wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 01:43 pm GMT

PDB ID	:	4V5E
Title	:	Insights into translational termination from the structure of RF2 bound to the ribosome
Authors	:	Weixlbaumer, A.; Jin, H.; Neubauer, C.; Voorhees, R.M.; Petry, S.; Kelley, A.C.; Ramakrishnan, V.
Deposited on	:	2009-04-30
Resolution	:	3.45 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

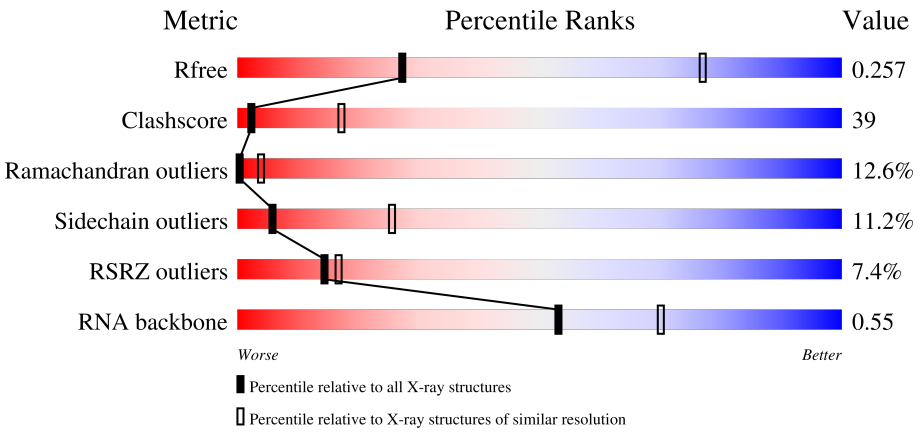
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)
RNA backbone	3102	1036 (3.96-2.96)

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	1522	2% 26% 60% 12% •
1	CA	1522	3% 26% 60% 12% ••
2	AB	256	17% 21% 58% 12% • 8%
2	CB	256	6% 21% 57% 12% • 8%

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Mol	Chain	Length	Quality of chain
3	AC	239	12% 22% 55% 9% 13%
3	CC	239	.% 24% 53% 9% 13%
4	AD	209	10% 24% 61% 12%
4	CD	209	2% 23% 62% 13%
5	AE	162	9% 26% 56% 11% 7%
5	CE	162	2% 27% 56% 10% 7%
6	AF	101	15% 31% 60% 9%
6	CF	101	7% 30% 61% 9%
7	AG	156	16% 40% 49% 10%
7	CG	156	7% 38% 52% 10%
8	AH	138	4% 25% 60% 14%
8	CH	138	.% 26% 58% 15%
9	AI	128	29% 21% 63% 15%
9	CI	128	11% 22% 63% 14%
10	AJ	105	30% 16% 61% 16% 6%
10	CJ	105	19% 16% 61% 16% 6%
11	AK	129	14% 28% 59% 5% 8%
11	CK	129	8% 29% 57% 5% 8%
12	AL	132	5% 30% 55% 9% 5%
12	CL	132	5% 32% 52% 11% 5%
13	AM	126	9% 28% 51% 17%
13	CM	126	4% 27% 52% 17%
14	AN	61	10% 26% 62% 8%
14	CN	61	25% 62% 10%
15	AO	89	4% 51% 43% 6%

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Mol	Chain	Length	Quality of chain
15	CO	89	3% 52% 42% 6%
16	AP	88	10% 18% 65% 13% 5%
16	CP	88	17% 19% 64% 13% 5%
17	AQ	105	10% 33% 50% 10% 5%
17	CQ	105	6% 34% 50% 10% 5%
18	AR	88	3% 18% 52% 8% 20%
18	CR	88	8% 19% 51% 8% 20%
19	AS	93	9% 16% 53% 15% 15%
19	CS	93	11% 16% 52% 16% 15%
20	AT	106	11% 23% 57% 14% 7%
20	CT	106	20% 20% 59% 14% 7%
21	AU	27	44% 33% 56% 7%
21	CU	27	33% 59% 7%
22	AV	76	30% 53% 17%
22	AW	76	37% 20% 61% 16%
22	CV	76	% 29% 47% 22%
22	CW	76	18% 17% 62% 17%
23	AX	8	12% 25% 50% 12% 12%
23	CX	8	12% 50% 38% 12%
24	AY	351	14% 27% 58% 14%
24	CY	351	12% 29% 58% 12%
25	B0	85	2% 26% 55% 8% 11%
25	D0	85	2% 28% 52% 9% 11%
26	B1	98	2% 29% 53% 12%
26	D1	98	% 35% 47% 11%

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Mol	Chain	Length	Quality of chain
27	B2	72	7% 17% 54% 28%
27	D2	72	4% 29% 49% 18%
28	B3	60	5% 40% 45% 15%
28	D3	60	5% 40% 50% 10%
29	B4	71	11% 10% 27% 7% 56%
29	D4	71	3% 13% 23% 8% 56%
30	B5	60	5% 38% 43% 10% 7%
30	D5	60	8% 35% 45% 12% 7%
31	B6	54	13% 43% 33% 7% 17%
31	D6	54	4% 44% 31% 7% 17%
32	B7	49	6% 61% 37%
32	D7	49	2% 57% 41%
33	B8	65	2% 22% 52% 17% 8%
33	D8	65	23% 51% 17% 8%
34	B9	37	5% 32% 54% 11%
34	D9	37	14% 32% 51% 14%
35	BA	2901	3% 34% 52% 13%
35	DA	2901	4% 34% 51% 13%
36	BB	122	31% 56% 9%
36	DB	122	31% 55% 11%
37	BC	229	59% 34% 35% 13% 17%
37	DC	229	68% 36% 34% 13% 17%
38	BD	276	2% 35% 49% 13%
38	DD	276	% 37% 48% 13%
39	BE	206	3% 24% 51% 22%

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Mol	Chain	Length	Quality of chain
39	DE	206	3% 23% 52% 22%
40	BF	210	2% 30% 51% 17%
40	DF	210	3% 33% 50% 16%
41	BG	182	11% 13% 61% 23%
41	DG	182	4% 18% 59% 20%
42	BH	180	19% 13% 61% 13% 11%
42	DH	180	23% 13% 62% 12% 11%
43	BI	148	8% 32% 59% 7%
44	BJ	130	65% 35%
44	DJ	130	65% 35%
45	BK	147	38% 22% 60% 13%
45	DK	147	39% 22% 60% 14%
46	BN	140	% 33% 44% 23%
46	DN	140	34% 43% 22%
47	BO	122	41% 51% 8%
47	DO	122	39% 52% 7%
48	BP	150	7% 20% 39% 33% 5%
48	DP	150	3% 21% 39% 33% 5%
49	BQ	141	3% 40% 51% 9%
49	DQ	141	2% 40% 50% 9%
50	BR	118	20% 59% 17%
50	DR	118	% 25% 55% 17%
51	BS	112	15% 19% 46% 19% 12%
51	DS	112	17% 48% 19% 12%
52	BT	146	8% 16% 51% 26% 5%

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Mol	Chain	Length	Quality of chain
52	DT	146	5% 16% 51% 26% 5%
53	BU	118	% 35% 53% 12%
53	DU	118	% 32% 55% 12%
54	BV	101	7% 35% 47% 16%
54	DV	101	2% 33% 50% 15%
55	BW	113	2% 42% 47% 11%
55	DW	113	% 40% 50% 10%
56	BX	96	% 34% 54% 8%
56	DX	96	34% 55% 7%
57	BY	110	15% 17% 40% 29% 5% 8%
57	DY	110	9% 16% 41% 28% 6% 8%
58	BZ	206	5% 19% 44% 21% 14%
58	DZ	206	% 20% 43% 22% 14%
59	DI	148	8% 24% 59% 16%

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
60	MG	AA	1616	-	-	-	X
60	MG	AA	1637	-	-	-	X
60	MG	AA	1653	-	-	-	X
60	MG	AA	1668	-	-	-	X
60	MG	AA	1683	-	-	-	X
60	MG	AA	1688	-	-	-	X
60	MG	AA	1689	-	-	-	X
60	MG	AA	1692	-	-	-	X
60	MG	AA	1699	-	-	-	X
60	MG	AA	1716	-	-	-	X
60	MG	AA	1720	-	-	-	X
60	MG	AA	1730	-	-	-	X
60	MG	AA	1732	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	1748	-	-	-	X
60	MG	AM	201	-	-	-	X
60	MG	AV	107	-	-	-	X
60	MG	BA	3105	-	-	-	X
60	MG	BA	3135	-	-	-	X
60	MG	BA	3199	-	-	-	X
60	MG	BA	3201	-	-	-	X
60	MG	BA	3212	-	-	-	X
60	MG	BA	3227	-	-	-	X
60	MG	BA	3234	-	-	-	X
60	MG	BA	3287	-	-	-	X
60	MG	BA	3301	-	-	-	X
60	MG	BA	3320	-	-	-	X
60	MG	BA	3328	-	-	-	X
60	MG	BA	3336	-	-	-	X
60	MG	BA	3341	-	-	-	X
60	MG	BC	301	-	-	-	X
60	MG	BS	201	-	-	-	X
60	MG	CA	1615	-	-	-	X
60	MG	CA	1625	-	-	-	X
60	MG	CA	1631	-	-	-	X
60	MG	CA	1643	-	-	-	X
60	MG	CA	1651	-	-	-	X
60	MG	CA	1655	-	-	-	X
60	MG	CA	1670	-	-	-	X
60	MG	CA	1676	-	-	-	X
60	MG	CA	1681	-	-	-	X
60	MG	CA	1687	-	-	-	X
60	MG	CA	1705	-	-	-	X
60	MG	CA	1717	-	-	-	X
60	MG	CA	1718	-	-	-	X
60	MG	CA	1733	-	-	-	X
60	MG	CW	101	-	-	-	X
60	MG	CW	105	-	-	-	X
60	MG	DA	3003	-	-	-	X
60	MG	DA	3100	-	-	-	X
60	MG	DA	3122	-	-	-	X
60	MG	DA	3134	-	-	-	X
60	MG	DA	3142	-	-	-	X
60	MG	DA	3143	-	-	-	X
60	MG	DA	3176	-	-	-	X
60	MG	DA	3177	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DA	3181	-	-	-	X
60	MG	DA	3193	-	-	-	X
60	MG	DA	3202	-	-	-	X
60	MG	DA	3224	-	-	-	X
60	MG	DA	3225	-	-	-	X
60	MG	DA	3231	-	-	-	X
60	MG	DA	3240	-	-	-	X
60	MG	DA	3260	-	-	-	X
60	MG	DA	3280	-	-	-	X
60	MG	DA	3283	-	-	-	X
60	MG	DA	3287	-	-	-	X
60	MG	DA	3294	-	-	-	X
60	MG	DA	3319	-	-	-	X
60	MG	DA	3327	-	-	-	X
60	MG	DA	3349	-	-	-	X
60	MG	DA	3351	-	-	-	X
60	MG	DA	3352	-	-	-	X
60	MG	DB	201	-	-	-	X
60	MG	DC	301	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 304505 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	1504	32329	14390	5992	10444	1503	0	0	0
1	CA	1504	32329	14390	5992	10444	1503	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	1011	639	198	174	0	0	0
9	CI	127	1011	639	198	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	126	976	614	197	164	1	0	0	1
12	CL	126	976	614	197	164	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	121	956	591	198	165	2	0	0	1
13	CM	121	956	591	198	165	2	0	0	1

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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	79	630	403	115	110	2	0	0	1
19	CS	79	630	403	115	110	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 RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	AV	76	1619	723	290	531	75	0	0	0
22	AW	76	1619	723	290	531	75	0	0	0
22	CV	76	1619	723	290	531	75	0	0	0
22	CW	76	1619	723	290	531	75	0	0	0

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	AX	8	166	76	29	54	7	0	0	0
23	CX	8	166	76	29	54	7	0	0	0

- Molecule 24 is a protein called PEPTIDE CHAIN RELEASE FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	AY	351	2799	1751	503	537	8	0	0	0
24	CY	351	2799	1751	503	537	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	303	GLU	ARG	conflict	UNP Q5SM01
CY	303	GLU	ARG	conflict	UNP Q5SM01

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	B0	76	607	376	128	102	1	0	0	0
25	D0	76	607	376	128	102	1	0	0	0

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	B3	60	468	298	91	78	1	0	0	1
28	D3	60	468	298	91	78	1	0	0	1

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	B6	45	381	235	78	64	4	0	0	1
31	D6	45	381	235	78	64	4	0	0	1

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
35	BA	2886	62154	27663	11625	19981	2885	0	0	0
35	DA	2886	62154	27663	11625	19981	2885	0	0	0

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	BH	160	1223	773	229	220	1	0	0	1
42	DH	160	1223	773	229	220	1	0	0	1

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
44	BJ	130	651	390	130	131	0	0	0
44	DJ	130	651	390	130	131	0	0	0

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BK	141	1038	661	184	187	6	0	0	1
45	DK	141	1038	661	184	187	6	0	0	1

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	BQ	141	1122	715	212	188	7	0	0	0
49	DQ	141	1122	715	212	188	7	0	0	0

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
57	BY	101	776	500	149	123	4	0	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
57	DY	101	776	500	149	123	4	0	0	1

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 59 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
59	DI	146	1133	724	201	207	1	0	0	1

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
60	AA	157	157	157	0	0
60	AE	1	1	1	0	0
60	AL	1	1	1	0	0
60	AM	1	1	1	0	0
60	AV	7	7	7	0	0
60	AW	5	5	5	0	0
60	AY	1	1	1	0	0
60	B1	1	1	1	0	0
60	B3	1	1	1	0	0
60	B5	2	2	2	0	0
60	B7	2	2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
60	BA	354	354	354	0	0
60	BB	4	4	4	0	0
60	BC	1	1	1	0	0
60	BD	2	2	2	0	0
60	BF	1	1	1	0	0
60	BH	1	1	1	0	0
60	BP	1	1	1	0	0
60	BQ	1	1	1	0	0
60	BS	1	1	1	0	0
60	BU	1	1	1	0	0
60	CA	157	157	157	0	0
60	CL	1	1	1	0	0
60	CN	1	1	1	0	0
60	CV	7	7	7	0	0
60	CW	5	5	5	0	0
60	CY	1	1	1	0	0
60	D1	1	1	1	0	0
60	D3	1	1	1	0	0
60	D5	2	2	2	0	0
60	D7	1	1	1	0	0
60	DA	353	353	353	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
60	DB	4	4	4	0	0
60	DC	1	1	1	0	0
60	DD	2	2	2	0	0
60	DF	3	3	3	0	0
60	DH	1	1	1	0	0
60	DQ	1	1	1	0	0
60	DR	1	1	1	0	0
60	DU	1	1	1	0	0
60	DX	1	1	1	0	0
60	DY	1	1	1	0	0

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

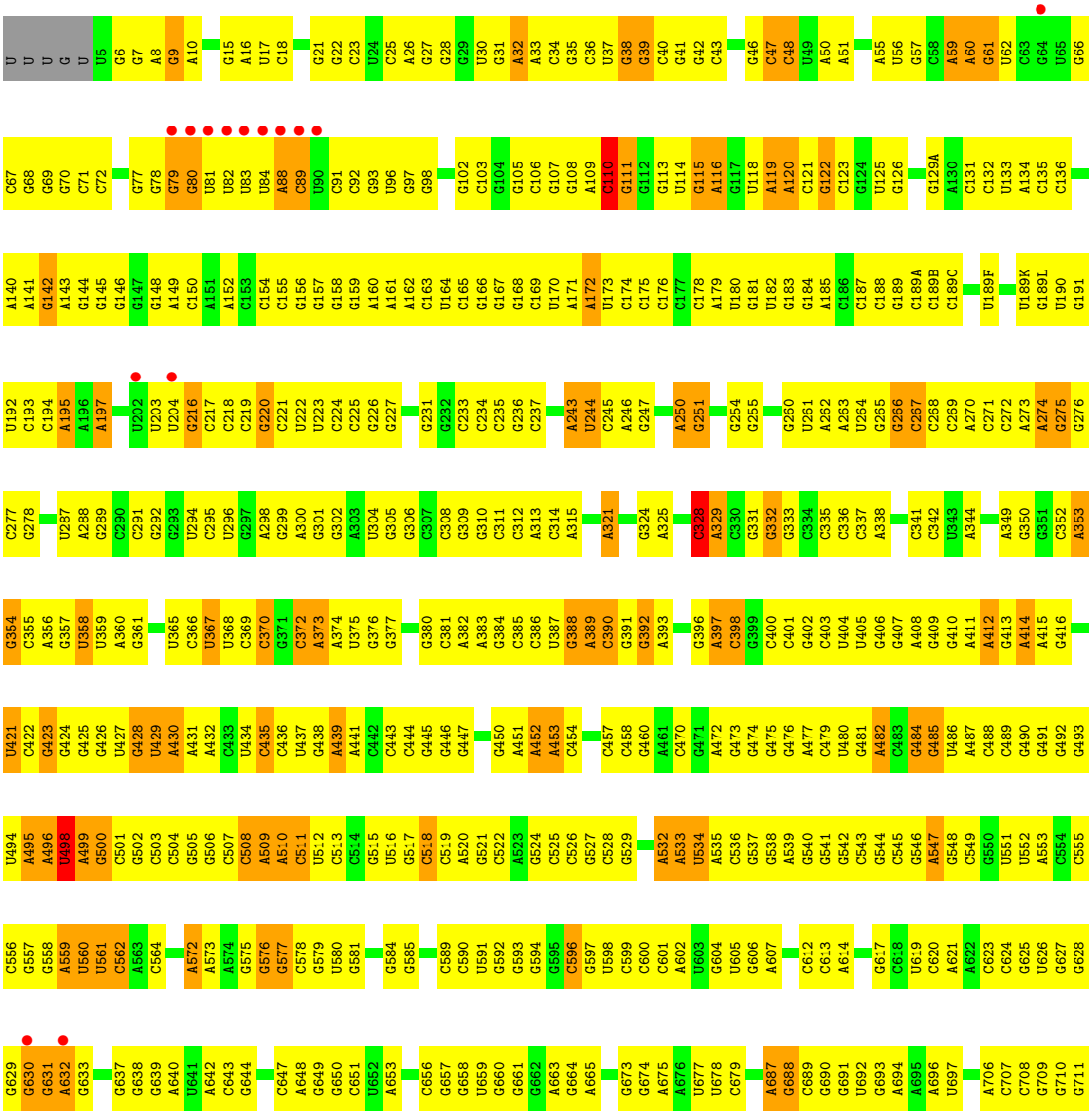
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
61	AD	1	1	1	0	0
61	AN	1	1	1	0	0
61	B9	1	1	1	0	0
61	CD	1	1	1	0	0
61	CN	1	1	1	0	0
61	D9	1	1	1	0	0

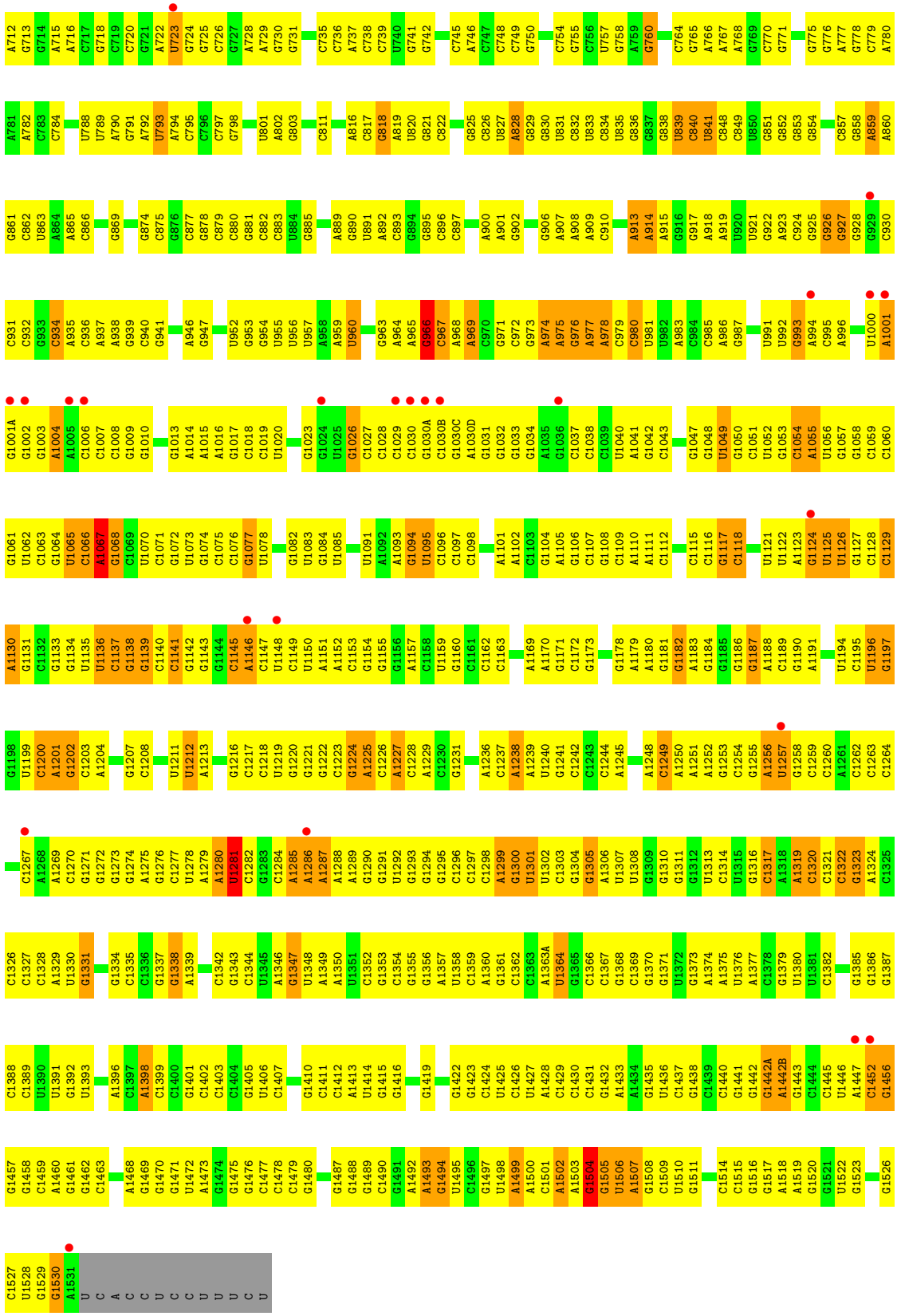
3 Residue-property plots (i)

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

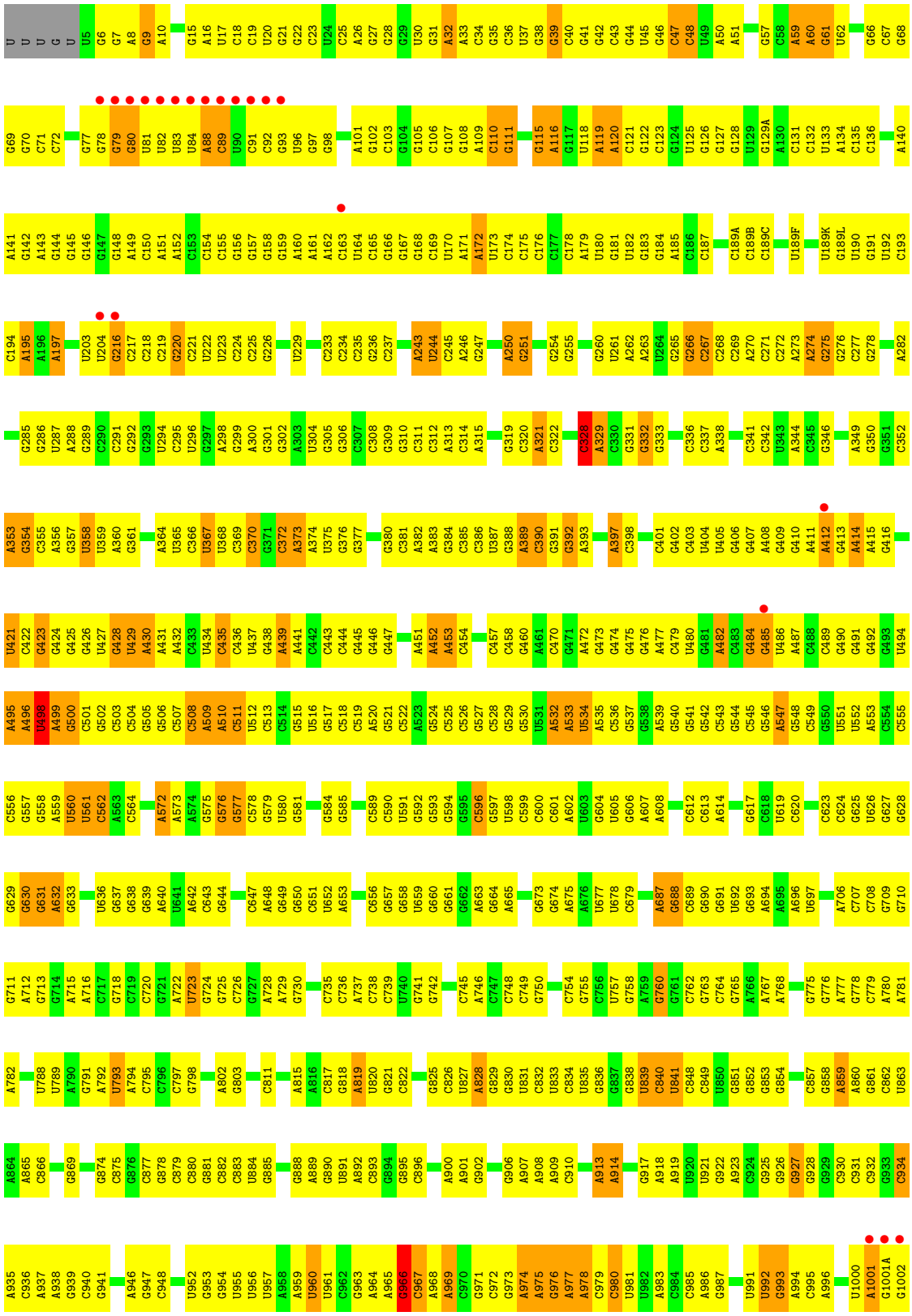
Chain AA:

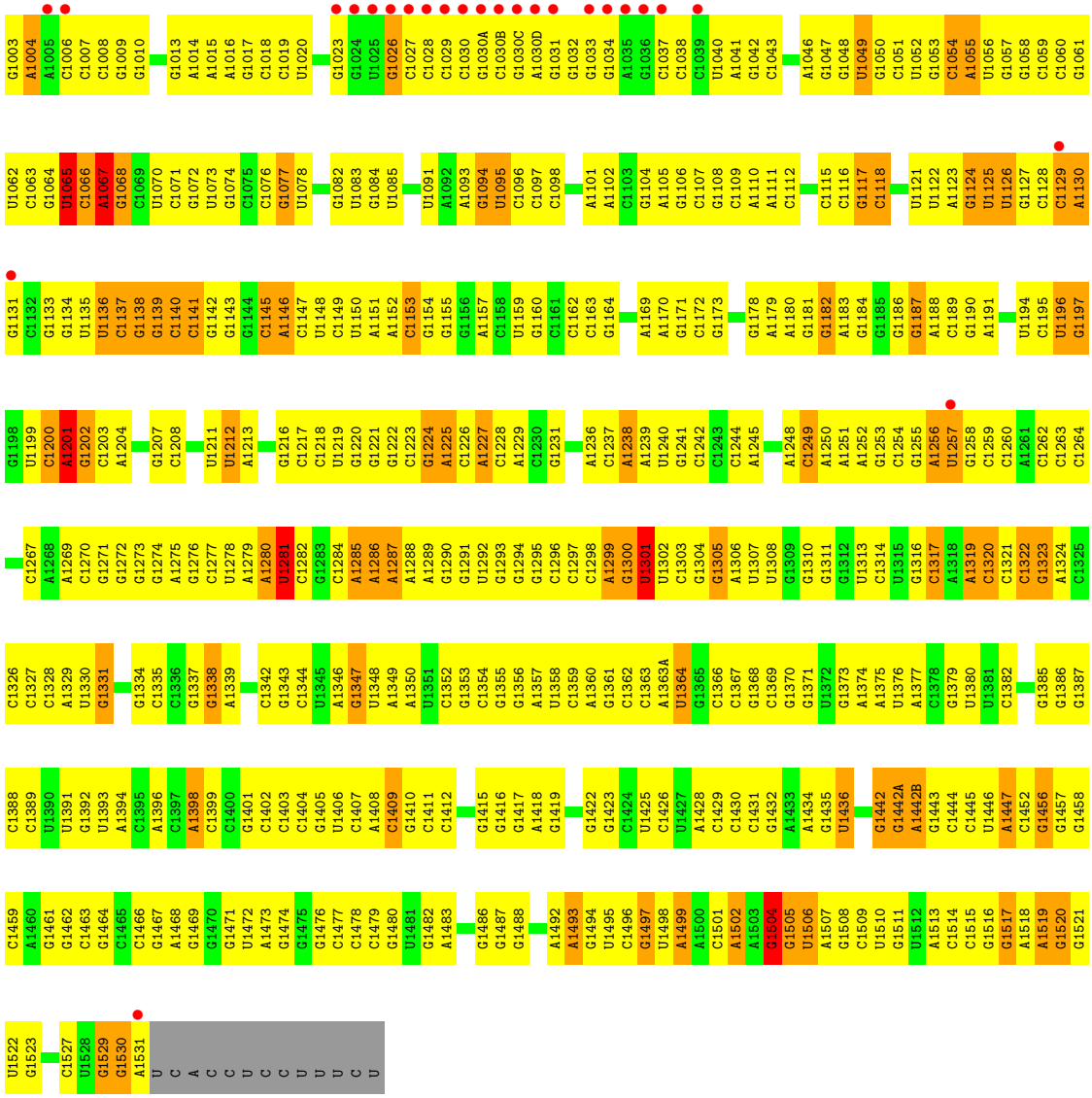




- Molecule 1: 16S ribosomal RNA

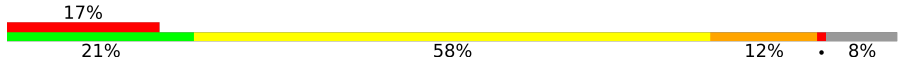
Chain CA: 3% 26% 60% 12%

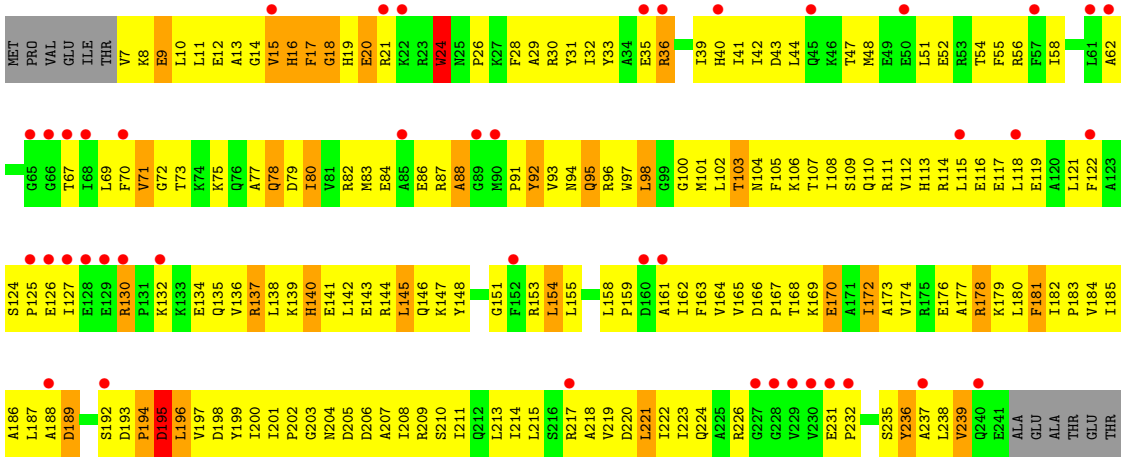




• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB:





PRO GLU GLY GLU SER GLU VAL GLU ALA

- Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain CB: 6% 21% 57% 12% • 8%

MET PRO VAL GLU ILE THR V7 K8 E9 L10 L11 E12 A13 G14 V15 H16 F17 G18 H19 E20 R21 W24 N25 P26 K27 F28 A29 R30 Y31 I32 Y33 A34 E35 R36 I39 H40 I41 I42 D43 L44 T47 M48 E49 E50 L51 E52 R53 T54 F55 R56 F57 I58 A62 T67 I68

L69 F70 V71 G72 T73 K74 K75 Q76 A77 Q78 D79 I80 V81 R82 M83 E84 A85 E86 R87 A88 P91 Y92 V93 N94 Q95 R96 W97 L98 G99 G100 M101 L102 T103 N104 F105 K106 T107 I108 S109 Q110 R111 V112 H113 R114 L115 E116 E117 L118 E119 A120 L121 F122 A123 S124 P125 E129 R130 P131

K132 K133 E134 Q135 V136 R137 L138 K139 H140 E141 L142 E143 R144 L145 Q146 K147 Y148 G151 F152 R153 L154 L155 L158 P159 D160 A161 I162 F163 V164 V165 D166 P167 T168 K169 E170 A171 I172 A173 V174 R175 E176 A177 R178 K179 L180 F181 I182 P183 V184 I185 A186 L187 A188 D189 S192 D193 P194

D195 L196 V197 D198 Y199 I200 I201 P202 G203 N204 D205 D206 A207 I208 R209 S210 I211 Q212 L213 I214 L215 S216 R217 A218 V219 D220 L221 I222 I223 Q224 A225 R226 E231 P232 S235 Y236 A237 L238 V239 Q240 E241 ALA GLU ALA THR GLU THR PRO GLU GLY GLU SER GLU VAL GLU ALA

- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC: 12% 22% 55% 9% • 13%

MET G2 N3 K4 I5 H6 P7 I8 G9 F10 R11 L12 T15 R16 D17 W18 E19 S20 R21 W22 Y23 A24 G25 K26 K27 Q28 Y29 R30 H31 L32 L33 L34 E35 D36 Q37 R38 I39 R40 G41 L42 K45 E46 L47 G51 L52 A53 R54 V55 D56 I57 E58 R59 A60 A61 D62 N63 V64

A65 V66 T67 V68 H69 V70 A71 K72 P73 G74 V75 V76 I77 G78 R79 G80 G81 E82 R83 I84 R85 V86 L87 R88 E89 E90 L91 A92 K93 L94 T95 G96 K97 N98 V99 A100 L101 N102 V103 Q104 E105 V106 Q107 N108 P109 N110 L111 S112 A113 P114 L115 Q118 R119 V120 A121 E122 Q123 I124 E125

R126 R127 F128 A129 V130 R131 R132 A133 I134 K135 V138 Q139 R140 V141 M142 E143 S144 G145 A146 K147 G148 A149 K150 V151 I152 V153 S154 G155 R156 I157 G158 G159 A163 R164 T165 E166 W167 A168 A169 Q170 G171 R172 V173 P174 L175 H176 T177 L178 R179 A180 N181 I182 D183 Y184 G185 F186 A187 L188

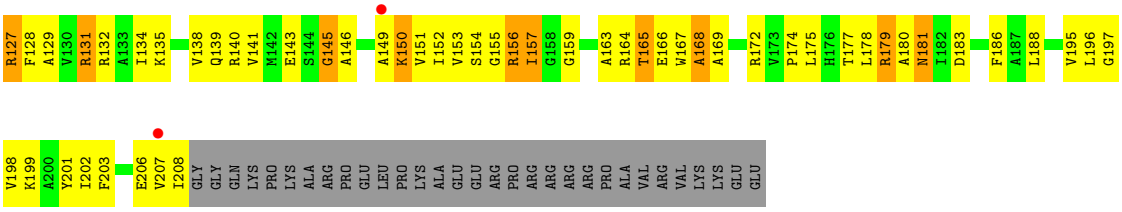
V195 L196 G197 V198 K199 A200 Y201 I202 F203 L204 G205 E206 V207 I208 GLY GLY GLN LYS PRO LYS ALA ARG PRO GLU LEU PRO LYS ALA GLU GLU ARG PRO ARG ARG ARG ARG PRO ALA VAL ARG VAL LYS LYS GLU GLU

- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC: % 24% 53% 9% • 13%

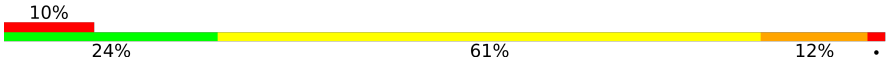
MET G2 N3 K4 I5 H6 P7 I8 G9 F10 R11 L12 T15 R16 D17 W18 E19 S20 R21 W22 Y23 A24 G25 K26 K27 Q28 Y29 R30 H31 L32 L33 L34 E35 D36 Q37 R38 I39 R40 G41 L42 K45 E46 L47 G51 L52 A53 R54 V55 D56 I57 E58 R59 A60 A61 D62 N63 V64

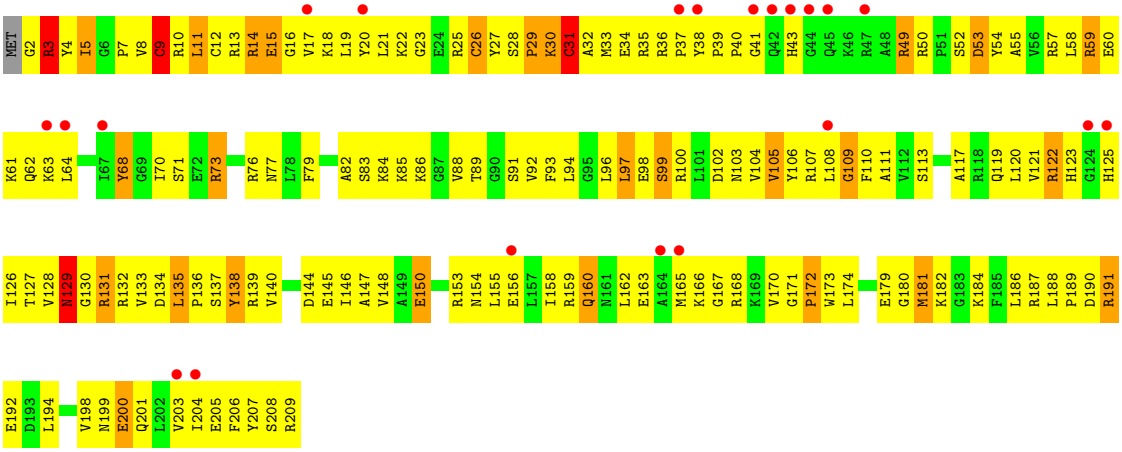
A65 V66 T67 V70 A71 K72 P73 G74 V75 V76 I77 G78 R79 G80 G81 E82 R83 I84 R85 V86 L87 R88 E89 E90 L91 A92 K93 L94 T95 G96 K97 N98 V99 A100 L101 N102 V103 Q104 E105 V106 Q107 N108 P109 N110 L111 S112 A113 P114 L115 Q118 R119 V120 A121 E122 Q123 I124 E125 R126



• Molecule 4: 30S RIBOSOMAL PROTEIN S4

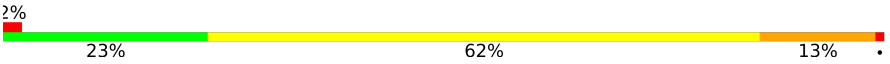
Chain AD:

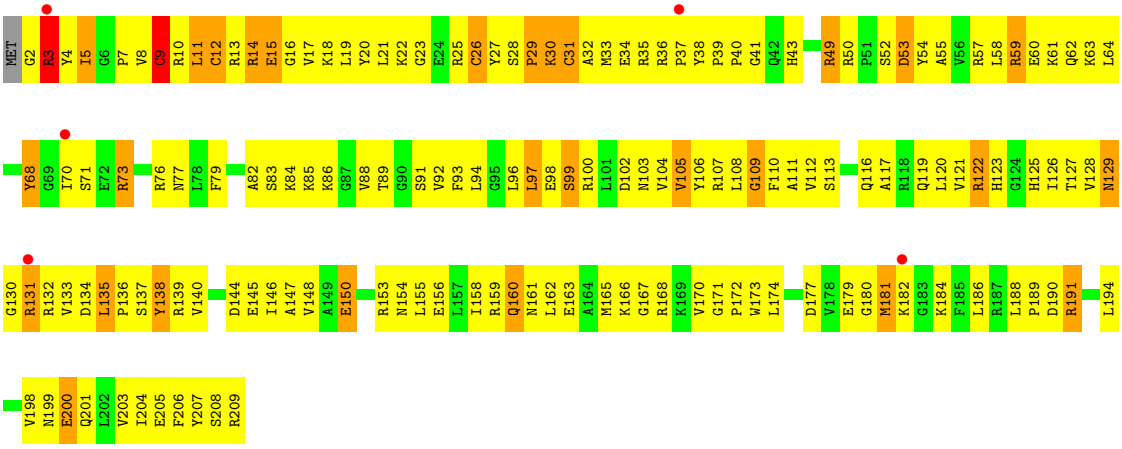




• Molecule 4: 30S RIBOSOMAL PROTEIN S4

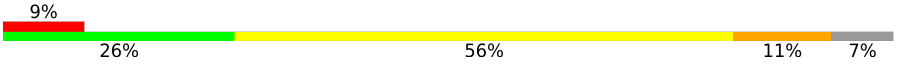
Chain CD:

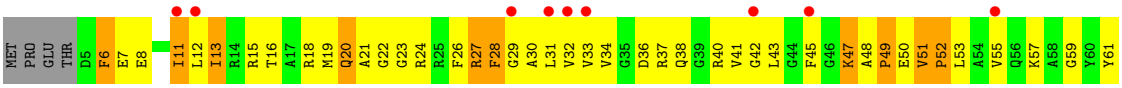


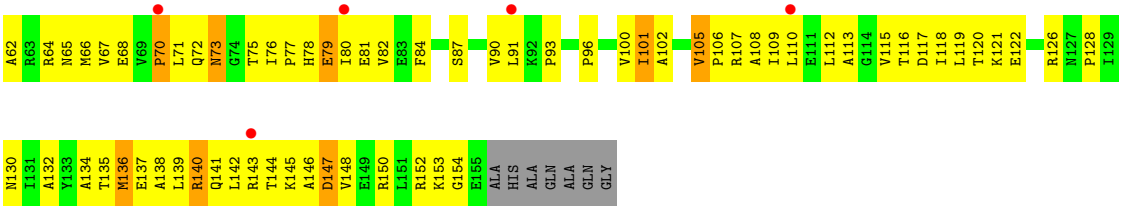


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

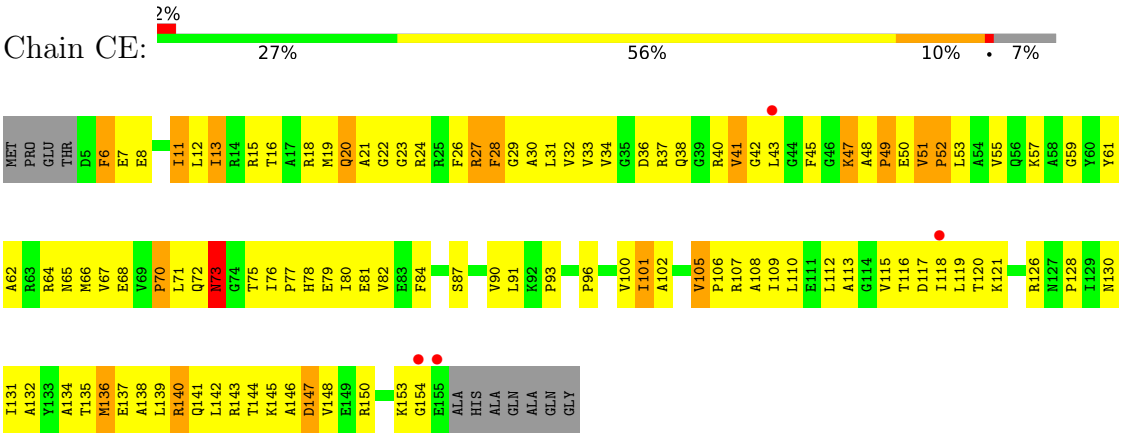
Chain AE:



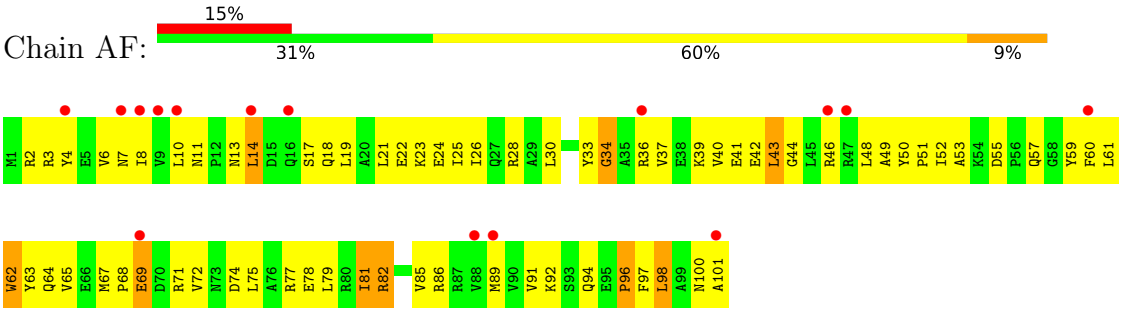




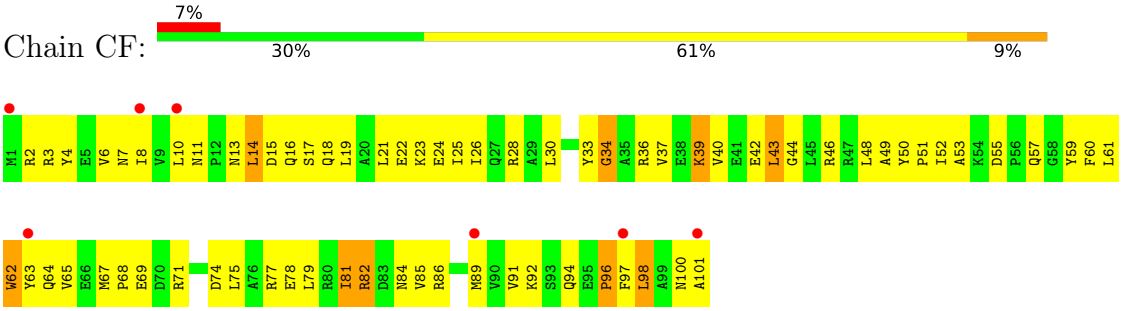
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



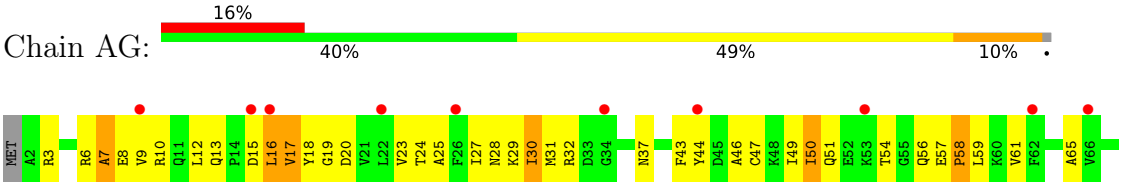
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

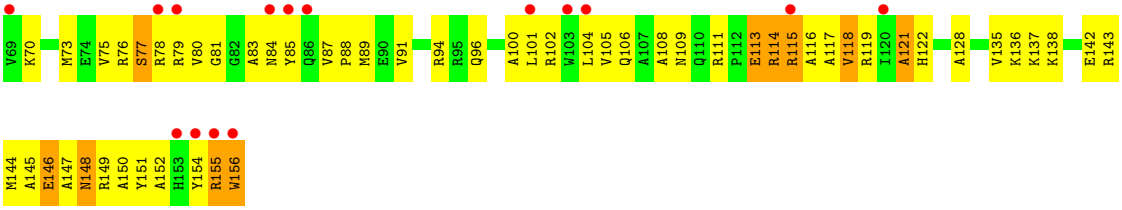


• Molecule 6: 30S RIBOSOMAL PROTEIN S6



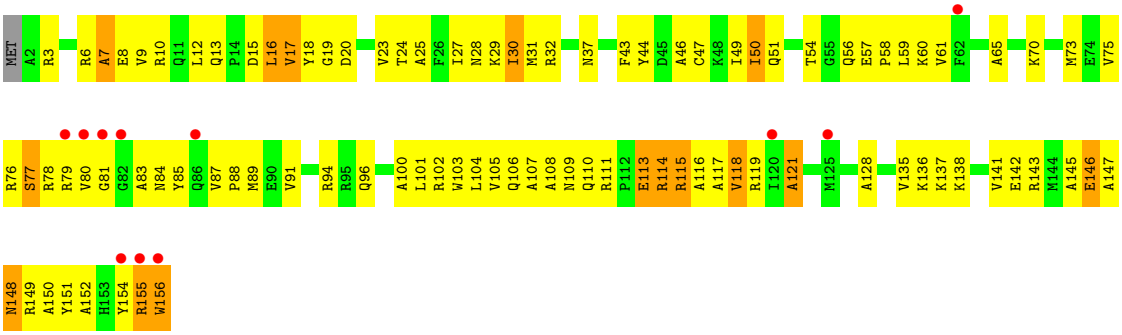
• Molecule 7: 30S RIBOSOMAL PROTEIN S7





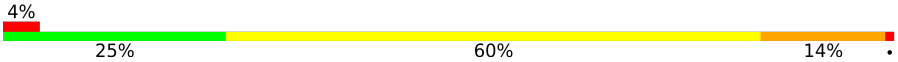
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

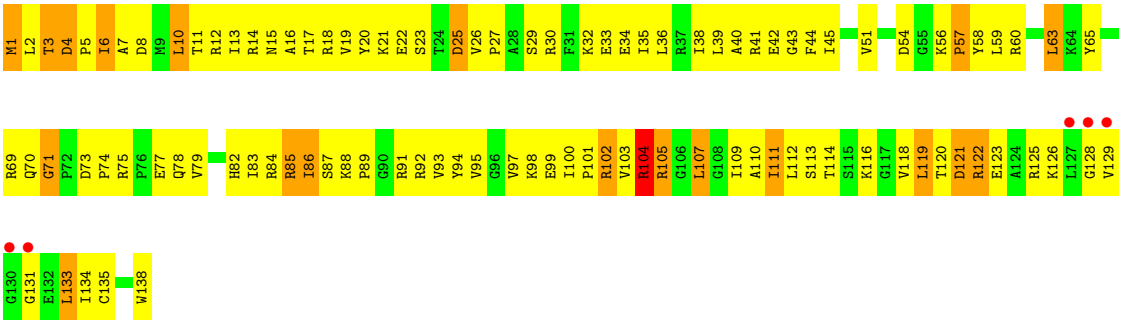
Chain CG:



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

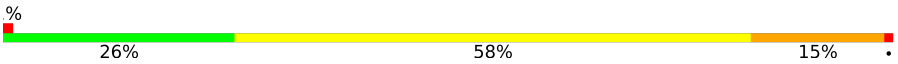
Chain AH:

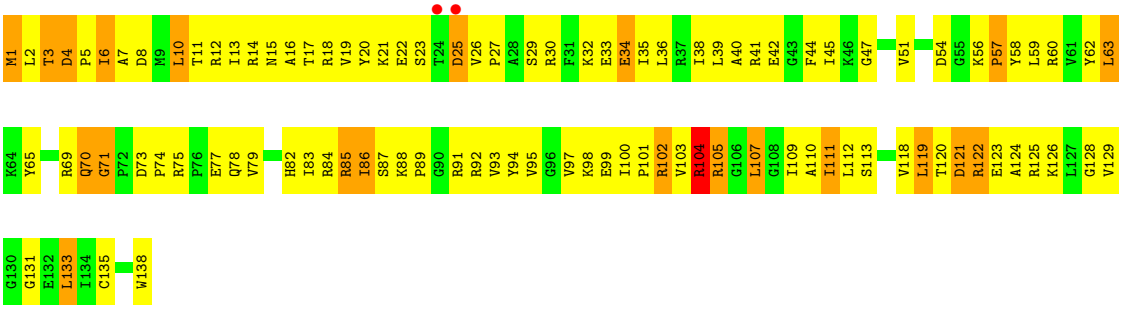




• Molecule 8: 30S RIBOSOMAL PROTEIN S8

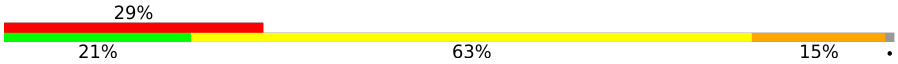
Chain CH:

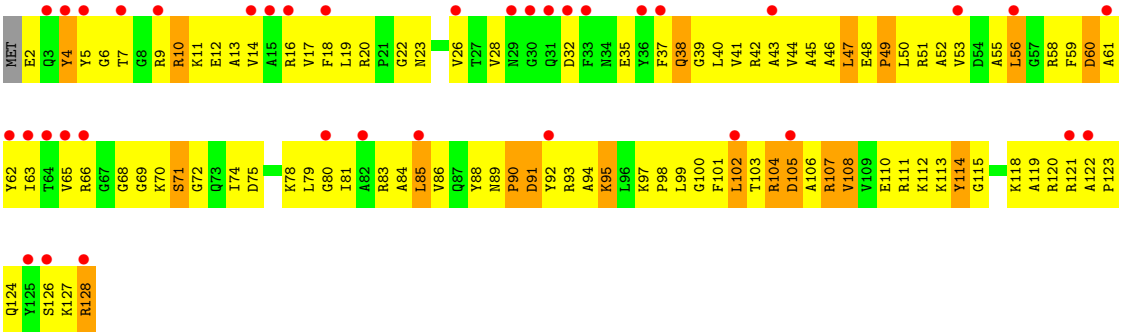




• Molecule 9: 30S RIBOSOMAL PROTEIN S9

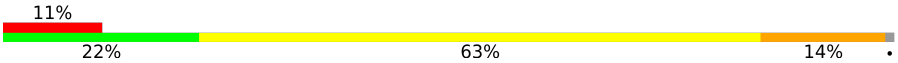
Chain AI:

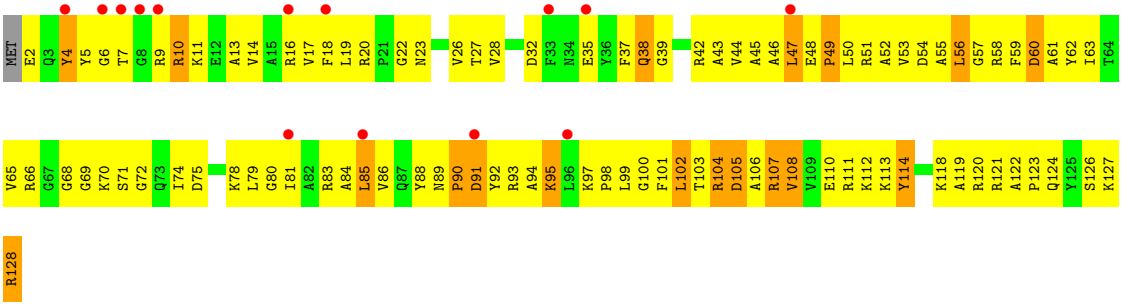




- Molecule 9: 30S RIBOSOMAL PROTEIN S9

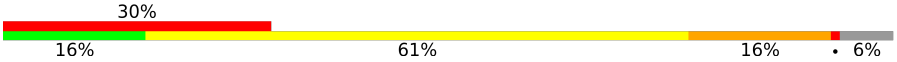
Chain CI:

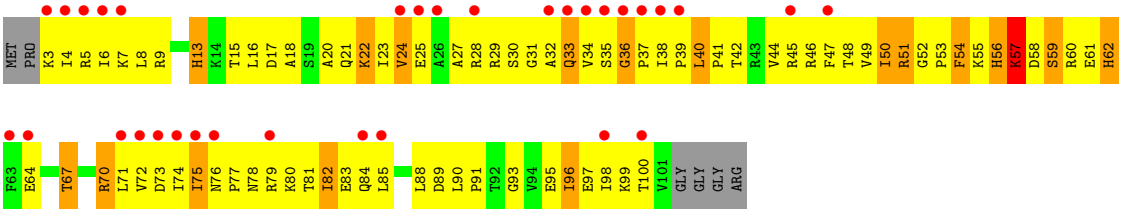




- Molecule 10: 30S RIBOSOMAL PROTEIN S10

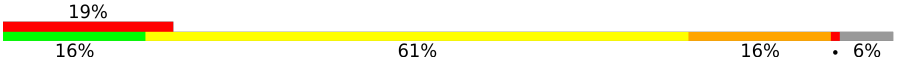
Chain AJ:

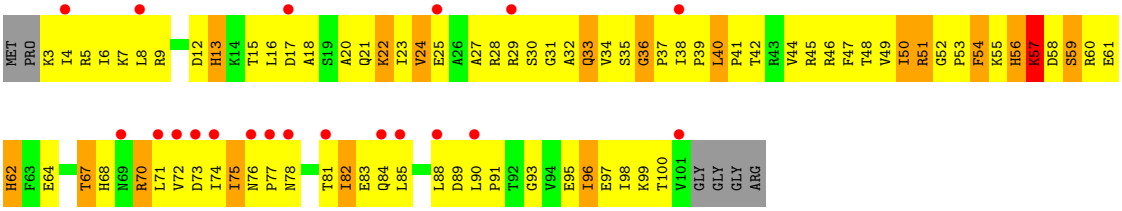




- Molecule 10: 30S RIBOSOMAL PROTEIN S10

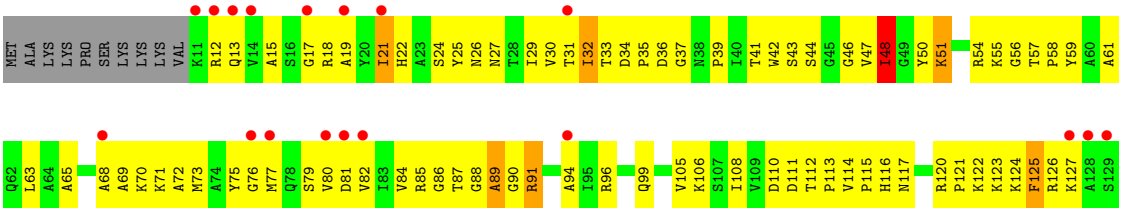
Chain CJ:





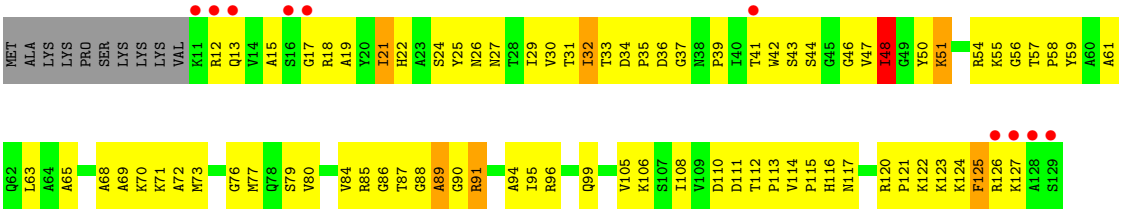
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



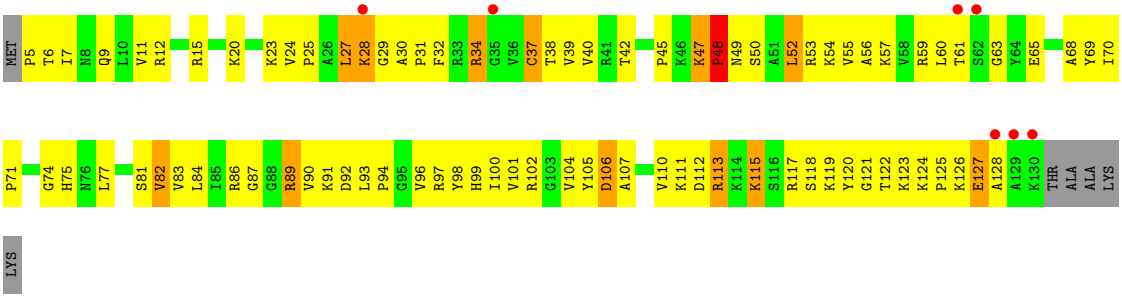
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



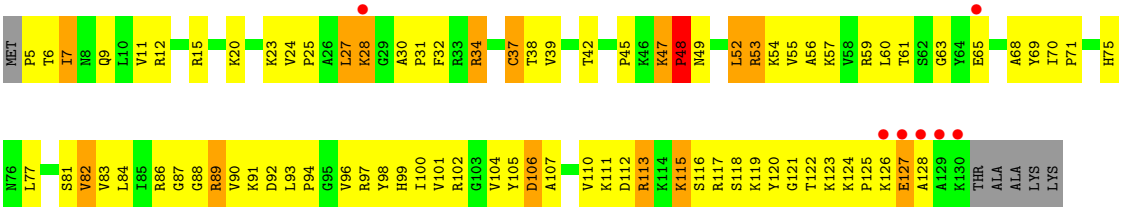
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



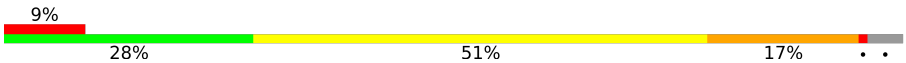
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

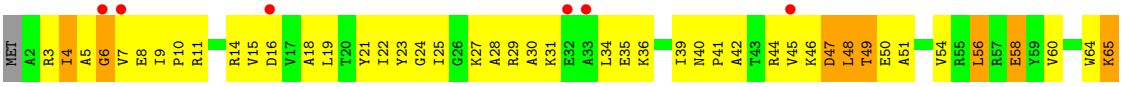
Chain CL:

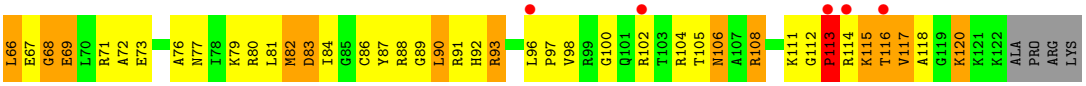


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:

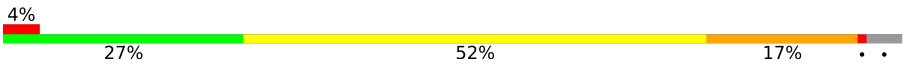


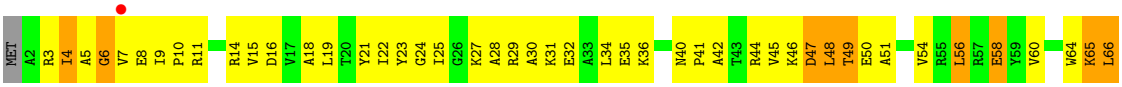


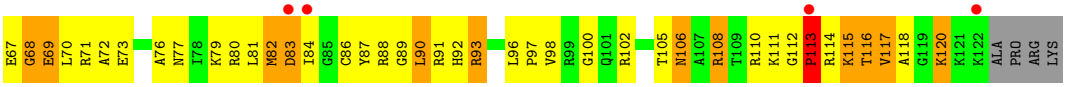


• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:

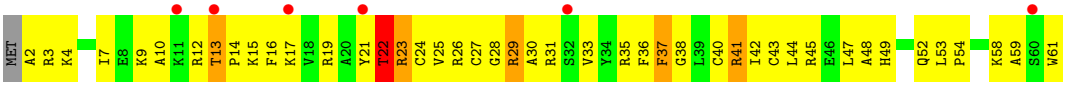






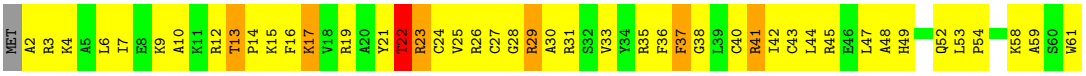
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:



• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN:

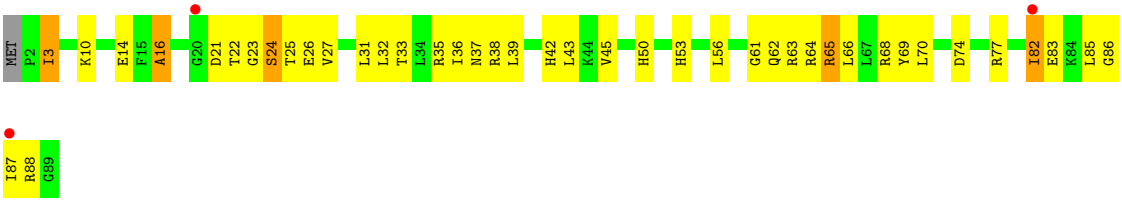


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:

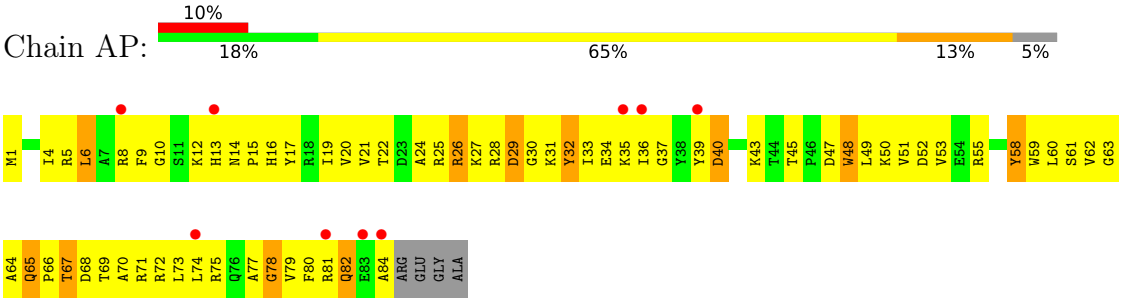
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



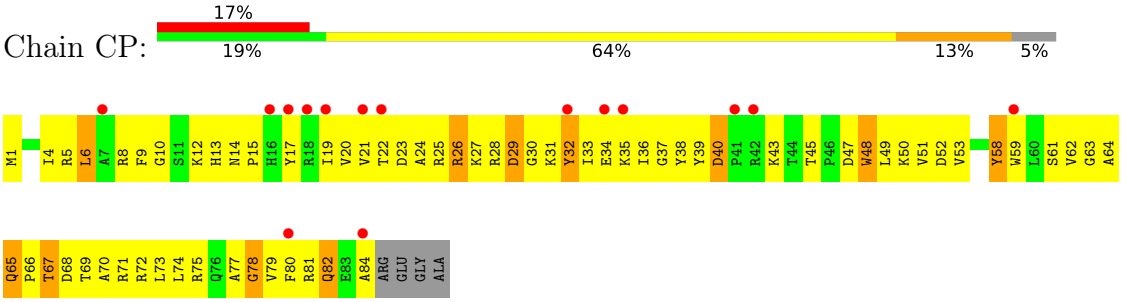
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



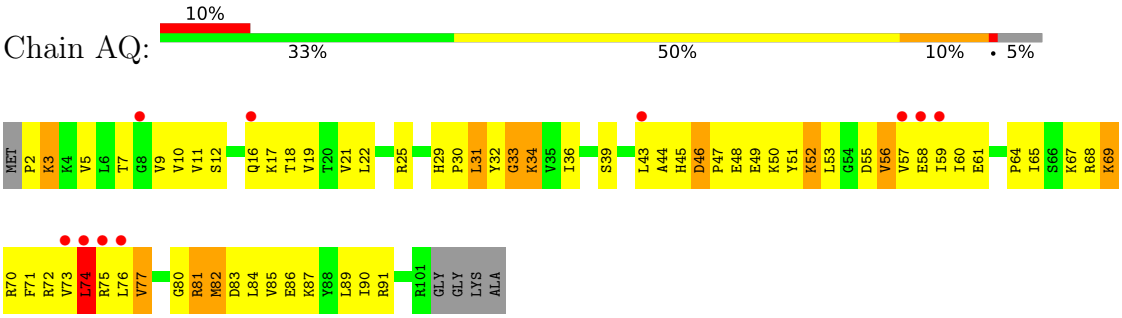
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



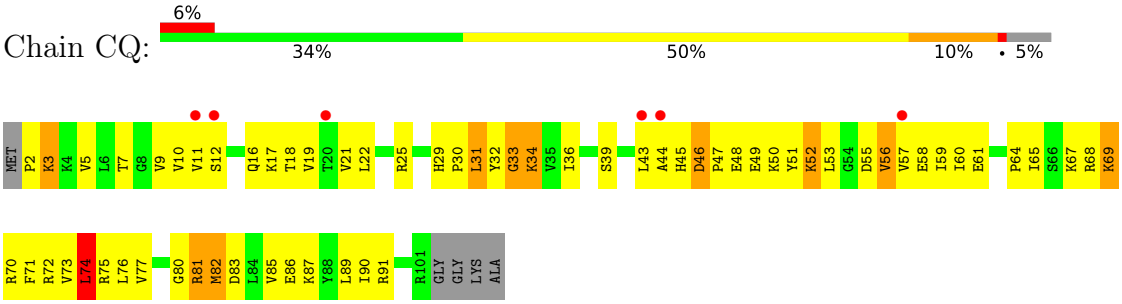
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



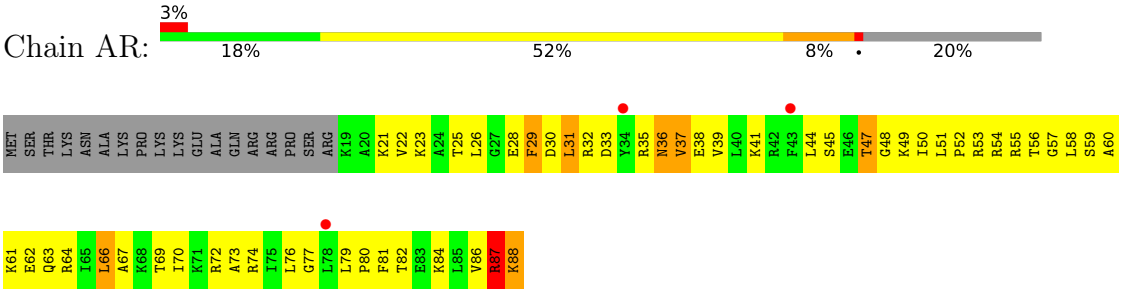
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



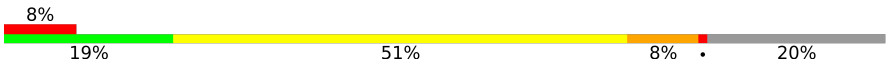
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

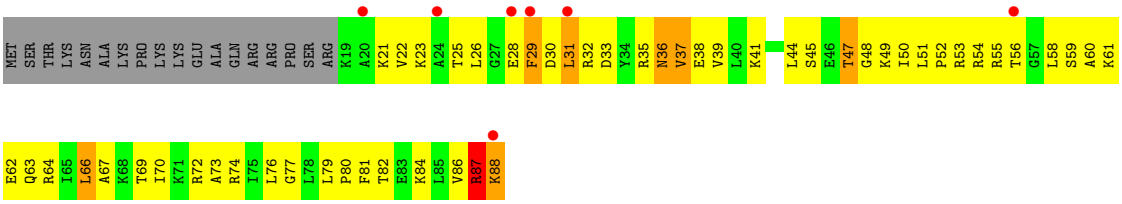
Chain AR:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

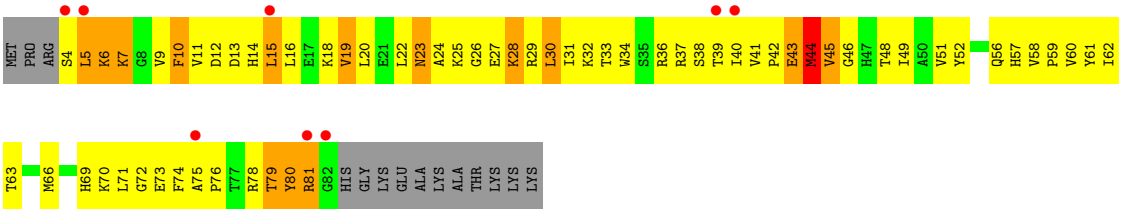
Chain CR:





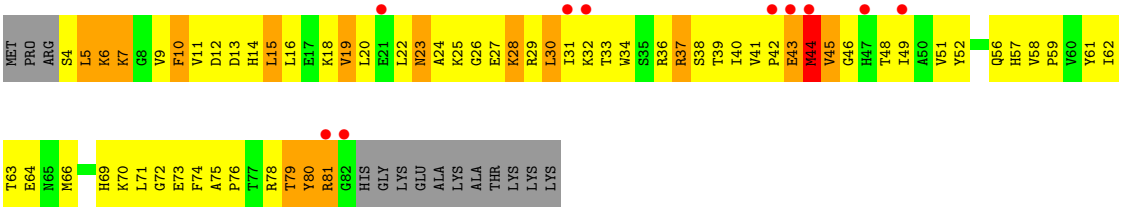
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



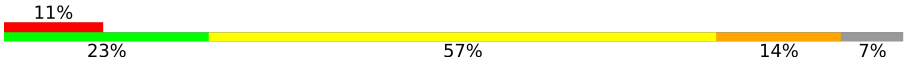
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

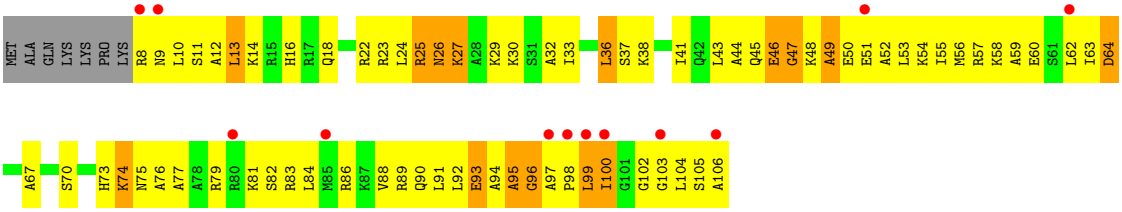
Chain CS:



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

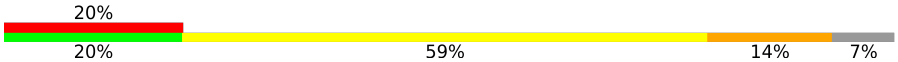
Chain AT:

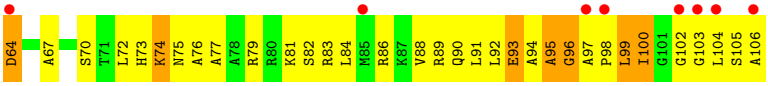




• Molecule 20: 30S RIBOSOMAL PROTEIN S20

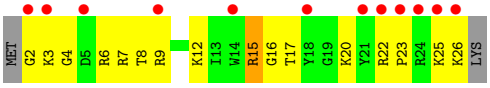
Chain CT:





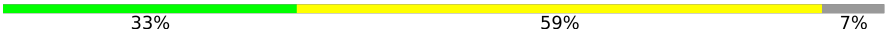
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



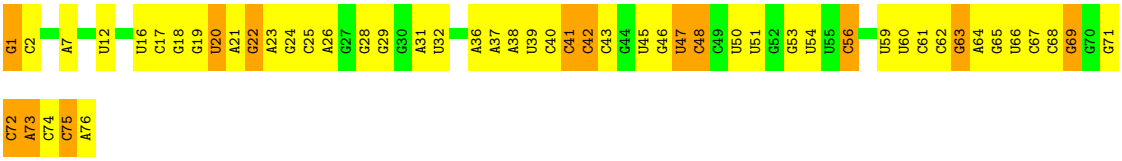
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:



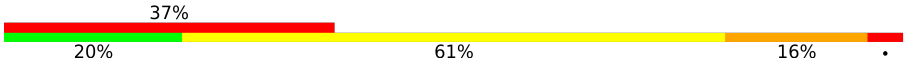
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

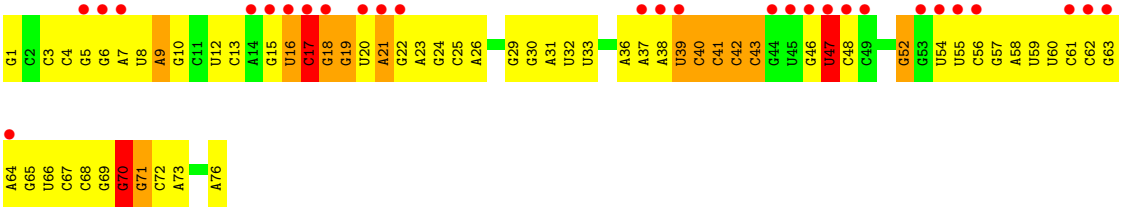
Chain AV:



• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

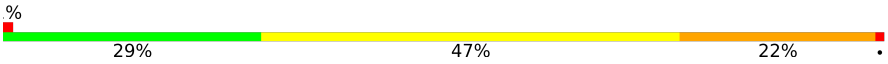
Chain AW:

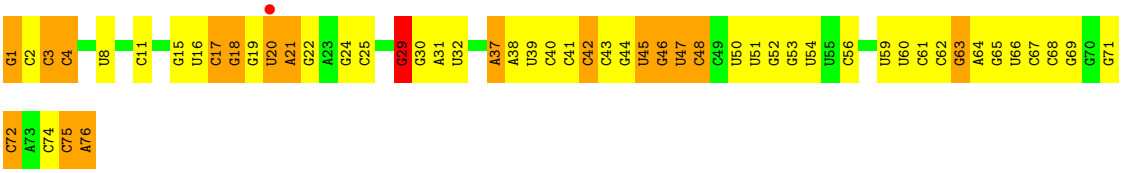




• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

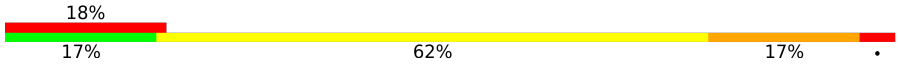
Chain CV:

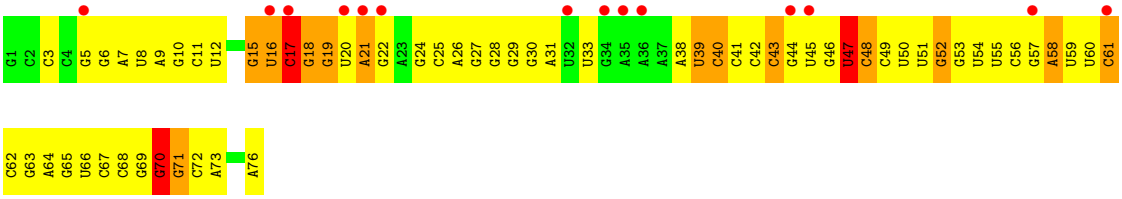




• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

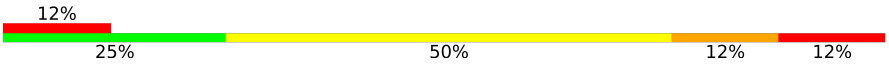
Chain CW:

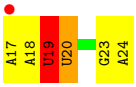




- Molecule 23: MRNA

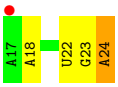
Chain AX:





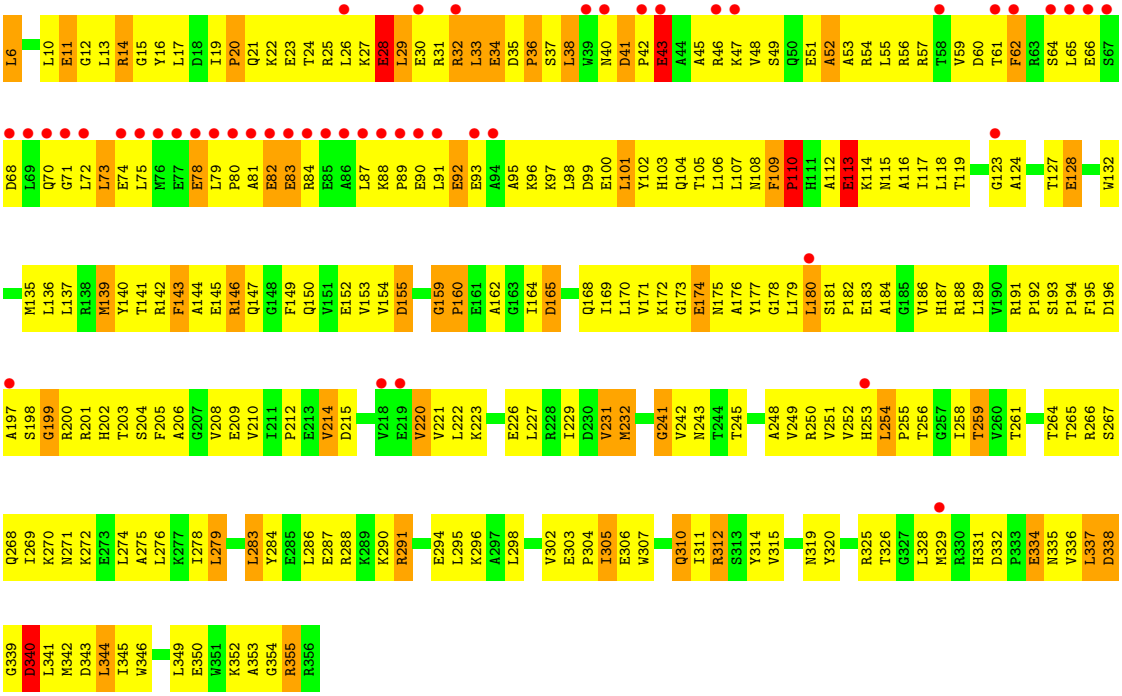
- Molecule 23: MRNA

Chain CX:



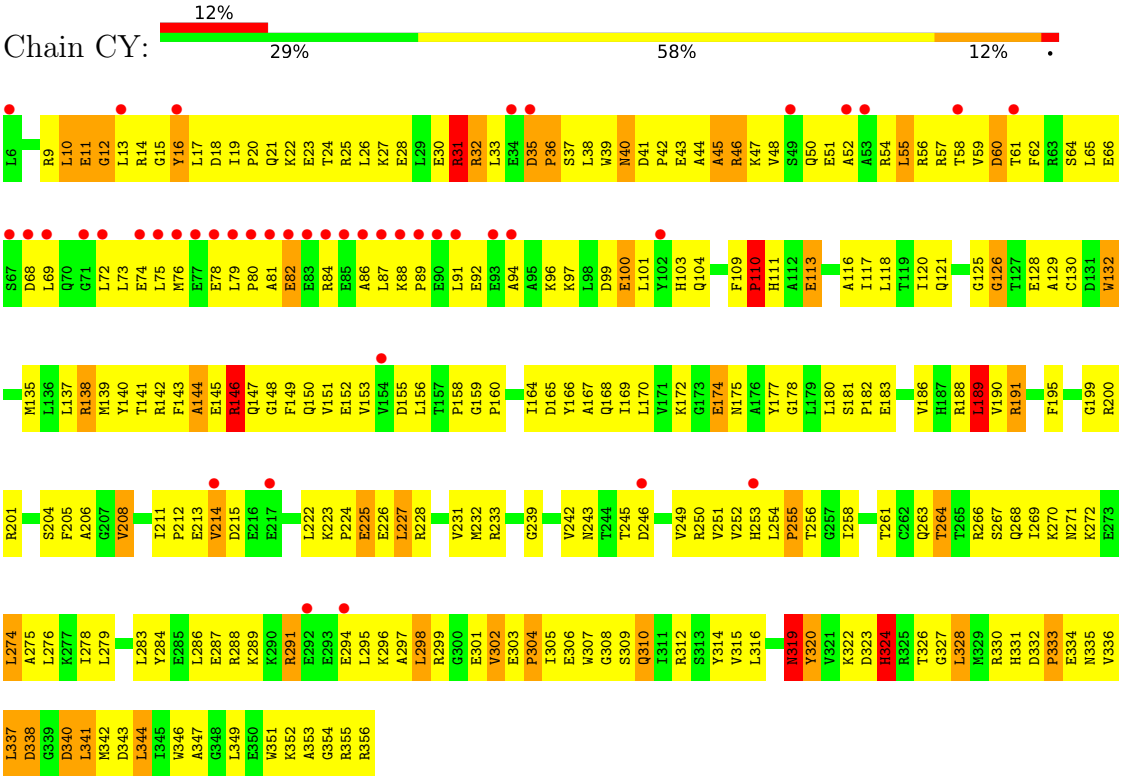
- Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2

Chain AY:



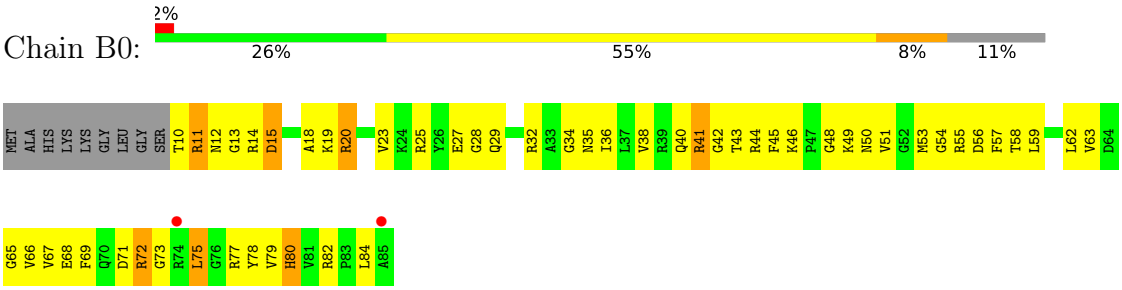
- Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2

Chain CY:



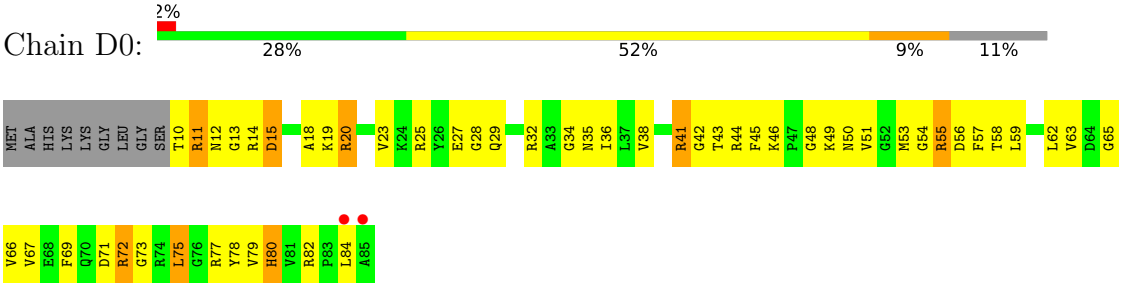
- Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain B0:



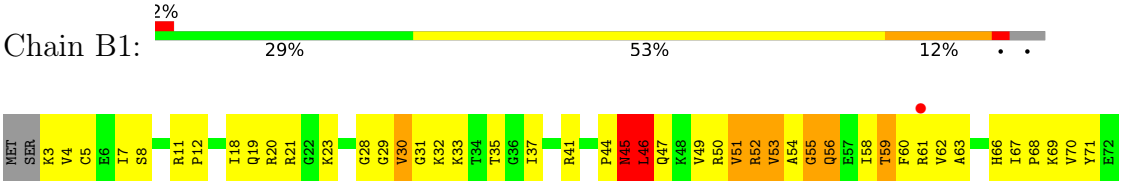
- Molecule 25: 50S RIBOSOMAL PROTEIN L27

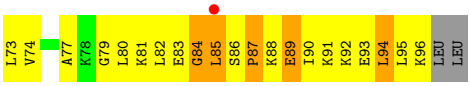
Chain D0:



- Molecule 26: 50S RIBOSOMAL PROTEIN L28

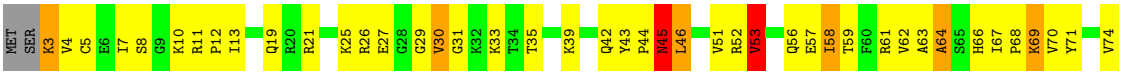
Chain B1:





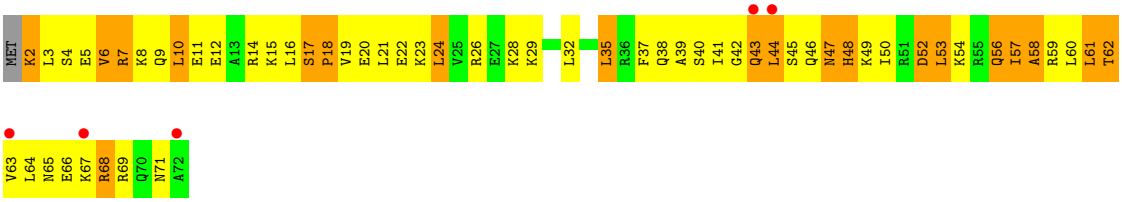
• Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain D1:



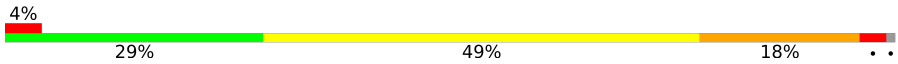
• Molecule 27: 50S RIBOSOMAL PROTEIN L29

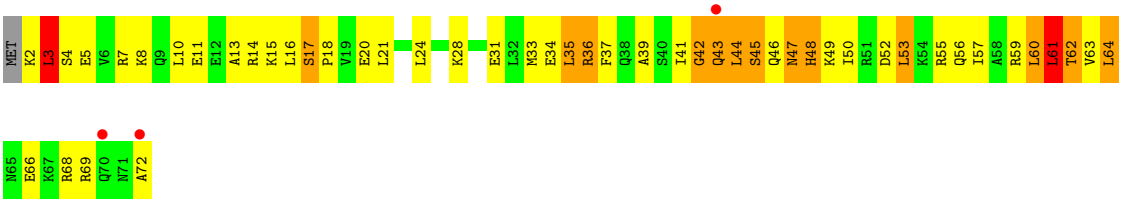
Chain B2:



• Molecule 27: 50S RIBOSOMAL PROTEIN L29

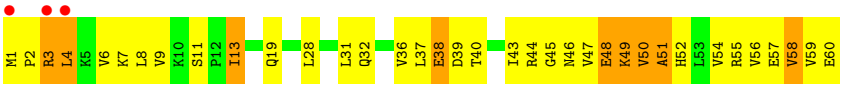
Chain D2:





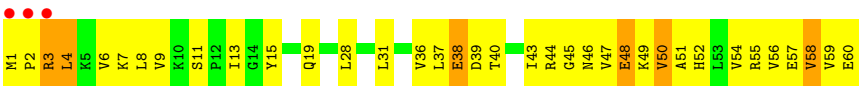
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain B3:



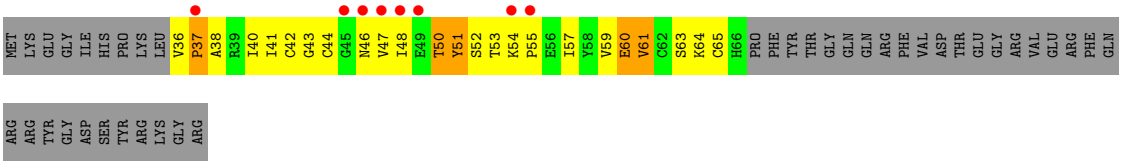
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain D3:



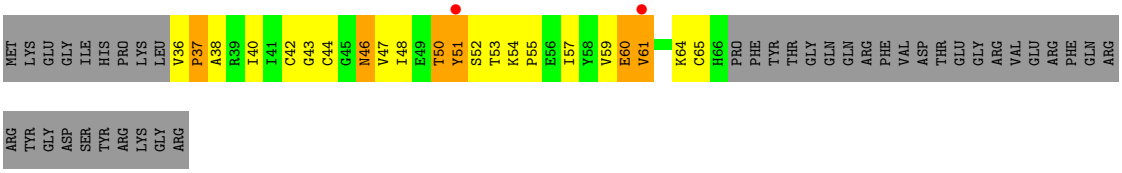
• Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain B4:



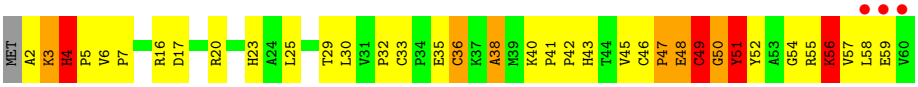
- Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain D4:



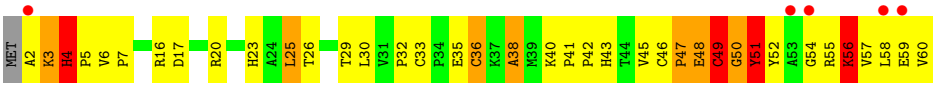
- Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain B5:



- Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain D5:



- Molecule 31: 50S RIBOSOMAL PROTEIN L33

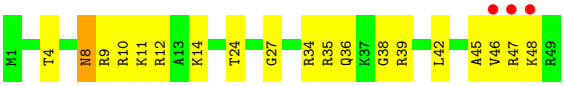
Chain B6:

- Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain D6:

- Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain B7:

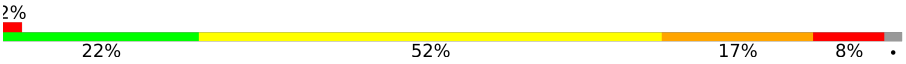


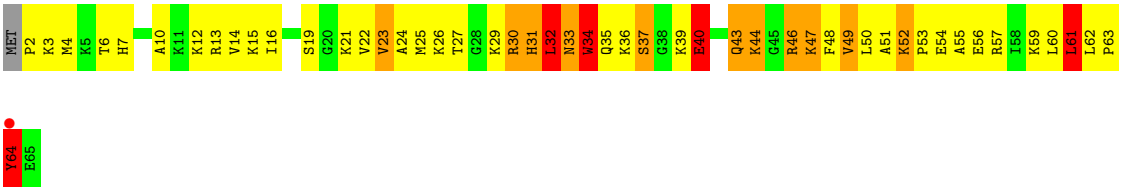
• Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain D7:

• Molecule 33: 50S RIBOSOMAL PROTEIN L35

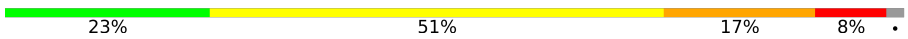
Chain B8:

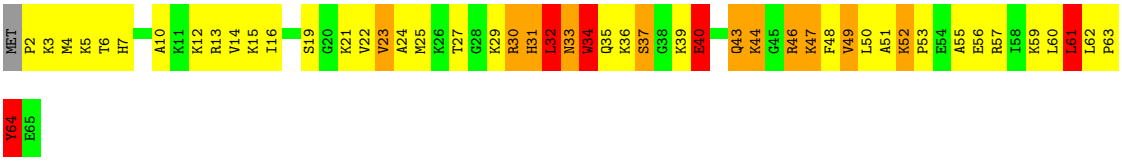




• Molecule 33: 50S RIBOSOMAL PROTEIN L35

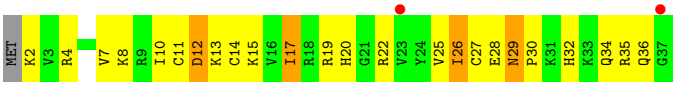
Chain D8:





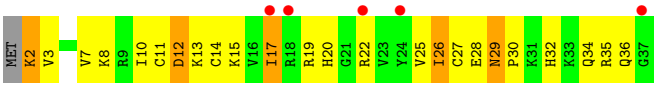
• Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain B9:



• Molecule 34: 50S RIBOSOMAL PROTEIN L36

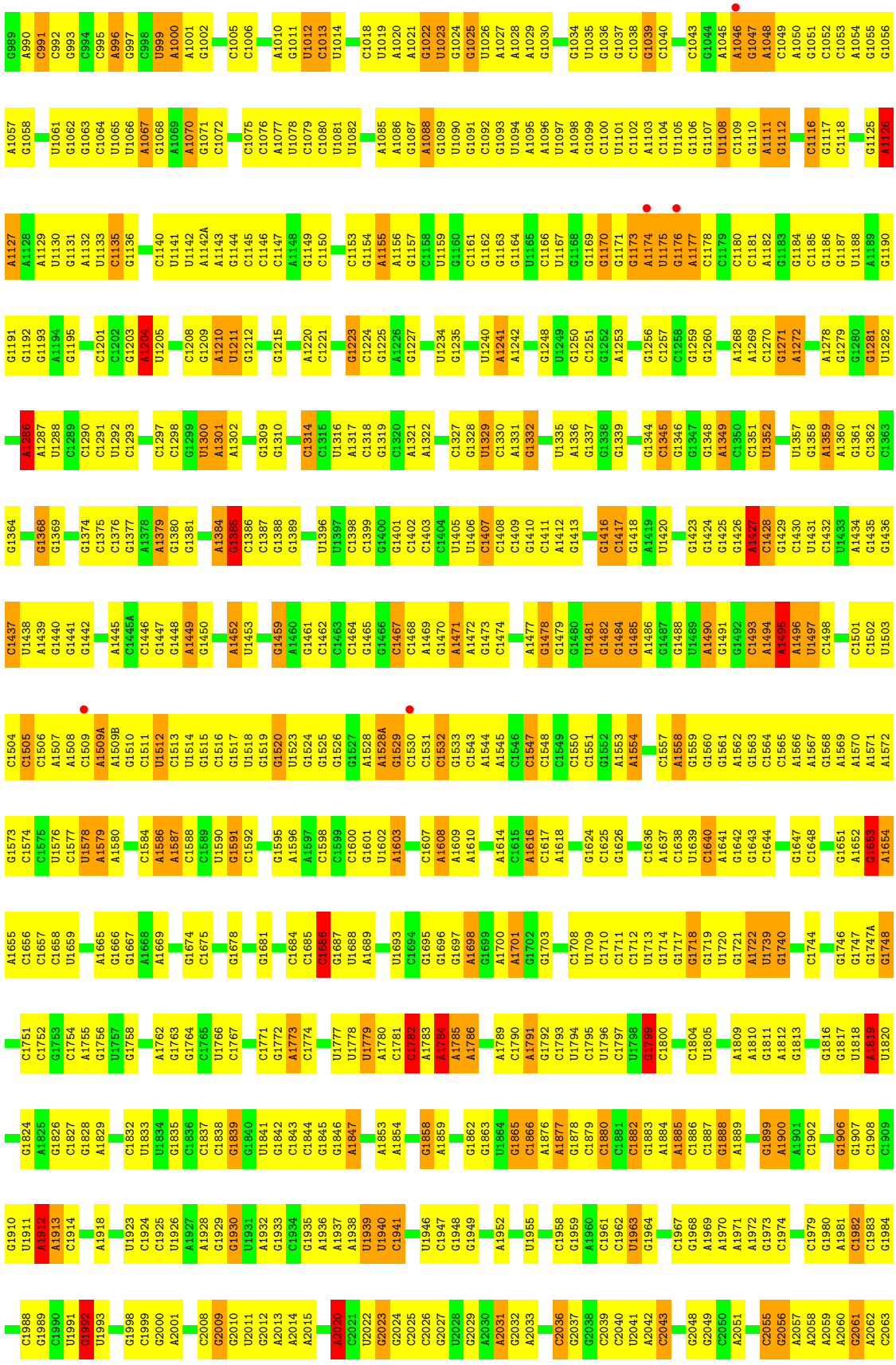
Chain D9:

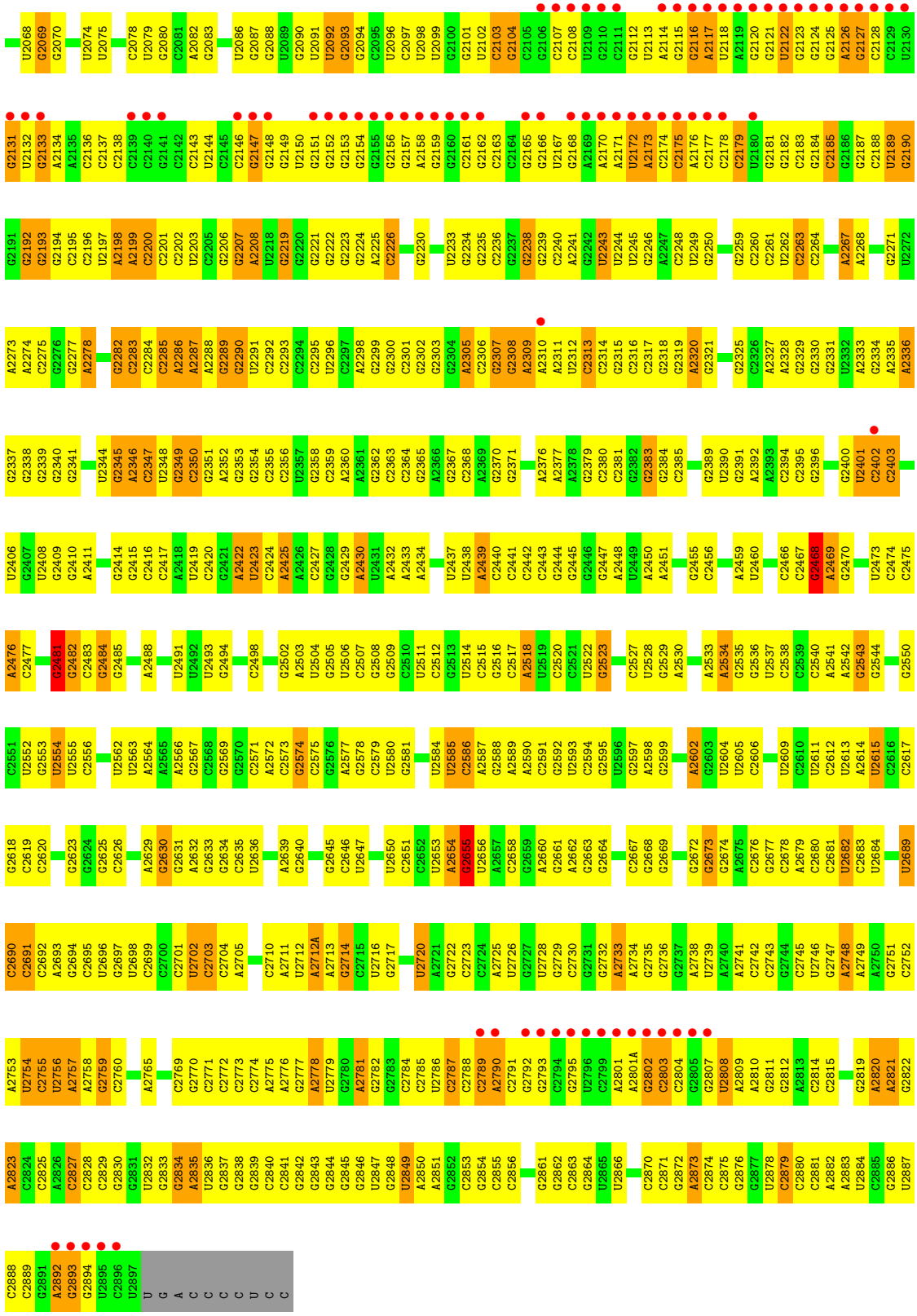


• Molecule 35: 23S RIBOSOMAL RNA

Chain BA:

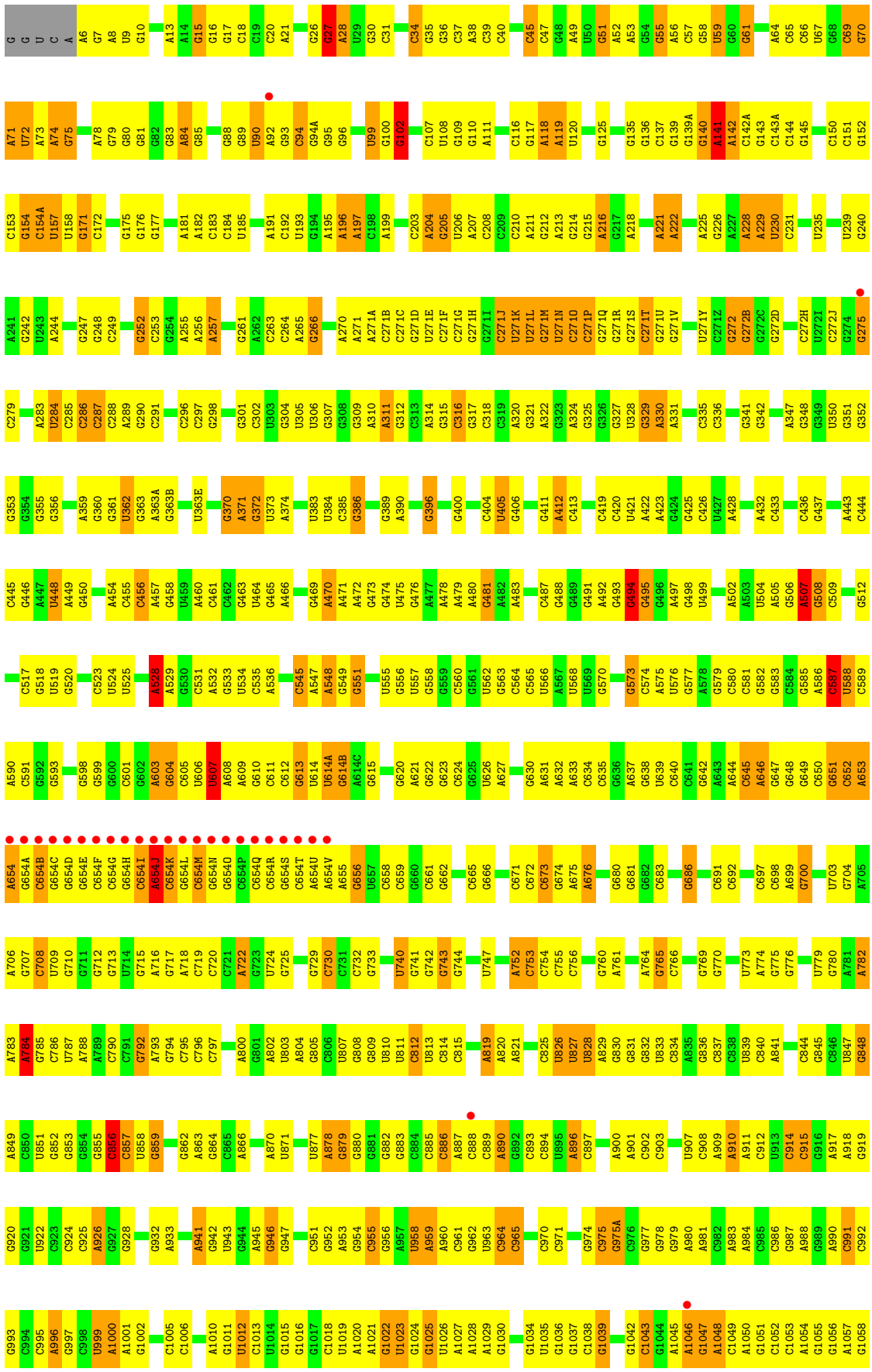
G
G
U
C
A
A6 G7 A8 U9 G10 A13 A14 G15 G16 G17 C18 C19 C20 A21 G26 G27 A28 U29 G30 C31 C34 G35 G36 C37 A38 C39 C40 C45 A49 U50 G51 A52 A53 G54 G55 A56 C57 G58 U59 G60 G61 A64 C65 C66 U67 G68 C69 G70 A71
U72 A73 A74 G75 A78 G79 G80 G81 G82 G83 A84 G85 G88 G89 U90 A92 G93 G94 G94A G95 G96 G97 G98 U99 G100 G102 C107 U108 G109 C110 A111 C116 G117 A118 A119 U120 G125 G135 G136 C137 G139 G139A G140 A141 A142 G142A G143 G143A C144 G145 C150 C151 G152
C153 G154 C154A U157 U158 G171 C172 G175 G176 G177 A182 C183 C184 U185 A191 C192 U193 G194 A195 A196 A197 C198 A199 U200 C201 U202 C203 A204 G205 U206 A207 C208 G212 A213 G214 G215 A216 G217 A218 A221 A222 A225 G226 A227 A228 A229 U230 C231 C234 U235 C236 C237 C238
U239 G240 A241 G242 U243 A244 G247 G248 C249 G252 A255 A256 A257 G258 G259 G260 G261 A262 C263 C264 A265 G266 A270 A271 A271A C271B C271C G271D U271E C271F C271G C271H G271I C271J U271K U271L G271M U271N C271O C271P G271Q G271R G271S G271T G271U G271V U271Y C271Z G272 G272B G272C G272D C272H U272I
C272J G274 G275 C279 A283 U284 C285 C286 C287 C288 A289 G290 C291 C296 C297 G298 G301 C302 U303 G304 U305 U306 G307 G308 G309 A310 A311 A314 G315 C316 G317 C318 C319 A320 G321 A322 G323 A324 G325 G326 G327 U328 G329 A330 A331 C335 C336 G341 G342 A347 G348 G349 U350
G351 G352 G353 G354 G355 G356 A359 G360 G361 U362 G363 A363A G363B U363E G370 A371 G372 U373 A374 U380 U383 U384 C385 G386 G389 A390 U395 G396 G400 C404 U405 G406 C409 G410 G411 A412 C413 C419 C420 U421 A422 A423 G424 G425 C426 U427 A428 U431
A432 C433 C436 G437 A443 C444 C445 G446 A447 U448 A449 G450 A454 C455 C456 A457 G458 U459 A460 C461 U464 G465 A466 G469 A470 A471 A472 G473 G474 U475 G476 A477 A478 A479 A480 G481 A482 A483 A492 G493 G494 G495 G496 A497 G498 U499 A502 A503 U504 A505 G506 A507 G508
C509 G512 C517 G518 U519 G520 C523 U524 U525 A528 A529 G530 C531 A532 G533 U534 C535 A536 C545 A547 A548 G549 G551 U555 G556 U557 G558 G559 C560 G563 C564 C565 U566 A567 U568 G573 C574 A575 U576 G577 C580 C581 G582 G583 C584 G585 A586 C587 U588 C589 A590
C591 G592 G593 G598 G599 G600 C601 G602 A603 G604 C605 U606 U607 A608 A609 G610 C611 C612 G613 U614 U614A G614B A614C G615 G620 A621 G622 G623 C624 G625 U626 A627 G630 A631 A632 A633 C634 C635 G636 A637 G638 U639 C640 C641 G642 A643 A644 C645 A646 G647 G648 G649 C650 G651 C652 A653 A654
G654A C654B G654C G654D G654E C654F C654G G654H C654I A654J C654K G654L C654M G654N C654O C654P C654Q C654R G654S C654T A654U A654V A655 G656 U657 C658 C659 G660 C661 G662 C665 G666 C671 C672 C673 G674 A675 A676 G680 G681 G682 C683 G686 C691 C692 G697 C698 A699 G700 U703 C704 A705 A706
G707 C708 U709 G710 G711 G712 G713 U714 G715 A716 G717 A718 C719 C720 C721 A722 G723 U724 G725 G729 C730 C731 C732 G733 U740 G741 C742 G743 G744 U747 A752 C753 C754 C755 C756 G760 A761 A764 G765 C766 G769 G770 U773 A774 G775 G776 U779 G780 A781 A782 A783
A784 G785 C786 U787 A788 A789 C790 C791 G792 A793 G794 C795 C796 C797 A800 G801 A802 U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 A813 C814 C815 C816 C817 G818 A819 A820 A821 C825 U826 U827 U828 A829 G830 G831 U832 U833 C834 A835 G836 C837 C838 U839 C840 A841 C844 G845 C846 U847
G848 A849 C850 U851 G852 G853 G854 G855 C856 C857 U858 G859 G862 A863 G864 C865 A866 C867 U868 G869 A870 U871 G875 C876 U877 A878 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 A900 A901 C902 C903 U907 C908 A909 A910 A911 C912 U913 C914
C915 G916 A917 A918 G919 U922 C923 C924 C925 A926 G927 G928 G932 A933 A941 G942 U943 G944 A945 G946 G947 C951 G952 A953 G954 C955 G956 A957 U958 A959 A960 C961 G962 U963 C964 C965 C970 C971 G974 C975 G975A C976 G977 G978 G979 A980 A981 C982 A983 A984 C985 C986 G987 A988





• Molecule 35: 23S RIBOSOMAL RNA

Chain DA: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G920 G921 U922 C923 C924 C925 A926 G927 G928 G932 A933 A941 G942 U943 G944 A945 G946 G947 C951 G952 A953 G954 C955 G956 A957 U958 A959 A960 C961 G962 U963 C964 C965 C970 C971 G974 C975 G975A C976 G977 G978 G979 A980 A981 C982 A983 A984 C985 C986 G987 A988 G989 A990 C991 C992
A849 C850 U851 G852 G853 G854 G855 G856 C857 U858 G859 G862 A863 G864 C865 A866 A870 U871 U877 A878 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 A900 A901 C902 C903 U907 C908 A909 A910 A911 C912 U913 C914 C915 G916 A917 A918 G919
A783 A784 G785 C786 U787 A788 A789 C790 C791 G792 A793 G794 C795 C796 C797 A800 G801 A802 U803 A804 G805 C806 U807 G808 G809 U810 U811 C812 U813 C814 C815 A819 A820 A821 C825 U826 U827 U828 A829 G830 G831 G832 U833 C834 A835 G836 C837 C838 U839 C840 A841 C844 G845 C846 U847 G848
A706 G707 C708 U709 G710 G711 G712 G713 U714 G715 A716 A717 A718 C719 C720 C721 A722 G723 U724 G725 G729 C730 C731 C732 G733 U740 G741 G742 G743 G744 U747 A752 C753 C754 C755 C756 G760 A761 A764 G765 C766 G769 G770 U773 A774 G775 G776 U779 G780 A781 A782
A654 G654A C654B G654C G654D G654E C654F C654G G654H C654I A654J C654K G654L C654M G654N G654O C654P C654Q G654R G654S C654T A654U A654V A655 G656 U657 C658 C659 G660 C661 G662 C665 G666 C671 C672 C673 G674 A675 A676 G680 G681 G682 C683 G686 C691 C692 C697 C698 A699 G700 U703 G704 A705
A590 C591 G592 G593 G598 G599 G600 C601 G602 A603 G604 C605 U606 W607 A608 A609 G610 C611 C612 G613 U614 G614A G614B A614C G615 G620 A621 G622 G623 C624 G625 U626 A627 G630 A631 A632 A633 C634 C635 G636 A637 G638 U639 C640 C641 G642 A643 A644 C645 A646 G647 G648 G649 C650 G651 C652 A653
C517 G518 U519 G520 C523 U524 U525 A528 A529 G530 C531 A532 G533 U534 C535 A536 C545 A547 A548 G549 G551 U555 G556 U557 G558 G559 C560 G561 U562 G563 C564 C565 U566 A567 U568 U569 G570 G573 C574 A575 U576 G577 A578 G579 C580 C581 U582 G583 C584 G585 A586 C587 U588 G589
C445 G446 A447 U448 A449 G450 A454 C455 C456 A457 G458 U459 A460 C461 C462 G463 U464 G465 A466 G469 A470 A471 A472 G473 G474 U475 G476 A477 A478 A479 A480 G481 A482 A483 C487 G488 G489 G491 A492 G493 G494 G495 G496 A497 G498 U499 A502 A503 U504 A505 G506 A507 G508 C509 G512
G353 G354 G355 G356 A359 G360 G361 U362 G363 A363A A363B U363E G370 A371 G372 U373 A374 U383 U384 C385 G386 G389 A390 G396 G400 C404 U405 G406 G411 A412 C413 C419 C420 U421 A422 A423 G424 G425 C426 U427 A428 A432 C433 C436 G437 A443 C444
C279 A283 U284 C285 C286 C287 C288 A289 G290 C291 C296 C297 G298 G301 C302 U303 G304 U305 U306 G307 G308 G309 A310 A311 G312 C313 A314 G315 C316 G317 C318 C319 A320 G321 A322 G323 A324 G325 G326 G327 U328 G329 A330 A331 C335 C336 G341 G342 A347 G348 G349 U350 G351 G352
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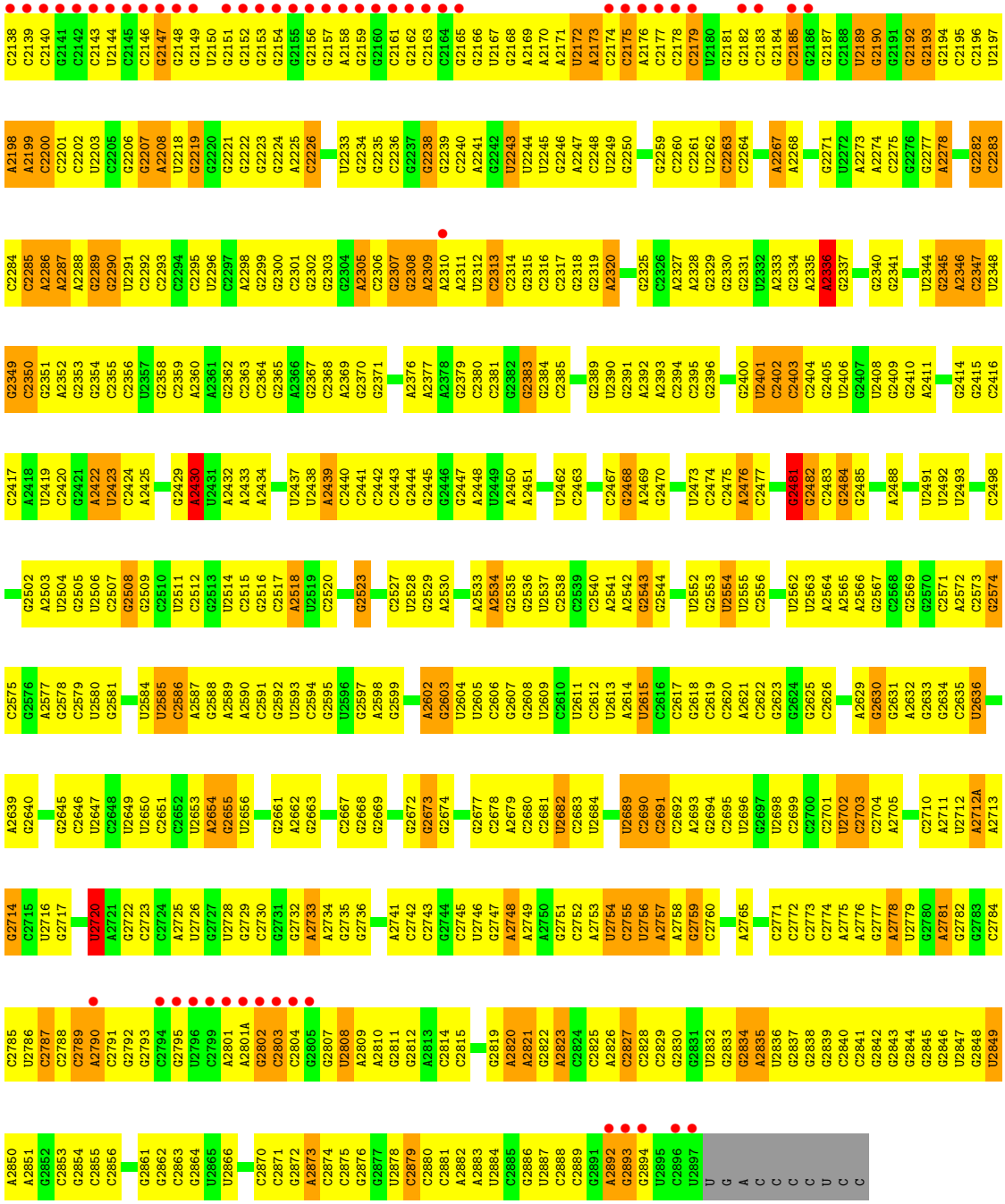
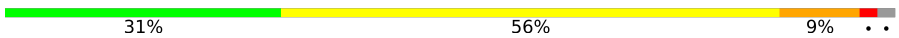
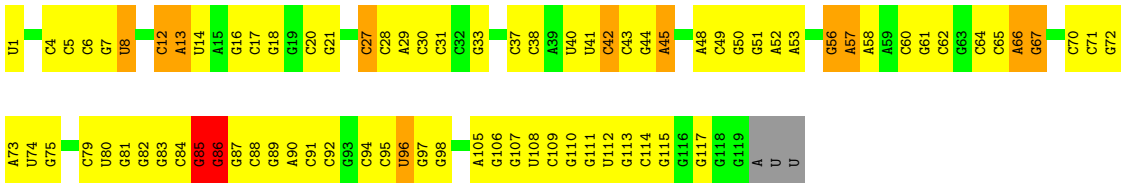
C153 G154 C154A U157 U158 G171 C172 G175 G176 G177 A181 A182 C183 C184 U185 A191 C192 U193 G194 A195 A196 A197 C198 A199 C203 A204 G205 U206 A207 C208 C209 C210 A211 G212 A213 G214 G215 A216 G217 A218 A221 A222 A225 G226 A227 A228 A229 U230 C231 U235 U239 G240
A71 U72 A73 A74 G75 A78 G79 G80 G81 G82 G83 A84 G85 G88 G89 U90 A92 G93 G94 G94A G95 G96 U99 G100 G102 C107 U108 G109 C110 A111 C116 G117 A118 A119 U120 G125 G135 G136 C137 G139 G139A G140 A141 A142 G142A G143 G143A C144 G145 C150 C151 G152
G C U A A6 G7 A8 U9 G10 A13 A14 G15 G16 G17 C18 C19 C20 A21 G26 G27 A28 U29 G30 C31 C34 G35 G36 C37 A38 C39 C40 C45 C47 G48 A49 U50 G51 A52 A53 G54 G55 A56 C57 G58 U59 G60 G61 A64 C65 C66 U67 G68 C69 G70



• Molecule 36: 5S RIBOSOMAL RNA

Chain BB:



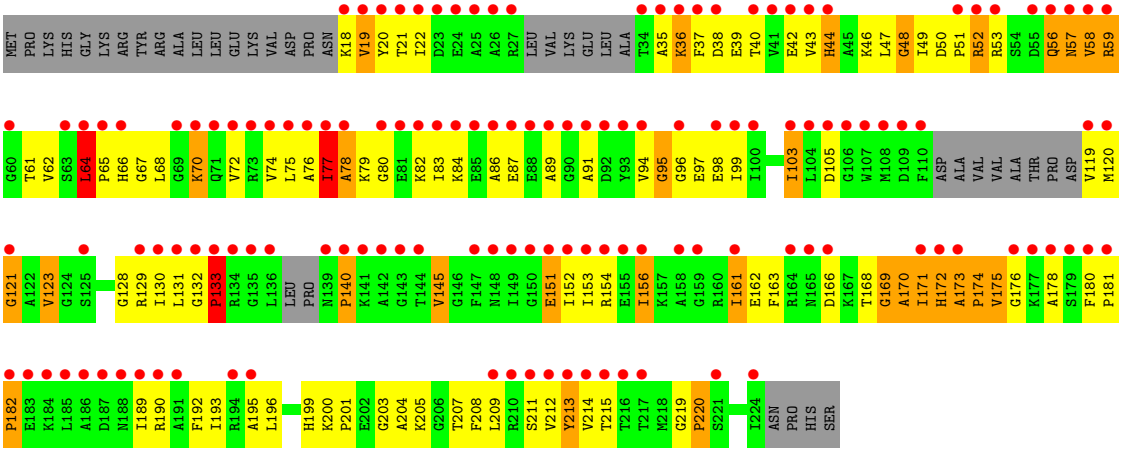


• Molecule 36: 5S RIBOSOMAL RNA

Chain DB: 31% 55% 11%

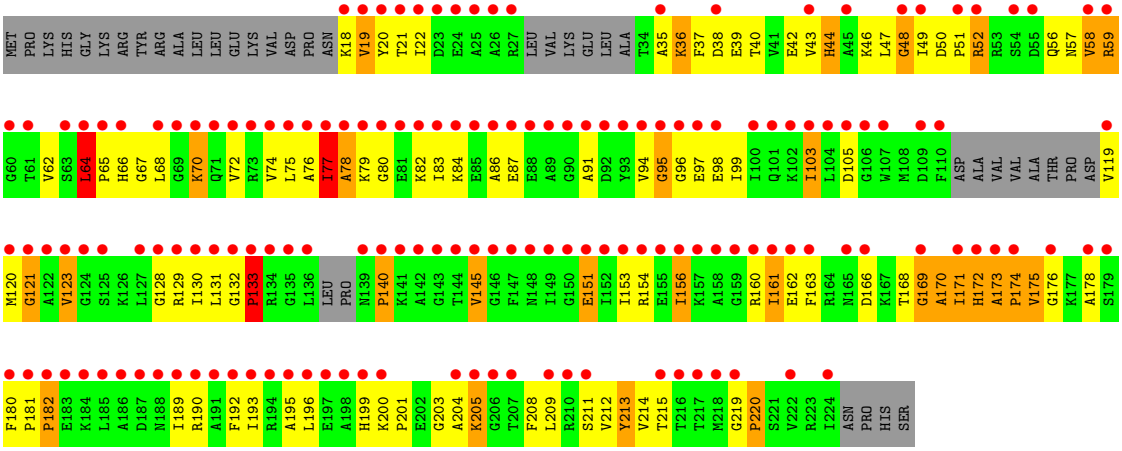
- Molecule 37: 50S RIBOSOMAL PROTEIN L1

Chain BC: 59% 34% 35% 13% 17%



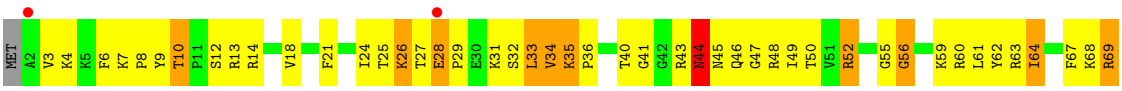
- Molecule 37: 50S RIBOSOMAL PROTEIN L1

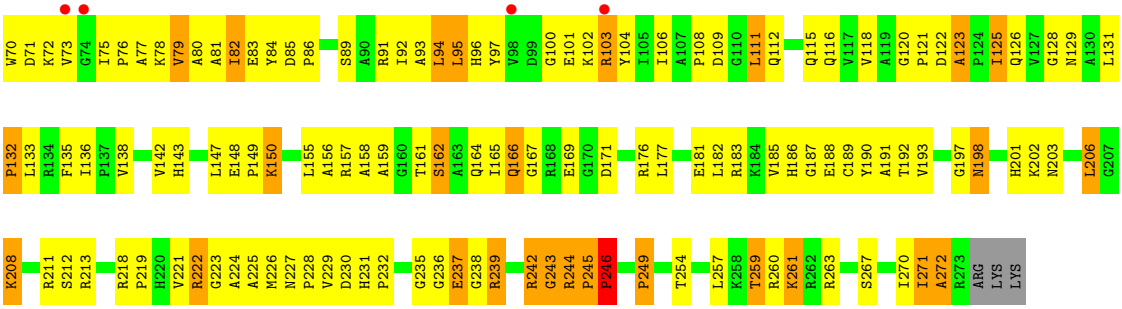
Chain DC: 68% 36% 34% 13% 17%



- Molecule 38: 50S RIBOSOMAL PROTEIN L2

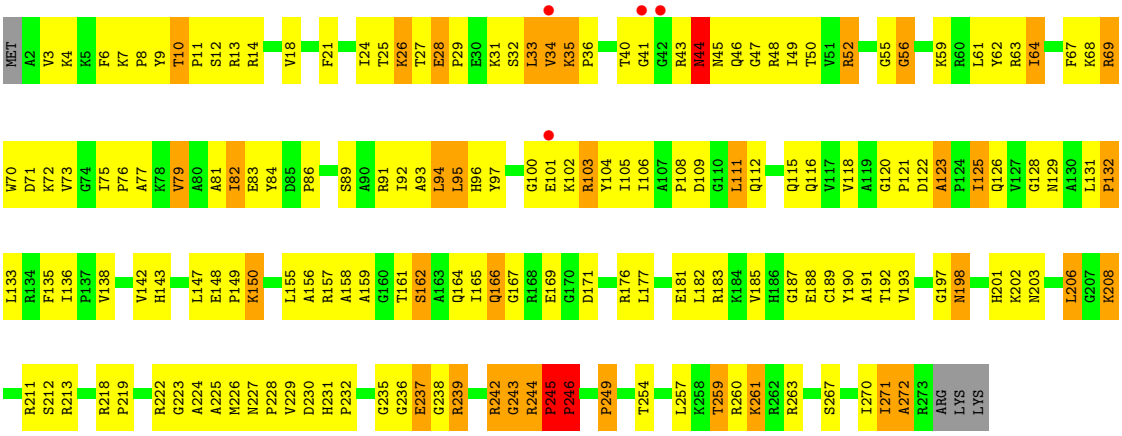
Chain BD: 2% 35% 49% 13%





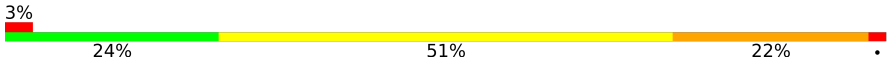
- Molecule 38: 50S RIBOSOMAL PROTEIN L2

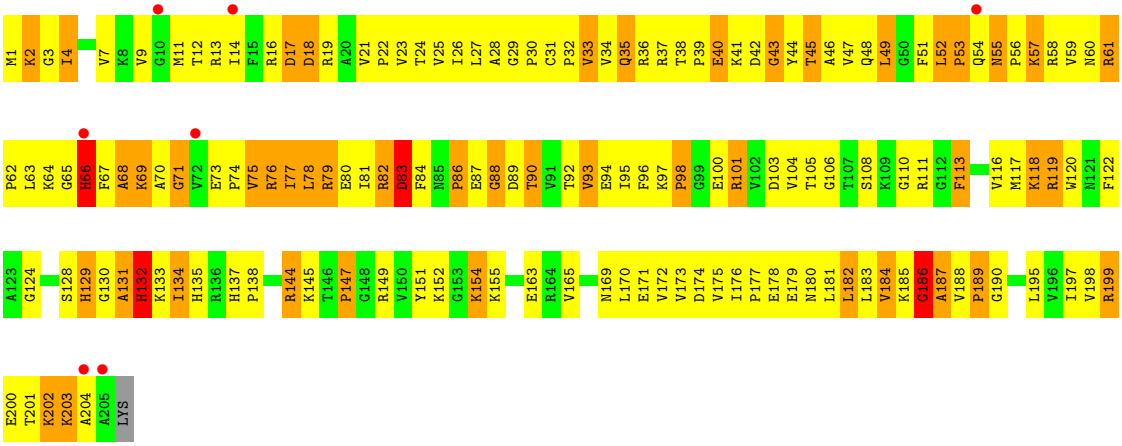
Chain DD:



- Molecule 39: 50S RIBOSOMAL PROTEIN L3

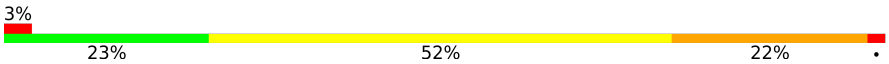
Chain BE:

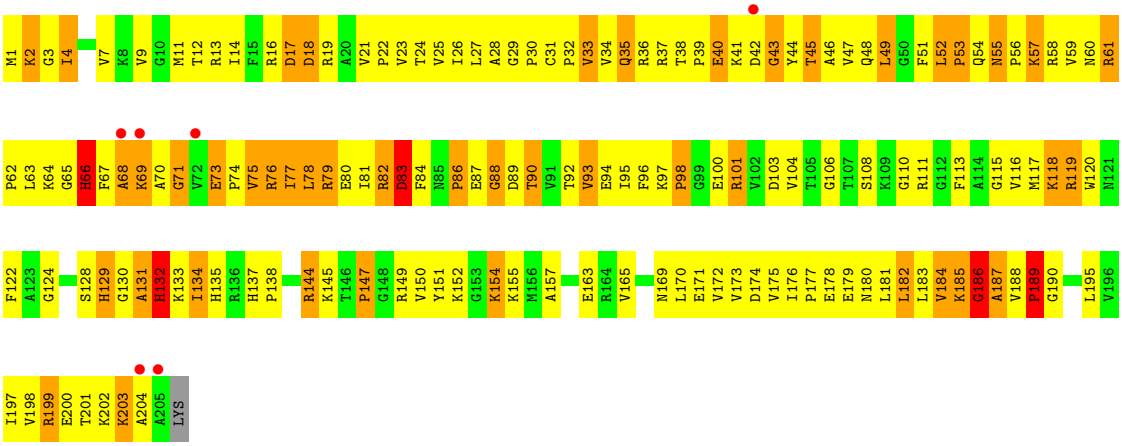




- Molecule 39: 50S RIBOSOMAL PROTEIN L3

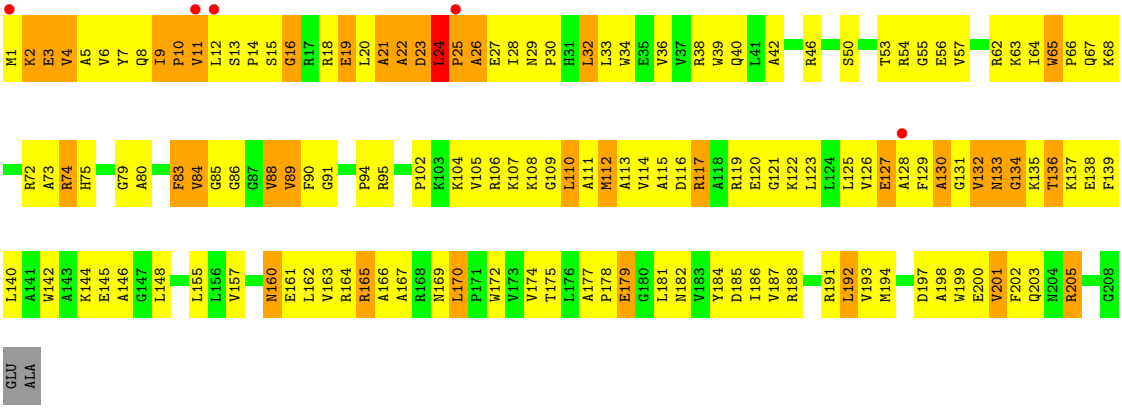
Chain DE:





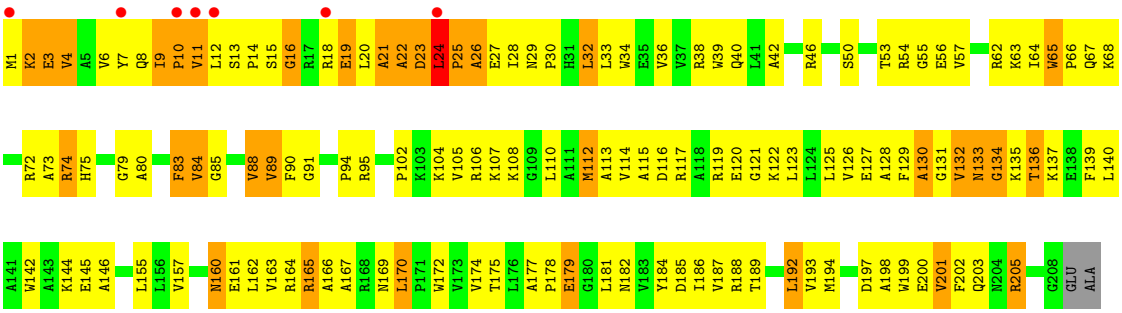
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain BF: 2% 30% 51% 17%



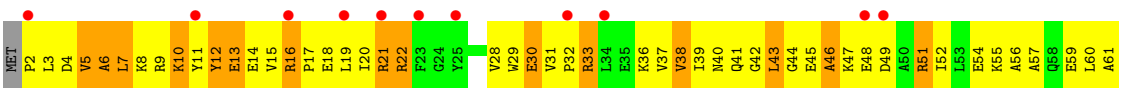
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

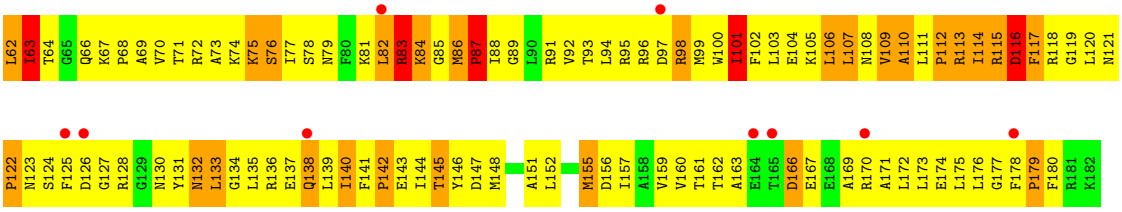
Chain DF: 3% 33% 50% 16%



• Molecule 41: 50S RIBOSOMAL PROTEIN L5

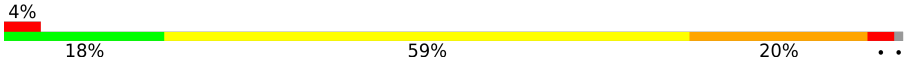
Chain BG: 11% 13% 61% 23%

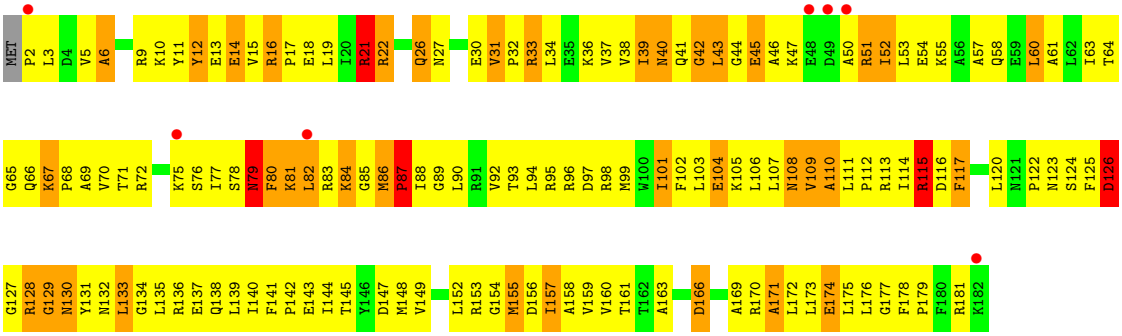




• Molecule 41: 50S RIBOSOMAL PROTEIN L5

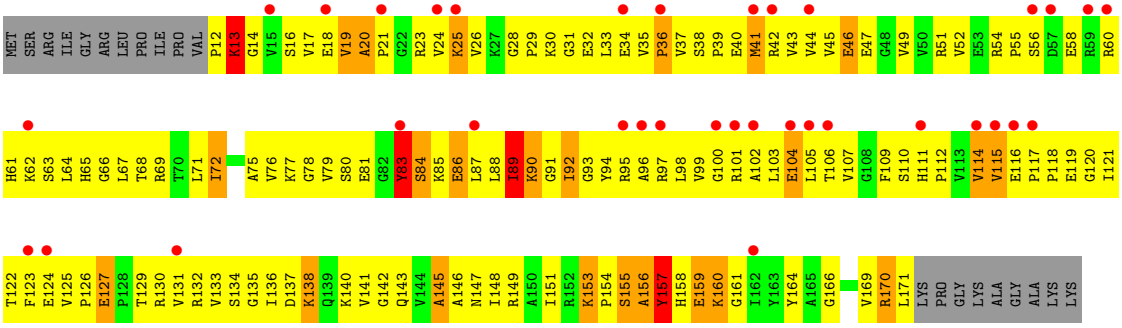
Chain DG:





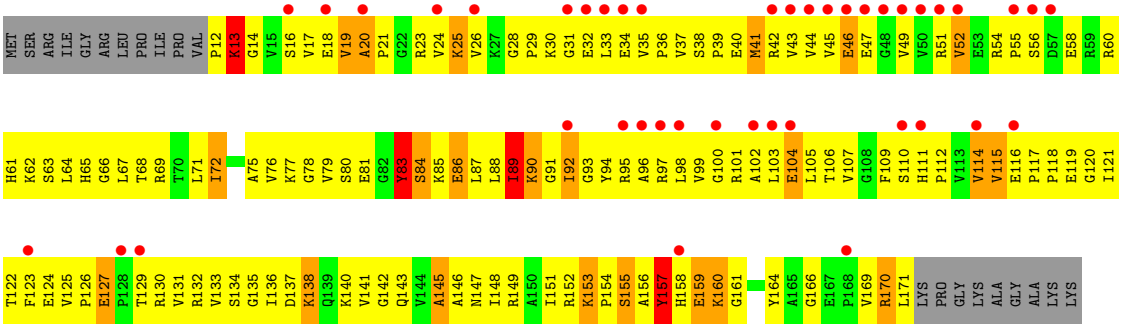
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain BH:



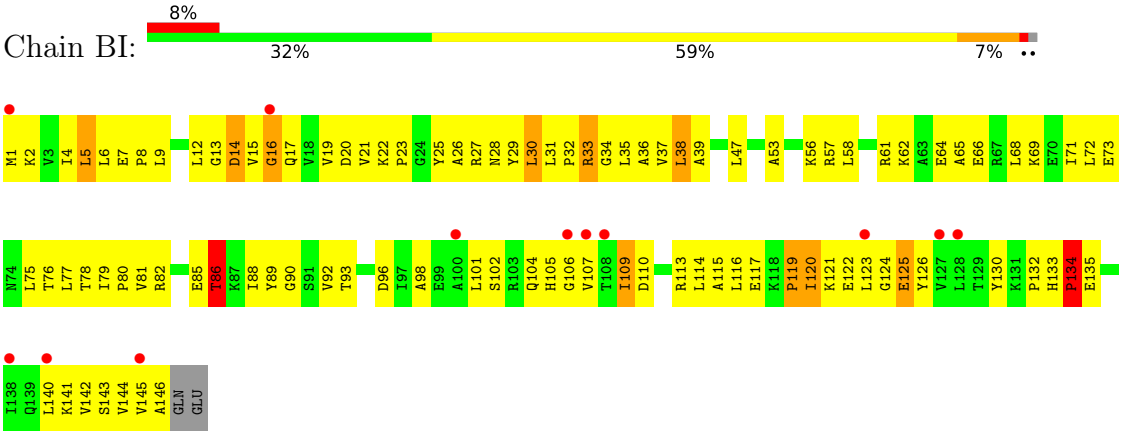
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain DH:



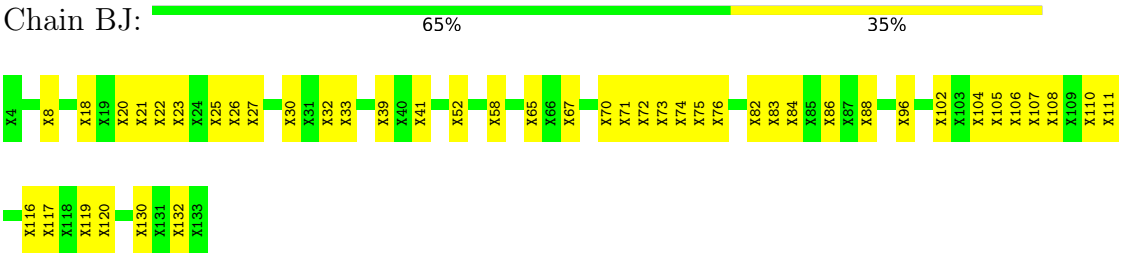
• Molecule 43: 50S RIBOSOMAL PROTEIN L9

Chain BI:



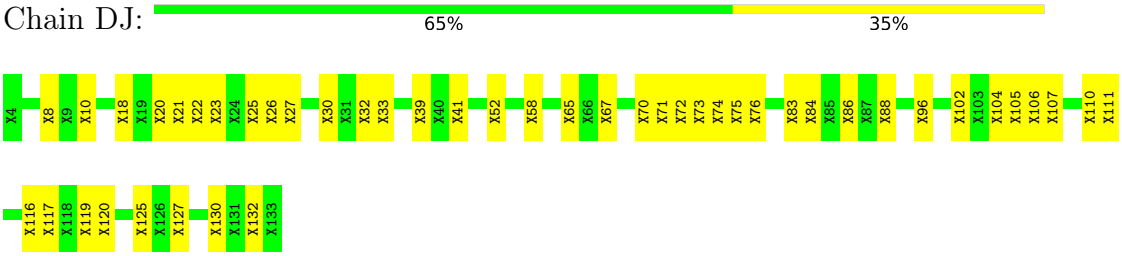
- Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



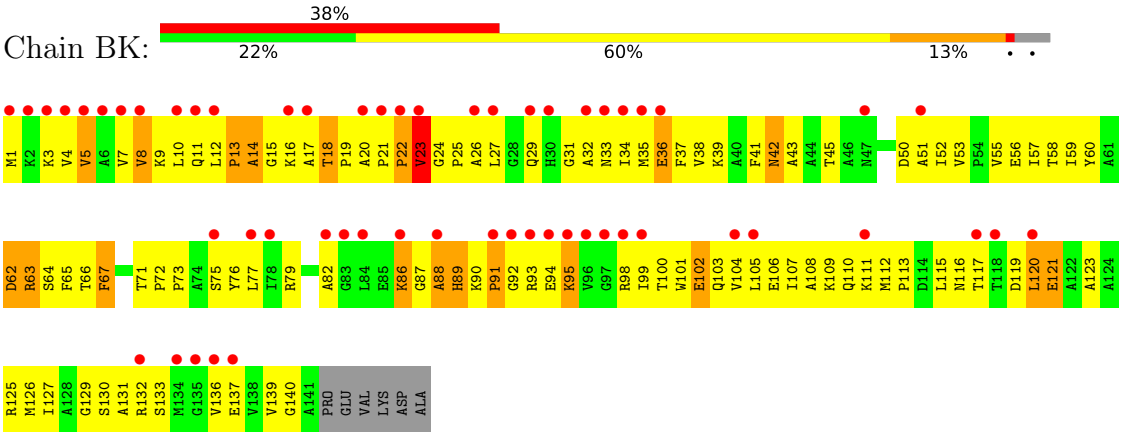
- Molecule 44: 50S RIBOSOMAL PROTEIN L10

Chain DJ:



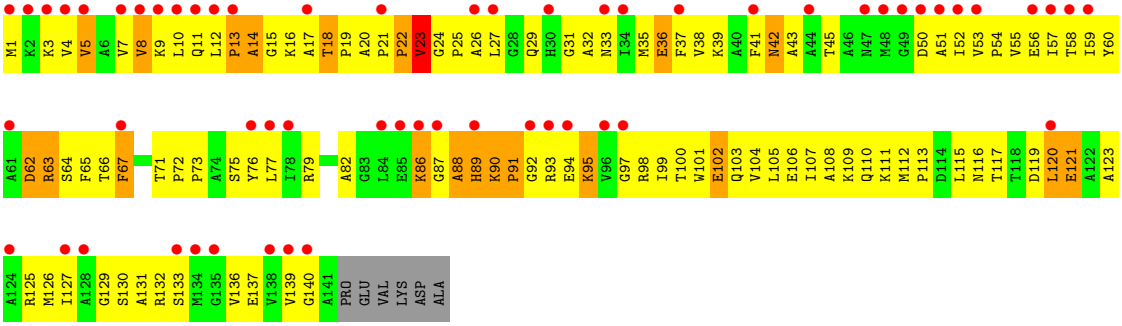
- Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain BK:



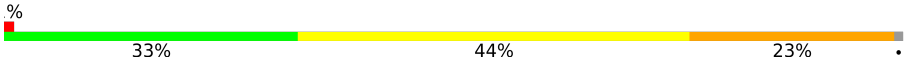
- Molecule 45: 50S RIBOSOMAL PROTEIN L11

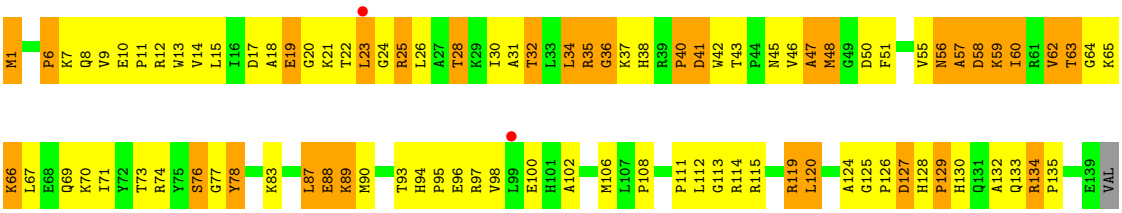
Chain DK:



- Molecule 46: 50S RIBOSOMAL PROTEIN L13

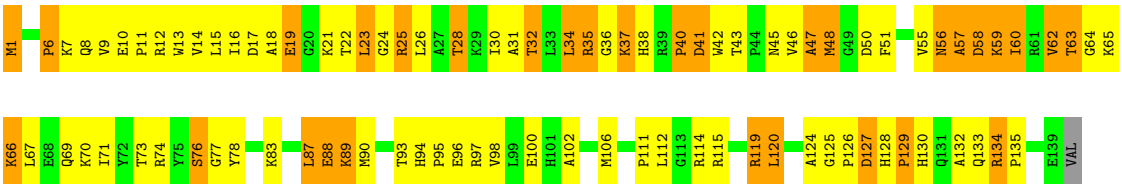
Chain BN:





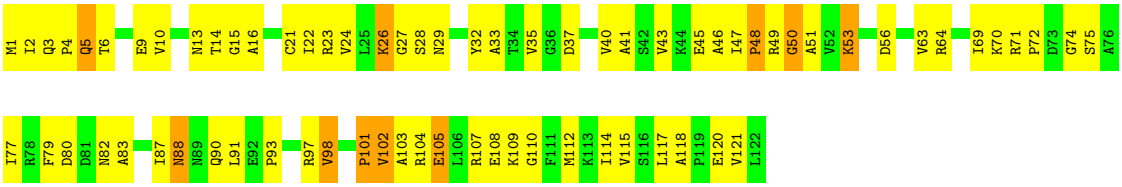
- Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN:



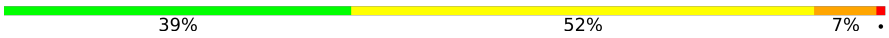
- Molecule 47: 50S RIBOSOMAL PROTEIN L14

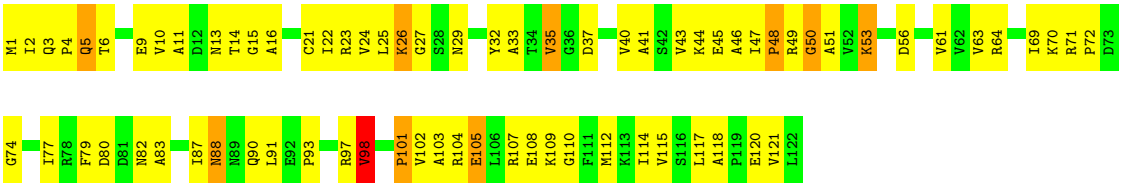
Chain BO:



- Molecule 47: 50S RIBOSOMAL PROTEIN L14

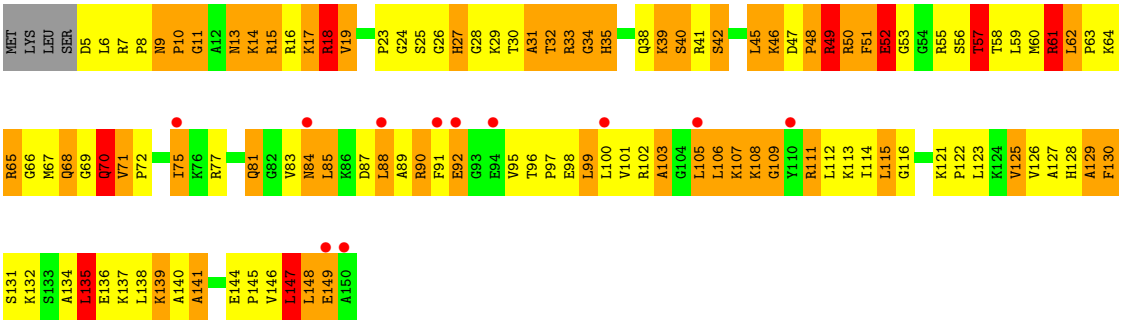
Chain DO:





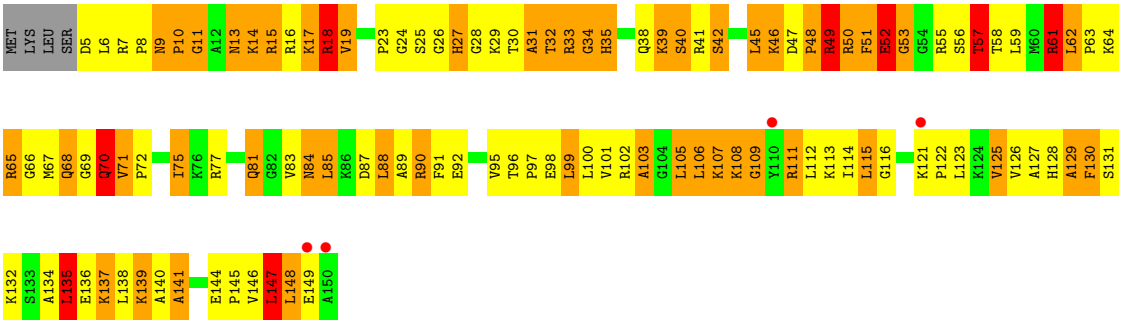
- Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP:



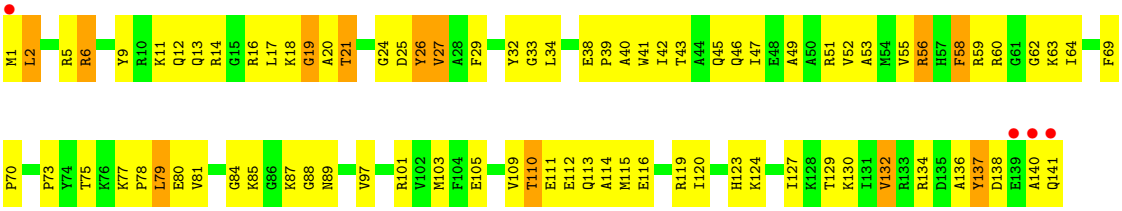
- Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP:



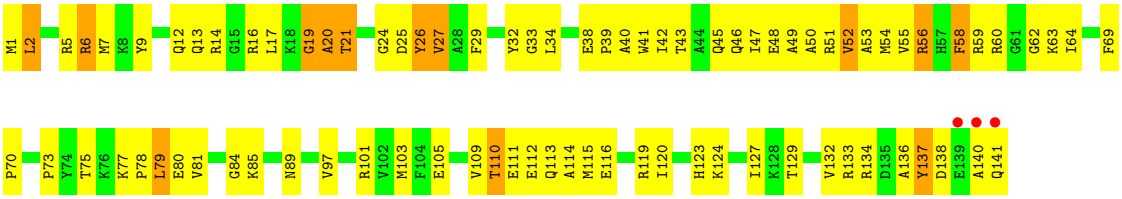
- Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



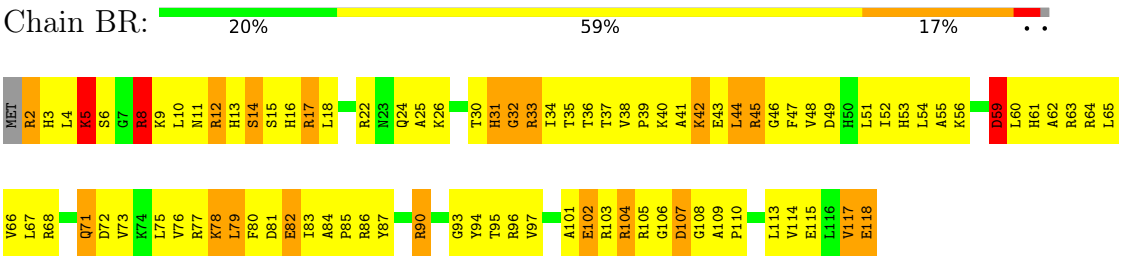
- Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain DQ:



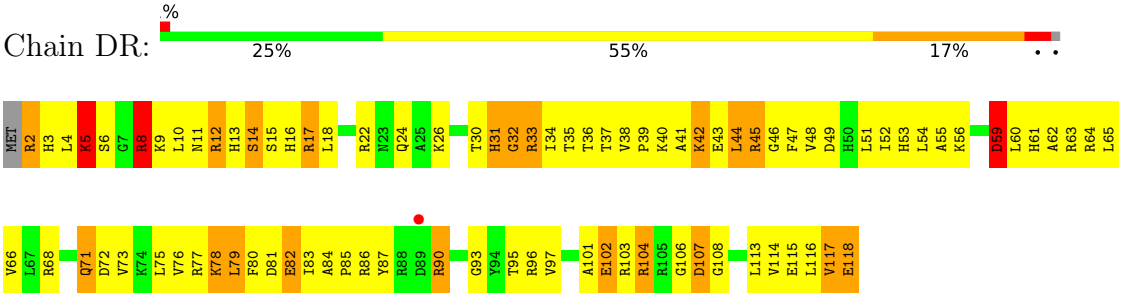
- Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain BR:



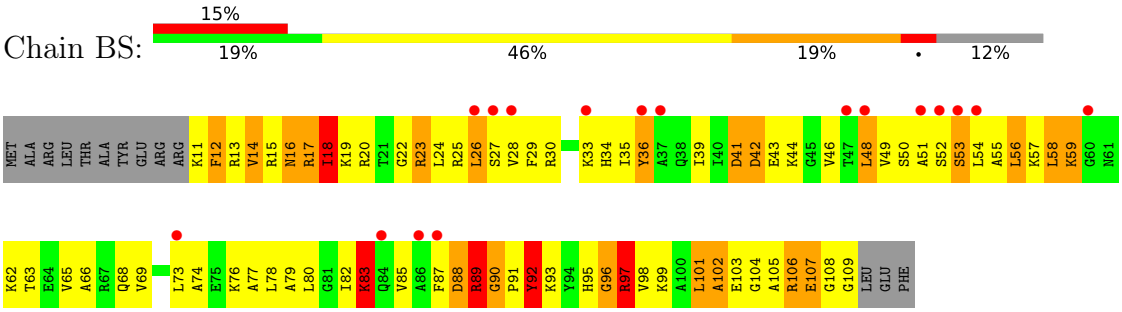
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain DR:



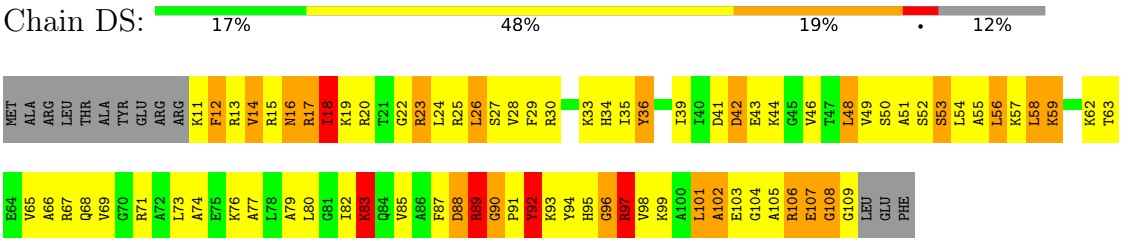
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS:



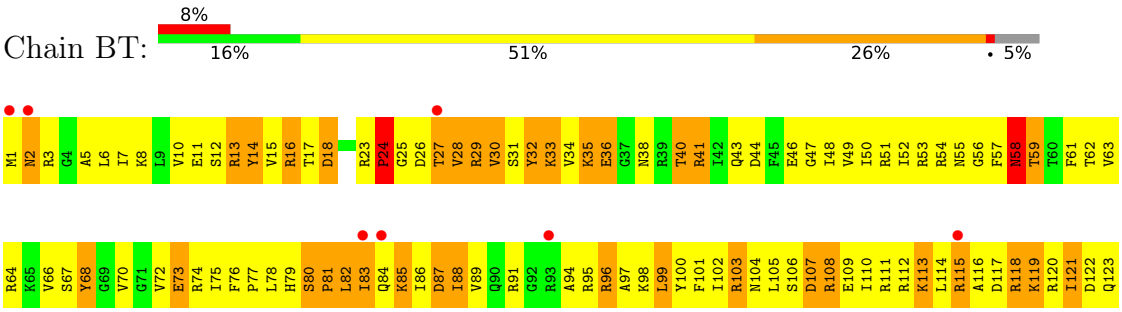
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

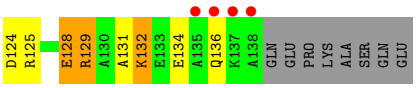
Chain DS:



• Molecule 52: 50S RIBOSOMAL PROTEIN L19

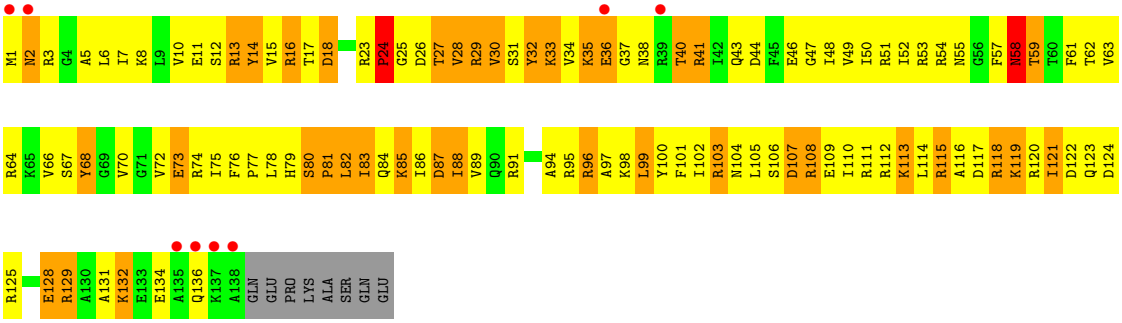
Chain BT:





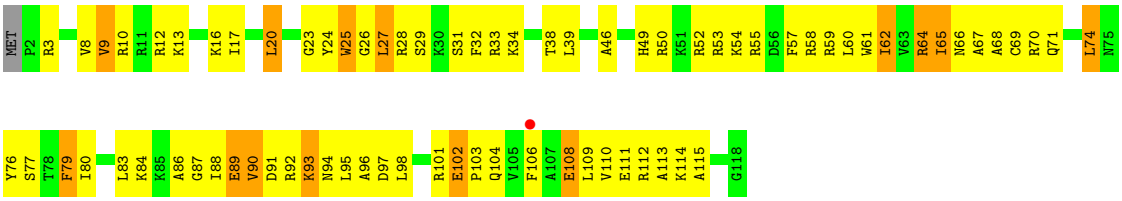
• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain DT:



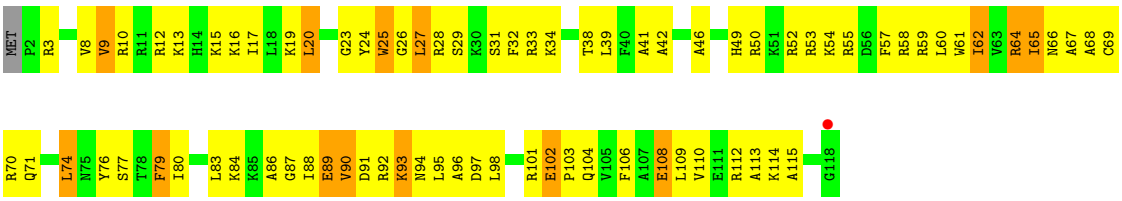
• Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU:



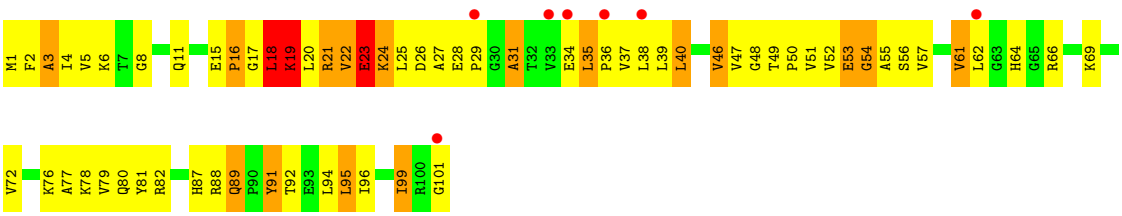
• Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain DU:



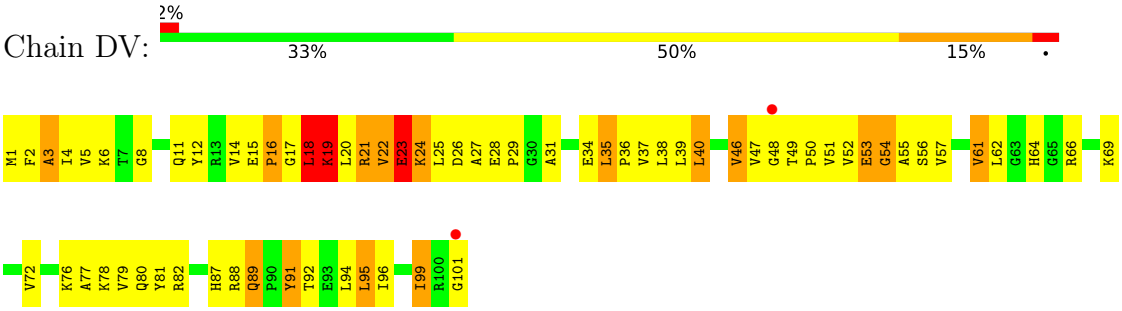
• Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain BV:



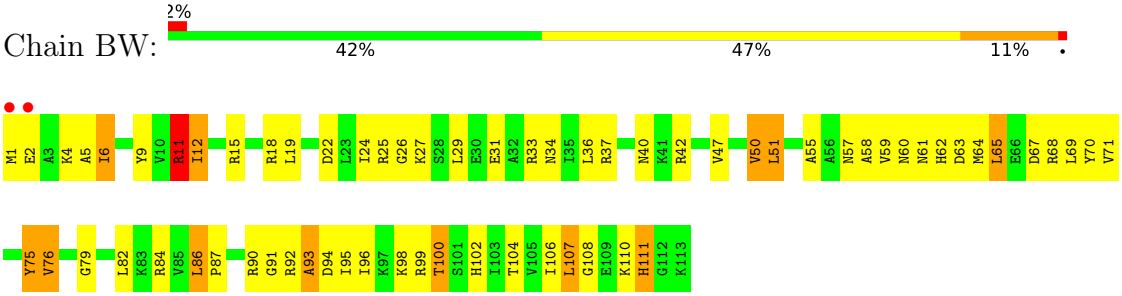
• Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain DV:



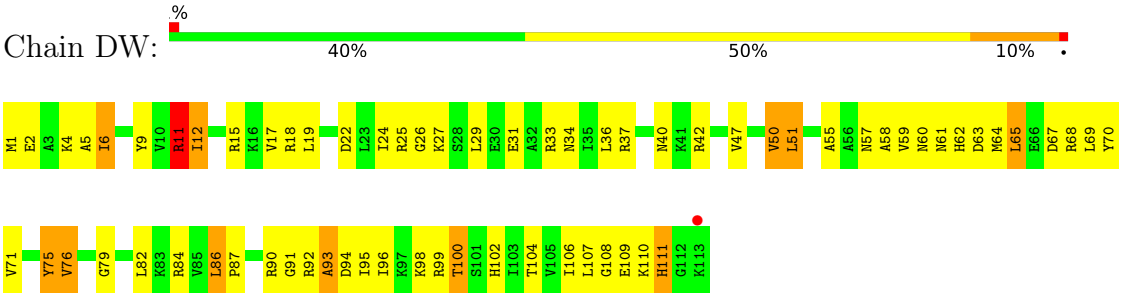
- Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain BW:



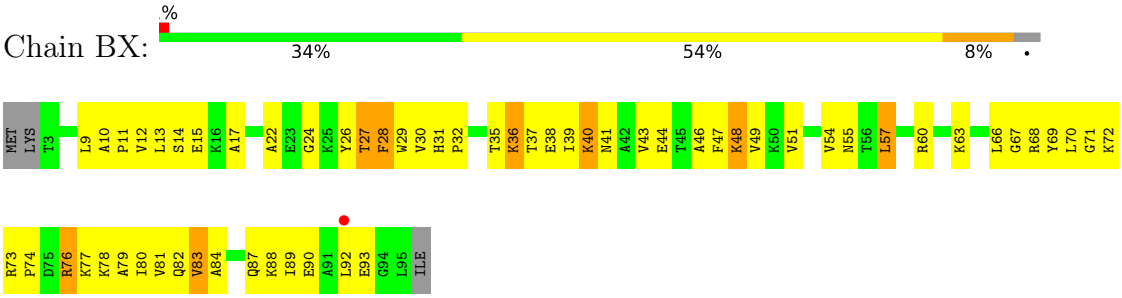
- Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain DW:



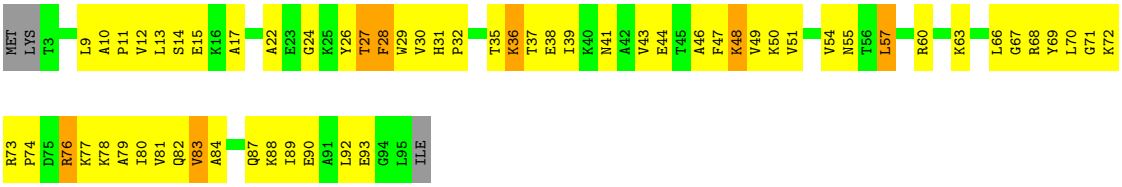
- Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



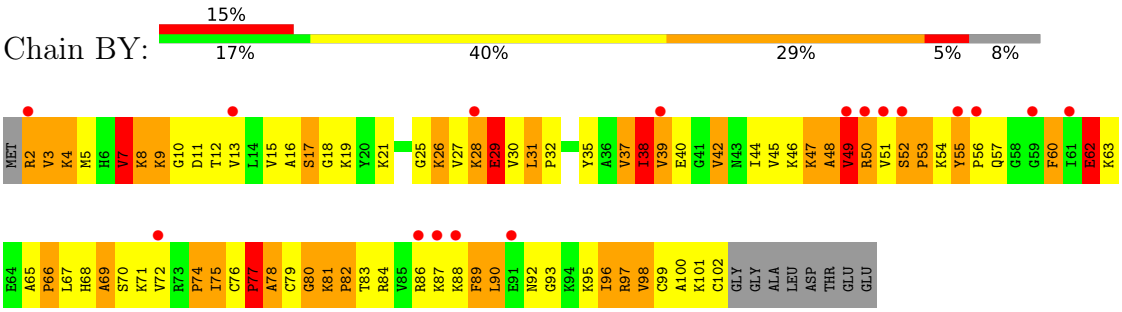
- Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain DX:



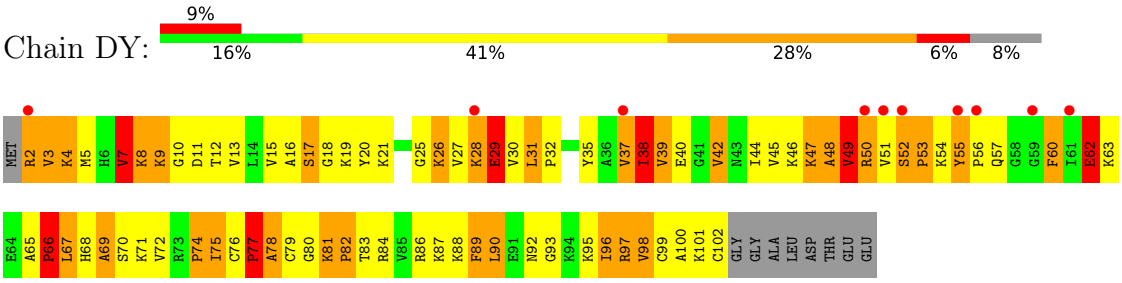
- Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY:



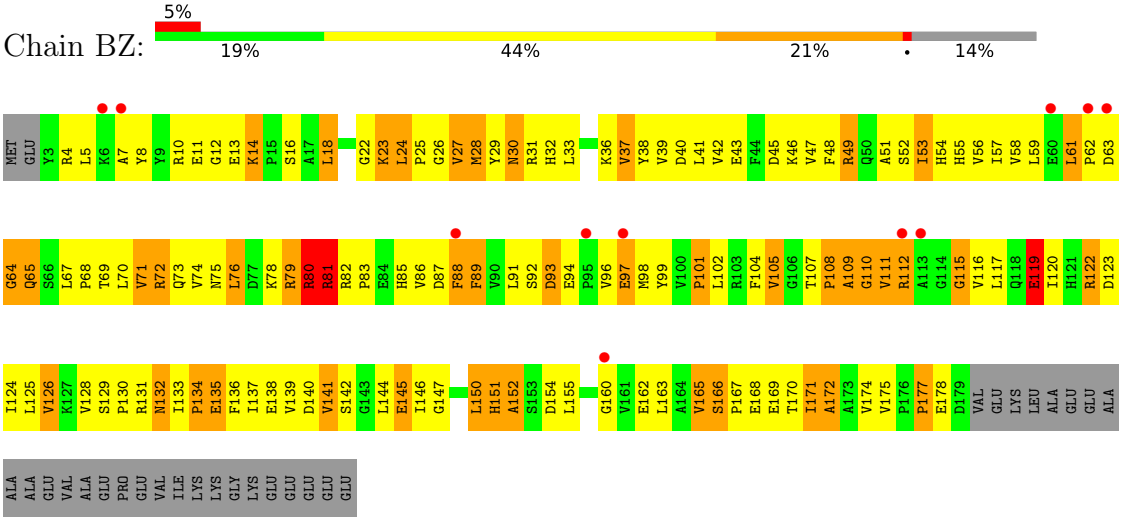
- Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain DY:



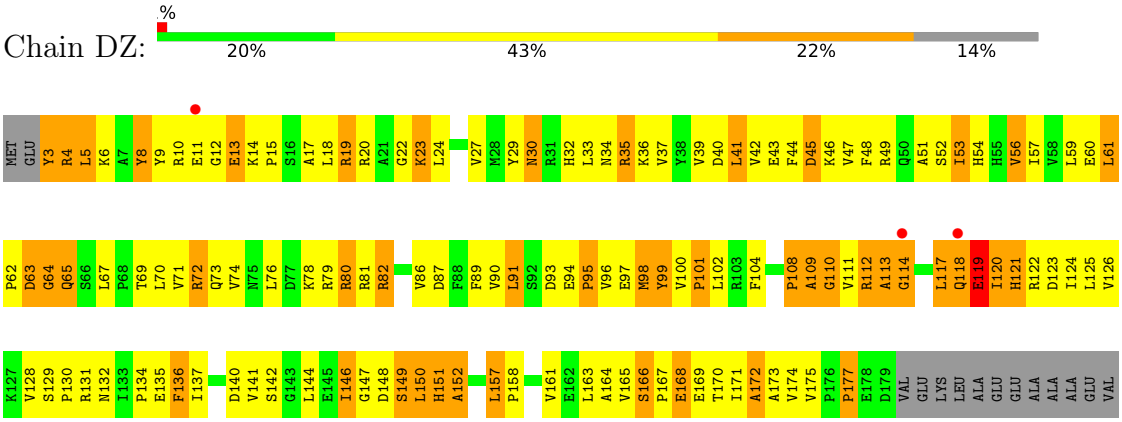
- Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain BZ:



- Molecule 58: 50S RIBOSOMAL PROTEIN L25

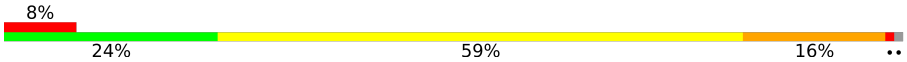
Chain DZ:



ALA GLU PRO GLU VAL ILE LYS LYS GLY LYS GLU GLU GLU GLU GLU

- Molecule 59: 50S RIBOSOMAL PROTEIN L9

Chain DI:



M1 K2 V3 I4 L5 L6 E7 P8 L9 E10 N11 L12 G13 D14 V15 G16 Q17 V18 V19 D20 V21 K22 P23 A26 R27 N28 Y29 L30 L31 P32 R33 G34 L35 A36 V37 L38 A39 T40 N43 L44 K45 A46 L47 E48 A49 R50 I51 R52 A53 Q54 A55 K56 R57 L58 A59 E60 R61 K62

A63 E66 R67 L68 K69 L72 E73 N74 L75 T76 L77 T78 T79 P80 W81 R82 A83 G84 E85 T86 K87 I88 Y89 G90 S91 V92 T93 A94 K95 D96 I97 A98 E99 A100 L101 S102 R103 I107 T108 I109 D110 P111 K112 R113 L114 A115 L116 E117 K118 P119 I120 K121 E122 L123 G124 E125 Y126

V127 L128 T129 Y130 K131 P132 H133 P134 E135 V136 P137 I138 Q139 L140 K141 V142 S143 V144 V145 A146 GLN GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	211.34Å 450.91Å 614.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 3.45 49.57 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.57-3.45) 99.6 (49.57-3.45)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.257 0.209 , 0.257	Depositor DCC
R_{free} test set	33081 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å^2)	76.9	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 88.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	304505	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% 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: MG, ZN

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	0.39	0/36190	0.69	9/56486 (0.0%)
1	CA	0.41	0/36190	0.69	11/56486 (0.0%)
2	AB	0.32	0/1936	0.61	0/2611
2	CB	0.32	0/1936	0.61	0/2611
3	AC	0.32	0/1637	0.57	0/2207
3	CC	0.35	0/1637	0.57	0/2207
4	AD	0.34	0/1733	0.58	0/2318
4	CD	0.36	0/1733	0.59	0/2318
5	AE	0.36	0/1163	0.61	0/1566
5	CE	0.37	0/1163	0.62	0/1566
6	AF	0.29	0/856	0.58	0/1154
6	CF	0.29	0/856	0.58	0/1154
7	AG	0.30	0/1276	0.54	0/1709
7	CG	0.33	0/1276	0.56	0/1709
8	AH	0.32	0/1136	0.62	0/1527
8	CH	0.33	0/1136	0.63	0/1527
9	AI	0.31	0/1029	0.60	0/1378
9	CI	0.33	0/1029	0.61	0/1378
10	AJ	0.33	0/808	0.60	0/1087
10	CJ	0.34	0/808	0.61	0/1087
11	AK	0.32	0/900	0.60	0/1213
11	CK	0.33	0/900	0.60	0/1213
12	AL	0.40	0/992	0.74	0/1329
12	CL	0.40	0/992	0.75	0/1329
13	AM	0.32	0/966	0.65	0/1294
13	CM	0.34	0/966	0.66	0/1294
14	AN	0.35	0/501	0.58	0/664
14	CN	0.38	0/501	0.60	0/664
15	AO	0.31	0/745	0.54	0/992
15	CO	0.32	0/745	0.55	0/992
16	AP	0.37	0/717	0.63	0/965
16	CP	0.37	0/717	0.63	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.37	0/837	0.60	0/1119
17	CQ	0.37	0/837	0.60	0/1119
18	AR	0.32	0/579	0.61	0/768
18	CR	0.32	0/579	0.62	0/768
19	AS	0.37	0/643	0.60	0/867
19	CS	0.39	0/643	0.60	0/867
20	AT	0.29	0/765	0.55	0/1007
20	CT	0.29	0/765	0.56	0/1007
21	AU	0.44	0/213	0.53	0/279
21	CU	0.43	0/213	0.54	0/279
22	AV	0.52	0/1809	0.77	1/2819 (0.0%)
22	AW	0.42	0/1809	0.78	5/2819 (0.2%)
22	CV	0.53	0/1809	0.78	2/2819 (0.1%)
22	CW	0.39	0/1809	0.76	4/2819 (0.1%)
23	AX	0.53	0/185	0.79	1/286 (0.3%)
23	CX	0.56	0/185	0.71	0/286
24	AY	0.34	0/2847	0.66	0/3846
24	CY	0.36	0/2847	0.70	1/3846 (0.0%)
25	B0	0.42	0/615	0.72	0/819
25	D0	0.44	0/615	0.73	0/819
26	B1	0.44	0/739	0.79	1/983 (0.1%)
26	D1	0.49	0/739	0.77	0/983
27	B2	0.39	0/600	0.73	0/793
27	D2	0.44	0/600	0.75	1/793 (0.1%)
28	B3	0.44	0/473	0.74	0/636
28	D3	0.45	0/473	0.73	0/636
29	B4	0.38	0/229	0.53	0/311
29	D4	0.41	0/229	0.53	0/311
30	B5	0.46	0/473	0.83	0/639
30	D5	0.45	0/473	0.85	0/639
31	B6	0.62	1/388 (0.3%)	0.97	0/520
31	D6	0.71	1/388 (0.3%)	1.00	0/520
32	B7	0.48	0/427	0.70	0/563
32	D7	0.48	0/427	0.69	0/563
33	B8	0.63	0/516	0.88	0/681
33	D8	0.67	0/516	0.91	0/681
34	B9	0.42	0/302	0.77	1/397 (0.3%)
34	D9	0.45	0/302	0.77	1/397 (0.3%)
35	BA	0.53	1/69614 (0.0%)	0.74	40/108679 (0.0%)
35	DA	0.56	3/69614 (0.0%)	0.75	40/108679 (0.0%)
36	BB	0.50	2/2853 (0.1%)	0.87	4/4451 (0.1%)
36	DB	0.52	1/2853 (0.0%)	0.84	3/4451 (0.1%)
37	BC	0.36	0/1145	0.65	7/1556 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	DC	0.35	0/1145	0.66	7/1556 (0.4%)
38	BD	0.45	0/2155	0.68	1/2907 (0.0%)
38	DD	0.47	0/2155	0.68	1/2907 (0.0%)
39	BE	0.43	0/1597	0.76	1/2155 (0.0%)
39	DE	0.44	0/1597	0.76	1/2155 (0.0%)
40	BF	0.48	0/1659	0.77	0/2246
40	DF	0.49	0/1659	0.77	0/2246
41	BG	0.37	0/1499	0.69	0/2016
41	DG	0.41	0/1499	0.76	1/2016 (0.0%)
42	BH	0.36	0/1246	0.69	1/1684 (0.1%)
42	DH	0.37	0/1246	0.69	1/1684 (0.1%)
43	BI	0.31	0/1147	0.60	0/1553
45	BK	0.31	0/1057	0.57	0/1432
45	DK	0.31	0/1057	0.57	0/1432
46	BN	0.38	0/1132	0.69	0/1527
46	DN	0.41	0/1132	0.70	0/1527
47	BO	0.42	0/943	0.71	0/1269
47	DO	0.40	0/943	0.71	0/1269
48	BP	0.41	0/1131	0.78	1/1504 (0.1%)
48	DP	0.44	0/1131	0.78	1/1504 (0.1%)
49	BQ	0.44	0/1143	0.71	0/1527
49	DQ	0.46	0/1143	0.72	0/1527
50	BR	0.36	0/974	0.71	1/1302 (0.1%)
50	DR	0.37	0/974	0.72	1/1302 (0.1%)
51	BS	0.45	0/779	0.85	1/1038 (0.1%)
51	DS	0.56	0/779	0.89	1/1038 (0.1%)
52	BT	0.40	0/1156	0.74	0/1544
52	DT	0.41	0/1156	0.75	0/1544
53	BU	0.47	0/975	0.77	1/1297 (0.1%)
53	DU	0.47	0/975	0.80	1/1297 (0.1%)
54	BV	0.42	0/790	0.73	0/1057
54	DV	0.46	0/790	0.76	0/1057
55	BW	0.39	0/907	0.67	0/1216
55	DW	0.41	0/907	0.69	0/1216
56	BX	0.43	0/740	0.71	0/995
56	DX	0.44	0/740	0.72	0/995
57	BY	0.50	0/789	0.80	0/1053
57	DY	0.49	0/789	0.81	0/1053
58	BZ	0.41	0/1436	0.72	0/1951
58	DZ	0.41	0/1436	0.77	0/1951
59	DI	0.36	0/1148	0.73	0/1554
All	All	0.47	9/327803 (0.0%)	0.72	154/489223 (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	9
1	CA	0	10
22	AW	3	0
22	CV	0	2
22	CW	3	0
23	AX	0	1
30	B5	0	1
30	D5	0	2
35	BA	2	40
35	DA	3	46
All	All	11	111

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	DB	86	G	P-OP2	-7.68	1.35	1.49
35	BA	568	U	C4-O4	7.25	1.29	1.23
36	BB	86	G	P-OP1	-7.23	1.36	1.49
36	BB	96	U	C2-O2	-6.42	1.16	1.22
31	D6	42	TRP	CB-CG	6.09	1.61	1.50

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	BB	85	G	OP1-P-O3'	-22.67	55.33	105.20
36	DB	85	G	OP2-P-O3'	-19.05	63.30	105.20
36	BB	85	G	OP2-P-O3'	13.54	134.99	105.20
36	DB	85	G	OP1-P-O3'	12.71	133.15	105.20
36	DB	86	G	O5'-P-OP2	11.85	124.92	110.70

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	AW	17	C	C1'
22	AW	47	U	C1'
22	AW	70	G	C3'
35	BA	1784	A	C3'
35	BA	1799	G	C3'

5 of 111 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	110	C	Sidechain
1	AA	324	G	Sidechain
1	AA	38	G	Sidechain
1	AA	388	G	Sidechain
1	AA	498	U	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	32329	0	16318	1300	0
1	CA	32329	0	16318	1291	0
2	AB	1901	0	1951	253	0
2	CB	1901	0	1951	256	0
3	AC	1613	0	1677	193	0
3	CC	1613	0	1677	190	0
4	AD	1703	0	1763	215	0
4	CD	1703	0	1763	213	0
5	AE	1147	0	1207	140	0
5	CE	1147	0	1207	134	0
6	AF	843	0	857	93	0
6	CF	843	0	857	98	0
7	AG	1257	0	1296	112	0
7	CG	1257	0	1296	112	0
8	AH	1116	0	1177	160	0
8	CH	1116	0	1177	152	0
9	AI	1011	0	1043	164	0
9	CI	1011	0	1043	172	0
10	AJ	795	0	840	170	0
10	CJ	795	0	840	165	0
11	AK	885	0	904	101	0
11	CK	885	0	904	104	0
12	AL	976	0	1062	99	0
12	CL	976	0	1062	93	0
13	AM	956	0	1021	104	0
13	CM	956	0	1021	106	0
14	AN	492	0	529	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	529	57	0
15	AO	734	0	771	52	0
15	CO	734	0	771	48	0
16	AP	701	0	720	100	0
16	CP	701	0	720	106	0
17	AQ	824	0	891	69	0
17	CQ	824	0	891	70	0
18	AR	574	0	644	78	0
18	CR	574	0	644	78	0
19	AS	630	0	652	97	0
19	CS	630	0	652	97	0
20	AT	763	0	861	112	0
20	CT	763	0	861	110	0
21	AU	209	0	221	18	0
21	CU	209	0	221	18	0
22	AV	1619	0	822	76	0
22	AW	1619	0	822	98	0
22	CV	1619	0	822	83	0
22	CW	1619	0	822	92	0
23	AX	166	0	87	17	0
23	CX	166	0	87	7	0
24	AY	2799	0	2809	362	0
24	CY	2799	0	2809	344	0
25	B0	607	0	628	82	0
25	D0	607	0	628	82	0
26	B1	732	0	808	113	0
26	D1	732	0	808	108	0
27	B2	598	0	653	85	0
27	D2	598	0	653	78	0
28	B3	468	0	523	59	3
28	D3	468	0	523	60	0
29	B4	226	0	229	33	0
29	D4	226	0	229	36	0
30	B5	459	0	480	64	0
30	D5	459	0	480	72	0
31	B6	381	0	391	117	0
31	D6	381	0	391	123	0
32	B7	419	0	467	25	0
32	D7	419	0	467	29	0
33	B8	508	0	576	122	0
33	D8	508	0	576	130	0
34	B9	299	0	324	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D9	299	0	324	31	0
35	BA	62154	0	31337	2153	0
35	DA	62154	0	31337	2168	9
36	BB	2551	0	1295	103	6
36	DB	2551	0	1295	103	0
37	BC	1142	0	865	110	0
37	DC	1142	0	865	103	0
38	BD	2105	0	2182	255	0
38	DD	2105	0	2182	246	0
39	BE	1564	0	1629	245	0
39	DE	1564	0	1629	252	0
40	BF	1624	0	1677	227	0
40	DF	1624	0	1677	226	0
41	BG	1474	0	1535	288	0
41	DG	1474	0	1535	249	0
42	BH	1223	0	1282	214	0
42	DH	1223	0	1282	212	0
43	BI	1132	0	1218	120	0
44	BJ	651	0	146	35	0
44	DJ	651	0	146	36	0
45	BK	1038	0	1089	157	0
45	DK	1038	0	1089	184	0
46	BN	1105	0	1180	129	0
46	DN	1105	0	1180	122	0
47	BO	933	0	996	92	0
47	DO	933	0	996	94	0
48	BP	1114	0	1187	261	0
48	DP	1114	0	1187	259	0
49	BQ	1122	0	1179	121	0
49	DQ	1122	0	1179	123	0
50	BR	960	0	1021	134	0
50	DR	960	0	1020	134	0
51	BS	771	0	832	147	0
51	DS	771	0	832	149	0
52	BT	1142	0	1202	231	0
52	DT	1142	0	1202	231	0
53	BU	958	0	1015	134	0
53	DU	958	0	1015	139	0
54	BV	779	0	852	144	0
54	DV	779	0	852	149	0
55	BW	896	0	953	76	0
55	DW	896	0	953	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BX	726	0	778	67	0
56	DX	726	0	778	65	0
57	BY	776	0	870	181	0
57	DY	776	0	870	182	0
58	BZ	1404	0	1432	232	0
58	DZ	1404	0	1432	245	0
59	DI	1133	0	1220	185	0
60	AA	157	0	0	0	0
60	AE	1	0	0	0	0
60	AL	1	0	0	0	0
60	AM	1	0	0	0	0
60	AV	7	0	0	0	0
60	AW	5	0	0	0	0
60	AY	1	0	0	0	0
60	B1	1	0	0	0	0
60	B3	1	0	0	0	0
60	B5	2	0	0	0	0
60	B7	2	0	0	0	0
60	BA	354	0	0	0	0
60	BB	4	0	0	0	0
60	BC	1	0	0	0	0
60	BD	2	0	0	0	0
60	BF	1	0	0	0	0
60	BH	1	0	0	0	0
60	BP	1	0	0	0	0
60	BQ	1	0	0	0	0
60	BS	1	0	0	0	0
60	BU	1	0	0	0	0
60	CA	157	0	0	0	0
60	CL	1	0	0	0	0
60	CN	1	0	0	0	0
60	CV	7	0	0	0	0
60	CW	5	0	0	0	0
60	CY	1	0	0	0	0
60	D1	1	0	0	0	0
60	D3	1	0	0	0	0
60	D5	2	0	0	0	0
60	D7	1	0	0	0	0
60	DA	353	0	0	0	0
60	DB	4	0	0	0	0
60	DC	1	0	0	0	0
60	DD	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	DF	3	0	0	0	0
60	DH	1	0	0	0	0
60	DQ	1	0	0	0	0
60	DR	1	0	0	0	0
60	DU	1	0	0	0	0
60	DX	1	0	0	0	0
60	DY	1	0	0	0	0
61	AD	1	0	0	0	0
61	AN	1	0	0	0	0
61	B9	1	0	0	0	0
61	CD	1	0	0	0	0
61	CN	1	0	0	0	0
61	D9	1	0	0	0	0
All	All	304505	0	207553	19769	9

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 39.

The worst 5 of 19769 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)
26:D1:81:LYS:CE	35:DA:271(H):G:H5'	1.21	1.60
26:B1:81:LYS:HE2	35:BA:271(H):G:C5'	1.23	1.59
26:D1:81:LYS:HE2	35:DA:271(H):G:C5'	1.31	1.54
26:B1:81:LYS:CE	35:BA:271(H):G:H5'	1.10	1.53
35:BA:1887:C:H2'	35:BA:1888:G:H5"	1.22	1.18

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B3:48:GLU:O	35:DA:654(L):G:OP2[3_455]	1.99	0.21
36:BB:97:G:N7	35:DA:654(J):A:OP1[3_455]	2.05	0.15
36:BB:97:G:OP2	35:DA:654(I):C:O2'[3_455]	2.06	0.14
36:BB:96:U:C3'	35:DA:654(I):C:O2'[3_455]	2.09	0.11
36:BB:96:U:O2	35:DA:654(K):C:OP1[3_455]	2.10	0.10

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%)	155 (66%)	58 (25%)	20 (9%)	1 8
2	CB	233/256 (91%)	156 (67%)	56 (24%)	21 (9%)	1 7
3	AC	205/239 (86%)	125 (61%)	57 (28%)	23 (11%)	0 5
3	CC	205/239 (86%)	128 (62%)	55 (27%)	22 (11%)	0 5
4	AD	206/209 (99%)	134 (65%)	49 (24%)	23 (11%)	0 5
4	CD	206/209 (99%)	135 (66%)	49 (24%)	22 (11%)	0 5
5	AE	149/162 (92%)	98 (66%)	36 (24%)	15 (10%)	0 6
5	CE	149/162 (92%)	100 (67%)	34 (23%)	15 (10%)	0 6
6	AF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1 11
6	CF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1 11
7	AG	153/156 (98%)	108 (71%)	34 (22%)	11 (7%)	1 10
7	CG	153/156 (98%)	108 (71%)	34 (22%)	11 (7%)	1 10
8	AH	136/138 (99%)	92 (68%)	32 (24%)	12 (9%)	1 7
8	CH	136/138 (99%)	92 (68%)	32 (24%)	12 (9%)	1 7
9	AI	125/128 (98%)	83 (66%)	30 (24%)	12 (10%)	0 7
9	CI	125/128 (98%)	82 (66%)	31 (25%)	12 (10%)	0 7
10	AJ	97/105 (92%)	64 (66%)	21 (22%)	12 (12%)	0 4
10	CJ	97/105 (92%)	64 (66%)	21 (22%)	12 (12%)	0 4
11	AK	117/129 (91%)	89 (76%)	24 (20%)	4 (3%)	3 27
11	CK	117/129 (91%)	89 (76%)	24 (20%)	4 (3%)	3 27
12	AL	124/132 (94%)	89 (72%)	26 (21%)	9 (7%)	1 10
12	CL	124/132 (94%)	90 (73%)	25 (20%)	9 (7%)	1 10
13	AM	119/126 (94%)	82 (69%)	23 (19%)	14 (12%)	0 4
13	CM	119/126 (94%)	84 (71%)	21 (18%)	14 (12%)	0 4
14	AN	58/61 (95%)	39 (67%)	12 (21%)	7 (12%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	58/61 (95%)	38 (66%)	12 (21%)	8 (14%)	0	3
15	AO	86/89 (97%)	59 (69%)	23 (27%)	4 (5%)	2	19
15	CO	86/89 (97%)	57 (66%)	25 (29%)	4 (5%)	2	19
16	AP	82/88 (93%)	51 (62%)	22 (27%)	9 (11%)	0	5
16	CP	82/88 (93%)	53 (65%)	20 (24%)	9 (11%)	0	5
17	AQ	98/105 (93%)	68 (69%)	17 (17%)	13 (13%)	0	3
17	CQ	98/105 (93%)	69 (70%)	17 (17%)	12 (12%)	0	4
18	AR	68/88 (77%)	45 (66%)	16 (24%)	7 (10%)	0	6
18	CR	68/88 (77%)	45 (66%)	16 (24%)	7 (10%)	0	6
19	AS	77/93 (83%)	36 (47%)	30 (39%)	11 (14%)	0	3
19	CS	77/93 (83%)	36 (47%)	30 (39%)	11 (14%)	0	3
20	AT	97/106 (92%)	68 (70%)	18 (19%)	11 (11%)	0	5
20	CT	97/106 (92%)	68 (70%)	18 (19%)	11 (11%)	0	5
21	AU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	1	8
21	CU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	1	8
24	AY	349/351 (99%)	246 (70%)	70 (20%)	33 (10%)	0	7
24	CY	349/351 (99%)	256 (73%)	61 (18%)	32 (9%)	1	7
25	B0	74/85 (87%)	58 (78%)	10 (14%)	6 (8%)	1	9
25	D0	74/85 (87%)	58 (78%)	10 (14%)	6 (8%)	1	9
26	B1	92/98 (94%)	65 (71%)	15 (16%)	12 (13%)	0	3
26	D1	92/98 (94%)	72 (78%)	12 (13%)	8 (9%)	1	8
27	B2	69/72 (96%)	40 (58%)	17 (25%)	12 (17%)	0	2
27	D2	69/72 (96%)	39 (56%)	20 (29%)	10 (14%)	0	2
28	B3	58/60 (97%)	43 (74%)	9 (16%)	6 (10%)	0	6
28	D3	58/60 (97%)	43 (74%)	9 (16%)	6 (10%)	0	6
29	B4	29/71 (41%)	14 (48%)	11 (38%)	4 (14%)	0	3
29	D4	29/71 (41%)	14 (48%)	11 (38%)	4 (14%)	0	3
30	B5	57/60 (95%)	40 (70%)	7 (12%)	10 (18%)	0	1
30	D5	57/60 (95%)	40 (70%)	7 (12%)	10 (18%)	0	1
31	B6	43/54 (80%)	17 (40%)	12 (28%)	14 (33%)	0	0
31	D6	43/54 (80%)	17 (40%)	13 (30%)	13 (30%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	B7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
32	D7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
33	B8	62/65 (95%)	38 (61%)	15 (24%)	9 (14%)	0	2
33	D8	62/65 (95%)	38 (61%)	15 (24%)	9 (14%)	0	2
34	B9	34/37 (92%)	23 (68%)	11 (32%)	0	100	100
34	D9	34/37 (92%)	24 (71%)	10 (29%)	0	100	100
37	BC	183/229 (80%)	64 (35%)	71 (39%)	48 (26%)	0	0
37	DC	183/229 (80%)	65 (36%)	72 (39%)	46 (25%)	0	0
38	BD	270/276 (98%)	199 (74%)	39 (14%)	32 (12%)	0	4
38	DD	270/276 (98%)	198 (73%)	40 (15%)	32 (12%)	0	4
39	BE	203/206 (98%)	124 (61%)	45 (22%)	34 (17%)	0	2
39	DE	203/206 (98%)	123 (61%)	44 (22%)	36 (18%)	0	1
40	BF	206/210 (98%)	149 (72%)	33 (16%)	24 (12%)	0	4
40	DF	206/210 (98%)	149 (72%)	33 (16%)	24 (12%)	0	4
41	BG	179/182 (98%)	92 (51%)	54 (30%)	33 (18%)	0	1
41	DG	179/182 (98%)	107 (60%)	46 (26%)	26 (14%)	0	2
42	BH	158/180 (88%)	90 (57%)	38 (24%)	30 (19%)	0	1
42	DH	158/180 (88%)	91 (58%)	36 (23%)	31 (20%)	0	1
43	BI	144/148 (97%)	100 (69%)	28 (19%)	16 (11%)	0	5
45	BK	139/147 (95%)	88 (63%)	33 (24%)	18 (13%)	0	3
45	DK	139/147 (95%)	87 (63%)	34 (24%)	18 (13%)	0	3
46	BN	137/140 (98%)	97 (71%)	20 (15%)	20 (15%)	0	2
46	DN	137/140 (98%)	99 (72%)	18 (13%)	20 (15%)	0	2
47	BO	120/122 (98%)	97 (81%)	17 (14%)	6 (5%)	2	18
47	DO	120/122 (98%)	98 (82%)	14 (12%)	8 (7%)	1	12
48	BP	144/150 (96%)	68 (47%)	36 (25%)	40 (28%)	0	0
48	DP	144/150 (96%)	68 (47%)	36 (25%)	40 (28%)	0	0
49	BQ	139/141 (99%)	111 (80%)	19 (14%)	9 (6%)	1	12
49	DQ	139/141 (99%)	114 (82%)	16 (12%)	9 (6%)	1	12
50	BR	115/118 (98%)	72 (63%)	29 (25%)	14 (12%)	0	4
50	DR	115/118 (98%)	70 (61%)	31 (27%)	14 (12%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	BS	97/112 (87%)	55 (57%)	22 (23%)	20 (21%)	0	1
51	DS	97/112 (87%)	54 (56%)	22 (23%)	21 (22%)	0	1
52	BT	136/146 (93%)	84 (62%)	23 (17%)	29 (21%)	0	1
52	DT	136/146 (93%)	85 (62%)	22 (16%)	29 (21%)	0	1
53	BU	115/118 (98%)	78 (68%)	27 (24%)	10 (9%)	1	8
53	DU	115/118 (98%)	77 (67%)	28 (24%)	10 (9%)	1	8
54	BV	99/101 (98%)	72 (73%)	13 (13%)	14 (14%)	0	3
54	DV	99/101 (98%)	72 (73%)	14 (14%)	13 (13%)	0	3
55	BW	111/113 (98%)	83 (75%)	22 (20%)	6 (5%)	2	16
55	DW	111/113 (98%)	83 (75%)	22 (20%)	6 (5%)	2	16
56	BX	91/96 (95%)	75 (82%)	14 (15%)	2 (2%)	6	35
56	DX	91/96 (95%)	74 (81%)	16 (18%)	1 (1%)	14	50
57	BY	99/110 (90%)	46 (46%)	20 (20%)	33 (33%)	0	0
57	DY	99/110 (90%)	47 (48%)	20 (20%)	32 (32%)	0	0
58	BZ	175/206 (85%)	102 (58%)	41 (23%)	32 (18%)	0	1
58	DZ	175/206 (85%)	110 (63%)	36 (21%)	29 (17%)	0	2
59	DI	144/148 (97%)	81 (56%)	42 (29%)	21 (15%)	0	2
All	All	12652/13582 (93%)	8336 (66%)	2725 (22%)	1591 (13%)	0	4

5 of 1591 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	20	GLU
2	AB	88	ALA
2	AB	95	GLN
2	AB	195	ASP

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%)	184 (91%)	18 (9%)	9	36
2	CB	202/220 (92%)	184 (91%)	18 (9%)	9	36
3	AC	160/188 (85%)	149 (93%)	11 (7%)	15	47
3	CC	160/188 (85%)	150 (94%)	10 (6%)	18	50
4	AD	180/181 (99%)	159 (88%)	21 (12%)	5	24
4	CD	180/181 (99%)	159 (88%)	21 (12%)	5	24
5	AE	115/123 (94%)	103 (90%)	12 (10%)	7	29
5	CE	115/123 (94%)	101 (88%)	14 (12%)	5	22
6	AF	90/90 (100%)	86 (96%)	4 (4%)	28	61
6	CF	90/90 (100%)	86 (96%)	4 (4%)	28	61
7	AG	126/127 (99%)	117 (93%)	9 (7%)	14	46
7	CG	126/127 (99%)	118 (94%)	8 (6%)	18	50
8	AH	119/119 (100%)	105 (88%)	14 (12%)	5	23
8	CH	119/119 (100%)	105 (88%)	14 (12%)	5	23
9	AI	98/99 (99%)	88 (90%)	10 (10%)	7	30
9	CI	98/99 (99%)	88 (90%)	10 (10%)	7	30
10	AJ	88/92 (96%)	78 (89%)	10 (11%)	5	24
10	CJ	88/92 (96%)	78 (89%)	10 (11%)	5	24
11	AK	90/99 (91%)	84 (93%)	6 (7%)	16	48
11	CK	90/99 (91%)	84 (93%)	6 (7%)	16	48
12	AL	104/109 (95%)	98 (94%)	6 (6%)	20	52
12	CL	104/109 (95%)	96 (92%)	8 (8%)	13	42
13	AM	96/101 (95%)	83 (86%)	13 (14%)	4	19
13	CM	96/101 (95%)	83 (86%)	13 (14%)	4	19
14	AN	49/50 (98%)	46 (94%)	3 (6%)	18	51
14	CN	49/50 (98%)	46 (94%)	3 (6%)	18	51
15	AO	79/80 (99%)	76 (96%)	3 (4%)	33	64
15	CO	79/80 (99%)	76 (96%)	3 (4%)	33	64
16	AP	72/74 (97%)	64 (89%)	8 (11%)	6	26
16	CP	72/74 (97%)	64 (89%)	8 (11%)	6	26
17	AQ	94/97 (97%)	92 (98%)	2 (2%)	53	78
17	CQ	94/97 (97%)	92 (98%)	2 (2%)	53	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	61/77 (79%)	57 (93%)	4 (7%)	16	48
18	CR	61/77 (79%)	57 (93%)	4 (7%)	16	48
19	AS	69/80 (86%)	61 (88%)	8 (12%)	5	24
19	CS	69/80 (86%)	61 (88%)	8 (12%)	5	24
20	AT	76/82 (93%)	70 (92%)	6 (8%)	12	41
20	CT	76/82 (93%)	70 (92%)	6 (8%)	12	41
21	AU	19/22 (86%)	18 (95%)	1 (5%)	22	54
21	CU	19/22 (86%)	19 (100%)	0	100	100
24	AY	298/298 (100%)	264 (89%)	34 (11%)	5	24
24	CY	298/298 (100%)	264 (89%)	34 (11%)	5	24
25	B0	61/67 (91%)	58 (95%)	3 (5%)	25	57
25	D0	61/67 (91%)	58 (95%)	3 (5%)	25	57
26	B1	78/83 (94%)	70 (90%)	8 (10%)	7	30
26	D1	78/83 (94%)	66 (85%)	12 (15%)	2	14
27	B2	66/67 (98%)	55 (83%)	11 (17%)	2	11
27	D2	66/67 (98%)	59 (89%)	7 (11%)	6	28
28	B3	51/52 (98%)	47 (92%)	4 (8%)	12	41
28	D3	51/52 (98%)	48 (94%)	3 (6%)	19	52
29	B4	27/63 (43%)	25 (93%)	2 (7%)	13	43
29	D4	27/63 (43%)	24 (89%)	3 (11%)	6	26
30	B5	51/52 (98%)	45 (88%)	6 (12%)	5	23
30	D5	51/52 (98%)	44 (86%)	7 (14%)	3	18
31	B6	43/52 (83%)	32 (74%)	11 (26%)	0	2
31	D6	43/52 (83%)	32 (74%)	11 (26%)	0	2
32	B7	41/42 (98%)	39 (95%)	2 (5%)	25	57
32	D7	41/42 (98%)	39 (95%)	2 (5%)	25	57
33	B8	53/55 (96%)	41 (77%)	12 (23%)	1	3
33	D8	53/55 (96%)	41 (77%)	12 (23%)	1	3
34	B9	33/34 (97%)	28 (85%)	5 (15%)	3	15
34	D9	33/34 (97%)	28 (85%)	5 (15%)	3	15
37	BC	61/181 (34%)	55 (90%)	6 (10%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DC	61/181 (34%)	55 (90%)	6 (10%)	8	31
38	BD	213/218 (98%)	192 (90%)	21 (10%)	8	31
38	DD	213/218 (98%)	191 (90%)	22 (10%)	7	30
39	BE	165/166 (99%)	137 (83%)	28 (17%)	2	10
39	DE	165/166 (99%)	136 (82%)	29 (18%)	2	9
40	BF	165/166 (99%)	144 (87%)	21 (13%)	4	20
40	DF	165/166 (99%)	146 (88%)	19 (12%)	5	24
41	BG	155/156 (99%)	131 (84%)	24 (16%)	2	14
41	DG	155/156 (99%)	129 (83%)	26 (17%)	2	11
42	BH	132/148 (89%)	122 (92%)	10 (8%)	13	42
42	DH	132/148 (89%)	122 (92%)	10 (8%)	13	42
43	BI	122/124 (98%)	116 (95%)	6 (5%)	25	57
45	BK	106/111 (96%)	97 (92%)	9 (8%)	10	38
45	DK	106/111 (96%)	97 (92%)	9 (8%)	10	38
46	BN	117/119 (98%)	101 (86%)	16 (14%)	3	18
46	DN	117/119 (98%)	101 (86%)	16 (14%)	3	18
47	BO	100/100 (100%)	94 (94%)	6 (6%)	19	51
47	DO	100/100 (100%)	95 (95%)	5 (5%)	24	56
48	BP	112/116 (97%)	84 (75%)	28 (25%)	0	3
48	DP	112/116 (97%)	84 (75%)	28 (25%)	0	3
49	BQ	111/111 (100%)	97 (87%)	14 (13%)	4	21
49	DQ	111/111 (100%)	96 (86%)	15 (14%)	4	19
50	BR	100/101 (99%)	88 (88%)	12 (12%)	5	23
50	DR	100/101 (99%)	88 (88%)	12 (12%)	5	23
51	BS	77/88 (88%)	61 (79%)	16 (21%)	1	5
51	DS	77/88 (88%)	61 (79%)	16 (21%)	1	5
52	BT	120/127 (94%)	102 (85%)	18 (15%)	3	15
52	DT	120/127 (94%)	102 (85%)	18 (15%)	3	15
53	BU	92/94 (98%)	85 (92%)	7 (8%)	13	42
53	DU	92/94 (98%)	85 (92%)	7 (8%)	13	42
54	BV	82/82 (100%)	73 (89%)	9 (11%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
54	DV	82/82 (100%)	72 (88%)	10 (12%)	5 22
55	BW	91/92 (99%)	79 (87%)	12 (13%)	4 19
55	DW	91/92 (99%)	80 (88%)	11 (12%)	5 22
56	BX	74/78 (95%)	65 (88%)	9 (12%)	5 22
56	DX	74/78 (95%)	65 (88%)	9 (12%)	5 22
57	BY	84/91 (92%)	67 (80%)	17 (20%)	1 5
57	DY	84/91 (92%)	67 (80%)	17 (20%)	1 5
58	BZ	155/179 (87%)	128 (83%)	27 (17%)	2 9
58	DZ	155/179 (87%)	129 (83%)	26 (17%)	2 11
59	DI	122/124 (98%)	118 (97%)	4 (3%)	38 68
All	All	10446/11246 (93%)	9279 (89%)	1167 (11%)	6 25

5 of 1167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	DF	201	VAL
58	DZ	19	ARG
41	DG	166	ASP
40	DF	197	ASP
49	DQ	137	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 327 such sidechains are listed below:

Mol	Chain	Res	Type
20	CT	73	HIS
42	DH	147	ASN
24	CY	243	ASN
33	D8	33	ASN
49	DQ	12	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	222 (14%)	34 (2%)
1	CA	1503/1522 (98%)	217 (14%)	34 (2%)
22	AV	75/76 (98%)	17 (22%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	AW	75/76 (98%)	15 (20%)	3 (4%)
22	CV	75/76 (98%)	18 (24%)	0
22	CW	75/76 (98%)	16 (21%)	4 (5%)
23	AX	7/8 (87%)	1 (14%)	1 (14%)
23	CX	7/8 (87%)	1 (14%)	0
35	BA	2885/2901 (99%)	515 (17%)	58 (2%)
35	DA	2885/2901 (99%)	516 (17%)	57 (1%)
36	BB	118/122 (96%)	15 (12%)	3 (2%)
36	DB	118/122 (96%)	14 (11%)	3 (2%)
All	All	9326/9410 (99%)	1567 (16%)	198 (2%)

5 of 1567 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 198 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	508	C
35	DA	221	A
1	CA	687	A
1	CA	1224	G
35	DA	587	C

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 1098 ligands modelled in this entry, 1098 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	1504/1522 (98%)	0.12	38 (2%)	57	54	43, 106, 183, 201	0
1	CA	1504/1522 (98%)	0.03	46 (3%)	49	47	35, 87, 183, 201	0
2	AB	235/256 (91%)	0.77	43 (18%)	1	2	76, 137, 191, 201	0
2	CB	235/256 (91%)	0.32	16 (6%)	17	19	51, 117, 180, 201	0
3	AC	207/239 (86%)	0.84	28 (13%)	3	4	71, 130, 177, 201	0
3	CC	207/239 (86%)	0.07	2 (0%)	82	79	48, 96, 159, 200	0
4	AD	208/209 (99%)	0.55	21 (10%)	7	9	53, 116, 168, 199	0
4	CD	208/209 (99%)	0.15	5 (2%)	59	56	41, 95, 158, 183	0
5	AE	151/162 (93%)	0.41	14 (9%)	8	11	48, 102, 156, 179	0
5	CE	151/162 (93%)	-0.05	4 (2%)	56	53	29, 86, 145, 193	0
6	AF	101/101 (100%)	0.87	15 (14%)	2	3	75, 120, 170, 189	0
6	CF	101/101 (100%)	0.35	7 (6%)	16	19	60, 116, 162, 184	0
7	AG	155/156 (99%)	0.82	25 (16%)	1	2	64, 137, 182, 201	0
7	CG	155/156 (99%)	0.22	11 (7%)	16	18	42, 89, 143, 193	0
8	AH	138/138 (100%)	0.38	5 (3%)	42	41	50, 101, 152, 201	0
8	CH	138/138 (100%)	0.11	2 (1%)	75	72	50, 97, 148, 188	0
9	AI	127/128 (99%)	1.41	37 (29%)	0	0	66, 148, 192, 201	0
9	CI	127/128 (99%)	0.61	14 (11%)	5	7	43, 97, 148, 183	0
10	AJ	99/105 (94%)	1.83	32 (32%)	0	0	64, 154, 198, 201	0
10	CJ	99/105 (94%)	0.98	20 (20%)	1	1	44, 122, 197, 201	0
11	AK	119/129 (92%)	0.87	18 (15%)	2	3	52, 100, 155, 172	0
11	CK	119/129 (92%)	0.32	10 (8%)	11	13	49, 89, 165, 183	0
12	AL	126/132 (95%)	0.46	7 (5%)	24	24	42, 81, 146, 193	0
12	CL	126/132 (95%)	0.41	7 (5%)	24	24	37, 75, 148, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AM	121/126 (96%)	0.83	11 (9%) 9 11	69, 133, 191, 201	0
13	CM	121/126 (96%)	0.27	5 (4%) 37 36	26, 96, 156, 189	0
14	AN	60/61 (98%)	0.79	6 (10%) 7 9	76, 124, 173, 187	0
14	CN	60/61 (98%)	-0.03	0 100 100	40, 82, 118, 155	0
15	AO	88/89 (98%)	0.54	4 (4%) 33 32	43, 100, 153, 177	0
15	CO	88/89 (98%)	0.43	3 (3%) 45 43	55, 92, 138, 155	0
16	AP	84/88 (95%)	0.71	9 (10%) 6 8	59, 104, 142, 201	0
16	CP	84/88 (95%)	1.16	15 (17%) 1 2	56, 106, 157, 201	0
17	AQ	100/105 (95%)	0.50	10 (10%) 7 9	54, 96, 137, 165	0
17	CQ	100/105 (95%)	0.43	6 (6%) 21 22	53, 99, 152, 162	0
18	AR	70/88 (79%)	0.47	3 (4%) 35 34	62, 116, 160, 183	0
18	CR	70/88 (79%)	0.67	7 (10%) 7 9	51, 101, 157, 183	0
19	AS	79/93 (84%)	0.95	8 (10%) 7 9	91, 140, 191, 201	0
19	CS	79/93 (84%)	0.84	10 (12%) 3 5	51, 103, 193, 201	0
20	AT	99/106 (93%)	0.83	12 (12%) 4 6	55, 112, 165, 201	0
20	CT	99/106 (93%)	1.04	21 (21%) 0 1	68, 115, 177, 201	0
21	AU	25/27 (92%)	1.79	12 (48%) 0 0	78, 131, 167, 178	0
21	CU	25/27 (92%)	0.45	0 100 100	58, 85, 117, 123	0
22	AV	76/76 (100%)	-0.09	0 100 100	42, 85, 152, 176	0
22	AW	76/76 (100%)	1.60	28 (36%) 0 0	48, 184, 201, 201	0
22	CV	76/76 (100%)	-0.27	1 (1%) 77 73	35, 65, 135, 185	0
22	CW	76/76 (100%)	1.15	14 (18%) 1 2	30, 166, 198, 201	0
23	AX	8/8 (100%)	0.43	1 (12%) 3 6	67, 76, 160, 166	0
23	CX	8/8 (100%)	0.17	1 (12%) 3 6	46, 62, 153, 170	0
24	AY	351/351 (100%)	0.79	48 (13%) 3 4	31, 109, 190, 201	0
24	CY	351/351 (100%)	0.66	43 (12%) 4 6	25, 95, 188, 201	0
25	B0	76/85 (89%)	0.09	2 (2%) 56 53	25, 64, 105, 177	0
25	D0	76/85 (89%)	0.20	2 (2%) 56 53	10, 43, 103, 179	0
26	B1	94/98 (95%)	0.09	2 (2%) 63 61	23, 61, 123, 173	0
26	D1	94/98 (95%)	-0.08	1 (1%) 80 77	18, 52, 109, 155	0
27	B2	71/72 (98%)	0.35	5 (7%) 16 18	36, 85, 156, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
27	D2	71/72 (98%)	0.03	3 (4%) 36 35	27, 76, 144, 186	0
28	B3	60/60 (100%)	0.33	3 (5%) 28 28	19, 56, 131, 197	0
28	D3	60/60 (100%)	0.31	3 (5%) 28 28	20, 51, 112, 201	0
29	B4	31/71 (43%)	1.24	8 (25%) 0 0	99, 184, 201, 201	0
29	D4	31/71 (43%)	0.38	2 (6%) 18 19	51, 140, 184, 200	0
30	B5	59/60 (98%)	0.01	3 (5%) 28 27	22, 74, 170, 190	0
30	D5	59/60 (98%)	0.26	5 (8%) 10 13	7, 55, 183, 201	0
31	B6	45/54 (83%)	1.00	7 (15%) 2 3	39, 85, 140, 198	0
31	D6	45/54 (83%)	0.45	2 (4%) 34 33	24, 65, 117, 183	0
32	B7	49/49 (100%)	0.13	3 (6%) 21 22	7, 48, 129, 165	0
32	D7	49/49 (100%)	-0.01	1 (2%) 65 63	7, 37, 113, 189	0
33	B8	64/65 (98%)	-0.05	1 (1%) 72 69	17, 51, 125, 160	0
33	D8	64/65 (98%)	-0.20	0 100 100	8, 40, 120, 162	0
34	B9	36/37 (97%)	0.50	2 (5%) 24 24	45, 69, 127, 147	0
34	D9	36/37 (97%)	0.76	5 (13%) 2 4	40, 74, 133, 162	0
35	BA	2886/2901 (99%)	-0.06	91 (3%) 47 46	16, 58, 179, 201	0
35	DA	2886/2901 (99%)	-0.02	102 (3%) 44 42	14, 51, 181, 201	0
36	BB	119/122 (97%)	-0.07	0 100 100	46, 105, 160, 186	0
36	DB	119/122 (97%)	-0.21	0 100 100	34, 65, 99, 129	0
37	BC	191/229 (83%)	4.65	136 (71%) 0 0	91, 174, 201, 201	0
37	DC	191/229 (83%)	4.56	156 (81%) 0 0	104, 177, 201, 201	0
38	BD	272/276 (98%)	0.12	6 (2%) 62 59	27, 71, 122, 165	0
38	DD	272/276 (98%)	0.00	4 (1%) 73 71	25, 66, 108, 168	0
39	BE	205/206 (99%)	0.13	7 (3%) 45 43	22, 69, 152, 201	0
39	DE	205/206 (99%)	0.25	6 (2%) 51 49	16, 67, 144, 197	0
40	BF	208/210 (99%)	-0.19	5 (2%) 59 56	9, 52, 134, 194	0
40	DF	208/210 (99%)	-0.12	7 (3%) 45 43	9, 48, 140, 179	0
41	BG	181/182 (99%)	0.66	20 (11%) 5 7	64, 118, 173, 200	0
41	DG	181/182 (99%)	0.05	7 (3%) 39 38	30, 76, 137, 201	0
42	BH	160/180 (88%)	1.00	35 (21%) 0 1	50, 123, 181, 201	0
42	DH	160/180 (88%)	1.21	42 (26%) 0 0	63, 137, 186, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
43	BI	146/148 (98%)	0.69	12 (8%) 11 14	41, 138, 187, 200	0
44	BJ	0/130	-	-	-	-
44	DJ	0/130	-	-	-	-
45	BK	141/147 (95%)	1.97	56 (39%) 0 0	85, 158, 195, 201	0
45	DK	141/147 (95%)	1.98	58 (41%) 0 0	99, 158, 197, 201	0
46	BN	139/140 (99%)	-0.01	2 (1%) 75 72	30, 70, 129, 164	0
46	DN	139/140 (99%)	-0.06	0 100 100	24, 62, 122, 186	0
47	BO	122/122 (100%)	-0.23	0 100 100	28, 64, 101, 158	0
47	DO	122/122 (100%)	-0.12	0 100 100	25, 68, 101, 120	0
48	BP	146/150 (97%)	0.76	11 (7%) 14 16	27, 89, 163, 200	0
48	DP	146/150 (97%)	0.27	4 (2%) 54 52	25, 72, 147, 201	0
49	BQ	141/141 (100%)	0.01	4 (2%) 53 51	23, 65, 127, 198	0
49	DQ	141/141 (100%)	-0.18	3 (2%) 63 61	14, 53, 105, 196	0
50	BR	117/118 (99%)	-0.08	0 100 100	33, 72, 126, 156	0
50	DR	117/118 (99%)	0.05	1 (0%) 84 81	26, 68, 122, 150	0
51	BS	99/112 (88%)	0.88	17 (17%) 1 2	60, 104, 165, 188	0
51	DS	99/112 (88%)	-0.14	0 100 100	25, 61, 120, 171	0
52	BT	138/146 (94%)	0.27	11 (7%) 12 14	44, 87, 164, 201	0
52	DT	138/146 (94%)	0.26	8 (5%) 23 23	39, 87, 172, 199	0
53	BU	117/118 (99%)	-0.22	1 (0%) 84 81	18, 55, 112, 140	0
53	DU	117/118 (99%)	-0.32	1 (0%) 84 81	12, 45, 111, 190	0
54	BV	101/101 (100%)	0.28	7 (6%) 16 19	34, 79, 137, 185	0
54	DV	101/101 (100%)	0.07	2 (1%) 65 63	25, 66, 141, 201	0
55	BW	113/113 (100%)	-0.03	2 (1%) 68 65	25, 57, 114, 201	0
55	DW	113/113 (100%)	-0.17	1 (0%) 84 81	16, 47, 115, 170	0
56	BX	93/96 (96%)	0.16	1 (1%) 80 77	31, 74, 129, 155	0
56	DX	93/96 (96%)	-0.10	0 100 100	33, 67, 114, 160	0
57	BY	101/110 (91%)	0.89	17 (16%) 1 2	27, 84, 157, 201	0
57	DY	101/110 (91%)	0.61	10 (9%) 7 9	25, 81, 162, 201	0
58	BZ	177/206 (85%)	0.38	11 (6%) 20 21	36, 98, 156, 201	0
58	DZ	177/206 (85%)	-0.02	3 (1%) 70 67	30, 83, 130, 192	0
59	DI	146/148 (98%)	0.56	12 (8%) 11 14	28, 109, 155, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	22210/23252 (95%)	0.32	1644 (7%)	14	17	7, 84, 181, 201	0

The worst 5 of 1644 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	BC	215	THR	21.9
37	BC	214	VAL	21.7
37	BC	165	ASN	20.9
37	BC	108	MET	15.9
48	BP	150	ALA	15.8

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
60	MG	DA	3240	1/1	0.24	0.90	55,55,55,55	1
60	MG	DA	3134	1/1	0.36	0.65	64,64,64,64	0
60	MG	DC	301	1/1	0.45	0.64	52,52,52,52	1
60	MG	DA	3177	1/1	0.46	0.56	49,49,49,49	0
60	MG	AA	1642	1/1	0.47	0.32	55,55,55,55	0
60	MG	AV	107	1/1	0.53	0.67	54,54,54,54	1
60	MG	AA	1657	1/1	0.54	0.27	54,54,54,54	0
60	MG	CA	1670	1/1	0.54	0.72	69,69,69,69	0
60	MG	BC	301	1/1	0.56	0.53	52,52,52,52	1
60	MG	BA	3201	1/1	0.56	0.44	52,52,52,52	0
60	MG	DA	3193	1/1	0.57	0.41	65,65,65,65	0
60	MG	AA	1659	1/1	0.57	0.30	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	1716	1/1	0.57	1.12	52,52,52,52	0
60	MG	AA	1616	1/1	0.58	0.55	64,64,64,64	0
60	MG	CA	1643	1/1	0.58	0.56	49,49,49,49	0
60	MG	AA	1689	1/1	0.59	0.97	59,59,59,59	1
60	MG	BA	3212	1/1	0.59	0.49	55,55,55,55	0
60	MG	CV	103	1/1	0.60	0.30	54,54,54,54	0
60	MG	AA	1613	1/1	0.60	0.27	56,56,56,56	0
60	MG	DA	3202	1/1	0.62	0.61	52,52,52,52	1
60	MG	DA	3319	1/1	0.63	0.47	55,55,55,55	0
60	MG	AA	1694	1/1	0.64	0.21	56,56,56,56	0
60	MG	DA	3143	1/1	0.64	0.45	47,47,47,47	1
60	MG	BA	3287	1/1	0.64	0.41	51,51,51,51	0
60	MG	AA	1675	1/1	0.64	0.18	48,48,48,48	0
60	MG	AA	1732	1/1	0.65	0.52	55,55,55,55	0
60	MG	CA	1676	1/1	0.65	0.49	58,58,58,58	0
60	MG	CA	1687	1/1	0.65	0.44	58,58,58,58	0
60	MG	AA	1748	1/1	0.65	0.40	55,55,55,55	0
60	MG	BA	3135	1/1	0.66	0.71	58,58,58,58	0
60	MG	DA	3144	1/1	0.66	0.29	57,57,57,57	0
60	MG	BA	3227	1/1	0.66	0.66	55,55,55,55	0
60	MG	CA	1615	1/1	0.66	0.69	64,64,64,64	0
60	MG	CA	1677	1/1	0.67	0.20	55,55,55,55	1
60	MG	BA	3199	1/1	0.67	0.70	58,58,58,58	0
60	MG	DA	3327	1/1	0.67	0.46	55,55,55,55	0
60	MG	DA	3328	1/1	0.67	0.34	55,55,55,55	1
60	MG	CA	1651	1/1	0.67	0.42	47,47,47,47	0
60	MG	BA	3301	1/1	0.68	0.54	55,55,55,55	0
60	MG	AA	1718	1/1	0.68	0.23	55,55,55,55	0
60	MG	AA	1683	1/1	0.68	0.45	47,47,47,47	0
60	MG	AA	1747	1/1	0.69	0.36	55,55,55,55	1
60	MG	CA	1709	1/1	0.69	0.37	65,65,65,65	0
60	MG	CA	1729	1/1	0.69	0.35	55,55,55,55	1
60	MG	CA	1655	1/1	0.69	0.67	52,52,52,52	0
60	MG	DA	3294	1/1	0.69	0.51	49,49,49,49	1
60	MG	CW	101	1/1	0.69	0.58	56,56,56,56	1
60	MG	CA	1613	1/1	0.69	0.23	52,52,52,52	0
60	MG	AA	1637	1/1	0.69	0.52	53,53,53,53	0
60	MG	BA	3338	1/1	0.69	0.33	55,55,55,55	0
60	MG	AM	201	1/1	0.70	0.57	47,47,47,47	0
60	MG	DA	3183	1/1	0.70	0.23	53,53,53,53	0
60	MG	DA	3260	1/1	0.70	0.52	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	3336	1/1	0.70	0.62	55,55,55,55	0
60	MG	DA	3231	1/1	0.71	0.51	54,54,54,54	1
60	MG	BA	3161	1/1	0.71	0.28	47,47,47,47	0
60	MG	BA	3237	1/1	0.71	0.27	67,67,67,67	0
60	MG	AA	1648	1/1	0.71	0.13	62,62,62,62	0
60	MG	DA	3225	1/1	0.72	0.76	51,51,51,51	0
60	MG	BA	3328	1/1	0.72	0.60	55,55,55,55	0
60	MG	DA	3142	1/1	0.72	0.54	49,49,49,49	0
60	MG	AA	1699	1/1	0.72	0.47	54,54,54,54	1
60	MG	CA	1719	1/1	0.72	0.39	55,55,55,55	1
60	MG	BA	3181	1/1	0.72	0.27	53,53,53,53	0
60	MG	CA	1730	1/1	0.72	0.40	55,55,55,55	0
60	MG	BA	3142	1/1	0.72	0.40	47,47,47,47	0
60	MG	CA	1681	1/1	0.72	0.54	66,66,66,66	0
60	MG	AA	1720	1/1	0.73	0.51	58,58,58,58	1
60	MG	AA	1692	1/1	0.73	0.70	59,59,59,59	0
60	MG	BA	3319	1/1	0.74	0.33	55,55,55,55	0
60	MG	BA	3105	1/1	0.74	0.49	47,47,47,47	0
60	MG	AA	1730	1/1	0.74	0.46	55,55,55,55	0
60	MG	DA	3083	1/1	0.74	0.29	51,51,51,51	0
60	MG	DA	3122	1/1	0.74	0.44	50,50,50,50	0
60	MG	DA	3337	1/1	0.74	0.25	55,55,55,55	0
60	MG	DA	3181	1/1	0.74	0.64	59,59,59,59	0
60	MG	CA	1722	1/1	0.75	0.40	55,55,55,55	0
60	MG	DA	3180	1/1	0.75	0.22	52,52,52,52	0
60	MG	AA	1668	1/1	0.75	0.61	58,58,58,58	0
60	MG	BS	201	1/1	0.75	0.50	55,55,55,55	0
60	MG	DA	3334	1/1	0.75	0.29	55,55,55,55	0
60	MG	CA	1733	1/1	0.75	0.53	55,55,55,55	0
60	MG	DB	201	1/1	0.75	0.89	67,67,67,67	0
60	MG	DA	3287	1/1	0.75	0.45	51,51,51,51	0
60	MG	BA	3294	1/1	0.76	0.12	52,52,52,52	0
60	MG	BA	3179	1/1	0.76	0.34	59,59,59,59	0
60	MG	DA	3003	1/1	0.76	0.43	67,67,67,67	0
60	MG	DA	3219	1/1	0.76	0.38	66,66,66,66	0
60	MG	DA	3176	1/1	0.76	0.41	58,58,58,58	0
60	MG	AA	1698	1/1	0.76	0.35	53,53,53,53	1
60	MG	DA	3239	1/1	0.76	0.24	67,67,67,67	1
60	MG	CA	1663	1/1	0.76	0.24	51,51,51,51	0
60	MG	BA	3341	1/1	0.76	0.60	55,55,55,55	0
60	MG	DA	3238	1/1	0.77	0.24	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	3162	1/1	0.77	0.35	47,47,47,47	0
60	MG	AA	1688	1/1	0.77	0.47	63,63,63,63	1
60	MG	CV	106	1/1	0.77	0.18	57,57,57,57	1
60	MG	DA	3283	1/1	0.77	0.47	65,65,65,65	0
60	MG	CA	1705	1/1	0.77	0.45	49,49,49,49	1
60	MG	BA	3320	1/1	0.77	0.45	55,55,55,55	0
60	MG	CA	1718	1/1	0.77	0.43	66,66,66,66	0
60	MG	CA	1625	1/1	0.77	0.62	53,53,53,53	0
60	MG	CA	1641	1/1	0.77	0.38	55,55,55,55	0
60	MG	DA	3333	1/1	0.77	0.38	55,55,55,55	0
60	MG	AL	201	1/1	0.77	0.25	51,51,51,51	1
60	MG	CA	1679	1/1	0.77	0.39	53,53,53,53	1
60	MG	DA	3351	1/1	0.77	0.67	55,55,55,55	0
60	MG	DA	3227	1/1	0.77	0.34	56,56,56,56	0
60	MG	AA	1653	1/1	0.77	0.87	60,60,60,60	0
60	MG	CA	1740	1/1	0.78	0.33	55,55,55,55	0
60	MG	DA	3280	1/1	0.78	0.68	57,57,57,57	0
60	MG	CA	1631	1/1	0.78	0.83	53,53,53,53	0
60	MG	DA	3190	1/1	0.78	0.26	59,59,59,59	0
60	MG	BA	3309	1/1	0.78	0.22	55,55,55,55	0
60	MG	BA	3239	1/1	0.78	0.38	55,55,55,55	0
60	MG	AA	1705	1/1	0.78	0.22	51,51,51,51	0
60	MG	BA	3222	1/1	0.79	0.29	49,49,49,49	0
60	MG	CA	1675	1/1	0.79	0.19	48,48,48,48	1
60	MG	CW	105	1/1	0.79	0.65	53,53,53,53	0
60	MG	BA	3091	1/1	0.79	0.39	51,51,51,51	0
60	MG	CA	1720	1/1	0.79	0.15	56,56,56,56	0
60	MG	DA	3167	1/1	0.79	0.23	47,47,47,47	0
60	MG	DA	3106	1/1	0.79	0.40	47,47,47,47	0
60	MG	DA	3349	1/1	0.79	0.55	55,55,55,55	0
60	MG	DA	3282	1/1	0.79	0.35	57,57,57,57	0
60	MG	DA	3352	1/1	0.79	0.55	55,55,55,55	0
60	MG	DA	3224	1/1	0.79	0.42	52,52,52,52	0
60	MG	BA	3241	1/1	0.79	0.32	61,61,61,61	1
60	MG	BA	3214	1/1	0.80	0.33	48,48,48,48	0
60	MG	AA	1696	1/1	0.80	0.31	62,62,62,62	0
60	MG	AW	101	1/1	0.80	0.70	56,56,56,56	1
60	MG	DA	3281	1/1	0.80	0.37	57,57,57,57	0
60	MG	BA	3234	1/1	0.80	0.81	52,52,52,52	0
60	MG	BA	3032	1/1	0.80	0.17	53,53,53,53	0
60	MG	CA	1647	1/1	0.80	0.24	62,62,62,62	0
60	MG	CA	1716	1/1	0.80	0.28	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	1717	1/1	0.80	0.41	52,52,52,52	0
60	MG	DA	3100	1/1	0.80	0.69	55,55,55,55	0
60	MG	DA	3105	1/1	0.80	0.83	48,48,48,48	0
60	MG	DA	3330	1/1	0.80	0.20	55,55,55,55	0
60	MG	AA	1693	1/1	0.80	0.47	61,61,61,61	0
60	MG	AA	1635	1/1	0.80	0.19	47,47,47,47	0
60	MG	DA	3127	1/1	0.80	0.32	52,52,52,52	0
60	MG	BA	3249	1/1	0.80	0.43	56,56,56,56	0
60	MG	DA	3229	1/1	0.80	0.38	52,52,52,52	0
60	MG	BA	3269	1/1	0.80	0.53	52,52,52,52	0
60	MG	BA	3133	1/1	0.80	0.40	64,64,64,64	0
60	MG	AA	1733	1/1	0.80	0.28	55,55,55,55	0
60	MG	BA	3129	1/1	0.81	0.36	56,56,56,56	0
60	MG	CA	1644	1/1	0.81	0.13	57,57,57,57	0
60	MG	AA	1697	1/1	0.81	0.35	52,52,52,52	0
60	MG	CA	1648	1/1	0.81	0.29	53,53,53,53	1
60	MG	AA	1655	1/1	0.81	0.41	52,52,52,52	0
60	MG	BA	3324	1/1	0.81	0.37	55,55,55,55	0
60	MG	BA	3139	1/1	0.81	0.47	50,50,50,50	0
60	MG	AA	1647	1/1	0.81	0.36	62,62,62,62	0
60	MG	BA	3236	1/1	0.81	0.14	47,47,47,47	0
60	MG	CA	1753	1/1	0.81	0.89	55,55,55,55	1
60	MG	AA	1686	1/1	0.81	0.47	58,58,58,58	1
60	MG	BA	3175	1/1	0.81	0.31	49,49,49,49	1
60	MG	AA	1746	1/1	0.81	0.32	55,55,55,55	1
60	MG	BA	3082	1/1	0.81	0.67	51,51,51,51	0
60	MG	BA	3183	1/1	0.81	0.63	56,56,56,56	0
60	MG	DA	3033	1/1	0.81	0.27	53,53,53,53	0
60	MG	CA	1688	1/1	0.81	0.15	48,48,48,48	0
60	MG	DA	3087	1/1	0.81	0.58	48,48,48,48	0
60	MG	BA	3189	1/1	0.81	0.37	59,59,59,59	0
60	MG	DA	3103	1/1	0.81	0.49	47,47,47,47	0
60	MG	AA	1687	1/1	0.81	0.21	48,48,48,48	0
60	MG	AA	1673	1/1	0.81	0.12	52,52,52,52	0
60	MG	DA	3205	1/1	0.82	0.55	57,57,57,57	0
60	MG	DA	3285	1/1	0.82	0.27	55,55,55,55	0
60	MG	CA	1674	1/1	0.82	0.21	50,50,50,50	0
60	MG	BA	3126	1/1	0.82	0.29	52,52,52,52	0
60	MG	DA	3302	1/1	0.82	0.53	55,55,55,55	0
60	MG	DA	3309	1/1	0.82	0.49	55,55,55,55	1
60	MG	DA	3317	1/1	0.82	0.31	55,55,55,55	0
60	MG	DA	3011	1/1	0.82	0.56	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	3253	1/1	0.82	0.54	54,54,54,54	0
60	MG	BA	3141	1/1	0.82	0.57	49,49,49,49	0
60	MG	AA	1737	1/1	0.82	0.67	55,55,55,55	0
60	MG	AA	1638	1/1	0.82	0.25	52,52,52,52	0
60	MG	CA	1621	1/1	0.82	0.21	48,48,48,48	0
60	MG	CA	1652	1/1	0.82	0.91	60,60,60,60	0
60	MG	AA	1666	1/1	0.82	0.58	57,57,57,57	0
60	MG	DA	3272	1/1	0.82	0.33	59,59,59,59	1
60	MG	CA	1660	1/1	0.82	0.20	58,58,58,58	0
60	MG	CA	1629	1/1	0.82	0.46	51,51,51,51	0
60	MG	BA	3303	1/1	0.82	0.73	55,55,55,55	0
60	MG	BA	3337	1/1	0.83	0.16	55,55,55,55	0
60	MG	AA	1679	1/1	0.83	0.19	53,53,53,53	0
60	MG	DA	3188	1/1	0.83	0.39	48,48,48,48	0
60	MG	BA	3187	1/1	0.83	0.40	48,48,48,48	0
60	MG	BA	3122	1/1	0.83	0.39	64,64,64,64	1
60	MG	CA	1731	1/1	0.83	0.37	55,55,55,55	0
60	MG	AA	1667	1/1	0.83	0.27	47,47,47,47	0
60	MG	CA	1734	1/1	0.83	0.21	55,55,55,55	1
60	MG	DA	3222	1/1	0.83	0.71	53,53,53,53	0
60	MG	BU	201	1/1	0.83	0.41	48,48,48,48	0
60	MG	DA	3318	1/1	0.83	0.21	55,55,55,55	0
60	MG	CA	1744	1/1	0.83	0.44	55,55,55,55	0
60	MG	BA	3200	1/1	0.83	0.26	60,60,60,60	0
60	MG	CA	1693	1/1	0.83	0.74	59,59,59,59	0
60	MG	AA	1735	1/1	0.83	0.54	55,55,55,55	0
60	MG	CA	1659	1/1	0.83	0.23	57,57,57,57	0
60	MG	AA	1650	1/1	0.83	0.45	47,47,47,47	0
60	MG	AA	1742	1/1	0.83	0.34	55,55,55,55	0
60	MG	DA	3247	1/1	0.83	0.32	55,55,55,55	1
60	MG	BA	3258	1/1	0.83	0.32	58,58,58,58	0
60	MG	DA	3262	1/1	0.83	0.32	52,52,52,52	0
60	MG	BA	3137	1/1	0.83	0.59	52,52,52,52	0
60	MG	DA	3274	1/1	0.83	0.51	63,63,63,63	0
60	MG	DA	3133	1/1	0.84	0.33	57,57,57,57	0
60	MG	AA	1617	1/1	0.84	0.17	54,54,54,54	0
60	MG	BA	3292	1/1	0.84	0.68	55,55,55,55	0
60	MG	DA	3263	1/1	0.84	0.44	63,63,63,63	0
60	MG	BA	3131	1/1	0.84	0.38	59,59,59,59	0
60	MG	BA	3296	1/1	0.84	0.67	55,55,55,55	0
60	MG	CA	1606	1/1	0.84	0.32	58,58,58,58	0
60	MG	CA	1612	1/1	0.84	0.29	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	1704	1/1	0.84	0.26	49,49,49,49	1
60	MG	BA	3080	1/1	0.84	0.65	52,52,52,52	0
60	MG	BA	3307	1/1	0.84	0.33	55,55,55,55	0
60	MG	AA	1677	1/1	0.84	0.35	55,55,55,55	1
60	MG	CV	107	1/1	0.84	0.28	54,54,54,54	0
60	MG	BA	3315	1/1	0.84	0.41	55,55,55,55	1
60	MG	CW	104	1/1	0.84	0.37	56,56,56,56	0
60	MG	BA	3318	1/1	0.84	0.29	55,55,55,55	0
60	MG	DA	3001	1/1	0.84	0.30	57,57,57,57	0
60	MG	CA	1632	1/1	0.84	0.12	55,55,55,55	0
60	MG	DA	3213	1/1	0.84	0.32	55,55,55,55	0
60	MG	AA	1754	1/1	0.84	0.26	55,55,55,55	0
60	MG	CA	1708	1/1	0.84	0.25	49,49,49,49	0
60	MG	AA	1729	1/1	0.84	0.22	55,55,55,55	0
60	MG	CA	1710	1/1	0.84	0.27	50,50,50,50	0
60	MG	DA	3336	1/1	0.84	0.27	55,55,55,55	1
60	MG	AA	1708	1/1	0.84	0.30	65,65,65,65	0
60	MG	DA	3343	1/1	0.84	0.53	55,55,55,55	0
60	MG	BA	3251	1/1	0.84	0.52	61,61,61,61	0
60	MG	BA	3143	1/1	0.84	0.30	57,57,57,57	0
60	MG	BA	3152	1/1	0.84	0.12	50,50,50,50	0
60	MG	AA	1743	1/1	0.84	0.61	55,55,55,55	0
60	MG	BA	3339	1/1	0.84	0.24	55,55,55,55	0
60	MG	DA	3191	1/1	0.85	0.31	54,54,54,54	0
60	MG	DA	3259	1/1	0.85	0.35	58,58,58,58	0
60	MG	BA	3030	1/1	0.85	0.61	47,47,47,47	0
60	MG	DA	3138	1/1	0.85	0.47	52,52,52,52	0
60	MG	BA	3351	1/1	0.85	0.49	55,55,55,55	0
60	MG	BA	3225	1/1	0.85	0.33	51,51,51,51	0
60	MG	BA	3259	1/1	0.85	0.28	59,59,59,59	0
60	MG	BA	3265	1/1	0.85	0.47	47,47,47,47	0
60	MG	DA	3097	1/1	0.85	0.50	56,56,56,56	0
60	MG	CV	105	1/1	0.85	0.23	50,50,50,50	0
60	MG	CA	1637	1/1	0.85	0.26	52,52,52,52	0
60	MG	AA	1712	1/1	0.85	0.41	54,54,54,54	0
60	MG	BA	3274	1/1	0.85	0.67	63,63,63,63	0
60	MG	CA	1707	1/1	0.85	0.63	51,51,51,51	0
60	MG	AA	1727	1/1	0.85	0.65	55,55,55,55	0
60	MG	BA	3153	1/1	0.85	0.45	53,53,53,53	0
60	MG	DF	301	1/1	0.85	0.27	47,47,47,47	0
60	MG	BA	3314	1/1	0.86	0.33	55,55,55,55	0
60	MG	DA	3012	1/1	0.86	0.34	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	3030	1/1	0.86	0.41	55,55,55,55	0
60	MG	BA	3151	1/1	0.86	0.31	47,47,47,47	0
60	MG	DA	3185	1/1	0.86	0.53	56,56,56,56	0
60	MG	DA	3059	1/1	0.86	0.77	55,55,55,55	0
60	MG	AA	1695	1/1	0.86	0.30	62,62,62,62	0
60	MG	AA	1755	1/1	0.86	0.62	55,55,55,55	0
60	MG	DA	3092	1/1	0.86	0.42	51,51,51,51	1
60	MG	DA	3301	1/1	0.86	0.63	55,55,55,55	0
60	MG	CA	1691	1/1	0.86	0.72	52,52,52,52	0
60	MG	AA	1622	1/1	0.86	0.20	48,48,48,48	0
60	MG	DA	3316	1/1	0.86	0.60	55,55,55,55	0
60	MG	DA	3210	1/1	0.86	0.59	66,66,66,66	0
60	MG	CA	1695	1/1	0.86	0.38	56,56,56,56	0
60	MG	CA	1700	1/1	0.86	0.26	54,54,54,54	0
60	MG	CA	1747	1/1	0.86	0.39	55,55,55,55	1
60	MG	CA	1751	1/1	0.86	0.27	55,55,55,55	0
60	MG	BA	3284	1/1	0.86	0.68	57,57,57,57	0
60	MG	BA	3173	1/1	0.86	0.33	56,56,56,56	0
60	MG	AA	1676	1/1	0.86	0.38	58,58,58,58	0
60	MG	BA	3209	1/1	0.86	0.55	66,66,66,66	0
60	MG	CA	1665	1/1	0.86	0.50	50,50,50,50	0
60	MG	AV	106	1/1	0.86	0.05	57,57,57,57	0
60	MG	BA	3180	1/1	0.86	0.42	56,56,56,56	0
60	MG	DA	3149	1/1	0.86	0.24	47,47,47,47	0
60	MG	AA	1656	1/1	0.86	0.67	47,47,47,47	0
60	MG	DA	3353	1/1	0.86	0.70	55,55,55,55	0
60	MG	DA	3166	1/1	0.86	0.65	47,47,47,47	0
60	MG	BA	3254	1/1	0.86	0.60	60,60,60,60	0
60	MG	BA	3224	1/1	0.86	0.43	51,51,51,51	0
60	MG	DF	303	1/1	0.86	0.69	59,59,59,59	0
60	MG	CA	1627	1/1	0.87	0.20	70,70,70,70	0
60	MG	DA	3269	1/1	0.87	0.60	52,52,52,52	0
60	MG	D7	101	1/1	0.87	0.38	54,54,54,54	0
60	MG	CA	1673	1/1	0.87	0.48	52,52,52,52	1
60	MG	AA	1643	1/1	0.87	0.17	56,56,56,56	0
60	MG	AA	1651	1/1	0.87	0.72	54,54,54,54	0
60	MG	BA	3123	1/1	0.87	0.62	53,53,53,53	0
60	MG	CA	1726	1/1	0.87	0.79	54,54,54,54	0
60	MG	BA	3247	1/1	0.87	0.20	59,59,59,59	0
60	MG	DA	3046	1/1	0.87	0.74	47,47,47,47	0
60	MG	AA	1670	1/1	0.87	0.29	69,69,69,69	0
60	MG	BA	3346	1/1	0.87	0.46	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	CA	1683	1/1	0.87	0.25	47,47,47,47	0
60	MG	DA	3200	1/1	0.87	0.97	58,58,58,58	0
60	MG	AW	105	1/1	0.87	0.20	53,53,53,53	0
60	MG	CA	1736	1/1	0.87	0.61	55,55,55,55	0
60	MG	AA	1709	1/1	0.87	0.55	50,50,50,50	0
60	MG	AA	1684	1/1	0.87	0.17	49,49,49,49	0
60	MG	DA	3323	1/1	0.87	0.50	55,55,55,55	0
60	MG	BA	3178	1/1	0.87	0.29	52,52,52,52	0
60	MG	CA	1749	1/1	0.87	0.38	55,55,55,55	0
60	MG	DA	3118	1/1	0.87	0.41	52,52,52,52	0
60	MG	BA	3039	1/1	0.87	0.24	68,68,68,68	0
60	MG	BA	3072	1/1	0.87	0.72	53,53,53,53	0
60	MG	DA	3228	1/1	0.87	0.37	55,55,55,55	0
60	MG	CA	1754	1/1	0.87	0.24	55,55,55,55	0
60	MG	AA	1713	1/1	0.87	0.16	64,64,64,64	0
60	MG	AA	1744	1/1	0.87	0.27	55,55,55,55	0
60	MG	CA	1661	1/1	0.87	0.59	52,52,52,52	0
60	MG	BA	3282	1/1	0.87	0.43	57,57,57,57	0
60	MG	CA	1664	1/1	0.87	0.49	60,60,60,60	0
60	MG	DA	3249	1/1	0.87	0.20	56,56,56,56	0
60	MG	CW	103	1/1	0.87	0.49	54,54,54,54	1
60	MG	DA	3158	1/1	0.87	0.45	53,53,53,53	0
60	MG	DF	302	1/1	0.87	0.24	53,53,53,53	0
60	MG	AV	105	1/1	0.87	0.22	50,50,50,50	1
60	MG	DA	3242	1/1	0.88	0.22	58,58,58,58	1
60	MG	AA	1610	1/1	0.88	0.28	55,55,55,55	0
60	MG	CA	1685	1/1	0.88	0.35	47,47,47,47	0
60	MG	DA	3253	1/1	0.88	0.35	49,49,49,49	0
60	MG	AA	1621	1/1	0.88	0.22	56,56,56,56	0
60	MG	BA	3045	1/1	0.88	0.80	47,47,47,47	0
60	MG	BA	3248	1/1	0.88	0.26	56,56,56,56	1
60	MG	BA	3195	1/1	0.88	0.42	52,52,52,52	0
60	MG	BA	3054	1/1	0.88	0.77	47,47,47,47	0
60	MG	AA	1717	1/1	0.88	0.26	66,66,66,66	0
60	MG	AA	1736	1/1	0.88	0.25	55,55,55,55	0
60	MG	BA	3325	1/1	0.88	0.34	55,55,55,55	0
60	MG	CA	1645	1/1	0.88	0.69	50,50,50,50	0
60	MG	BA	3207	1/1	0.88	0.55	60,60,60,60	0
60	MG	DA	3002	1/1	0.88	0.95	54,54,54,54	1
60	MG	DA	3182	1/1	0.88	0.27	56,56,56,56	0
60	MG	BA	3335	1/1	0.88	0.54	55,55,55,55	0
60	MG	DA	3293	1/1	0.88	0.24	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	1649	1/1	0.88	0.14	53,53,53,53	0
60	MG	DA	3299	1/1	0.88	0.37	55,55,55,55	0
60	MG	AA	1739	1/1	0.88	0.21	55,55,55,55	1
60	MG	BA	3099	1/1	0.88	0.80	55,55,55,55	0
60	MG	BA	3273	1/1	0.88	0.46	58,58,58,58	0
60	MG	DA	3314	1/1	0.88	0.25	55,55,55,55	1
60	MG	DA	3037	1/1	0.88	0.36	53,53,53,53	0
60	MG	BA	3220	1/1	0.88	0.64	54,54,54,54	0
60	MG	BA	3344	1/1	0.88	0.89	55,55,55,55	0
60	MG	BA	3276	1/1	0.88	0.45	58,58,58,58	0
60	MG	DA	3206	1/1	0.88	0.33	50,50,50,50	0
60	MG	AA	1644	1/1	0.88	0.36	49,49,49,49	0
60	MG	BB	201	1/1	0.88	0.56	67,67,67,67	0
60	MG	DA	3215	1/1	0.88	0.50	48,48,48,48	0
60	MG	DA	3216	1/1	0.88	0.54	60,60,60,60	0
60	MG	DA	3093	1/1	0.88	0.74	50,50,50,50	0
60	MG	CA	1666	1/1	0.88	0.56	57,57,57,57	0
60	MG	DA	3223	1/1	0.88	0.35	49,49,49,49	0
60	MG	AA	1681	1/1	0.88	0.28	66,66,66,66	0
60	MG	BA	3286	1/1	0.88	0.24	60,60,60,60	0
60	MG	AA	1710	1/1	0.88	0.13	55,55,55,55	0
60	MG	AW	102	1/1	0.88	0.13	60,60,60,60	1
60	MG	BA	3230	1/1	0.88	0.78	54,54,54,54	0
60	MG	CA	1745	1/1	0.88	0.24	55,55,55,55	0
60	MG	DA	3235	1/1	0.88	0.28	49,49,49,49	0
60	MG	AA	1645	1/1	0.88	0.16	57,57,57,57	0
60	MG	BA	3002	1/1	0.88	0.30	67,67,67,67	0
60	MG	AA	1731	1/1	0.88	0.24	55,55,55,55	0
60	MG	BA	3194	1/1	0.89	0.26	53,53,53,53	0
60	MG	DA	3178	1/1	0.89	0.49	48,48,48,48	0
60	MG	DA	3008	1/1	0.89	0.35	52,52,52,52	0
60	MG	BA	3140	1/1	0.89	0.49	56,56,56,56	0
60	MG	BA	3001	1/1	0.89	0.33	54,54,54,54	0
60	MG	CA	1721	1/1	0.89	0.27	58,58,58,58	0
60	MG	CA	1667	1/1	0.89	0.41	47,47,47,47	0
60	MG	AA	1701	1/1	0.89	0.31	51,51,51,51	0
60	MG	DA	3040	1/1	0.89	0.31	68,68,68,68	0
60	MG	AA	1611	1/1	0.89	0.49	48,48,48,48	0
60	MG	DA	3047	1/1	0.89	0.35	47,47,47,47	0
60	MG	BA	3117	1/1	0.89	0.39	52,52,52,52	0
60	MG	AA	1646	1/1	0.89	0.74	50,50,50,50	0
60	MG	DA	3085	1/1	0.89	0.42	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AE	201	1/1	0.89	0.79	57,57,57,57	0
60	MG	DA	3209	1/1	0.89	0.49	51,51,51,51	0
60	MG	BA	3124	1/1	0.89	0.31	49,49,49,49	0
60	MG	BA	3217	1/1	0.89	0.70	51,51,51,51	0
60	MG	CA	1739	1/1	0.89	0.13	55,55,55,55	0
60	MG	BA	3266	1/1	0.89	0.55	59,59,59,59	0
60	MG	BA	3167	1/1	0.89	0.31	53,53,53,53	0
60	MG	CA	1684	1/1	0.89	0.14	49,49,49,49	0
60	MG	BA	3327	1/1	0.89	0.48	55,55,55,55	0
60	MG	BA	3272	1/1	0.89	0.26	59,59,59,59	1
60	MG	BA	3329	1/1	0.89	0.35	55,55,55,55	1
60	MG	AA	1627	1/1	0.89	0.31	53,53,53,53	0
60	MG	DA	3132	1/1	0.89	0.30	59,59,59,59	0
60	MG	AW	103	1/1	0.89	0.09	54,54,54,54	0
60	MG	CA	1694	1/1	0.89	0.62	61,61,61,61	0
60	MG	BA	3275	1/1	0.89	0.39	59,59,59,59	0
60	MG	BA	3057	1/1	0.89	0.47	47,47,47,47	0
60	MG	BA	3132	1/1	0.89	0.35	57,57,57,57	0
60	MG	BA	3067	1/1	0.89	0.32	50,50,50,50	0
60	MG	BA	3285	1/1	0.89	0.25	55,55,55,55	0
60	MG	BA	3134	1/1	0.89	0.26	54,54,54,54	0
60	MG	AA	1725	1/1	0.89	1.06	54,54,54,54	0
60	MG	CA	1715	1/1	0.89	0.65	59,59,59,59	0
60	MG	DA	3258	1/1	0.89	0.83	51,51,51,51	1
60	MG	AY	401	1/1	0.89	0.55	55,55,55,55	0
60	MG	B7	102	1/1	0.89	0.35	54,54,54,54	0
60	MG	CA	1614	1/1	0.90	0.81	53,53,53,53	0
60	MG	BA	3094	1/1	0.90	0.60	47,47,47,47	0
60	MG	DA	3140	1/1	0.90	0.38	50,50,50,50	1
60	MG	CA	1617	1/1	0.90	0.29	51,51,51,51	0
60	MG	BA	3174	1/1	0.90	0.32	58,58,58,58	0
60	MG	CA	1624	1/1	0.90	0.38	51,51,51,51	0
60	MG	BA	3095	1/1	0.90	0.61	60,60,60,60	0
60	MG	BA	3096	1/1	0.90	0.43	56,56,56,56	0
60	MG	BA	3097	1/1	0.90	0.34	47,47,47,47	0
60	MG	CA	1690	1/1	0.90	0.20	59,59,59,59	0
60	MG	AA	1634	1/1	0.90	0.68	52,52,52,52	0
60	MG	BA	3100	1/1	0.90	0.83	51,51,51,51	0
60	MG	DA	3275	1/1	0.90	0.64	59,59,59,59	0
60	MG	CA	1633	1/1	0.90	0.93	52,52,52,52	0
60	MG	CA	1635	1/1	0.90	0.42	49,49,49,49	0
60	MG	CA	1698	1/1	0.90	0.33	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	3226	1/1	0.90	0.46	56,56,56,56	0
60	MG	B7	101	1/1	0.90	0.54	49,49,49,49	0
60	MG	BA	3229	1/1	0.90	0.17	49,49,49,49	0
60	MG	DA	3288	1/1	0.90	0.20	66,66,66,66	0
60	MG	DA	3290	1/1	0.90	0.44	57,57,57,57	0
60	MG	BA	3112	1/1	0.90	0.33	48,48,48,48	0
60	MG	BA	3231	1/1	0.90	0.40	51,51,51,51	0
60	MG	CA	1646	1/1	0.90	0.45	62,62,62,62	0
60	MG	CA	1713	1/1	0.90	0.36	54,54,54,54	0
60	MG	BA	3280	1/1	0.90	0.48	57,57,57,57	0
60	MG	AA	1715	1/1	0.90	0.23	55,55,55,55	0
60	MG	BA	3283	1/1	0.90	0.30	65,65,65,65	0
60	MG	DA	3315	1/1	0.90	0.29	55,55,55,55	0
60	MG	BA	3192	1/1	0.90	0.26	65,65,65,65	0
60	MG	CA	1654	1/1	0.90	0.72	57,57,57,57	0
60	MG	DA	3055	1/1	0.90	0.58	47,47,47,47	0
60	MG	AA	1723	1/1	0.90	0.33	57,57,57,57	0
60	MG	DA	3321	1/1	0.90	0.22	55,55,55,55	0
60	MG	DA	3068	1/1	0.90	0.40	50,50,50,50	0
60	MG	DA	3325	1/1	0.90	0.91	55,55,55,55	0
60	MG	DA	3326	1/1	0.90	0.55	55,55,55,55	0
60	MG	BA	3150	1/1	0.90	0.47	51,51,51,51	0
60	MG	BA	3349	1/1	0.90	0.50	55,55,55,55	0
60	MG	BA	3350	1/1	0.90	0.32	55,55,55,55	0
60	MG	DA	3331	1/1	0.90	0.09	55,55,55,55	1
60	MG	AA	1662	1/1	0.90	0.14	52,52,52,52	0
60	MG	BA	3244	1/1	0.90	0.25	60,60,60,60	0
60	MG	DA	3335	1/1	0.90	0.50	55,55,55,55	0
60	MG	BA	3246	1/1	0.90	0.38	55,55,55,55	0
60	MG	BA	3004	1/1	0.90	0.30	53,53,53,53	0
60	MG	BA	3029	1/1	0.90	0.34	55,55,55,55	0
60	MG	DA	3344	1/1	0.90	0.54	55,55,55,55	0
60	MG	DA	3347	1/1	0.90	0.25	55,55,55,55	0
60	MG	CA	1605	1/1	0.90	0.60	59,59,59,59	0
60	MG	CA	1737	1/1	0.90	0.40	55,55,55,55	1
60	MG	DA	3230	1/1	0.90	0.12	49,49,49,49	0
60	MG	CA	1738	1/1	0.90	0.94	55,55,55,55	0
60	MG	AA	1658	1/1	0.90	0.28	49,49,49,49	0
60	MG	DB	203	1/1	0.90	0.73	55,55,55,55	0
60	MG	DA	3237	1/1	0.90	0.69	60,60,60,60	0
60	MG	CA	1610	1/1	0.90	0.50	48,48,48,48	0
60	MG	BA	3250	1/1	0.90	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
60	MG	AA	1753	1/1	0.90	0.45	55,55,55,55	1
60	MG	DX	101	1/1	0.90	0.22	55,55,55,55	0
60	MG	BA	3188	1/1	0.91	0.36	57,57,57,57	0
60	MG	DA	3170	1/1	0.91	0.48	49,49,49,49	1
60	MG	AA	1601	1/1	0.91	0.19	56,56,56,56	0
60	MG	BA	3354	1/1	0.91	0.40	55,55,55,55	0
60	MG	BA	3290	1/1	0.91	0.37	57,57,57,57	0
60	MG	DA	3276	1/1	0.91	0.78	58,58,58,58	0
60	MG	AA	1714	1/1	0.91	0.55	59,59,59,59	0
60	MG	BA	3245	1/1	0.91	0.39	53,53,53,53	0
60	MG	AA	1734	1/1	0.91	0.16	55,55,55,55	0
60	MG	BA	3010	1/1	0.91	0.60	52,52,52,52	0
60	MG	BA	3024	1/1	0.91	0.65	56,56,56,56	0
60	MG	DA	3045	1/1	0.91	0.44	56,56,56,56	0
60	MG	CA	1607	1/1	0.91	0.32	47,47,47,47	0
60	MG	CA	1727	1/1	0.91	0.21	56,56,56,56	0
60	MG	DA	3054	1/1	0.91	0.35	51,51,51,51	0
60	MG	DA	3194	1/1	0.91	0.49	53,53,53,53	0
60	MG	CA	1668	1/1	0.91	0.82	58,58,58,58	0
60	MG	BA	3148	1/1	0.91	0.17	47,47,47,47	0
60	MG	BA	3104	1/1	0.91	0.71	48,48,48,48	0
60	MG	DA	3306	1/1	0.91	0.10	55,55,55,55	0
60	MG	BA	3310	1/1	0.91	0.21	55,55,55,55	0
60	MG	BA	3311	1/1	0.91	0.38	55,55,55,55	0
60	MG	AA	1700	1/1	0.91	0.27	51,51,51,51	0
60	MG	BA	3208	1/1	0.91	0.44	51,51,51,51	0
60	MG	AA	1639	1/1	0.91	0.21	53,53,53,53	0
60	MG	AA	1682	1/1	0.91	0.14	53,53,53,53	0
60	MG	DA	3098	1/1	0.91	0.27	47,47,47,47	0
60	MG	DA	3220	1/1	0.91	0.84	49,49,49,49	0
60	MG	BA	3159	1/1	0.91	0.32	55,55,55,55	0
60	MG	AA	1641	1/1	0.91	0.43	47,47,47,47	0
60	MG	BA	3162	1/1	0.91	0.82	50,50,50,50	0
60	MG	BA	3326	1/1	0.91	0.81	55,55,55,55	0
60	MG	CA	1748	1/1	0.91	0.45	55,55,55,55	1
60	MG	DA	3329	1/1	0.91	0.29	55,55,55,55	0
60	MG	AA	1706	1/1	0.91	0.24	51,51,51,51	0
60	MG	DA	3123	1/1	0.91	0.25	64,64,64,64	1
60	MG	AA	1707	1/1	0.91	0.46	49,49,49,49	0
60	MG	AA	1652	1/1	0.91	0.39	47,47,47,47	0
60	MG	DA	3232	1/1	0.91	0.18	51,51,51,51	0
60	MG	AA	1660	1/1	0.91	0.11	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	3177	1/1	0.91	0.84	47,47,47,47	0
60	MG	AA	1603	1/1	0.91	0.23	57,57,57,57	0
60	MG	BA	3277	1/1	0.91	0.74	57,57,57,57	0
60	MG	AA	1711	1/1	0.91	0.29	47,47,47,47	0
60	MG	B5	102	1/1	0.91	0.61	53,53,53,53	0
60	MG	AA	1750	1/1	0.91	0.23	55,55,55,55	0
60	MG	DA	3145	1/1	0.91	0.40	49,49,49,49	0
60	MG	DA	3250	1/1	0.91	0.44	56,56,56,56	0
60	MG	DA	3251	1/1	0.91	0.19	52,52,52,52	0
60	MG	BA	3345	1/1	0.91	0.24	55,55,55,55	0
60	MG	DA	3257	1/1	0.91	0.67	55,55,55,55	0
60	MG	BA	3092	1/1	0.91	0.61	50,50,50,50	0
60	MG	AA	1632	1/1	0.91	0.47	53,53,53,53	0
60	MG	DA	3165	1/1	0.91	0.27	47,47,47,47	0
60	MG	CA	1711	1/1	0.91	0.15	55,55,55,55	0
60	MG	BA	3215	1/1	0.92	0.71	60,60,60,60	0
60	MG	BA	3216	1/1	0.92	0.28	49,49,49,49	0
60	MG	AA	1602	1/1	0.92	0.37	52,52,52,52	0
60	MG	DA	3254	1/1	0.92	0.24	54,54,54,54	0
60	MG	BA	3219	1/1	0.92	0.86	49,49,49,49	0
60	MG	DA	3136	1/1	0.92	0.93	58,58,58,58	0
60	MG	AA	1633	1/1	0.92	0.12	55,55,55,55	0
60	MG	B1	101	1/1	0.92	0.56	55,55,55,55	0
60	MG	CA	1755	1/1	0.92	0.54	55,55,55,55	0
60	MG	CA	1756	1/1	0.92	0.35	55,55,55,55	1
60	MG	CA	1757	1/1	0.92	0.20	55,55,55,55	0
60	MG	CN	101	1/1	0.92	0.36	55,55,55,55	0
60	MG	BA	3036	1/1	0.92	0.24	53,53,53,53	0
60	MG	AA	1691	1/1	0.92	0.47	59,59,59,59	0
60	MG	DA	3160	1/1	0.92	0.32	55,55,55,55	0
60	MG	DA	3279	1/1	0.92	0.28	55,55,55,55	0
60	MG	BA	3044	1/1	0.92	0.84	56,56,56,56	0
60	MG	AV	103	1/1	0.92	0.26	54,54,54,54	1
60	MG	BA	3330	1/1	0.92	0.25	55,55,55,55	0
60	MG	BA	3332	1/1	0.92	0.11	55,55,55,55	0
60	MG	BA	3333	1/1	0.92	0.71	55,55,55,55	0
60	MG	CA	1634	1/1	0.92	0.16	47,47,47,47	0
60	MG	BA	3334	1/1	0.92	0.29	55,55,55,55	0
60	MG	CA	1702	1/1	0.92	0.38	51,51,51,51	0
60	MG	BA	3228	1/1	0.92	0.80	52,52,52,52	0
60	MG	CA	1639	1/1	0.92	0.30	48,48,48,48	0
60	MG	BA	3138	1/1	0.92	0.34	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	3047	1/1	0.92	0.30	47,47,47,47	0
60	MG	BA	3185	1/1	0.92	0.61	50,50,50,50	0
60	MG	DA	3303	1/1	0.92	0.73	55,55,55,55	0
60	MG	DA	3017	1/1	0.92	0.66	47,47,47,47	0
60	MG	DA	3018	1/1	0.92	0.47	52,52,52,52	0
60	MG	DA	3025	1/1	0.92	0.76	56,56,56,56	0
60	MG	BA	3102	1/1	0.92	0.77	47,47,47,47	0
60	MG	DA	3031	1/1	0.92	0.73	47,47,47,47	0
60	MG	AA	1726	1/1	0.92	0.29	56,56,56,56	0
60	MG	BA	3343	1/1	0.92	0.53	55,55,55,55	0
60	MG	AA	1664	1/1	0.92	0.29	60,60,60,60	0
60	MG	DA	3043	1/1	0.92	1.02	47,47,47,47	0
60	MG	BA	3111	1/1	0.92	0.26	52,52,52,52	0
60	MG	AA	1618	1/1	0.92	0.22	51,51,51,51	1
60	MG	AA	1620	1/1	0.92	0.29	55,55,55,55	0
60	MG	BA	3119	1/1	0.92	0.78	49,49,49,49	0
60	MG	CA	1656	1/1	0.92	0.82	47,47,47,47	0
60	MG	DA	3217	1/1	0.92	0.16	49,49,49,49	0
60	MG	BA	3120	1/1	0.92	0.62	50,50,50,50	0
60	MG	DA	3066	1/1	0.92	0.53	52,52,52,52	0
60	MG	DA	3221	1/1	0.92	0.55	54,54,54,54	0
60	MG	BA	3077	1/1	0.92	0.54	51,51,51,51	0
60	MG	BA	3205	1/1	0.92	0.17	50,50,50,50	0
60	MG	CA	1662	1/1	0.92	0.27	52,52,52,52	0
60	MG	BB	203	1/1	0.92	0.67	55,55,55,55	0
60	MG	DA	3338	1/1	0.92	0.71	55,55,55,55	0
60	MG	DA	3090	1/1	0.92	0.66	48,48,48,48	0
60	MG	BB	204	1/1	0.92	0.23	55,55,55,55	0
60	MG	BA	3304	1/1	0.92	0.65	55,55,55,55	0
60	MG	BD	302	1/1	0.92	0.62	47,47,47,47	0
60	MG	BA	3306	1/1	0.92	0.18	55,55,55,55	0
60	MG	BA	3078	1/1	0.92	0.68	56,56,56,56	0
60	MG	CA	1602	1/1	0.92	0.26	52,52,52,52	0
60	MG	AA	1741	1/1	0.92	0.49	55,55,55,55	0
60	MG	AA	1630	1/1	0.92	0.70	51,51,51,51	0
60	MG	DB	204	1/1	0.92	0.20	55,55,55,55	0
60	MG	DA	3111	1/1	0.92	0.25	49,49,49,49	0
60	MG	DD	301	1/1	0.92	0.58	47,47,47,47	0
60	MG	DA	3112	1/1	0.92	0.31	52,52,52,52	0
60	MG	CA	1741	1/1	0.92	0.53	55,55,55,55	0
60	MG	BA	3127	1/1	0.92	0.24	56,56,56,56	0
60	MG	DQ	201	1/1	0.92	0.77	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	3168	1/1	0.92	0.39	47,47,47,47	0
60	MG	BA	3064	1/1	0.93	0.52	53,53,53,53	0
60	MG	DA	3264	1/1	0.93	0.14	56,56,56,56	0
60	MG	DA	3266	1/1	0.93	0.52	47,47,47,47	0
60	MG	DA	3267	1/1	0.93	0.32	54,54,54,54	0
60	MG	DA	3169	1/1	0.93	0.39	47,47,47,47	0
60	MG	AA	1703	1/1	0.93	0.26	62,62,62,62	0
60	MG	DA	3173	1/1	0.93	0.23	58,58,58,58	0
60	MG	BA	3204	1/1	0.93	0.40	57,57,57,57	0
60	MG	CA	1743	1/1	0.93	0.28	55,55,55,55	0
60	MG	DA	3049	1/1	0.93	0.43	47,47,47,47	0
60	MG	AA	1740	1/1	0.93	0.38	55,55,55,55	0
60	MG	CA	1697	1/1	0.93	0.15	62,62,62,62	0
60	MG	BA	3144	1/1	0.93	0.42	49,49,49,49	0
60	MG	BA	3232	1/1	0.93	0.52	53,53,53,53	0
60	MG	CA	1658	1/1	0.93	0.25	49,49,49,49	0
60	MG	DA	3073	1/1	0.93	0.61	53,53,53,53	0
60	MG	DA	3079	1/1	0.93	0.47	56,56,56,56	0
60	MG	DA	3081	1/1	0.93	0.55	52,52,52,52	0
60	MG	AA	1615	1/1	0.93	0.81	53,53,53,53	0
60	MG	CA	1706	1/1	0.93	0.19	51,51,51,51	0
60	MG	DA	3296	1/1	0.93	0.60	55,55,55,55	0
60	MG	DA	3199	1/1	0.93	0.54	53,53,53,53	0
60	MG	DA	3300	1/1	0.93	0.48	55,55,55,55	0
60	MG	BA	3340	1/1	0.93	0.59	55,55,55,55	0
60	MG	BA	3103	1/1	0.93	0.58	50,50,50,50	0
60	MG	CA	1618	1/1	0.93	0.31	49,49,49,49	0
60	MG	DA	3305	1/1	0.93	0.24	55,55,55,55	0
60	MG	BA	3211	1/1	0.93	0.26	59,59,59,59	1
60	MG	DA	3308	1/1	0.93	0.15	55,55,55,55	0
60	MG	CL	201	1/1	0.93	0.59	51,51,51,51	1
60	MG	DA	3312	1/1	0.93	0.16	55,55,55,55	0
60	MG	BA	3312	1/1	0.93	0.74	55,55,55,55	0
60	MG	CA	1712	1/1	0.93	0.50	47,47,47,47	0
60	MG	CV	104	1/1	0.93	0.08	54,54,54,54	0
60	MG	AA	1623	1/1	0.93	0.53	57,57,57,57	0
60	MG	BA	3213	1/1	0.93	0.43	58,58,58,58	0
60	MG	BA	3042	1/1	0.93	1.00	47,47,47,47	0
60	MG	BA	3281	1/1	0.93	0.39	57,57,57,57	0
60	MG	DA	3113	1/1	0.93	0.31	48,48,48,48	0
60	MG	DA	3324	1/1	0.93	0.51	55,55,55,55	0
60	MG	DA	3115	1/1	0.93	0.23	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	AA	1752	1/1	0.93	0.20	55,55,55,55	0
60	MG	DA	3120	1/1	0.93	0.89	49,49,49,49	0
60	MG	BA	3322	1/1	0.93	0.38	55,55,55,55	0
60	MG	DA	3226	1/1	0.93	0.42	51,51,51,51	0
60	MG	AV	104	1/1	0.93	0.11	54,54,54,54	0
60	MG	DA	3125	1/1	0.93	0.22	49,49,49,49	0
60	MG	DA	3332	1/1	0.93	0.49	55,55,55,55	0
60	MG	BA	3113	1/1	0.93	0.52	47,47,47,47	0
60	MG	DA	3128	1/1	0.93	0.30	56,56,56,56	0
60	MG	BA	3016	1/1	0.93	0.89	47,47,47,47	0
60	MG	CA	1723	1/1	0.93	0.10	55,55,55,55	0
60	MG	CA	1725	1/1	0.93	0.38	59,59,59,59	0
60	MG	DA	3006	1/1	0.93	0.75	47,47,47,47	0
60	MG	CA	1638	1/1	0.93	0.59	53,53,53,53	0
60	MG	CA	1678	1/1	0.93	0.13	49,49,49,49	0
60	MG	DA	3346	1/1	0.93	0.82	55,55,55,55	0
60	MG	BA	3190	1/1	0.93	0.43	54,54,54,54	0
60	MG	AA	1612	1/1	0.93	0.13	52,52,52,52	0
60	MG	CA	1642	1/1	0.93	0.61	56,56,56,56	0
60	MG	CA	1732	1/1	0.93	0.20	55,55,55,55	0
60	MG	DA	3146	1/1	0.93	0.46	47,47,47,47	0
60	MG	DA	3027	1/1	0.93	0.45	47,47,47,47	0
60	MG	DA	3252	1/1	0.93	0.54	61,61,61,61	1
60	MG	DA	3153	1/1	0.93	0.12	50,50,50,50	0
60	MG	DA	3157	1/1	0.93	0.35	48,48,48,48	0
60	MG	DA	3256	1/1	0.93	0.61	55,55,55,55	0
60	MG	BF	301	1/1	0.93	0.29	47,47,47,47	0
60	MG	AA	1606	1/1	0.93	0.30	59,59,59,59	0
60	MG	BA	3171	1/1	0.93	0.15	58,58,58,58	0
60	MG	CA	1601	1/1	0.93	0.30	56,56,56,56	0
60	MG	BA	3058	1/1	0.93	0.69	55,55,55,55	0
60	MG	DY	201	1/1	0.93	0.28	55,55,55,55	0
60	MG	CA	1620	1/1	0.94	0.19	56,56,56,56	0
60	MG	BA	3191	1/1	0.94	0.17	61,61,61,61	0
60	MG	DA	3268	1/1	0.94	0.85	59,59,59,59	0
60	MG	CA	1622	1/1	0.94	0.84	57,57,57,57	0
60	MG	AA	1745	1/1	0.94	0.66	55,55,55,55	0
60	MG	BA	3084	1/1	0.94	0.38	47,47,47,47	0
60	MG	DA	3050	1/1	0.94	0.52	47,47,47,47	0
60	MG	DA	3174	1/1	0.94	0.37	52,52,52,52	0
60	MG	AA	1757	1/1	0.94	0.34	55,55,55,55	0
60	MG	BA	3233	1/1	0.94	0.62	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	3057	1/1	0.94	0.67	47,47,47,47	0
60	MG	DA	3179	1/1	0.94	0.90	47,47,47,47	0
60	MG	CA	1742	1/1	0.94	0.69	55,55,55,55	0
60	MG	DA	3063	1/1	0.94	0.55	47,47,47,47	0
60	MG	BA	3154	1/1	0.94	0.34	48,48,48,48	0
60	MG	CA	1686	1/1	0.94	0.33	57,57,57,57	0
60	MG	BA	3235	1/1	0.94	0.21	60,60,60,60	0
60	MG	DA	3076	1/1	0.94	0.37	47,47,47,47	0
60	MG	DA	3077	1/1	0.94	0.35	48,48,48,48	0
60	MG	AA	1721	1/1	0.94	0.41	55,55,55,55	1
60	MG	DA	3297	1/1	0.94	0.45	55,55,55,55	0
60	MG	DA	3298	1/1	0.94	0.30	55,55,55,55	0
60	MG	BA	3003	1/1	0.94	0.30	61,61,61,61	0
60	MG	BA	3289	1/1	0.94	0.42	54,54,54,54	0
60	MG	DA	3197	1/1	0.94	0.58	47,47,47,47	0
60	MG	CA	1692	1/1	0.94	0.49	59,59,59,59	0
60	MG	CA	1636	1/1	0.94	0.65	53,53,53,53	0
60	MG	BA	3238	1/1	0.94	0.09	55,55,55,55	1
60	MG	DA	3091	1/1	0.94	0.40	48,48,48,48	0
60	MG	DA	3307	1/1	0.94	0.27	55,55,55,55	0
60	MG	BA	3291	1/1	0.94	0.38	54,54,54,54	0
60	MG	BA	3128	1/1	0.94	0.21	50,50,50,50	0
60	MG	DA	3310	1/1	0.94	0.23	55,55,55,55	0
60	MG	BA	3166	1/1	0.94	0.10	47,47,47,47	0
60	MG	DA	3313	1/1	0.94	0.77	55,55,55,55	0
60	MG	BA	3243	1/1	0.94	0.57	53,53,53,53	0
60	MG	AA	1665	1/1	0.94	0.76	50,50,50,50	0
60	MG	CV	102	1/1	0.94	0.35	54,54,54,54	0
60	MG	AW	104	1/1	0.94	0.13	56,56,56,56	0
60	MG	BA	3353	1/1	0.94	0.54	55,55,55,55	0
60	MG	BA	3012	1/1	0.94	0.59	49,49,49,49	0
60	MG	BA	3172	1/1	0.94	0.34	52,52,52,52	0
60	MG	AA	1663	1/1	0.94	0.28	51,51,51,51	0
60	MG	CA	1649	1/1	0.94	0.42	47,47,47,47	0
60	MG	DA	3116	1/1	0.94	0.34	50,50,50,50	0
60	MG	DA	3117	1/1	0.94	0.28	47,47,47,47	0
60	MG	AA	1672	1/1	0.94	0.25	53,53,53,53	0
60	MG	BA	3025	1/1	0.94	0.44	55,55,55,55	0
60	MG	BD	301	1/1	0.94	0.50	47,47,47,47	0
60	MG	D3	101	1/1	0.94	0.48	58,58,58,58	0
60	MG	DA	3124	1/1	0.94	0.46	53,53,53,53	0
60	MG	BA	3065	1/1	0.94	0.24	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	3026	1/1	0.94	0.39	47,47,47,47	0
60	MG	DA	3233	1/1	0.94	0.63	53,53,53,53	0
60	MG	BA	3071	1/1	0.94	0.40	47,47,47,47	0
60	MG	DA	3129	1/1	0.94	0.21	50,50,50,50	0
60	MG	BA	3257	1/1	0.94	0.36	51,51,51,51	0
60	MG	BA	3316	1/1	0.94	0.46	55,55,55,55	0
60	MG	BA	3218	1/1	0.94	0.58	66,66,66,66	0
60	MG	AA	1640	1/1	0.94	0.41	48,48,48,48	0
60	MG	BA	3075	1/1	0.94	0.38	47,47,47,47	0
60	MG	DA	3139	1/1	0.94	0.65	50,50,50,50	0
60	MG	BA	3221	1/1	0.94	0.68	53,53,53,53	0
60	MG	DA	3350	1/1	0.94	0.43	55,55,55,55	0
60	MG	DA	3141	1/1	0.94	0.37	56,56,56,56	0
60	MG	CA	1609	1/1	0.94	0.36	55,55,55,55	0
60	MG	DA	3024	1/1	0.94	0.98	49,49,49,49	0
60	MG	BA	3268	1/1	0.94	0.72	59,59,59,59	0
60	MG	DA	3255	1/1	0.94	0.46	60,60,60,60	0
60	MG	AA	1728	1/1	0.94	0.30	55,55,55,55	0
60	MG	AA	1674	1/1	0.94	0.21	50,50,50,50	0
60	MG	BA	3118	1/1	0.94	0.51	49,49,49,49	0
60	MG	DD	302	1/1	0.94	0.46	47,47,47,47	0
60	MG	DA	3032	1/1	0.94	0.29	50,50,50,50	0
60	MG	BA	3146	1/1	0.94	0.65	47,47,47,47	0
60	MG	DA	3261	1/1	0.94	0.22	57,57,57,57	0
60	MG	DH	201	1/1	0.94	0.12	50,50,50,50	0
60	MG	DA	3035	1/1	0.94	0.41	50,50,50,50	0
60	MG	BA	3079	1/1	0.94	0.44	49,49,49,49	0
60	MG	BA	3034	1/1	0.94	0.35	50,50,50,50	0
60	MG	BA	3115	1/1	0.95	0.52	50,50,50,50	0
60	MG	DA	3245	1/1	0.95	0.58	53,53,53,53	0
60	MG	BA	3074	1/1	0.95	0.40	47,47,47,47	0
60	MG	AA	1608	1/1	0.95	0.26	47,47,47,47	0
60	MG	BA	3156	1/1	0.95	0.50	48,48,48,48	0
60	MG	BA	3206	1/1	0.95	0.30	47,47,47,47	0
60	MG	CA	1611	1/1	0.95	0.25	52,52,52,52	0
60	MG	BA	3313	1/1	0.95	0.18	55,55,55,55	0
60	MG	BA	3076	1/1	0.95	0.24	48,48,48,48	0
60	MG	AA	1628	1/1	0.95	0.37	70,70,70,70	0
60	MG	AV	102	1/1	0.95	0.28	54,54,54,54	0
60	MG	CA	1616	1/1	0.95	0.37	54,54,54,54	0
60	MG	BA	3210	1/1	0.95	0.41	57,57,57,57	0
60	MG	BA	3165	1/1	0.95	0.70	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	3033	1/1	0.95	0.56	47,47,47,47	0
60	MG	CY	401	1/1	0.95	0.56	55,55,55,55	0
60	MG	DA	3130	1/1	0.95	0.24	56,56,56,56	0
60	MG	BA	3321	1/1	0.95	0.20	55,55,55,55	0
60	MG	D5	101	1/1	0.95	0.16	49,49,49,49	0
60	MG	D5	102	1/1	0.95	0.35	53,53,53,53	0
60	MG	DA	3135	1/1	0.95	0.51	54,54,54,54	0
60	MG	AA	1629	1/1	0.95	0.27	56,56,56,56	0
60	MG	BA	3323	1/1	0.95	0.84	55,55,55,55	0
60	MG	DA	3270	1/1	0.95	0.60	67,67,67,67	0
60	MG	AA	1724	1/1	0.95	0.55	59,59,59,59	0
60	MG	DA	3273	1/1	0.95	0.29	58,58,58,58	0
60	MG	CA	1699	1/1	0.95	0.16	53,53,53,53	1
60	MG	DA	3004	1/1	0.95	0.38	61,61,61,61	0
60	MG	DA	3005	1/1	0.95	0.43	53,53,53,53	0
60	MG	CA	1626	1/1	0.95	0.17	53,53,53,53	0
60	MG	DA	3007	1/1	0.95	0.70	53,53,53,53	0
60	MG	BA	3260	1/1	0.95	0.18	57,57,57,57	0
60	MG	DA	3009	1/1	0.95	0.54	55,55,55,55	0
60	MG	DA	3010	1/1	0.95	0.64	47,47,47,47	0
60	MG	DA	3151	1/1	0.95	0.52	51,51,51,51	0
60	MG	DA	3152	1/1	0.95	0.46	47,47,47,47	0
60	MG	BA	3261	1/1	0.95	0.53	52,52,52,52	0
60	MG	CA	1630	1/1	0.95	0.27	47,47,47,47	0
60	MG	DA	3292	1/1	0.95	0.53	55,55,55,55	0
60	MG	DA	3013	1/1	0.95	0.55	49,49,49,49	0
60	MG	DA	3159	1/1	0.95	0.83	49,49,49,49	0
60	MG	DA	3295	1/1	0.95	0.75	55,55,55,55	0
60	MG	BA	3263	1/1	0.95	0.15	56,56,56,56	0
60	MG	DA	3161	1/1	0.95	0.31	47,47,47,47	0
60	MG	BA	3169	1/1	0.95	0.57	51,51,51,51	0
60	MG	DA	3164	1/1	0.95	0.68	53,53,53,53	0
60	MG	DA	3019	1/1	0.95	0.59	54,54,54,54	0
60	MG	BA	3170	1/1	0.95	0.40	50,50,50,50	0
60	MG	AA	1685	1/1	0.95	0.26	57,57,57,57	0
60	MG	DA	3026	1/1	0.95	0.44	55,55,55,55	0
60	MG	BA	3331	1/1	0.95	0.22	55,55,55,55	0
60	MG	AA	1636	1/1	0.95	0.20	49,49,49,49	0
60	MG	BA	3270	1/1	0.95	0.73	67,67,67,67	0
60	MG	BA	3271	1/1	0.95	0.61	51,51,51,51	0
60	MG	AA	1738	1/1	0.95	0.10	55,55,55,55	0
60	MG	DA	3034	1/1	0.95	0.58	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	3005	1/1	0.95	0.70	47,47,47,47	0
60	MG	BA	3007	1/1	0.95	0.49	52,52,52,52	0
60	MG	BA	3176	1/1	0.95	0.57	48,48,48,48	0
60	MG	BA	3223	1/1	0.95	0.39	52,52,52,52	0
60	MG	BA	3053	1/1	0.95	0.19	51,51,51,51	0
60	MG	AA	1624	1/1	0.95	0.34	48,48,48,48	0
60	MG	BA	3342	1/1	0.95	0.28	55,55,55,55	0
60	MG	AA	1671	1/1	0.95	0.31	47,47,47,47	0
60	MG	AA	1625	1/1	0.95	0.28	51,51,51,51	0
60	MG	DA	3322	1/1	0.95	0.74	55,55,55,55	0
60	MG	CA	1650	1/1	0.95	0.66	54,54,54,54	0
60	MG	BA	3101	1/1	0.95	0.68	47,47,47,47	0
60	MG	DA	3196	1/1	0.95	0.35	52,52,52,52	0
60	MG	BA	3062	1/1	0.95	0.51	47,47,47,47	0
60	MG	BA	3348	1/1	0.95	0.59	55,55,55,55	0
60	MG	DA	3061	1/1	0.95	0.49	47,47,47,47	0
60	MG	DA	3201	1/1	0.95	0.42	60,60,60,60	0
60	MG	BA	3019	1/1	0.95	0.54	47,47,47,47	0
60	MG	DA	3064	1/1	0.95	0.41	56,56,56,56	0
60	MG	DA	3065	1/1	0.95	0.56	53,53,53,53	0
60	MG	AA	1756	1/1	0.95	0.16	55,55,55,55	1
60	MG	DA	3067	1/1	0.95	0.61	50,50,50,50	0
60	MG	DA	3211	1/1	0.95	0.50	57,57,57,57	0
60	MG	DA	3212	1/1	0.95	0.22	59,59,59,59	0
60	MG	AA	1690	1/1	0.95	0.66	52,52,52,52	0
60	MG	BA	3352	1/1	0.95	0.34	55,55,55,55	0
60	MG	BA	3288	1/1	0.95	0.21	66,66,66,66	0
60	MG	BA	3106	1/1	0.95	0.73	51,51,51,51	0
60	MG	BA	3107	1/1	0.95	0.37	51,51,51,51	0
60	MG	BA	3109	1/1	0.95	0.30	48,48,48,48	0
60	MG	DA	3348	1/1	0.95	0.32	55,55,55,55	0
60	MG	BA	3147	1/1	0.95	0.42	51,51,51,51	0
60	MG	BA	3193	1/1	0.95	0.27	53,53,53,53	0
60	MG	DA	3086	1/1	0.95	0.14	47,47,47,47	0
60	MG	BA	3295	1/1	0.95	0.15	49,49,49,49	0
60	MG	DA	3088	1/1	0.95	0.42	49,49,49,49	0
60	MG	AA	1719	1/1	0.95	0.14	56,56,56,56	0
60	MG	BA	3298	1/1	0.95	0.44	55,55,55,55	0
60	MG	BH	201	1/1	0.95	0.13	50,50,50,50	0
60	MG	CA	1671	1/1	0.95	0.19	47,47,47,47	0
60	MG	CA	1672	1/1	0.95	0.45	53,53,53,53	0
60	MG	CA	1750	1/1	0.95	0.24	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	3027	1/1	0.95	0.31	50,50,50,50	0
60	MG	DA	3101	1/1	0.95	0.52	51,51,51,51	0
60	MG	BA	3196	1/1	0.95	0.47	47,47,47,47	0
60	MG	BA	3242	1/1	0.95	0.39	47,47,47,47	0
60	MG	BA	3073	1/1	0.95	0.44	52,52,52,52	0
60	MG	DA	3109	1/1	0.95	0.41	52,52,52,52	0
60	MG	DA	3110	1/1	0.95	0.30	48,48,48,48	0
60	MG	DA	3284	1/1	0.96	0.89	57,57,57,57	0
60	MG	DA	3204	1/1	0.96	0.33	52,52,52,52	0
60	MG	DA	3286	1/1	0.96	0.24	60,60,60,60	0
60	MG	DA	3056	1/1	0.96	0.43	47,47,47,47	0
60	MG	BA	3256	1/1	0.96	0.68	55,55,55,55	0
60	MG	DA	3208	1/1	0.96	0.25	60,60,60,60	0
60	MG	BA	3023	1/1	0.96	0.78	49,49,49,49	0
60	MG	BA	3006	1/1	0.96	0.82	53,53,53,53	0
60	MG	DA	3062	1/1	0.96	0.43	48,48,48,48	0
60	MG	BA	3317	1/1	0.96	0.75	55,55,55,55	0
60	MG	CA	1689	1/1	0.96	0.26	63,63,63,63	1
60	MG	DA	3214	1/1	0.96	0.37	58,58,58,58	0
60	MG	BA	3055	1/1	0.96	0.66	47,47,47,47	0
60	MG	AA	1604	1/1	0.96	0.39	61,61,61,61	0
60	MG	CA	1735	1/1	0.96	0.16	55,55,55,55	1
60	MG	BA	3009	1/1	0.96	0.65	47,47,47,47	0
60	MG	DA	3070	1/1	0.96	0.35	48,48,48,48	0
60	MG	CA	1619	1/1	0.96	0.25	55,55,55,55	0
60	MG	DA	3304	1/1	0.96	0.70	55,55,55,55	0
60	MG	DA	3075	1/1	0.96	0.52	47,47,47,47	0
60	MG	BA	3116	1/1	0.96	0.39	47,47,47,47	0
60	MG	CA	1657	1/1	0.96	0.28	54,54,54,54	0
60	MG	B3	101	1/1	0.96	0.56	58,58,58,58	0
60	MG	DA	3147	1/1	0.96	0.42	47,47,47,47	0
60	MG	DA	3080	1/1	0.96	0.55	49,49,49,49	0
60	MG	DA	3311	1/1	0.96	0.64	55,55,55,55	0
60	MG	BA	3240	1/1	0.96	0.60	58,58,58,58	1
60	MG	BA	3267	1/1	0.96	0.24	54,54,54,54	0
60	MG	BA	3198	1/1	0.96	0.69	53,53,53,53	0
60	MG	DA	3154	1/1	0.96	0.25	53,53,53,53	0
60	MG	CA	1701	1/1	0.96	0.45	51,51,51,51	0
60	MG	BB	202	1/1	0.96	0.44	55,55,55,55	0
60	MG	BA	3136	1/1	0.96	0.79	50,50,50,50	0
60	MG	CA	1628	1/1	0.96	0.31	56,56,56,56	0
60	MG	BA	3043	1/1	0.96	0.79	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	3297	1/1	0.96	0.49	55,55,55,55	0
60	MG	DA	3163	1/1	0.96	0.64	50,50,50,50	0
60	MG	BA	3158	1/1	0.96	0.86	49,49,49,49	0
60	MG	DA	3244	1/1	0.96	0.49	47,47,47,47	0
60	MG	DA	3094	1/1	0.96	0.45	51,51,51,51	0
60	MG	BA	3300	1/1	0.96	0.32	55,55,55,55	0
60	MG	CA	1669	1/1	0.96	0.30	47,47,47,47	0
60	MG	DA	3168	1/1	0.96	0.19	53,53,53,53	0
60	MG	DA	3099	1/1	0.96	0.36	54,54,54,54	0
60	MG	AA	1680	1/1	0.96	0.39	49,49,49,49	0
60	MG	BA	3302	1/1	0.96	0.63	55,55,55,55	0
60	MG	CA	1714	1/1	0.96	0.47	64,64,64,64	0
60	MG	DA	3175	1/1	0.96	0.46	56,56,56,56	0
60	MG	DA	3104	1/1	0.96	0.42	50,50,50,50	0
60	MG	BA	3066	1/1	0.96	0.94	50,50,50,50	0
60	MG	AA	1669	1/1	0.96	0.29	47,47,47,47	0
60	MG	BA	3305	1/1	0.96	0.71	55,55,55,55	0
60	MG	DA	3339	1/1	0.96	0.38	55,55,55,55	0
60	MG	DA	3341	1/1	0.96	0.49	55,55,55,55	0
60	MG	DA	3342	1/1	0.96	0.27	55,55,55,55	0
60	MG	DA	3036	1/1	0.96	0.40	55,55,55,55	0
60	MG	BA	3182	1/1	0.96	0.38	49,49,49,49	0
60	MG	DA	3039	1/1	0.96	0.38	51,51,51,51	0
60	MG	CA	1604	1/1	0.96	0.21	50,50,50,50	0
60	MG	DA	3114	1/1	0.96	0.38	47,47,47,47	0
60	MG	DA	3265	1/1	0.96	0.61	53,53,53,53	0
60	MG	DA	3186	1/1	0.96	0.54	50,50,50,50	0
60	MG	DA	3042	1/1	0.96	0.78	47,47,47,47	0
60	MG	DA	3189	1/1	0.96	0.17	57,57,57,57	0
60	MG	BA	3163	1/1	0.96	0.40	53,53,53,53	0
60	MG	BA	3086	1/1	0.96	0.54	48,48,48,48	0
60	MG	DB	202	1/1	0.96	0.74	55,55,55,55	0
60	MG	DA	3271	1/1	0.96	0.48	51,51,51,51	0
60	MG	DA	3192	1/1	0.96	0.20	61,61,61,61	1
60	MG	BA	3279	1/1	0.96	0.19	55,55,55,55	0
60	MG	AV	101	1/1	0.96	0.41	49,49,49,49	0
60	MG	CW	102	1/1	0.96	0.29	60,60,60,60	0
60	MG	CA	1724	1/1	0.96	0.14	57,57,57,57	1
60	MG	DA	3278	1/1	0.96	0.66	51,51,51,51	0
60	MG	DA	3052	1/1	0.96	0.56	51,51,51,51	0
60	MG	BA	3048	1/1	0.96	0.59	47,47,47,47	0
60	MG	DA	3126	1/1	0.96	0.80	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	3108	1/1	0.96	0.71	52,52,52,52	0
60	MG	DA	3203	1/1	0.96	0.46	47,47,47,47	0
60	MG	BA	3052	1/1	0.97	0.53	47,47,47,47	0
60	MG	BA	3145	1/1	0.97	0.29	47,47,47,47	0
60	MG	BA	3114	1/1	0.97	0.25	48,48,48,48	0
60	MG	DA	3038	1/1	0.97	0.58	47,47,47,47	0
60	MG	BA	3184	1/1	0.97	0.43	47,47,47,47	0
60	MG	AA	1654	1/1	0.97	0.15	53,53,53,53	0
60	MG	DA	3121	1/1	0.97	0.41	50,50,50,50	0
60	MG	DA	3041	1/1	0.97	0.34	47,47,47,47	0
60	MG	DA	3291	1/1	0.97	0.69	54,54,54,54	0
60	MG	CA	1752	1/1	0.97	0.19	55,55,55,55	1
60	MG	BA	3186	1/1	0.97	0.90	51,51,51,51	0
60	MG	BA	3008	1/1	0.97	0.41	55,55,55,55	0
60	MG	BA	3149	1/1	0.97	0.53	54,54,54,54	0
60	MG	BP	201	1/1	0.97	0.22	49,49,49,49	0
60	MG	BQ	201	1/1	0.97	0.79	55,55,55,55	0
60	MG	CA	1703	1/1	0.97	0.29	47,47,47,47	0
60	MG	DA	3051	1/1	0.97	0.19	47,47,47,47	0
60	MG	DA	3131	1/1	0.97	0.20	48,48,48,48	0
60	MG	CA	1704	1/1	0.97	0.64	62,62,62,62	0
60	MG	DA	3053	1/1	0.97	0.61	47,47,47,47	0
60	MG	CV	101	1/1	0.97	0.58	49,49,49,49	0
60	MG	DA	3218	1/1	0.97	0.53	51,51,51,51	0
60	MG	BA	3085	1/1	0.97	0.17	47,47,47,47	0
60	MG	AA	1614	1/1	0.97	0.07	52,52,52,52	0
60	MG	DA	3137	1/1	0.97	0.65	50,50,50,50	0
60	MG	BA	3087	1/1	0.97	0.32	49,49,49,49	0
60	MG	BA	3089	1/1	0.97	0.59	48,48,48,48	0
60	MG	DA	3060	1/1	0.97	0.47	48,48,48,48	0
60	MG	CA	1603	1/1	0.97	0.35	61,61,61,61	0
60	MG	BA	3121	1/1	0.97	0.27	50,50,50,50	0
60	MG	BA	3278	1/1	0.97	0.29	51,51,51,51	0
60	MG	BA	3155	1/1	0.97	0.30	51,51,51,51	0
60	MG	AA	1722	1/1	0.97	0.27	55,55,55,55	0
60	MG	BA	3031	1/1	0.97	0.26	50,50,50,50	0
60	MG	BA	3197	1/1	0.97	0.45	58,58,58,58	0
60	MG	BA	3093	1/1	0.97	0.42	51,51,51,51	0
60	MG	BA	3160	1/1	0.97	0.31	47,47,47,47	0
60	MG	DA	3320	1/1	0.97	0.20	55,55,55,55	0
60	MG	DA	3234	1/1	0.97	0.54	47,47,47,47	0
60	MG	BA	3125	1/1	0.97	0.71	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DA	3236	1/1	0.97	0.87	52,52,52,52	0
60	MG	DA	3074	1/1	0.97	0.42	52,52,52,52	0
60	MG	BA	3060	1/1	0.97	0.57	47,47,47,47	0
60	MG	DA	3156	1/1	0.97	0.34	51,51,51,51	0
60	MG	BA	3202	1/1	0.97	0.35	47,47,47,47	0
60	MG	DA	3241	1/1	0.97	0.10	55,55,55,55	0
60	MG	BA	3203	1/1	0.97	0.37	52,52,52,52	0
60	MG	DA	3243	1/1	0.97	0.13	61,61,61,61	1
60	MG	BA	3061	1/1	0.97	0.45	48,48,48,48	0
60	MG	BA	3011	1/1	0.97	0.30	47,47,47,47	0
60	MG	AA	1631	1/1	0.97	0.23	47,47,47,47	0
60	MG	DA	3082	1/1	0.97	0.74	47,47,47,47	0
60	MG	BA	3130	1/1	0.97	0.19	48,48,48,48	0
60	MG	BA	3014	1/1	0.97	0.58	53,53,53,53	0
60	MG	AA	1626	1/1	0.97	0.30	53,53,53,53	0
60	MG	CA	1728	1/1	0.97	0.52	55,55,55,55	0
60	MG	CA	1623	1/1	0.97	0.41	48,48,48,48	0
60	MG	DA	3089	1/1	0.97	0.64	48,48,48,48	0
60	MG	BA	3017	1/1	0.97	0.43	52,52,52,52	0
60	MG	BA	3069	1/1	0.97	0.35	48,48,48,48	0
60	MG	DA	3171	1/1	0.97	0.70	51,51,51,51	0
60	MG	DA	3345	1/1	0.97	0.37	55,55,55,55	0
60	MG	BA	3252	1/1	0.97	0.34	49,49,49,49	0
60	MG	BA	3299	1/1	0.97	0.42	55,55,55,55	0
60	MG	DA	3016	1/1	0.97	0.50	47,47,47,47	0
60	MG	DA	3096	1/1	0.97	0.44	60,60,60,60	0
60	MG	BA	3040	1/1	0.97	0.60	47,47,47,47	0
60	MG	CA	1680	1/1	0.97	0.30	49,49,49,49	0
60	MG	BA	3018	1/1	0.97	0.54	54,54,54,54	0
60	MG	DA	3021	1/1	0.97	0.53	47,47,47,47	0
60	MG	BA	3347	1/1	0.97	0.31	55,55,55,55	0
60	MG	DA	3102	1/1	0.97	0.74	47,47,47,47	0
60	MG	AA	1607	1/1	0.97	0.42	58,58,58,58	0
60	MG	DA	3184	1/1	0.97	0.50	49,49,49,49	0
60	MG	BA	3020	1/1	0.97	0.57	47,47,47,47	0
60	MG	AA	1619	1/1	0.97	0.60	49,49,49,49	0
60	MG	DA	3028	1/1	0.97	0.37	50,50,50,50	0
60	MG	DA	3107	1/1	0.97	0.60	51,51,51,51	0
60	MG	AA	1605	1/1	0.97	0.11	50,50,50,50	0
60	MG	AA	1661	1/1	0.97	0.48	52,52,52,52	0
60	MG	BA	3049	1/1	0.97	0.66	47,47,47,47	0
60	MG	BA	3051	1/1	0.97	0.35	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	DU	201	1/1	0.97	0.51	48,48,48,48	0
60	MG	BA	3264	1/1	0.97	0.58	53,53,53,53	0
60	MG	DA	3195	1/1	0.97	0.25	53,53,53,53	0
60	MG	DA	3020	1/1	0.98	0.54	47,47,47,47	0
60	MG	BA	3022	1/1	0.98	0.99	47,47,47,47	0
60	MG	DA	3108	1/1	0.98	0.21	51,51,51,51	0
60	MG	DA	3022	1/1	0.98	0.22	47,47,47,47	0
60	MG	DA	3023	1/1	0.98	0.80	47,47,47,47	0
60	MG	CA	1640	1/1	0.98	0.73	47,47,47,47	0
60	MG	BA	3164	1/1	0.98	0.25	47,47,47,47	0
60	MG	AA	1702	1/1	0.98	0.34	47,47,47,47	0
60	MG	AA	1678	1/1	0.98	0.05	49,49,49,49	0
60	MG	BA	3255	1/1	0.98	0.30	55,55,55,55	0
60	MG	DA	3029	1/1	0.98	0.32	52,52,52,52	0
60	MG	DA	3071	1/1	0.98	0.30	50,50,50,50	0
60	MG	DA	3072	1/1	0.98	0.24	47,47,47,47	0
60	MG	DA	3119	1/1	0.98	0.50	49,49,49,49	0
60	MG	BA	3046	1/1	0.98	0.43	47,47,47,47	0
60	MG	BA	3081	1/1	0.98	0.36	47,47,47,47	0
60	MG	DA	3172	1/1	0.98	0.50	50,50,50,50	0
60	MG	DA	3277	1/1	0.98	0.78	57,57,57,57	0
60	MG	AA	1749	1/1	0.98	0.35	55,55,55,55	0
60	MG	BA	3308	1/1	0.98	0.51	55,55,55,55	0
60	MG	BA	3083	1/1	0.98	0.51	47,47,47,47	0
60	MG	DA	3078	1/1	0.98	0.86	51,51,51,51	0
60	MG	D1	101	1/1	0.98	0.41	55,55,55,55	0
60	MG	BA	3035	1/1	0.98	0.38	55,55,55,55	0
60	MG	AA	1609	1/1	0.98	0.25	52,52,52,52	0
60	MG	BA	3262	1/1	0.98	0.18	63,63,63,63	1
60	MG	CA	1682	1/1	0.98	0.11	53,53,53,53	0
60	MG	DA	3084	1/1	0.98	0.36	47,47,47,47	0
60	MG	CA	1653	1/1	0.98	0.07	53,53,53,53	0
60	MG	DA	3289	1/1	0.98	0.45	54,54,54,54	0
60	MG	CA	1746	1/1	0.98	0.23	55,55,55,55	0
60	MG	BA	3050	1/1	0.98	0.33	47,47,47,47	0
60	MG	BA	3068	1/1	0.98	0.49	47,47,47,47	0
60	MG	DA	3187	1/1	0.98	0.53	51,51,51,51	0
60	MG	DA	3044	1/1	0.98	0.54	47,47,47,47	0
60	MG	BA	3110	1/1	0.98	0.41	49,49,49,49	0
60	MG	BA	3037	1/1	0.98	0.40	47,47,47,47	0
60	MG	BA	3090	1/1	0.98	0.46	48,48,48,48	0
60	MG	DA	3048	1/1	0.98	0.25	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	MG	BA	3070	1/1	0.98	0.39	50,50,50,50	0
60	MG	DA	3246	1/1	0.98	0.24	60,60,60,60	0
60	MG	DA	3095	1/1	0.98	0.75	47,47,47,47	0
60	MG	DA	3248	1/1	0.98	0.15	59,59,59,59	1
60	MG	BA	3293	1/1	0.98	0.45	55,55,55,55	1
60	MG	BA	3038	1/1	0.98	0.45	51,51,51,51	0
60	MG	B5	101	1/1	0.98	0.35	49,49,49,49	0
60	MG	BA	3013	1/1	0.98	0.40	47,47,47,47	0
60	MG	CA	1608	1/1	0.98	0.38	52,52,52,52	0
60	MG	DA	3148	1/1	0.98	0.38	51,51,51,51	0
60	MG	BA	3041	1/1	0.98	0.65	47,47,47,47	0
60	MG	CA	1696	1/1	0.98	0.10	62,62,62,62	0
60	MG	BA	3056	1/1	0.98	0.61	47,47,47,47	0
60	MG	DA	3058	1/1	0.98	0.62	47,47,47,47	0
60	MG	BA	3021	1/1	0.98	0.40	47,47,47,47	0
61	ZN	AD	301	1/1	0.98	0.20	52,52,52,52	0
61	ZN	AN	101	1/1	0.98	0.10	60,60,60,60	1
60	MG	BA	3028	1/1	0.99	0.45	52,52,52,52	0
60	MG	DA	3340	1/1	0.99	0.38	55,55,55,55	0
60	MG	BA	3157	1/1	0.99	0.11	53,53,53,53	0
60	MG	DA	3014	1/1	0.99	0.31	47,47,47,47	0
60	MG	DA	3207	1/1	0.99	0.48	47,47,47,47	0
60	MG	DA	3015	1/1	0.99	0.54	53,53,53,53	0
60	MG	DA	3155	1/1	0.99	0.40	48,48,48,48	0
60	MG	BA	3088	1/1	0.99	0.57	48,48,48,48	0
60	MG	BA	3063	1/1	0.99	0.27	56,56,56,56	0
60	MG	BA	3059	1/1	0.99	0.31	48,48,48,48	0
60	MG	DA	3198	1/1	0.99	0.49	58,58,58,58	0
60	MG	DR	201	1/1	0.99	0.33	47,47,47,47	0
60	MG	DA	3069	1/1	0.99	0.33	47,47,47,47	0
60	MG	AA	1751	1/1	0.99	0.07	55,55,55,55	0
60	MG	BA	3098	1/1	0.99	0.28	54,54,54,54	0
60	MG	BA	3015	1/1	0.99	0.48	47,47,47,47	0
60	MG	DA	3150	1/1	0.99	0.60	54,54,54,54	0
61	ZN	B9	101	1/1	0.99	0.06	55,55,55,55	0
61	ZN	CD	301	1/1	0.99	0.27	52,52,52,52	0
61	ZN	CN	102	1/1	1.00	0.12	60,60,60,60	0
61	ZN	D9	101	1/1	1.00	0.11	55,55,55,55	1

6.5 Other polymers (i)

There are no such residues in this entry.