wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2023 – 05:58 AM EDT

PDB ID	:	4V6A
Title	:	Structure of EF-P bound to the 70S ribosome.
Authors	:	Stanley, R.E.; Blaha, G.
Deposited on	:	2009-06-15
Resolution	:	3.10 Å(reported)

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

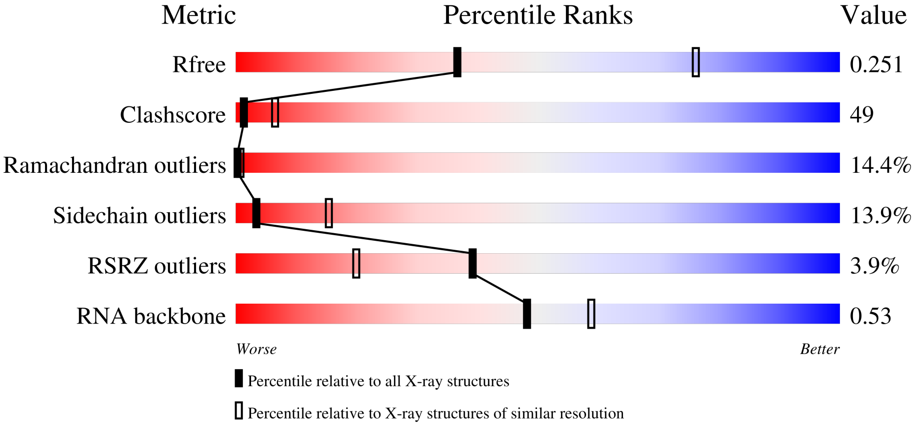
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

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

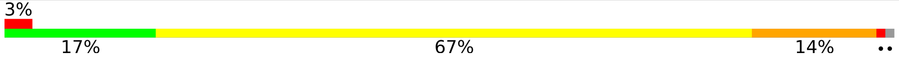
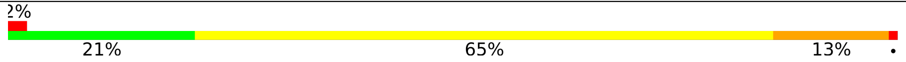
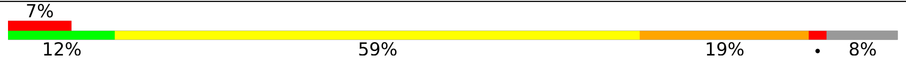
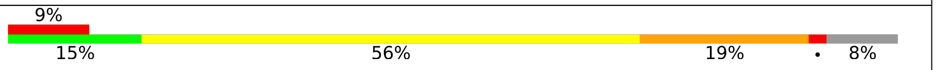
The reported resolution of this entry is 3.10 Å.

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



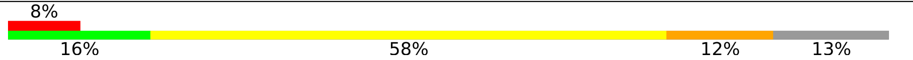
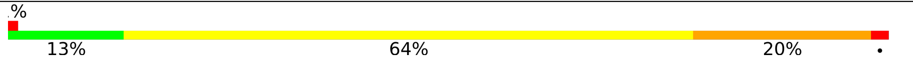
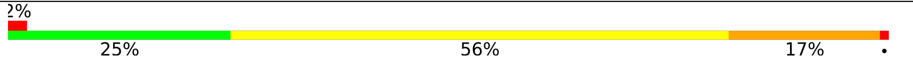
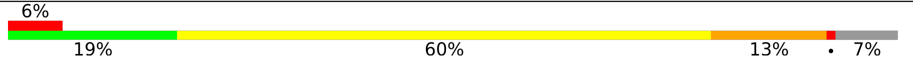
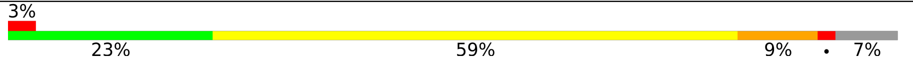
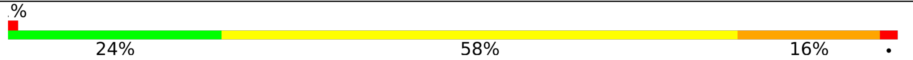
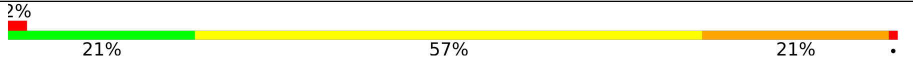
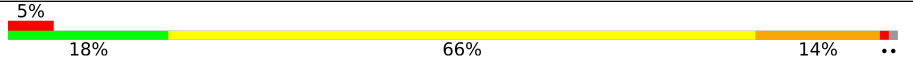
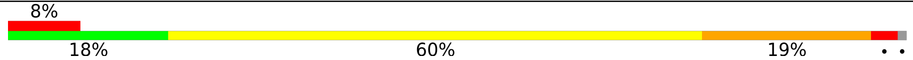
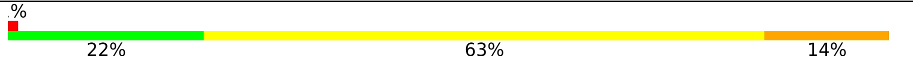
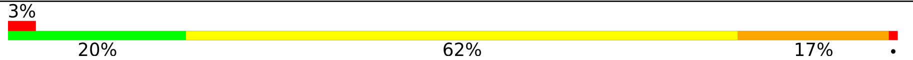
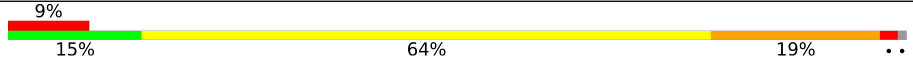
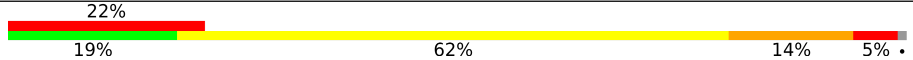
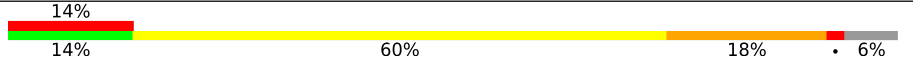
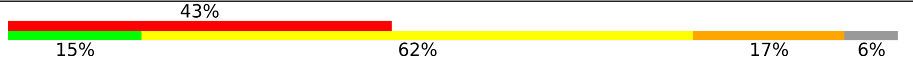
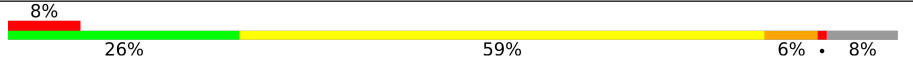
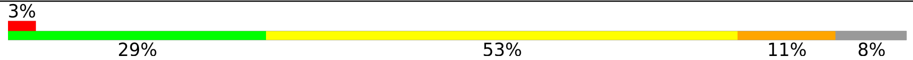
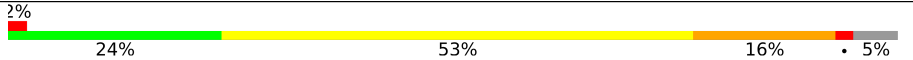
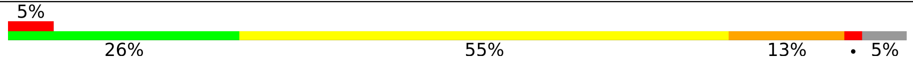
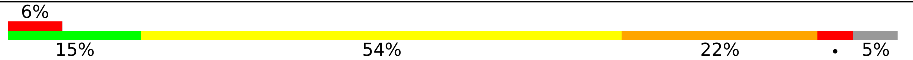
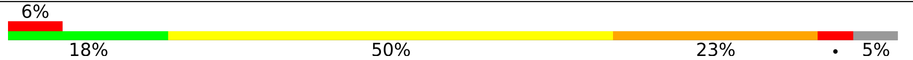
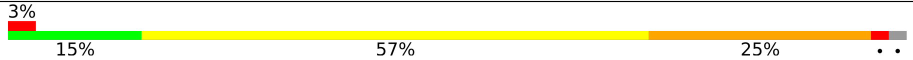
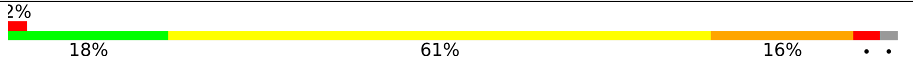
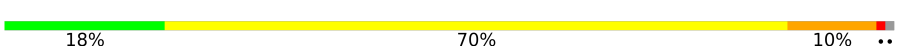
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1509	
1	CA	1509	
2	AB	256	
2	CB	256	

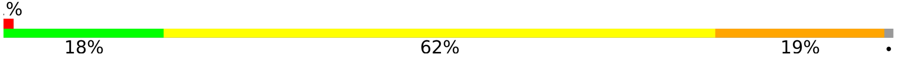
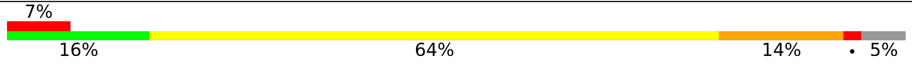
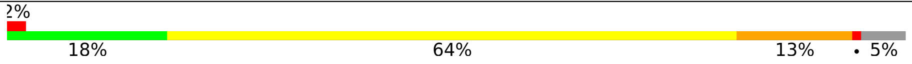
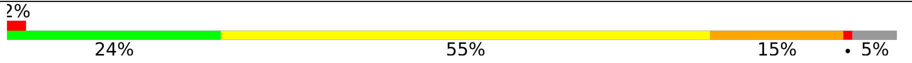
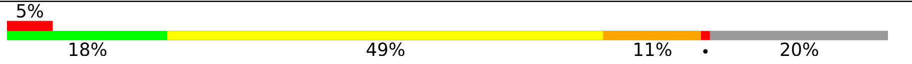
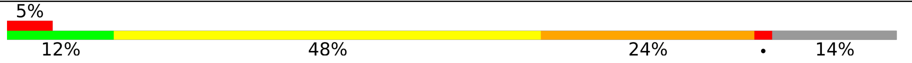
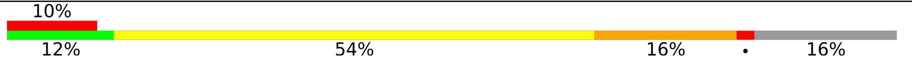
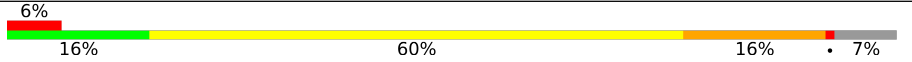
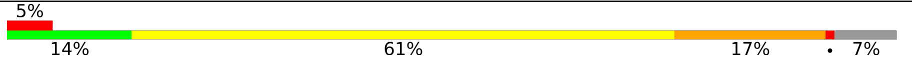
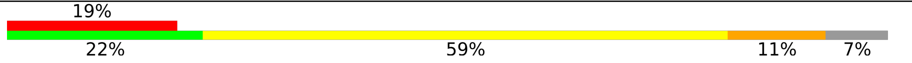
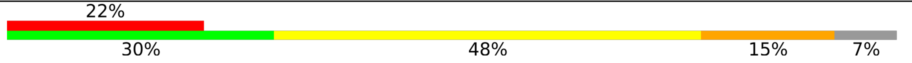
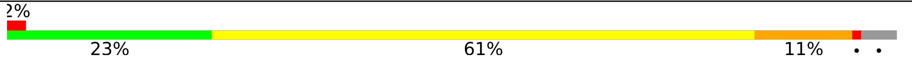
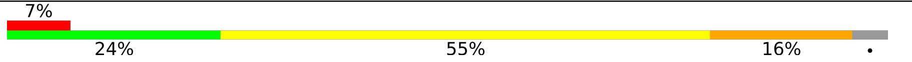
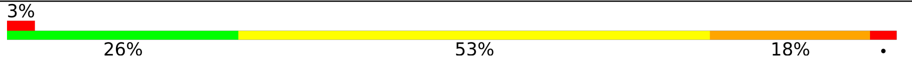
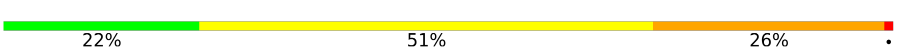
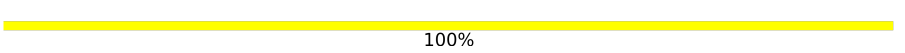
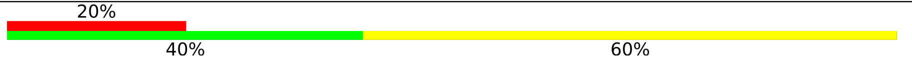
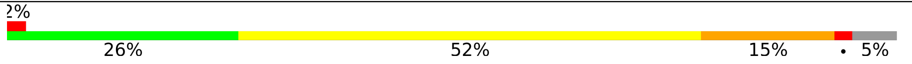
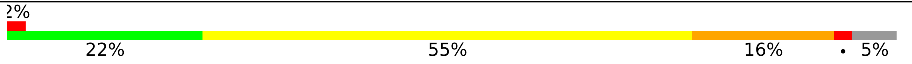
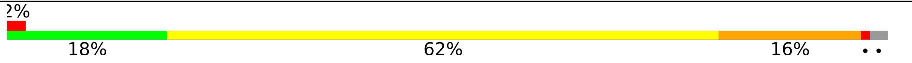
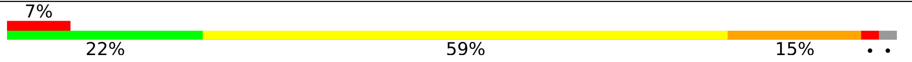
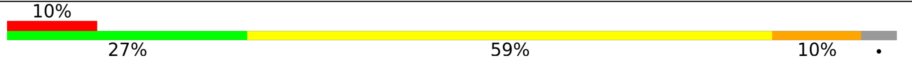
Continued on next page...

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	

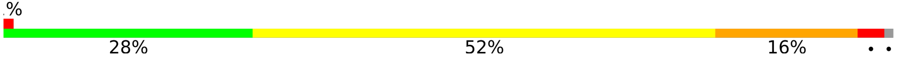
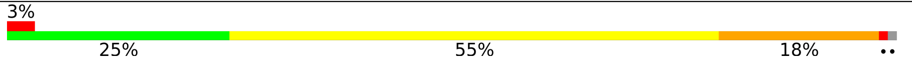
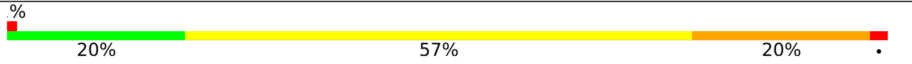
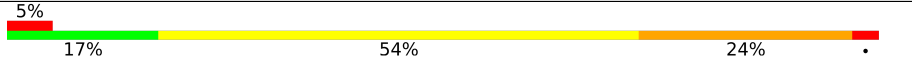
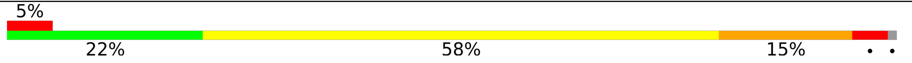
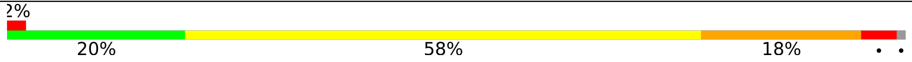
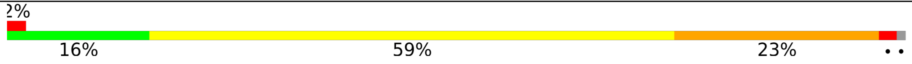
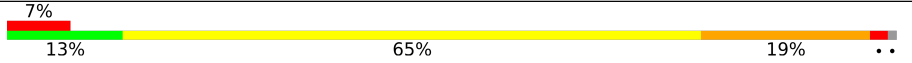
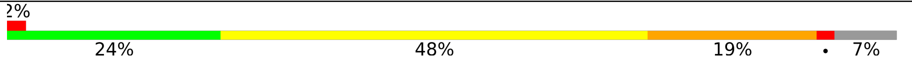
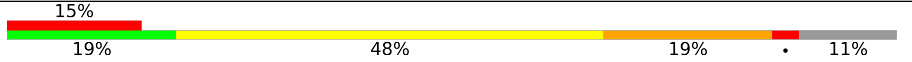
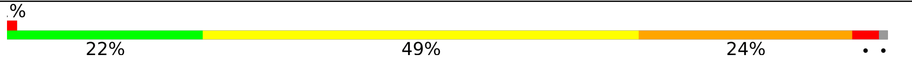
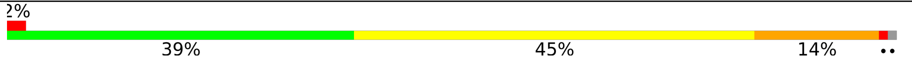
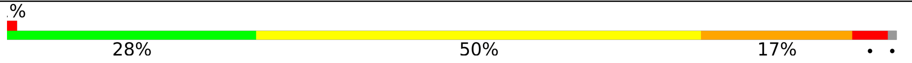
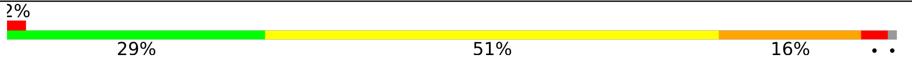
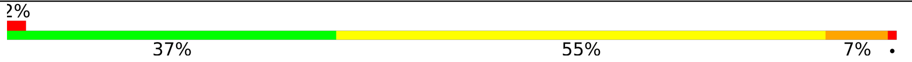
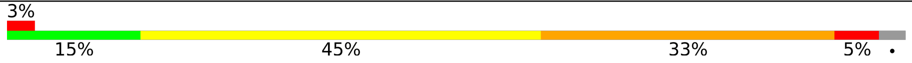
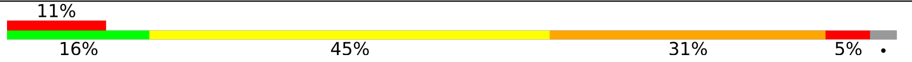
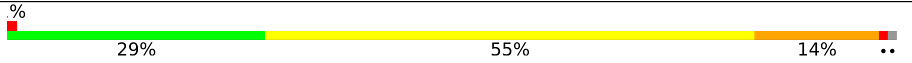
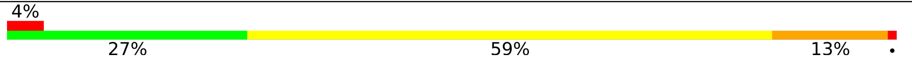
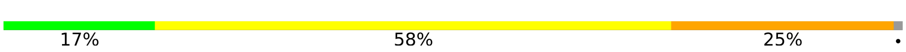
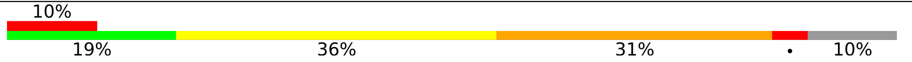
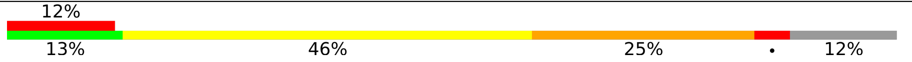
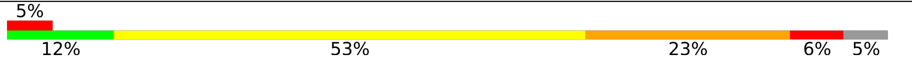
Continued on next page...

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

Continued on next page...

Continued from previous page...

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

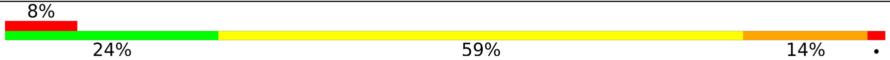
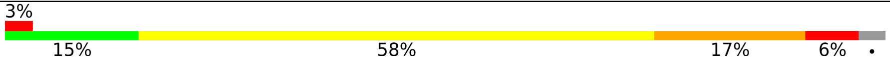
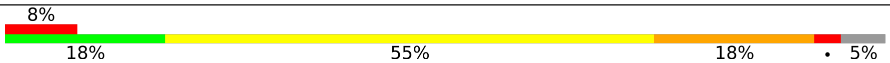
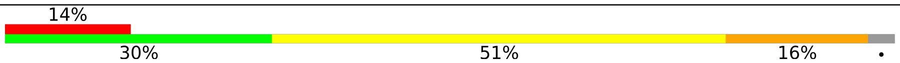
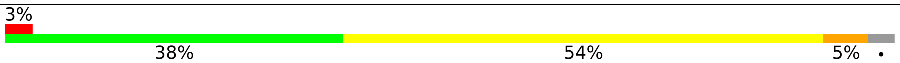
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	DT	146	4% 12% 51% 27% • 5%
41	BU	118	3% 35% 51% 11% • •
41	DU	118	3% 19% 63% 16% • •
42	BV	101	% 26% 46% 23% 6%
42	DV	101	3% 13% 58% 25% •
43	BW	113	% 34% 50% 14% •
43	DW	113	% 20% 67% 12% •
44	BX	96	33% 51% 12% • •
44	DX	96	4% 19% 64% 14% • •
45	BY	110	3% 13% 43% 29% 7% 8%
45	DY	110	7% 5% 53% 25% 9% 8%
46	BZ	206	% 22% 50% 12% • 12%
46	DZ	206	7% 12% 55% 17% • 14%
47	B0	85	2% 26% 58% 7% 9%
47	D0	85	7% 28% 55% 14% ••
48	B1	98	20% 54% 22% • •
48	D1	98	6% 28% 53% 15% •
49	B2	72	31% 53% 12% • •
49	D2	72	3% 14% 62% 19% • •
50	B3	60	8% 37% 53% 8% •
50	D3	60	13% 17% 68% 15%
51	B4	71	% 7% 23% 13% • 56%
51	D4	71	3% 13% 20% 11% 56%
52	B5	60	22% 42% 27% 5% 5%
52	D5	60	8% 33% 38% 23% • •

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	1604	-	-	-	X
57	MG	AA	1611	-	-	-	X
57	MG	AA	1619	-	-	-	X
57	MG	AA	1664	-	-	-	X
57	MG	BA	3022	-	-	-	X
57	MG	BA	3038	-	-	-	X
57	MG	BA	3052	-	-	-	X
57	MG	BA	3086	-	-	-	X
57	MG	BA	3118	-	-	-	X
57	MG	BA	3139	-	-	-	X
57	MG	BA	3188	-	-	-	X
57	MG	BA	3268	-	-	-	X
57	MG	BA	3300	-	-	-	X
57	MG	BA	3323	-	-	-	X
57	MG	BA	3355	-	-	-	X
57	MG	BA	3388	-	-	-	X
57	MG	BA	3432	-	-	-	X
57	MG	BA	3442	-	-	-	X
57	MG	BA	3444	-	-	-	X
57	MG	BA	3448	-	-	-	X
57	MG	BP	201	-	-	-	X
57	MG	CA	1608	-	-	-	X
57	MG	CA	1652	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	CA	1708	-	-	-	X
57	MG	CW	102	-	-	-	X
57	MG	DA	3033	-	-	-	X
57	MG	DA	3072	-	-	-	X
57	MG	DA	3094	-	-	-	X
57	MG	DA	3108	-	-	-	X
57	MG	DA	3111	-	-	-	X
57	MG	DA	3144	-	-	-	X
57	MG	DA	3164	-	-	-	X
57	MG	DA	3175	-	-	-	X
57	MG	DA	3195	-	-	-	X
57	MG	DA	3267	-	-	-	X
57	MG	DB	208	-	-	-	X
58	ZN	AD	301	-	-	-	X
58	ZN	D9	101	-	-	X	-

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 290405 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1495	32144	14306	5964	10379	1495	0	0	0
1	CA	1504	32332	14390	5992	10446	1504	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AB	235	1901	1213	342	341	5	0	0	1
2	CB	235	1901	1213	342	341	5	0	0	1

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total 1147	C 724	N 218	O 201	S 4	0	0	1
5	CE	151	Total 1147	C 724	N 218	O 201	S 4	0	0	1

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total 1004	C 635	N 195	O 174	0	0	0
9	CI	127	Total 1004	C 635	N 195	O 174	0	0	0

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total 971	C 611	N 196	O 163	S 1	0	0	1
12	CL	125	Total 971	C 611	N 196	O 163	S 1	0	0	1

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	80	Total	C	N	O	S	0	0	1
			613	392	110	109	2			
19	CS	78	Total	C	N	O	S	0	0	1
			619	397	111	109	2			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total 209	C 128	N 51	O 30	0	0	1
21	CU	25	Total 209	C 128	N 51	O 30	0	0	1

- Molecule 22 is a protein called Elongation factor P.

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

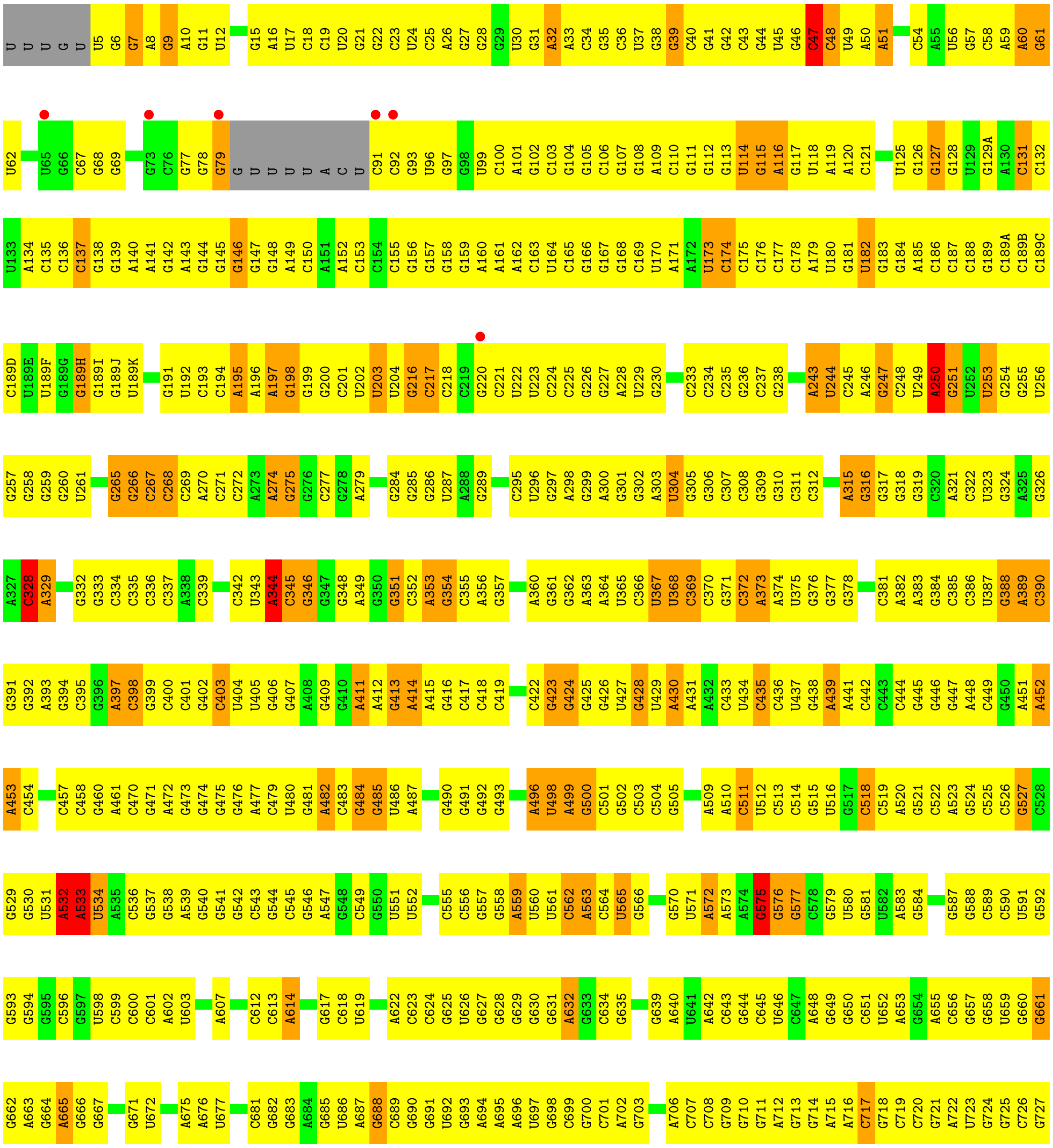
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

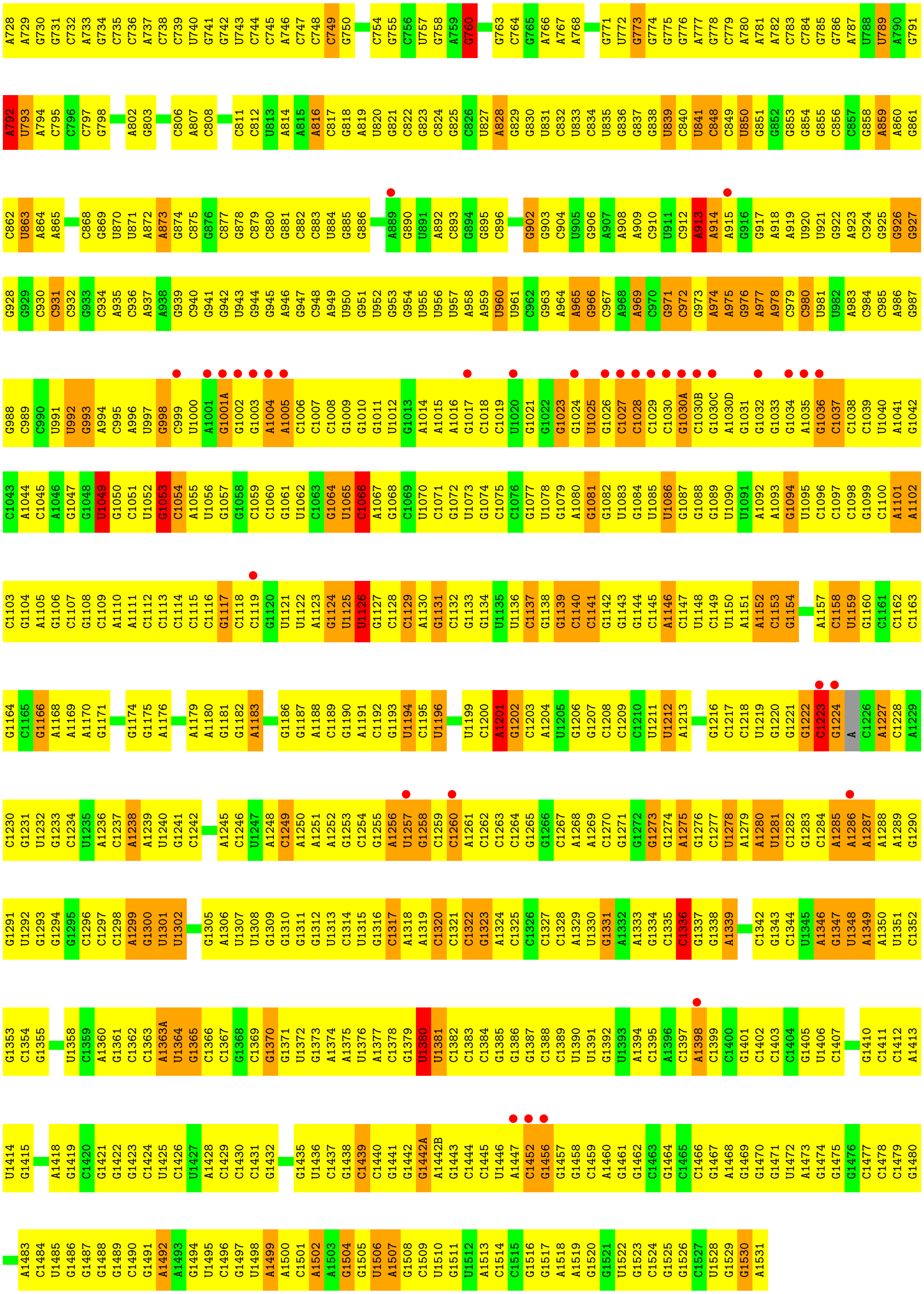
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AD	1	Total Zn 1 1	0	0
58	B5	1	Total Zn 1 1	0	0
58	B9	1	Total Zn 1 1	0	0
58	CD	1	Total Zn 1 1	0	0
58	D5	1	Total Zn 1 1	0	0
58	D9	1	Total Zn 1 1	0	0

3 Residue-property plots ⓘ

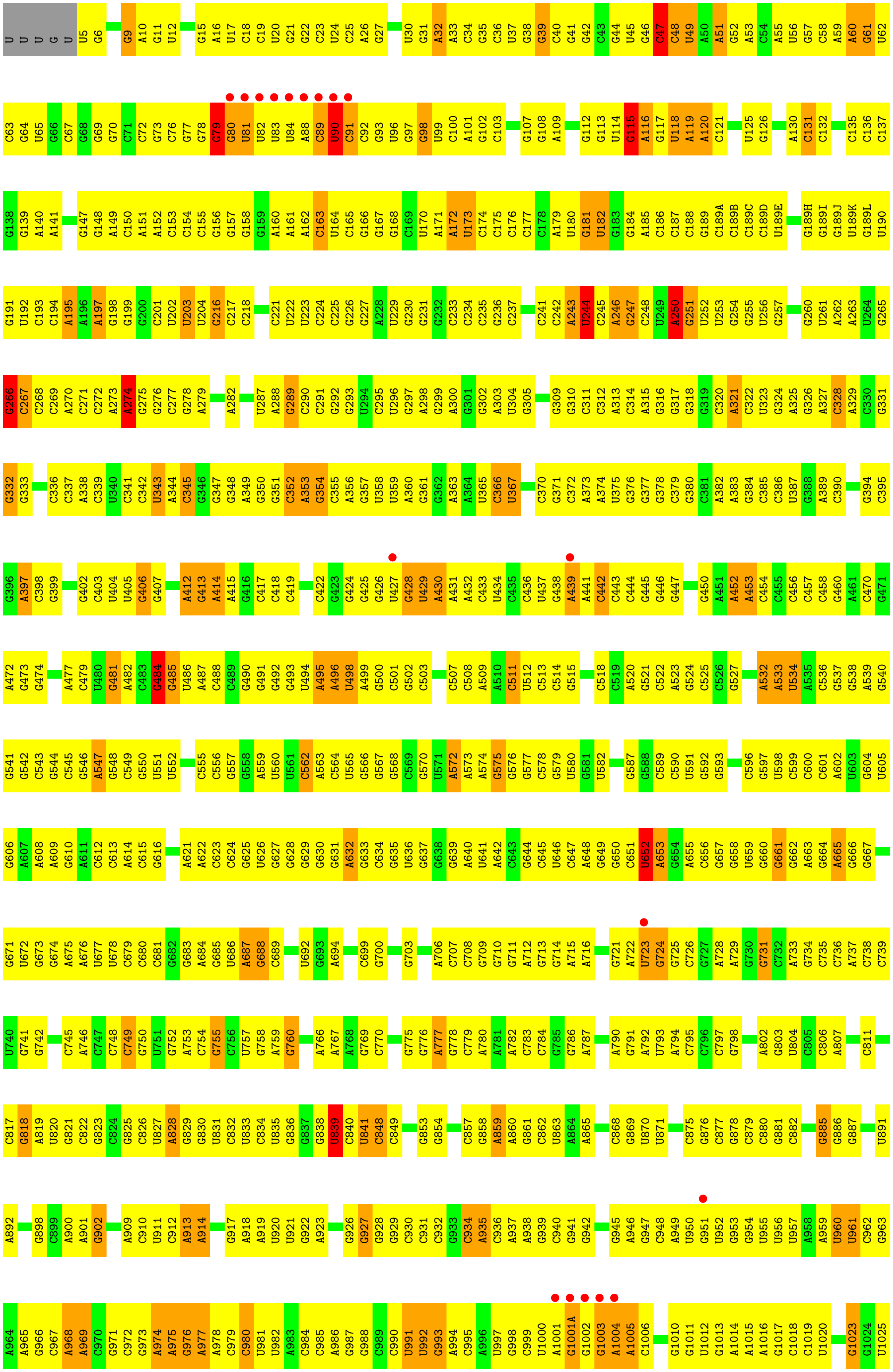
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

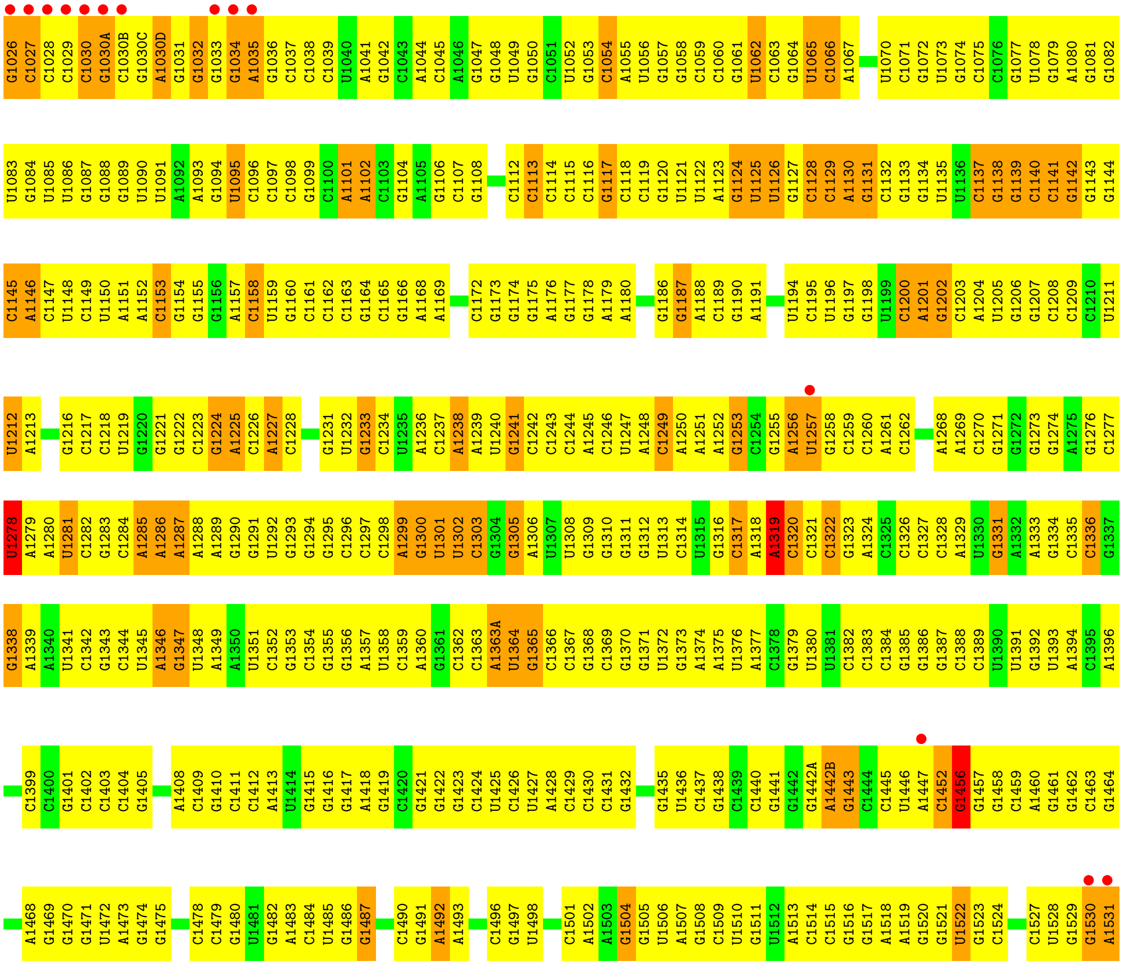
- Molecule 1: 16S ribosomal RNA





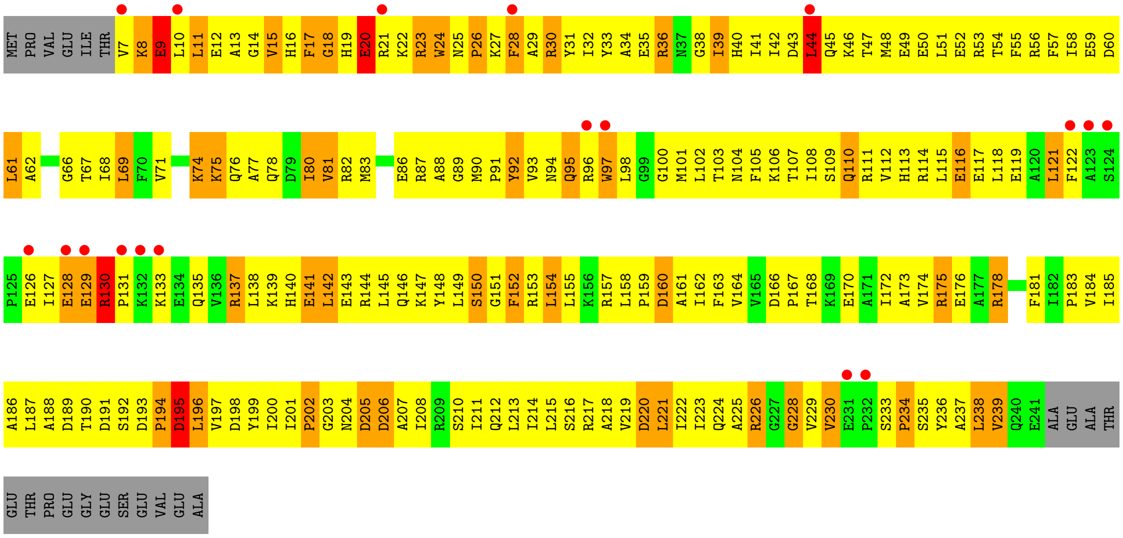
- Molecule 1: 16S ribosomal RNA


U U U G U U5 G6 G9 A10 G11 U12 G15 A16 U17 C18 C19 U20 G21 G22 C23 U24 C25 A26 G27 U30 G31 A32 A33 C34 G35 C36 U37 G38 G39 C40 G41 G42 C43 G44 U45 G46 C47 C48 U49 A50 A51 G52 A53 C54 A55 U56 G57 C58 A59 A60 G61 U62
C63 G64 U65 G66 C67 G68 G69 G70 C71 C72 G73 C76 G77 G78 G79 G80 U81 U82 U83 U84 A88 C89 U90 C91 C92 G93 U96 G97 G98 U99 C100 A101 G102 C103 G107 G108 A109 G112 G113 U114 G115 A116 G117 U118 A119 A120 C121 U125 G126 A130 C131 C132 C135 C136 C137
G138 G139 A140 A141 G147 G148 A149 C150 A151 A152 C153 C154 C155 G156 G157 G158 G159 A160 A161 A162 C163 U164 C165 G166 G167 G168 C169 U170 A171 A172 U173 C174 C175 C176 C177 C178 A179 U180 G181 U182 G183 G184 A185 C186 C187 C188 G189 C189A C189B C189C C189D U189E G189H G189I G189J U189K G189L U190
G191 U192 C193 C194 A195 A196 A197 G198 G199 G200 C201 U202 U203 U204 G216 C217 C218 C221 U222 U223 C224 C225 G226 G227 A228 U229 G230 G231 G232 C233 C234 C235 G236 C237 C241 C242 A243 U244 C245 A246 G247 C248 U249 A250 G251 U252 U253 G254 G255 G256 G257 C260 U261 A262 A263 U264 G265
G266 C267 C268 C269 A270 C271 C272 A273 A274 G275 C276 C277 G278 A279 A282 U287 A288 G289 C290 C291 G292 G293 U294 C295 U296 G297 A298 G299 A300 G301 C302 A303 U304 G305 G309 G310 C311 C312 A313 C314 A315 G316 G317 G318 G319 C320 A321 C322 U323 G324 A325 G326 A327 C328 A329 C330 G331
G332 G333 C336 C337 A338 C339 U340 C341 C342 U343 A344 C345 G346 G347 G348 A349 G350 G351 C352 A353 G354 C355 A356 G357 U358 U359 A360 G361 G362 A363 A364 U365 C366 U367 C370 G371 C372 A373 A374 U375 G376 G377 G378 C379 G380 C381 A382 A383 G384 C385 C386 U387 G388 A389 C390 G394 C395
G396 A397 C398 G399 G402 C403 U404 U405 G406 G407 A412 G413 A414 A415 G416 C417 C418 C419 C422 G423 G424 G425 C426 U427 G428 U429 A430 A431 A432 C433 U434 C435 C436 U437 G438 A439 A441 C442 C443 C444 G445 G446 G447 G450 A451 A452 A453 C454 C455 C456 G457 C458 G460 A461 C470 G471
A472 G473 G474 A477 C479 U480 G481 A482 C483 G484 G485 U486 A487 C488 G489 G490 G491 G492 G493 U494 A495 A496 U498 A499 G500 C501 G502 C503 C507 C508 A509 A510 C511 U512 C513 C514 G515 C518 C519 A520 G521 C522 A523 G524 C525 C526 G527 A532 A533 U534 A535 C536 G537 C538 A539 G540
G541 G542 C543 G544 C545 G546 A547 G548 C549 G550 U551 U552 C555 C556 G557 G558 A559 U560 U561 C562 A563 C564 U565 G566 G567 G568 C569 G570 U571 A572 A573 A574 G575 G576 G577 C578 G579 U580 G581 U582 G587 G588 C589 C590 U591 G592 G593 C596 G597 U598 C599 C600 C601 A602 U603 G604 U605
G606 A607 A608 A609 G610 A611 C612 C613 A614 C615 G616 A621 A622 C623 C624 G625 U626 G627 G628 G629 C630 G631 A632 G633 C634 G635 U636 G637 G638 G639 A640 U641 A642 C643 G644 C645 U646 C647 A648 G649 G650 C651 U652 A653 G654 A655 C656 G657 G658 U659 G660 G661 G662 A663 G664 A665 G666 G667
G671 U672 G673 G674 A675 A676 U677 U678 C679 C680 C681 G682 G683 A684 G685 U686 A687 G688 C689 U692 G693 A694 C699 G700 G703 A706 C707 G708 G709 G710 G711 A712 G713 G714 A715 A716 G721 A722 U723 G724 G725 C726 G727 A728 A729 G730 G731 C732 A733 G734 C735 C736 A737 C738 C739
U740 G741 G742 C745 A746 C747 C748 C749 G750 U751 G752 A753 C754 G755 C756 U757 G758 A759 G760 A766 A767 A768 G769 C770 G775 G776 A777 G778 C779 A780 A781 A782 C783 C784 G785 G786 A787 A790 G791 A792 U793 A794 C795 C796 C797 G798 A802 G803 U804 C805 C806 A807 C811
C817 G818 A819 U820 G821 C822 G823 C824 G825 C826 U827 A828 G829 G830 U831 C832 U833 C834 G835 G836 G837 G838 U839 C840 U841 C848 C849 G853 G854 C857 G858 A859 A860 G861 C862 U863 A864 A865 C868 G869 U870 U871 C875 G876 C877 G878 C879 C880 G881 C882 G885 G886 G887 U891
A892 G898 C899 A900 A901 G902 A909 C910 U911 C912 A913 A914 G917 A918 A919 U920 U921 G922 A923 G926 G927 G928 G929 C930 C931 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 G945 A946 G947 C948 A949 U950 G951 U952 G953 G954 U955 G956 U957 A958 A959 U960 U961 C962 G963
A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 G980 U981 U982 A983 C984 C985 A986 G987 G988 C989 C990 U991 U992 G993 A994 C995 A996 U997 G998 C999 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 G1010 G1011 U1012 G1013 A1014 A1015 A1016 G1017 C1018 C1019 U1020 G1023 G1024 U1025



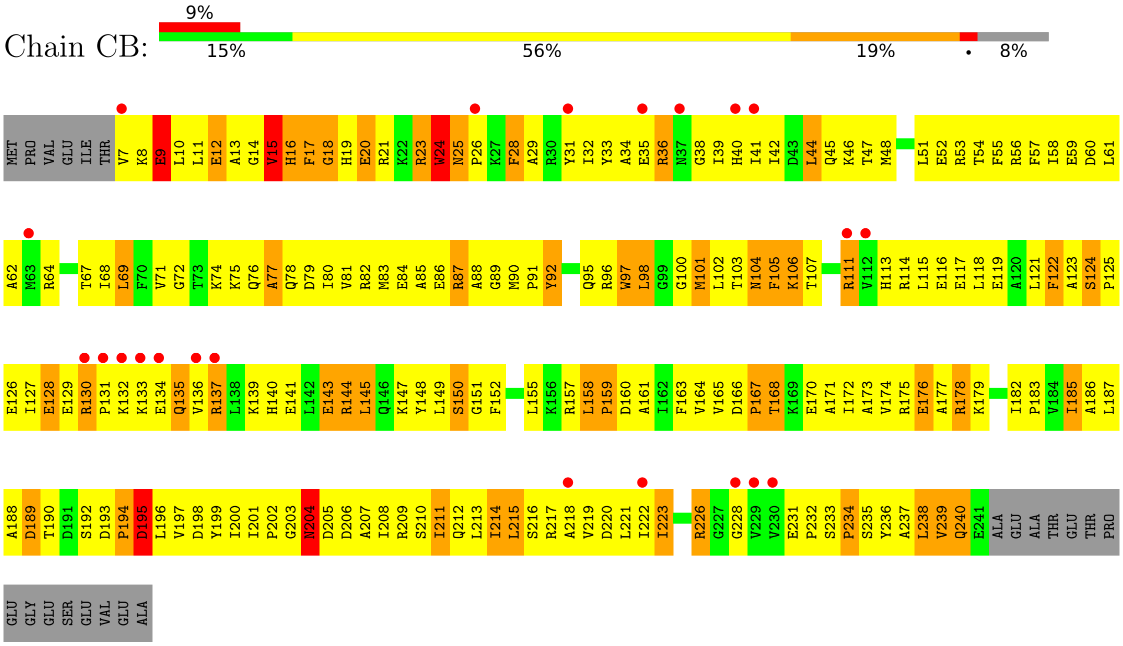
- Molecule 2: 30S ribosomal protein S2

Chain AB:



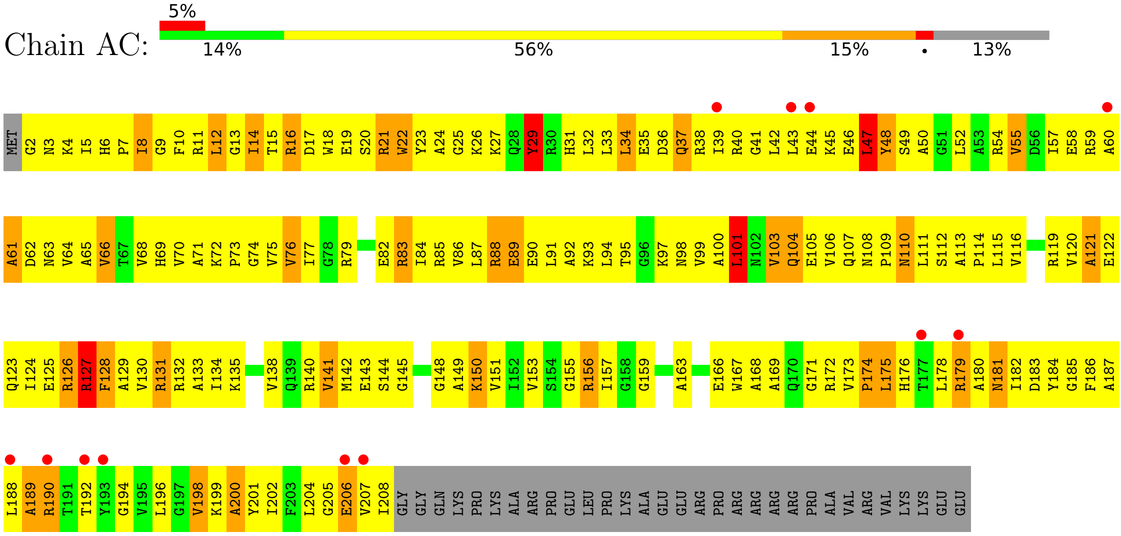
- Molecule 2: 30S ribosomal protein S2

Chain CB:



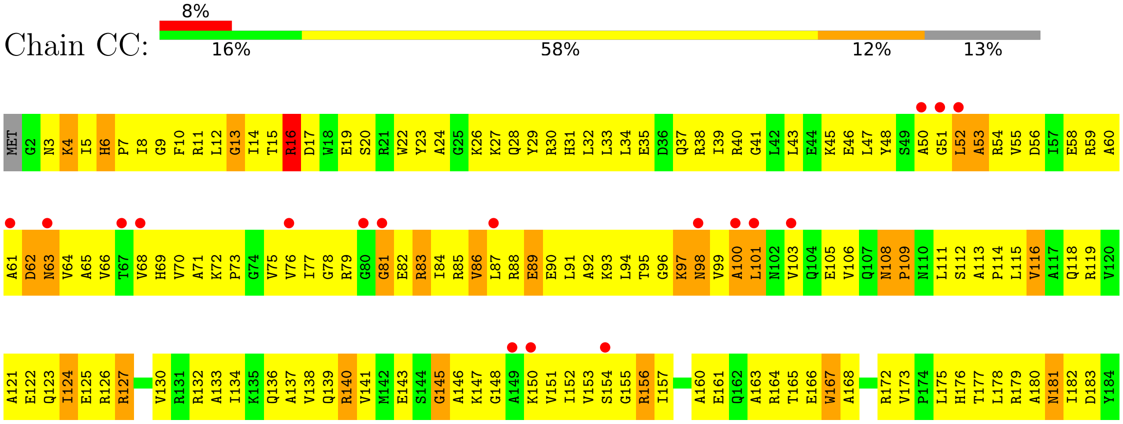
- Molecule 3: 30S ribosomal protein S3

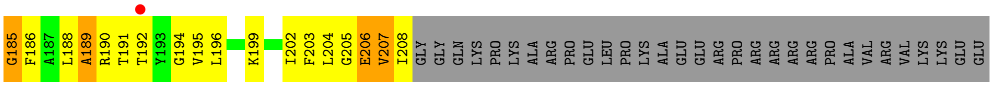
Chain AC:



- Molecule 3: 30S ribosomal protein S3

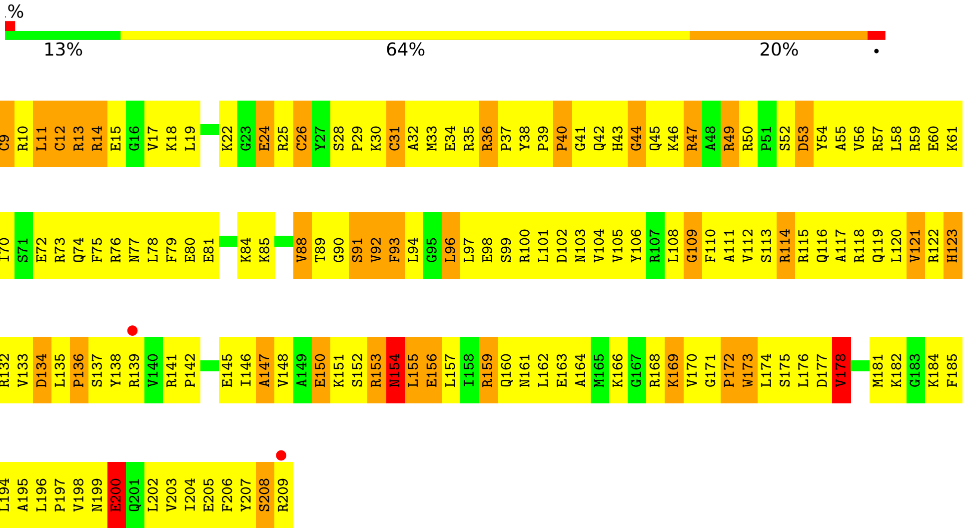
Chain CC:





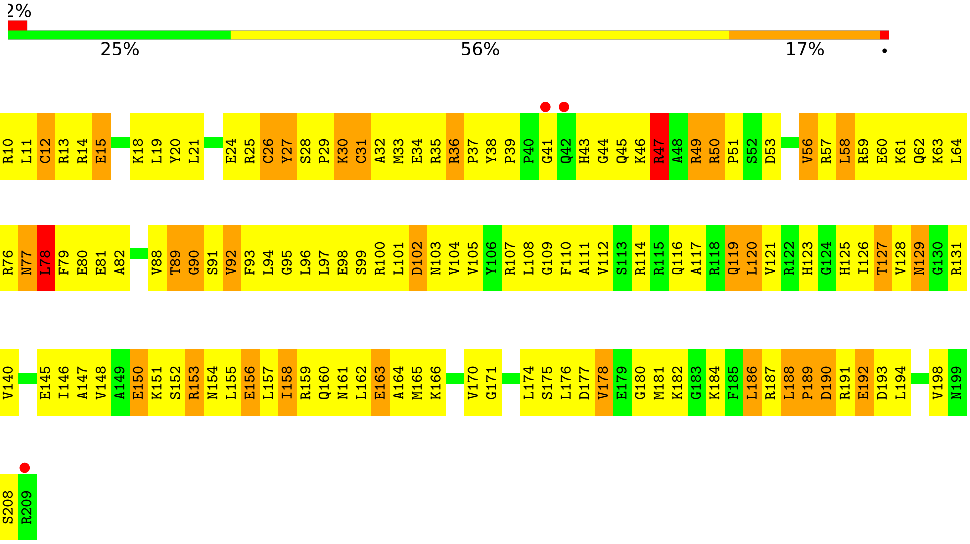
- Molecule 4: 30S ribosomal protein S4

Chain AD:



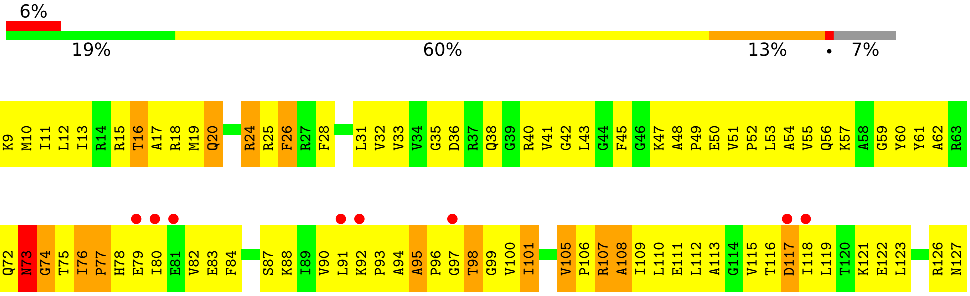
- Molecule 4: 30S ribosomal protein S4

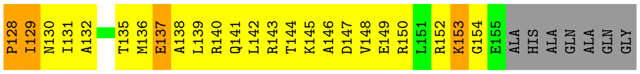
Chain CD:



- Molecule 5: 30S ribosomal protein S5

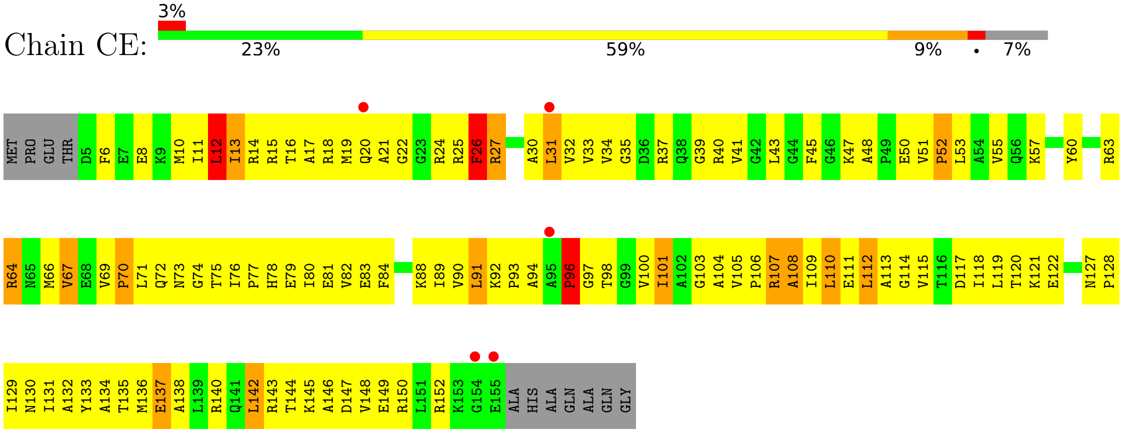
Chain AE:





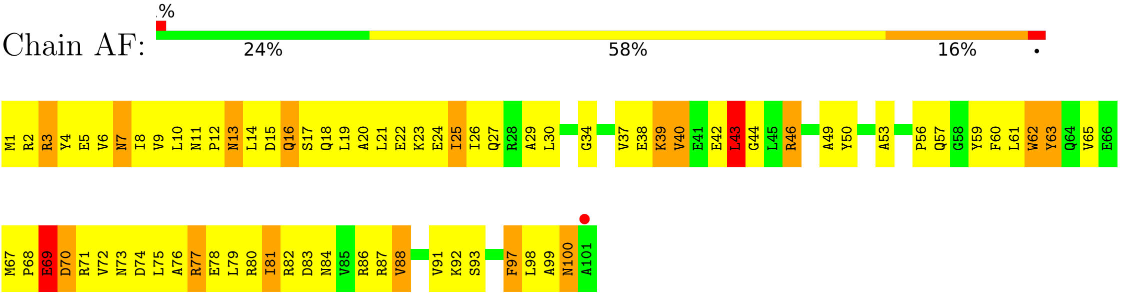
- Molecule 5: 30S ribosomal protein S5

Chain CE:



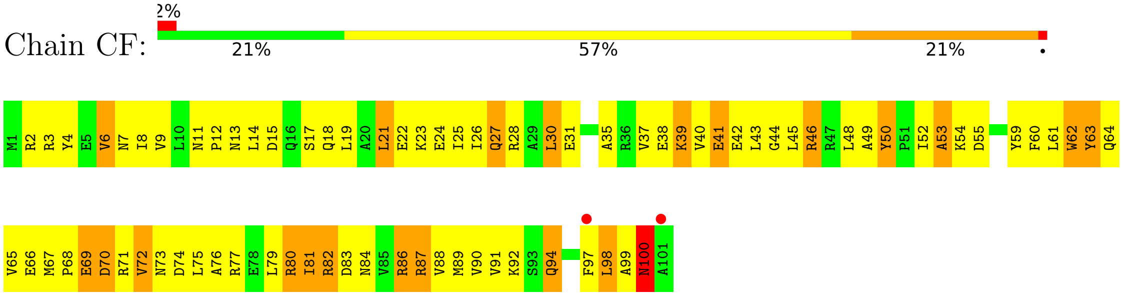
- Molecule 6: 30S ribosomal protein S6

Chain AF:



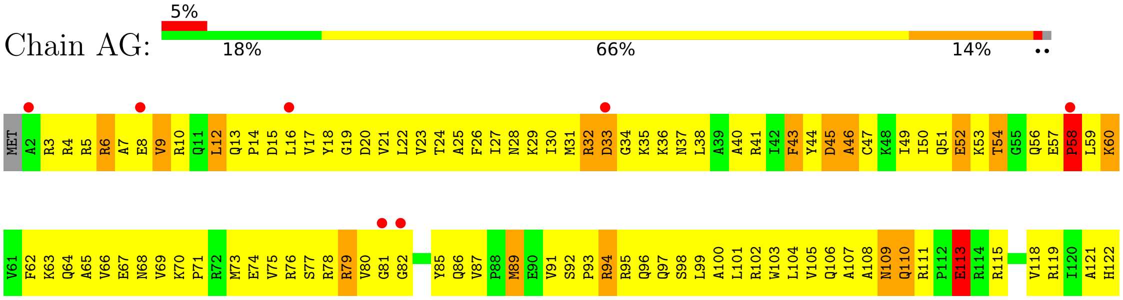
- Molecule 6: 30S ribosomal protein S6

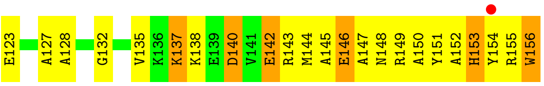
Chain CF:



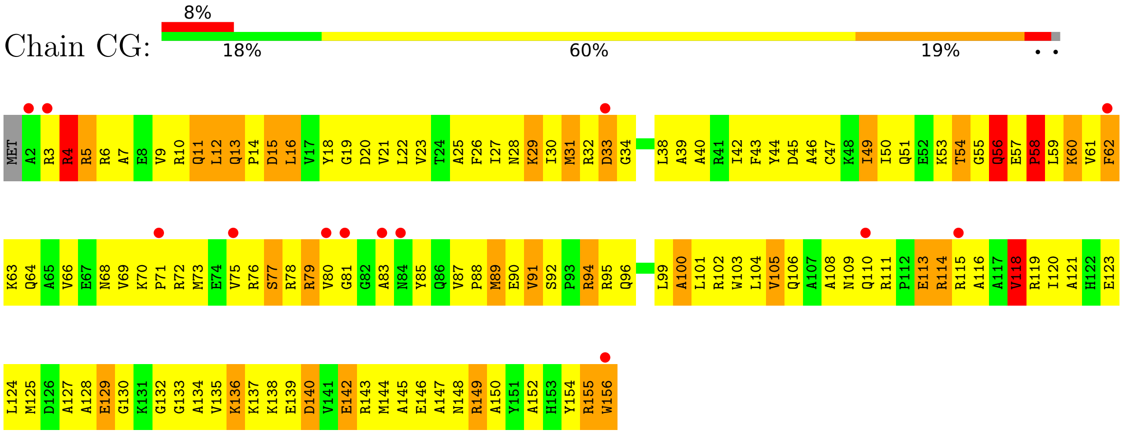
- Molecule 7: 30S ribosomal protein S7

Chain AG:

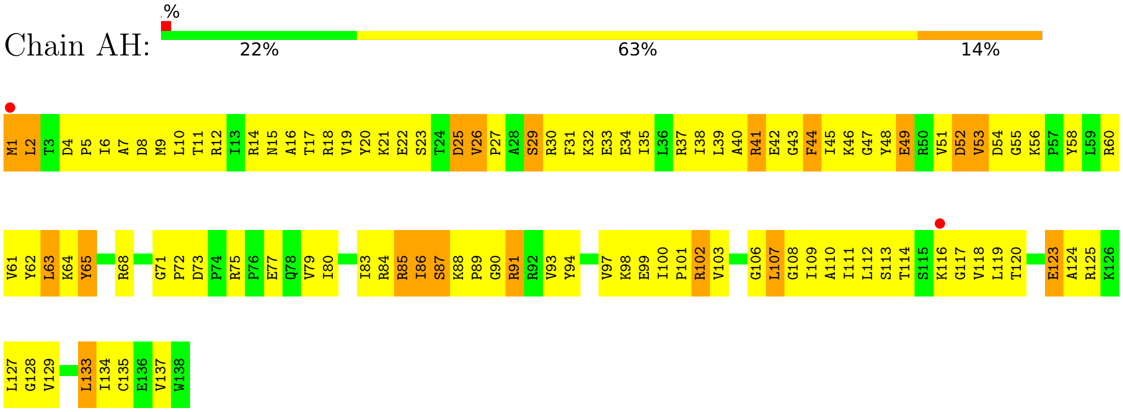




- Molecule 7: 30S ribosomal protein S7

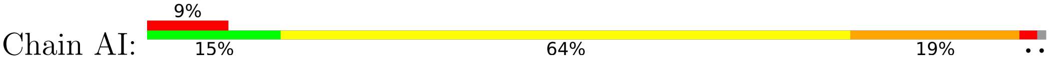


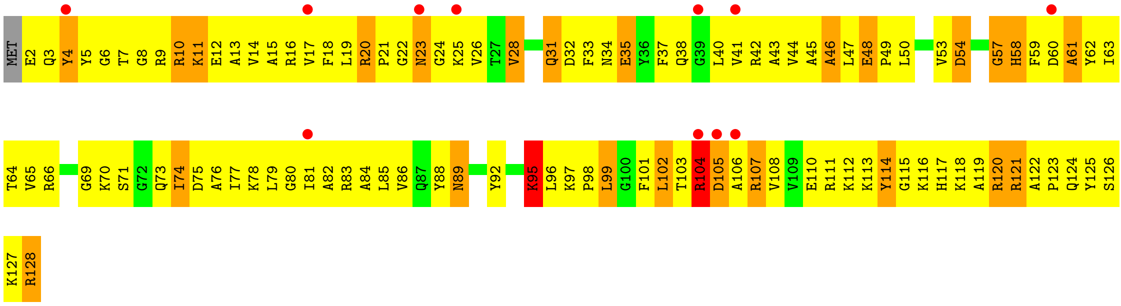
- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8

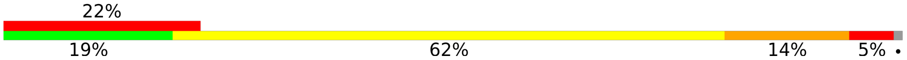
- Molecule 9: 30S ribosomal protein S9

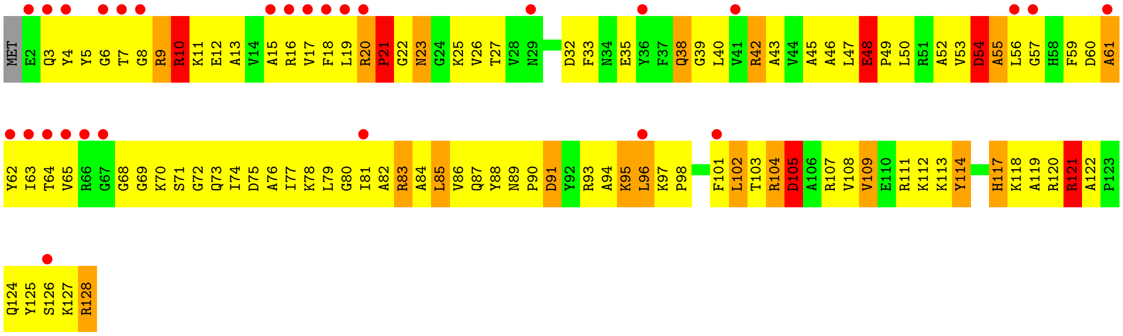




- Molecule 9: 30S ribosomal protein S9

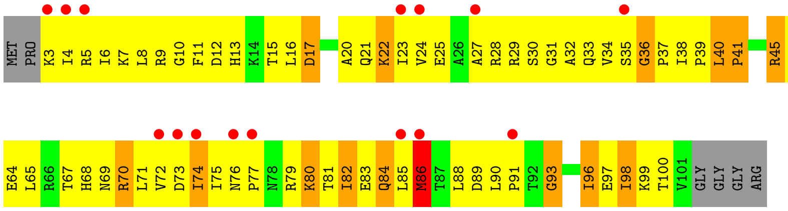
Chain CI:





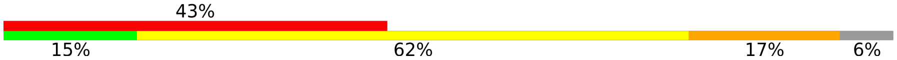
- Molecule 10: 30S ribosomal protein S10

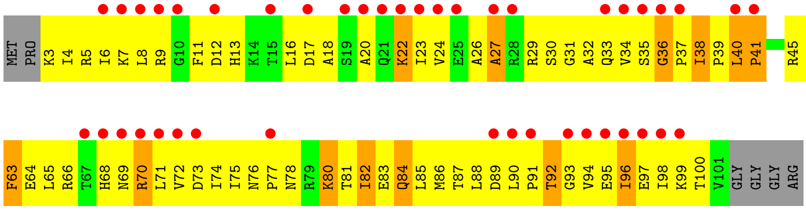
Chain AJ:



- Molecule 10: 30S ribosomal protein S10

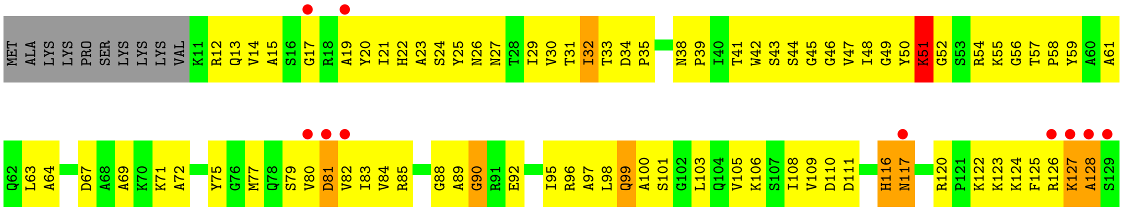
Chain CJ:





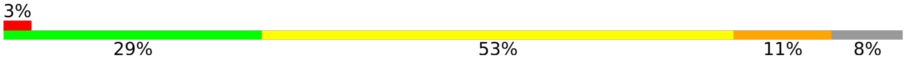
- Molecule 11: 30S ribosomal protein S11

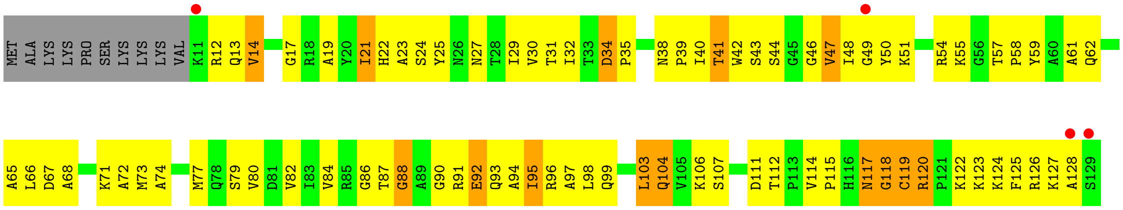
Chain AK:



- Molecule 11: 30S ribosomal protein S11

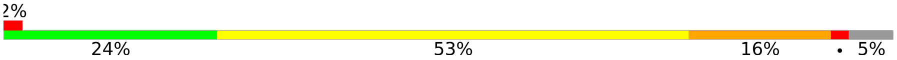
Chain CK:

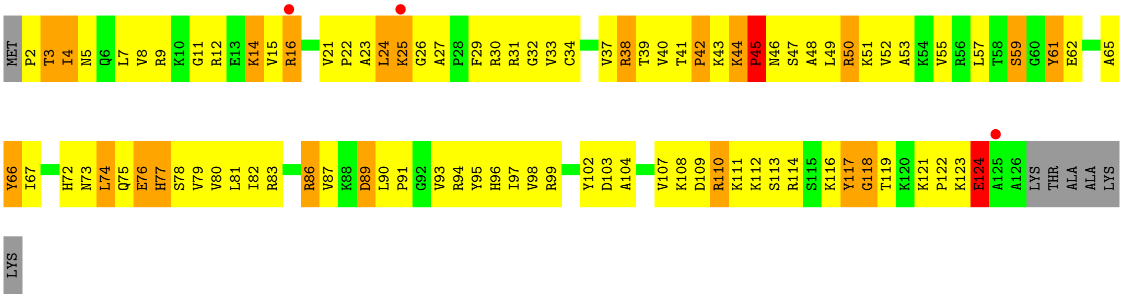




- Molecule 12: 30S ribosomal protein S12

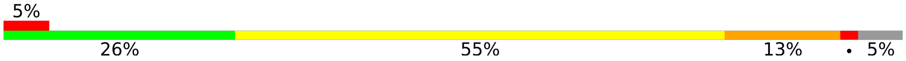
Chain AL:

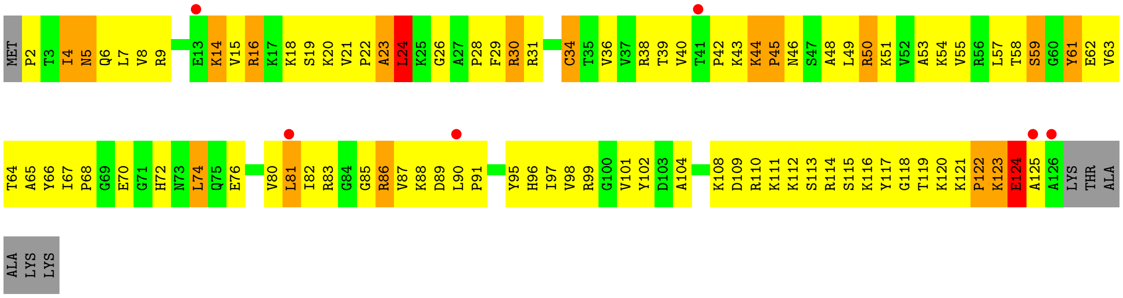




- Molecule 12: 30S ribosomal protein S12

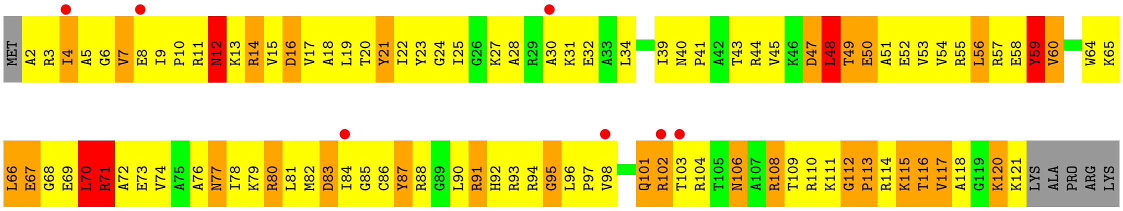
Chain CL:





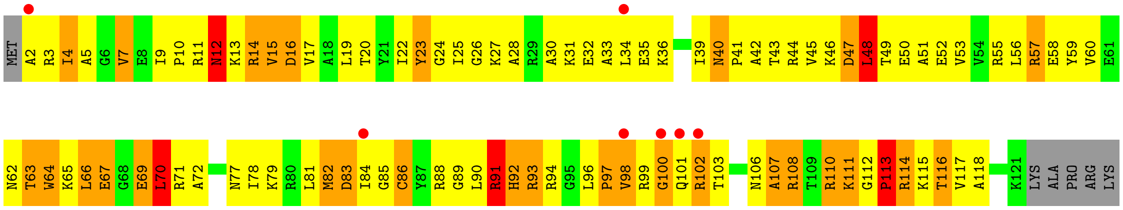
- Molecule 13: 30S ribosomal protein S13

Chain AM:



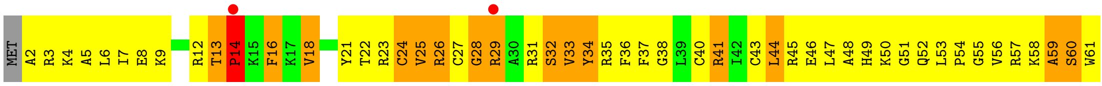
- Molecule 13: 30S ribosomal protein S13

Chain CM:



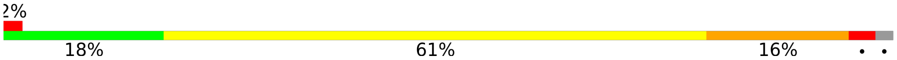
- Molecule 14: 30S ribosomal protein S14

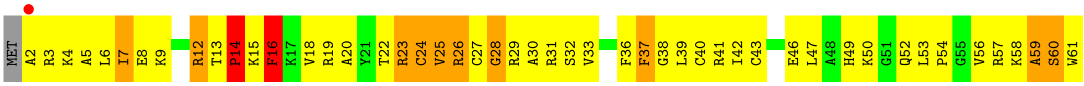
Chain AN:



- Molecule 14: 30S ribosomal protein S14

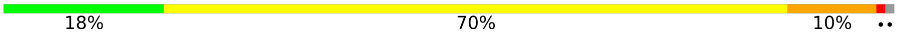
Chain CN:

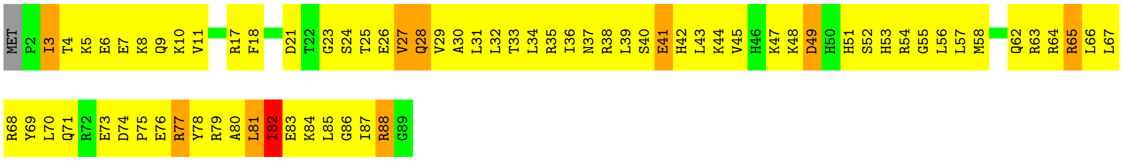




- Molecule 15: 30S ribosomal protein S15

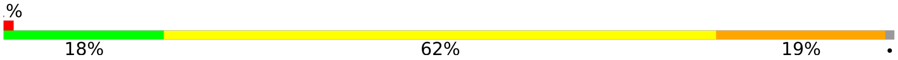
Chain AO:

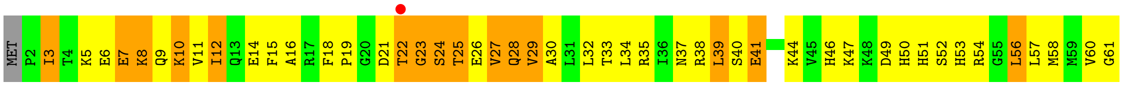




- Molecule 15: 30S ribosomal protein S15

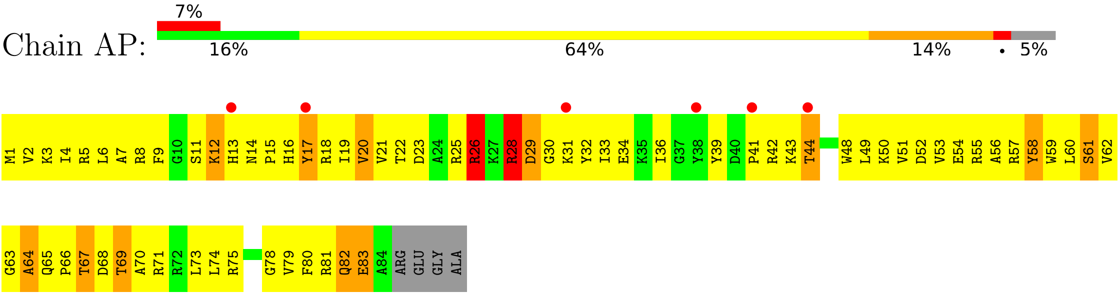
Chain CO:





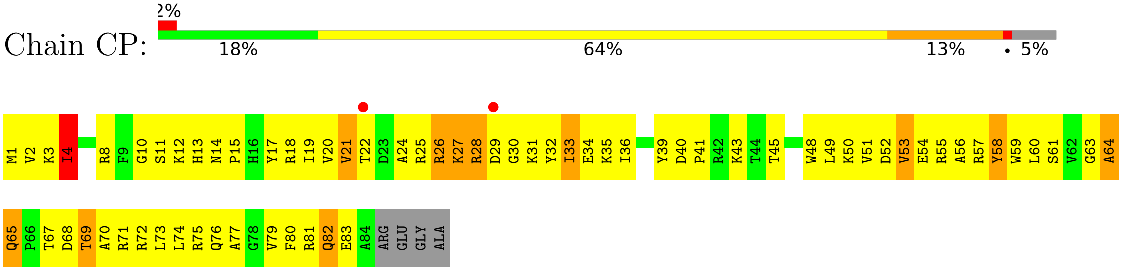
- Molecule 16: 30S ribosomal protein S16

Chain AP:



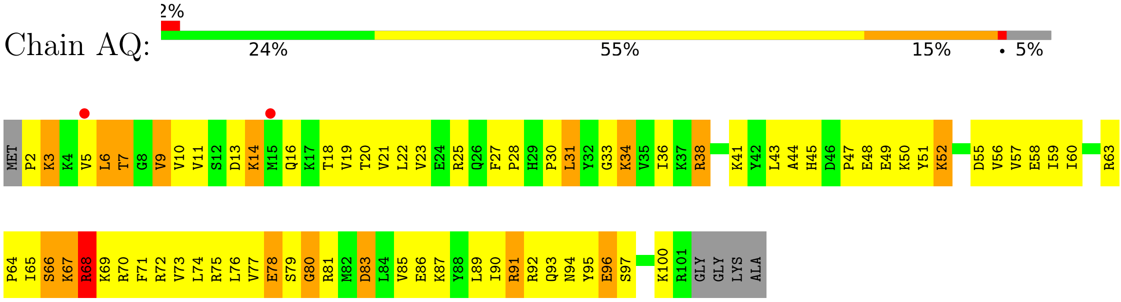
- Molecule 16: 30S ribosomal protein S16

Chain CP:



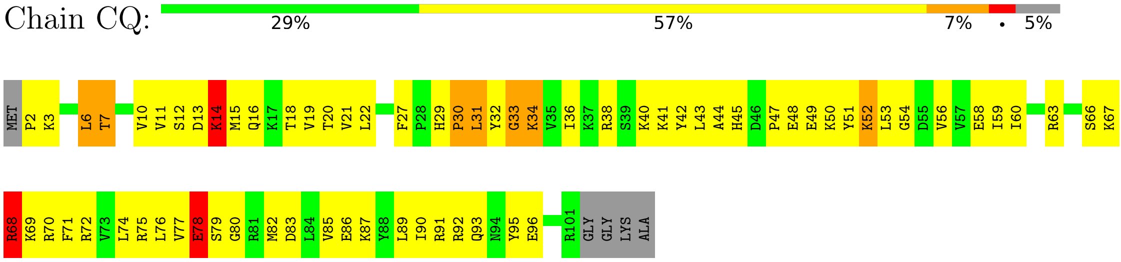
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



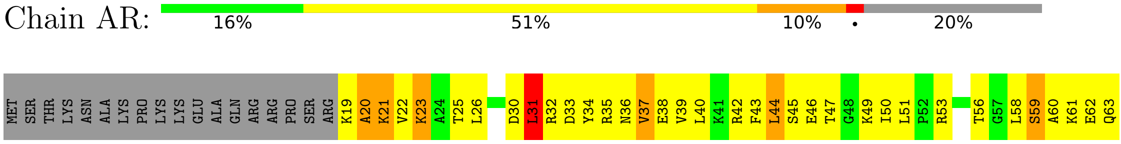
- Molecule 17: 30S ribosomal protein S17

Chain CQ:



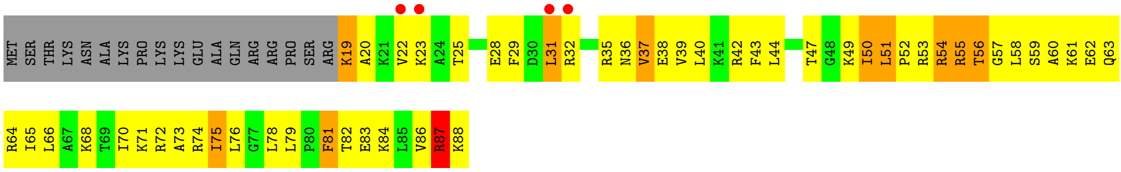
- Molecule 18: 30S ribosomal protein S18

Chain AR:



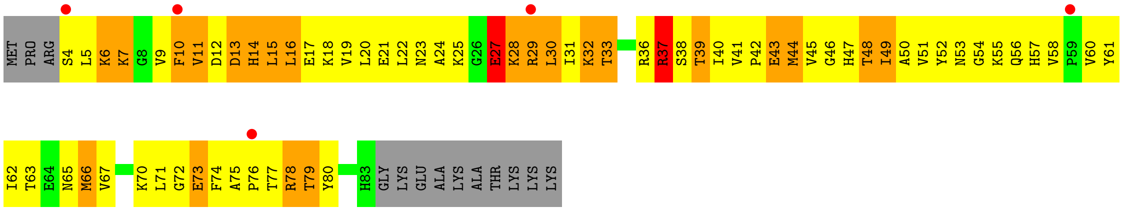
- Molecule 18: 30S ribosomal protein S18

Chain CR:



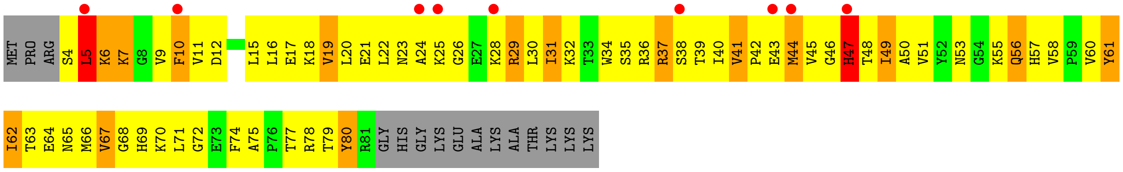
- Molecule 19: 30S ribosomal protein S19

Chain AS:



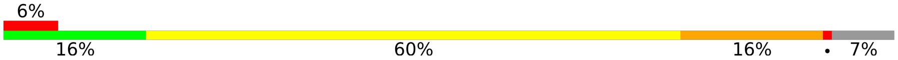
- Molecule 19: 30S ribosomal protein S19

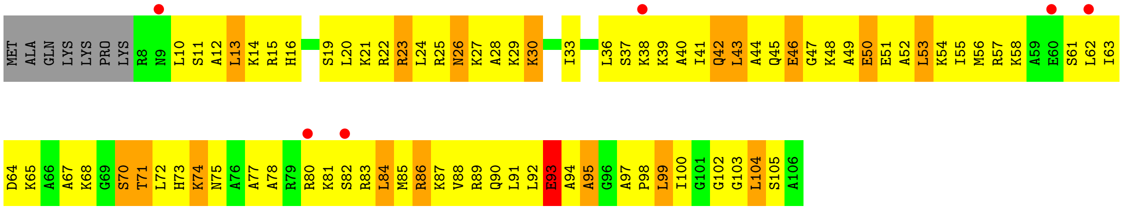
Chain CS:



- Molecule 20: 30S ribosomal protein S20

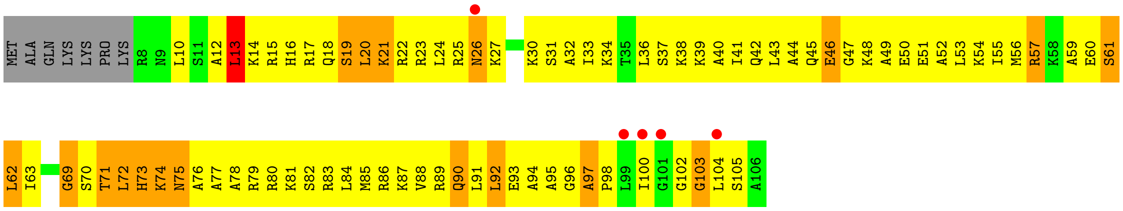
Chain AT:





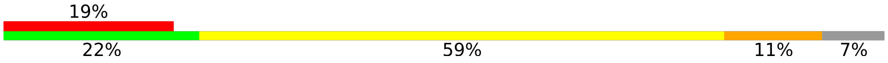
- Molecule 20: 30S ribosomal protein S20

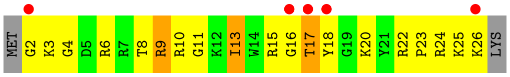
Chain CT:



- Molecule 21: 30S ribosomal protein Thx

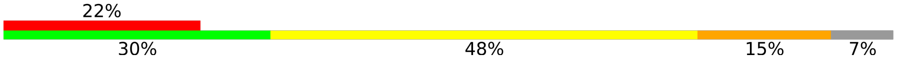
Chain AU:

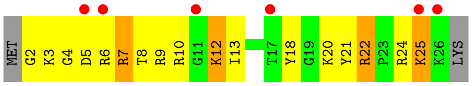




- Molecule 21: 30S ribosomal protein Thx

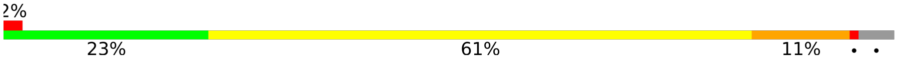
Chain CU:

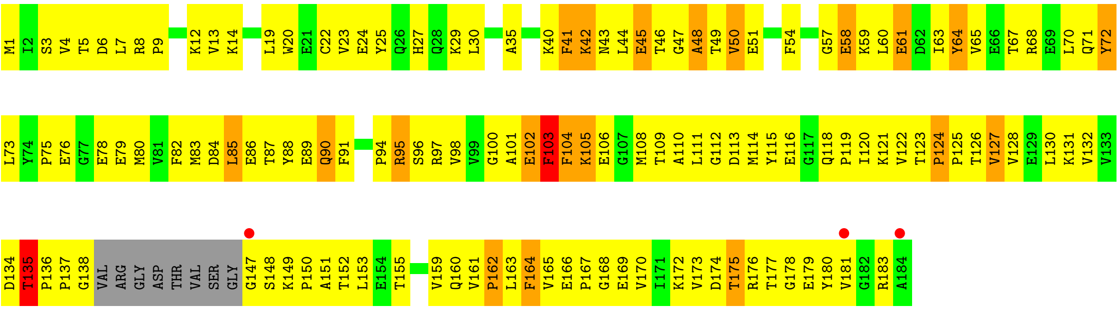




- Molecule 22: Elongation factor P

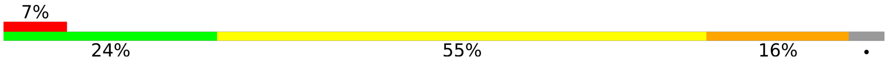
Chain AV:

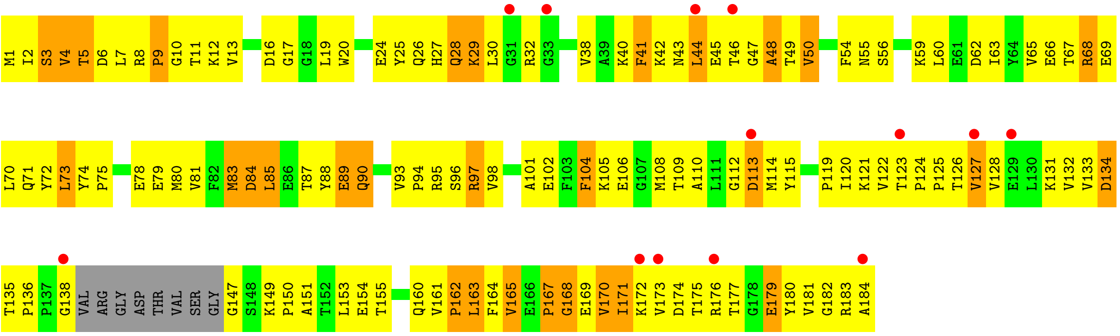




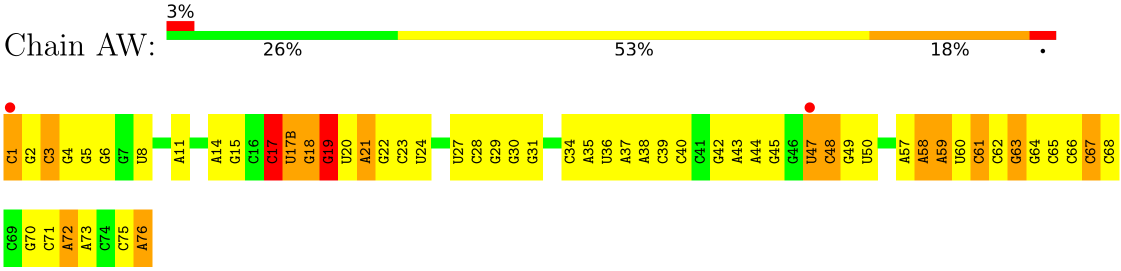
- Molecule 22: Elongation factor P

Chain CV:

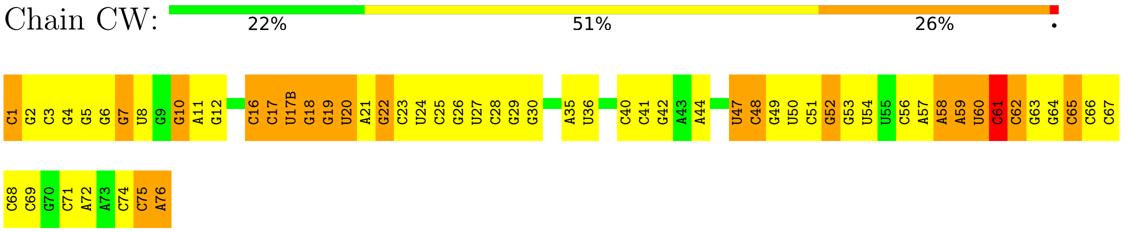




- Molecule 23: tRNA-Met

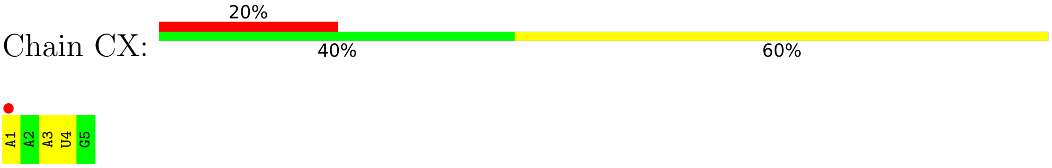


- Molecule 23: tRNA-Met

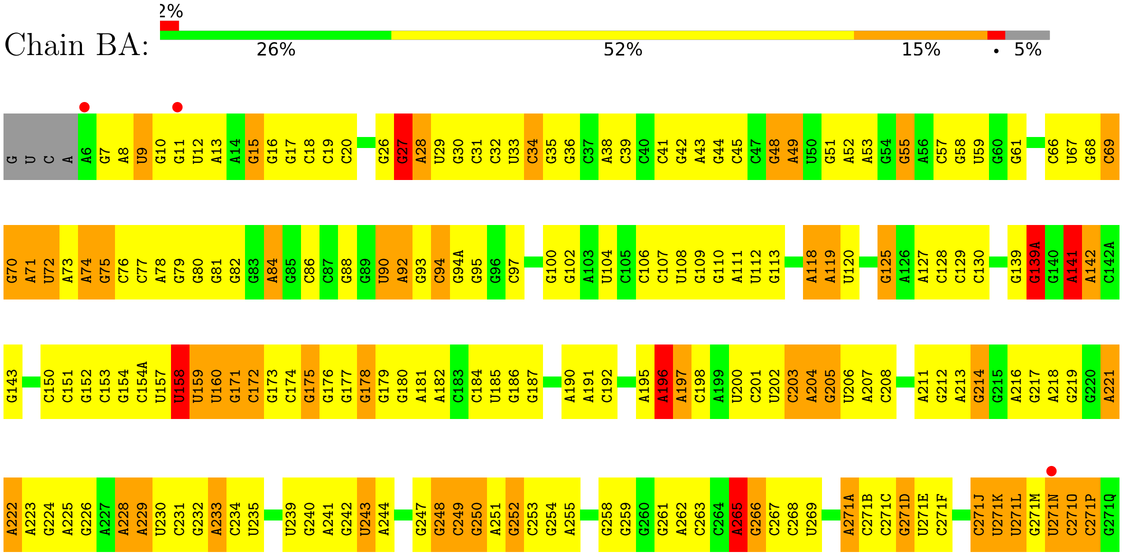


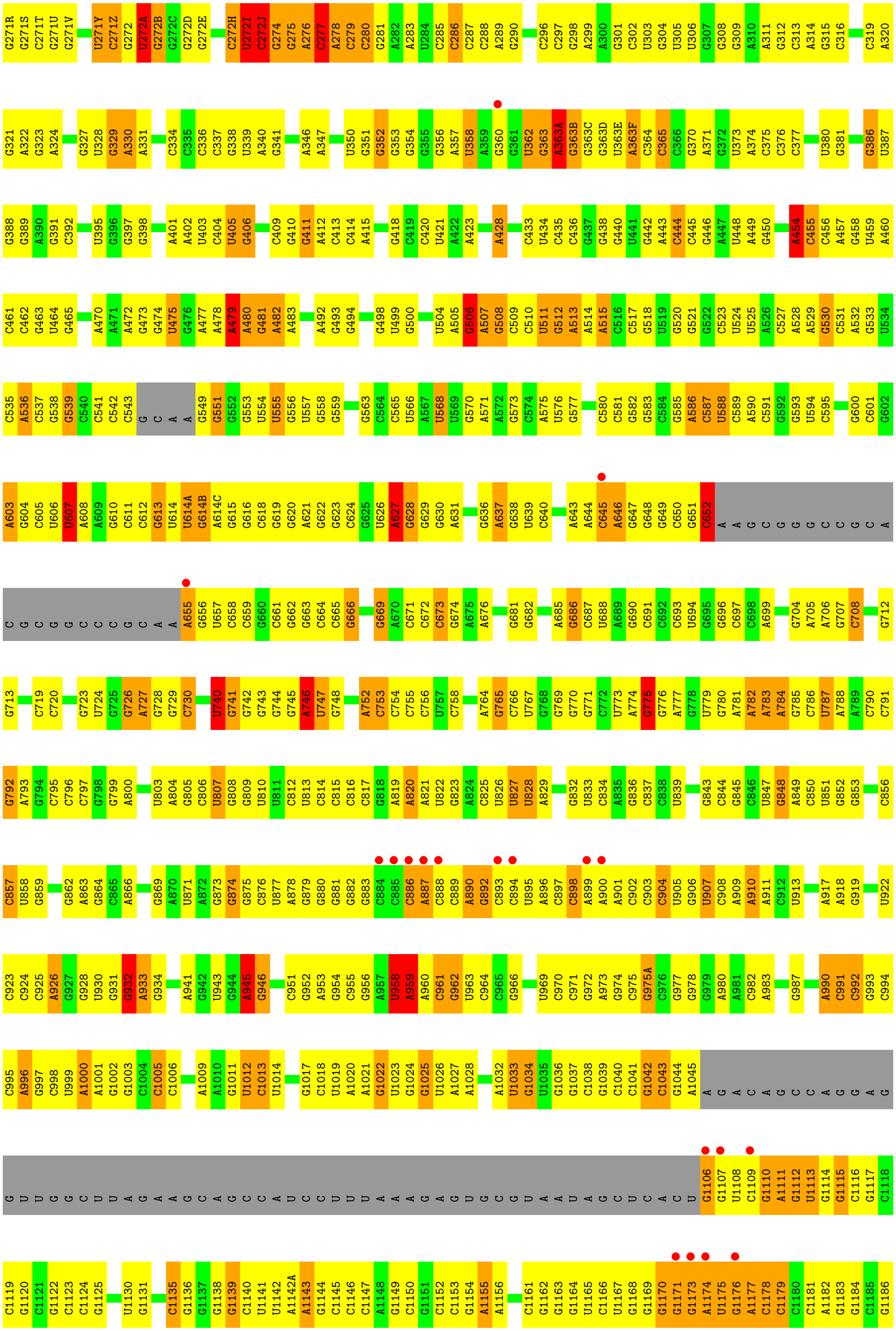
- Molecule 24: RNA (5'-R(P*AP*AP*AP*UP*G)-3')

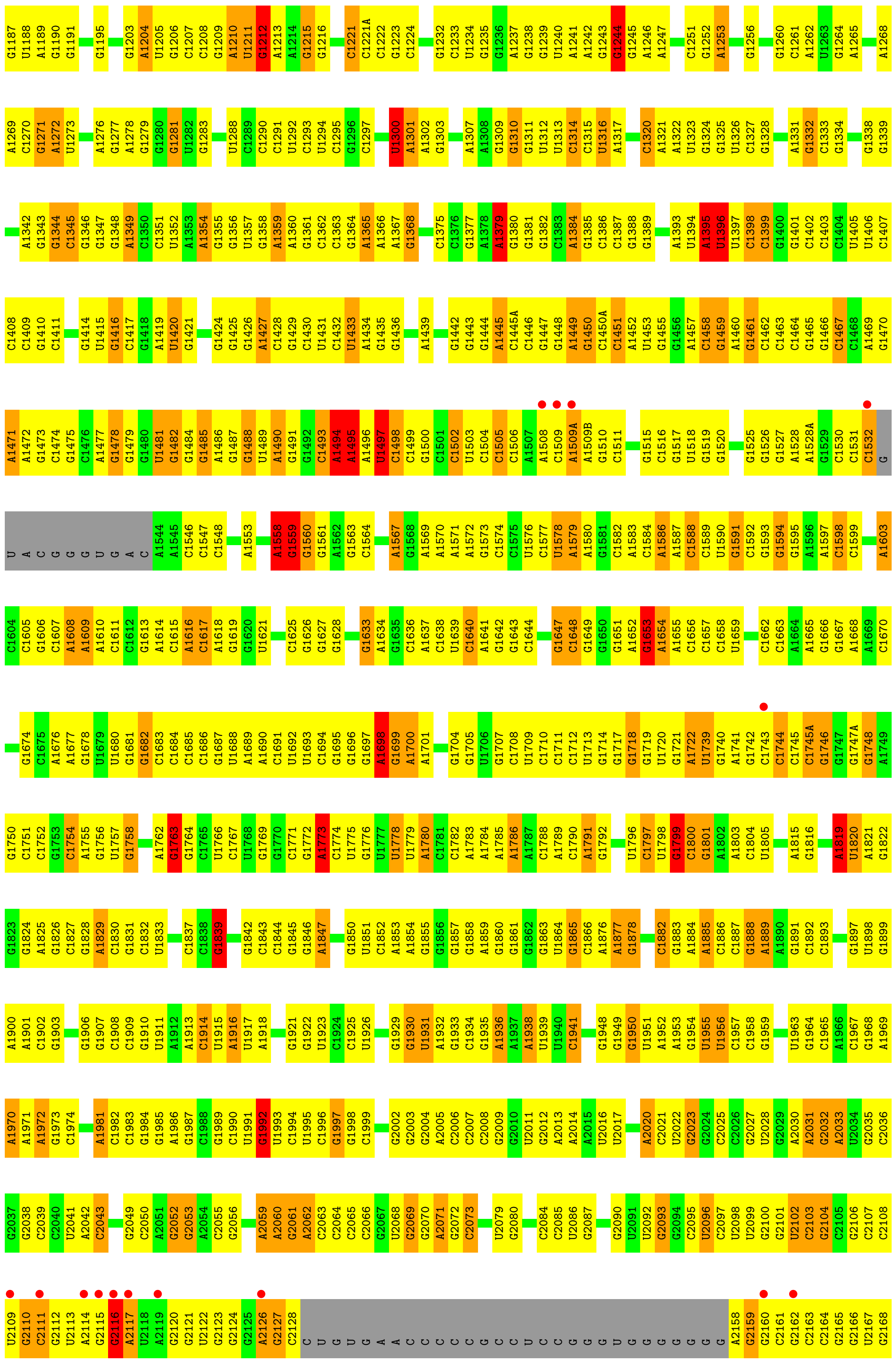
- Molecule 24: RNA (5'-R(P*AP*AP*AP*UP*G)-3')

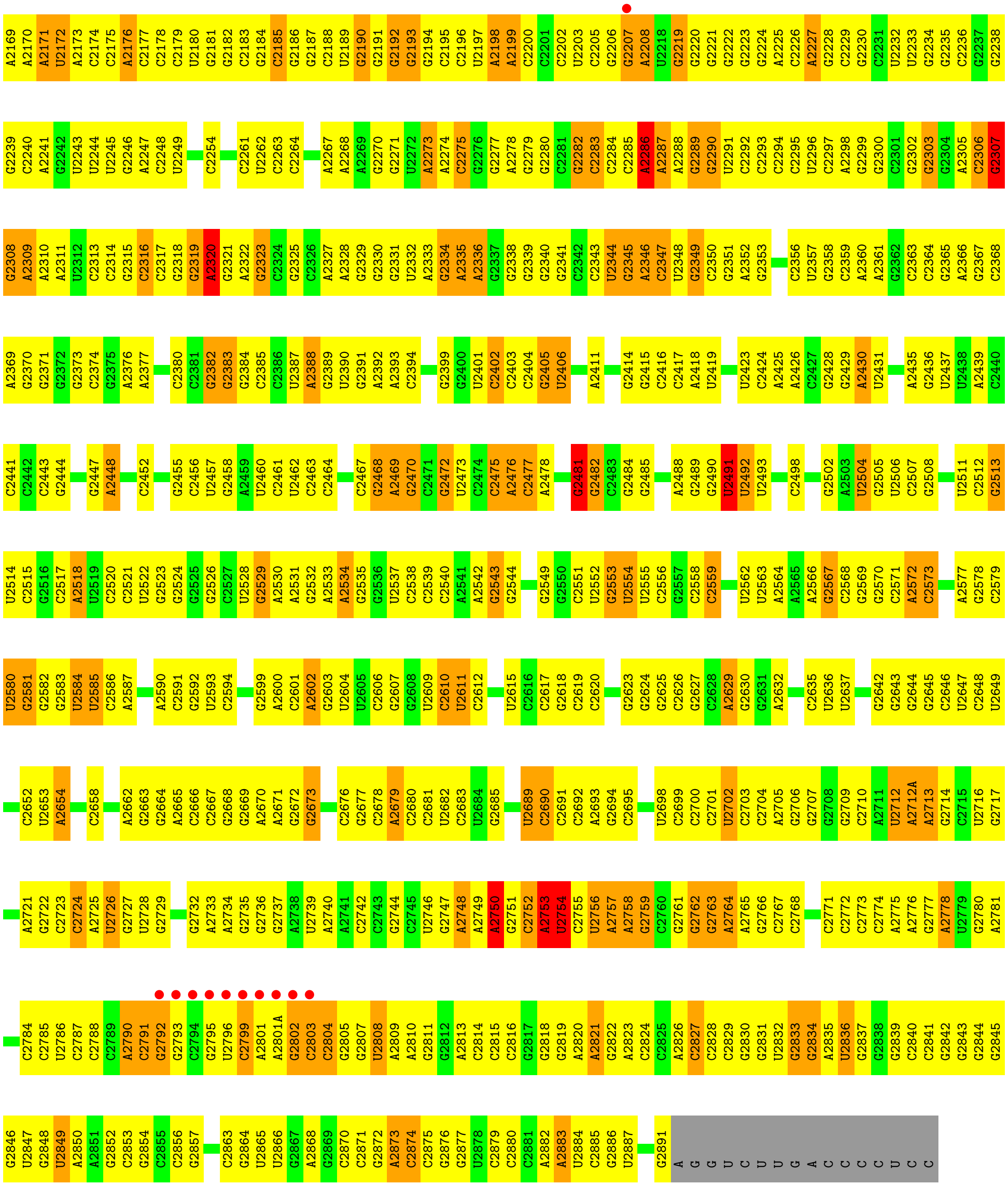


- Molecule 25: 23S ribosomal RNA



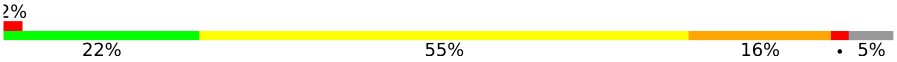

G271R G271S C271T G271U G271V U271Y C271Z G272 U272A G272B G272C G272D G272E C272H U272I C272J G274 G275 A276 C277 A278 C279 C280 G281 A282 A283 U284 C285 C286 C287 G288 A289 G290 C296 C297 G298 A299 A300 G301 C302 U303 G304 U305 U306 G307 G308 G309 A310 A311 G312 C313 A314 G315 C316 C319 A320
G321 A322 G323 A324 G327 U328 G329 A330 A331 C334 C335 C336 C337 G338 U339 A340 G341 A346 A347 U350 G351 G352 G353 G354 G355 G356 A357 U358 A359 G360 G361 U362 G363 A363A G363B G363C G363D U363E A363F C364 C365 C366 G370 A371 G372 U373 A374 C375 C376 C377 U380 G381 G386 U387
G388 G389 A390 G391 C392 U395 G396 G397 G398 A401 A402 U403 C404 U405 G406 C409 G410 G411 A412 C413 C414 A415 G418 C419 C420 U421 A422 A423 A428 C433 U434 C435 C436 G437 G438 G440 U441 G442 A443 C444 C445 G446 A447 U448 A449 G450 A454 C455 C456 A457 G458 U459 A460
C461 C462 G463 U464 G465 A470 A471 A472 G473 G474 U475 G476 A477 A478 A479 A480 G481 A482 A483 A492 G493 G494 G498 U499 G500 U504 A505 G506 A507 G508 C509 C510 U511 G512 A513 A514 A515 C516 C517 G518 U519 G520 G521 G522 C523 U524 U525 A526 C527 A528 A529 G530 C531 A532 G533 U534
C535 A536 C537 G538 G539 C540 C541 C542 C543 G C A A G549 G551 G552 G553 U554 U555 G556 U557 G558 G559 G563 C564 C565 U566 A567 U568 U569 G570 A571 A572 G573 C574 A575 U576 G577 C580 C581 G582 G583 C584 G585 A586 C587 U588 C589 A590 C591 G592 G593 U594 C595 G600 C601 G602
A603 G604 C605 U606 U607 A608 A609 G610 C611 C612 G613 U614 U614A G614B A614C G615 G616 C618 G619 C620 A621 C622 G623 C624 G625 U626 A627 G628 G629 G630 A631 G636 A637 G638 U639 C640 A643 A644 C645 A646 G647 G648 G649 C650 G651 C652 A A G C G G G C C G C A
C G C G G C C C C G C A A A655 G656 U657 C658 C659 G660 C661 G662 G663 C664 C665 G666 G669 A670 C671 C672 C673 G674 A675 A676 G681 G682 A685 G686 C687 U688 A689 G690 C691 C692 C693 U694 G695 G696 C697 C698 A699 G704 A705 A706 G707 C708 G712
G713 C719 C720 G723 U724 G725 G726 A727 G728 G729 C730 U740 G741 G742 G743 G744 G745 A746 U747 G748 A752 C753 C754 C755 C756 U757 C758 A764 G765 C766 U767 G768 G769 G770 G771 C772 U773 A774 G775 G776 A777 G778 U779 C780 A781 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791
G792 A793 G794 C795 C796 C797 G798 G799 A800 U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 U813 C814 C815 C816 C817 G818 A819 A820 A821 U822 G823 A824 C825 U826 U827 U828 A829 G832 U833 C834 A835 G836 C837 C838 U839 G843 C844 G845 C846 U847 G848 A849 C850 U851 G852 G853 C856
C857 U858 G859 G862 A863 G864 C865 A866 G869 A870 U871 A872 G873 G874 G875 C876 U877 A878 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 G898 A899 A900 A901 C902 C903 G904 U905 G906 U907 C908 A909 A910 A911 C912 U913 A917 A918 G919 U922
C923 C924 C925 A926 G927 G928 U930 G931 G932 A933 G934 A941 G942 U943 G944 A945 G946 C951 G952 A953 G954 C955 G956 A957 U958 A959 A960 C961 G962 U963 C964 C965 G966 U969 C970 C971 G972 A973 G974 C975 G975A C976 G977 G978 G979 A980 A981 C982 A983 G987 A990 C991 C992 G993 C994
C995 A996 G997 C998 U999 A1000 A1001 G1002 G1003 C1004 C1005 C1006 A1009 A1010 G1011 U1012 C1013 U1014 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1032 U1033 G1034 U1035 G1036 G1037 C1038 G1039 C1040 C1041 G1042 C1043 G1044 A1045 A G A C A G C C C A G G A G
G U U G G C U U A G A A G C A G C C A U C C U U U A A A G A G U G C G U A A U A G C U C A C U G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 G1114 G1115 C1116 G1117 C1118
C1119 G1120 C1121 G1122 C1123 C1124 G1125 U1130 G1131 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A A1143 G1144 C1145 C1146 C1147 A1148 G1149 C1150 G1151 C1152 C1153 G1154 A1155 A1156 C1161 G1162 G1163 G1164 U1165 C1166 U1167 G1168 G1169 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 G1183 G1184 C1185 G1186

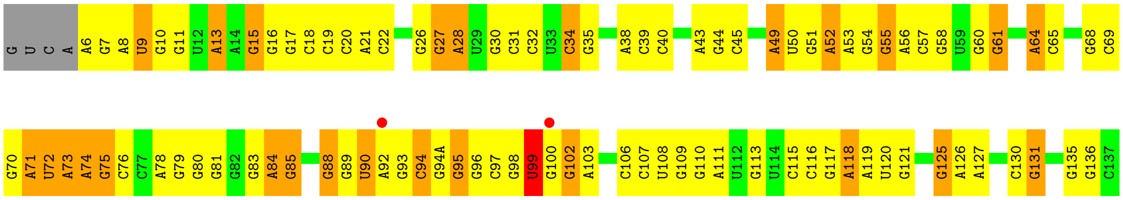

G1187 U1188 A1189 G1190 G1191 G1195 G1203 A1204 U1205 G1206 C1207 G1208 G1209 A1210 U1211 G1212 A1213 A1214 G1215 G1216 C1221 C1221A C1222 G1223 C1224 G1232 C1233 U1234 G1235 G1236 A1237 G1238 G1239 U1240 A1241 A1242 G1243 G1244 G1245 A1246 A1247 C1251 G1252 A1253 G1256 G1260 C1261 A1262 U1263 G1264 A1265 A1268
A1269 C1270 G1271 A1272 U1273 A1276 G1277 A1278 G1279 G1280 G1281 U1282 G1283 U1288 C1289 C1290 C1291 U1292 C1293 U1294 C1295 G1296 C1297 U1300 A1301 A1302 G1303 A1307 A1308 G1309 G1310 G1311 U1312 U1313 C1314 C1315 U1316 A1317 C1320 A1321 A1322 U1323 G1324 G1325 U1326 C1327 G1328 A1331 G1332 C1333 G1334 G1338 G1339
A1342 G1343 G1344 C1345 G1346 G1347 G1348 A1349 C1350 C1351 U1352 A1353 A1354 G1355 G1356 U1357 G1358 A1359 A1360 C1361 C1362 C1363 G1364 A1365 A1366 A1367 G1368 C1375 C1376 G1377 A1378 A1379 G1380 G1381 G1382 C1383 A1384 G1385 C1386 C1387 G1388 G1389 A1393 U1394 A1395 U1396 U1397 C1398 C1399 G1400 G1401 C1402 C1403 C1404 U1405 U1406 C1407
C1408 C1409 G1410 C1411 G1414 U1415 G1416 C1417 G1418 A1419 U1420 G1421 G1424 G1425 G1426 A1427 C1428 G1429 C1430 U1431 C1432 U1433 A1434 G1435 G1436 A1439 G1442 G1443 G1444 A1445 C1445A C1446 G1447 G1448 A1449 G1450 C1450A C1451 A1452 U1453 G1455 G1456 A1457 C1458 G1459 A1460 G1461 C1462 C1463 C1464 G1465 G1466 C1467 C1468 A1469 G1470
A1471 A1472 G1473 C1474 G1475 C1476 A1477 G1478 G1479 G1480 U1481 G1482 G1484 G1485 A1486 G1487 G1488 U1489 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1498 C1499 G1500 C1501 C1502 U1503 C1504 C1505 C1506 A1507 A1508 C1509 A1509A A1509B G1510 C1511 G1515 C1516 G1517 U1518 U1519 G1520 G1525 G1526 G1527 A1528 A1528A G1529 C1530 C1531 C1532 G
U A C G G G U G A C A1544 A1545 C1546 C1547 C1548 A1553 A1558 G1559 G1560 G1561 A1562 G1563 C1564 A1567 G1568 A1569 A1570 A1571 G1572 G1573 C1574 C1575 U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 C1584 A1586 A1587 C1588 C1589 U1590 G1591 C1592 G1593 G1594 G1595 A1596 A1597 C1598 C1599 A1603
C1604 C1605 G1606 C1607 A1608 A1609 A1610 C1611 C1612 G1613 A1614 C1615 A1616 C1617 A1618 G1619 G1620 U1621 C1625 G1626 G1627 G1628 G1633 A1634 G1635 C1636 A1637 C1638 U1639 C1640 A1641 G1642 G1643 C1644 G1647 C1648 G1649 G1650 G1651 A1652 G1653 A1654 A1655 C1656 C1657 C1658 U1659 C1662 C1663 A1664 A1665 G1666 G1667 A1668 A1669 C1670
G1674 C1675 A1676 A1677 G1678 U1679 U1680 G1681 G1682 C1683 C1684 C1685 C1686 C1687 U1688 A1689 A1690 C1691 U1692 U1693 C1694 G1695 G1696 G1697 A1698 G1699 A1700 A1701 G1704 G1705 U1706 G1707 C1708 U1709 C1710 C1711 C1712 U1713 G1714 G1717 G1718 G1719 U1720 G1721 A1722 U1739 G1740 A1741 G1742 C1743 C1744 C1745 C1745A G1746 G1747 G1747A G1748 A1749
G1750 C1751 C1752 G1753 C1754 A1755 G1756 U1757 G1758 A1762 G1763 G1764 C1765 U1766 C1767 U1768 G1769 G1770 C1771 G1772 A1773 C1774 U1775 G1776 U1777 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 G1792 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 U1805 A1815 G1816 A1819 U1820 A1821 G1822
G1823 G1824 A1825 G1826 C1827 G1828 A1829 C1830 G1831 C1832 U1833 C1837 C1838 G1839 G1842 C1843 C1844 G1845 G1846 A1847 G1850 U1851 C1852 A1853 A1854 G1855 G1856 G1857 G1858 A1859 G1860 G1861 G1862 G1863 U1864 G1865 C1866 A1876 A1877 G1878 C1882 G1883 A1884 A1885 C1886 C1887 G1888 A1889 A1890 G1891 C1892 C1893 G1897 U1898 G1899
A1900 A1901 C1902 G1903 G1906 G1907 C1908 G1909 G1910 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 G1921 G1922 U1923 C1924 C1925 U1926 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 U1940 C1941 G1948 G1949 G1950 U1951 A1952 G1953 G1954 U1955 U1956 C1957 C1958 G1959 U1963 G1964 C1965 A1966 C1967 G1968 A1969
A1970 A1971 A1972 G1973 C1974 A1981 C1982 G1983 G1984 G1985 A1986 G1987 C1988 G1989 C1990 U1991 G1992 U1993 C1994 U1995 C1996 G1997 G1998 C1999 G2002 G2003 G2004 A2005 C2006 C2007 C2008 G2009 G2010 U2011 G2012 A2013 A2014 A2015 U2016 U2017 A2020 C2021 U2022 G2023 G2024 C2025 C2026 G2027 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036
G2037 G2038 C2039 C2040 U2041 A2042 C2043 G2049 C2050 A2051 G2052 G2053 A2054 C2055 G2056 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2067 U2068 G2069 G2070 A2071 G2072 C2073 U2079 G2080 C2084 C2085 U2086 G2087 G2090 U2091 U2092 G2093 G2094 C2095 U2096 C2097 U2098 G2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108
U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C U G U G A A C C C C C G C C U C C G G G U G G G G G G G A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 C2166 U2167 G2168

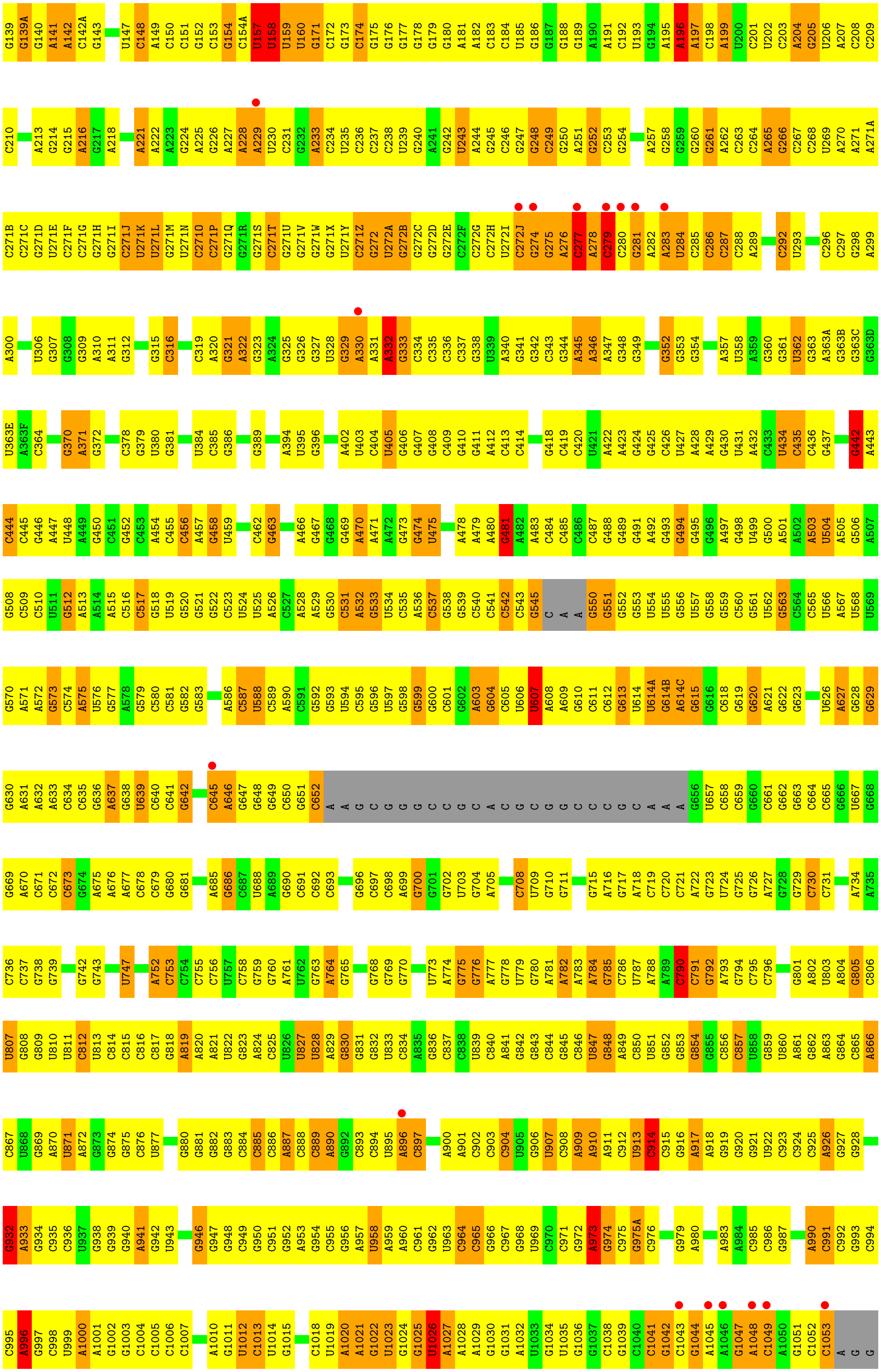


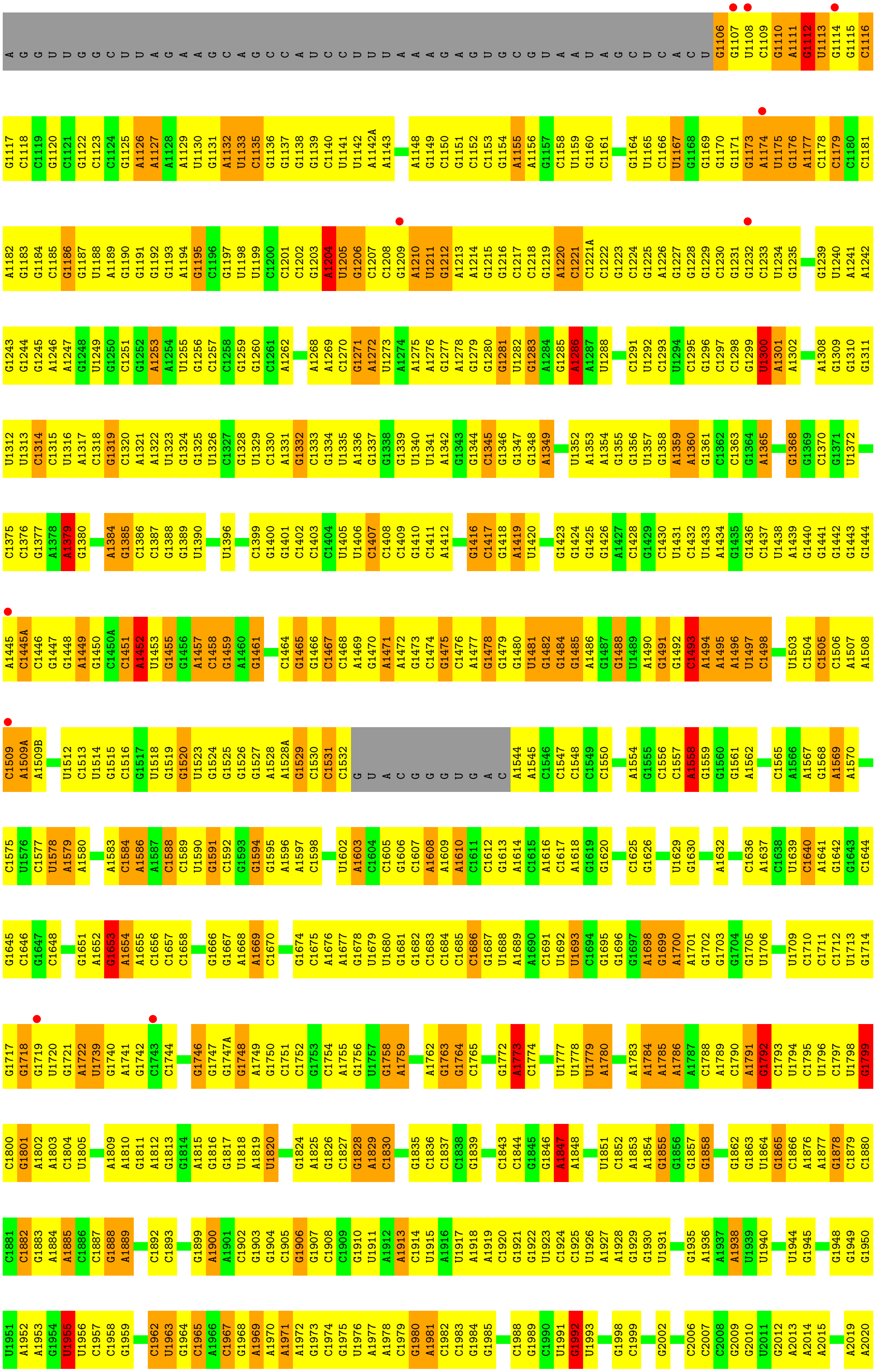
- Molecule 25: 23S ribosomal RNA

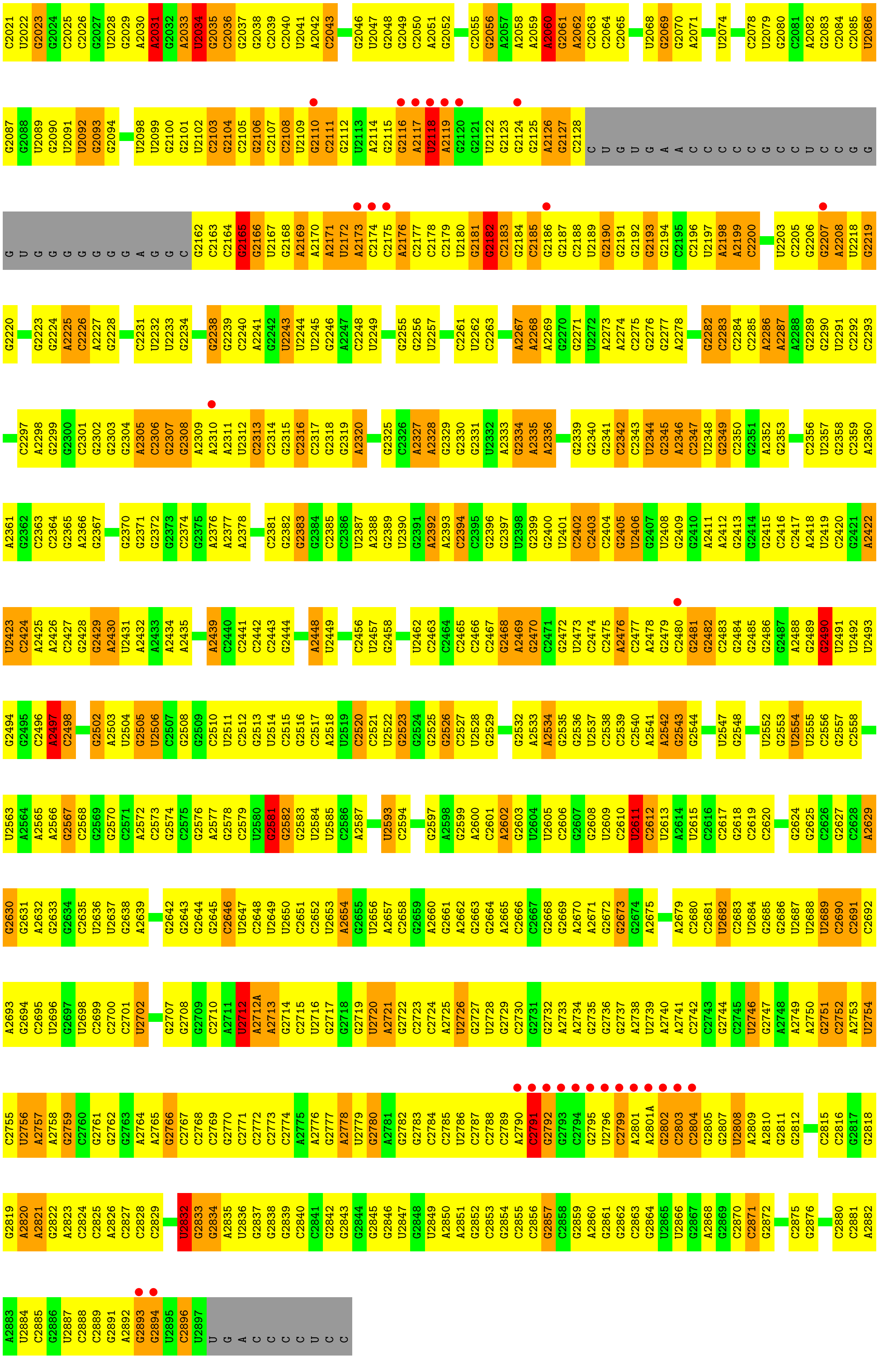
Chain DA:





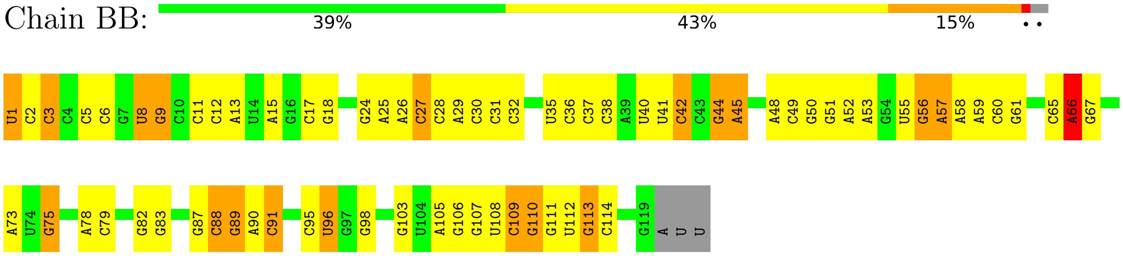

G139 G139A G140 A141 A142 C142A G143 U147 C148 A149 C150 C151 G152 C153 G154 C154A U157 U158 U159 U160 G171 C172 G173 C174 G175 G176 G177 G178 G179 G180 A181 A182 C183 C184 U185 G186 G187 G188 G189 A190 A191 C192 U193 G194 A195 A196 A197 C198 A199 U200 C201 U202 C203 A204 G205 U206 A207 C208 C209
C210 A213 G214 G215 A216 G217 A218 A221 A222 A223 G224 A225 G226 A227 A228 A229 U230 C231 G232 A233 C234 U235 C236 C237 C238 U239 G240 A241 G242 U243 A244 G245 C246 G247 G248 C249 G250 A251 G252 C253 G254 A257 G258 G259 G260 G261 A262 C263 C264 A265 G266 C267 C268 U269 A270 A271 A271A
C271B C271C G271D U271E C271F C271G C271H G271I C271J U271K U271L G271M U271N C271O C271P G271Q G271R G271S C271T G271U G271V G271W G271X U271Y C271Z G272 U272A G272B G272C G272D G272E C272F C272G C272H U272I C272J G274 G275 A276 C277 A278 C279 C280 G281 A282 A283 U284 C285 C286 C287 C288 A289 C292 U293 C296 C297 G298 A299
A300 U306 G307 G308 G309 A310 A311 G312 G315 C316 C319 A320 G321 A322 G323 A324 G325 G326 U327 U328 G329 A330 A331 A332 G333 C334 C335 C336 C337 G338 U339 A340 G341 G342 C343 G344 A345 A346 A347 G348 G349 G352 G353 G354 A357 U358 A359 G360 G361 U362 G363 A363A G363B G363C G363D
U363E A363F C364 G370 A371 G372 C378 G379 U380 G381 U384 C385 G386 G389 A394 U395 G396 A402 U403 C404 U405 G406 G407 G408 C409 G410 G411 A412 C413 C414 G418 C419 C420 U421 A422 A423 G424 G425 C426 U427 A428 A429 G430 U431 A432 C433 U434 C435 C436 G437 G442 A443
C444 C445 G446 A447 U448 A449 G450 C451 G452 C453 A454 C455 C456 A457 G458 U459 C462 G463 A466 G467 G468 G469 A470 A471 A472 G473 G474 U475 A478 A479 A480 G481 A482 A483 C484 C485 C486 C487 G488 G489 G491 A492 G493 G494 G495 G496 A497 G498 U499 G500 A501 A502 A503 U504 A505 G506 A507
G508 C509 C510 U511 G512 A513 A514 A515 C516 C517 G518 U519 G520 G521 G522 C523 U524 U525 A526 C527 A528 A529 G530 C531 A532 G533 U534 C535 A536 C537 G538 G539 C540 C541 C542 C543 G545 C A A G550 G551 G552 C553 U554 U555 G556 U557 G558 G559 C560 G561 U562 G563 C564 C565 U566 A567 U568 U569
G570 A571 A572 G573 C574 A575 U576 G577 A578 G579 C580 C581 G582 G583 A586 C587 U588 C589 A590 C591 G592 G593 U594 C595 G596 U597 G598 G599 G600 C601 G602 A603 G604 C605 U606 U607 A608 A609 G610 C611 C612 G613 U614 U614A G614B A614C G615 G616 C618 G619 G620 A621 G622 G623 U626 A627 G628 G629
G630 A631 A632 A633 C634 C635 G636 A637 G638 U639 C640 C641 G642 C645 A646 G647 G648 G649 C650 G651 C652 A A G C G G G C C G C A C G C G G C C C G C A A A G656 U657 C658 C659 G660 C661 G662 G663 C664 C665 G666 U667 G668
G669 A670 C671 C672 C673 G674 A675 A676 A677 C678 C679 G680 G681 A685 G686 C687 U688 A689 G690 C691 C692 C693 G696 C697 C698 A699 G700 G701 G702 U703 G704 A705 C708 U709 G710 G711 G715 A716 G717 A718 C719 C720 C721 A722 G723 U724 G725 G726 A727 G728 G729 C730 C731 A734 A735
C736 C737 G738 G739 G742 G743 U747 A752 C753 C754 C755 C756 U757 C758 G759 G760 A761 U762 G763 A764 G765 G768 G769 G770 U773 A774 G775 G776 A777 G778 U779 G780 A781 A782 A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 A793 G794 C795 C796 G801 A802 U803 A804 G805 C806
U807 G808 G809 U810 U811 C812 U813 C814 C815 C816 C817 G818 A819 A820 A821 U822 G823 A824 C825 U826 U827 U828 A829 G830 G831 G832 U833 C834 A835 G836 C837 C838 U839 C840 A841 G842 G843 C844 G845 C846 U847 G848 A849 C850 U851 G852 G853 G854 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 C865 A866
C867 U868 G869 A870 U871 A872 G873 G874 G875 C876 U877 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 A900 A901 C902 C903 C904 U905 G906 U907 C908 A909 A910 A911 C912 U913 C914 C915 G916 A917 A918 G919 G920 G921 U922 C923 C924 C925 A926 G927 G928
G932 A933 G934 C935 C936 U937 G938 G939 G940 A941 G942 U943 G946 G947 G948 C949 G950 C951 G952 A953 G954 C955 G956 A957 U958 A959 A960 C961 G962 U963 C964 C965 G966 C967 G968 U969 C970 C971 G972 A973 G974 C975 G975A C976 G979 A980 A983 A984 C985 C986 G987 A990 C991 C992 G993 C994
C995 A996 G997 C998 U999 A1000 A1001 G1002 G1003 C1004 C1005 C1006 C1007 A1010 G1011 U1012 C1013 U1014 G1015 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 A1029 G1030 G1031 A1032 U1033 G1034 U1035 G1036 G1037 C1038 G1039 C1040 C1041 G1042 C1043 G1044 A1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 A G G


A G G U U G G C U U A G A A G C A G C C A U C C U U U A A A G A G U G C G U A A U A G C U C A C U G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 G1114 G1115 C1116
G1117 C1118 C1119 G1120 C1121 G1122 C1123 C1124 G1125 A1126 A1127 A1128 A1129 U1130 G1131 A1132 U1133 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A A1143 A1148 G1149 C1150 G1151 C1152 C1153 G1154 A1155 A1156 G1157 C1158 U1159 G1160 C1161 G1164 U1165 C1166 U1167 G1168 G1169 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181
A1182 G1183 G1184 C1185 G1186 G1187 U1188 A1189 G1190 G1191 G1192 G1193 A1194 G1195 C1196 G1197 U1198 U1199 C1200 C1201 C1202 G1203 A1204 U1205 G1206 C1207 C1208 G1209 A1210 U1211 G1212 A1213 A1214 G1215 G1216 C1217 C1218 G1219 A1220 C1221 C1221A C1222 G1223 C1224 G1225 A1226 G1227 G1228 G1229 C1230 G1231 G1232 C1233 U1234 G1235 G1239 U1240 A1241 A1242
G1243 G1244 G1245 A1246 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 C1258 G1259 G1260 C1261 A1262 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 A1276 G1277 A1278 G1279 G1280 G1281 U1282 G1283 A1284 G1285 A1286 A1287 U1288 C1291 U1292 C1293 U1294 C1295 G1296 C1297 C1298 G1299 U1300 A1301 A1302 A1308 G1309 G1310 G1311
U1312 U1313 C1314 C1315 U1316 A1317 C1318 G1319 C1320 A1321 A1322 U1323 G1324 G1325 U1326 C1327 G1328 U1329 C1330 A1331 G1332 C1333 G1334 U1335 A1336 G1337 G1338 G1339 U1340 U1341 A1342 G1343 G1344 C1345 G1346 G1347 G1348 A1349 U1352 A1353 A1354 G1355 G1356 U1357 G1358 A1359 A1360 G1361 C1362 C1363 G1364 A1365 G1368 G1369 C1370 G1371 U1372
C1375 C1376 G1377 A1378 A1379 G1380 A1384 G1385 C1386 C1387 G1388 G1389 U1390 U1396 C1399 G1400 G1401 C1402 C1403 C1404 U1405 U1406 C1407 C1408 C1409 G1410 C1411 A1412 G1416 C1417 G1418 A1419 U1420 G1423 G1424 G1425 G1426 A1427 C1428 G1429 C1430 U1431 C1432 U1433 A1434 G1435 G1436 C1437 U1438 A1439 G1440 G1441 G1442 G1443 G1444
A1445 C1445A C1446 G1447 G1448 A1449 G1450 C1450A C1451 A1452 U1453 G1455 G1456 A1457 C1458 G1459 A1460 G1461 C1464 G1465 G1466 C1467 C1468 A1469 G1470 A1471 A1472 G1473 C1474 G1475 C1476 A1477 G1478 G1479 G1480 U1481 G1482 G1484 G1485 A1486 G1487 G1488 U1489 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1498 U1503 C1504 C1505 C1506 A1507 A1508
C1509 A1509A A1509B U1512 C1513 U1514 G1515 C1516 G1517 U1518 G1519 G1520 U1523 G1524 G1525 G1526 G1527 A1528 A1528A G1529 C1530 C1531 C1532 G U A C G G G U G A C A1544 A1545 C1546 C1547 C1548 C1549 C1550 A1554 G1555 C1556 C1557 A1558 G1559 G1560 G1561 A1562 C1565 A1566 A1567 G1568 A1569 A1570
C1575 U1576 C1577 U1578 A1579 A1580 A1583 C1584 A1586 A1587 C1588 C1589 U1590 G1591 C1592 G1593 G1594 G1595 A1596 A1597 C1598 U1602 A1603 C1604 C1605 G1606 C1607 A1608 A1609 A1610 C1611 C1612 G1613 A1614 C1615 A1616 C1617 A1618 G1619 G1620 C1625 G1626 U1629 G1630 A1632 C1636 A1637 C1638 U1639 C1640 A1641 G1642 G1643 C1644
G1645 C1646 G1647 C1648 G1651 A1652 G1653 A1654 A1655 C1656 C1657 C1658 G1666 G1667 A1668 A1669 C1670 G1674 C1675 A1676 A1677 G1678 U1679 U1680 G1681 G1682 C1683 C1684 C1685 C1686 G1687 U1688 A1689 A1690 C1691 U1692 U1693 C1694 G1695 G1696 G1697 A1698 G1699 A1700 A1701 G1702 G1703 G1704 G1705 U1706 U1709 C1710 C1711 C1712 U1713 G1714
G1717 G1718 G1719 U1720 G1721 A1722 U1739 G1740 A1741 G1742 C1743 C1744 G1746 G1747 G1747A G1748 A1749 G1750 C1751 C1752 G1753 C1754 A1755 G1756 U1757 G1758 A1759 A1762 G1763 G1764 C1765 G1772 A1773 C1774 U1777 U1778 U1779 A1780 A1783 A1784 A1785 A1786 A1787 C1788 A1789 C1790 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799
C1800 G1801 A1802 A1803 C1804 U1805 A1809 A1810 G1811 A1812 G1813 G1814 A1815 G1816 G1817 U1818 A1819 U1820 G1824 A1825 G1826 C1827 G1828 A1829 C1830 G1835 C1836 C1837 C1838 G1839 C1843 C1844 G1845 G1846 A1847 A1848 U1851 C1852 A1853 A1854 G1855 G1856 G1857 G1858 G1862 G1863 U1864 G1865 C1866 A1876 A1877 G1878 C1879 C1880
C1881 C1882 G1883 A1884 A1885 C1886 C1887 G1888 A1889 C1892 C1893 G1899 A1900 A1901 C1902 G1903 G1904 C1905 G1906 G1907 C1908 C1909 G1910 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1921 G1922 U1923 C1924 C1925 U1926 A1927 G1928 G1929 G1930 U1931 G1935 A1936 A1937 A1938 U1939 U1940 U1944 G1945 G1948 G1949 G1950
U1951 A1952 A1953 G1954 U1955 U1956 C1957 C1958 G1959 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 G1973 C1974 G1975 U1976 A1977 A1978 C1979 G1980 A1981 C1982 C1983 G1984 G1985 C1988 G1989 C1990 U1991 G1992 U1993 G1998 C1999 G2002 C2006 C2007 C2008 G2009 G2010 U2011 G2012 A2013 A2014 A2015 A2019 A2020


C2021 U2022 G2023 G2024 C2025 C2026 G2027 U2028 G2029 A2030 A2031 G2032 A2033 U2034 G2035 C2036 G2037 G2038 C2039 C2040 U2041 A2042 C2043 G2046 U2047 G2048 G2049 C2050 A2051 G2052 C2055 G2056 A2057 A2058 A2059 A2060 G2061 A2062 C2063 C2064 C2065 U2068 G2069 G2070 A2071 U2074 C2078 U2079 G2080 C2081 A2082 G2083 C2084 C2085 U2086
G2087 G2088 U2089 U2090 U2091 U2092 G2093 G2094 U2098 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C U G U G A A C C C C C G C C U C C G G
G U G G G G G G A G G C G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 G2193 G2194 C2195 C2196 U2197 A2198 A2199 C2200 U2203 C2205 G2206 G2207 A2208 U2218 G2219
G2220 G2223 G2224 A2225 C2226 A2227 G2228 C2231 U2232 U2233 G2234 G2238 G2239 C2240 A2241 G2242 U2243 U2244 U2245 G2246 A2247 C2248 U2249 G2255 G2256 U2257 C2261 U2262 C2263 A2267 A2268 A2269 G2270 G2271 U2272 A2273 A2274 C2275 G2276 G2277 A2278 G2282 C2283 C2284 C2285 A2286 A2287 A2288 G2289 G2290 U2291 C2292 C2293
C2297 A2298 G2299 G2300 C2301 G2302 G2303 G2304 A2305 C2306 G2307 G2308 A2309 A2310 A2311 U2312 C2313 C2314 C2315 C2316 C2317 G2318 G2319 A2320 G2325 C2326 A2327 A2328 G2329 C2330 G2331 U2332 A2333 G2334 A2335 A2336 G2339 G2340 C2341 C2342 C2343 U2344 G2345 A2346 C2347 U2348 G2349 C2350 G2351 A2352 G2353 C2356 U2357 G2358 C2359 A2360
A2361 G2362 C2363 C2364 G2365 A2366 G2367 G2370 G2371 G2372 G2373 C2374 G2375 A2376 A2377 A2378 C2381 G2382 G2383 G2384 C2385 C2386 U2387 A2388 G2389 U2390 G2391 A2392 A2393 C2394 C2395 G2396 G2397 U2398 G2399 G2400 U2401 C2402 C2403 C2404 G2405 U2406 G2407 U2408 G2409 G2410 A2411 A2412 G2413 G2414 G2415 C2416 C2417 A2418 U2419 C2420 G2421 A2422
U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 U2431 A2432 A2433 A2434 A2435 A2439 C2440 C2441 C2442 C2443 G2444 A2448 U2449 C2456 U2457 G2458 U2462 C2463 C2464 C2465 C2466 C2467 G2468 A2469 G2470 C2471 G2472 U2473 C2474 C2475 A2476 C2477 A2478 G2479 C2480 G2481 G2482 C2483 G2484 G2485 G2486 G2487 A2488 G2489 G2490 U2491 U2492 U2493
G2494 G2495 C2496 A2497 C2498 G2502 A2503 U2504 G2505 U2506 C2507 G2508 G2509 C2510 U2511 C2512 G2513 U2514 C2515 G2516 C2517 A2518 U2519 C2520 C2521 U2522 G2523 G2524 G2525 G2526 C2527 U2528 G2529 G2532 A2533 A2534 G2535 C2536 U2537 C2538 C2539 C2540 A2541 A2542 G2543 G2544 U2547 G2548 U2552 G2553 U2554 U2555 C2556 G2557 C2558
U2563 A2564 A2565 A2566 G2567 C2568 G2569 G2570 C2571 A2572 C2573 G2574 C2575 G2576 A2577 G2578 C2579 U2580 G2581 G2582 G2583 U2584 U2585 C2586 A2587 U2593 C2594 G2597 A2598 G2599 A2600 C2601 A2602 G2603 U2604 U2605 C2606 G2607 G2608 U2609 C2610 U2611 C2612 U2613 A2614 U2615 C2616 C2617 G2618 C2619 C2620 G2624 G2625 C2626 G2627 C2628 A2629
G2630 G2631 A2632 G2633 G2634 C2635 U2636 U2637 G2638 A2639 G2642 G2643 G2644 G2645 C2646 U2647 C2648 U2649 U2650 C2651 C2652 U2653 A2654 G2655 U2656 A2657 C2658 G2659 A2660 G2661 A2662 G2663 G2664 A2665 C2666 C2667 G2668 G2669 A2670 G2671 C2672 G2673 G2674 A2675 A2679 C2680 C2681 U2682 C2683 U2684 G2685 G2686 U2687 U2688 U2689 C2690 C2691 C2692
A2693 G2694 C2695 U2696 G2697 U2698 C2699 C2700 C2701 U2702 G2707 G2708 G2709 C2710 A2711 U2712 A2712A A2713 G2714 C2715 U2716 G2717 G2718 G2719 U2720 A2721 G2722 C2723 C2724 A2725 U2726 G2727 U2728 G2729 C2730 G2731 G2732 A2733 A2734 G2735 G2736 G2737 A2738 U2739 A2740 A2741 C2742 C2743 G2744 C2745 U2746 G2747 A2748 A2749 A2750 G2751 C2752 A2753 U2754
C2755 U2756 A2757 A2758 G2759 C2760 G2761 G2762 G2763 A2764 A2765 G2766 C2767 C2768 C2769 G2770 C2771 C2772 C2773 C2774 A2775 A2776 G2777 A2778 U2779 G2780 A2781 G2782 G2783 C2784 C2785 U2786 C2787 C2788 C2789 A2790 C2791 G2792 G2793 C2794 G2795 U2796 C2799 A2801 A2801A G2802 C2803 C2804 G2805 G2807 U2808 A2809 A2810 G2811 C2812 C2815 C2816 G2817 G2818
G2819 A2820 A2821 G2822 A2823 C2824 C2825 A2826 C2827 C2828 C2829 U2832 G2833 G2834 A2835 U2836 G2837 G2838 G2839 C2840 C2841 C2842 G2843 G2844 G2845 G2846 U2847 G2848 U2849 A2850 A2851 C2852 C2853 G2854 C2855 C2856 G2857 C2858 G2859 A2860 G2861 G2862 C2863 G2864 U2865 U2866 G2867 A2868 G2869 C2870 C2871 G2872 C2875 G2876 C2880 C2881 A2882
A2883 U2884 C2885 G2886 U2887 C2888 C2889 G2891 A2892 G2893 G2894 U2895 C2896 U2897 U G A C C C C U C C

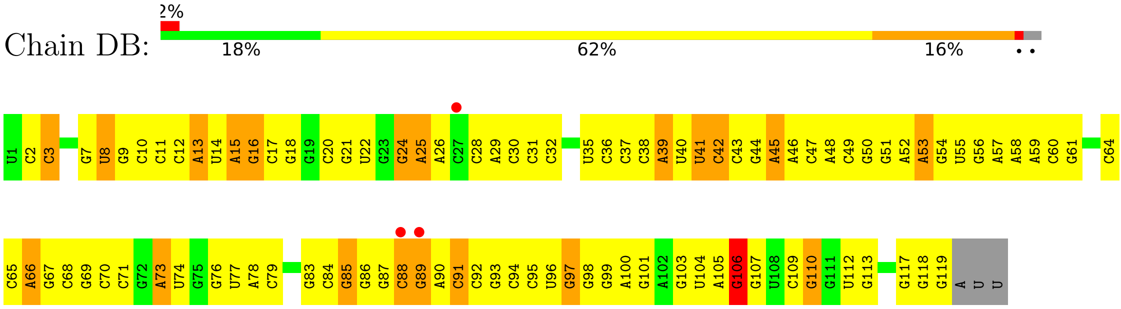
- Molecule 26: 5S ribosomal RNA

Chain BB:



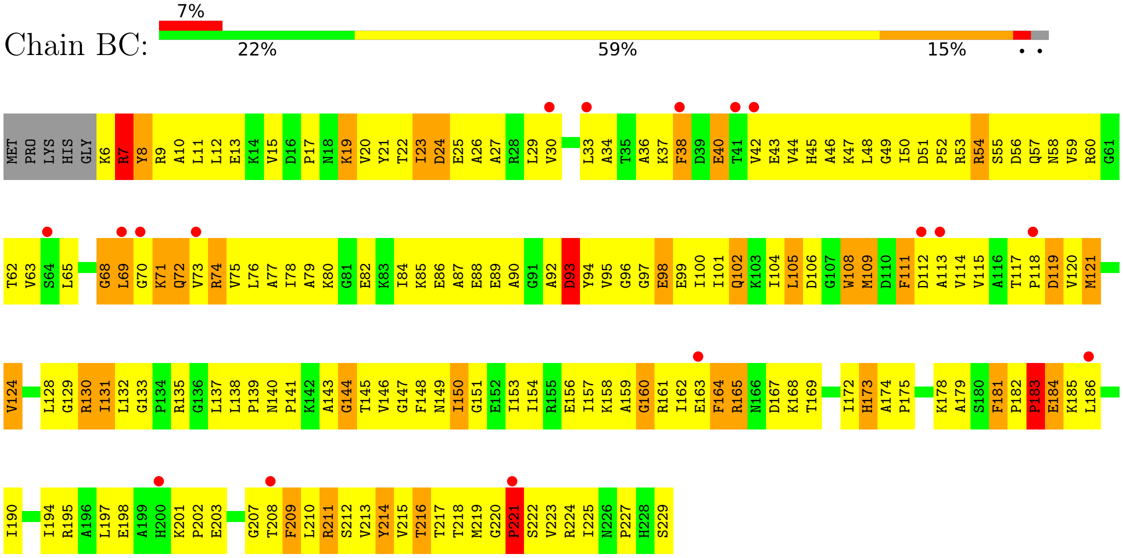
- Molecule 26: 5S ribosomal RNA

Chain DB:



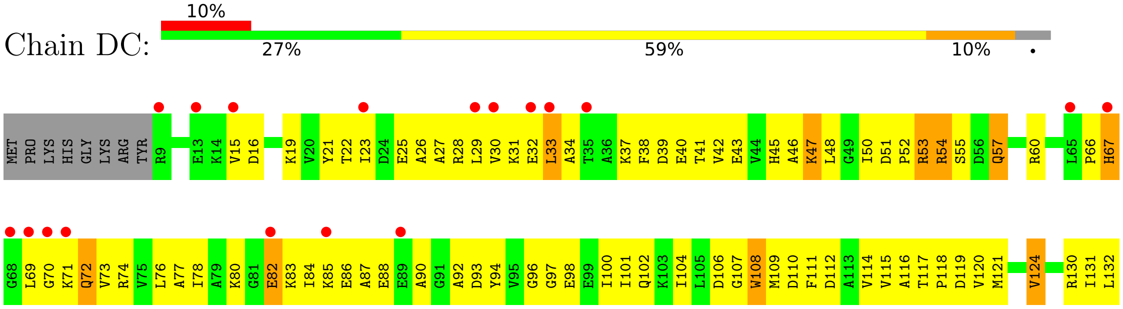
- Molecule 27: 50S ribosomal protein L1

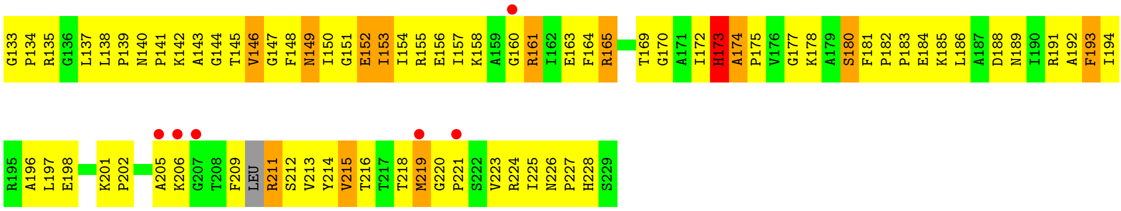
Chain BC:



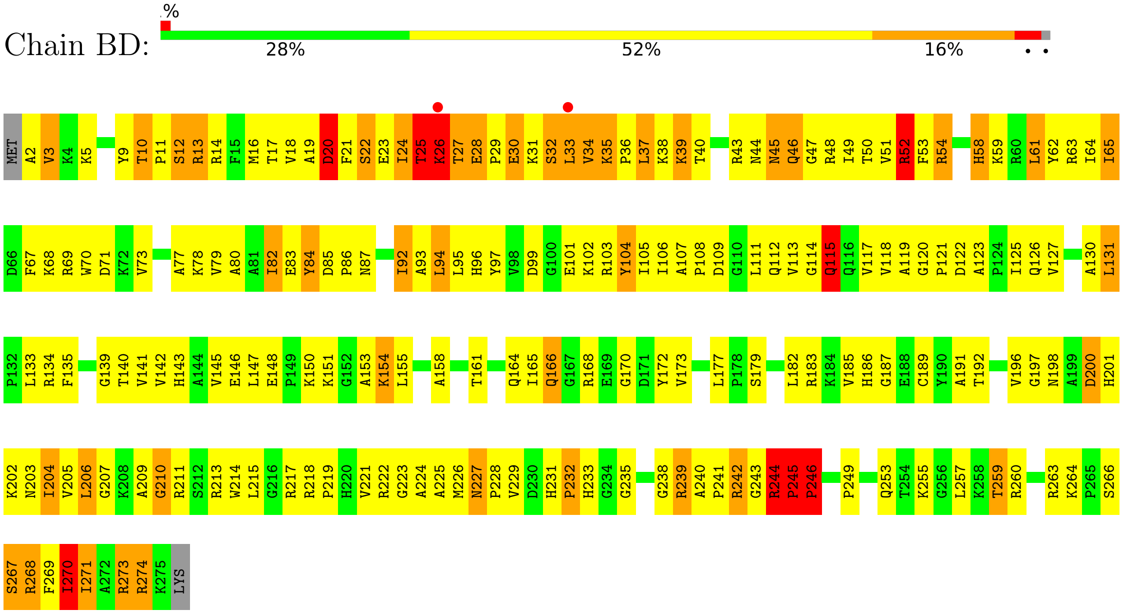
- Molecule 27: 50S ribosomal protein L1

Chain DC:

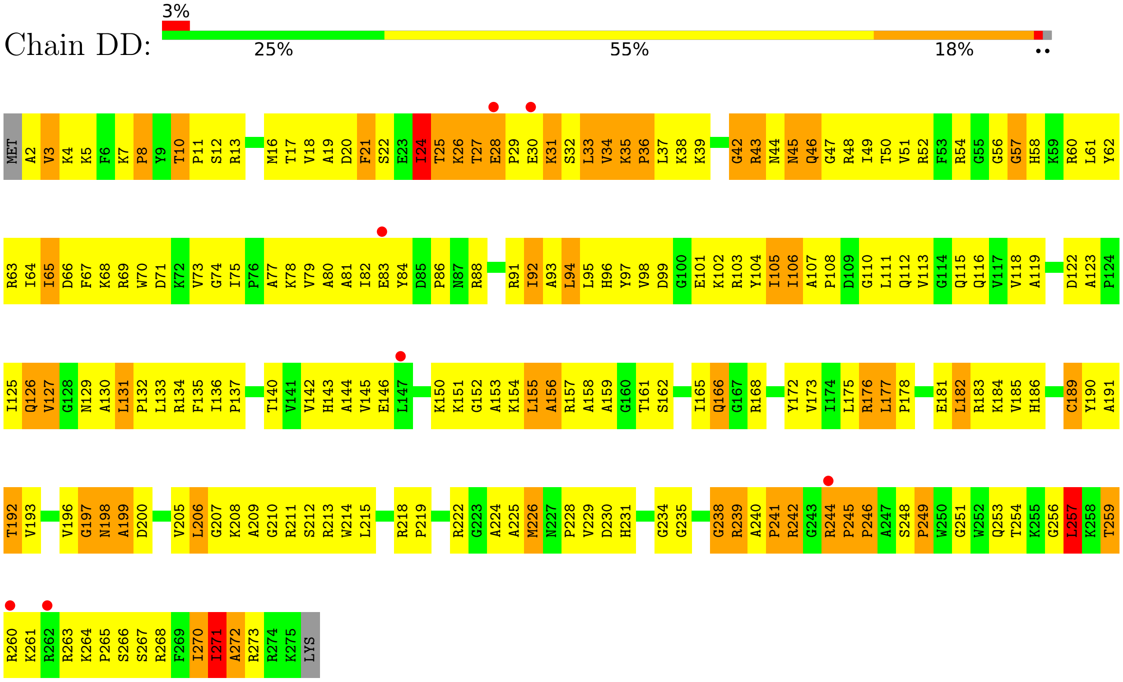




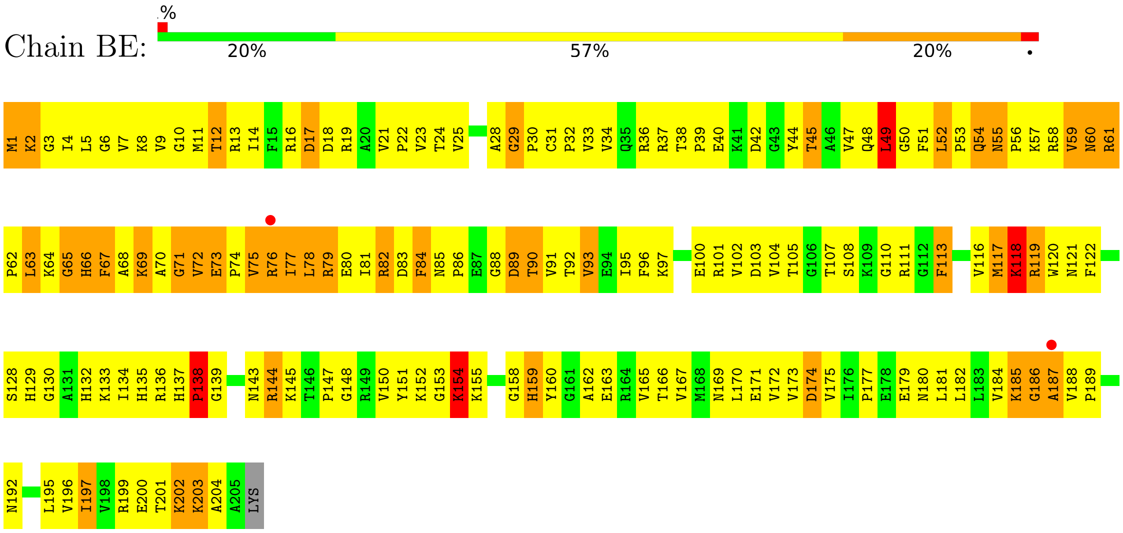
- Molecule 28: 50S ribosomal protein L2



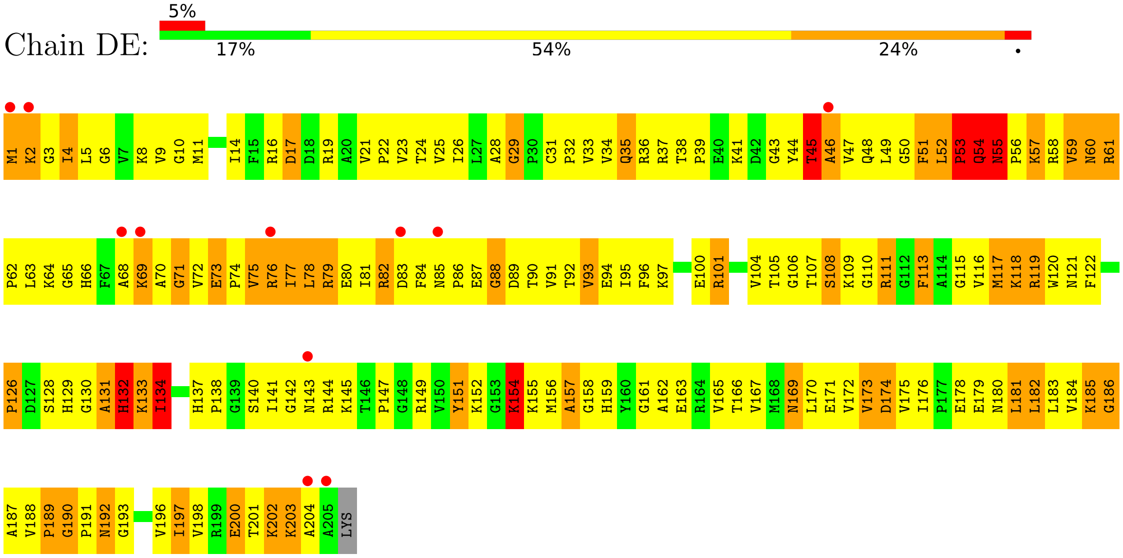
- Molecule 28: 50S ribosomal protein L2



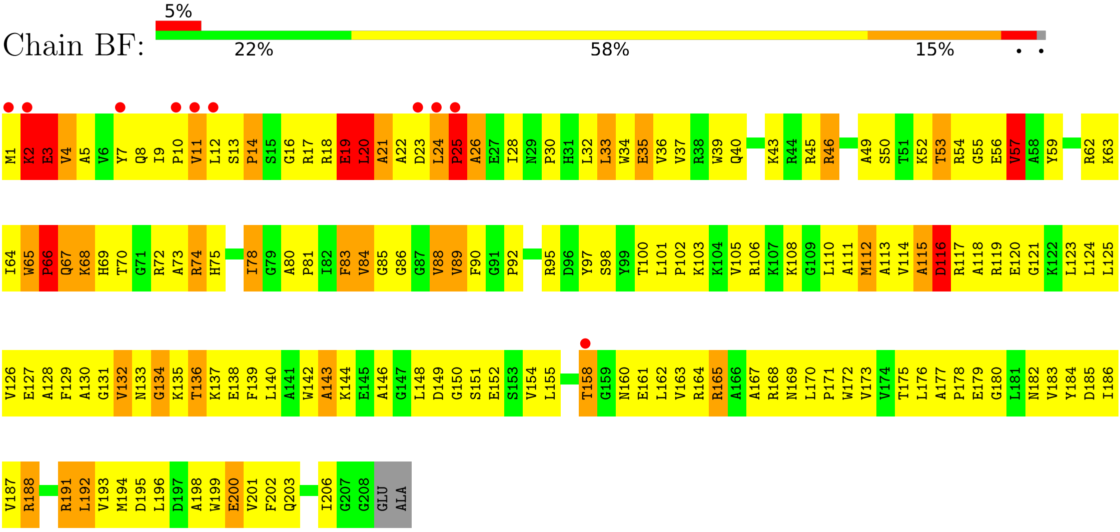
- Molecule 29: 50S ribosomal protein L3



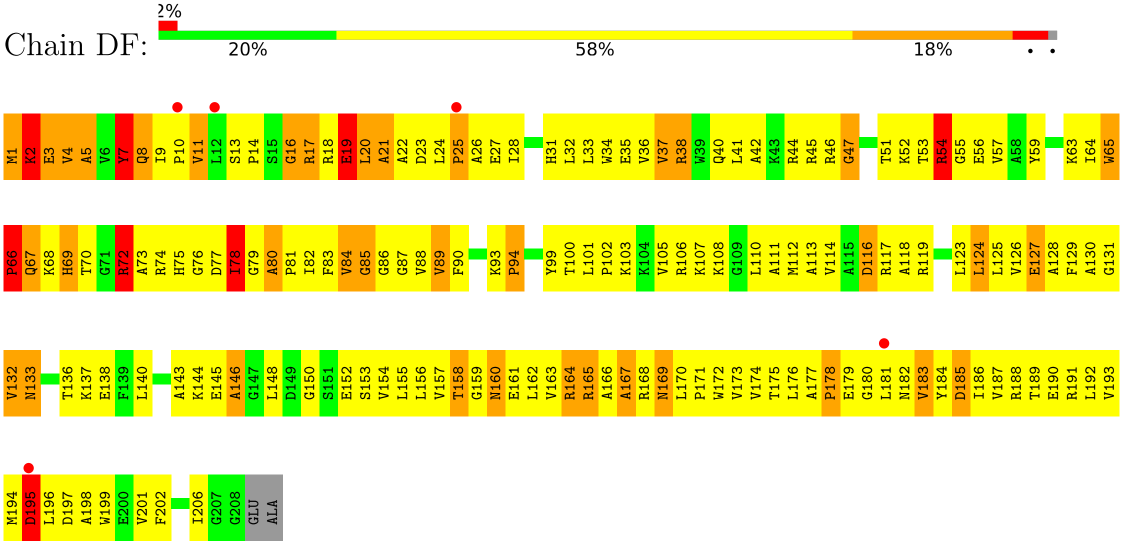
- Molecule 29: 50S ribosomal protein L3



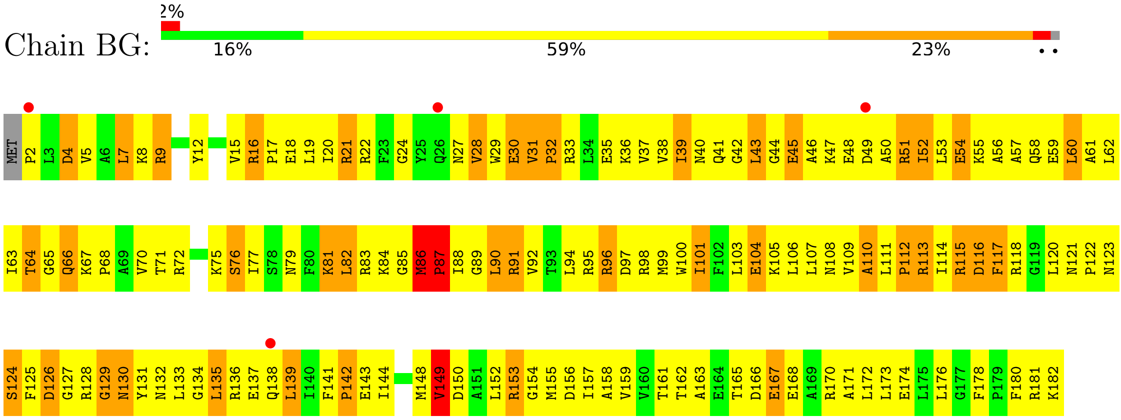
- Molecule 30: 50S ribosomal protein L4



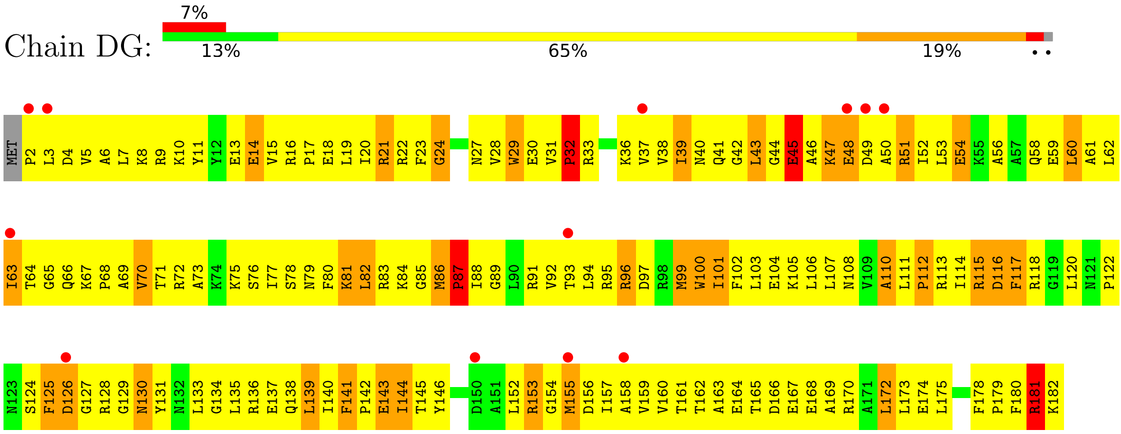
- Molecule 30: 50S ribosomal protein L4



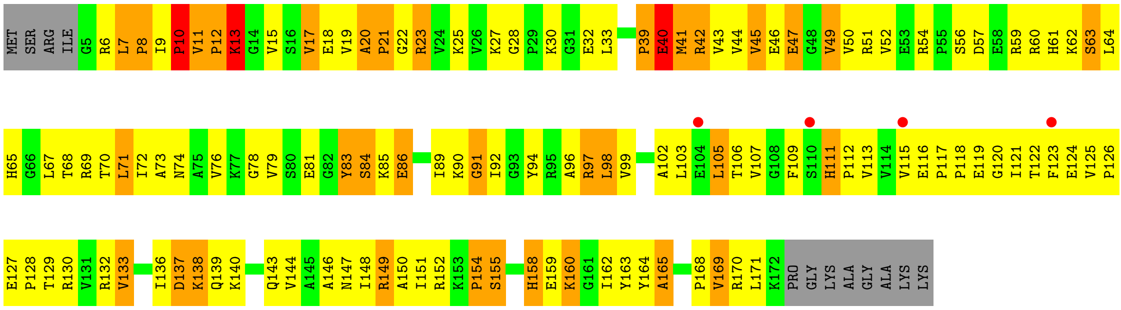
- Molecule 31: 50S ribosomal protein L5



- Molecule 31: 50S ribosomal protein L5

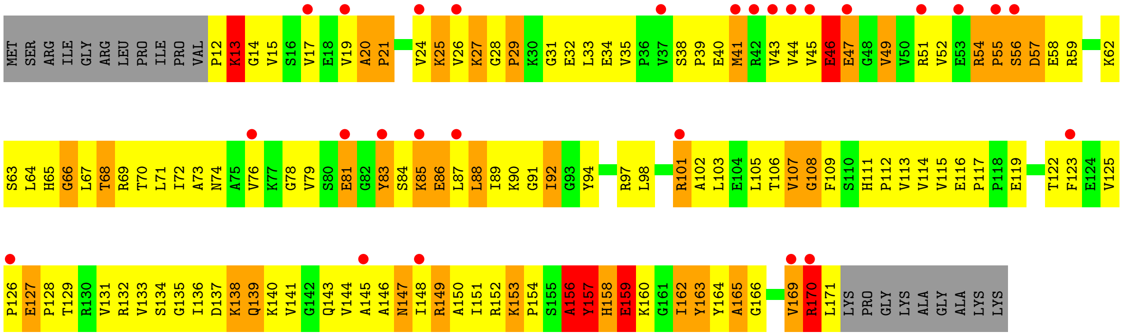


- Molecule 32: 50S ribosomal protein L6



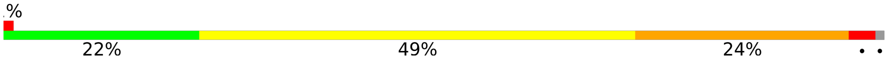
- Molecule 32: 50S ribosomal protein L6

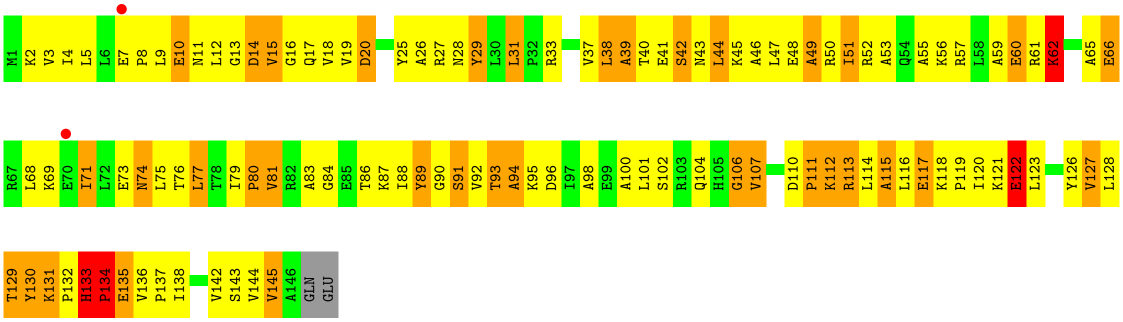
Chain DH:



- Molecule 33: 50S ribosomal protein L9

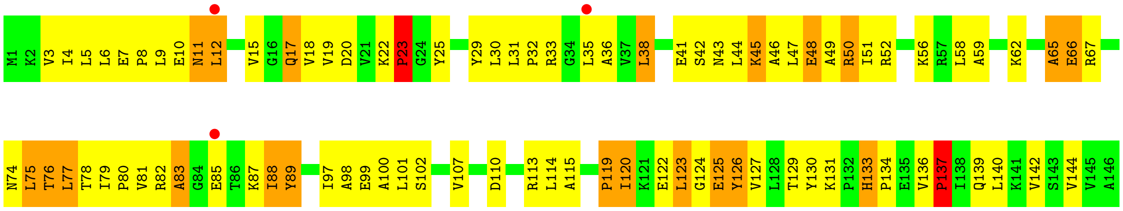
Chain BI:





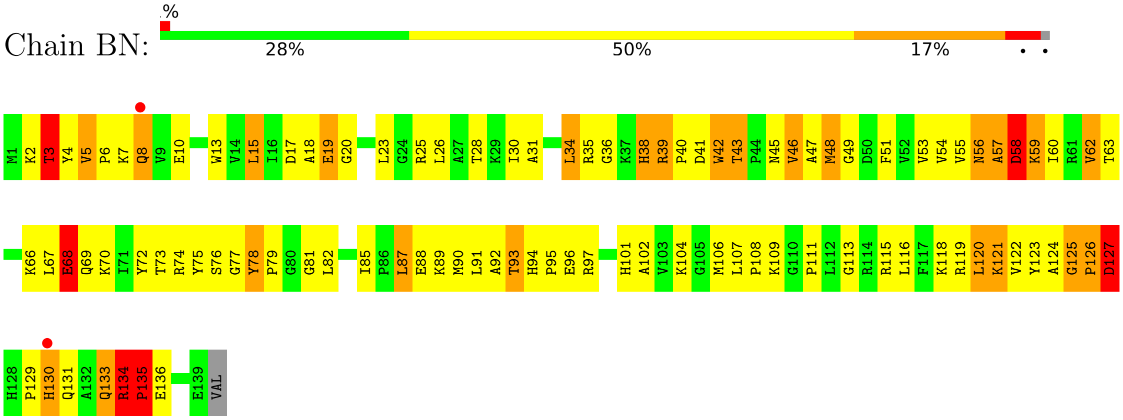
- Molecule 33: 50S ribosomal protein L9

Chain DI:



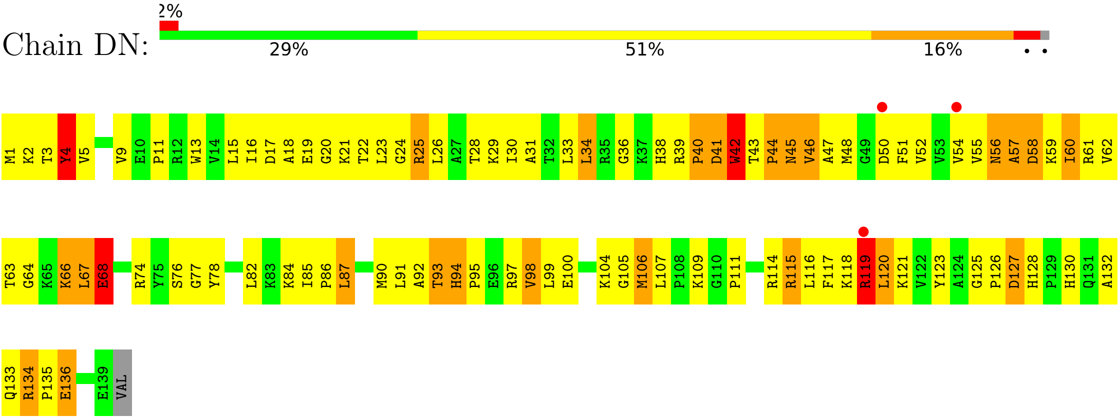
- Molecule 34: 50S ribosomal protein L13

Chain BN:



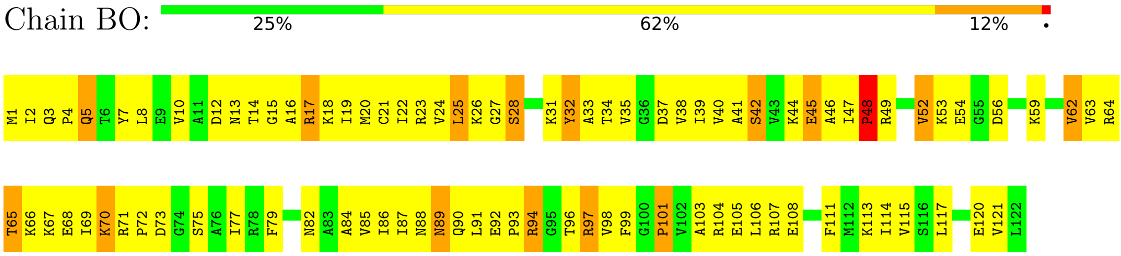
- Molecule 34: 50S ribosomal protein L13

Chain DN:



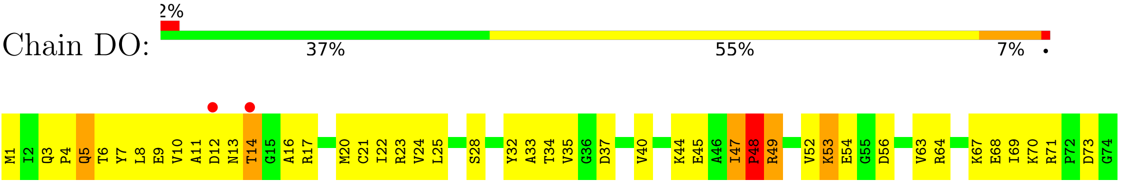
- Molecule 35: 50S ribosomal protein L14

Chain BO:

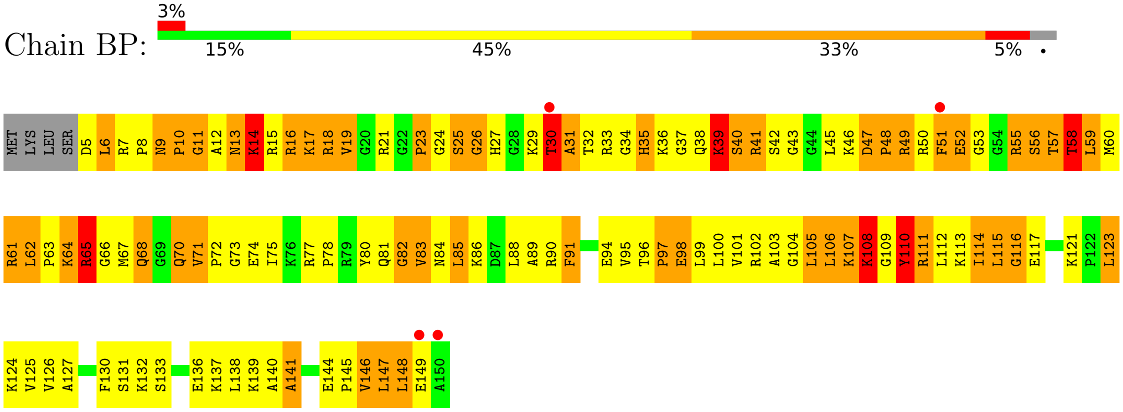


- Molecule 35: 50S ribosomal protein L14

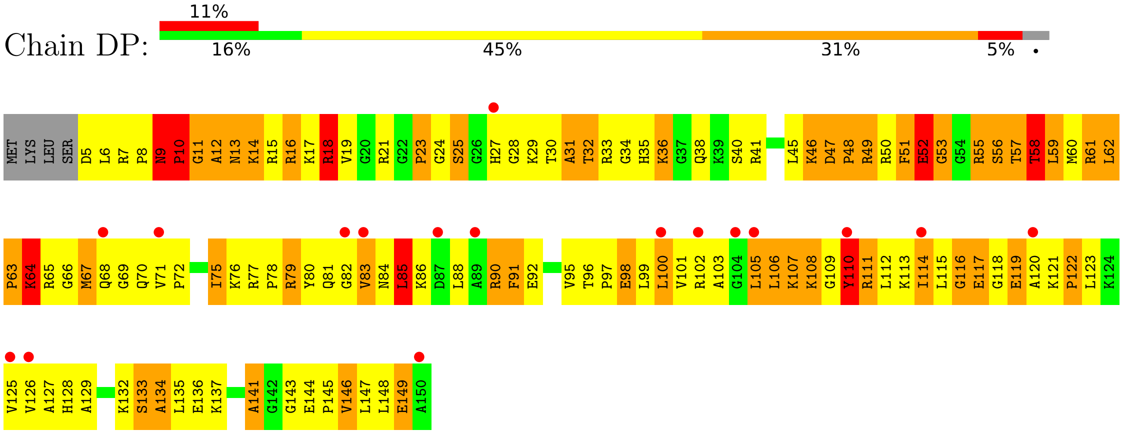
Chain DO:



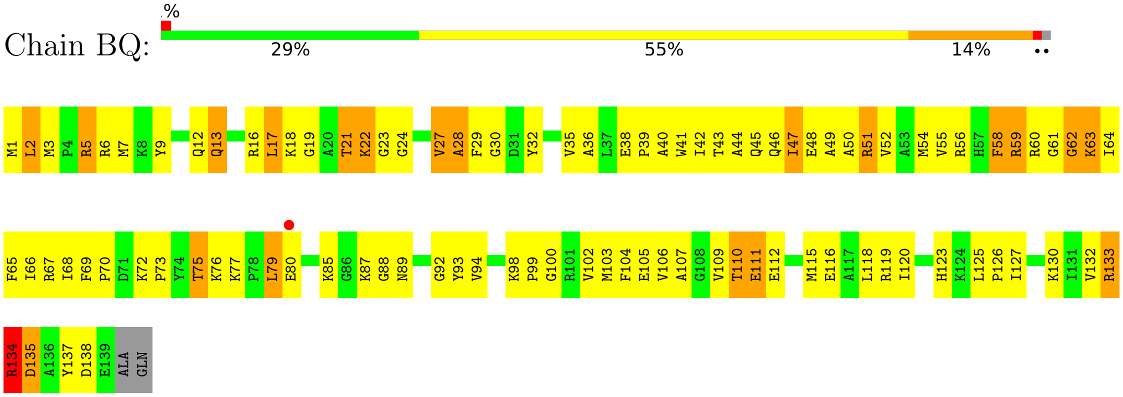
- Molecule 36: 50S ribosomal protein L15



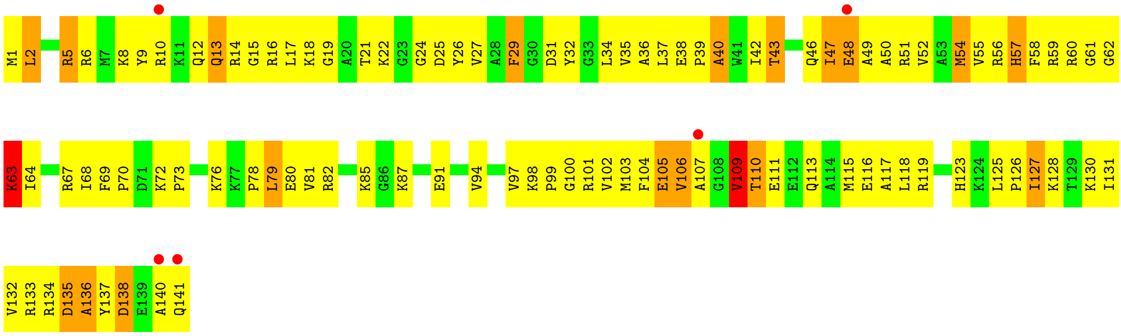
- Molecule 36: 50S ribosomal protein L15



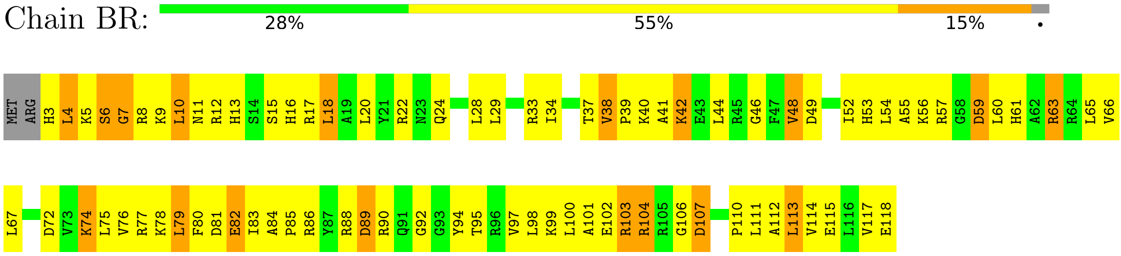
- Molecule 37: 50S ribosomal protein L16



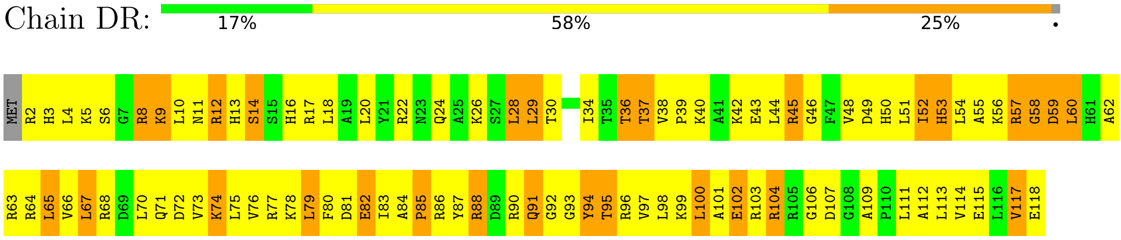
- Molecule 37: 50S ribosomal protein L16



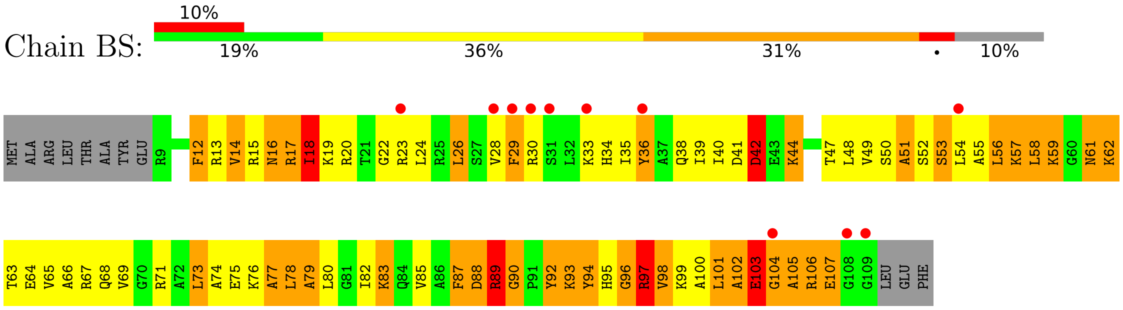
- Molecule 38: 50S ribosomal protein L17



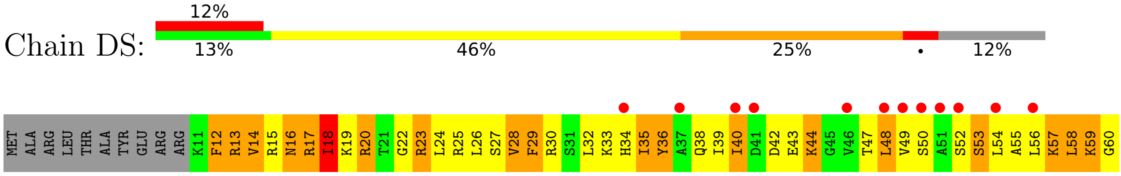
- Molecule 38: 50S ribosomal protein L17

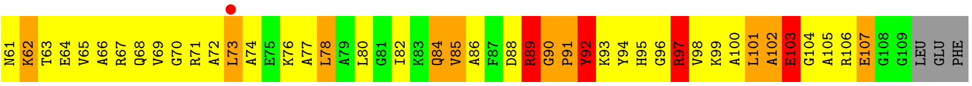


- Molecule 39: 50S ribosomal protein L18



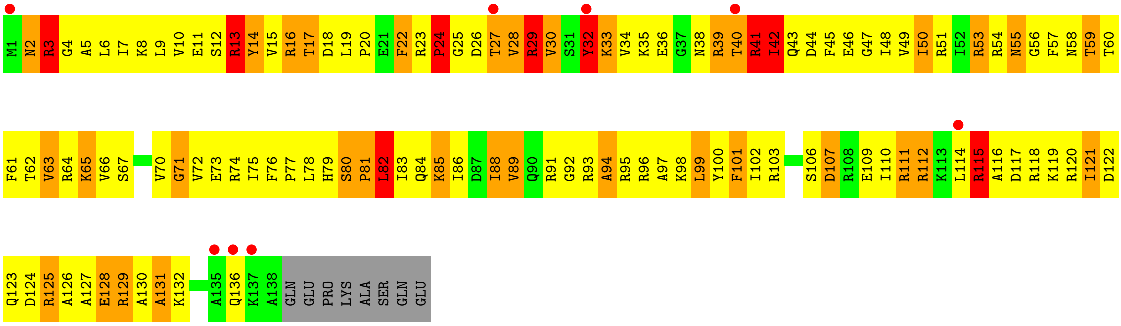
- Molecule 39: 50S ribosomal protein L18





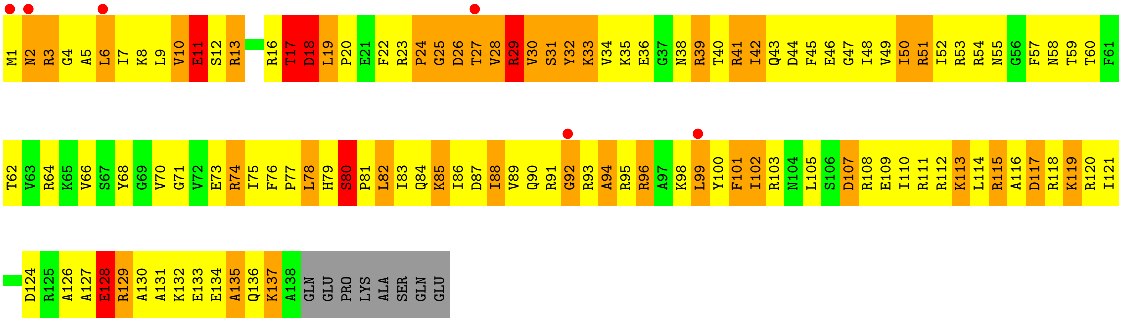
- Molecule 40: 50S ribosomal protein L19

Chain BT:



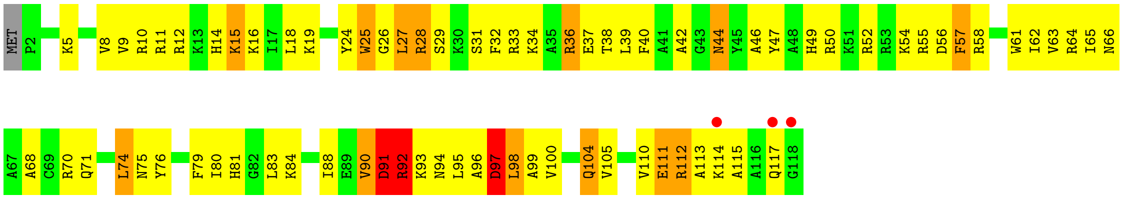
- Molecule 40: 50S ribosomal protein L19

Chain DT:



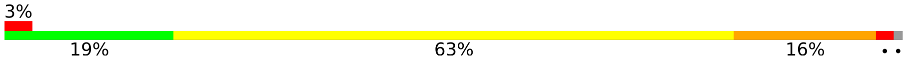
- Molecule 41: 50S ribosomal protein L20

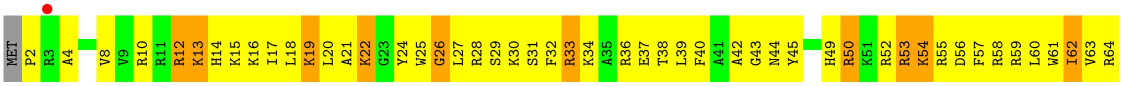
Chain BU:

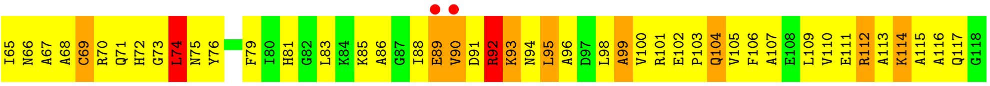


- Molecule 41: 50S ribosomal protein L20

Chain DU:

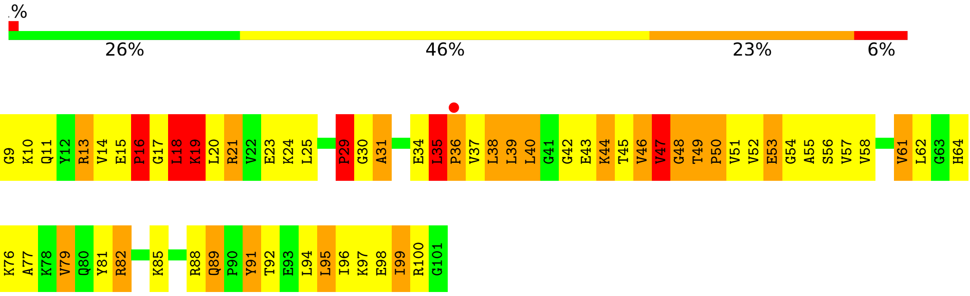






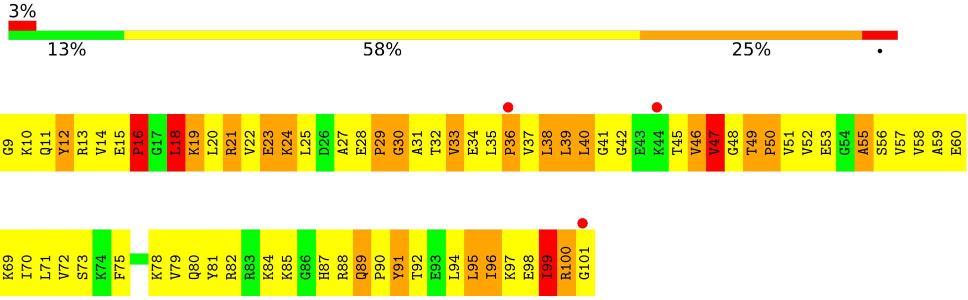
- Molecule 42: 50S ribosomal protein L21

Chain BV:



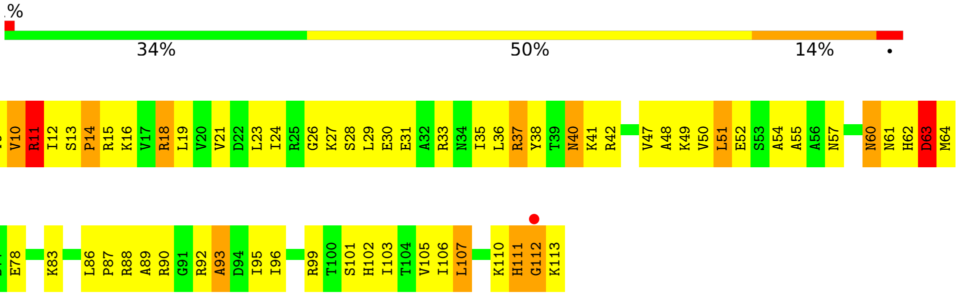
- Molecule 42: 50S ribosomal protein L21

Chain DV:



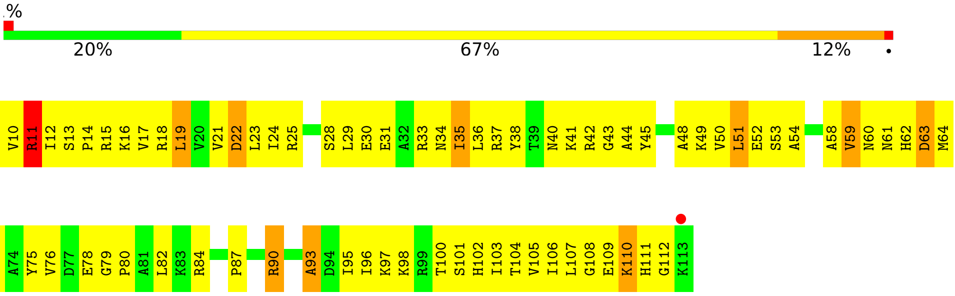
- Molecule 43: 50S ribosomal protein L22

Chain BW:



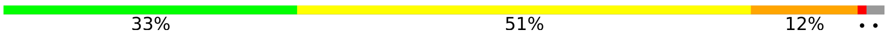
- Molecule 43: 50S ribosomal protein L22

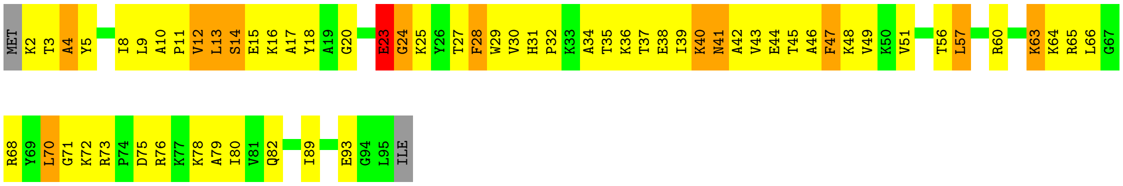
Chain DW:



- Molecule 44: 50S ribosomal protein L23

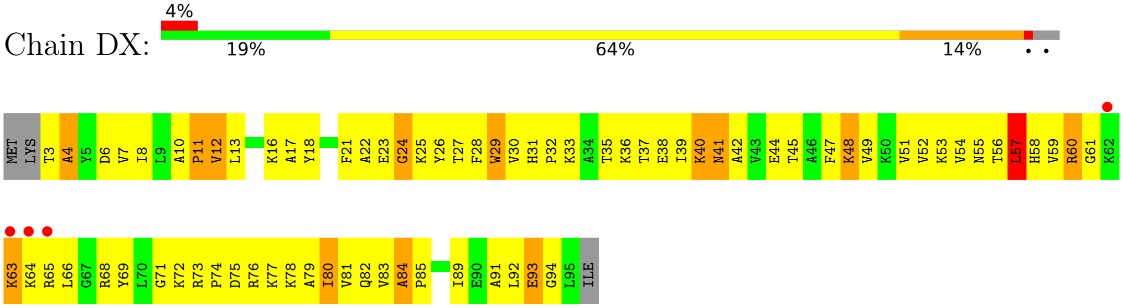
Chain BX:





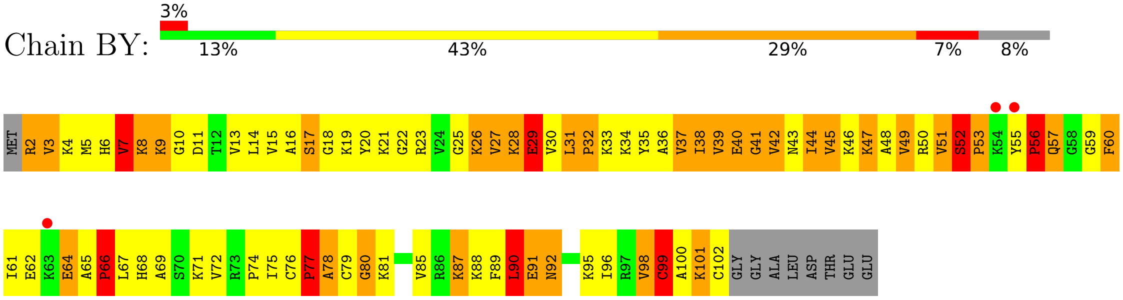
- Molecule 44: 50S ribosomal protein L23

Chain DX:



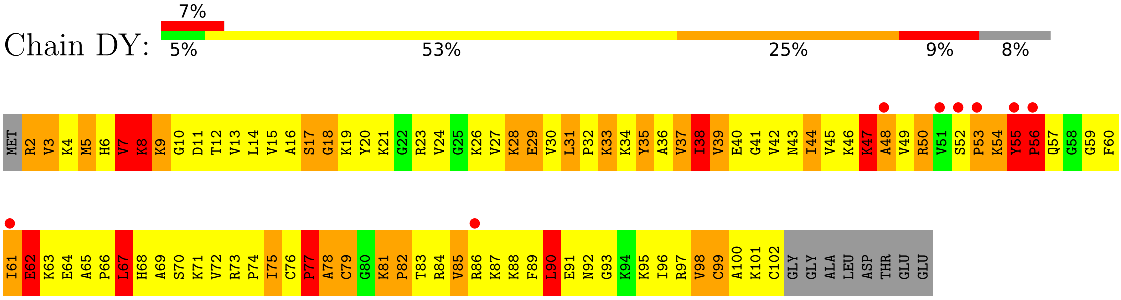
- Molecule 45: 50S ribosomal protein L24

Chain BY:



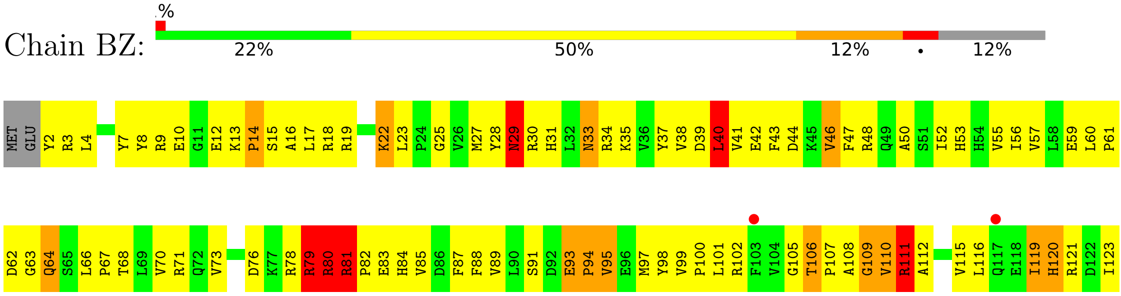
- Molecule 45: 50S ribosomal protein L24

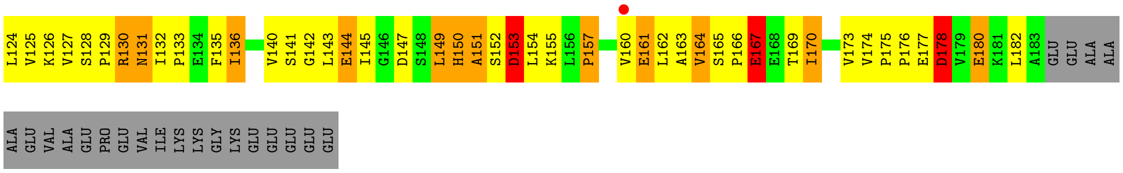
Chain DY:



- Molecule 46: 50S ribosomal protein L25

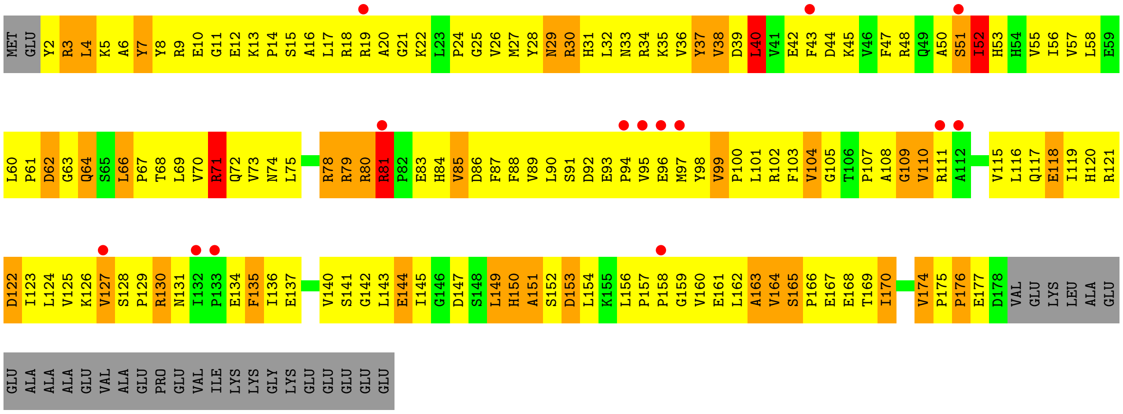
Chain BZ:





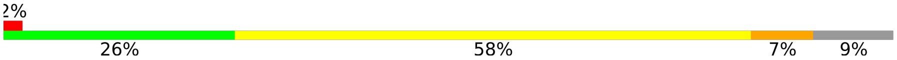
- Molecule 46: 50S ribosomal protein L25

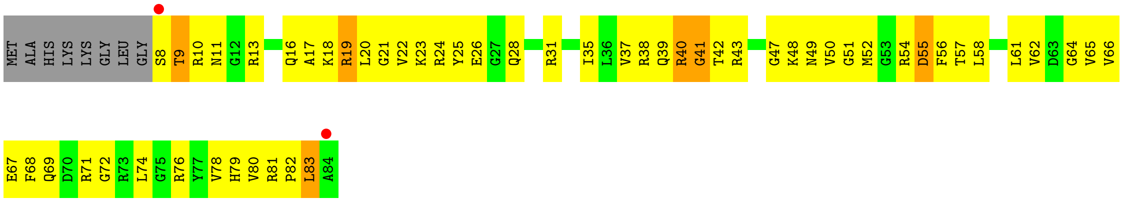
Chain DZ:



- Molecule 47: 50S ribosomal protein L27

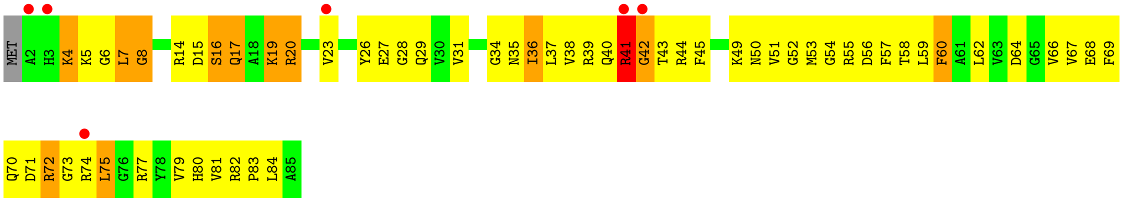
Chain B0:





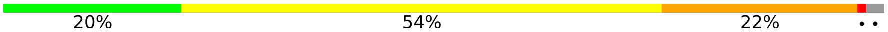
- Molecule 47: 50S ribosomal protein L27

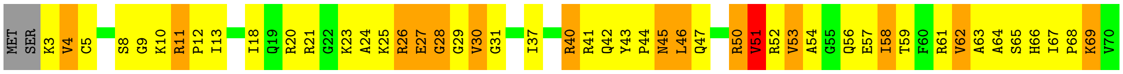
Chain D0:



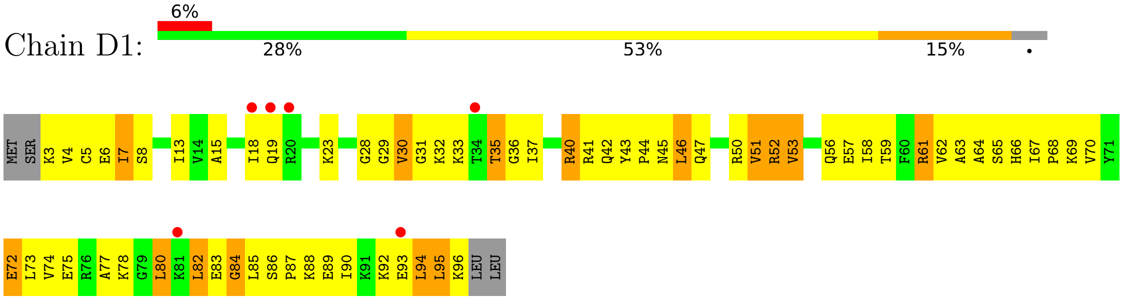
- Molecule 48: 50S ribosomal protein L28

Chain B1:

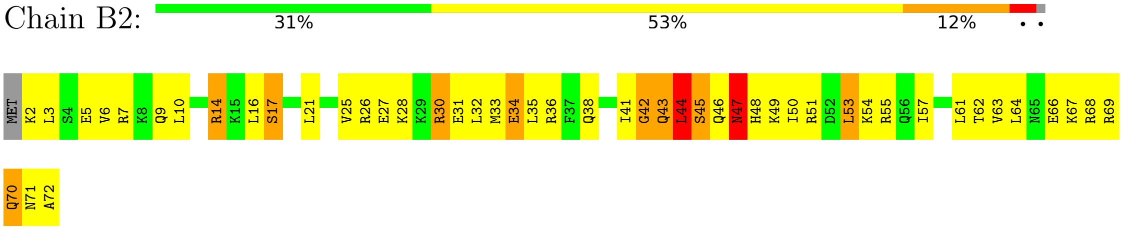




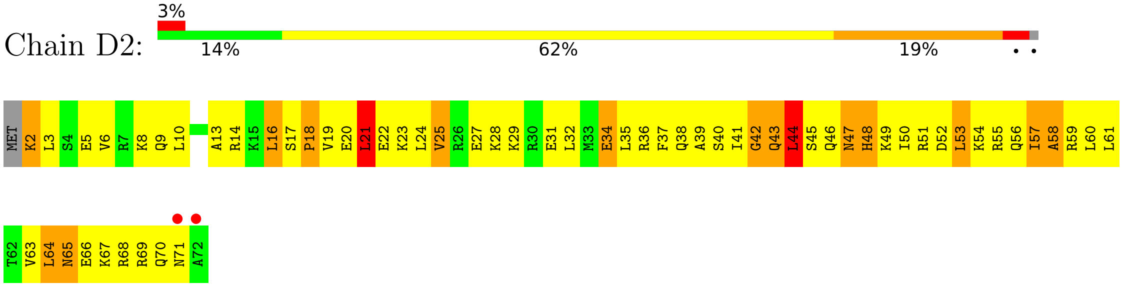
- Molecule 48: 50S ribosomal protein L28



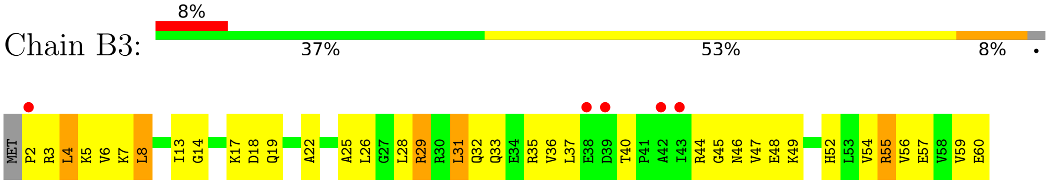
- Molecule 49: 50S ribosomal protein L29



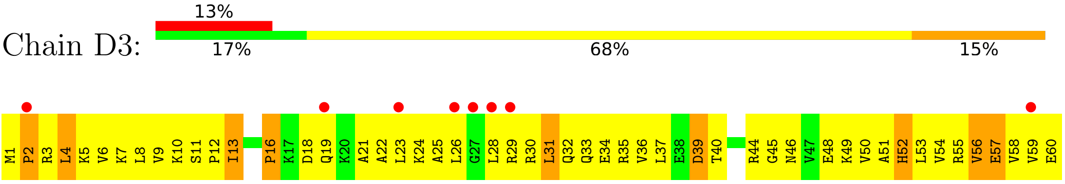
- Molecule 49: 50S ribosomal protein L29



- Molecule 50: 50S ribosomal protein L30

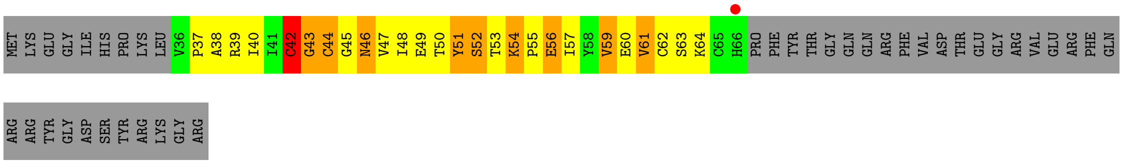


- Molecule 50: 50S ribosomal protein L30



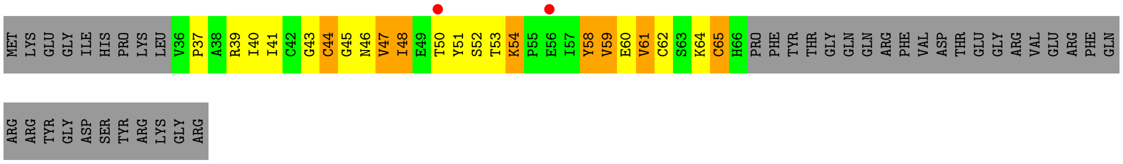
- Molecule 51: 50S ribosomal protein L31

Chain B4:



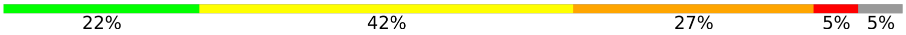
- Molecule 51: 50S ribosomal protein L31

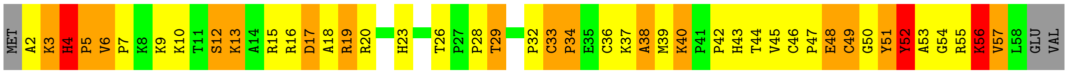
Chain D4:



- Molecule 52: 50S ribosomal protein L32

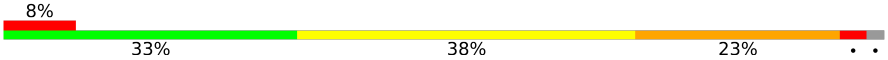
Chain B5:

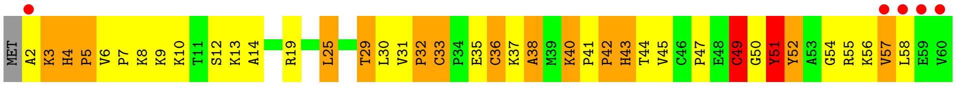




- Molecule 52: 50S ribosomal protein L32

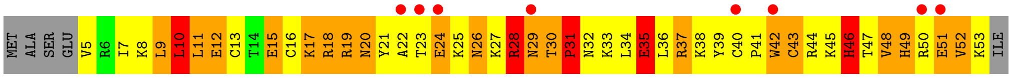
Chain D5:





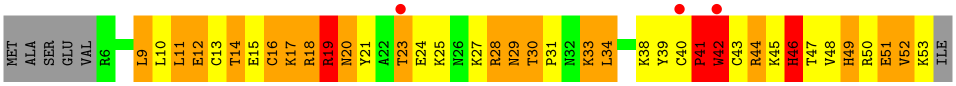
- Molecule 53: 50S ribosomal protein L33

Chain B6:



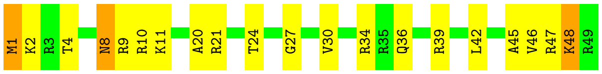
- Molecule 53: 50S ribosomal protein L33

Chain D6:



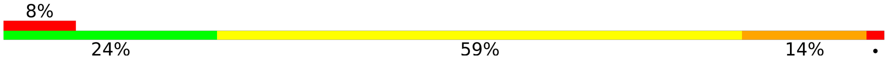
- Molecule 54: 50S ribosomal protein L34

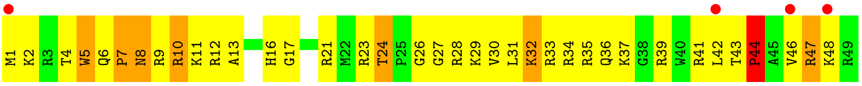
Chain B7:



- Molecule 54: 50S ribosomal protein L34

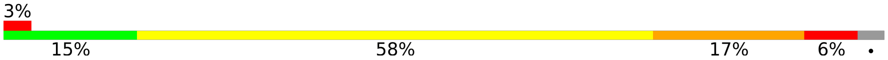
Chain D7:





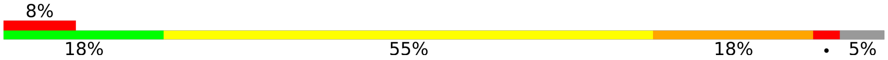
- Molecule 55: 50S ribosomal protein L35

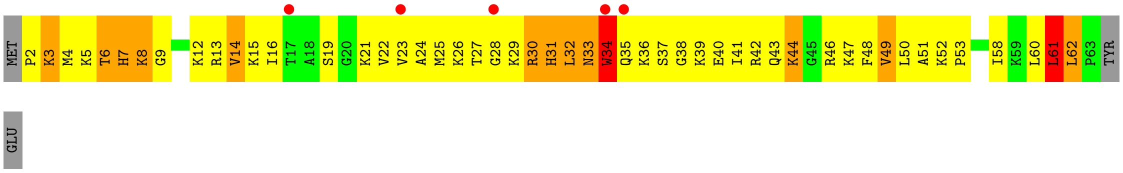
Chain B8:



- Molecule 55: 50S ribosomal protein L35

Chain D8:



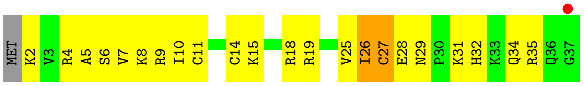


- Molecule 56: 50S ribosomal protein L36

Chain B9:

- Molecule 56: 50S ribosomal protein L36

Chain D9:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.53Å 447.03Å 622.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.10 49.65 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-3.10) 94.7 (49.65-3.10)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.302 0.254 , 0.251	Depositor DCC
R_{free} test set	49631 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	72.6	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 56.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	290405	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

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

---

[1] Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z|>5$	RMSZ	$\#|Z|>5$
1	AA	0.82	6/35982 (0.0%)	0.78	24/56156 (0.0%)
1	CA	0.47	0/36193	0.72	9/56490 (0.0%)
2	AB	0.41	0/1936	0.69	0/2611
2	CB	0.43	0/1936	0.73	1/2611 (0.0%)
3	AC	0.41	0/1637	0.66	0/2207
3	CC	0.40	0/1637	0.66	0/2207
4	AD	0.41	0/1733	0.69	0/2318
4	CD	0.42	0/1733	0.72	1/2318 (0.0%)
5	AE	0.42	0/1163	0.68	0/1566
5	CE	0.40	0/1163	0.69	0/1566
6	AF	0.44	0/856	0.71	0/1154
6	CF	0.40	0/856	0.70	0/1154
7	AG	0.42	0/1276	0.67	0/1709
7	CG	0.42	0/1276	0.67	0/1709
8	AH	0.41	0/1136	0.72	0/1527
8	CH	0.39	0/1136	0.67	0/1527
9	AI	0.46	0/1022	0.69	0/1369
9	CI	0.43	0/1022	0.70	0/1369
10	AJ	0.43	0/808	0.71	0/1087
10	CJ	0.45	0/808	0.72	0/1087
11	AK	0.41	0/900	0.72	1/1213 (0.1%)
11	CK	0.39	0/900	0.67	0/1213
12	AL	0.41	0/987	0.78	0/1322
12	CL	0.41	0/987	0.77	1/1322 (0.1%)
13	AM	0.41	0/957	0.78	1/1283 (0.1%)
13	CM	0.39	0/957	0.76	1/1283 (0.1%)
14	AN	0.43	0/501	0.69	0/664
14	CN	0.45	0/501	0.66	0/664
15	AO	0.42	0/745	0.66	0/992
15	CO	0.39	0/745	0.67	1/992 (0.1%)
16	AP	0.42	0/717	0.71	1/965 (0.1%)
16	CP	0.42	0/717	0.73	1/965 (0.1%)

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

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

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

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

The worst 5 of 32 bond length outliers are listed below:

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

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

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

All (4) chirality outliers are listed below:

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

5 of 247 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	114	U	Sidechain

Continued on next page...

Continued from previous page...

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32144	0	16225	1841	0
1	CA	32332	0	16317	1680	0
2	AB	1901	0	1951	360	0
2	CB	1901	0	1951	361	0
3	AC	1613	0	1677	329	0
3	CC	1613	0	1677	275	0
4	AD	1703	0	1763	325	0
4	CD	1703	0	1763	212	0
5	AE	1147	0	1207	168	0
5	CE	1147	0	1207	177	0
6	AF	843	0	857	111	0
6	CF	843	0	857	137	0
7	AG	1257	0	1296	192	0
7	CG	1257	0	1296	213	0
8	AH	1116	0	1177	183	0
8	CH	1116	0	1177	170	0
9	AI	1004	0	1031	187	0
9	CI	1004	0	1031	200	0
10	AJ	795	0	840	215	0
10	CJ	795	0	840	192	0
11	AK	885	0	904	130	0
11	CK	885	0	904	111	0
12	AL	971	0	1057	168	0
12	CL	971	0	1057	133	0
13	AM	947	0	1008	191	0
13	CM	947	0	1008	135	0
14	AN	492	0	533	111	0
14	CN	492	0	533	95	0
15	AO	734	0	771	102	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	DP	1079	0	1117	265	0
37	BQ	1099	0	1160	144	0
37	DQ	1122	0	1179	190	0
38	BR	923	0	949	105	0
38	DR	960	0	1021	156	0
39	BS	777	0	825	180	0
39	DS	771	0	832	159	0
40	BT	1142	0	1202	274	0
40	DT	1142	0	1202	231	0
41	BU	958	0	1015	150	0
41	DU	958	0	1015	224	0
42	BV	779	0	852	167	0
42	DV	779	0	852	217	0
43	BW	896	0	953	91	0
43	DW	896	0	953	126	0
44	BX	735	0	791	85	0
44	DX	726	0	778	122	0
45	BY	757	0	821	198	0
45	DY	776	0	870	199	0
46	BZ	1438	0	1455	202	0
46	DZ	1404	0	1432	302	0
47	B0	613	0	633	88	0
47	D0	662	0	688	109	0
48	B1	757	0	843	108	0
48	D1	732	0	808	99	0
49	B2	598	0	653	56	0
49	D2	598	0	653	101	0
50	B3	460	0	512	46	0
50	D3	468	0	523	91	0
51	B4	226	0	229	46	0
51	D4	226	0	229	39	0
52	B5	435	0	452	58	0
52	D5	459	0	477	64	0
53	B6	401	0	399	118	0
53	D6	322	0	250	85	0
54	B7	419	0	467	27	0
54	D7	419	0	467	49	0
55	B8	496	0	567	113	0
55	D8	467	0	519	114	0
56	B9	294	0	311	43	0
56	D9	299	0	325	31	0
57	AA	117	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	AL	1	0	0	0	0
57	AT	1	0	0	0	0
57	AW	2	0	0	0	0
57	B0	2	0	0	0	0
57	B1	1	0	0	0	0
57	B5	4	0	0	0	0
57	B7	1	0	0	0	0
57	BA	459	0	0	1	0
57	BB	9	0	0	0	0
57	BD	1	0	0	0	0
57	BE	1	0	0	0	0
57	BF	1	0	0	0	0
57	BH	1	0	0	0	0
57	BP	3	0	0	0	0
57	BQ	3	0	0	0	0
57	BR	1	0	0	0	0
57	BT	1	0	0	0	0
57	BU	1	0	0	0	0
57	BX	1	0	0	0	0
57	CA	109	0	0	0	0
57	CE	1	0	0	0	0
57	CW	5	0	0	0	0
57	CX	1	0	0	0	0
57	D5	2	0	0	0	0
57	D6	2	0	0	0	0
57	DA	305	0	0	0	0
57	DB	10	0	0	0	0
57	DD	1	0	0	0	0
57	DF	1	0	0	0	0
57	DP	1	0	0	0	0
57	DR	1	0	0	0	0
58	AD	1	0	0	0	0
58	B5	1	0	0	0	0
58	B9	1	0	0	0	0
58	CD	1	0	0	0	0
58	D5	1	0	0	1	0
58	D9	1	0	0	2	0
All	All	290405	0	198457	23826	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

The worst 5 of 23826 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:D5:49:CYS:SG	58:D5:103:ZN:ZN	0.84	1.63
56:D9:14:CYS:SG	58:D9:101:ZN:ZN	1.23	1.27
27:DC:180:SER:CB	27:DC:180:SER:OG	1.82	1.25
36:BP:59:LEU:HA	36:BP:61:ARG:NH1	1.53	1.21
39:BS:97:ARG:NH2	39:BS:98:VAL:HA	1.55	1.20

There are no symmetry-related clashes.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

5 of 1742 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	173 (86%)	29 (14%)	3	14
2	CB	202/220 (92%)	179 (89%)	23 (11%)	5	23
3	AC	160/188 (85%)	142 (89%)	18 (11%)	6	23
3	CC	160/188 (85%)	146 (91%)	14 (9%)	10	36
4	AD	180/181 (99%)	157 (87%)	23 (13%)	4	18
4	CD	180/181 (99%)	158 (88%)	22 (12%)	5	19
5	AE	115/123 (94%)	102 (89%)	13 (11%)	6	23
5	CE	115/123 (94%)	104 (90%)	11 (10%)	8	31
6	AF	90/90 (100%)	77 (86%)	13 (14%)	3	14
6	CF	90/90 (100%)	81 (90%)	9 (10%)	7	28
7	AG	126/127 (99%)	112 (89%)	14 (11%)	6	24
7	CG	126/127 (99%)	110 (87%)	16 (13%)	4	18
8	AH	119/119 (100%)	109 (92%)	10 (8%)	11	38
8	CH	119/119 (100%)	108 (91%)	11 (9%)	9	33
9	AI	97/99 (98%)	80 (82%)	17 (18%)	2	8
9	CI	97/99 (98%)	78 (80%)	19 (20%)	1	6
10	AJ	88/92 (96%)	75 (85%)	13 (15%)	3	13
10	CJ	88/92 (96%)	79 (90%)	9 (10%)	7	27
11	AK	90/99 (91%)	85 (94%)	5 (6%)	21	52
11	CK	90/99 (91%)	81 (90%)	9 (10%)	7	28
12	AL	104/109 (95%)	94 (90%)	10 (10%)	8	31
12	CL	104/109 (95%)	92 (88%)	12 (12%)	5	22
13	AM	95/101 (94%)	74 (78%)	21 (22%)	1	4
13	CM	95/101 (94%)	79 (83%)	16 (17%)	2	9
14	AN	49/50 (98%)	40 (82%)	9 (18%)	1	7
14	CN	49/50 (98%)	44 (90%)	5 (10%)	7	27

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Res	Type
18	CR	19	LYS
35	DO	96	THR
20	CT	75	ASN
17	CQ	78	GLU
29	DE	173	VAL

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

Mol	Chain	Res	Type
19	CS	56	GLN
36	DP	84	ASN
22	CV	55	ASN
29	DE	159	HIS
41	DU	81	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1492/1509 (98%)	236 (15%)	40 (2%)
1	CA	1503/1509 (99%)	227 (15%)	33 (2%)
23	AW	76/77 (98%)	18 (23%)	2 (2%)
23	CW	76/77 (98%)	19 (25%)	6 (7%)
24	AX	4/5 (80%)	0	0
24	CX	4/5 (80%)	0	0
25	BA	2761/2915 (94%)	508 (18%)	77 (2%)
25	DA	2771/2915 (95%)	546 (19%)	84 (3%)
26	BB	118/122 (96%)	19 (16%)	2 (1%)
26	DB	118/122 (96%)	20 (16%)	2 (1%)
All	All	8923/9256 (96%)	1593 (17%)	246 (2%)

5 of 1593 RNA backbone outliers are listed below:

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

5 of 246 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2756	U
25	DA	2225	A
1	CA	968	A
25	DA	2171	A
25	DA	2611	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AA	1

All chain breaks are listed below:

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

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	1495/1509 (99%)	0.09	40 (2%)	54	31	43, 73, 89, 96	1 (0%)
1	CA	1504/1509 (99%)	0.16	32 (2%)	63	43	47, 71, 88, 97	1 (0%)
2	AB	235/256 (91%)	0.22	18 (7%)	13	5	65, 75, 82, 88	0
2	CB	235/256 (91%)	0.34	22 (9%)	8	3	66, 76, 82, 85	0
3	AC	207/239 (86%)	0.33	12 (5%)	23	10	67, 75, 82, 86	0
3	CC	207/239 (86%)	0.35	19 (9%)	9	3	67, 75, 81, 84	0
4	AD	208/209 (99%)	-0.08	2 (0%)	82	67	61, 72, 79, 85	0
4	CD	208/209 (99%)	-0.05	5 (2%)	59	37	55, 68, 75, 83	0
5	AE	151/162 (93%)	0.22	9 (5%)	21	10	60, 69, 76, 83	0
5	CE	151/162 (93%)	0.21	5 (3%)	46	24	60, 69, 77, 90	0
6	AF	101/101 (100%)	-0.36	1 (0%)	82	67	56, 67, 76, 81	0
6	CF	101/101 (100%)	-0.03	2 (1%)	65	44	61, 70, 78, 83	0
7	AG	155/156 (99%)	0.09	8 (5%)	27	12	63, 74, 80, 83	0
7	CG	155/156 (99%)	0.44	13 (8%)	11	4	67, 74, 81, 84	0
8	AH	138/138 (100%)	-0.04	2 (1%)	75	56	56, 69, 74, 79	0
8	CH	138/138 (100%)	0.02	4 (2%)	51	28	57, 70, 76, 82	0
9	AI	127/128 (99%)	0.55	11 (8%)	10	4	66, 77, 83, 87	0
9	CI	127/128 (99%)	1.02	28 (22%)	0	0	70, 77, 83, 86	0
10	AJ	99/105 (94%)	0.85	15 (15%)	2	1	66, 79, 84, 88	0
10	CJ	99/105 (94%)	1.96	45 (45%)	0	0	66, 79, 84, 87	0
11	AK	119/129 (92%)	0.57	10 (8%)	11	4	58, 68, 78, 82	0
11	CK	119/129 (92%)	0.07	4 (3%)	45	24	64, 72, 78, 84	0
12	AL	125/132 (94%)	-0.10	3 (2%)	59	37	53, 67, 76, 85	0
12	CL	125/132 (94%)	0.29	6 (4%)	30	14	56, 65, 74, 84	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	AM	120/126 (95%)	0.32	7 (5%)	23	10	66, 75, 81, 83	0
13	CM	120/126 (95%)	0.26	7 (5%)	23	10	65, 75, 81, 84	0
14	AN	60/61 (98%)	0.08	2 (3%)	46	24	65, 74, 80, 82	0
14	CN	60/61 (98%)	0.12	1 (1%)	70	49	62, 74, 78, 82	0
15	AO	88/89 (98%)	-0.05	0	100	100	52, 66, 74, 79	0
15	CO	88/89 (98%)	-0.06	1 (1%)	80	64	59, 68, 76, 78	0
16	AP	84/88 (95%)	0.21	6 (7%)	16	6	62, 69, 77, 80	0
16	CP	84/88 (95%)	0.38	2 (2%)	59	37	59, 66, 75, 83	0
17	AQ	100/105 (95%)	0.17	2 (2%)	65	44	59, 68, 75, 76	0
17	CQ	100/105 (95%)	-0.05	0	100	100	58, 68, 76, 78	0
18	AR	70/88 (79%)	0.07	0	100	100	58, 69, 78, 85	0
18	CR	70/88 (79%)	0.50	4 (5%)	23	11	63, 69, 77, 82	0
19	AS	80/93 (86%)	0.40	5 (6%)	20	8	66, 76, 83, 86	0
19	CS	78/93 (83%)	0.60	9 (11%)	4	2	70, 76, 82, 84	0
20	AT	99/106 (93%)	0.28	6 (6%)	21	9	62, 71, 79, 83	0
20	CT	99/106 (93%)	0.25	5 (5%)	28	13	63, 69, 77, 83	0
21	AU	25/27 (92%)	1.11	5 (20%)	1	0	67, 74, 81, 83	0
21	CU	25/27 (92%)	1.48	6 (24%)	0	0	68, 77, 83, 85	0
22	AV	176/184 (95%)	-0.04	3 (1%)	70	49	51, 71, 79, 83	0
22	CV	176/184 (95%)	0.34	13 (7%)	14	5	58, 72, 80, 84	0
23	AW	77/77 (100%)	0.21	2 (2%)	56	33	45, 69, 81, 92	0
23	CW	77/77 (100%)	-0.18	0	100	100	58, 72, 83, 87	0
24	AX	5/5 (100%)	0.66	0	100	100	65, 65, 83, 88	0
24	CX	5/5 (100%)	0.65	1 (20%)	1	0	68, 70, 82, 88	0
25	BA	2767/2915 (94%)	0.07	48 (1%)	70	49	25, 53, 82, 97	0
25	DA	2777/2915 (95%)	0.13	58 (2%)	63	43	38, 65, 85, 97	0
26	BB	119/122 (97%)	-0.17	0	100	100	53, 67, 77, 86	0
26	DB	119/122 (97%)	0.18	3 (2%)	57	34	68, 77, 83, 92	0
27	BC	224/229 (97%)	0.52	17 (7%)	13	5	67, 76, 81, 86	1 (0%)
27	DC	220/229 (96%)	0.55	24 (10%)	5	2	66, 76, 82, 87	1 (0%)
28	BD	274/276 (99%)	-0.06	2 (0%)	87	75	38, 53, 65, 74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	DD	274/276 (99%)	0.08	7 (2%)	56	33	42, 59, 70, 77	0
29	BE	205/206 (99%)	-0.04	2 (0%)	82	67	38, 58, 73, 77	0
29	DE	205/206 (99%)	0.15	11 (5%)	25	12	46, 65, 78, 82	0
30	BF	208/210 (99%)	0.18	10 (4%)	30	14	35, 58, 78, 88	0
30	DF	208/210 (99%)	0.14	5 (2%)	59	37	52, 69, 78, 90	0
31	BG	181/182 (99%)	0.03	4 (2%)	62	41	60, 71, 79, 86	0
31	DG	181/182 (99%)	0.38	12 (6%)	18	7	65, 73, 81, 85	0
32	BH	168/180 (93%)	0.11	4 (2%)	59	37	25, 66, 75, 82	0
32	DH	160/180 (88%)	0.71	27 (16%)	1	0	66, 76, 82, 87	0
33	BI	146/148 (98%)	-0.14	2 (1%)	75	56	55, 71, 77, 84	0
33	DI	146/148 (98%)	0.03	3 (2%)	63	43	60, 73, 80, 83	0
34	BN	139/140 (99%)	-0.15	2 (1%)	75	56	46, 59, 72, 77	0
34	DN	139/140 (99%)	0.23	3 (2%)	62	41	60, 70, 77, 82	0
35	BO	122/122 (100%)	-0.18	0	100	100	44, 59, 70, 73	0
35	DO	122/122 (100%)	0.14	2 (1%)	72	51	50, 63, 71, 75	0
36	BP	146/150 (97%)	0.33	4 (2%)	54	31	40, 65, 76, 81	0
36	DP	146/150 (97%)	0.66	17 (11%)	4	2	52, 70, 78, 82	0
37	BQ	139/141 (98%)	-0.14	1 (0%)	87	75	45, 61, 71, 80	0
37	DQ	141/141 (100%)	0.15	5 (3%)	44	23	54, 69, 77, 83	0
38	BR	116/118 (98%)	-0.00	0	100	100	39, 57, 69, 74	0
38	DR	117/118 (99%)	0.11	0	100	100	50, 63, 73, 78	0
39	BS	101/112 (90%)	0.60	11 (10%)	5	2	49, 69, 74, 80	0
39	DS	99/112 (88%)	0.57	13 (13%)	3	1	63, 72, 79, 86	0
40	BT	138/146 (94%)	0.14	8 (5%)	23	10	52, 65, 79, 83	0
40	DT	138/146 (94%)	0.15	6 (4%)	35	17	56, 67, 81, 84	0
41	BU	117/118 (99%)	0.07	3 (2%)	56	33	41, 54, 68, 78	0
41	DU	117/118 (99%)	0.10	3 (2%)	56	33	55, 67, 76, 81	0
42	BV	101/101 (100%)	-0.15	1 (0%)	82	67	41, 60, 71, 75	0
42	DV	101/101 (100%)	0.37	3 (2%)	50	27	58, 74, 79, 85	0
43	BW	113/113 (100%)	-0.01	1 (0%)	84	69	44, 53, 70, 86	0
43	DW	113/113 (100%)	-0.02	1 (0%)	84	69	56, 64, 78, 87	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
44	BX	94/96 (97%)	0.01	0	100	100	42, 57, 69, 79	0
44	DX	93/96 (96%)	0.11	4 (4%)	35	17	53, 67, 73, 81	0
45	BY	101/110 (91%)	0.06	3 (2%)	50	27	51, 64, 77, 81	0
45	DY	101/110 (91%)	0.43	8 (7%)	12	5	63, 74, 82, 85	0
46	BZ	182/206 (88%)	-0.02	3 (1%)	72	51	56, 70, 78, 83	0
46	DZ	177/206 (85%)	0.47	14 (7%)	12	5	68, 76, 83, 87	0
47	B0	77/85 (90%)	0.15	2 (2%)	56	33	49, 59, 72, 81	0
47	D0	84/85 (98%)	0.43	6 (7%)	16	6	59, 68, 78, 84	0
48	B1	96/98 (97%)	-0.09	0	100	100	42, 60, 72, 77	0
48	D1	94/98 (95%)	0.32	6 (6%)	19	8	50, 64, 75, 78	0
49	B2	71/72 (98%)	-0.20	0	100	100	50, 61, 75, 80	0
49	D2	71/72 (98%)	-0.23	2 (2%)	53	30	60, 71, 79, 87	0
50	B3	59/60 (98%)	0.13	5 (8%)	10	4	45, 59, 71, 74	0
50	D3	60/60 (100%)	0.90	8 (13%)	3	1	62, 72, 82, 85	0
51	B4	31/71 (43%)	-0.06	1 (3%)	47	25	69, 75, 80, 86	0
51	D4	31/71 (43%)	0.23	2 (6%)	18	8	67, 74, 81, 84	0
52	B5	57/60 (95%)	-0.22	0	100	100	40, 55, 71, 73	0
52	D5	59/60 (98%)	0.33	5 (8%)	10	4	55, 68, 78, 86	0
53	B6	49/54 (90%)	0.53	8 (16%)	1	1	39, 65, 75, 75	0
53	D6	48/54 (88%)	0.06	3 (6%)	20	8	54, 66, 73, 78	0
54	B7	49/49 (100%)	-0.01	0	100	100	35, 46, 69, 76	0
54	D7	49/49 (100%)	0.76	4 (8%)	11	4	47, 58, 77, 83	0
55	B8	63/65 (96%)	0.11	2 (3%)	47	25	43, 56, 69, 75	0
55	D8	62/65 (95%)	0.33	5 (8%)	12	5	54, 62, 68, 76	0
56	B9	36/37 (97%)	0.45	5 (13%)	2	1	52, 59, 69, 71	0
56	D9	36/37 (97%)	0.30	1 (2%)	53	30	60, 69, 76, 82	0
All	All	21272/22210 (95%)	0.17	823 (3%)	39	20	25, 68, 82, 97	4 (0%)

The worst 5 of 823 RSRZ outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3022	1/1	0.18	2.25	205,205,205,205	0
57	MG	BA	3442	1/1	0.39	3.28	205,205,205,205	0
57	MG	BA	3139	1/1	0.43	0.88	72,72,72,72	0
57	MG	AA	1611	1/1	0.47	0.91	58,58,58,58	0
57	MG	CW	102	1/1	0.47	0.48	93,93,93,93	0
57	MG	DA	3072	1/1	0.48	0.53	72,72,72,72	0
57	MG	DA	3164	1/1	0.50	0.65	83,83,83,83	0
57	MG	BA	3332	1/1	0.55	0.17	61,61,61,61	0
57	MG	BA	3448	1/1	0.56	0.42	54,54,54,54	0
57	MG	DA	3255	1/1	0.56	0.31	46,46,46,46	0
57	MG	DA	3277	1/1	0.56	0.27	57,57,57,57	0
57	MG	BA	3323	1/1	0.59	1.30	205,205,205,205	0
57	MG	BA	3207	1/1	0.61	0.26	74,74,74,74	0
57	MG	DA	3151	1/1	0.63	0.30	43,43,43,43	0
57	MG	DA	3211	1/1	0.64	0.35	55,55,55,55	0
57	MG	BA	3118	1/1	0.64	2.55	205,205,205,205	0
57	MG	CA	1618	1/1	0.64	0.25	39,39,39,39	0
57	MG	BP	201	1/1	0.65	1.32	205,205,205,205	0
57	MG	DA	3175	1/1	0.66	0.50	56,56,56,56	0
57	MG	AA	1664	1/1	0.66	0.52	77,77,77,77	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3449	1/1	0.76	0.21	53,53,53,53	0
57	MG	AA	1622	1/1	0.76	0.22	36,36,36,36	0
57	MG	CA	1652	1/1	0.76	0.47	59,59,59,59	0
57	MG	DA	3246	1/1	0.76	0.33	43,43,43,43	0
57	MG	BA	3388	1/1	0.76	0.40	37,37,37,37	0
57	MG	BA	3424	1/1	0.76	0.16	26,26,26,26	0
57	MG	DA	3266	1/1	0.77	0.36	46,46,46,46	0
57	MG	BA	3431	1/1	0.77	0.38	53,53,53,53	0
57	MG	CA	1655	1/1	0.77	0.19	34,34,34,34	0
57	MG	BA	3344	1/1	0.77	0.22	24,24,24,24	0
57	MG	BA	3268	1/1	0.78	0.61	46,46,46,46	0
57	MG	DA	3123	1/1	0.78	0.24	25,25,25,25	0
57	MG	DA	3142	1/1	0.78	0.26	51,51,51,51	0
57	MG	AA	1637	1/1	0.78	0.36	45,45,45,45	0
57	MG	BA	3175	1/1	0.78	0.23	71,71,71,71	0
57	MG	AA	1709	1/1	0.78	0.21	66,66,66,66	0
57	MG	AA	1621	1/1	0.78	0.19	48,48,48,48	0
57	MG	BA	3029	1/1	0.78	0.14	40,40,40,40	0
57	MG	BA	3038	1/1	0.78	1.44	163,163,163,163	0
57	MG	BA	3258	1/1	0.78	0.27	39,39,39,39	0
57	MG	DB	208	1/1	0.78	0.48	48,48,48,48	0
57	MG	CA	1695	1/1	0.78	0.26	38,38,38,38	0
58	ZN	AD	301	1/1	0.78	0.59	192,192,192,192	0
57	MG	CA	1629	1/1	0.79	0.24	25,25,25,25	0
57	MG	CA	1649	1/1	0.79	0.29	65,65,65,65	0
57	MG	DA	3192	1/1	0.79	0.27	43,43,43,43	0
57	MG	DA	3094	1/1	0.79	0.43	71,71,71,71	0
57	MG	DA	3200	1/1	0.79	0.28	66,66,66,66	0
57	MG	AA	1647	1/1	0.79	0.22	45,45,45,45	0
57	MG	AA	1619	1/1	0.79	0.47	66,66,66,66	0
57	MG	DB	209	1/1	0.79	0.23	41,41,41,41	0
57	MG	BA	3143	1/1	0.79	0.32	31,31,31,31	0
57	MG	DA	3067	1/1	0.79	0.19	56,56,56,56	0
57	MG	DA	3042	1/1	0.80	0.33	28,28,28,28	0
57	MG	BA	3354	1/1	0.80	0.39	25,25,25,25	0
57	MG	AA	1602	1/1	0.80	0.33	77,77,77,77	0
57	MG	DA	3152	1/1	0.80	0.33	61,61,61,61	0
57	MG	BA	3374	1/1	0.80	0.23	51,51,51,51	0
57	MG	BA	3428	1/1	0.80	0.20	24,24,24,24	0
57	MG	DA	3280	1/1	0.80	0.12	44,44,44,44	0
57	MG	BA	3378	1/1	0.80	0.22	55,55,55,55	0
57	MG	BA	3300	1/1	0.80	0.53	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	BA	3264	1/1	0.80	0.30	34,34,34,34	0
57	MG	DA	3117	1/1	0.80	0.18	42,42,42,42	0
57	MG	DA	3121	1/1	0.80	0.30	57,57,57,57	0
57	MG	BA	3444	1/1	0.80	0.99	101,101,101,101	0
57	MG	CA	1643	1/1	0.80	0.17	44,44,44,44	0
57	MG	AA	1645	1/1	0.81	0.36	52,52,52,52	0
57	MG	BA	3015	1/1	0.81	0.45	21,21,21,21	0
57	MG	BA	3254	1/1	0.81	0.27	37,37,37,37	0
57	MG	BA	3169	1/1	0.81	0.16	21,21,21,21	0
57	MG	CA	1640	1/1	0.81	0.62	61,61,61,61	0
57	MG	AA	1674	1/1	0.81	0.22	49,49,49,49	0
57	MG	CA	1646	1/1	0.81	0.20	59,59,59,59	0
57	MG	DB	203	1/1	0.81	0.20	66,66,66,66	0
57	MG	AA	1618	1/1	0.81	0.21	64,64,64,64	0
57	MG	DA	3204	1/1	0.81	0.12	41,41,41,41	0
57	MG	BA	3425	1/1	0.81	0.17	55,55,55,55	0
57	MG	AA	1659	1/1	0.81	0.19	58,58,58,58	0
57	MG	DF	301	1/1	0.81	0.54	49,49,49,49	0
57	MG	CA	1670	1/1	0.81	0.40	43,43,43,43	0
57	MG	AA	1704	1/1	0.82	0.15	64,64,64,64	0
57	MG	BA	3349	1/1	0.82	0.24	38,38,38,38	0
57	MG	BA	3153	1/1	0.82	0.14	42,42,42,42	0
57	MG	BA	3194	1/1	0.82	0.08	72,72,72,72	0
57	MG	BA	3361	1/1	0.82	0.24	31,31,31,31	0
57	MG	BA	3095	1/1	0.82	0.27	45,45,45,45	0
57	MG	BA	3434	1/1	0.82	0.29	28,28,28,28	0
57	MG	BA	3223	1/1	0.82	0.24	49,49,49,49	0
57	MG	BA	3236	1/1	0.82	0.27	62,62,62,62	0
57	MG	BA	3383	1/1	0.82	0.20	48,48,48,48	0
57	MG	BA	3239	1/1	0.82	0.24	46,46,46,46	0
57	MG	AA	1603	1/1	0.82	0.11	18,18,18,18	0
57	MG	BA	3459	1/1	0.83	0.18	35,35,35,35	0
57	MG	BA	3191	1/1	0.83	0.13	40,40,40,40	0
57	MG	DA	3269	1/1	0.83	0.27	47,47,47,47	0
57	MG	BA	3238	1/1	0.83	0.43	20,20,20,20	0
57	MG	DA	3045	1/1	0.83	0.26	59,59,59,59	0
57	MG	BA	3385	1/1	0.83	0.14	54,54,54,54	0
57	MG	DA	3297	1/1	0.83	0.17	48,48,48,48	0
57	MG	DA	3298	1/1	0.83	0.15	33,33,33,33	0
57	MG	BA	3292	1/1	0.83	0.43	24,24,24,24	0
57	MG	AA	1711	1/1	0.83	0.24	58,58,58,58	0
57	MG	BA	3180	1/1	0.83	0.31	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	AA	1657	1/1	0.83	0.16	54,54,54,54	0
57	MG	BA	3226	1/1	0.83	0.38	31,31,31,31	0
57	MG	DA	3248	1/1	0.83	0.21	36,36,36,36	0
57	MG	DA	3254	1/1	0.83	0.41	60,60,60,60	0
57	MG	DA	3161	1/1	0.83	0.78	50,50,50,50	0
57	MG	DA	3256	1/1	0.83	0.27	62,62,62,62	0
57	MG	DA	3282	1/1	0.84	0.24	65,65,65,65	0
57	MG	DA	3069	1/1	0.84	0.47	30,30,30,30	0
57	MG	DA	3149	1/1	0.84	0.49	38,38,38,38	0
57	MG	BA	3001	1/1	0.84	0.17	50,50,50,50	0
57	MG	DB	201	1/1	0.84	0.23	53,53,53,53	0
57	MG	BA	3195	1/1	0.84	0.20	47,47,47,47	0
57	MG	DA	3198	1/1	0.84	0.23	31,31,31,31	0
57	MG	BA	3190	1/1	0.84	0.21	34,34,34,34	0
57	MG	BA	3211	1/1	0.84	0.27	38,38,38,38	0
57	MG	DA	3129	1/1	0.84	0.23	47,47,47,47	0
57	MG	DA	3276	1/1	0.84	0.21	51,51,51,51	0
57	MG	DA	3220	1/1	0.84	0.35	31,31,31,31	0
57	MG	AA	1687	1/1	0.84	0.29	44,44,44,44	0
57	MG	AA	1686	1/1	0.85	0.15	42,42,42,42	0
57	MG	BA	3129	1/1	0.85	0.18	25,25,25,25	0
57	MG	CA	1602	1/1	0.85	0.19	35,35,35,35	0
57	MG	CA	1681	1/1	0.85	0.18	44,44,44,44	0
57	MG	AA	1636	1/1	0.85	0.17	62,62,62,62	0
57	MG	DA	3169	1/1	0.85	0.40	18,18,18,18	0
57	MG	AA	1654	1/1	0.85	0.26	29,29,29,29	0
57	MG	BA	3178	1/1	0.85	0.27	22,22,22,22	0
57	MG	DA	3185	1/1	0.85	0.37	37,37,37,37	0
57	MG	CA	1627	1/1	0.85	0.18	24,24,24,24	0
57	MG	BA	3408	1/1	0.85	0.43	57,57,57,57	0
57	MG	CW	105	1/1	0.85	0.33	61,61,61,61	0
57	MG	DA	3302	1/1	0.85	0.34	36,36,36,36	0
57	MG	DA	3010	1/1	0.85	0.41	66,66,66,66	0
57	MG	DA	3020	1/1	0.85	0.35	23,23,23,23	0
57	MG	BA	3446	1/1	0.85	0.69	60,60,60,60	0
57	MG	DA	3143	1/1	0.85	0.21	23,23,23,23	0
57	MG	DA	3227	1/1	0.85	0.35	37,37,37,37	0
57	MG	AA	1605	1/1	0.85	0.18	51,51,51,51	0
57	MG	BA	3381	1/1	0.85	0.43	66,66,66,66	0
57	MG	DA	3150	1/1	0.85	0.27	21,21,21,21	0
57	MG	BA	3427	1/1	0.85	0.18	40,40,40,40	0
57	MG	BA	3151	1/1	0.86	0.41	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BU	201	1/1	0.86	0.35	21,21,21,21	0
57	MG	CA	1672	1/1	0.86	0.23	29,29,29,29	0
57	MG	B0	101	1/1	0.86	0.38	30,30,30,30	0
57	MG	BA	3257	1/1	0.86	0.24	41,41,41,41	0
57	MG	AA	1661	1/1	0.86	0.22	67,67,67,67	0
57	MG	BA	3342	1/1	0.86	0.13	22,22,22,22	0
57	MG	DA	3278	1/1	0.86	0.27	59,59,59,59	0
57	MG	DA	3190	1/1	0.86	0.22	44,44,44,44	0
57	MG	BA	3262	1/1	0.86	0.51	32,32,32,32	0
57	MG	DA	3288	1/1	0.86	0.26	60,60,60,60	0
57	MG	BA	3346	1/1	0.86	0.50	50,50,50,50	0
57	MG	CA	1620	1/1	0.86	0.52	29,29,29,29	0
57	MG	AA	1617	1/1	0.86	0.27	43,43,43,43	0
57	MG	DA	3203	1/1	0.86	0.21	52,52,52,52	0
57	MG	BA	3014	1/1	0.86	0.37	24,24,24,24	0
57	MG	DA	3025	1/1	0.86	0.18	38,38,38,38	0
57	MG	DA	3028	1/1	0.86	0.14	34,34,34,34	0
57	MG	BA	3403	1/1	0.86	0.24	48,48,48,48	0
57	MG	DA	3245	1/1	0.86	0.28	52,52,52,52	0
57	MG	AA	1633	1/1	0.86	0.11	36,36,36,36	0
57	MG	BA	3251	1/1	0.86	0.27	23,23,23,23	0
57	MG	BA	3458	1/1	0.86	0.47	47,47,47,47	0
57	MG	D5	101	1/1	0.86	0.20	38,38,38,38	0
57	MG	BA	3372	1/1	0.86	0.25	59,59,59,59	0
57	MG	DA	3223	1/1	0.87	0.24	32,32,32,32	0
57	MG	BA	3390	1/1	0.87	0.20	48,48,48,48	0
57	MG	DA	3132	1/1	0.87	0.39	32,32,32,32	0
57	MG	CA	1635	1/1	0.87	0.25	22,22,22,22	0
57	MG	DA	3021	1/1	0.87	0.26	34,34,34,34	0
57	MG	CA	1638	1/1	0.87	0.39	35,35,35,35	0
57	MG	DA	3026	1/1	0.87	0.09	33,33,33,33	0
57	MG	BA	3270	1/1	0.87	0.31	43,43,43,43	0
57	MG	DA	3261	1/1	0.87	0.21	58,58,58,58	0
57	MG	BA	3243	1/1	0.87	0.27	51,51,51,51	0
57	MG	BA	3456	1/1	0.87	0.26	43,43,43,43	0
57	MG	DA	3044	1/1	0.87	0.42	69,69,69,69	0
57	MG	DA	3158	1/1	0.87	0.36	44,44,44,44	0
57	MG	DA	3273	1/1	0.87	0.30	55,55,55,55	0
57	MG	BA	3296	1/1	0.87	0.18	25,25,25,25	0
57	MG	DA	3049	1/1	0.87	0.25	15,15,15,15	0
57	MG	DA	3165	1/1	0.87	0.14	43,43,43,43	0
57	MG	BA	3204	1/1	0.87	0.45	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3412	1/1	0.87	0.27	35,35,35,35	0
57	MG	BA	3373	1/1	0.87	0.21	31,31,31,31	0
57	MG	AA	1646	1/1	0.87	0.15	49,49,49,49	0
57	MG	DA	3073	1/1	0.87	0.45	49,49,49,49	0
57	MG	DA	3088	1/1	0.87	0.20	20,20,20,20	0
57	MG	AA	1679	1/1	0.87	0.26	56,56,56,56	0
57	MG	BA	3092	1/1	0.87	0.34	36,36,36,36	0
57	MG	CA	1687	1/1	0.87	0.17	37,37,37,37	0
57	MG	BA	3380	1/1	0.87	0.31	37,37,37,37	0
57	MG	BA	3136	1/1	0.87	0.93	76,76,76,76	0
57	MG	AA	1685	1/1	0.87	0.29	42,42,42,42	0
57	MG	DA	3205	1/1	0.87	0.32	55,55,55,55	0
57	MG	DA	3208	1/1	0.87	0.09	59,59,59,59	0
57	MG	AA	1665	1/1	0.87	0.38	63,63,63,63	0
57	MG	DA	3213	1/1	0.87	0.17	28,28,28,28	0
57	MG	D6	101	1/1	0.87	0.26	57,57,57,57	0
57	MG	BA	3199	1/1	0.87	0.32	23,23,23,23	0
57	MG	CA	1680	1/1	0.88	0.18	31,31,31,31	0
57	MG	BA	3124	1/1	0.88	0.21	41,41,41,41	0
57	MG	AA	1609	1/1	0.88	0.21	48,48,48,48	0
57	MG	BA	3091	1/1	0.88	0.44	21,21,21,21	0
57	MG	DA	3081	1/1	0.88	0.25	37,37,37,37	0
57	MG	AA	1681	1/1	0.88	0.29	63,63,63,63	0
57	MG	DA	3177	1/1	0.88	0.48	52,52,52,52	0
57	MG	BA	3440	1/1	0.88	0.46	64,64,64,64	0
57	MG	BA	3093	1/1	0.88	0.17	23,23,23,23	0
57	MG	BA	3284	1/1	0.88	0.17	15,15,15,15	0
57	MG	BA	3290	1/1	0.88	0.22	22,22,22,22	0
57	MG	CA	1632	1/1	0.88	0.42	18,18,18,18	0
57	MG	DA	3016	1/1	0.88	0.44	24,24,24,24	0
57	MG	DA	3283	1/1	0.88	0.19	62,62,62,62	0
57	MG	DA	3286	1/1	0.88	0.27	52,52,52,52	0
57	MG	DA	3287	1/1	0.88	0.31	48,48,48,48	0
57	MG	AA	1706	1/1	0.88	0.12	47,47,47,47	0
57	MG	BA	3366	1/1	0.88	0.32	49,49,49,49	0
57	MG	DA	3125	1/1	0.88	0.27	26,26,26,26	0
57	MG	BA	3100	1/1	0.88	0.55	28,28,28,28	0
57	MG	BA	3253	1/1	0.88	0.54	41,41,41,41	0
57	MG	BA	3418	1/1	0.88	0.21	31,31,31,31	0
57	MG	DA	3031	1/1	0.88	0.26	24,24,24,24	0
57	MG	DA	3218	1/1	0.88	0.20	35,35,35,35	0
57	MG	BB	203	1/1	0.88	0.31	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3062	1/1	0.88	0.11	19,19,19,19	0
57	MG	DA	3043	1/1	0.88	0.23	39,39,39,39	0
57	MG	DA	3237	1/1	0.88	0.24	33,33,33,33	0
57	MG	BQ	203	1/1	0.88	0.21	27,27,27,27	0
57	MG	BA	3320	1/1	0.88	0.28	25,25,25,25	0
57	MG	BA	3224	1/1	0.88	0.31	31,31,31,31	0
57	MG	CA	1678	1/1	0.88	0.22	25,25,25,25	0
57	MG	BA	3013	1/1	0.89	0.16	56,56,56,56	0
57	MG	DA	3226	1/1	0.89	0.35	32,32,32,32	0
57	MG	CA	1603	1/1	0.89	0.21	49,49,49,49	0
57	MG	DA	3232	1/1	0.89	0.28	40,40,40,40	0
57	MG	CW	103	1/1	0.89	0.34	27,27,27,27	0
57	MG	BA	3301	1/1	0.89	0.22	33,33,33,33	0
57	MG	DA	3136	1/1	0.89	0.16	22,22,22,22	0
57	MG	DA	3001	1/1	0.89	0.32	61,61,61,61	0
57	MG	DA	3251	1/1	0.89	0.31	53,53,53,53	0
57	MG	CA	1605	1/1	0.89	0.42	62,62,62,62	0
57	MG	DA	3014	1/1	0.89	0.24	44,44,44,44	0
57	MG	BA	3311	1/1	0.89	0.18	31,31,31,31	0
57	MG	BA	3430	1/1	0.89	0.35	58,58,58,58	0
57	MG	AA	1632	1/1	0.89	0.44	57,57,57,57	0
57	MG	BA	3212	1/1	0.89	0.42	30,30,30,30	0
57	MG	BA	3218	1/1	0.89	0.39	23,23,23,23	0
57	MG	BA	3163	1/1	0.89	0.17	21,21,21,21	0
57	MG	BA	3384	1/1	0.89	0.25	42,42,42,42	0
57	MG	DA	3274	1/1	0.89	0.25	36,36,36,36	0
57	MG	BA	3111	1/1	0.89	0.15	20,20,20,20	0
57	MG	DA	3038	1/1	0.89	0.47	49,49,49,49	0
57	MG	BA	3445	1/1	0.89	0.14	36,36,36,36	0
57	MG	DA	3279	1/1	0.89	0.25	43,43,43,43	0
57	MG	BA	3171	1/1	0.89	0.44	41,41,41,41	0
57	MG	CA	1644	1/1	0.89	0.39	30,30,30,30	0
57	MG	DA	3176	1/1	0.89	0.32	24,24,24,24	0
57	MG	BA	3230	1/1	0.89	0.29	34,34,34,34	0
57	MG	BA	3232	1/1	0.89	0.43	38,38,38,38	0
57	MG	BA	3116	1/1	0.89	0.11	23,23,23,23	0
57	MG	DA	3291	1/1	0.89	0.23	31,31,31,31	0
57	MG	BA	3406	1/1	0.89	0.15	50,50,50,50	0
57	MG	CA	1660	1/1	0.89	0.41	22,22,22,22	0
57	MG	CA	1663	1/1	0.89	0.19	33,33,33,33	0
57	MG	CA	1665	1/1	0.89	0.25	30,30,30,30	0
57	MG	BA	3198	1/1	0.89	0.16	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	1675	1/1	0.89	0.18	50,50,50,50	0
57	MG	BB	209	1/1	0.89	0.12	37,37,37,37	0
57	MG	AA	1703	1/1	0.89	0.15	51,51,51,51	0
57	MG	BA	3417	1/1	0.89	0.24	62,62,62,62	0
57	MG	BA	3368	1/1	0.89	0.42	49,49,49,49	0
57	MG	BA	3421	1/1	0.89	0.16	32,32,32,32	0
57	MG	DA	3215	1/1	0.89	0.35	37,37,37,37	0
57	MG	B0	102	1/1	0.89	0.23	33,33,33,33	0
57	MG	BA	3248	1/1	0.89	0.31	34,34,34,34	0
57	MG	DA	3222	1/1	0.89	0.31	26,26,26,26	0
57	MG	BA	3281	1/1	0.90	0.25	29,29,29,29	0
57	MG	CA	1623	1/1	0.90	0.33	59,59,59,59	0
57	MG	DA	3194	1/1	0.90	0.21	61,61,61,61	0
57	MG	CA	1626	1/1	0.90	0.54	67,67,67,67	0
57	MG	AL	201	1/1	0.90	0.38	29,29,29,29	0
57	MG	BA	3233	1/1	0.90	0.69	53,53,53,53	0
57	MG	DA	3201	1/1	0.90	0.45	32,32,32,32	0
57	MG	BA	3370	1/1	0.90	0.10	48,48,48,48	0
57	MG	CA	1634	1/1	0.90	0.10	37,37,37,37	0
57	MG	BA	3291	1/1	0.90	0.34	24,24,24,24	0
57	MG	DA	3050	1/1	0.90	0.40	46,46,46,46	0
57	MG	DA	3061	1/1	0.90	0.25	22,22,22,22	0
57	MG	DA	3065	1/1	0.90	0.35	29,29,29,29	0
57	MG	BA	3157	1/1	0.90	0.15	38,38,38,38	0
57	MG	BA	3438	1/1	0.90	0.22	67,67,67,67	0
57	MG	BA	3294	1/1	0.90	0.33	29,29,29,29	0
57	MG	BA	3196	1/1	0.90	0.16	27,27,27,27	0
57	MG	BA	3123	1/1	0.90	0.25	43,43,43,43	0
57	MG	BA	3166	1/1	0.90	0.56	38,38,38,38	0
57	MG	BA	3028	1/1	0.90	0.22	29,29,29,29	0
57	MG	BA	3382	1/1	0.90	0.23	26,26,26,26	0
57	MG	DA	3098	1/1	0.90	0.40	32,32,32,32	0
57	MG	DA	3238	1/1	0.90	0.23	33,33,33,33	0
57	MG	DA	3101	1/1	0.90	0.23	35,35,35,35	0
57	MG	CA	1658	1/1	0.90	0.17	21,21,21,21	0
57	MG	BA	3315	1/1	0.90	0.16	17,17,17,17	0
57	MG	DA	3110	1/1	0.90	0.33	38,38,38,38	0
57	MG	CA	1661	1/1	0.90	0.26	26,26,26,26	0
57	MG	DA	3112	1/1	0.90	0.27	27,27,27,27	0
57	MG	BA	3450	1/1	0.90	0.41	44,44,44,44	0
57	MG	DA	3119	1/1	0.90	0.24	42,42,42,42	0
57	MG	BA	3205	1/1	0.90	0.10	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3318	1/1	0.90	0.39	41,41,41,41	0
57	MG	BA	3387	1/1	0.90	0.26	46,46,46,46	0
57	MG	AA	1701	1/1	0.90	0.32	33,33,33,33	0
57	MG	DA	3272	1/1	0.90	0.21	40,40,40,40	0
57	MG	BB	207	1/1	0.90	0.17	44,44,44,44	0
57	MG	DA	3131	1/1	0.90	0.31	39,39,39,39	0
57	MG	AA	1713	1/1	0.90	0.14	43,43,43,43	0
57	MG	BF	301	1/1	0.90	0.26	62,62,62,62	0
57	MG	DA	3137	1/1	0.90	0.20	30,30,30,30	0
57	MG	BA	3329	1/1	0.90	0.07	26,26,26,26	0
57	MG	AA	1715	1/1	0.90	0.14	62,62,62,62	0
57	MG	DA	3281	1/1	0.90	0.10	49,49,49,49	0
57	MG	CA	1700	1/1	0.90	0.30	56,56,56,56	0
57	MG	CA	1707	1/1	0.90	0.62	62,62,62,62	0
57	MG	BR	201	1/1	0.90	0.43	35,35,35,35	0
57	MG	BA	3217	1/1	0.90	0.23	34,34,34,34	0
57	MG	BA	3097	1/1	0.90	0.40	34,34,34,34	0
57	MG	DA	3290	1/1	0.90	0.55	50,50,50,50	0
57	MG	AA	1717	1/1	0.90	0.27	25,25,25,25	0
57	MG	DA	3293	1/1	0.90	0.23	39,39,39,39	0
57	MG	DA	3155	1/1	0.90	0.06	60,60,60,60	0
57	MG	CW	104	1/1	0.90	0.39	52,52,52,52	0
57	MG	DA	3299	1/1	0.90	0.15	42,42,42,42	0
57	MG	B5	103	1/1	0.90	0.18	20,20,20,20	0
57	MG	BA	3347	1/1	0.90	0.15	28,28,28,28	0
57	MG	BA	3141	1/1	0.90	0.30	45,45,45,45	0
57	MG	BA	3074	1/1	0.90	0.38	31,31,31,31	0
57	MG	BA	3077	1/1	0.90	0.82	63,63,63,63	0
57	MG	BA	3422	1/1	0.90	0.45	20,20,20,20	0
57	MG	BA	3358	1/1	0.90	0.15	38,38,38,38	0
57	MG	CA	1612	1/1	0.90	0.36	55,55,55,55	0
57	MG	DA	3178	1/1	0.90	0.09	30,30,30,30	0
57	MG	DA	3182	1/1	0.90	0.15	37,37,37,37	0
57	MG	CA	1613	1/1	0.90	0.43	42,42,42,42	0
57	MG	BA	3359	1/1	0.90	0.28	44,44,44,44	0
57	MG	DA	3187	1/1	0.90	0.33	48,48,48,48	0
57	MG	BA	3265	1/1	0.91	0.12	67,67,67,67	0
57	MG	DA	3207	1/1	0.91	0.12	26,26,26,26	0
57	MG	BA	3357	1/1	0.91	0.19	38,38,38,38	0
57	MG	CA	1689	1/1	0.91	0.18	39,39,39,39	0
57	MG	DA	3109	1/1	0.91	0.12	33,33,33,33	0
57	MG	DA	3214	1/1	0.91	0.34	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CA	1694	1/1	0.91	0.74	51,51,51,51	0
57	MG	DA	3217	1/1	0.91	0.57	54,54,54,54	0
57	MG	BA	3017	1/1	0.91	0.27	20,20,20,20	0
57	MG	CA	1698	1/1	0.91	0.18	33,33,33,33	0
57	MG	BA	3021	1/1	0.91	1.61	180,180,180,180	0
57	MG	CA	1703	1/1	0.91	0.41	34,34,34,34	0
57	MG	AA	1626	1/1	0.91	0.24	35,35,35,35	0
57	MG	CA	1609	1/1	0.91	0.29	27,27,27,27	0
57	MG	DA	3231	1/1	0.91	0.38	45,45,45,45	0
57	MG	BA	3025	1/1	0.91	0.35	31,31,31,31	0
57	MG	AA	1669	1/1	0.91	0.21	70,70,70,70	0
57	MG	BA	3167	1/1	0.91	0.32	65,65,65,65	0
57	MG	DA	3241	1/1	0.91	0.10	26,26,26,26	0
57	MG	AA	1650	1/1	0.91	0.16	28,28,28,28	0
57	MG	BA	3437	1/1	0.91	0.10	27,27,27,27	0
57	MG	DA	3133	1/1	0.91	0.16	31,31,31,31	0
57	MG	DA	3249	1/1	0.91	0.14	33,33,33,33	0
57	MG	DA	3135	1/1	0.91	0.26	42,42,42,42	0
57	MG	CA	1625	1/1	0.91	0.33	31,31,31,31	0
57	MG	DA	3003	1/1	0.91	0.18	30,30,30,30	0
57	MG	BA	3036	1/1	0.91	0.20	30,30,30,30	0
57	MG	AA	1653	1/1	0.91	0.24	28,28,28,28	0
57	MG	BA	3376	1/1	0.91	0.16	33,33,33,33	0
57	MG	BA	3051	1/1	0.91	0.44	51,51,51,51	0
57	MG	DA	3268	1/1	0.91	0.19	43,43,43,43	0
57	MG	BA	3002	1/1	0.91	0.18	39,39,39,39	0
57	MG	DA	3024	1/1	0.91	0.13	33,33,33,33	0
57	MG	BA	3053	1/1	0.91	0.47	63,63,63,63	0
57	MG	BA	3313	1/1	0.91	0.37	26,26,26,26	0
57	MG	BA	3184	1/1	0.91	0.25	53,53,53,53	0
57	MG	DA	3157	1/1	0.91	0.25	30,30,30,30	0
57	MG	DA	3030	1/1	0.91	0.14	46,46,46,46	0
57	MG	DA	3160	1/1	0.91	0.30	38,38,38,38	0
57	MG	BA	3060	1/1	0.91	0.38	47,47,47,47	0
57	MG	BA	3242	1/1	0.91	0.26	24,24,24,24	0
57	MG	DA	3037	1/1	0.91	0.42	45,45,45,45	0
57	MG	CA	1645	1/1	0.91	0.28	41,41,41,41	0
57	MG	DA	3167	1/1	0.91	0.44	38,38,38,38	0
57	MG	DA	3040	1/1	0.91	0.35	26,26,26,26	0
57	MG	DA	3171	1/1	0.91	0.47	27,27,27,27	0
57	MG	DA	3172	1/1	0.91	0.15	30,30,30,30	0
57	MG	DA	3174	1/1	0.91	0.55	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	BA	3126	1/1	0.91	0.30	66,66,66,66	0
57	MG	CA	1647	1/1	0.91	0.28	61,61,61,61	0
57	MG	BA	3322	1/1	0.91	0.34	29,29,29,29	0
57	MG	CA	1651	1/1	0.91	0.18	28,28,28,28	0
57	MG	BA	3127	1/1	0.91	0.24	30,30,30,30	0
57	MG	BA	3328	1/1	0.91	0.24	32,32,32,32	0
57	MG	DA	3301	1/1	0.91	0.11	33,33,33,33	0
57	MG	CA	1657	1/1	0.91	0.12	37,37,37,37	0
57	MG	DA	3303	1/1	0.91	0.23	54,54,54,54	0
57	MG	DA	3304	1/1	0.91	0.12	35,35,35,35	0
57	MG	AA	1678	1/1	0.91	0.10	33,33,33,33	0
57	MG	BA	3331	1/1	0.91	0.27	28,28,28,28	0
57	MG	BA	3064	1/1	0.91	0.40	44,44,44,44	0
57	MG	AA	1691	1/1	0.91	0.14	39,39,39,39	0
57	MG	BA	3197	1/1	0.91	0.34	20,20,20,20	0
57	MG	AA	1607	1/1	0.91	0.25	51,51,51,51	0
57	MG	DA	3199	1/1	0.91	0.23	67,67,67,67	0
57	MG	BA	3414	1/1	0.91	0.36	36,36,36,36	0
57	MG	DP	201	1/1	0.91	0.15	38,38,38,38	0
57	MG	BA	3016	1/1	0.91	0.48	20,20,20,20	0
57	MG	BA	3088	1/1	0.91	0.28	24,24,24,24	0
57	MG	BA	3148	1/1	0.91	0.23	64,64,64,64	0
57	MG	BA	3057	1/1	0.92	0.41	39,39,39,39	0
57	MG	BA	3235	1/1	0.92	0.26	51,51,51,51	0
57	MG	DA	3196	1/1	0.92	0.31	26,26,26,26	0
57	MG	AA	1716	1/1	0.92	0.11	31,31,31,31	0
57	MG	AA	1649	1/1	0.92	0.29	50,50,50,50	0
57	MG	BA	3326	1/1	0.92	0.17	21,21,21,21	0
57	MG	DA	3048	1/1	0.92	0.24	6,6,6,6	0
57	MG	AA	1625	1/1	0.92	0.20	37,37,37,37	0
57	MG	BA	3240	1/1	0.92	0.22	23,23,23,23	0
57	MG	DA	3059	1/1	0.92	0.24	26,26,26,26	0
57	MG	BA	3066	1/1	0.92	0.20	14,14,14,14	0
57	MG	BA	3426	1/1	0.92	0.11	26,26,26,26	0
57	MG	BA	3069	1/1	0.92	0.27	30,30,30,30	0
57	MG	BA	3187	1/1	0.92	0.41	45,45,45,45	0
57	MG	BA	3343	1/1	0.92	0.19	22,22,22,22	0
57	MG	BA	3071	1/1	0.92	0.34	25,25,25,25	0
57	MG	BA	3345	1/1	0.92	0.29	34,34,34,34	0
57	MG	DA	3080	1/1	0.92	0.28	24,24,24,24	0
57	MG	BA	3433	1/1	0.92	0.50	52,52,52,52	0
57	MG	DA	3087	1/1	0.92	0.39	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3024	1/1	0.92	0.34	20,20,20,20	0
57	MG	CA	1654	1/1	0.92	0.13	17,17,17,17	0
57	MG	BA	3252	1/1	0.92	0.14	25,25,25,25	0
57	MG	DA	3228	1/1	0.92	0.22	25,25,25,25	0
57	MG	DA	3099	1/1	0.92	0.43	23,23,23,23	0
57	MG	AW	101	1/1	0.92	0.19	6,6,6,6	0
57	MG	DA	3233	1/1	0.92	0.17	17,17,17,17	0
57	MG	DA	3234	1/1	0.92	0.30	33,33,33,33	0
57	MG	DA	3235	1/1	0.92	0.15	24,24,24,24	0
57	MG	BA	3439	1/1	0.92	0.17	32,32,32,32	0
57	MG	BA	3350	1/1	0.92	0.19	37,37,37,37	0
57	MG	DA	3239	1/1	0.92	0.23	32,32,32,32	0
57	MG	DA	3240	1/1	0.92	0.14	35,35,35,35	0
57	MG	BA	3352	1/1	0.92	0.27	22,22,22,22	0
57	MG	BA	3353	1/1	0.92	0.36	36,36,36,36	0
57	MG	CA	1664	1/1	0.92	0.28	42,42,42,42	0
57	MG	BA	3193	1/1	0.92	0.12	47,47,47,47	0
57	MG	AA	1616	1/1	0.92	0.27	30,30,30,30	0
57	MG	DA	3250	1/1	0.92	0.38	26,26,26,26	0
57	MG	BA	3087	1/1	0.92	0.35	23,23,23,23	0
57	MG	BA	3140	1/1	0.92	0.13	33,33,33,33	0
57	MG	AA	1688	1/1	0.92	0.16	56,56,56,56	0
57	MG	BA	3453	1/1	0.92	0.20	41,41,41,41	0
57	MG	DA	3259	1/1	0.92	0.20	47,47,47,47	0
57	MG	CA	1685	1/1	0.92	0.13	33,33,33,33	0
57	MG	BA	3009	1/1	0.92	0.20	16,16,16,16	0
57	MG	BA	3037	1/1	0.92	0.23	9,9,9,9	0
57	MG	BA	3269	1/1	0.92	0.25	27,27,27,27	0
57	MG	CA	1690	1/1	0.92	0.25	44,44,44,44	0
57	MG	CA	1692	1/1	0.92	0.17	48,48,48,48	0
57	MG	BA	3369	1/1	0.92	0.13	63,63,63,63	0
57	MG	AA	1660	1/1	0.92	0.23	31,31,31,31	0
57	MG	DA	3139	1/1	0.92	0.17	58,58,58,58	0
57	MG	BA	3277	1/1	0.92	0.24	29,29,29,29	0
57	MG	BA	3280	1/1	0.92	0.17	19,19,19,19	0
57	MG	CA	1702	1/1	0.92	0.32	29,29,29,29	0
57	MG	BA	3152	1/1	0.92	0.22	23,23,23,23	0
57	MG	CA	1706	1/1	0.92	0.23	59,59,59,59	0
57	MG	BA	3044	1/1	0.92	0.30	22,22,22,22	0
57	MG	BA	3288	1/1	0.92	0.19	18,18,18,18	0
57	MG	DA	3153	1/1	0.92	0.15	41,41,41,41	0
57	MG	BA	3289	1/1	0.92	0.31	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CW	101	1/1	0.92	0.24	22,22,22,22	0
57	MG	BA	3155	1/1	0.92	0.55	37,37,37,37	0
57	MG	AA	1673	1/1	0.92	0.12	40,40,40,40	0
57	MG	B5	102	1/1	0.92	0.38	40,40,40,40	0
57	MG	BA	3215	1/1	0.92	0.20	35,35,35,35	0
57	MG	BA	3158	1/1	0.92	0.28	37,37,37,37	0
57	MG	BA	3162	1/1	0.92	0.10	21,21,21,21	0
57	MG	BA	3297	1/1	0.92	0.23	21,21,21,21	0
57	MG	AA	1684	1/1	0.92	0.13	31,31,31,31	0
57	MG	BA	3107	1/1	0.92	0.13	40,40,40,40	0
57	MG	BA	3306	1/1	0.92	0.33	47,47,47,47	0
57	MG	BA	3394	1/1	0.92	0.12	28,28,28,28	0
57	MG	DA	3023	1/1	0.92	0.23	42,42,42,42	0
57	MG	BA	3395	1/1	0.92	0.46	39,39,39,39	0
57	MG	BA	3310	1/1	0.92	0.19	30,30,30,30	0
57	MG	CA	1615	1/1	0.92	0.37	63,63,63,63	0
57	MG	CA	1616	1/1	0.92	0.16	20,20,20,20	0
57	MG	DA	3180	1/1	0.92	0.30	49,49,49,49	0
57	MG	AA	1702	1/1	0.92	0.11	26,26,26,26	0
57	MG	CA	1619	1/1	0.92	0.15	34,34,34,34	0
57	MG	DA	3032	1/1	0.92	0.23	20,20,20,20	0
57	MG	BA	3113	1/1	0.92	0.37	32,32,32,32	0
57	MG	DA	3189	1/1	0.92	0.20	34,34,34,34	0
57	MG	BA	3231	1/1	0.92	0.38	54,54,54,54	0
57	MG	BA	3170	1/1	0.92	0.18	40,40,40,40	0
57	MG	AW	102	1/1	0.93	0.09	26,26,26,26	0
57	MG	AA	1648	1/1	0.93	0.14	40,40,40,40	0
57	MG	CA	1621	1/1	0.93	0.18	22,22,22,22	0
57	MG	CA	1622	1/1	0.93	0.31	24,24,24,24	0
57	MG	CA	1704	1/1	0.93	0.17	26,26,26,26	0
57	MG	DA	3116	1/1	0.93	0.35	33,33,33,33	0
57	MG	AA	1710	1/1	0.93	0.11	30,30,30,30	0
57	MG	CA	1624	1/1	0.93	0.60	39,39,39,39	0
57	MG	DA	3225	1/1	0.93	0.31	44,44,44,44	0
57	MG	BA	3181	1/1	0.93	0.56	19,19,19,19	0
57	MG	BA	3227	1/1	0.93	0.29	21,21,21,21	0
57	MG	BA	3182	1/1	0.93	0.45	27,27,27,27	0
57	MG	BA	3027	1/1	0.93	0.19	26,26,26,26	0
57	MG	BA	3447	1/1	0.93	0.42	27,27,27,27	0
57	MG	DA	3130	1/1	0.93	0.37	34,34,34,34	0
57	MG	BA	3336	1/1	0.93	0.16	29,29,29,29	0
57	MG	BA	3339	1/1	0.93	0.29	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CX	101	1/1	0.93	0.20	22,22,22,22	0
57	MG	CA	1637	1/1	0.93	0.15	26,26,26,26	0
57	MG	BA	3105	1/1	0.93	0.16	15,15,15,15	0
57	MG	CA	1639	1/1	0.93	0.11	22,22,22,22	0
57	MG	BA	3149	1/1	0.93	0.28	27,27,27,27	0
57	MG	DA	3244	1/1	0.93	0.31	26,26,26,26	0
57	MG	DA	3140	1/1	0.93	0.24	36,36,36,36	0
57	MG	DA	3141	1/1	0.93	0.19	25,25,25,25	0
57	MG	CA	1642	1/1	0.93	0.13	37,37,37,37	0
57	MG	DA	3017	1/1	0.93	0.39	21,21,21,21	0
57	MG	BA	3005	1/1	0.93	0.20	23,23,23,23	0
57	MG	DA	3147	1/1	0.93	0.50	18,18,18,18	0
57	MG	DA	3252	1/1	0.93	0.52	27,27,27,27	0
57	MG	BA	3393	1/1	0.93	0.09	61,61,61,61	0
57	MG	BA	3006	1/1	0.93	0.24	27,27,27,27	0
57	MG	BA	3030	1/1	0.93	0.42	37,37,37,37	0
57	MG	AA	1638	1/1	0.93	0.15	55,55,55,55	0
57	MG	CA	1648	1/1	0.93	0.10	28,28,28,28	0
57	MG	DA	3262	1/1	0.93	0.27	29,29,29,29	0
57	MG	BA	3156	1/1	0.93	0.09	26,26,26,26	0
57	MG	BA	3404	1/1	0.93	0.06	53,53,53,53	0
57	MG	BA	3241	1/1	0.93	0.18	50,50,50,50	0
57	MG	BA	3117	1/1	0.93	0.60	42,42,42,42	0
57	MG	BA	3075	1/1	0.93	0.21	24,24,24,24	0
57	MG	DA	3271	1/1	0.93	0.20	42,42,42,42	0
57	MG	BT	201	1/1	0.93	0.21	32,32,32,32	0
57	MG	AA	1629	1/1	0.93	0.15	56,56,56,56	0
57	MG	BX	101	1/1	0.93	0.14	36,36,36,36	0
57	MG	BA	3079	1/1	0.93	0.34	25,25,25,25	0
57	MG	CA	1662	1/1	0.93	0.43	26,26,26,26	0
57	MG	BA	3356	1/1	0.93	0.17	21,21,21,21	0
57	MG	BA	3305	1/1	0.93	0.34	41,41,41,41	0
57	MG	DA	3046	1/1	0.93	0.40	26,26,26,26	0
57	MG	BA	3081	1/1	0.93	0.48	16,16,16,16	0
57	MG	B5	104	1/1	0.93	0.23	33,33,33,33	0
57	MG	CA	1671	1/1	0.93	0.10	54,54,54,54	0
57	MG	DA	3053	1/1	0.93	0.36	21,21,21,21	0
57	MG	BA	3308	1/1	0.93	0.31	22,22,22,22	0
57	MG	CA	1675	1/1	0.93	0.47	33,33,33,33	0
57	MG	DA	3062	1/1	0.93	0.17	33,33,33,33	0
57	MG	DA	3183	1/1	0.93	0.23	54,54,54,54	0
57	MG	DA	3292	1/1	0.93	0.13	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	1651	1/1	0.93	0.11	49,49,49,49	0
57	MG	BA	3362	1/1	0.93	0.32	30,30,30,30	0
57	MG	BA	3363	1/1	0.93	0.21	23,23,23,23	0
57	MG	CA	1684	1/1	0.93	0.21	42,42,42,42	0
57	MG	BA	3365	1/1	0.93	0.34	23,23,23,23	0
57	MG	AA	1644	1/1	0.93	0.27	40,40,40,40	0
57	MG	AA	1635	1/1	0.93	0.42	31,31,31,31	0
57	MG	AA	1631	1/1	0.93	0.16	29,29,29,29	0
57	MG	DA	3085	1/1	0.93	0.46	49,49,49,49	0
57	MG	DA	3305	1/1	0.93	0.38	35,35,35,35	0
57	MG	BA	3174	1/1	0.93	0.18	53,53,53,53	0
57	MG	CA	1691	1/1	0.93	0.59	67,67,67,67	0
57	MG	DA	3090	1/1	0.93	0.23	31,31,31,31	0
57	MG	AA	1615	1/1	0.93	0.17	46,46,46,46	0
57	MG	DB	205	1/1	0.93	0.33	42,42,42,42	0
57	MG	DA	3096	1/1	0.93	0.20	34,34,34,34	0
57	MG	CA	1693	1/1	0.93	0.21	36,36,36,36	0
57	MG	BA	3319	1/1	0.93	0.07	28,28,28,28	0
57	MG	DA	3206	1/1	0.93	0.17	49,49,49,49	0
57	MG	BA	3263	1/1	0.93	0.09	36,36,36,36	0
57	MG	DA	3104	1/1	0.93	0.23	21,21,21,21	0
57	MG	DA	3209	1/1	0.93	0.26	33,33,33,33	0
57	MG	CA	1696	1/1	0.93	0.30	54,54,54,54	0
58	ZN	D5	103	1/1	0.93	0.16	30,30,30,30	0
57	MG	CA	1659	1/1	0.94	0.36	32,32,32,32	0
57	MG	BA	3131	1/1	0.94	0.33	26,26,26,26	0
57	MG	BA	3309	1/1	0.94	0.07	20,20,20,20	0
57	MG	BA	3132	1/1	0.94	0.28	28,28,28,28	0
57	MG	BB	201	1/1	0.94	0.30	59,59,59,59	0
57	MG	BA	3082	1/1	0.94	0.32	24,24,24,24	0
57	MG	BB	205	1/1	0.94	0.25	19,19,19,19	0
57	MG	DA	3075	1/1	0.94	0.32	27,27,27,27	0
57	MG	DA	3078	1/1	0.94	0.31	44,44,44,44	0
57	MG	CA	1668	1/1	0.94	0.22	27,27,27,27	0
57	MG	DA	3210	1/1	0.94	0.24	41,41,41,41	0
57	MG	BA	3042	1/1	0.94	0.31	10,10,10,10	0
57	MG	BB	208	1/1	0.94	0.33	36,36,36,36	0
57	MG	DA	3086	1/1	0.94	0.34	25,25,25,25	0
57	MG	BA	3137	1/1	0.94	0.41	46,46,46,46	0
57	MG	DA	3216	1/1	0.94	0.41	23,23,23,23	0
57	MG	BA	3183	1/1	0.94	0.12	22,22,22,22	0
57	MG	CA	1677	1/1	0.94	0.36	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BH	201	1/1	0.94	0.19	21,21,21,21	0
57	MG	DA	3221	1/1	0.94	0.36	38,38,38,38	0
57	MG	AA	1680	1/1	0.94	0.33	49,49,49,49	0
57	MG	BA	3046	1/1	0.94	0.31	32,32,32,32	0
57	MG	BA	3386	1/1	0.94	0.29	68,68,68,68	0
57	MG	BA	3050	1/1	0.94	0.30	24,24,24,24	0
57	MG	BA	3189	1/1	0.94	0.09	14,14,14,14	0
57	MG	AA	1667	1/1	0.94	0.22	62,62,62,62	0
57	MG	BA	3391	1/1	0.94	0.22	44,44,44,44	0
57	MG	BA	3146	1/1	0.94	0.26	22,22,22,22	0
57	MG	B1	101	1/1	0.94	0.41	63,63,63,63	0
57	MG	BA	3192	1/1	0.94	0.26	27,27,27,27	0
57	MG	AA	1608	1/1	0.94	0.17	65,65,65,65	0
57	MG	DA	3236	1/1	0.94	0.10	30,30,30,30	0
57	MG	DA	3114	1/1	0.94	0.30	30,30,30,30	0
57	MG	DA	3115	1/1	0.94	0.08	36,36,36,36	0
57	MG	BA	3397	1/1	0.94	0.23	44,44,44,44	0
57	MG	B7	101	1/1	0.94	0.14	12,12,12,12	0
57	MG	DA	3118	1/1	0.94	0.18	33,33,33,33	0
57	MG	AT	201	1/1	0.94	0.23	22,22,22,22	0
57	MG	BA	3401	1/1	0.94	0.13	46,46,46,46	0
57	MG	BA	3402	1/1	0.94	0.13	24,24,24,24	0
57	MG	DA	3247	1/1	0.94	0.14	23,23,23,23	0
57	MG	CA	1701	1/1	0.94	0.23	25,25,25,25	0
57	MG	DA	3124	1/1	0.94	0.17	26,26,26,26	0
57	MG	BA	3256	1/1	0.94	0.19	25,25,25,25	0
57	MG	DA	3126	1/1	0.94	0.20	6,6,6,6	0
57	MG	BA	3333	1/1	0.94	0.59	77,77,77,77	0
57	MG	CA	1607	1/1	0.94	0.12	37,37,37,37	0
57	MG	BA	3405	1/1	0.94	0.09	25,25,25,25	0
57	MG	BA	3150	1/1	0.94	0.46	29,29,29,29	0
57	MG	BA	3054	1/1	0.94	0.46	33,33,33,33	0
57	MG	DA	3260	1/1	0.94	0.13	31,31,31,31	0
57	MG	BA	3260	1/1	0.94	0.22	24,24,24,24	0
57	MG	BA	3410	1/1	0.94	0.14	30,30,30,30	0
57	MG	DA	3264	1/1	0.94	0.11	25,25,25,25	0
57	MG	DA	3265	1/1	0.94	0.40	54,54,54,54	0
57	MG	BA	3411	1/1	0.94	0.38	53,53,53,53	0
57	MG	DA	3138	1/1	0.94	0.25	17,17,17,17	0
57	MG	BA	3261	1/1	0.94	0.40	28,28,28,28	0
57	MG	AA	1672	1/1	0.94	0.20	33,33,33,33	0
57	MG	BA	3058	1/1	0.94	0.47	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	AA	1612	1/1	0.94	0.39	25,25,25,25	0
57	MG	BA	3419	1/1	0.94	0.40	44,44,44,44	0
57	MG	BA	3200	1/1	0.94	0.33	20,20,20,20	0
57	MG	DA	3004	1/1	0.94	0.17	21,21,21,21	0
57	MG	DA	3275	1/1	0.94	0.25	48,48,48,48	0
57	MG	DA	3008	1/1	0.94	0.27	6,6,6,6	0
57	MG	BA	3348	1/1	0.94	0.35	55,55,55,55	0
57	MG	BA	3201	1/1	0.94	0.12	24,24,24,24	0
57	MG	BA	3061	1/1	0.94	0.39	25,25,25,25	0
57	MG	AA	1656	1/1	0.94	0.12	28,28,28,28	0
57	MG	BA	3271	1/1	0.94	0.22	40,40,40,40	0
57	MG	CA	1631	1/1	0.94	0.29	34,34,34,34	0
57	MG	DA	3022	1/1	0.94	0.20	21,21,21,21	0
57	MG	BA	3026	1/1	0.94	0.25	31,31,31,31	0
57	MG	CA	1633	1/1	0.94	0.44	45,45,45,45	0
57	MG	BA	3209	1/1	0.94	0.25	23,23,23,23	0
57	MG	DA	3162	1/1	0.94	0.20	24,24,24,24	0
57	MG	BA	3161	1/1	0.94	0.21	25,25,25,25	0
57	MG	AA	1662	1/1	0.94	0.14	22,22,22,22	0
57	MG	DA	3029	1/1	0.94	0.14	22,22,22,22	0
57	MG	DA	3296	1/1	0.94	0.35	40,40,40,40	0
57	MG	AA	1640	1/1	0.94	0.24	19,19,19,19	0
57	MG	BA	3121	1/1	0.94	0.19	20,20,20,20	0
57	MG	BA	3436	1/1	0.94	0.28	48,48,48,48	0
57	MG	AA	1690	1/1	0.94	0.09	26,26,26,26	0
57	MG	DA	3034	1/1	0.94	0.24	57,57,57,57	0
57	MG	BA	3220	1/1	0.94	0.23	30,30,30,30	0
57	MG	BA	3008	1/1	0.94	0.41	16,16,16,16	0
57	MG	BA	3032	1/1	0.94	0.25	6,6,6,6	0
57	MG	BA	3225	1/1	0.94	0.16	16,16,16,16	0
57	MG	AA	1712	1/1	0.94	0.19	56,56,56,56	0
57	MG	BA	3298	1/1	0.94	0.15	20,20,20,20	0
57	MG	BA	3172	1/1	0.94	0.52	22,22,22,22	0
57	MG	BA	3371	1/1	0.94	0.15	48,48,48,48	0
57	MG	BA	3173	1/1	0.94	0.13	40,40,40,40	0
57	MG	CA	1653	1/1	0.94	0.19	36,36,36,36	0
57	MG	AA	1658	1/1	0.94	0.15	23,23,23,23	0
57	MG	DA	3052	1/1	0.94	0.27	21,21,21,21	0
57	MG	DD	301	1/1	0.94	0.19	18,18,18,18	0
57	MG	DA	3191	1/1	0.94	0.21	18,18,18,18	0
57	MG	AA	1697	1/1	0.94	0.16	27,27,27,27	0
57	MG	DA	3055	1/1	0.94	0.26	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	D5	102	1/1	0.94	0.44	44,44,44,44	0
57	MG	BA	3451	1/1	0.94	0.20	23,23,23,23	0
57	MG	DA	3060	1/1	0.94	0.28	27,27,27,27	0
57	MG	BA	3375	1/1	0.94	0.41	36,36,36,36	0
57	MG	BA	3330	1/1	0.95	0.17	21,21,21,21	0
57	MG	AA	1671	1/1	0.95	0.23	42,42,42,42	0
57	MG	AA	1698	1/1	0.95	0.35	37,37,37,37	0
57	MG	BA	3145	1/1	0.95	0.35	29,29,29,29	0
57	MG	BA	3334	1/1	0.95	0.18	24,24,24,24	0
57	MG	DA	3243	1/1	0.95	0.12	44,44,44,44	0
57	MG	BA	3011	1/1	0.95	0.22	6,6,6,6	0
57	MG	DA	3063	1/1	0.95	0.17	29,29,29,29	0
57	MG	BA	3338	1/1	0.95	0.09	18,18,18,18	0
57	MG	BA	3279	1/1	0.95	0.07	26,26,26,26	0
57	MG	CA	1697	1/1	0.95	0.08	39,39,39,39	0
57	MG	BA	3112	1/1	0.95	0.23	23,23,23,23	0
57	MG	DA	3071	1/1	0.95	0.31	20,20,20,20	0
57	MG	BA	3454	1/1	0.95	0.14	25,25,25,25	0
57	MG	AA	1700	1/1	0.95	0.19	44,44,44,44	0
57	MG	BA	3282	1/1	0.95	0.40	22,22,22,22	0
57	MG	DA	3077	1/1	0.95	0.39	22,22,22,22	0
57	MG	BA	3114	1/1	0.95	0.38	24,24,24,24	0
57	MG	BA	3286	1/1	0.95	0.36	24,24,24,24	0
57	MG	BA	3115	1/1	0.95	0.24	19,19,19,19	0
57	MG	AA	1683	1/1	0.95	0.31	31,31,31,31	0
57	MG	BB	206	1/1	0.95	0.32	31,31,31,31	0
57	MG	DA	3263	1/1	0.95	0.18	28,28,28,28	0
57	MG	CA	1709	1/1	0.95	0.33	28,28,28,28	0
57	MG	BA	3234	1/1	0.95	0.05	38,38,38,38	0
57	MG	BA	3080	1/1	0.95	0.29	32,32,32,32	0
57	MG	DA	3179	1/1	0.95	0.33	30,30,30,30	0
57	MG	DA	3093	1/1	0.95	0.26	19,19,19,19	0
57	MG	AA	1666	1/1	0.95	0.14	24,24,24,24	0
57	MG	DA	3095	1/1	0.95	0.30	62,62,62,62	0
57	MG	BA	3120	1/1	0.95	0.29	35,35,35,35	0
57	MG	BA	3295	1/1	0.95	0.26	20,20,20,20	0
57	MG	BA	3055	1/1	0.95	0.26	24,24,24,24	0
57	MG	DA	3188	1/1	0.95	0.11	27,27,27,27	0
57	MG	BP	203	1/1	0.95	0.21	27,27,27,27	0
57	MG	DA	3102	1/1	0.95	0.41	32,32,32,32	0
57	MG	DA	3103	1/1	0.95	0.53	19,19,19,19	0
57	MG	BQ	201	1/1	0.95	0.20	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3105	1/1	0.95	0.37	30,30,30,30	0
57	MG	DA	3106	1/1	0.95	0.50	25,25,25,25	0
57	MG	BQ	202	1/1	0.95	0.27	30,30,30,30	0
57	MG	BA	3083	1/1	0.95	0.14	22,22,22,22	0
57	MG	BA	3084	1/1	0.95	0.69	61,61,61,61	0
57	MG	DA	3285	1/1	0.95	0.23	38,38,38,38	0
57	MG	AA	1624	1/1	0.95	0.33	33,33,33,33	0
57	MG	DA	3013	1/1	0.95	0.33	20,20,20,20	0
57	MG	BA	3033	1/1	0.95	0.22	34,34,34,34	0
57	MG	BA	3415	1/1	0.95	0.22	36,36,36,36	0
57	MG	CA	1656	1/1	0.95	0.43	43,43,43,43	0
57	MG	BA	3165	1/1	0.95	0.19	25,25,25,25	0
57	MG	AA	1714	1/1	0.95	0.26	42,42,42,42	0
57	MG	DA	3295	1/1	0.95	0.25	40,40,40,40	0
57	MG	AA	1614	1/1	0.95	0.38	29,29,29,29	0
57	MG	B5	101	1/1	0.95	0.40	78,78,78,78	0
57	MG	AA	1693	1/1	0.95	0.11	45,45,45,45	0
57	MG	BA	3063	1/1	0.95	0.24	17,17,17,17	0
57	MG	DA	3212	1/1	0.95	0.20	18,18,18,18	0
57	MG	BA	3367	1/1	0.95	0.39	33,33,33,33	0
57	MG	BA	3206	1/1	0.95	0.25	22,22,22,22	0
57	MG	BA	3041	1/1	0.95	0.47	44,44,44,44	0
57	MG	BA	3135	1/1	0.95	0.16	23,23,23,23	0
57	MG	BA	3316	1/1	0.95	0.18	28,28,28,28	0
57	MG	BA	3210	1/1	0.95	0.30	24,24,24,24	0
57	MG	BA	3259	1/1	0.95	0.19	37,37,37,37	0
57	MG	CA	1674	1/1	0.95	0.27	41,41,41,41	0
57	MG	BA	3023	1/1	0.95	0.42	45,45,45,45	0
57	MG	CA	1676	1/1	0.95	0.20	48,48,48,48	0
57	MG	DA	3224	1/1	0.95	0.41	14,14,14,14	0
57	MG	BA	3007	1/1	0.95	0.38	19,19,19,19	0
57	MG	BA	3321	1/1	0.95	0.37	22,22,22,22	0
57	MG	CA	1679	1/1	0.95	0.12	29,29,29,29	0
57	MG	BA	3377	1/1	0.95	0.11	23,23,23,23	0
57	MG	BA	3138	1/1	0.95	0.13	39,39,39,39	0
57	MG	CA	1683	1/1	0.95	0.15	36,36,36,36	0
57	MG	BA	3103	1/1	0.95	0.32	21,21,21,21	0
57	MG	BA	3104	1/1	0.95	0.17	37,37,37,37	0
57	MG	BA	3179	1/1	0.95	0.48	23,23,23,23	0
57	MG	BA	3221	1/1	0.95	0.21	22,22,22,22	0
57	MG	DA	3019	1/1	0.96	0.46	35,35,35,35	0
57	MG	BA	3147	1/1	0.96	0.32	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	AA	1641	1/1	0.96	0.17	30,30,30,30	0
57	MG	BA	3185	1/1	0.96	0.24	17,17,17,17	0
57	MG	BA	3228	1/1	0.96	0.37	36,36,36,36	0
57	MG	DA	3120	1/1	0.96	0.23	25,25,25,25	0
57	MG	BA	3186	1/1	0.96	0.54	24,24,24,24	0
57	MG	BA	3012	1/1	0.96	0.38	22,22,22,22	0
57	MG	AA	1682	1/1	0.96	0.21	18,18,18,18	0
57	MG	DA	3027	1/1	0.96	0.13	33,33,33,33	0
57	MG	DA	3229	1/1	0.96	0.17	19,19,19,19	0
57	MG	DA	3230	1/1	0.96	0.31	23,23,23,23	0
57	MG	AA	1628	1/1	0.96	0.45	43,43,43,43	0
57	MG	AA	1692	1/1	0.96	0.23	51,51,51,51	0
57	MG	DA	3128	1/1	0.96	0.26	24,24,24,24	0
57	MG	BA	3416	1/1	0.96	0.13	42,42,42,42	0
57	MG	BA	3059	1/1	0.96	0.34	28,28,28,28	0
57	MG	BA	3085	1/1	0.96	0.18	17,17,17,17	0
57	MG	CA	1669	1/1	0.96	0.18	21,21,21,21	0
57	MG	BA	3122	1/1	0.96	0.38	41,41,41,41	0
57	MG	DA	3134	1/1	0.96	0.16	24,24,24,24	0
57	MG	DA	3035	1/1	0.96	0.51	22,22,22,22	0
57	MG	BA	3034	1/1	0.96	0.21	19,19,19,19	0
57	MG	DA	3242	1/1	0.96	0.09	32,32,32,32	0
57	MG	AA	1643	1/1	0.96	0.15	23,23,23,23	0
57	MG	BA	3360	1/1	0.96	0.16	27,27,27,27	0
57	MG	BA	3159	1/1	0.96	0.47	29,29,29,29	0
57	MG	AA	1707	1/1	0.96	0.23	20,20,20,20	0
57	MG	BA	3020	1/1	0.96	0.35	19,19,19,19	0
57	MG	BA	3302	1/1	0.96	0.10	37,37,37,37	0
57	MG	CA	1606	1/1	0.96	0.38	50,50,50,50	0
57	MG	DA	3047	1/1	0.96	0.34	26,26,26,26	0
57	MG	BA	3304	1/1	0.96	0.10	49,49,49,49	0
57	MG	BA	3244	1/1	0.96	0.25	47,47,47,47	0
57	MG	BA	3246	1/1	0.96	0.10	11,11,11,11	0
57	MG	CA	1611	1/1	0.96	0.10	25,25,25,25	0
57	MG	BA	3247	1/1	0.96	0.06	33,33,33,33	0
57	MG	DA	3258	1/1	0.96	0.21	64,64,64,64	0
57	MG	DA	3054	1/1	0.96	0.58	27,27,27,27	0
57	MG	AA	1694	1/1	0.96	0.18	23,23,23,23	0
57	MG	DA	3057	1/1	0.96	0.23	22,22,22,22	0
57	MG	DA	3156	1/1	0.96	0.83	58,58,58,58	0
57	MG	AA	1695	1/1	0.96	0.20	26,26,26,26	0
57	MG	CA	1688	1/1	0.96	0.12	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3130	1/1	0.96	0.39	35,35,35,35	0
57	MG	BA	3312	1/1	0.96	0.31	22,22,22,22	0
57	MG	BA	3203	1/1	0.96	0.35	29,29,29,29	0
57	MG	DA	3064	1/1	0.96	0.26	19,19,19,19	0
57	MG	BA	3314	1/1	0.96	0.07	22,22,22,22	0
57	MG	BA	3067	1/1	0.96	0.18	30,30,30,30	0
57	MG	DA	3068	1/1	0.96	0.22	19,19,19,19	0
57	MG	DA	3168	1/1	0.96	0.24	35,35,35,35	0
57	MG	BA	3068	1/1	0.96	0.23	30,30,30,30	0
57	MG	BA	3255	1/1	0.96	0.44	31,31,31,31	0
57	MG	BA	3099	1/1	0.96	0.48	29,29,29,29	0
57	MG	DA	3173	1/1	0.96	0.19	33,33,33,33	0
57	MG	AA	1696	1/1	0.96	0.22	26,26,26,26	0
57	MG	BA	3208	1/1	0.96	0.05	56,56,56,56	0
57	MG	BA	3070	1/1	0.96	0.15	23,23,23,23	0
57	MG	DA	3076	1/1	0.96	0.13	19,19,19,19	0
57	MG	CA	1628	1/1	0.96	0.12	26,26,26,26	0
57	MG	AA	1620	1/1	0.96	0.18	27,27,27,27	0
57	MG	DA	3079	1/1	0.96	0.21	45,45,45,45	0
57	MG	DA	3284	1/1	0.96	0.13	51,51,51,51	0
57	MG	DA	3181	1/1	0.96	0.31	36,36,36,36	0
57	MG	AA	1634	1/1	0.96	0.40	41,41,41,41	0
57	MG	BA	3106	1/1	0.96	0.34	23,23,23,23	0
57	MG	DA	3084	1/1	0.96	0.12	21,21,21,21	0
57	MG	CA	1705	1/1	0.96	0.26	48,48,48,48	0
57	MG	DA	3186	1/1	0.96	0.08	29,29,29,29	0
57	MG	BA	3214	1/1	0.96	0.11	29,29,29,29	0
57	MG	AA	1652	1/1	0.96	0.16	44,44,44,44	0
57	MG	BA	3457	1/1	0.96	0.16	35,35,35,35	0
57	MG	DA	3089	1/1	0.96	0.13	19,19,19,19	0
57	MG	BA	3177	1/1	0.96	0.30	21,21,21,21	0
57	MG	DA	3091	1/1	0.96	0.14	26,26,26,26	0
57	MG	DA	3092	1/1	0.96	0.36	25,25,25,25	0
57	MG	BA	3110	1/1	0.96	0.23	32,32,32,32	0
57	MG	BA	3076	1/1	0.96	0.34	24,24,24,24	0
57	MG	BB	202	1/1	0.96	0.32	21,21,21,21	0
57	MG	CA	1641	1/1	0.96	0.07	18,18,18,18	0
57	MG	BA	3144	1/1	0.96	0.20	24,24,24,24	0
57	MG	BA	3222	1/1	0.96	0.30	31,31,31,31	0
57	MG	DA	3202	1/1	0.96	0.58	38,38,38,38	0
57	MG	DA	3100	1/1	0.96	0.33	21,21,21,21	0
57	MG	BA	3273	1/1	0.96	0.21	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3337	1/1	0.96	0.25	37,37,37,37	0
57	MG	BA	3398	1/1	0.96	0.17	34,34,34,34	0
57	MG	DB	206	1/1	0.96	0.16	19,19,19,19	0
57	MG	BA	3275	1/1	0.96	0.28	27,27,27,27	0
57	MG	DA	3005	1/1	0.96	0.48	45,45,45,45	0
57	MG	DA	3007	1/1	0.96	0.43	54,54,54,54	0
57	MG	BD	301	1/1	0.96	0.25	34,34,34,34	0
57	MG	BE	301	1/1	0.96	0.29	43,43,43,43	0
57	MG	BA	3276	1/1	0.96	0.39	21,21,21,21	0
57	MG	DR	201	1/1	0.96	0.15	22,22,22,22	0
57	MG	AA	1627	1/1	0.96	0.15	21,21,21,21	0
57	MG	DA	3015	1/1	0.96	0.22	36,36,36,36	0
57	MG	BA	3278	1/1	0.96	0.17	33,33,33,33	0
57	MG	DA	3113	1/1	0.96	0.42	26,26,26,26	0
57	MG	BA	3078	1/1	0.96	0.38	29,29,29,29	0
57	MG	CA	1667	1/1	0.97	0.18	23,23,23,23	0
57	MG	DA	3018	1/1	0.97	0.45	21,21,21,21	0
57	MG	AA	1663	1/1	0.97	0.16	27,27,27,27	0
57	MG	DA	3170	1/1	0.97	0.27	22,22,22,22	0
57	MG	BA	3335	1/1	0.97	0.10	47,47,47,47	0
57	MG	BA	3441	1/1	0.97	0.41	37,37,37,37	0
57	MG	BA	3048	1/1	0.97	0.39	27,27,27,27	0
57	MG	BA	3443	1/1	0.97	0.23	24,24,24,24	0
57	MG	CA	1673	1/1	0.97	0.17	26,26,26,26	0
57	MG	BA	3089	1/1	0.97	0.37	24,24,24,24	0
57	MG	AA	1699	1/1	0.97	0.26	29,29,29,29	0
57	MG	BA	3119	1/1	0.97	0.42	23,23,23,23	0
57	MG	BA	3340	1/1	0.97	0.21	29,29,29,29	0
57	MG	CA	1617	1/1	0.97	0.25	35,35,35,35	0
57	MG	BA	3341	1/1	0.97	0.19	28,28,28,28	0
57	MG	BA	3213	1/1	0.97	0.29	43,43,43,43	0
57	MG	AA	1623	1/1	0.97	0.32	18,18,18,18	0
57	MG	CA	1682	1/1	0.97	0.26	40,40,40,40	0
57	MG	AA	1630	1/1	0.97	0.29	41,41,41,41	0
57	MG	BA	3216	1/1	0.97	0.44	20,20,20,20	0
57	MG	BA	3396	1/1	0.97	0.11	26,26,26,26	0
57	MG	BA	3299	1/1	0.97	0.21	22,22,22,22	0
57	MG	DA	3039	1/1	0.97	0.31	18,18,18,18	0
57	MG	BA	3072	1/1	0.97	0.43	23,23,23,23	0
57	MG	DA	3041	1/1	0.97	0.16	19,19,19,19	0
57	MG	BA	3096	1/1	0.97	0.45	24,24,24,24	0
57	MG	BA	3400	1/1	0.97	0.08	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3031	1/1	0.97	0.20	21,21,21,21	0
57	MG	BA	3098	1/1	0.97	0.24	25,25,25,25	0
57	MG	DA	3197	1/1	0.97	0.27	27,27,27,27	0
57	MG	CA	1630	1/1	0.97	0.11	29,29,29,29	0
57	MG	BA	3351	1/1	0.97	0.15	56,56,56,56	0
57	MG	BB	204	1/1	0.97	0.38	54,54,54,54	0
57	MG	BA	3003	1/1	0.97	0.12	25,25,25,25	0
57	MG	BA	3019	1/1	0.97	0.34	25,25,25,25	0
57	MG	BA	3307	1/1	0.97	0.46	24,24,24,24	0
57	MG	BA	3101	1/1	0.97	0.10	21,21,21,21	0
57	MG	BA	3056	1/1	0.97	0.42	26,26,26,26	0
57	MG	DA	3127	1/1	0.97	0.33	34,34,34,34	0
57	MG	BA	3160	1/1	0.97	0.15	30,30,30,30	0
57	MG	DA	3056	1/1	0.97	0.22	30,30,30,30	0
57	MG	AA	1639	1/1	0.97	0.15	27,27,27,27	0
57	MG	DA	3058	1/1	0.97	0.21	27,27,27,27	0
57	MG	DA	3289	1/1	0.97	0.15	27,27,27,27	0
57	MG	AA	1606	1/1	0.97	0.23	42,42,42,42	0
57	MG	BA	3413	1/1	0.97	0.29	24,24,24,24	0
57	MG	BA	3229	1/1	0.97	0.26	6,6,6,6	0
57	MG	AA	1676	1/1	0.97	0.30	30,30,30,30	0
57	MG	DA	3294	1/1	0.97	0.41	19,19,19,19	0
57	MG	BA	3164	1/1	0.97	0.16	35,35,35,35	0
57	MG	BA	3272	1/1	0.97	0.48	23,23,23,23	0
57	MG	BA	3134	1/1	0.97	0.17	22,22,22,22	0
57	MG	DA	3066	1/1	0.97	0.30	22,22,22,22	0
57	MG	DA	3219	1/1	0.97	0.45	34,34,34,34	0
57	MG	BA	3274	1/1	0.97	0.35	27,27,27,27	0
57	MG	AA	1677	1/1	0.97	0.13	48,48,48,48	0
57	MG	CA	1650	1/1	0.97	0.12	28,28,28,28	0
57	MG	BA	3108	1/1	0.97	0.23	35,35,35,35	0
57	MG	BA	3423	1/1	0.97	0.08	25,25,25,25	0
57	MG	DA	3145	1/1	0.97	0.73	57,57,57,57	0
57	MG	BA	3168	1/1	0.97	0.14	33,33,33,33	0
57	MG	BA	3109	1/1	0.97	0.29	21,21,21,21	0
57	MG	BA	3039	1/1	0.97	0.75	39,39,39,39	0
57	MG	BA	3324	1/1	0.97	0.17	25,25,25,25	0
57	MG	BA	3325	1/1	0.97	0.33	22,22,22,22	0
57	MG	BA	3202	1/1	0.97	0.16	19,19,19,19	0
57	MG	DB	207	1/1	0.97	0.18	27,27,27,27	0
57	MG	BA	3327	1/1	0.97	0.20	28,28,28,28	0
57	MG	AA	1610	1/1	0.97	0.45	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	3009	1/1	0.97	0.21	18,18,18,18	0
57	MG	DA	3082	1/1	0.97	0.29	21,21,21,21	0
57	MG	DA	3083	1/1	0.97	0.10	30,30,30,30	0
57	MG	AA	1670	1/1	0.97	0.24	30,30,30,30	0
57	MG	DA	3012	1/1	0.97	0.49	28,28,28,28	0
57	MG	BA	3283	1/1	0.97	0.34	20,20,20,20	0
57	MG	DA	3163	1/1	0.97	0.26	32,32,32,32	0
57	MG	AA	1708	1/1	0.97	0.11	46,46,46,46	0
57	MG	D6	102	1/1	0.97	0.18	23,23,23,23	0
57	MG	BA	3142	1/1	0.97	0.30	25,25,25,25	0
58	ZN	B5	105	1/1	0.97	0.17	90,90,90,90	0
58	ZN	CD	301	1/1	0.97	0.34	81,81,81,81	0
57	MG	BA	3045	1/1	0.97	0.22	6,6,6,6	0
57	MG	BA	3018	1/1	0.98	0.51	21,21,21,21	0
57	MG	BA	3154	1/1	0.98	0.31	38,38,38,38	0
57	MG	BP	202	1/1	0.98	0.14	22,22,22,22	0
57	MG	DA	3097	1/1	0.98	0.26	21,21,21,21	0
57	MG	BA	3065	1/1	0.98	0.31	24,24,24,24	0
57	MG	BA	3293	1/1	0.98	0.24	23,23,23,23	0
57	MG	BA	3047	1/1	0.98	0.39	62,62,62,62	0
57	MG	BA	3364	1/1	0.98	0.17	32,32,32,32	0
57	MG	BA	3389	1/1	0.98	0.24	21,21,21,21	0
57	MG	DA	3146	1/1	0.98	0.25	60,60,60,60	0
57	MG	DA	3193	1/1	0.98	0.31	27,27,27,27	0
57	MG	BA	3128	1/1	0.98	0.40	33,33,33,33	0
57	MG	DA	3148	1/1	0.98	0.33	24,24,24,24	0
57	MG	BA	3102	1/1	0.98	0.55	33,33,33,33	0
57	MG	BA	3392	1/1	0.98	0.14	52,52,52,52	0
57	MG	BA	3420	1/1	0.98	0.18	45,45,45,45	0
57	MG	CA	1699	1/1	0.98	0.23	32,32,32,32	0
57	MG	BA	3219	1/1	0.98	0.12	28,28,28,28	0
57	MG	BA	3040	1/1	0.98	0.24	24,24,24,24	0
57	MG	BA	3237	1/1	0.98	0.13	21,21,21,21	0
57	MG	CA	1666	1/1	0.98	0.41	18,18,18,18	0
57	MG	BA	3455	1/1	0.98	0.21	46,46,46,46	0
57	MG	BA	3049	1/1	0.98	0.43	24,24,24,24	0
57	MG	DA	3253	1/1	0.98	0.21	20,20,20,20	0
57	MG	DA	3159	1/1	0.98	0.49	38,38,38,38	0
57	MG	BA	3035	1/1	0.98	0.41	25,25,25,25	0
57	MG	AA	1668	1/1	0.98	0.13	40,40,40,40	0
57	MG	DA	3257	1/1	0.98	0.16	35,35,35,35	0
57	MG	BA	3303	1/1	0.98	0.34	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	DA	3074	1/1	0.98	0.26	21,21,21,21	0
57	MG	CA	1636	1/1	0.98	0.16	28,28,28,28	0
57	MG	BA	3094	1/1	0.98	0.30	34,34,34,34	0
57	MG	BA	3429	1/1	0.98	0.05	33,33,33,33	0
57	MG	DA	3036	1/1	0.98	0.49	27,27,27,27	0
57	MG	BA	3043	1/1	0.98	0.34	25,25,25,25	0
57	MG	BA	3010	1/1	0.98	0.24	23,23,23,23	0
57	MG	BA	3073	1/1	0.98	0.21	23,23,23,23	0
57	MG	BA	3245	1/1	0.98	0.18	27,27,27,27	0
57	MG	BA	3285	1/1	0.98	0.14	6,6,6,6	0
57	MG	BA	3435	1/1	0.98	0.05	30,30,30,30	0
57	MG	DA	3002	1/1	0.98	0.64	37,37,37,37	0
57	MG	CA	1610	1/1	0.98	0.34	30,30,30,30	0
57	MG	BA	3004	1/1	0.98	0.54	61,61,61,61	0
57	MG	BA	3266	1/1	0.98	0.46	26,26,26,26	0
57	MG	DA	3006	1/1	0.98	0.34	28,28,28,28	0
57	MG	BA	3267	1/1	0.98	0.16	19,19,19,19	0
57	MG	CA	1614	1/1	0.98	0.15	30,30,30,30	0
57	MG	BA	3409	1/1	0.98	0.11	24,24,24,24	0
57	MG	DA	3051	1/1	0.98	0.18	6,6,6,6	0
57	MG	BA	3287	1/1	0.99	0.17	20,20,20,20	0
57	MG	DA	3011	1/1	0.99	0.35	20,20,20,20	0
57	MG	BA	3452	1/1	0.99	0.15	16,16,16,16	0
57	MG	BA	3090	1/1	0.99	0.24	17,17,17,17	0
58	ZN	B9	101	1/1	0.99	0.12	75,75,75,75	0
57	MG	AA	1655	1/1	0.99	0.21	6,6,6,6	0
57	MG	BA	3250	1/1	0.99	0.50	22,22,22,22	0
58	ZN	D9	101	1/1	0.99	0.15	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.