	0.90	0.30	-	9,9,9,9	0
60	MG	BA	3089	1/1	0.95	0.20	-	12,12,12,12	0
60	MG	BA	3286	1/1	0.93	0.49	-	18,18,18,18	0
60	MG	AA	1696	1/1	0.98	0.46	-	20,20,20,20	0
60	MG	BA	3071	1/1	0.97	0.34	-	1,1,1,1	0
60	MG	AA	1619	1/1	0.94	0.20	-	10,10,10,10	0
60	MG	BA	3301	1/1	0.90	0.31	-	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.