wwPDB X-ray Structure Validation Summary Report (i)

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)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

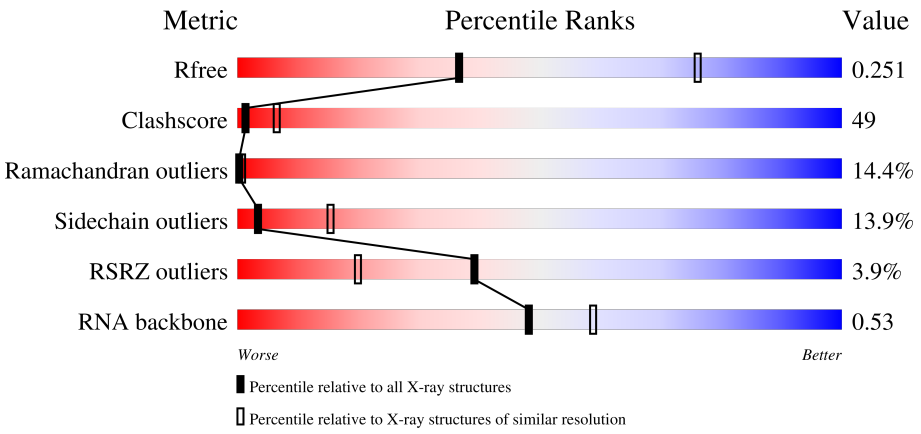
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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	3% 17% 67% 14% ••
1	CA	1509	2% 21% 65% 13% •
2	AB	256	7% 12% 59% 19% • 8%
2	CB	256	9% 15% 56% 19% • 8%

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Mol	Chain	Length	Quality of chain
3	AC	239	5% 14% 56% 15% • 13%
3	CC	239	8% 16% 58% 12% 13%
4	AD	209	% 13% 64% 20% •
4	CD	209	2% 25% 56% 17% •
5	AE	162	6% 19% 60% 13% • 7%
5	CE	162	3% 23% 59% 9% • 7%
6	AF	101	% 24% 58% 16% •
6	CF	101	2% 21% 57% 21% •
7	AG	156	5% 18% 66% 14% ••
7	CG	156	8% 18% 60% 19% • •
8	AH	138	% 22% 63% 14%
8	CH	138	3% 20% 62% 17% •
9	AI	128	9% 15% 64% 19% • •
9	CI	128	22% 19% 62% 14% 5% •
10	AJ	105	14% 14% 60% 18% • 6%
10	CJ	105	43% 15% 62% 17% 6%
11	AK	129	8% 26% 59% 6% • 8%
11	CK	129	3% 29% 53% 11% 8%
12	AL	132	2% 24% 53% 16% • 5%
12	CL	132	5% 26% 55% 13% • 5%
13	AM	126	6% 15% 54% 22% • 5%
13	CM	126	6% 18% 50% 23% • 5%
14	AN	61	3% 15% 57% 25% • •
14	CN	61	2% 18% 61% 16% • •
15	AO	89	18% 70% 10% ••

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Mol	Chain	Length	Quality of chain
15	CO	89	%, 18%, 62%, 19%
16	AP	88	7%, 16%, 64%, 14%, 5%
16	CP	88	2%, 18%, 64%, 13%, 5%
17	AQ	105	2%, 24%, 55%, 15%, 5%
17	CQ	105	29%, 57%, 7%, 5%
18	AR	88	16%, 51%, 10%, 20%
18	CR	88	5%, 18%, 49%, 11%, 20%
19	AS	93	5%, 12%, 48%, 24%, 14%
19	CS	93	10%, 12%, 54%, 16%, 16%
20	AT	106	6%, 16%, 60%, 16%, 7%
20	CT	106	5%, 14%, 61%, 17%, 7%
21	AU	27	19%, 22%, 59%, 11%, 7%
21	CU	27	22%, 30%, 48%, 15%, 7%
22	AV	184	2%, 23%, 61%, 11%
22	CV	184	7%, 24%, 55%, 16%
23	AW	77	3%, 26%, 53%, 18%
23	CW	77	22%, 51%, 26%
24	AX	5	100%
24	CX	5	20%, 40%, 60%
25	BA	2915	2%, 26%, 52%, 15%, 5%
25	DA	2915	2%, 22%, 55%, 16%, 5%
26	BB	122	39%, 43%, 15%
26	DB	122	2%, 18%, 62%, 16%
27	BC	229	7%, 22%, 59%, 15%
27	DC	229	10%, 27%, 59%, 10%

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Mol	Chain	Length	Quality of chain
28	BD	276	%; 28%; 52%; 16%
28	DD	276	3%; 25%; 55%; 18%
29	BE	206	%; 20%; 57%; 20%
29	DE	206	5%; 17%; 54%; 24%
30	BF	210	5%; 22%; 58%; 15%
30	DF	210	2%; 20%; 58%; 18%
31	BG	182	2%; 16%; 59%; 23%
31	DG	182	7%; 13%; 65%; 19%
32	BH	180	2%; 24%; 48%; 19%; 7%
32	DH	180	15%; 19%; 48%; 19%; 11%
33	BI	148	%; 22%; 49%; 24%
33	DI	148	2%; 39%; 45%; 14%
34	BN	140	%; 28%; 50%; 17%
34	DN	140	2%; 29%; 51%; 16%
35	BO	122	25%; 62%; 12%
35	DO	122	2%; 37%; 55%; 7%
36	BP	150	3%; 15%; 45%; 33%; 5%
36	DP	150	11%; 16%; 45%; 31%; 5%
37	BQ	141	%; 29%; 55%; 14%
37	DQ	141	4%; 27%; 59%; 13%
38	BR	118	28%; 55%; 15%
38	DR	118	17%; 58%; 25%
39	BS	112	10%; 19%; 36%; 31%; 10%
39	DS	112	12%; 13%; 46%; 25%; 12%
40	BT	146	5%; 12%; 53%; 23%; 6%; 5%

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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%

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Mol	Chain	Length	Quality of chain
53	B6	54	15% · 43% 35% 9% 9%
53	D6	54	6% 17% 31% 33% 7% 11%
54	B7	49	59% 35% 6%
54	D7	49	8% 24% 59% 14% ·
55	B8	65	3% 15% 58% 17% 6% ·
55	D8	65	8% 18% 55% 18% · 5%
56	B9	37	14% 30% 51% 16% ·
56	D9	37	3% 38% 54% 5% ·

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

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

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

2 Entry composition (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
			Total	C	N	O	S			
5	AE	151	1147	724	218	201	4	0	0	1
5	CE	151	1147	724	218	201	4	0	0	1

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a protein called Elongation factor P.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	AW	77	1644	732	297	538	77	0	0	0
23	CW	77	1644	732	297	538	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
			Total	C	N	O	P			
24	AX	5	110	49	22	34	5	0	0	0
24	CX	5	110	49	22	34	5	0	0	0

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

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

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

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

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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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
32	BH	168	1231	780	228	222	1	0	0	1
32	DH	160	1223	773	229	220	1	0	0	1

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	B1	96	757	478	149	129	1	0	0	0
48	D1	94	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
			Total	C	N	O	S			
49	B2	71	598	370	121	106	1	0	0	0
49	D2	71	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
			Total	C	N	O				
50	B3	59	460	293	90	77		0	0	1
50	D3	60	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
			Total	C	N	O	S			
51	B4	31	226	142	37	43	4	0	0	1
51	D4	31	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
			Total	C	N	O	S			
52	B5	57	435	272	88	70	5	0	0	1
52	D5	59	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

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

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

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

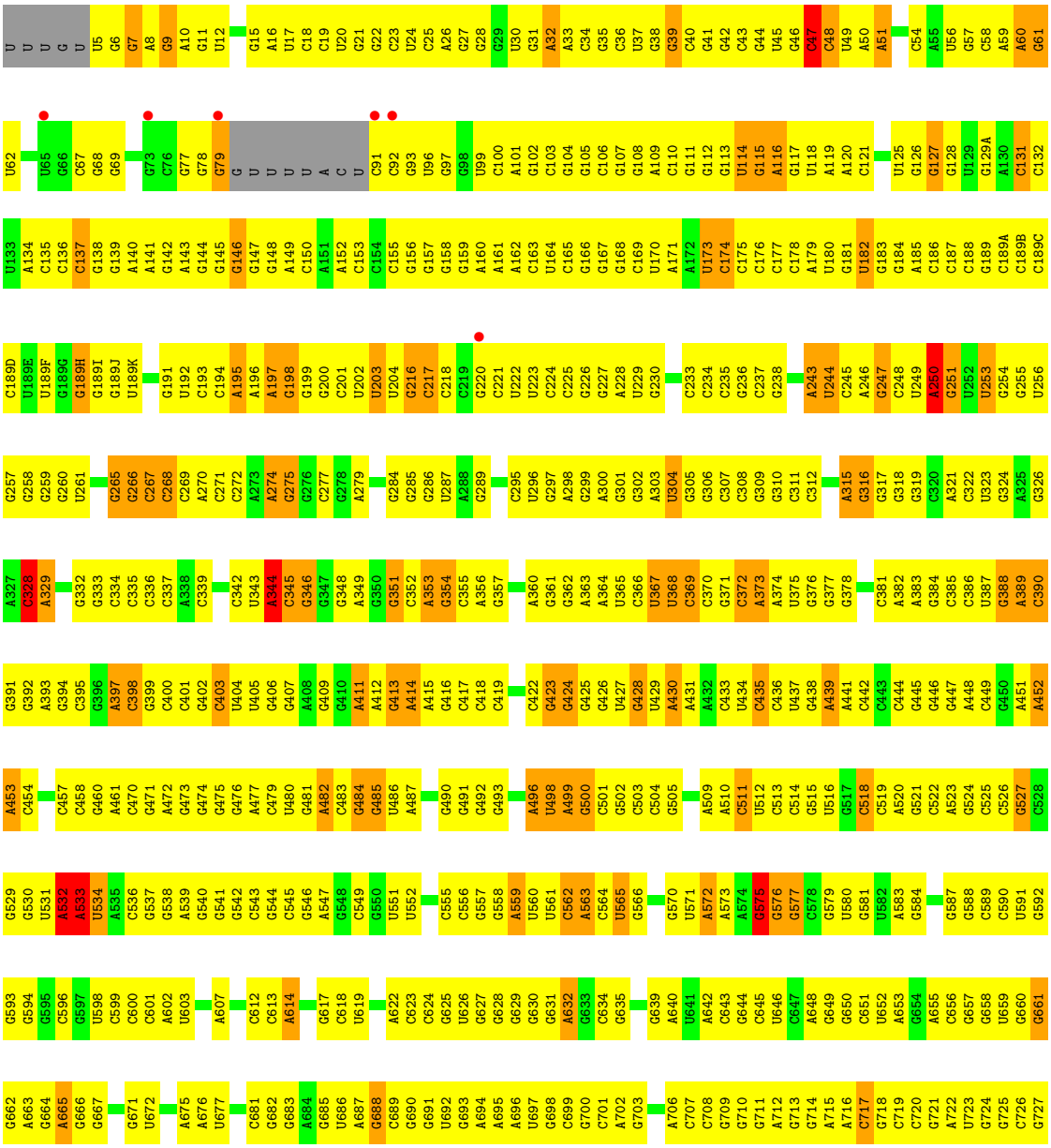
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
58	AD	1	1	1	0	0
			Total	Zn		
58	B5	1	1	1	0	0
			Total	Zn		
58	B9	1	1	1	0	0
			Total	Zn		
58	CD	1	1	1	0	0
			Total	Zn		
58	D5	1	1	1	0	0
			Total	Zn		
58	D9	1	1	1	0	0

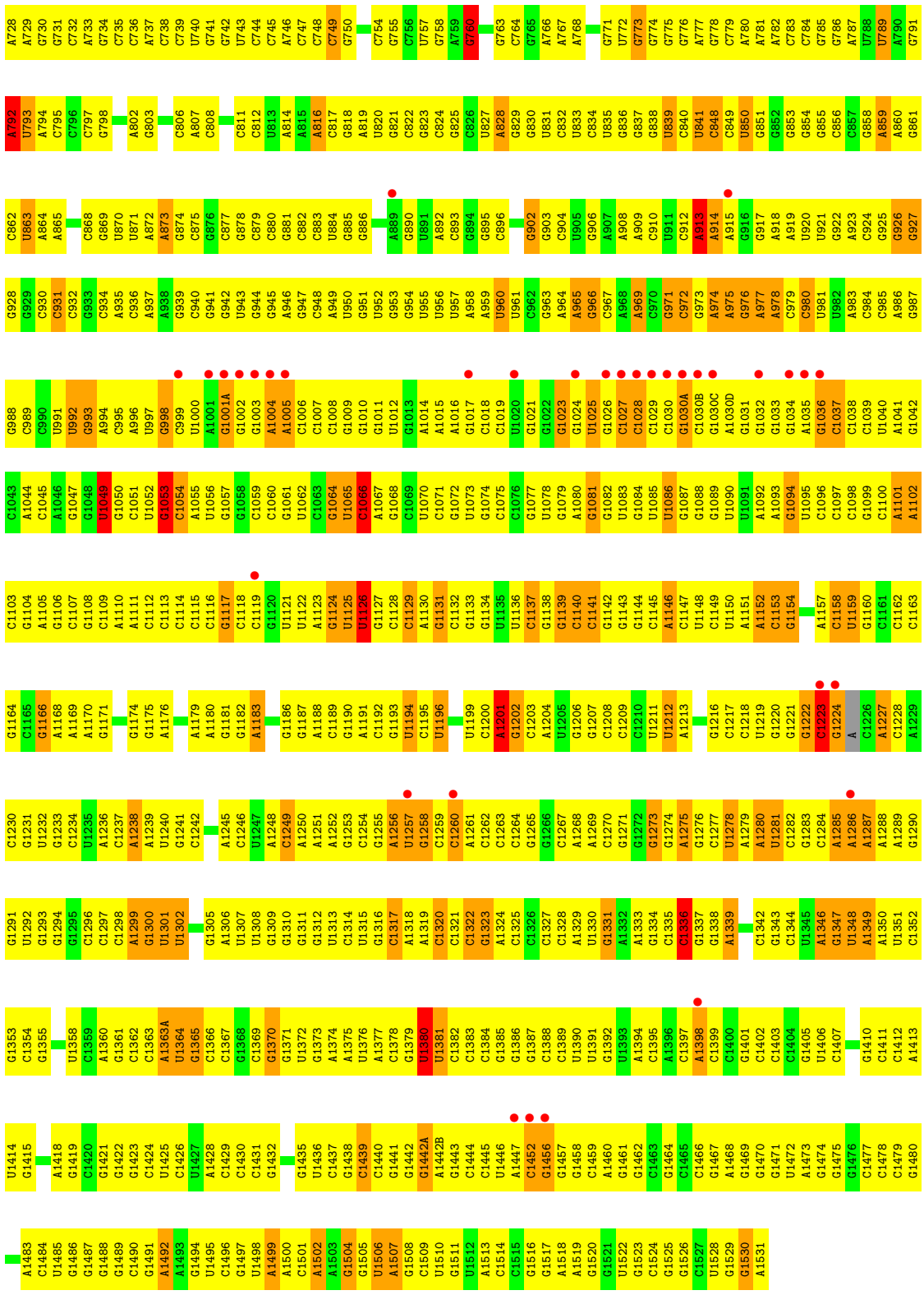
3 Residue-property plots (i)

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

- Molecule 1: 16S ribosomal RNA

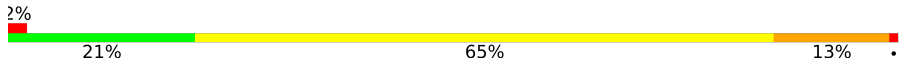
Chain AA: 3% 17% 67% 14%

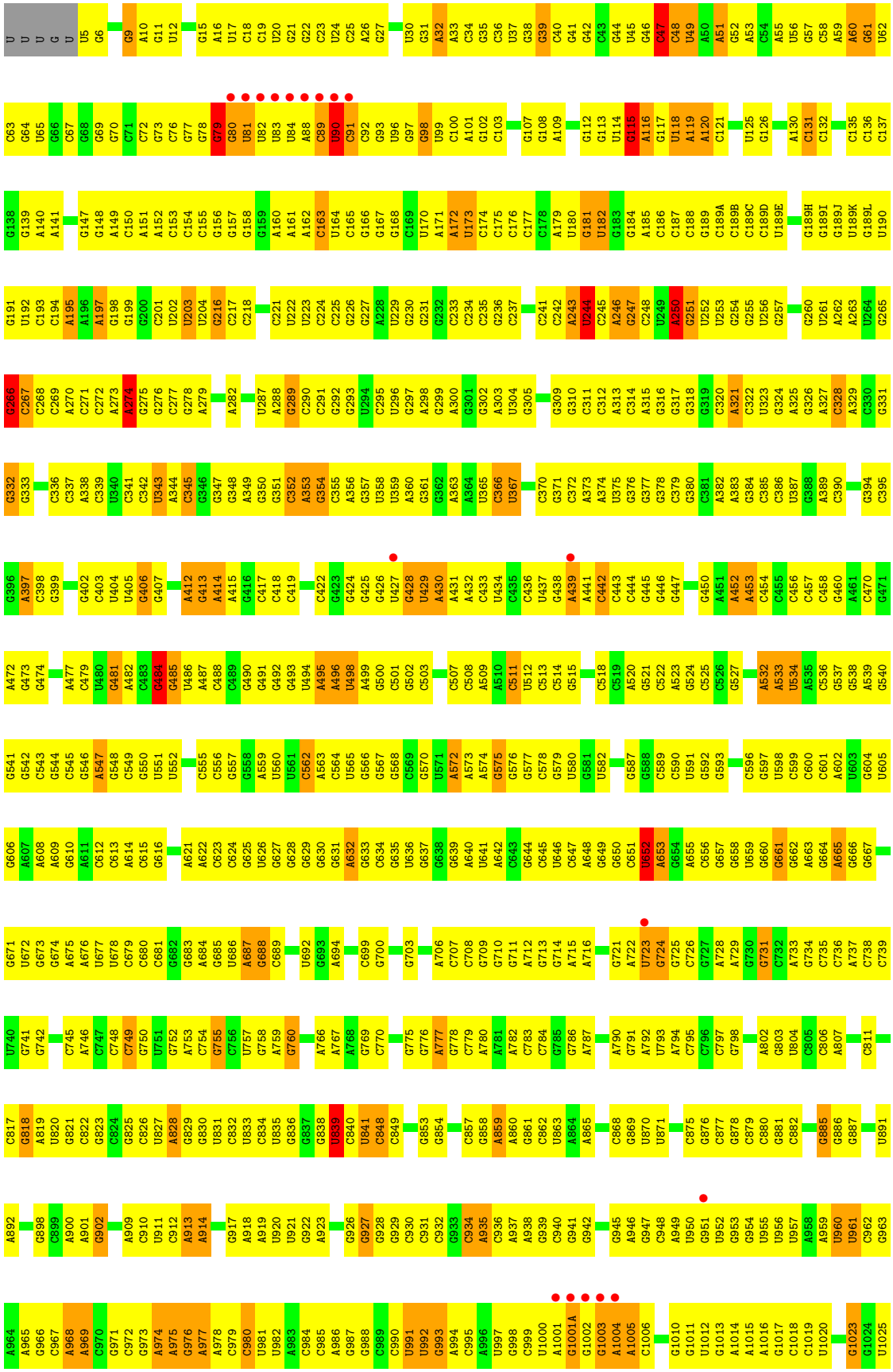


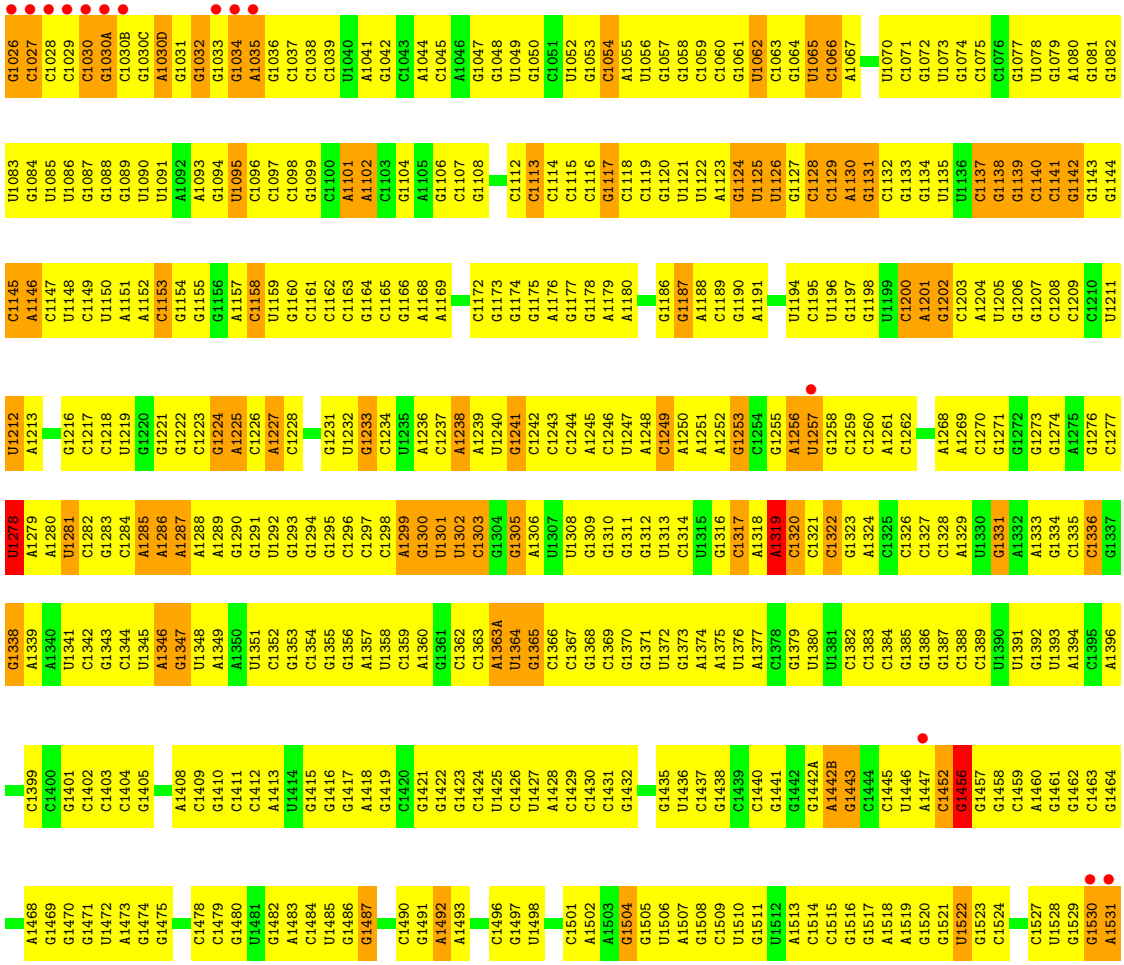


- Molecule 1: 16S ribosomal RNA

Chain CA:

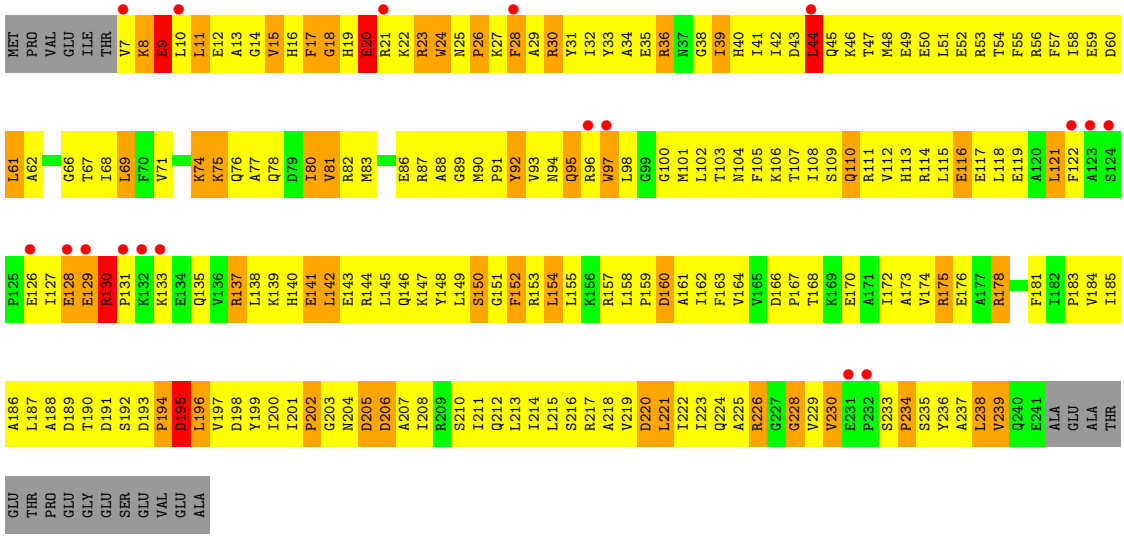



U U U G U
U5 G6 G9 A10 G11 U12 G15 A16 U17 C18 C19 U20 G21 G22 C23 U24 C25 A26 G27 U30 G31 A32 A33 C34 G35 C36 U37 G38 G39 C40 G41 G42 C43 G44 U45 G46 C47 C48 U49 A50 A51 G52 A53 C54 A55 U56 G57 C58 A59 A60 G61 U62
C63 G64 U65 G66 C67 G68 G69 G70 C71 C72 G73 C76 G77 G78 G79 G80 U81 U82 U83 U84 A88 C89 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 C156 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 C232 C233 C234 C235 G236 C237 C241 C242 A243 U244 C245 A246 G247 C248 U249 A250 G251 U252 U253 G254 G255 U256 G257 G260 U261 A262 A263 U264 G265
G266 C267 C268 C269 A270 C271 C272 A273 A274 G275 G276 C277 G278 A279 A282 U287 A288 G289 C290 C291 G292 C225 G293 U294 C295 U296 G297 A298 G299 A300 G301 G302 A303 U304 G305 G309 G310 C311 C312 A313 C314 A315 G316 G317 G318 G319 C320 A321 C322 U323 G324 A325 G326 A327 G328 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 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 G426 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 C457 C458 G460 A461 C470 G471
A472 G473 G474 A477 C479 U480 G481 A482 C483 G484 G485 U486 A487 C488 C489 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 G538 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 G630 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 C708 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 U835 G836 G837 G838 U839 C840 U841 C848 C849 G853 C854 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 U956 U957 A958 A959 U960 U961 C962 G963
A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 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



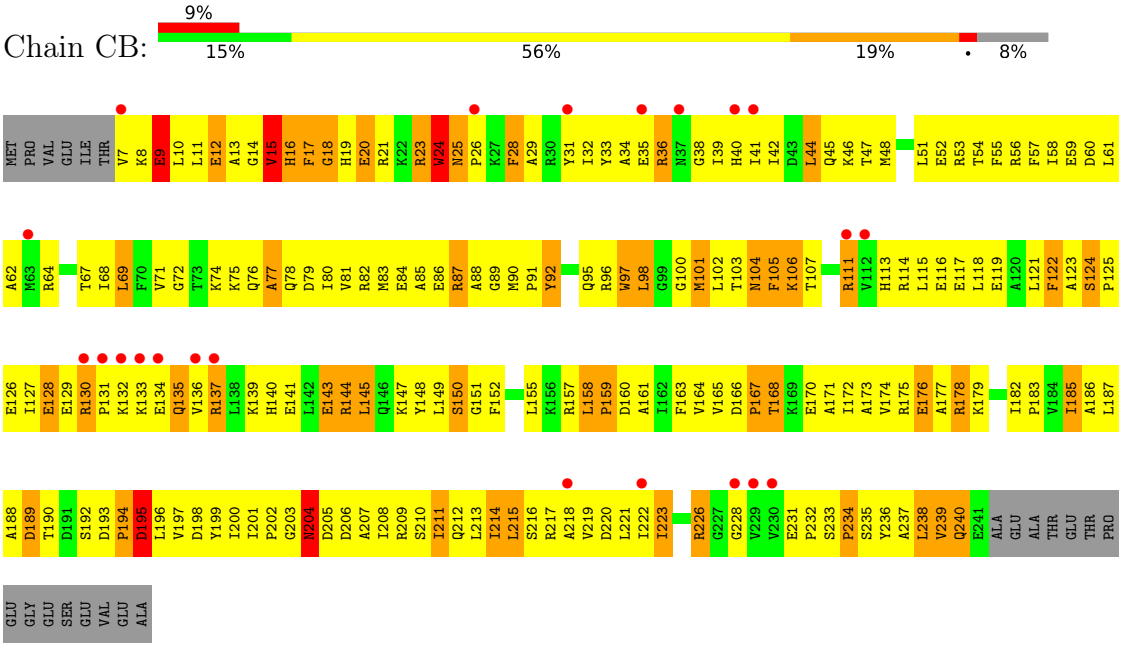
• Molecule 2: 30S ribosomal protein S2

Chain AB:



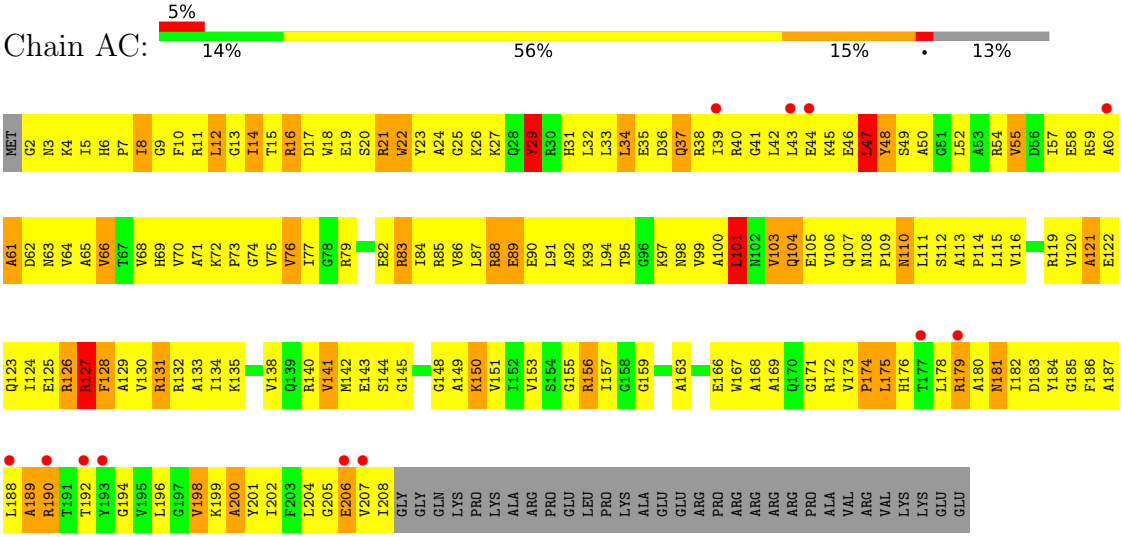
• Molecule 2: 30S ribosomal protein S2

Chain CB:



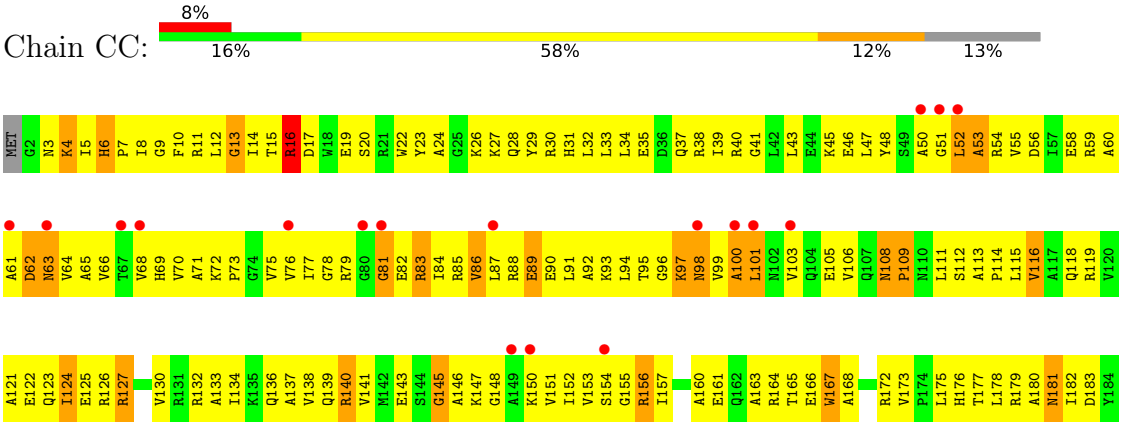
- Molecule 3: 30S ribosomal protein S3

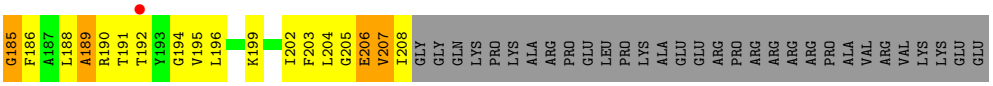
Chain AC:



- Molecule 3: 30S ribosomal protein S3

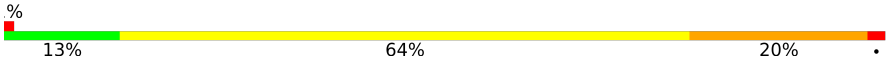
Chain CC:

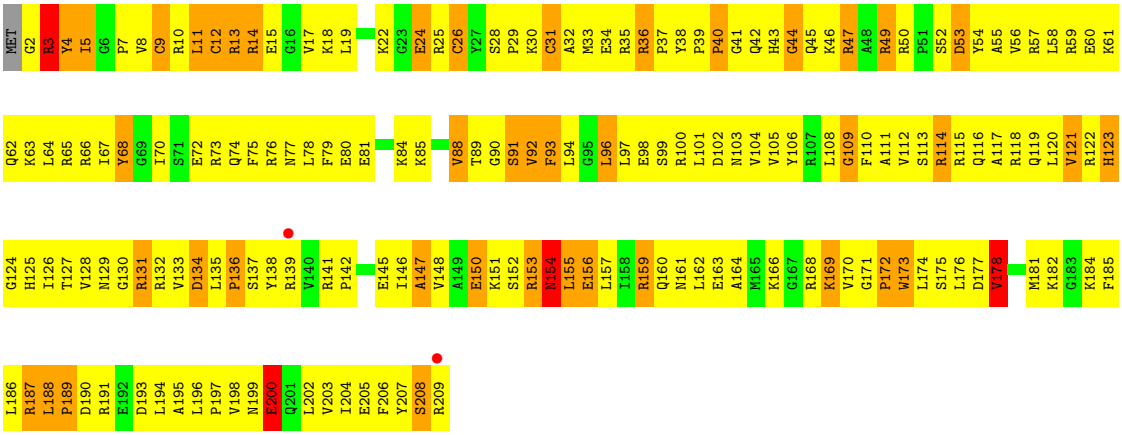




• Molecule 4: 30S ribosomal protein S4

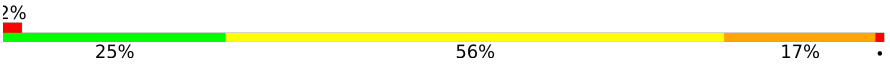
Chain AD:

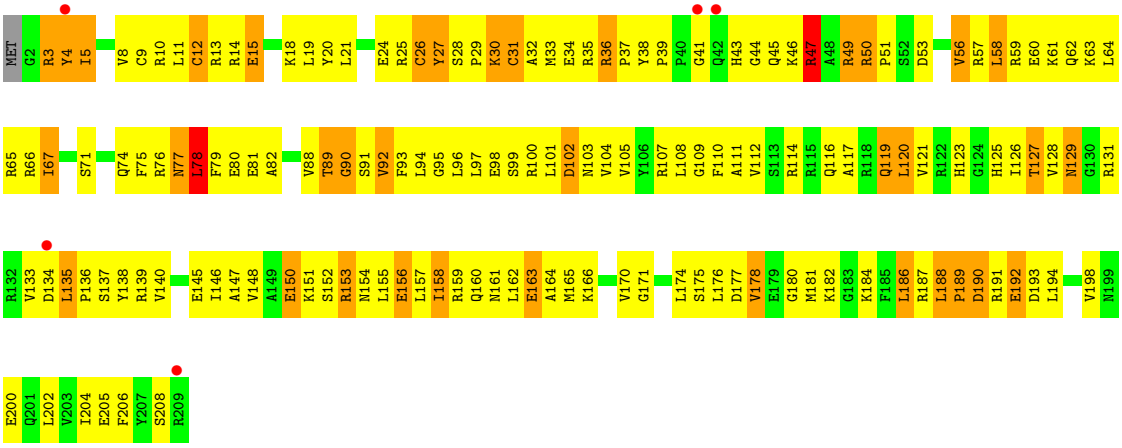




• Molecule 4: 30S ribosomal protein S4

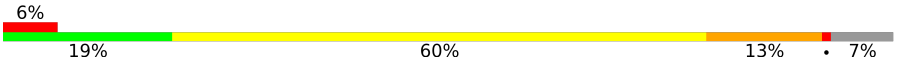
Chain CD:

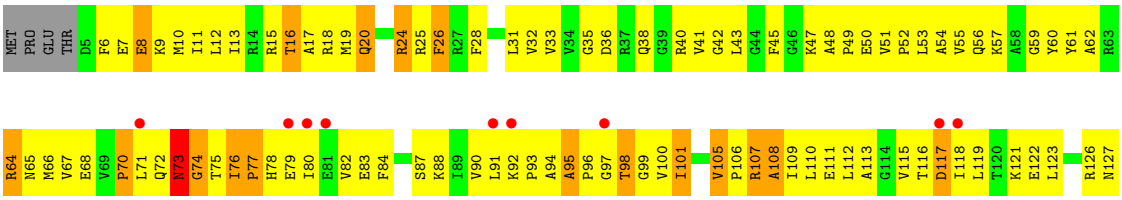


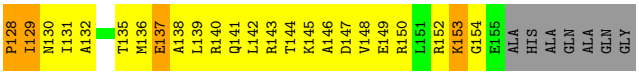


• Molecule 5: 30S ribosomal protein S5

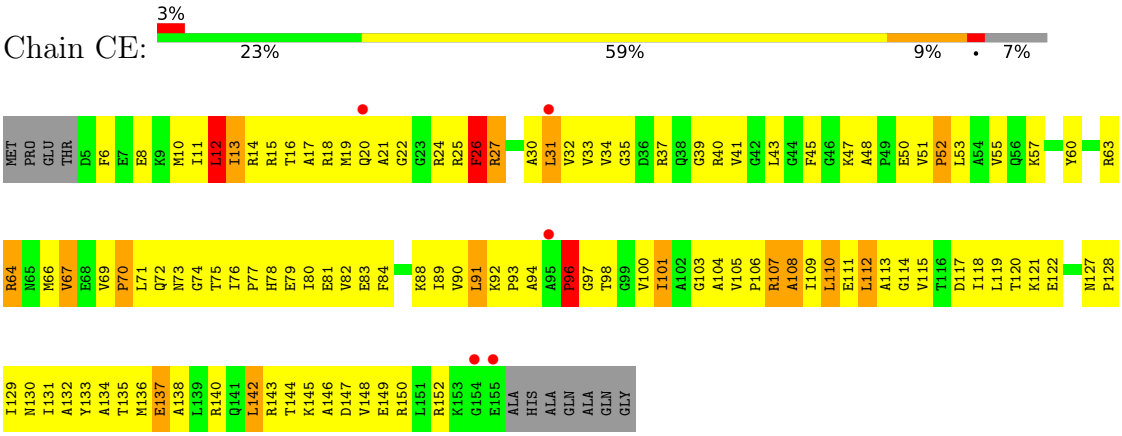
Chain AE:



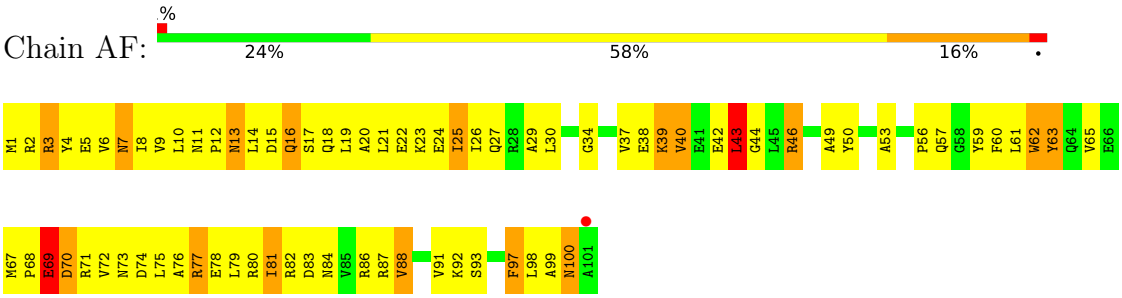




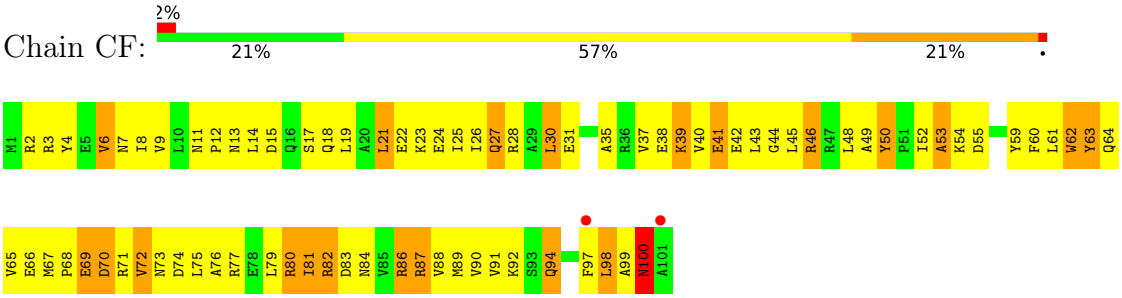
• Molecule 5: 30S ribosomal protein S5



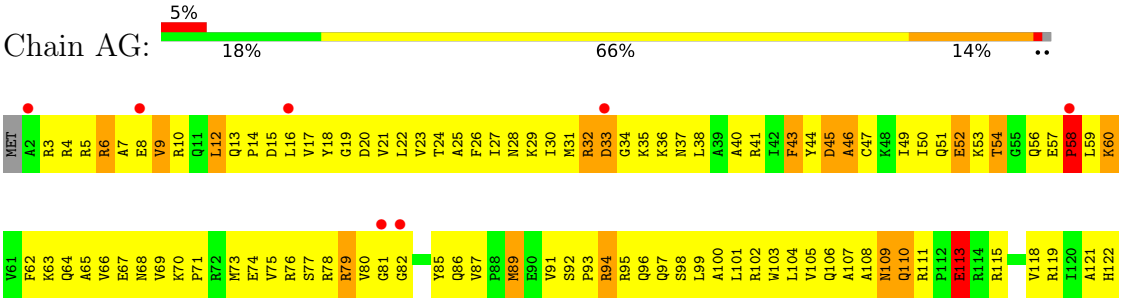
• Molecule 6: 30S ribosomal protein S6



• Molecule 6: 30S ribosomal protein S6

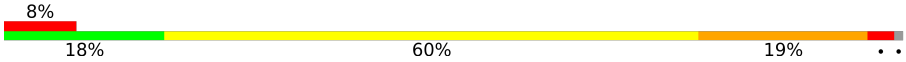


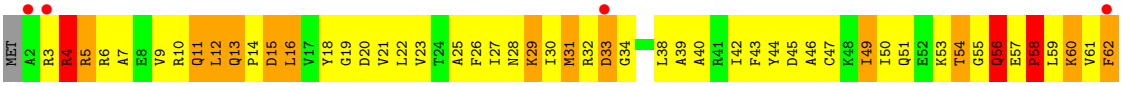
• Molecule 7: 30S ribosomal protein S7

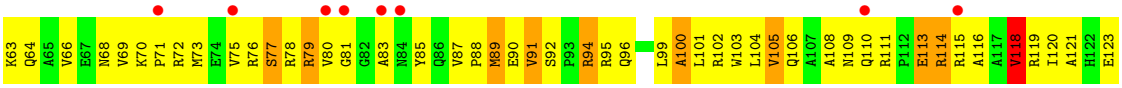


• Molecule 7: 30S ribosomal protein S7

Chain CG:

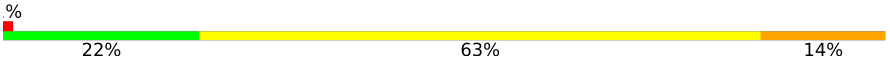


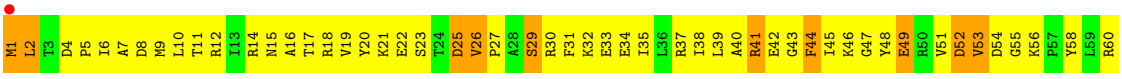


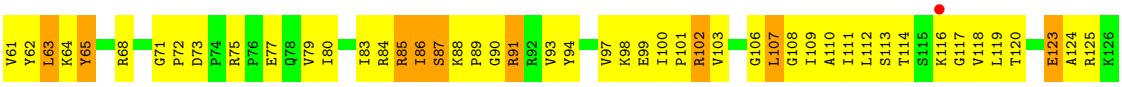


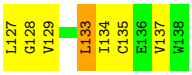
• Molecule 8: 30S ribosomal protein S8

Chain AH:



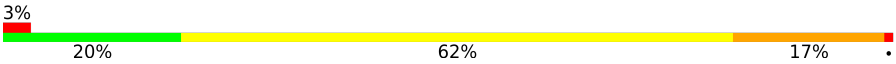


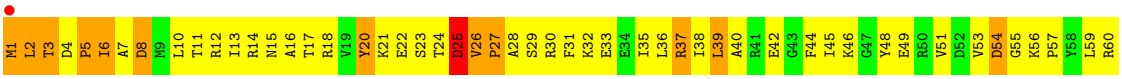


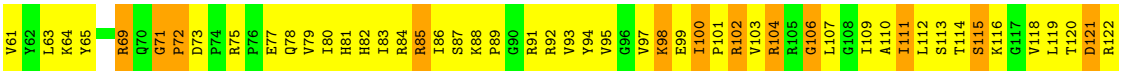


• Molecule 8: 30S ribosomal protein S8

Chain CH:

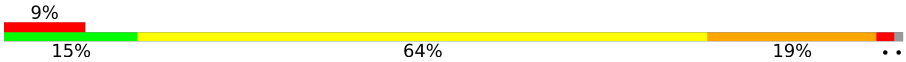


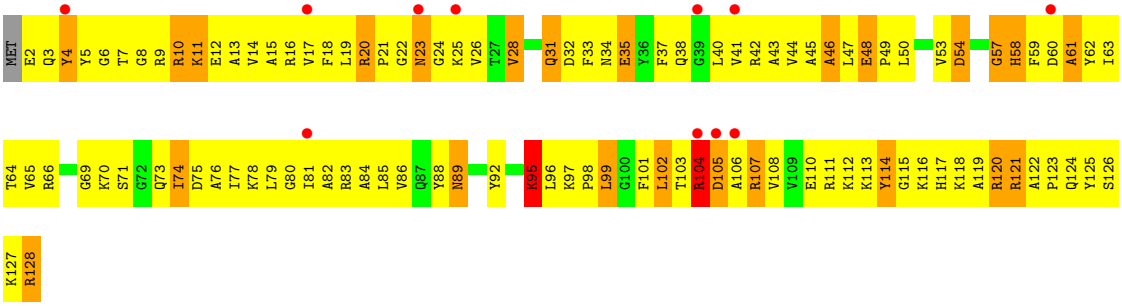




• Molecule 9: 30S ribosomal protein S9

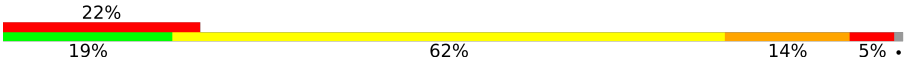
Chain AI:

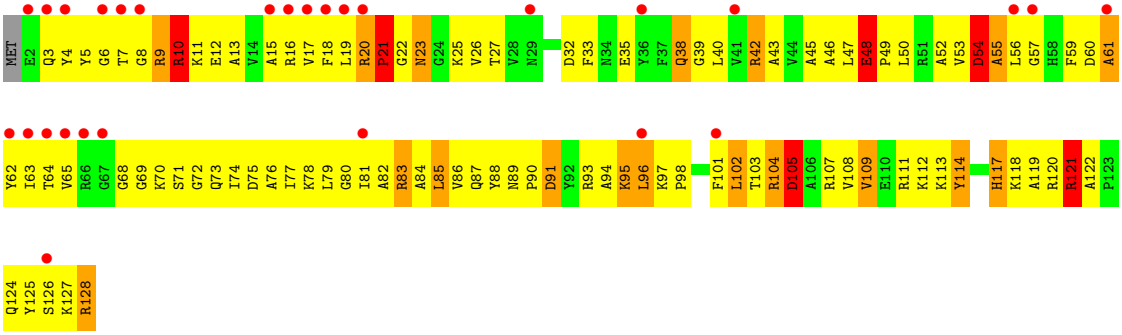




- Molecule 9: 30S ribosomal protein S9

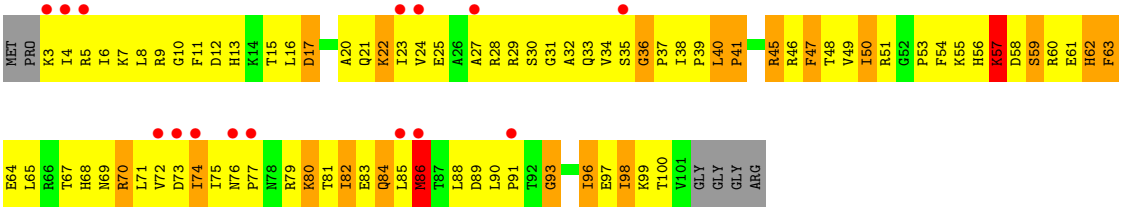
Chain CI:





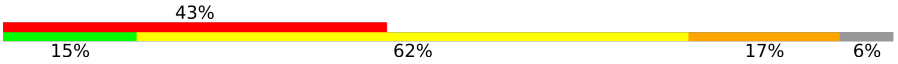
- Molecule 10: 30S ribosomal protein S10

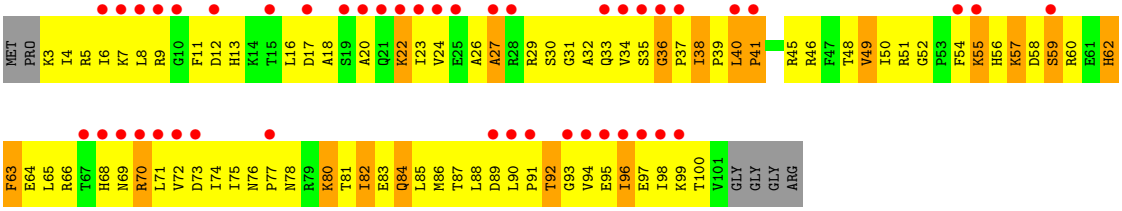
Chain AJ:



- Molecule 10: 30S ribosomal protein S10

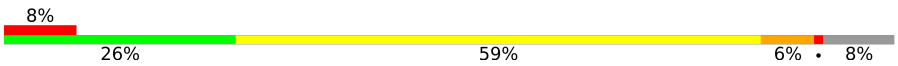
Chain CJ:

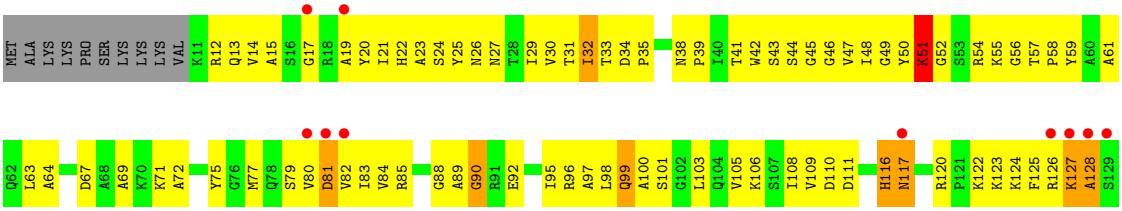




- Molecule 11: 30S ribosomal protein S11

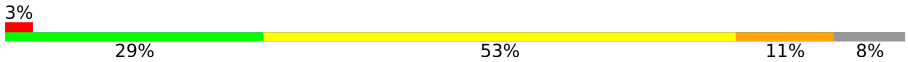
Chain AK:

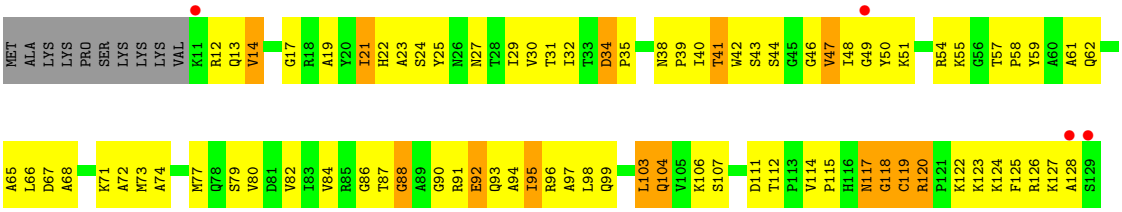




• Molecule 11: 30S ribosomal protein S11

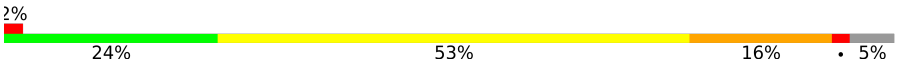
Chain CK:

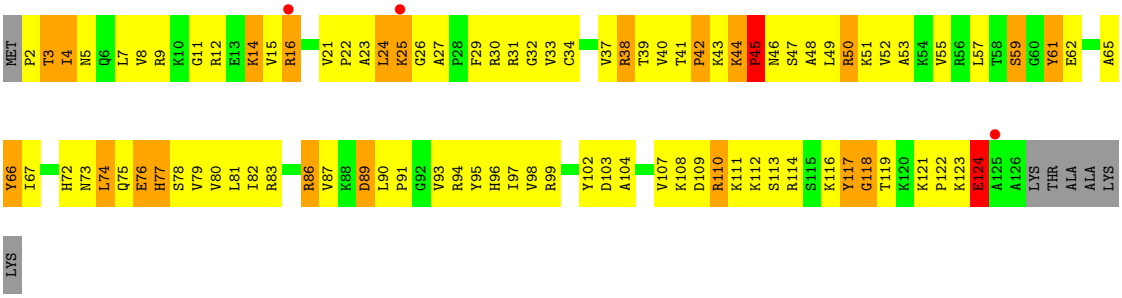




• Molecule 12: 30S ribosomal protein S12

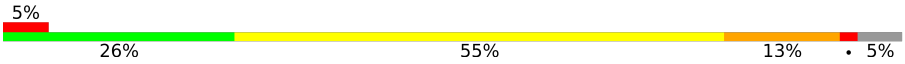
Chain AL:

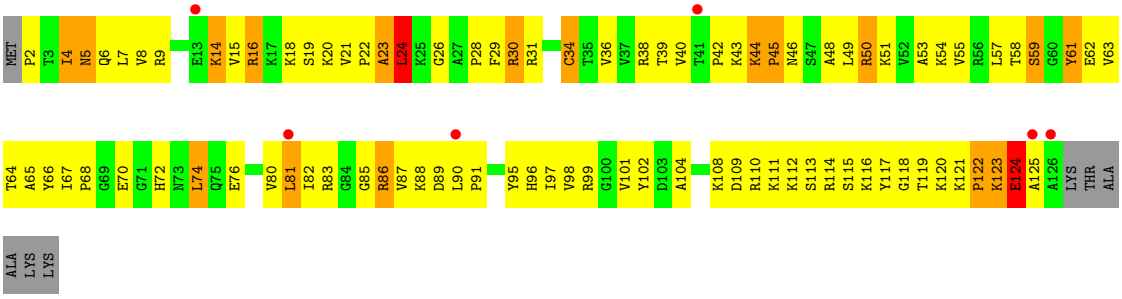




• Molecule 12: 30S ribosomal protein S12

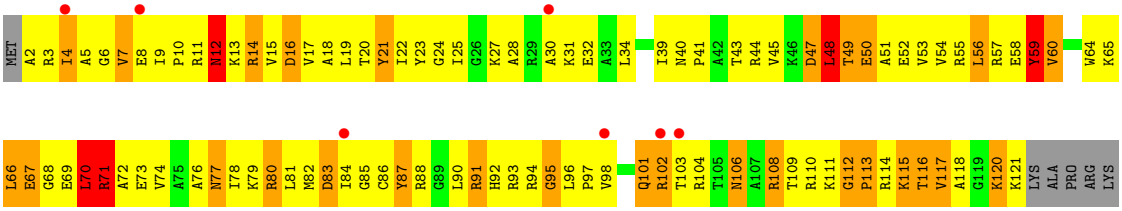
Chain CL:





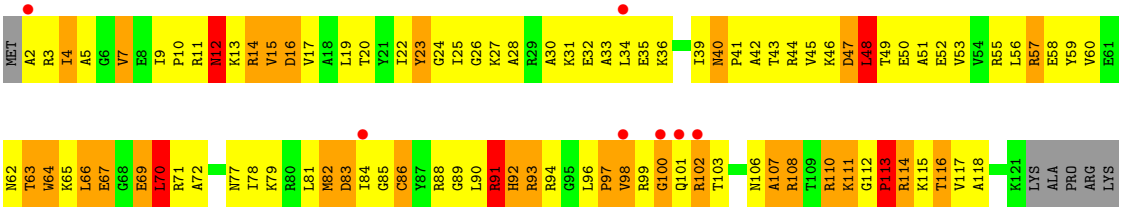
• Molecule 13: 30S ribosomal protein S13

Chain AM:



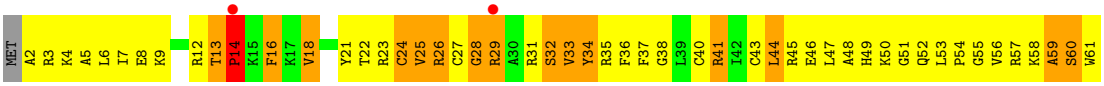
- Molecule 13: 30S ribosomal protein S13

Chain CM:



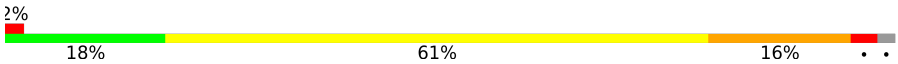
- Molecule 14: 30S ribosomal protein S14

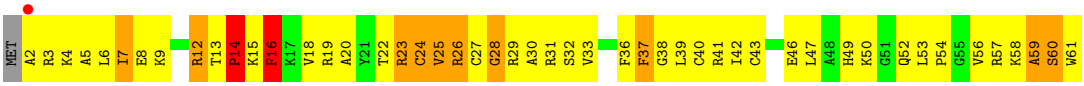
Chain AN:



- Molecule 14: 30S ribosomal protein S14

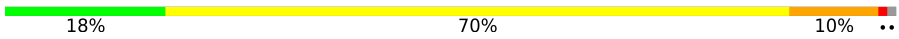
Chain CN:

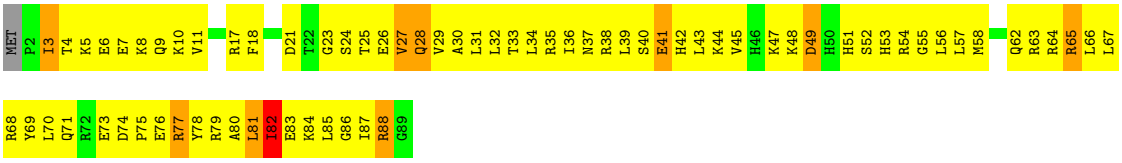




- Molecule 15: 30S ribosomal protein S15

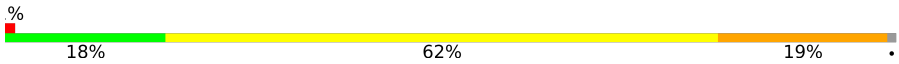
Chain AO:

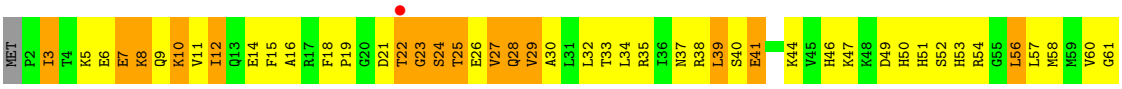


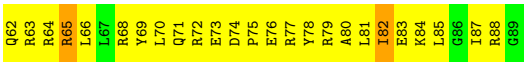


- Molecule 15: 30S ribosomal protein S15

Chain CO:

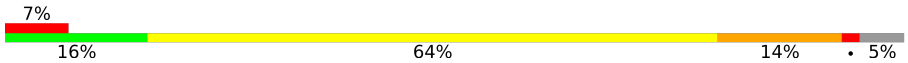


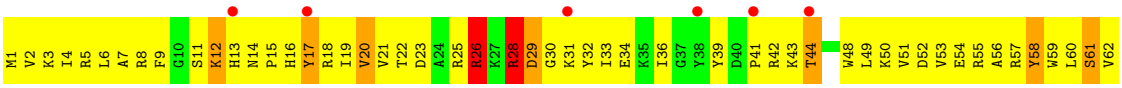


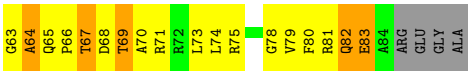


• Molecule 16: 30S ribosomal protein S16

Chain AP:

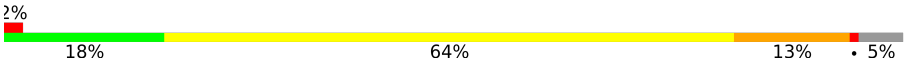






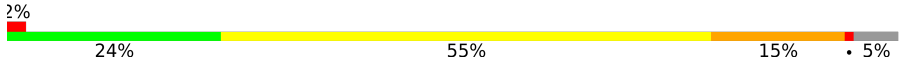
• Molecule 16: 30S ribosomal protein S16

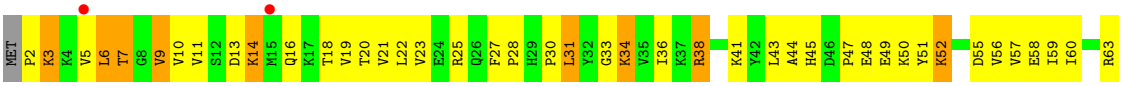
Chain CP:

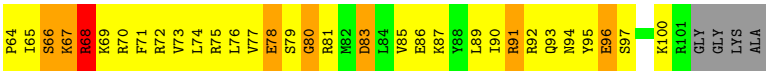


• Molecule 17: 30S ribosomal protein S17

Chain AQ:

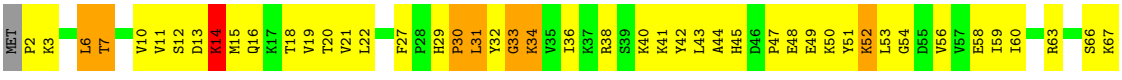






• Molecule 17: 30S ribosomal protein S17

Chain CQ:

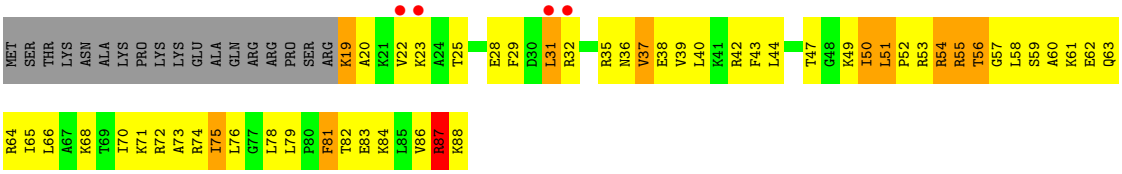


• Molecule 18: 30S ribosomal protein S18

Chain AR:

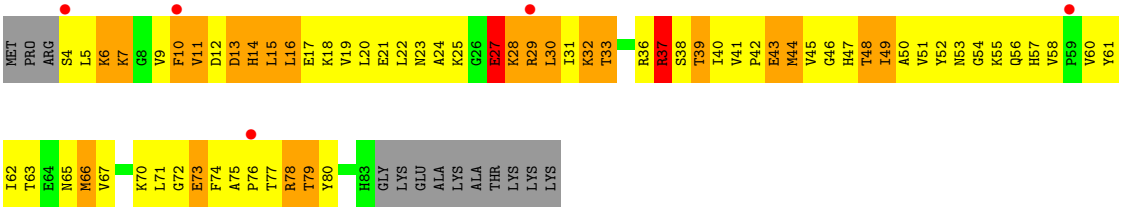
- Molecule 18: 30S ribosomal protein S18

Chain CR:



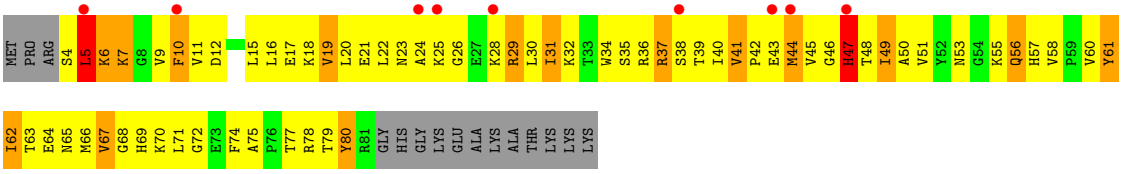
- Molecule 19: 30S ribosomal protein S19

Chain AS:



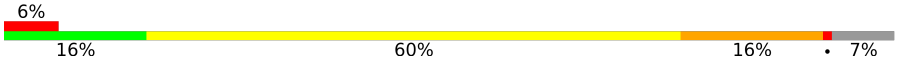
- Molecule 19: 30S ribosomal protein S19

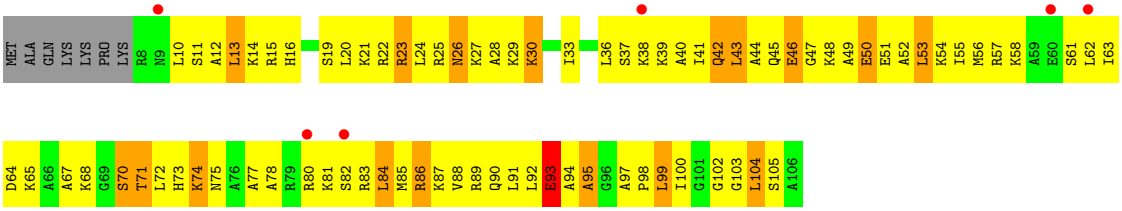
Chain CS:



- Molecule 20: 30S ribosomal protein S20

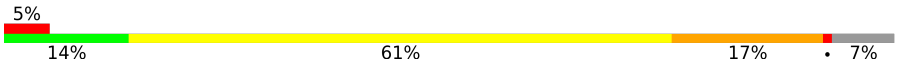
Chain AT:

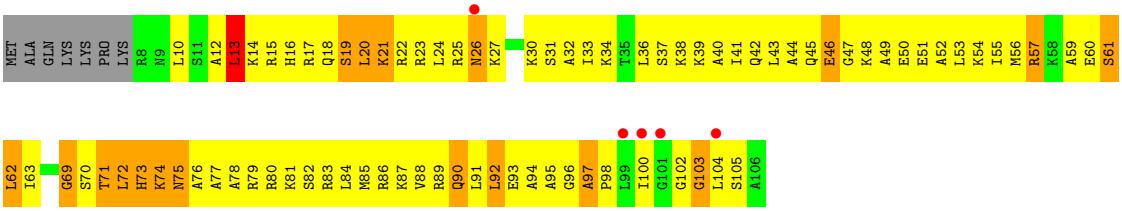




- Molecule 20: 30S ribosomal protein S20

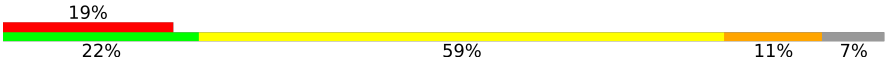
Chain CT:





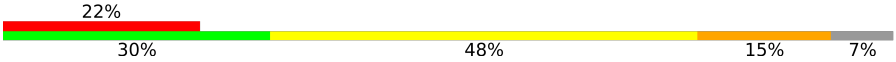
• Molecule 21: 30S ribosomal protein Thx

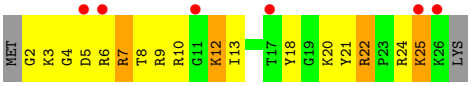
Chain AU:



• Molecule 21: 30S ribosomal protein Thx

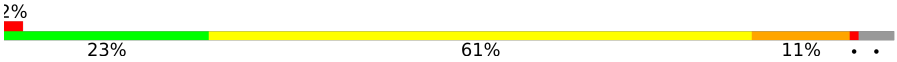
Chain CU:

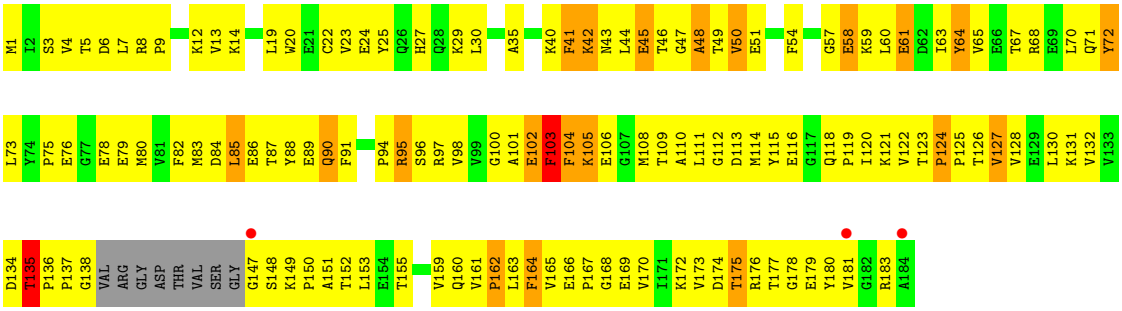




• Molecule 22: Elongation factor P

Chain AV:





• Molecule 22: Elongation factor P

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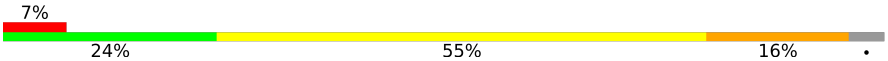

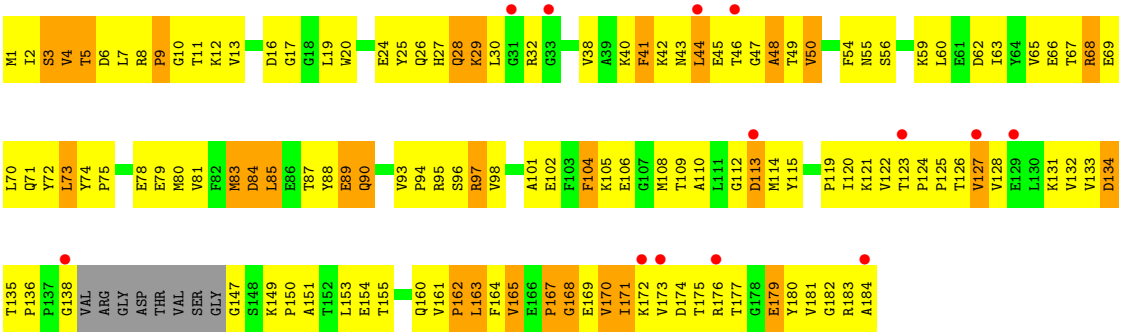

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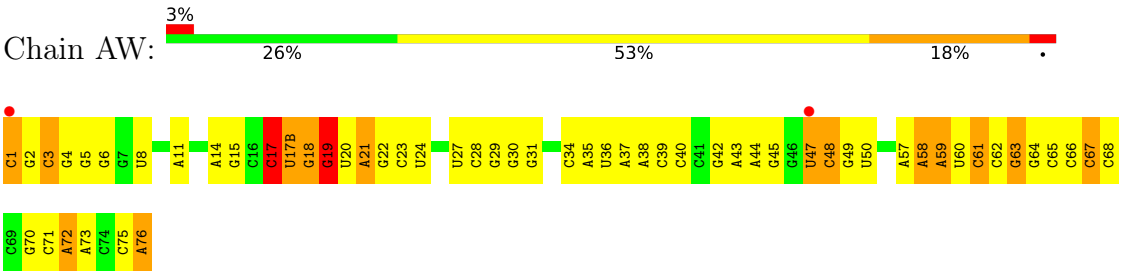

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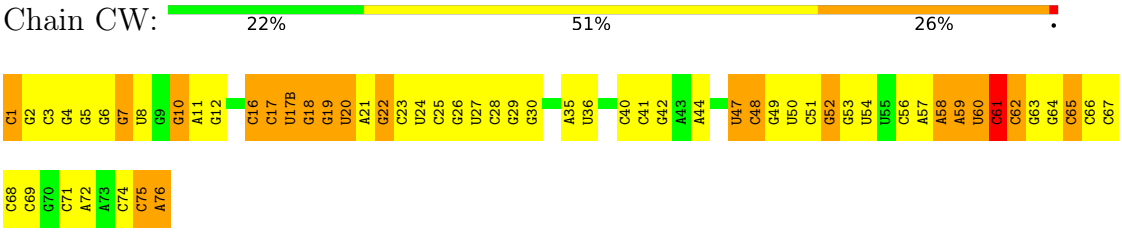
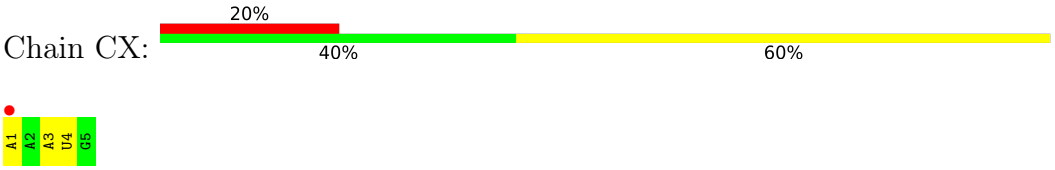


• Molecule 24: RNA (5'-R(P*AP*AP*AP*UP*G)-3')

Chain AX:

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

Chain CX:



• Molecule 25: 23S ribosomal RNA

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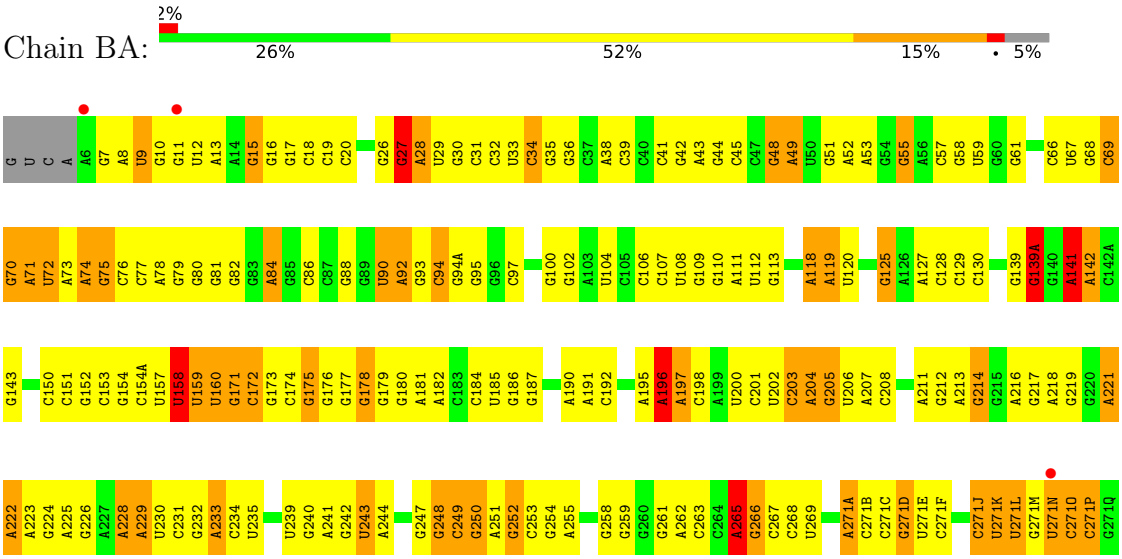

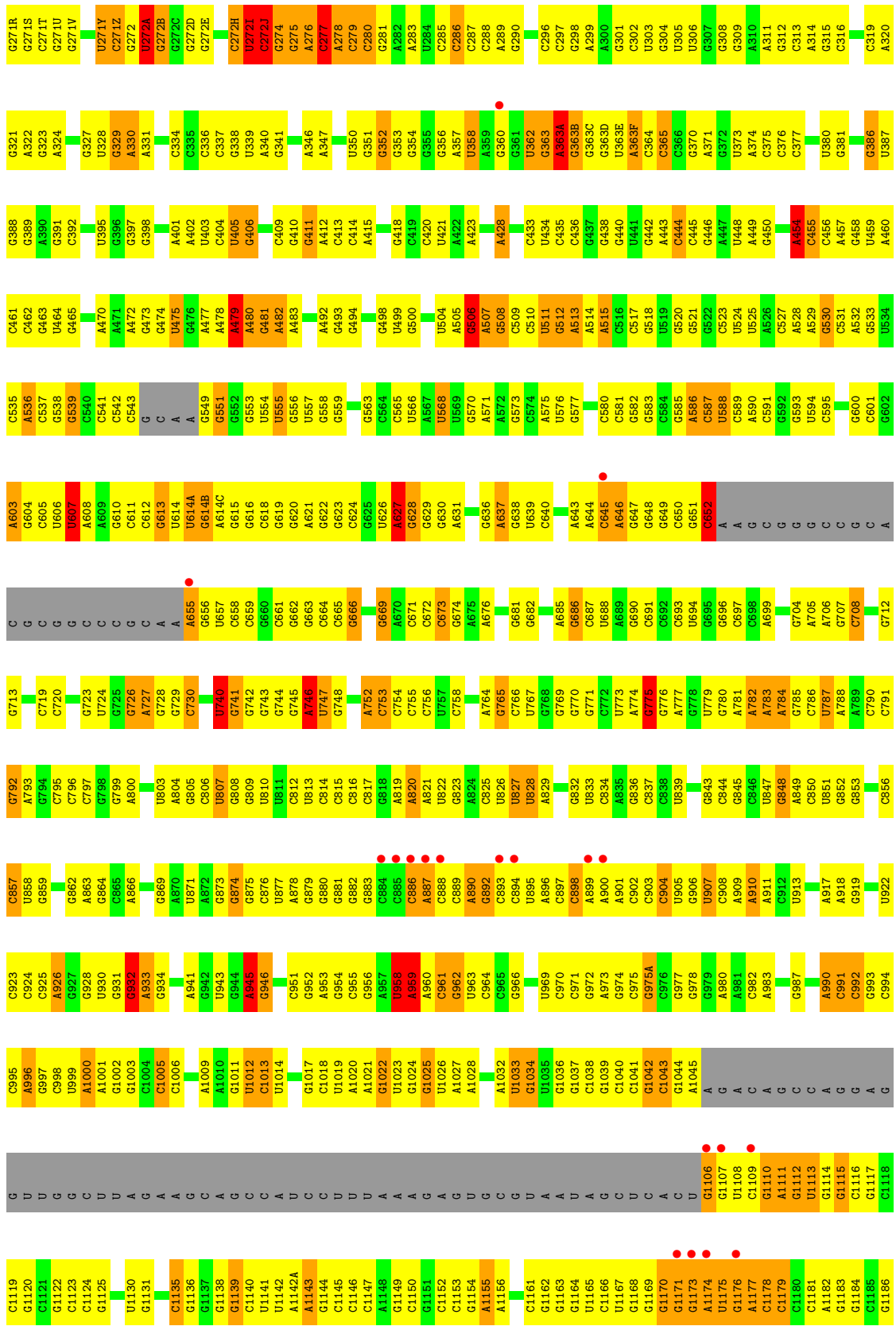
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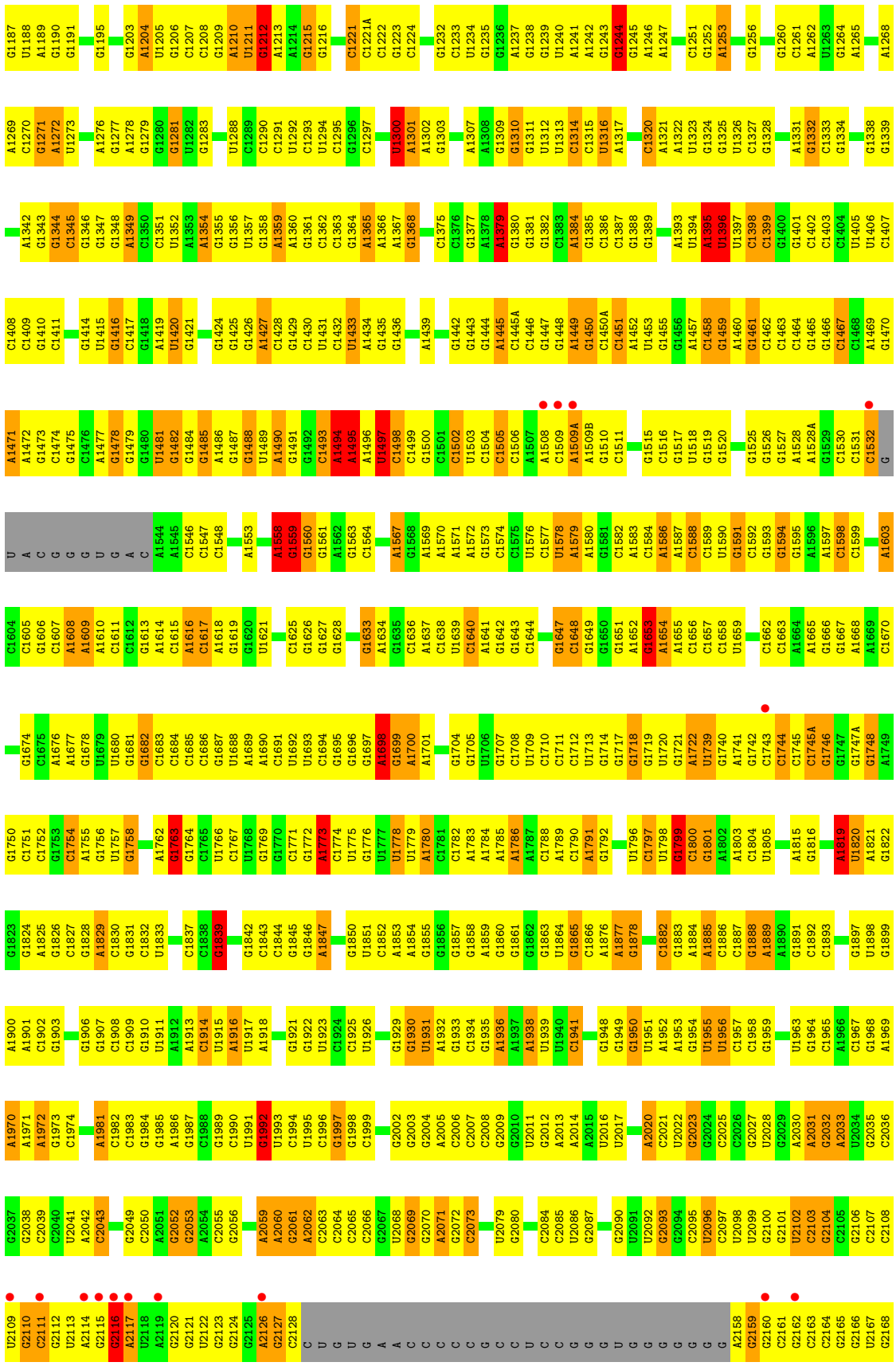
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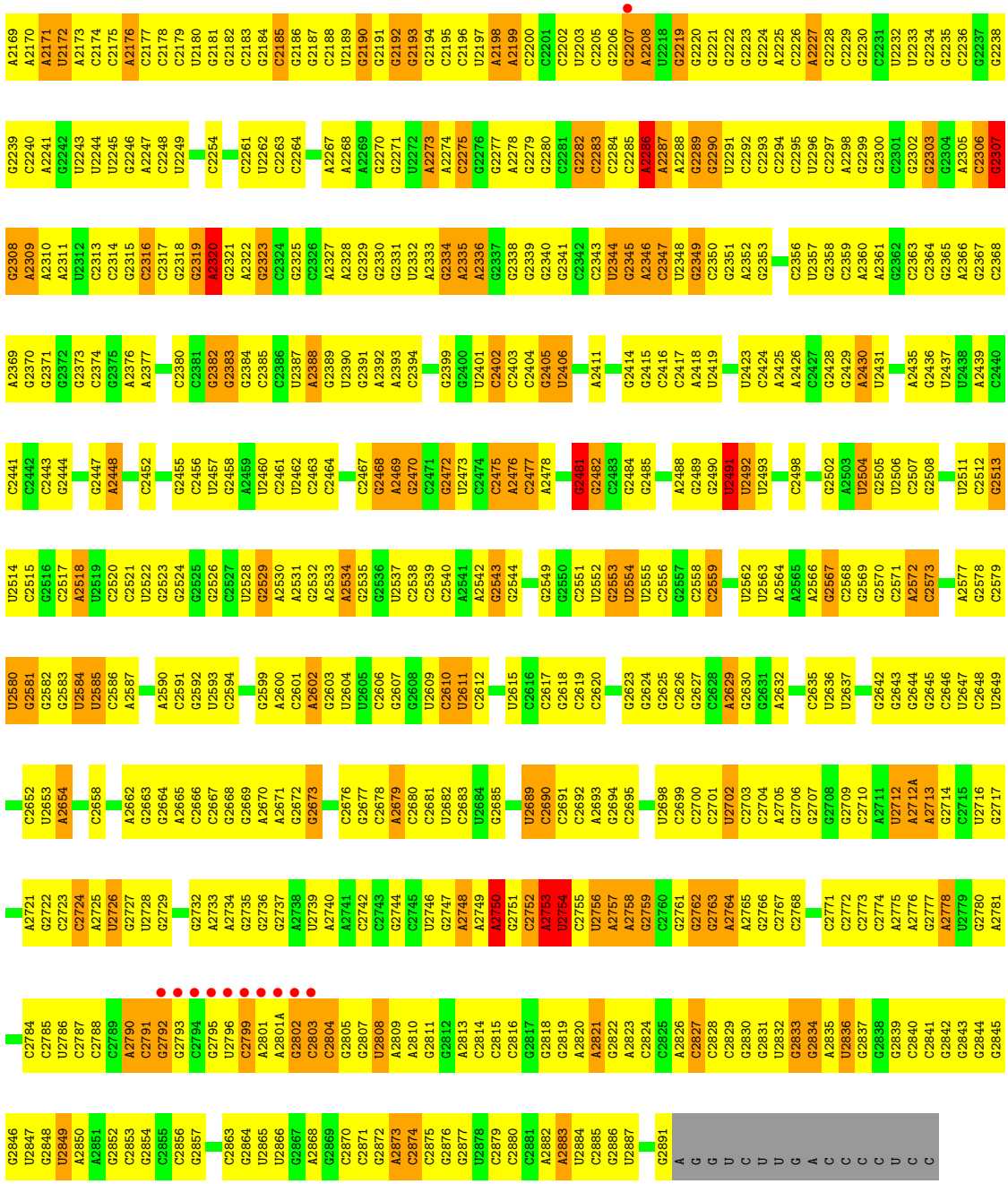

• Molecule 25: 23S ribosomal RNA

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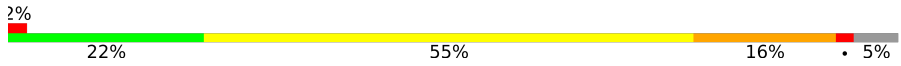

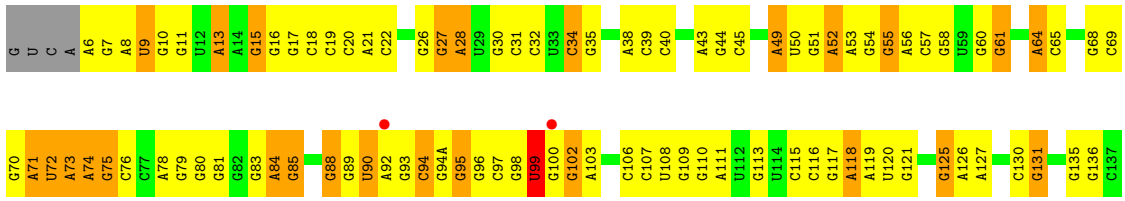

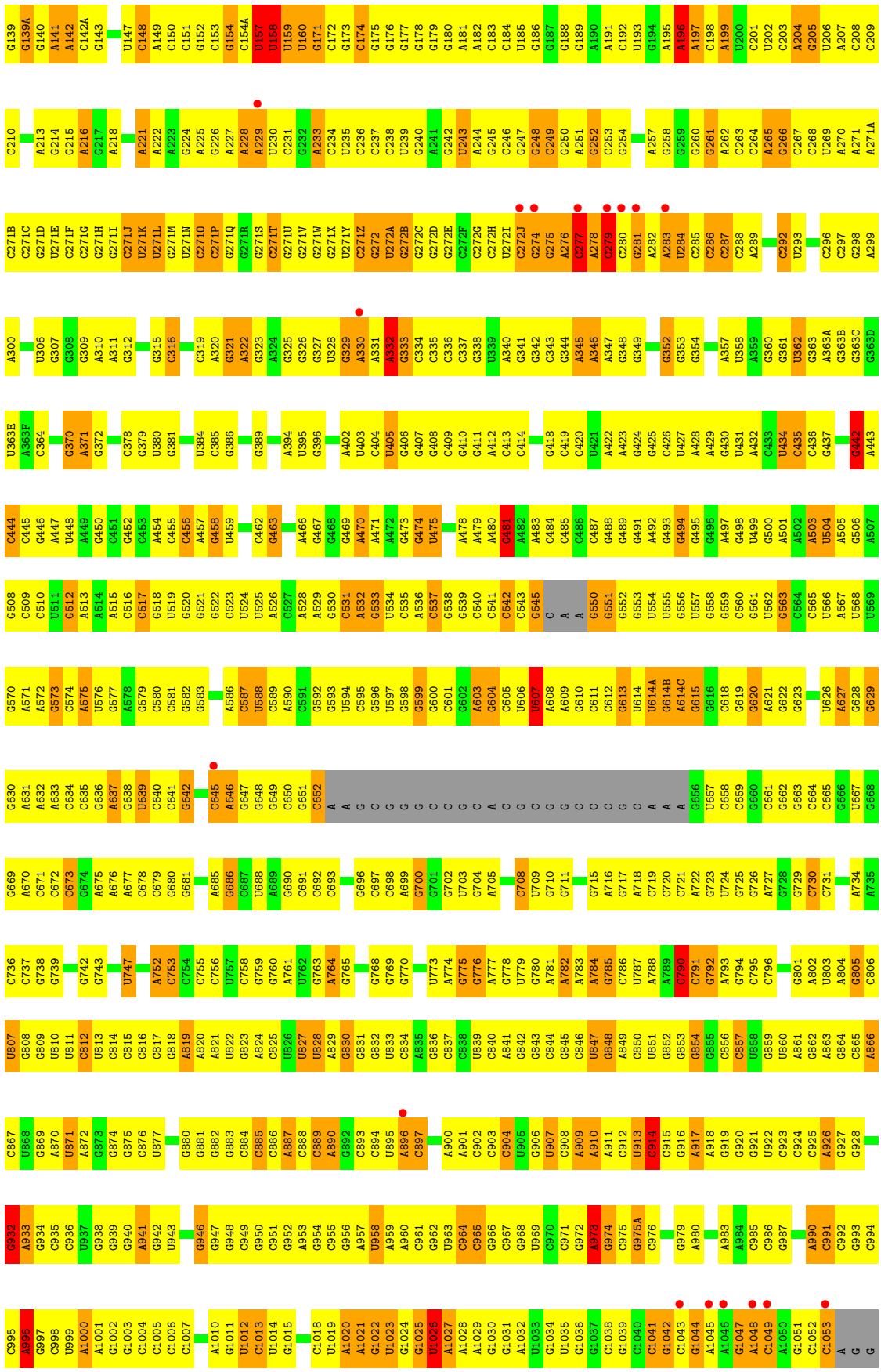
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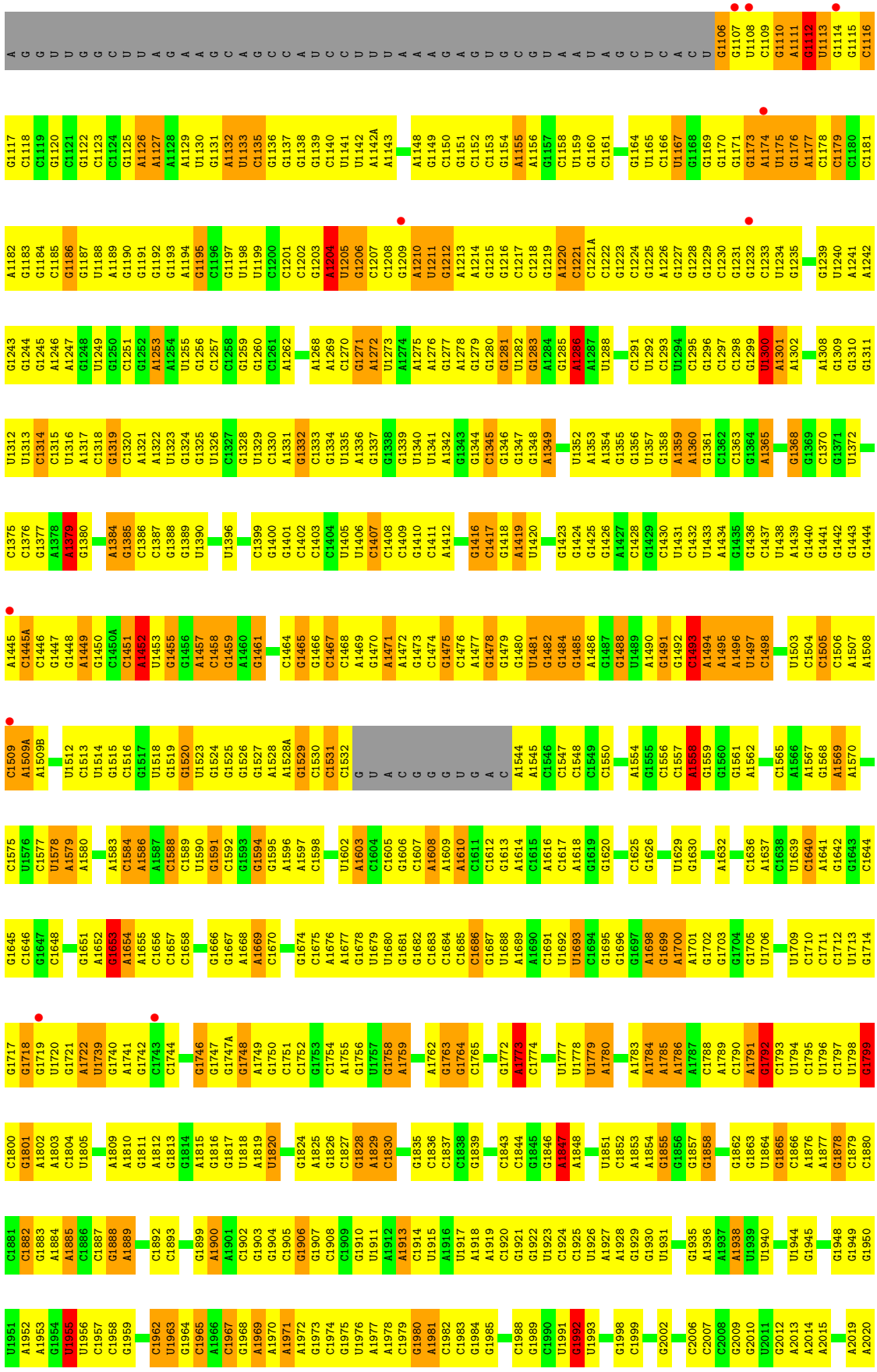

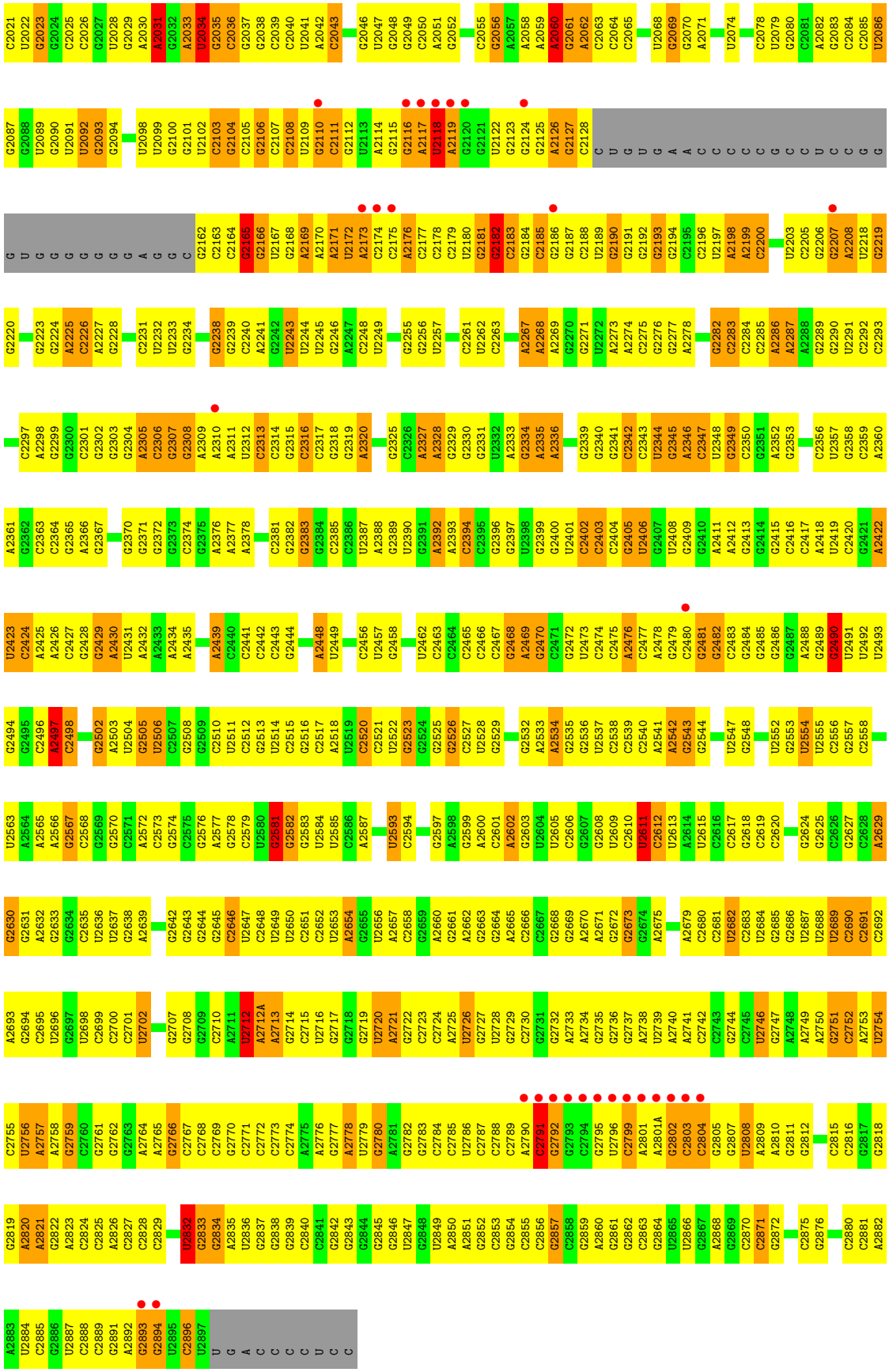
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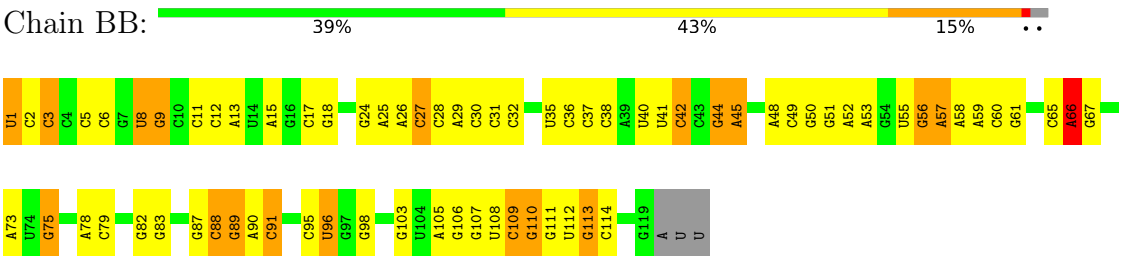
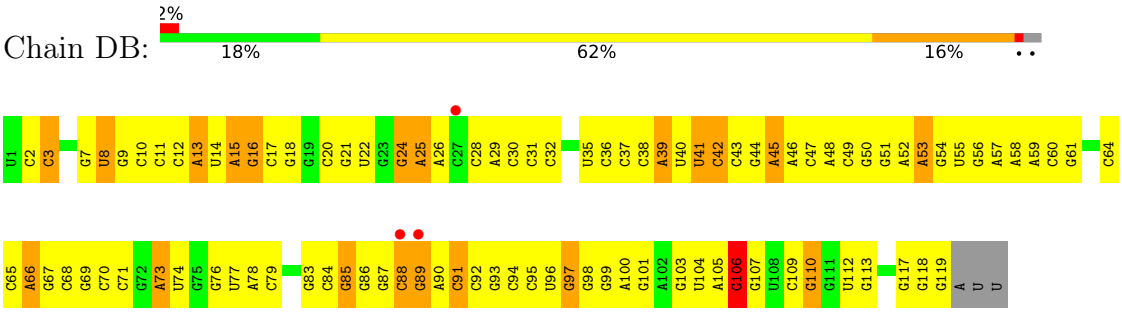
- Molecule 26: 5S ribosomal RNA

Chain BB:



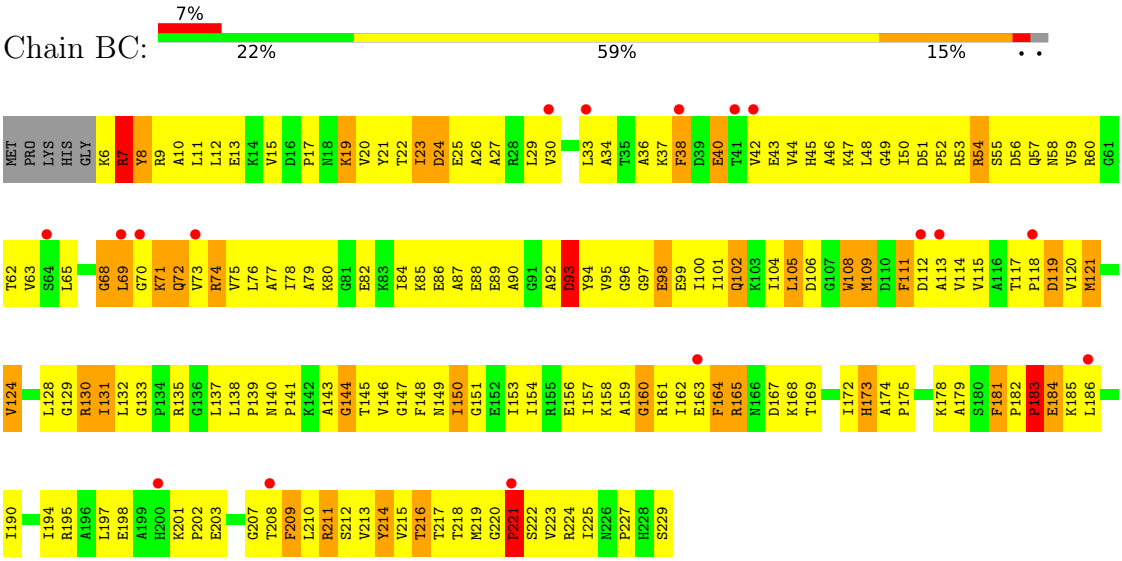
- Molecule 26: 5S ribosomal RNA

Chain DB:



- Molecule 27: 50S ribosomal protein L1

Chain BC:



- Molecule 27: 50S ribosomal protein L1

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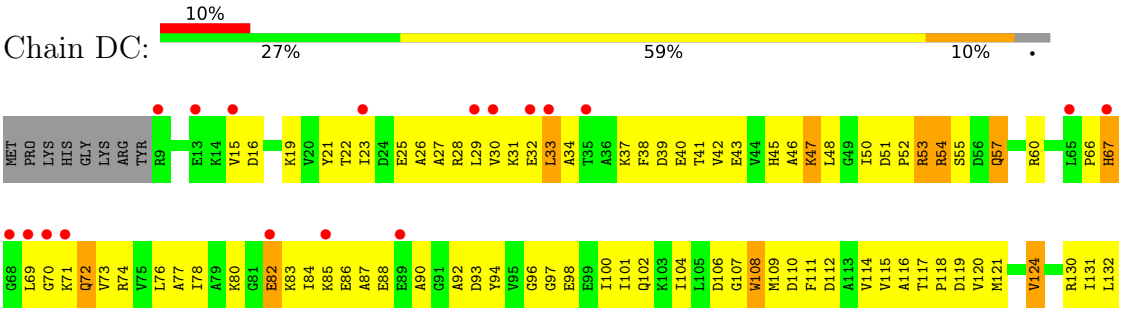
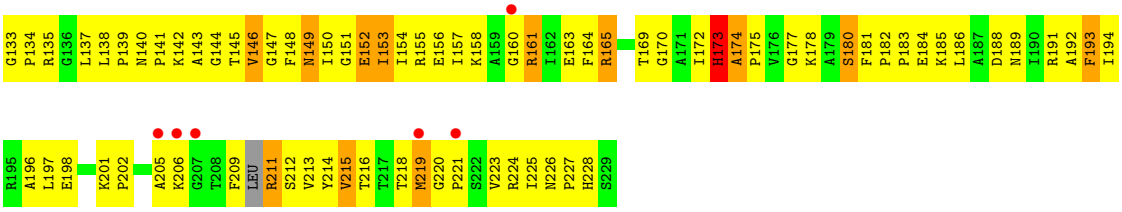
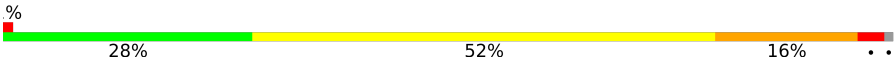
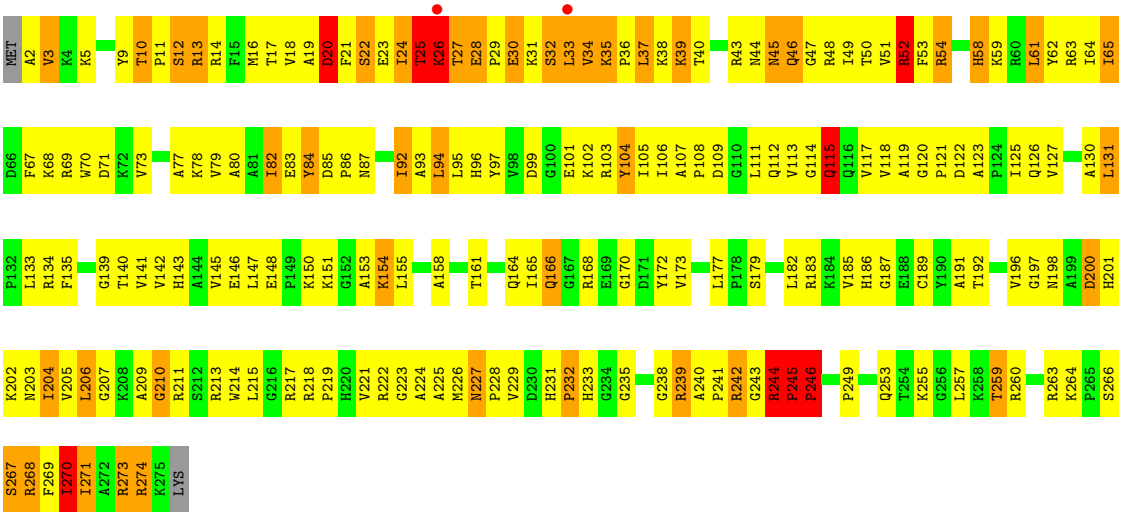




- Molecule 28: 50S ribosomal protein L2

Chain BD:





- Molecule 28: 50S ribosomal protein L2

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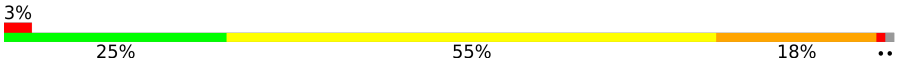
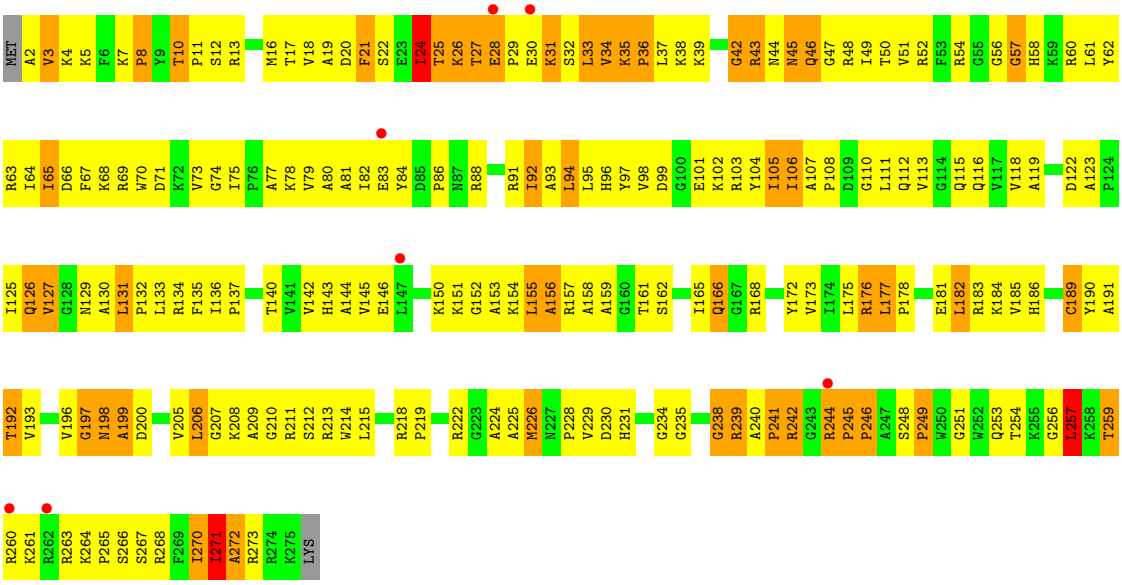
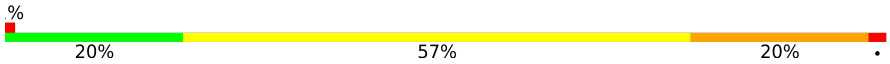
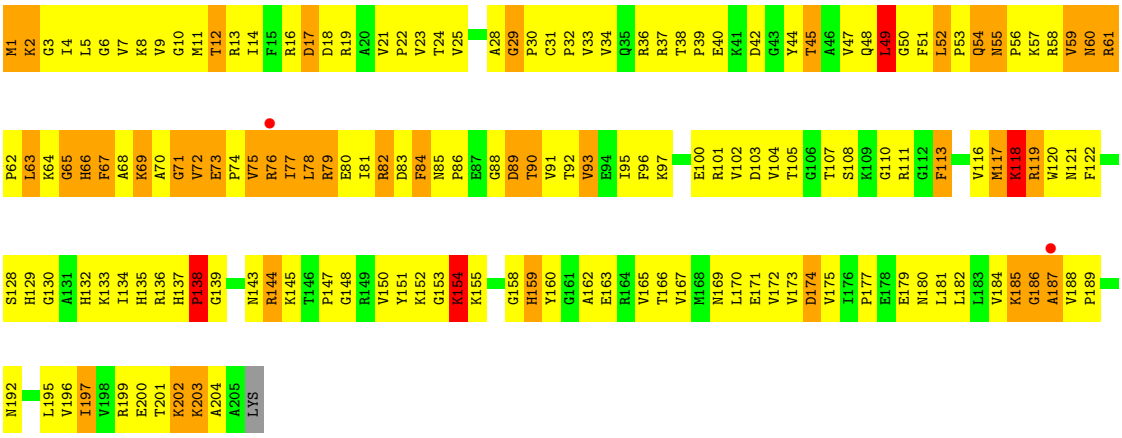




- Molecule 29: 50S ribosomal protein L3

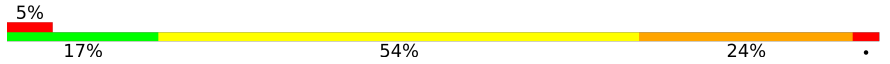
Chain BE:

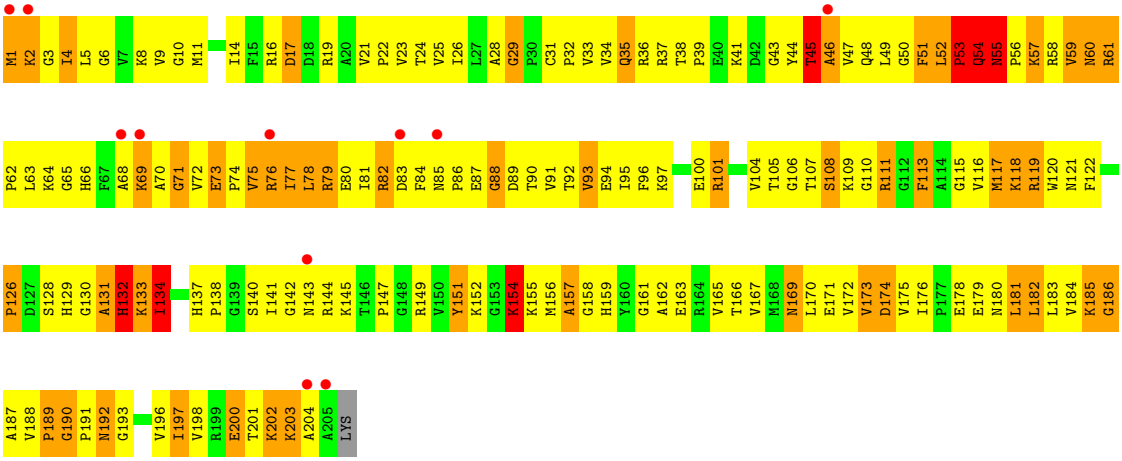




- Molecule 29: 50S ribosomal protein L3

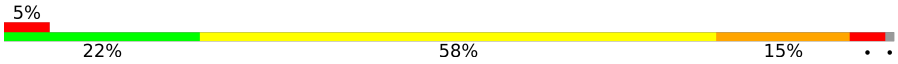
Chain DE:

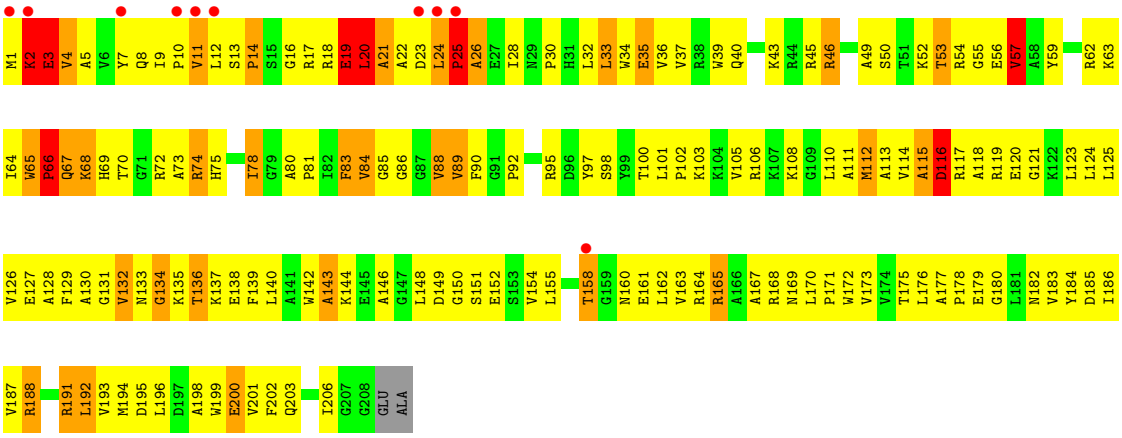




- Molecule 30: 50S ribosomal protein L4

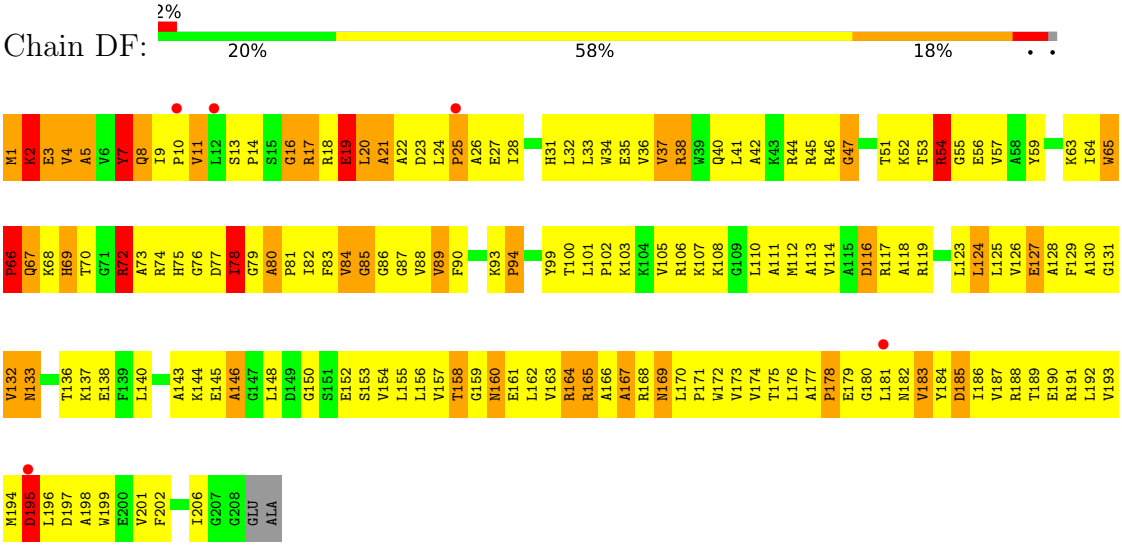
Chain BF:





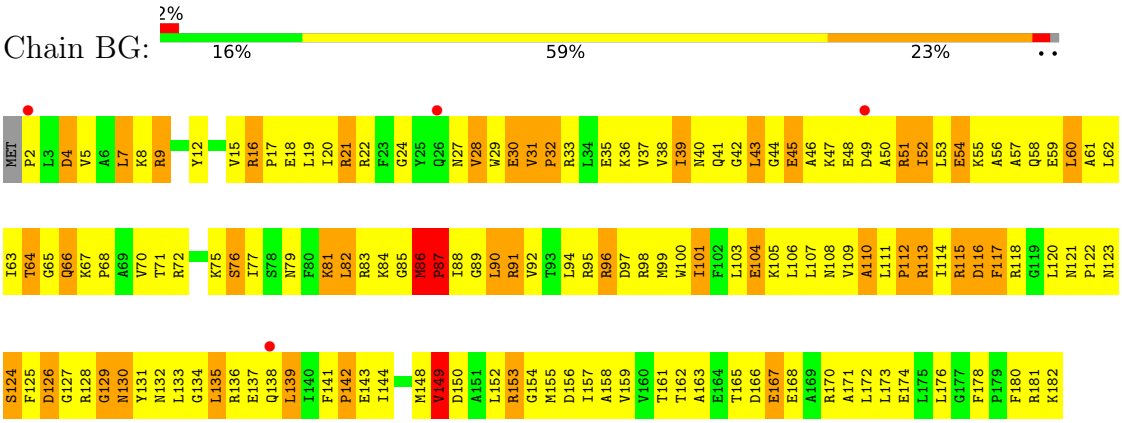
• Molecule 30: 50S ribosomal protein L4

Chain DF:



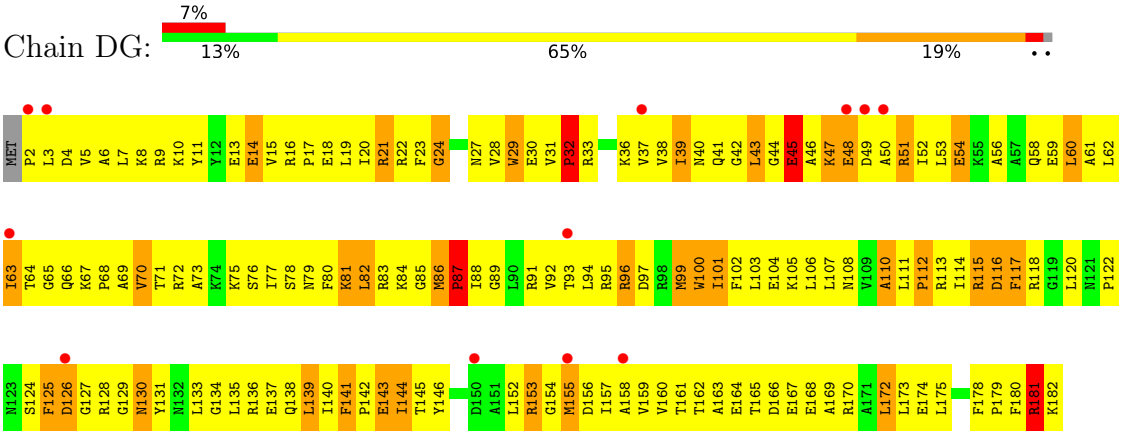
• Molecule 31: 50S ribosomal protein L5

Chain BG:



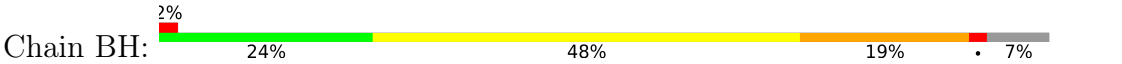
• Molecule 31: 50S ribosomal protein L5

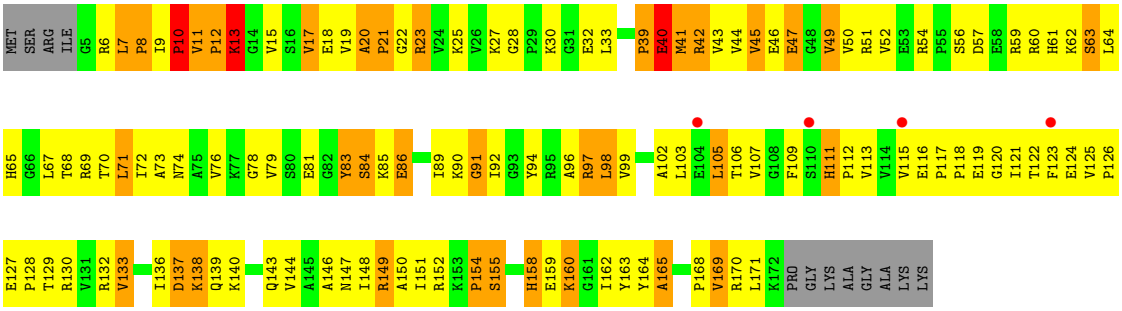
Chain DG:



• Molecule 32: 50S ribosomal protein L6

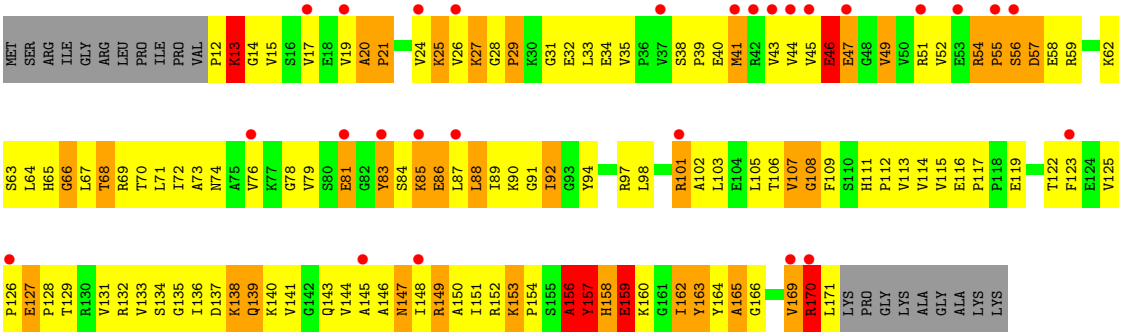
Chain BH:





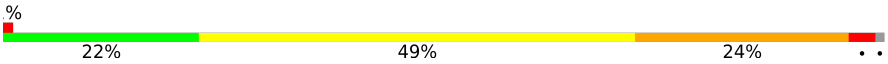
- Molecule 32: 50S ribosomal protein L6

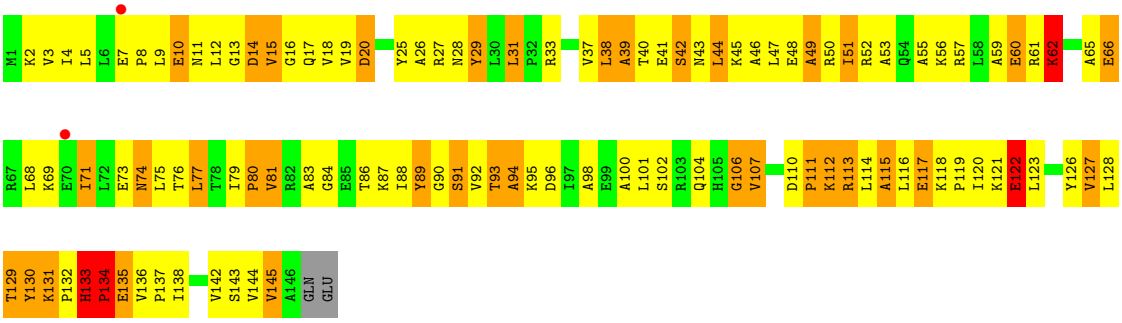
Chain DH:



- Molecule 33: 50S ribosomal protein L9

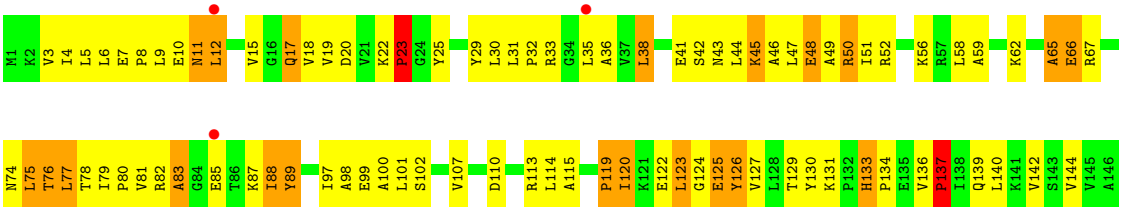
Chain BI:





- Molecule 33: 50S ribosomal protein L9

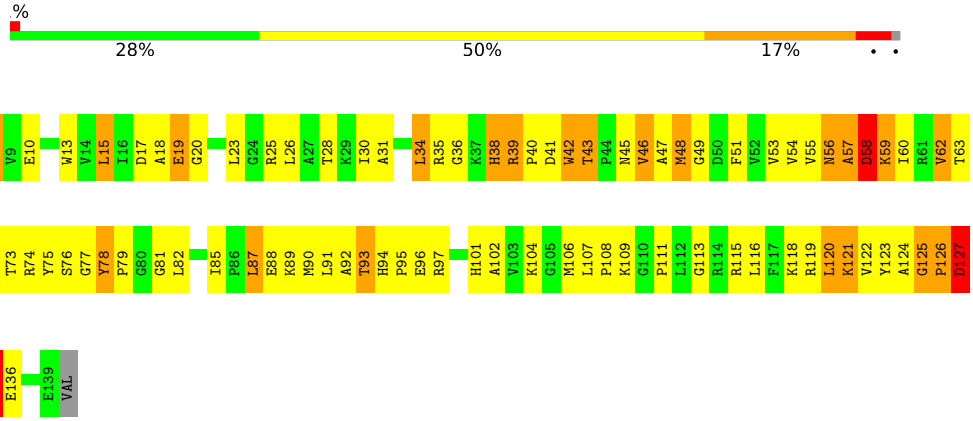
Chain DI:



GLN
GLU

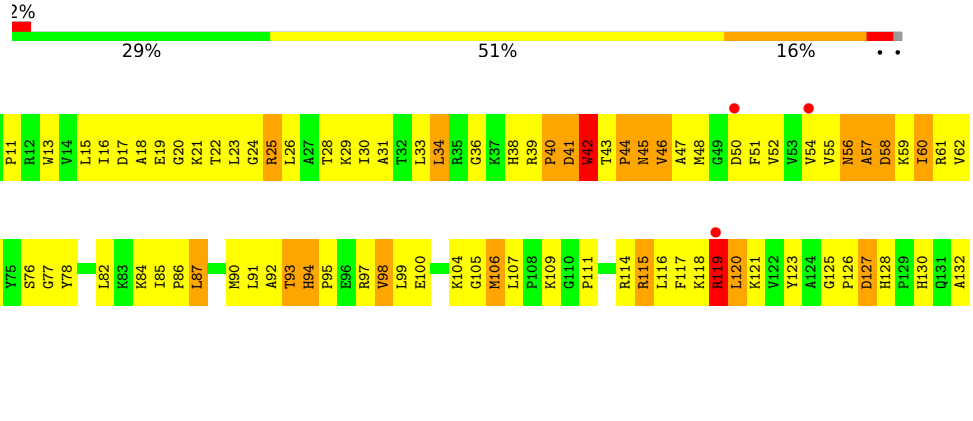
• Molecule 34: 50S ribosomal protein L13

Chain BN:



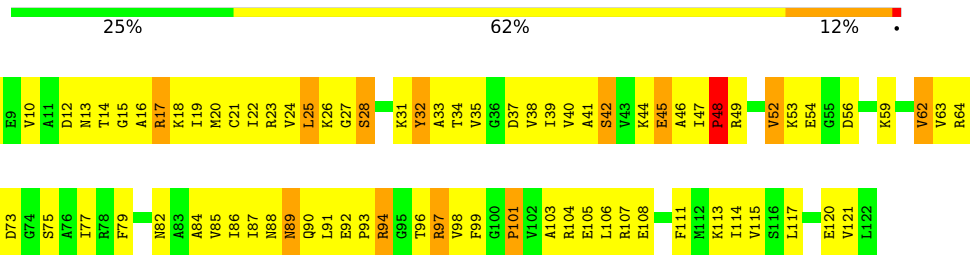
• Molecule 34: 50S ribosomal protein L13

Chain DN:



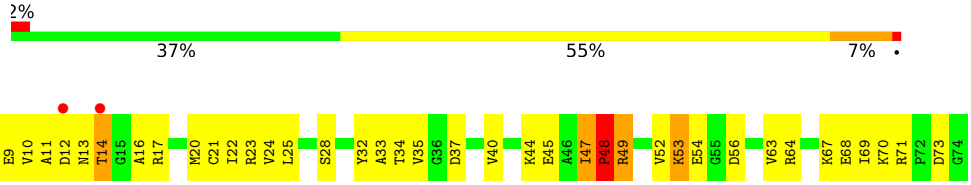
• Molecule 35: 50S ribosomal protein L14

Chain BO:



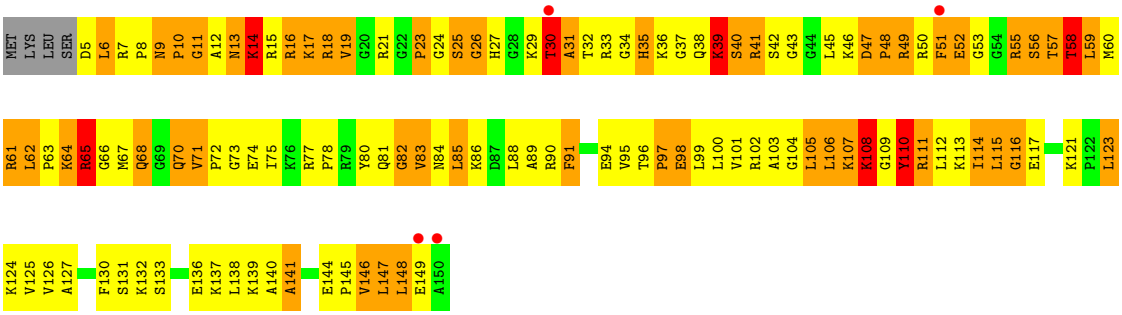
• Molecule 35: 50S ribosomal protein L14

Chain DO:



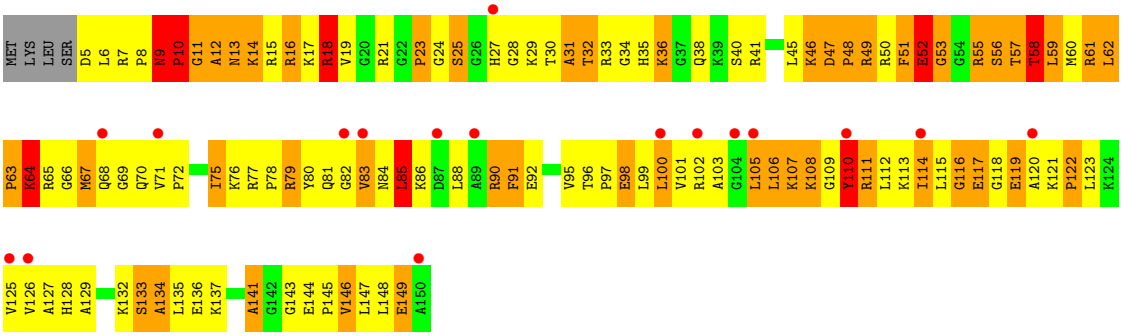
• Molecule 36: 50S ribosomal protein L15

Chain BP:



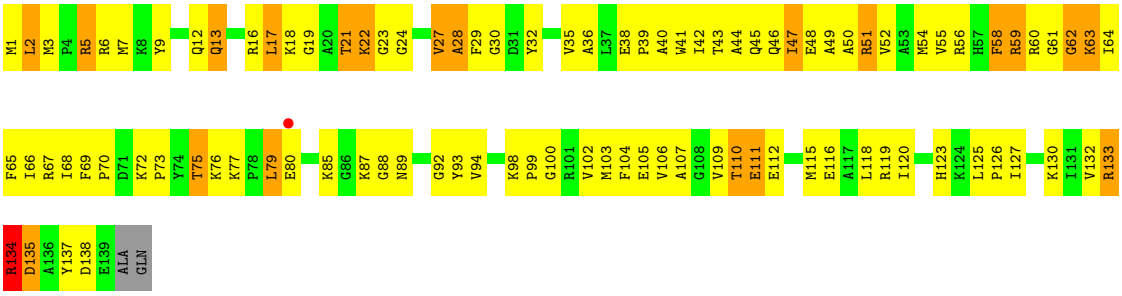
• Molecule 36: 50S ribosomal protein L15

Chain DP:



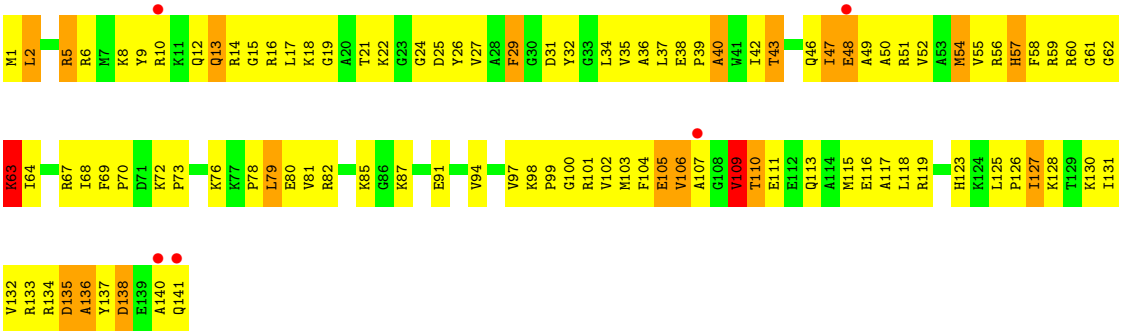
• Molecule 37: 50S ribosomal protein L16

Chain BQ:



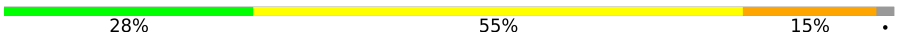
• Molecule 37: 50S ribosomal protein L16

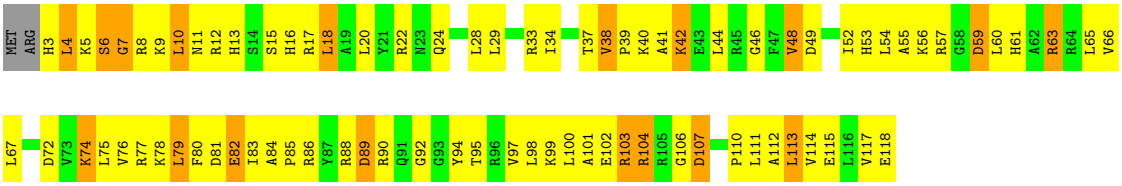
Chain DQ:



- Molecule 38: 50S ribosomal protein L17

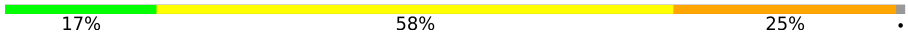
Chain BR:

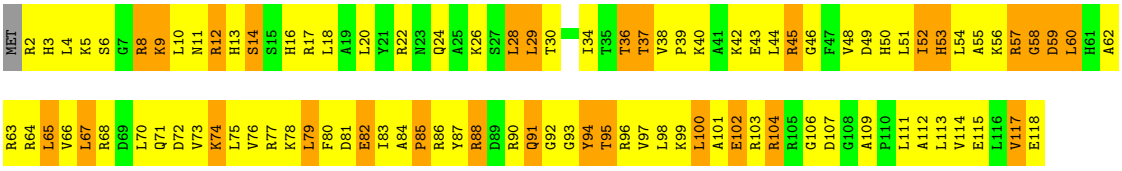




- Molecule 38: 50S ribosomal protein L17

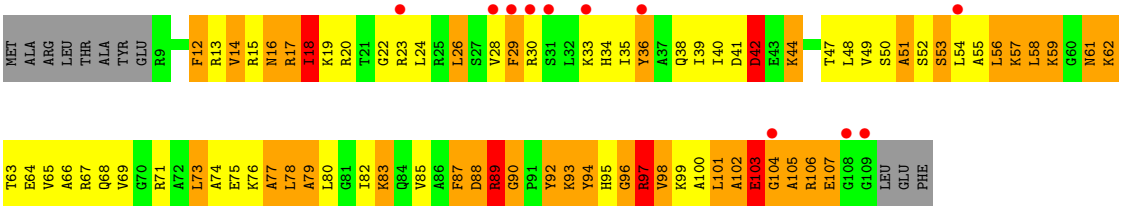
Chain DR:





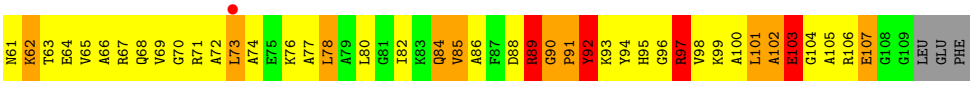
- Molecule 39: 50S ribosomal protein L18

Chain BS:



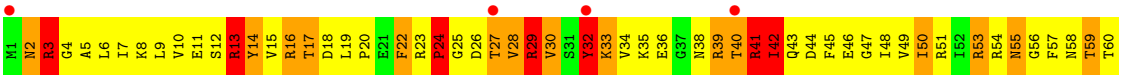
- Molecule 39: 50S ribosomal protein L18

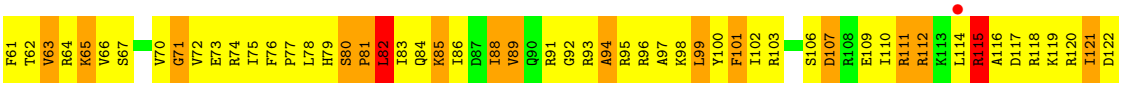
Chain DS:

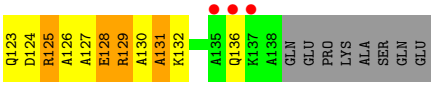


• Molecule 40: 50S ribosomal protein L19

Chain BT:

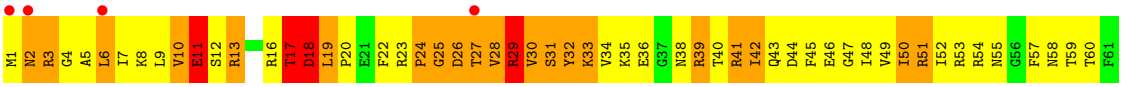


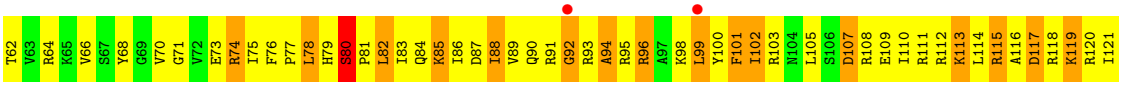




• Molecule 40: 50S ribosomal protein L19

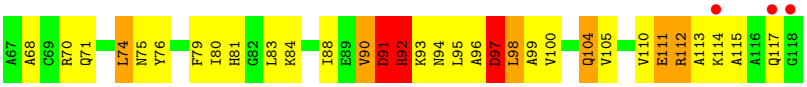
Chain DT:





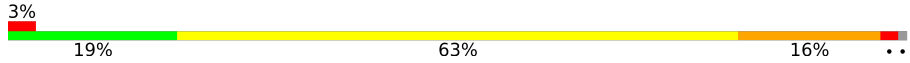
• Molecule 41: 50S ribosomal protein L20

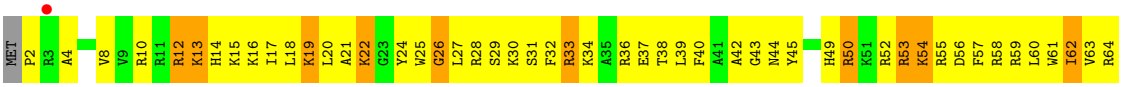
Chain BU:

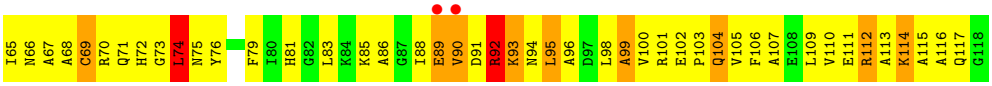


• Molecule 41: 50S ribosomal protein L20

Chain DU:

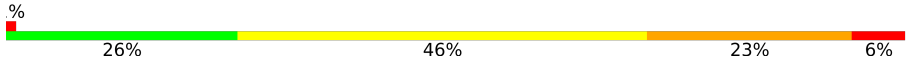


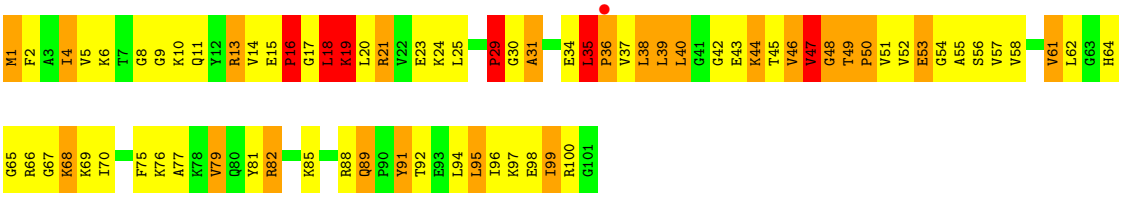




• Molecule 42: 50S ribosomal protein L21

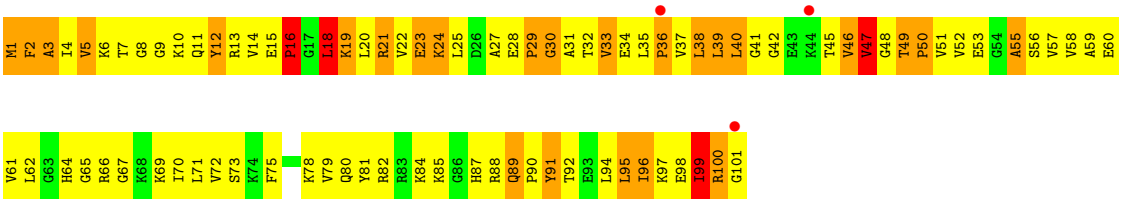
Chain BV:





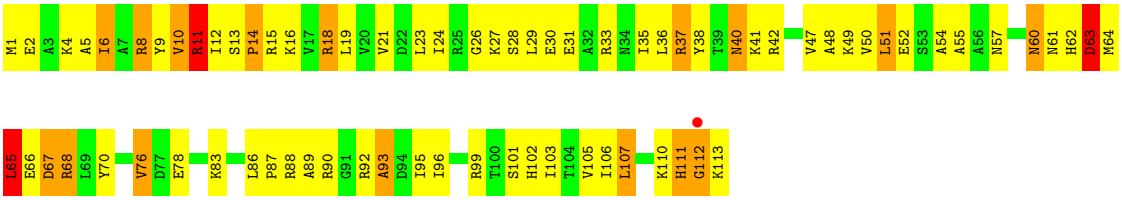
• Molecule 42: 50S ribosomal protein L21

Chain DV:



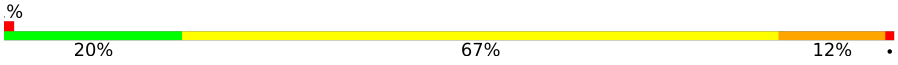
• Molecule 43: 50S ribosomal protein L22

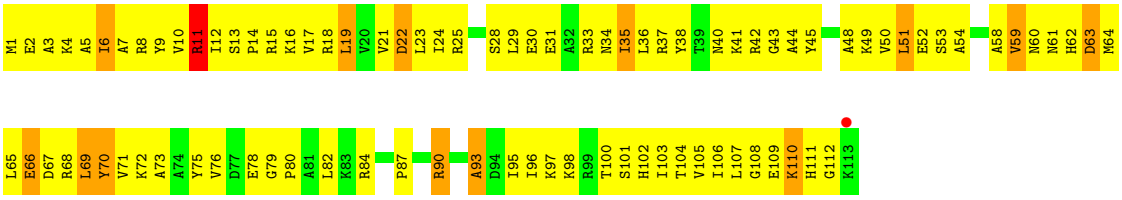
Chain BW:



• Molecule 43: 50S ribosomal protein L22

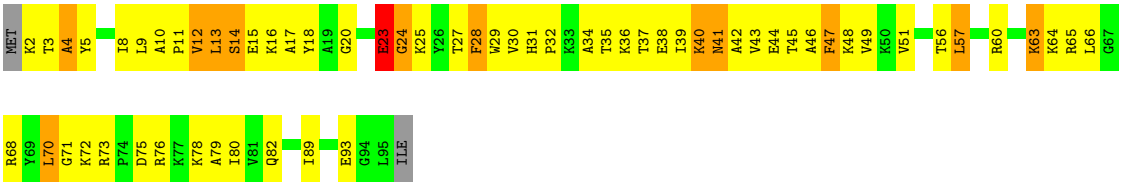
Chain DW:





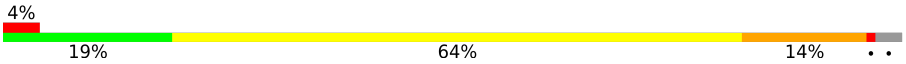
• Molecule 44: 50S ribosomal protein L23

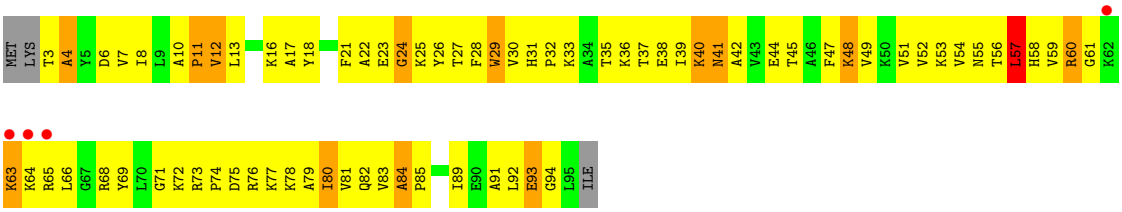
Chain BX:



- Molecule 44: 50S ribosomal protein L23

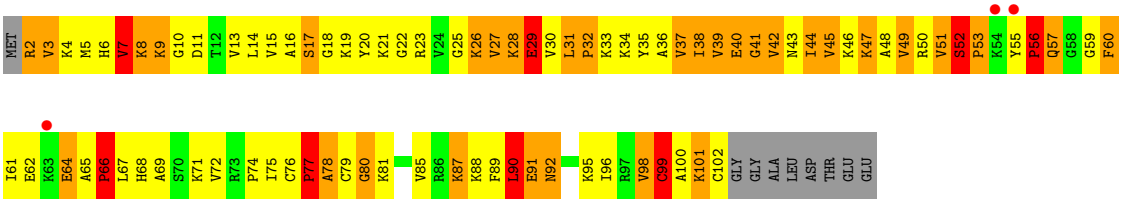
Chain DX:





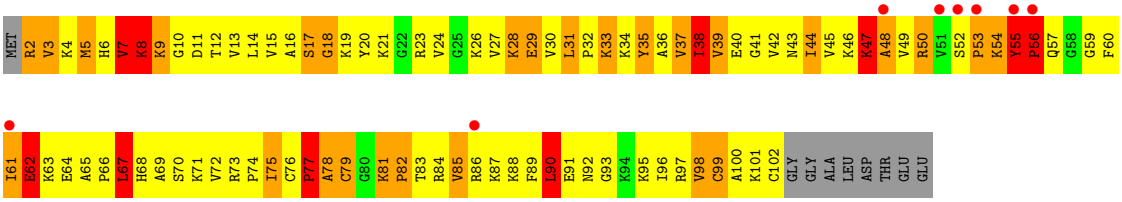
- Molecule 45: 50S ribosomal protein L24

Chain BY:



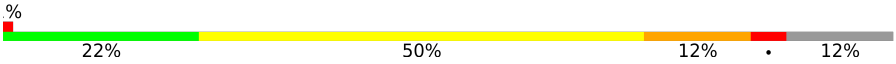
- Molecule 45: 50S ribosomal protein L24

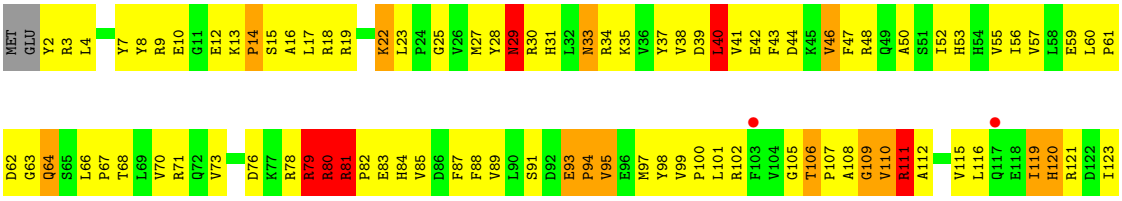
Chain DY:

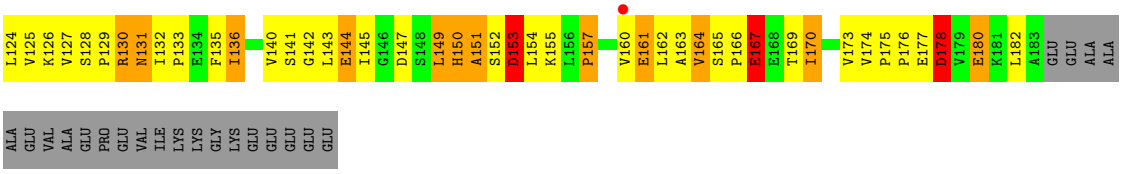


- Molecule 46: 50S ribosomal protein L25

Chain BZ:

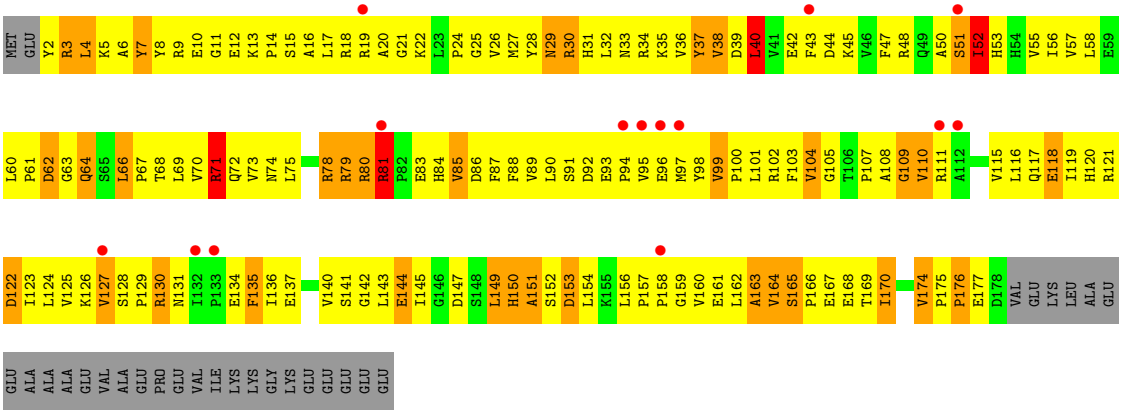






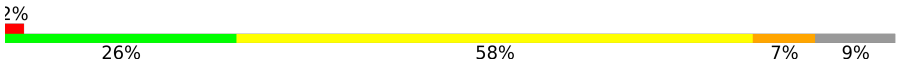
• Molecule 46: 50S ribosomal protein L25

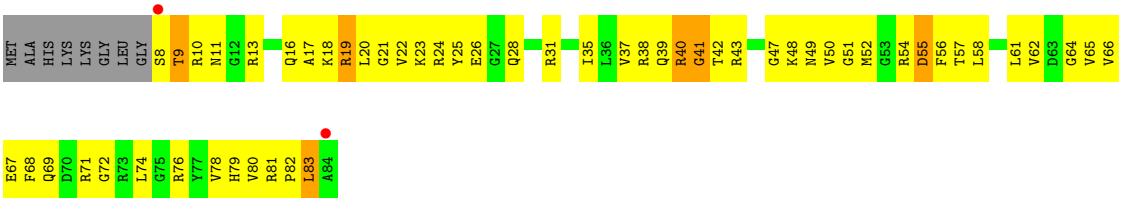
Chain DZ:



• Molecule 47: 50S ribosomal protein L27

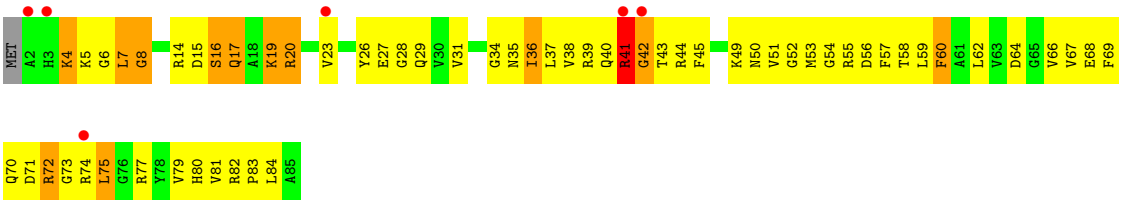
Chain B0:





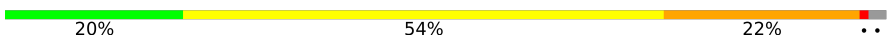
• Molecule 47: 50S ribosomal protein L27

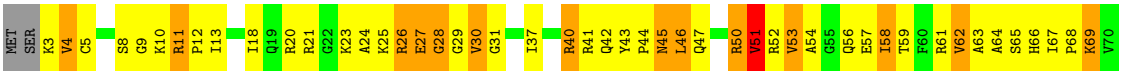
Chain D0:



• Molecule 48: 50S ribosomal protein L28

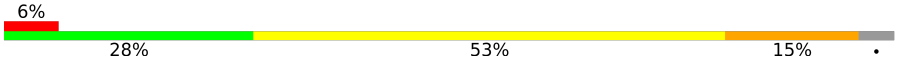
Chain B1:

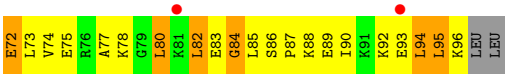




• Molecule 48: 50S ribosomal protein L28

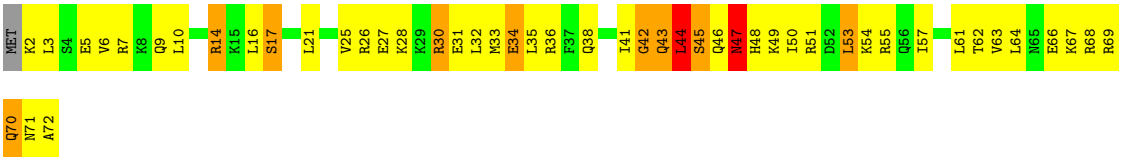
Chain D1:





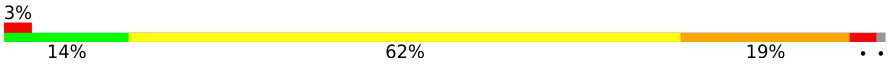
• Molecule 49: 50S ribosomal protein L29

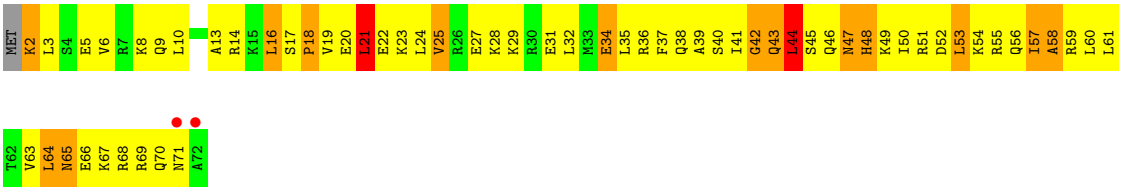
Chain B2:



• Molecule 49: 50S ribosomal protein L29

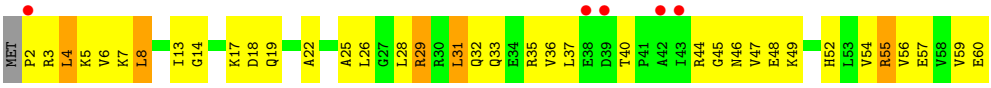
Chain D2:





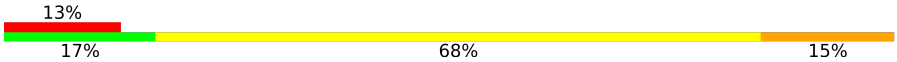
• Molecule 50: 50S ribosomal protein L30

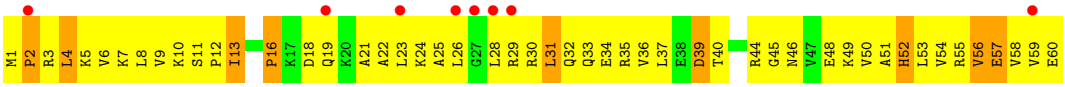
Chain B3:



• Molecule 50: 50S ribosomal protein L30

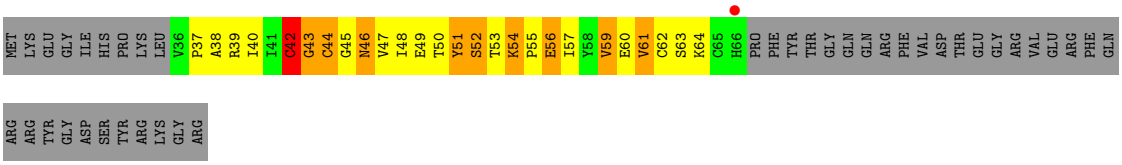
Chain D3:





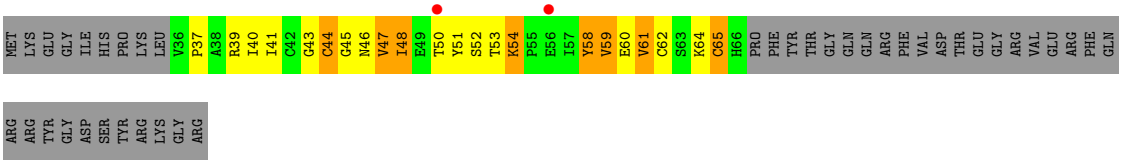
• Molecule 51: 50S ribosomal protein L31

Chain B4:



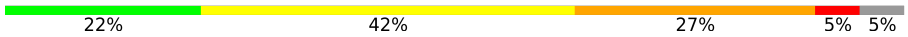
- Molecule 51: 50S ribosomal protein L31

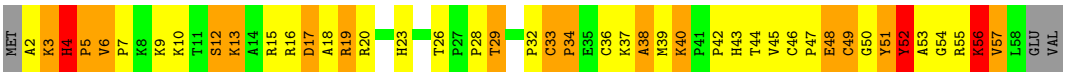
Chain D4:



- Molecule 52: 50S ribosomal protein L32

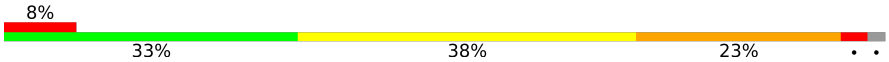
Chain B5:

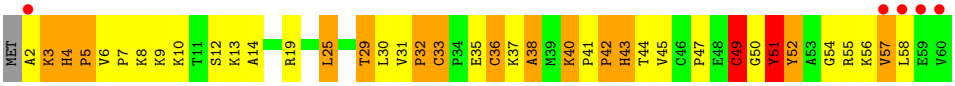




- Molecule 52: 50S ribosomal protein L32

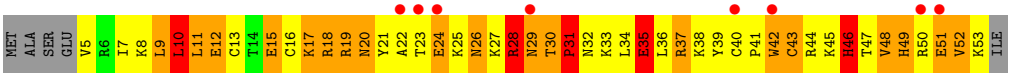
Chain D5:





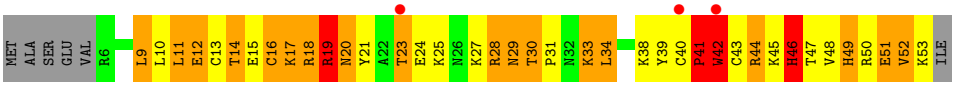
- Molecule 53: 50S ribosomal protein L33

Chain B6:



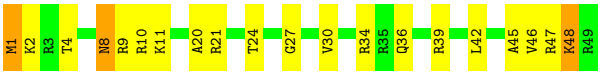
- Molecule 53: 50S ribosomal protein L33

Chain D6:



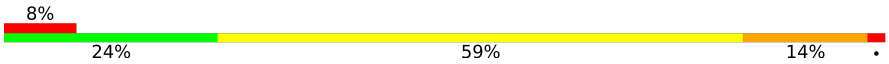
- Molecule 54: 50S ribosomal protein L34

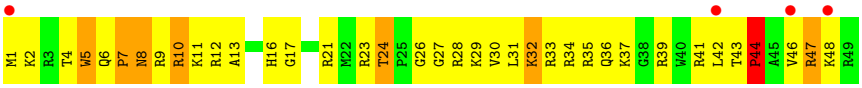
Chain B7:



• Molecule 54: 50S ribosomal protein L34

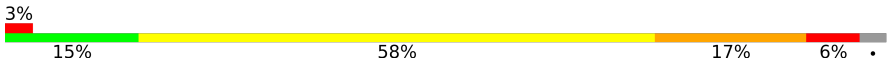
Chain D7:

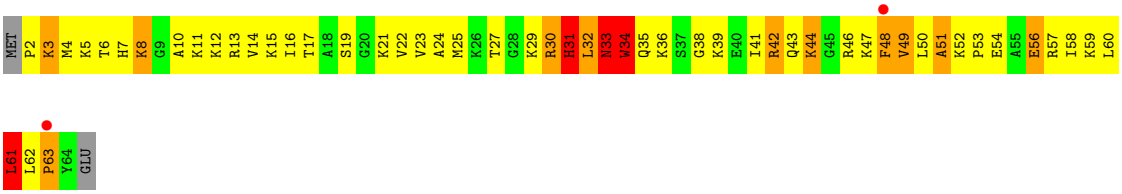




• Molecule 55: 50S ribosomal protein L35

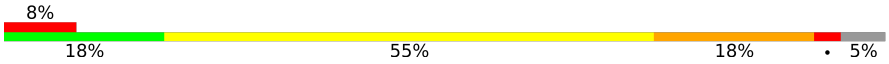
Chain B8:

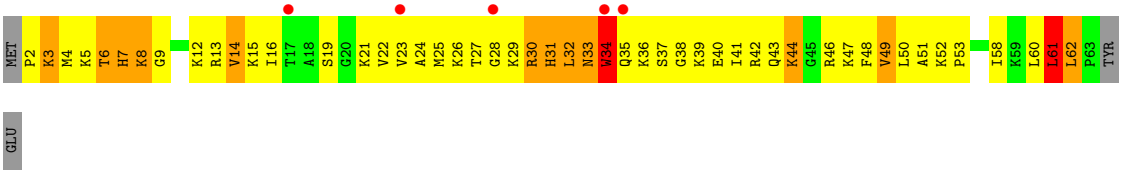




• Molecule 55: 50S ribosomal protein L35

Chain D8:



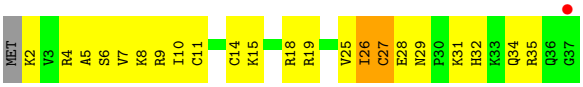


• Molecule 56: 50S ribosomal protein L36

Chain B9:

• Molecule 56: 50S ribosomal protein L36

Chain D9:



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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

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

5.2 Too-close contacts (i)

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

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

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

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

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

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

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

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

There are no symmetry-related clashes.

5.3 Torsion angles (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

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

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

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

5 of 1742 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

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

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

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

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

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

Mol	Chain	Res	Type
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 (i)

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

5 of 1593 RNA backbone outliers are listed below:

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

5 of 246 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AA	1

All chain breaks are listed below:

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

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

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

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

The worst 5 of 823 RSRZ outliers are listed below:

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

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

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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

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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

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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

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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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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.