wwPDB X-ray Structure Validation Summary Report ⓘ

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)

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

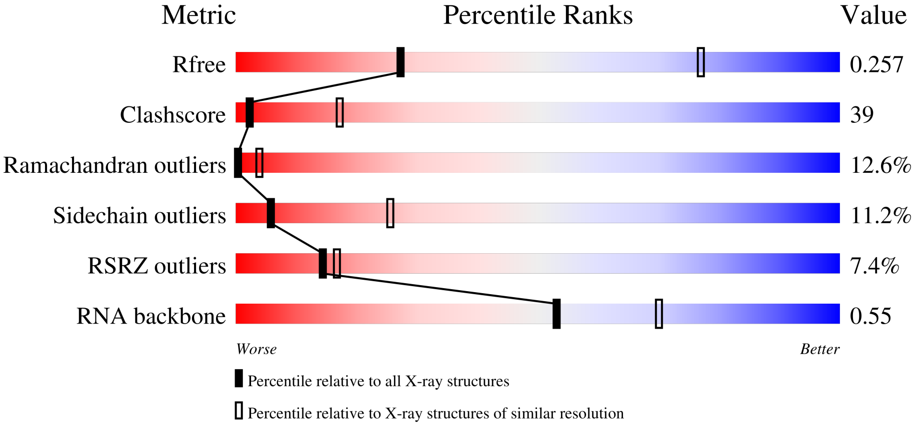
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

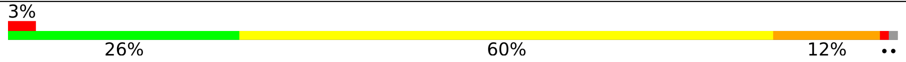
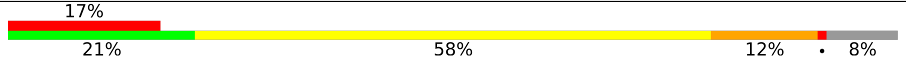
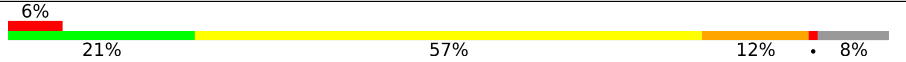
The reported resolution of this entry is 3.45 Å.

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	
1	CA	1522	
2	AB	256	
2	CB	256	

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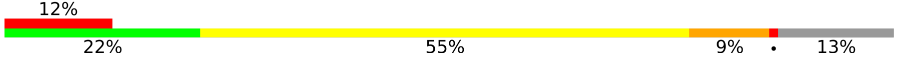
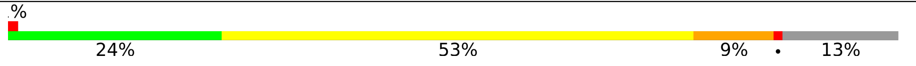
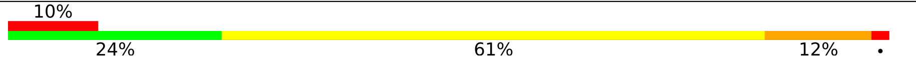
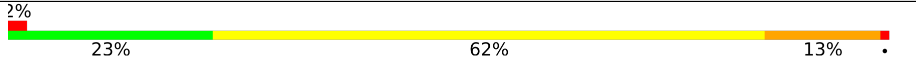
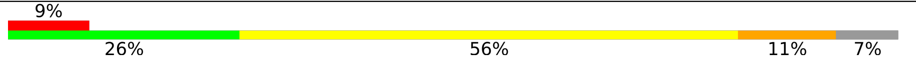
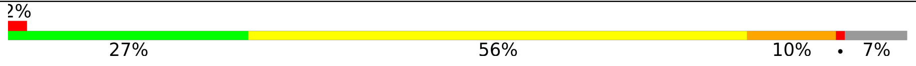
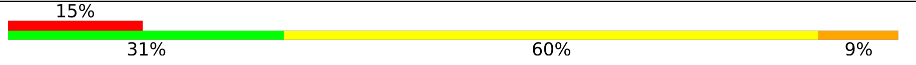
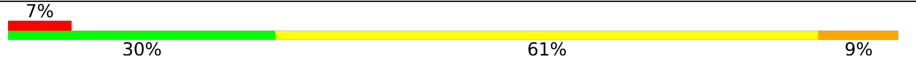
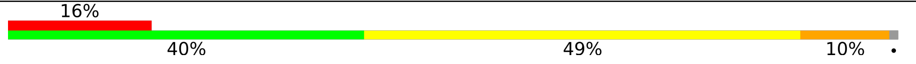
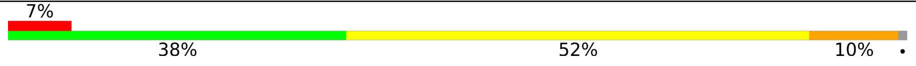
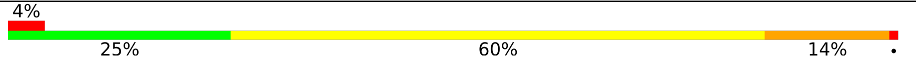
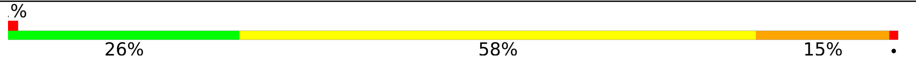
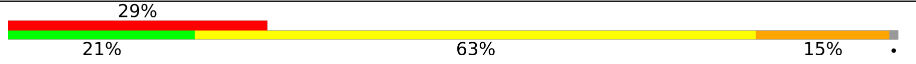
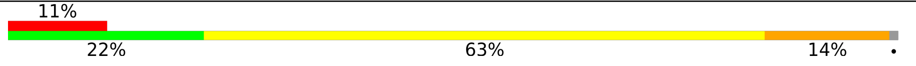
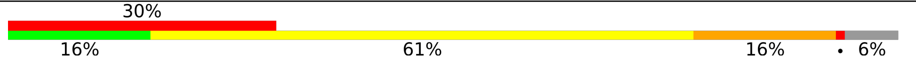
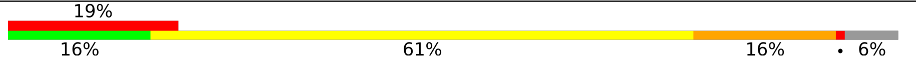
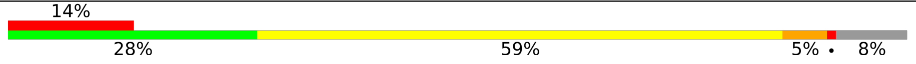
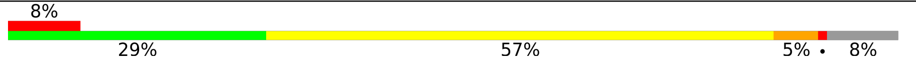
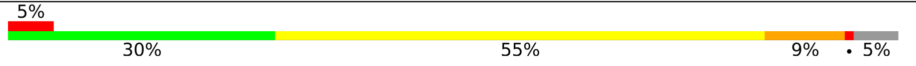
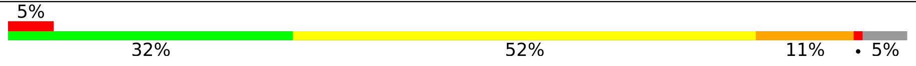
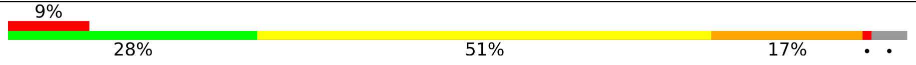
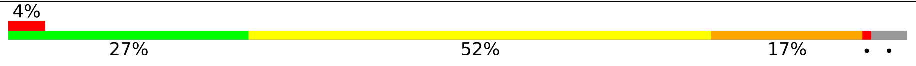
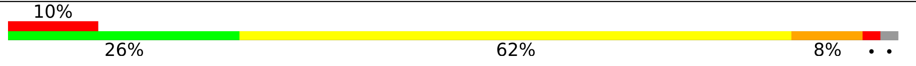
Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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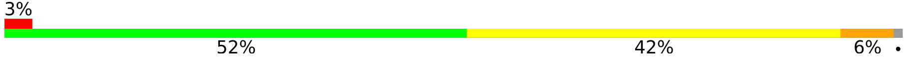
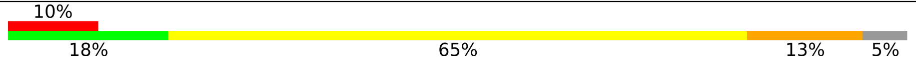
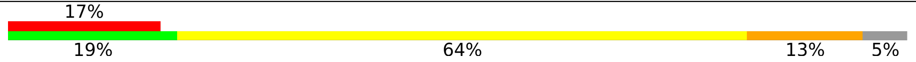
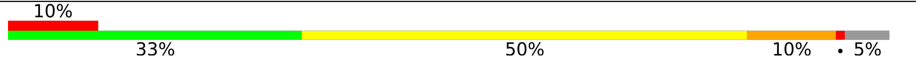
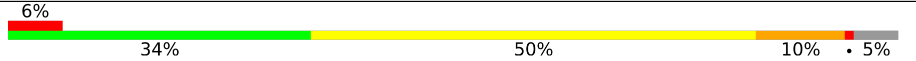
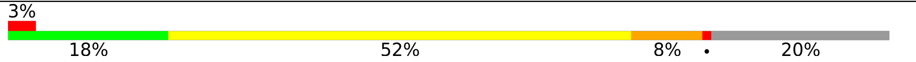
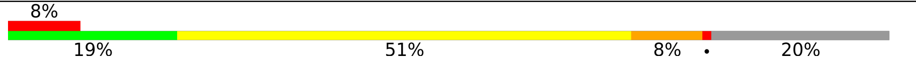
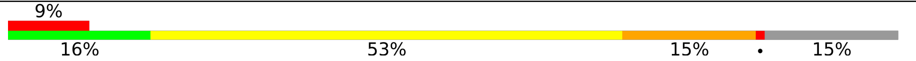
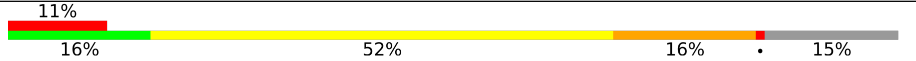
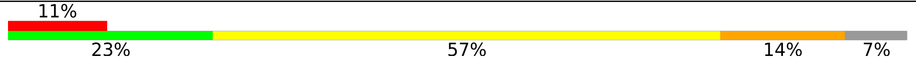
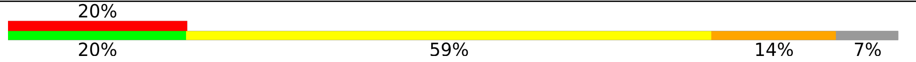
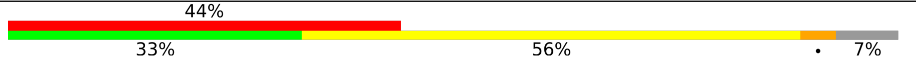
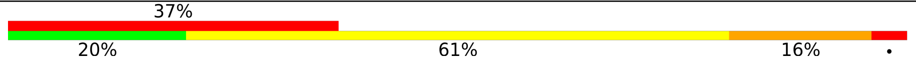
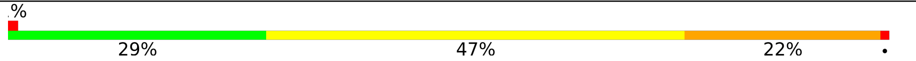
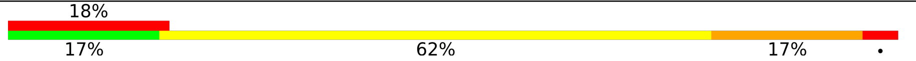
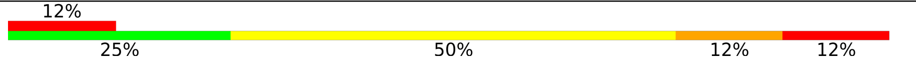
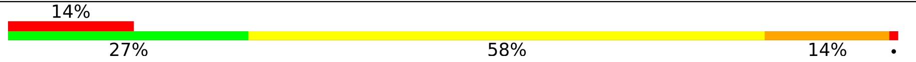
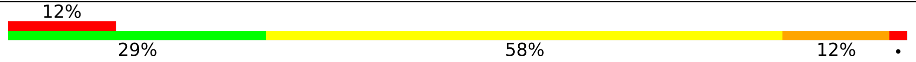
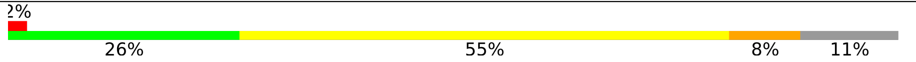
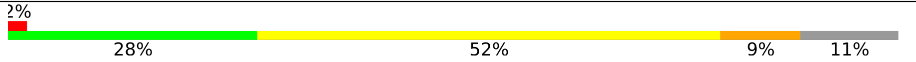
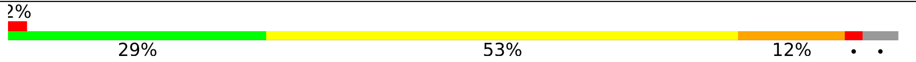
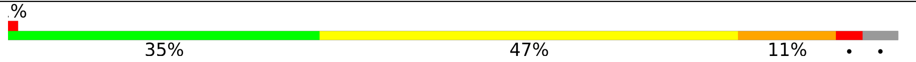
Mol	Chain	Length	Quality of chain
15	CO	89	 3% 52% 42% 6% •
16	AP	88	 10% 18% 65% 13% 5%
16	CP	88	 17% 19% 64% 13% 5%
17	AQ	105	 10% 33% 50% 10% • 5%
17	CQ	105	 6% 34% 50% 10% • 5%
18	AR	88	 3% 18% 52% 8% • 20%
18	CR	88	 8% 19% 51% 8% • 20%
19	AS	93	 9% 16% 53% 15% • 15%
19	CS	93	 11% 16% 52% 16% • 15%
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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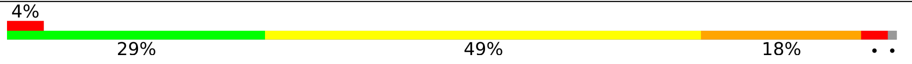
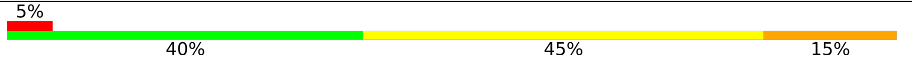
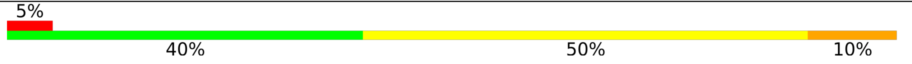
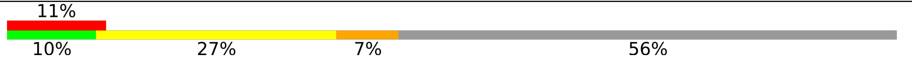
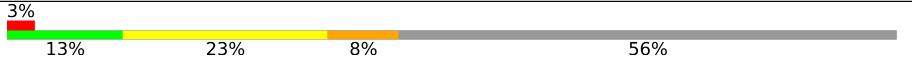
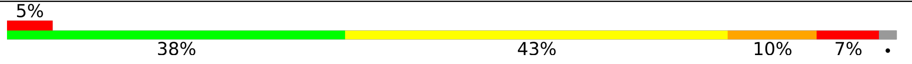
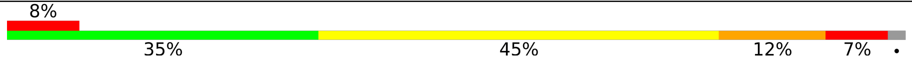
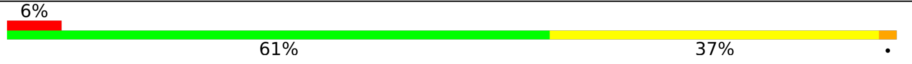
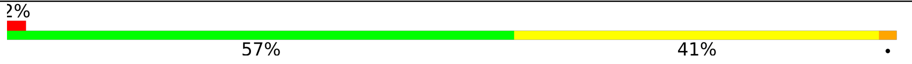
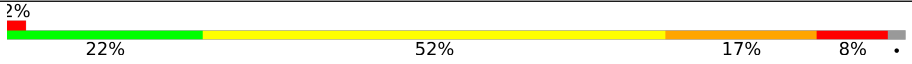
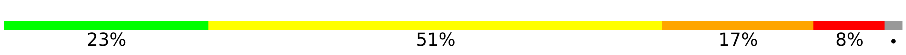
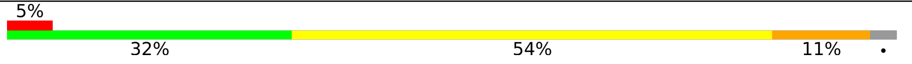
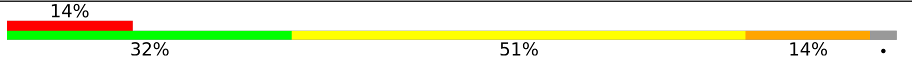
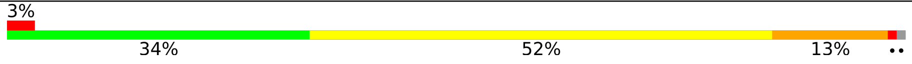
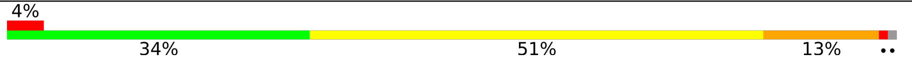
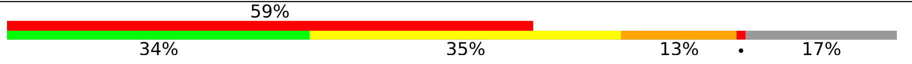
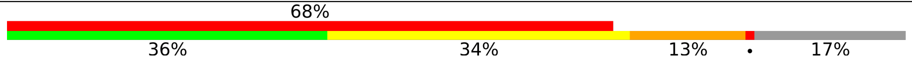
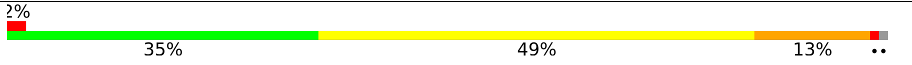
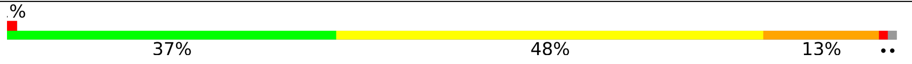
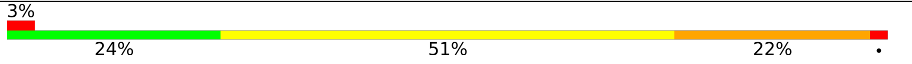
Mol	Chain	Length	Quality of chain
27	B2	72	 7% 17% 54% 28% •
27	D2	72	 4% 29% 49% 18% • •
28	B3	60	 5% 40% 45% 15%
28	D3	60	 5% 40% 50% 10%
29	B4	71	 11% 10% 27% 7% 56%
29	D4	71	 3% 13% 23% 8% 56%
30	B5	60	 5% 38% 43% 10% 7% •
30	D5	60	 8% 35% 45% 12% 7% •
31	B6	54	 13% 43% 33% 7% 17%
31	D6	54	 4% 44% 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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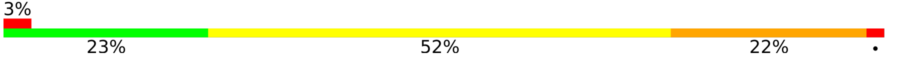
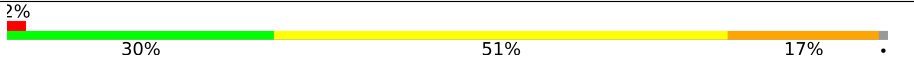
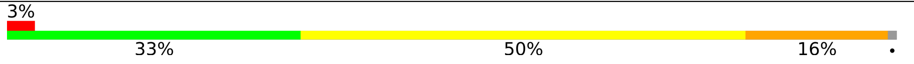
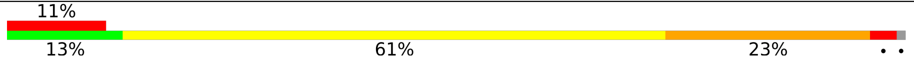
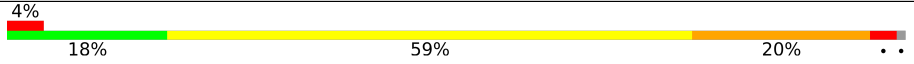
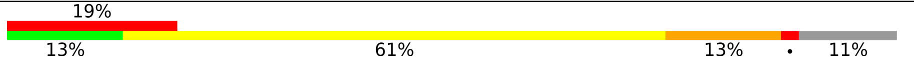
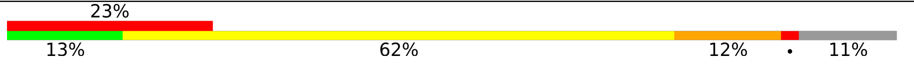
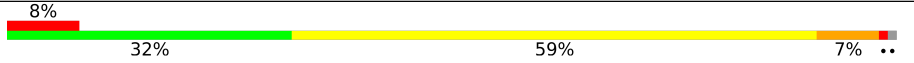
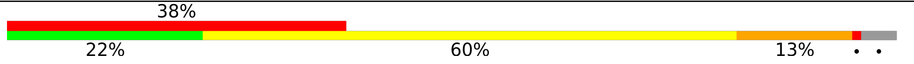
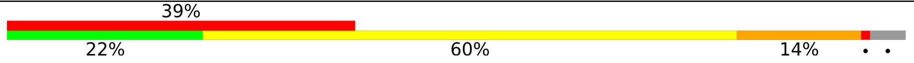
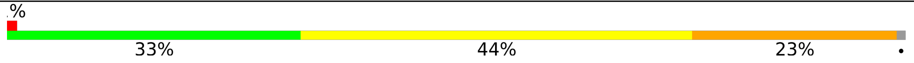
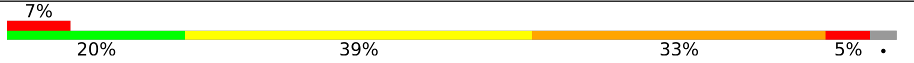
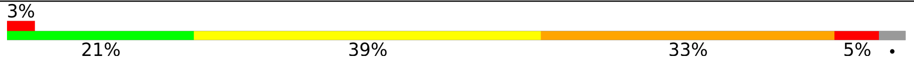
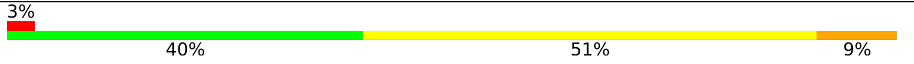
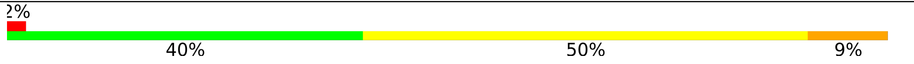
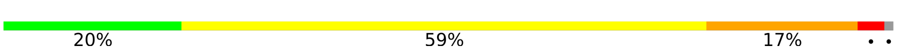
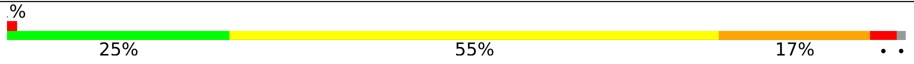
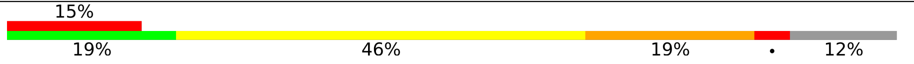
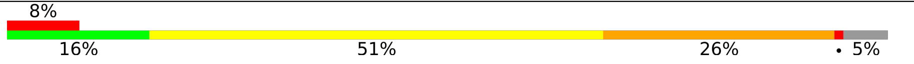
Mol	Chain	Length	Quality of chain
39	DE	206	 3% 23% 52% 22% •
40	BF	210	 2% 30% 51% 17% •
40	DF	210	 3% 33% 50% 16% •
41	BG	182	 11% 13% 61% 23% • •
41	DG	182	 4% 18% 59% 20% • •
42	BH	180	 19% 13% 61% 13% • 11%
42	DH	180	 23% 13% 62% 12% • 11%
43	BI	148	 8% 32% 59% 7% ••
44	BJ	130	 65% 35%
44	DJ	130	 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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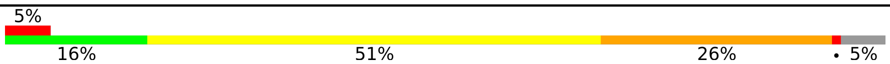
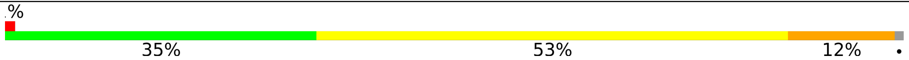
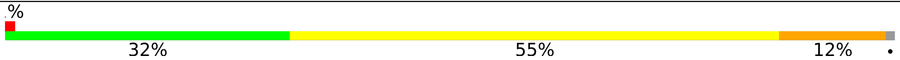
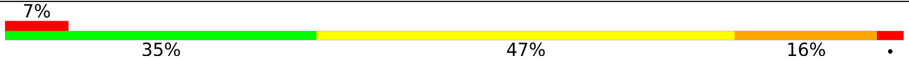
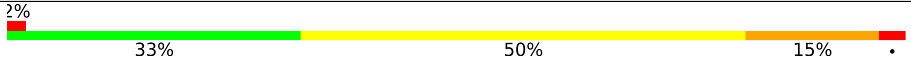
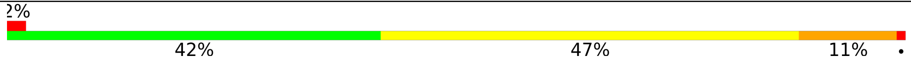
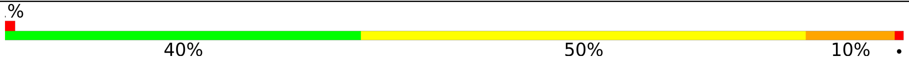
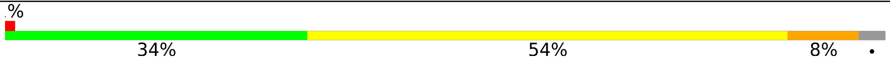
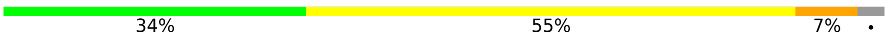
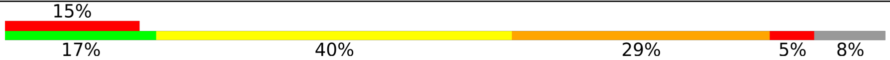
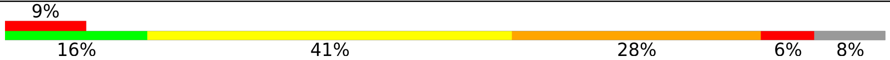
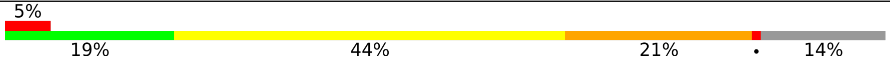
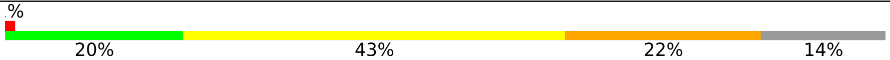
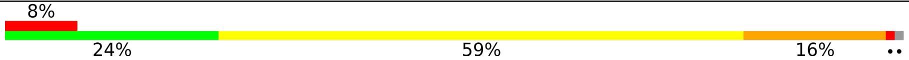
Mol	Chain	Length	Quality of chain
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	
59	DI	148	

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total 1011	C 639	N 198	O 174	0	0	0
9	CI	127	Total 1011	C 639	N 198	O 174	0	0	0

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

Continued on next page...

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	126	Total 976	C 614	N 197	O 164	S 1	0	0	1
12	CL	126	Total 976	C 614	N 197	O 164	S 1	0	0	1

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	121	Total 956	C 591	N 198	O 165	S 2	0	0	1
13	CM	121	Total 956	C 591	N 198	O 165	S 2	0	0	1

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

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total 630	C 403	N 115	O 110	S 2	0	0	1
19	CS	79	Total 630	C 403	N 115	O 110	S 2	0	0	1

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total 763	C 470	N 162	O 129	S 2	0	0	0
20	CT	99	Total 763	C 470	N 162	O 129	S 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
25	B0	76	Total C N O S 607 376 128 102 1	0	0	0
25	D0	76	Total C N O S 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
26	B1	94	Total C N O S 732 460 146 125 1	0	0	1
26	D1	94	Total C N O S 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
27	B2	71	Total C N O S 598 370 121 106 1	0	0	0
27	D2	71	Total C N O S 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
28	B3	60	Total C N O S 468 298 91 78 1	0	0	1
28	D3	60	Total C N O S 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
29	B4	31	Total C N O S 226 142 37 43 4	0	0	1
29	D4	31	Total C N O S 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
30	B5	59	Total C N O S 459 288 90 76 5	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
36	BB	119	Total C N O P 2551 1136 471 826 118	0	0	0
36	DB	119	Total C N O P 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
37	BC	191	Total C N O 1142 691 221 230	0	0	1
37	DC	191	Total C N O 1142 691 221 230	0	0	1

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
38	BD	272	Total C N O S 2105 1329 417 356 3	0	0	1
38	DD	272	Total C N O S 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
39	BE	205	Total C N O S 1564 988 300 270 6	0	0	1
39	DE	205	Total C N O S 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
40	BF	208	Total C N O S 1624 1035 304 282 3	0	0	1
40	DF	208	Total C N O S 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
41	BG	181	Total 1474	C 942	N 268	O 260	S 4	0	0	0
41	DG	181	Total 1474	C 942	N 268	O 260	S 4	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
52	BT	138	Total C N O S 1142 710 235 196 1	0	0	1
52	DT	138	Total C N O S 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
53	BU	117	Total C N O S 958 604 202 151 1	0	0	0
53	DU	117	Total C N O S 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
54	BV	101	Total C N O S 779 501 142 135 1	0	0	0
54	DV	101	Total C N O S 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
55	BW	113	Total C N O S 896 563 176 155 2	0	0	0
55	DW	113	Total C N O S 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
56	BX	93	Total C N O 726 471 132 123	0	0	1
56	DX	93	Total C N O 726 471 132 123	0	0	1

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
57	DY	101	Total C N O S 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
58	BZ	177	Total C N O S 1404 897 253 252 2	0	0	1
58	DZ	177	Total C N O S 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
59	DI	146	Total C N O S 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
60	AA	157	Total Mg 157 157	0	0
60	AE	1	Total Mg 1 1	0	0
60	AL	1	Total Mg 1 1	0	0
60	AM	1	Total Mg 1 1	0	0
60	AV	7	Total Mg 7 7	0	0
60	AW	5	Total Mg 5 5	0	0
60	AY	1	Total Mg 1 1	0	0
60	B1	1	Total Mg 1 1	0	0
60	B3	1	Total Mg 1 1	0	0
60	B5	2	Total Mg 2 2	0	0
60	B7	2	Total Mg 2 2	0	0

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

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

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

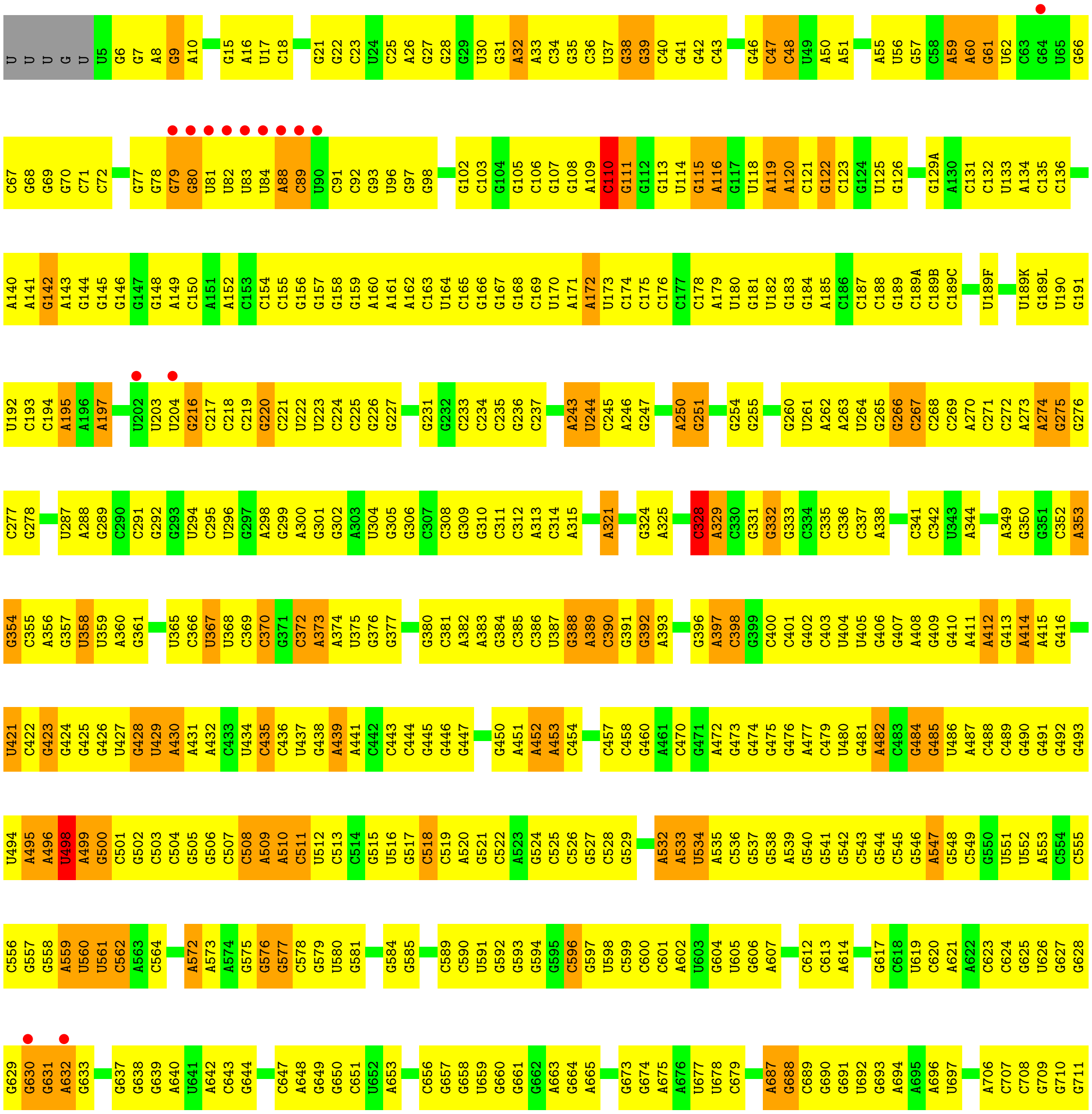
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AD	1	Total Zn 1 1	0	0
61	AN	1	Total Zn 1 1	0	0
61	B9	1	Total Zn 1 1	0	0
61	CD	1	Total Zn 1 1	0	0
61	CN	1	Total Zn 1 1	0	0
61	D9	1	Total Zn 1 1	0	0

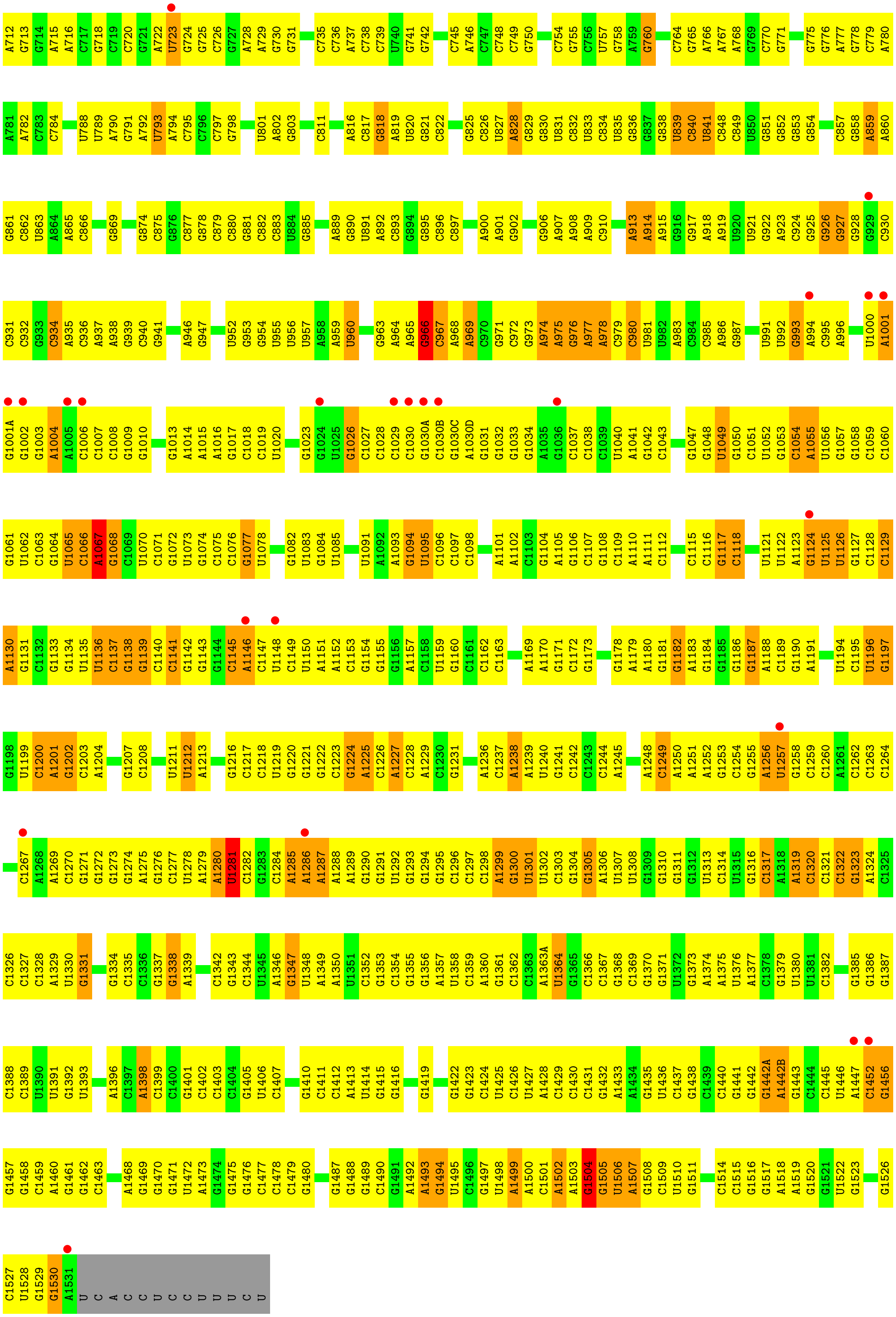
3 Residue-property plots ⓘ

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

- Molecule 1: 16S ribosomal RNA

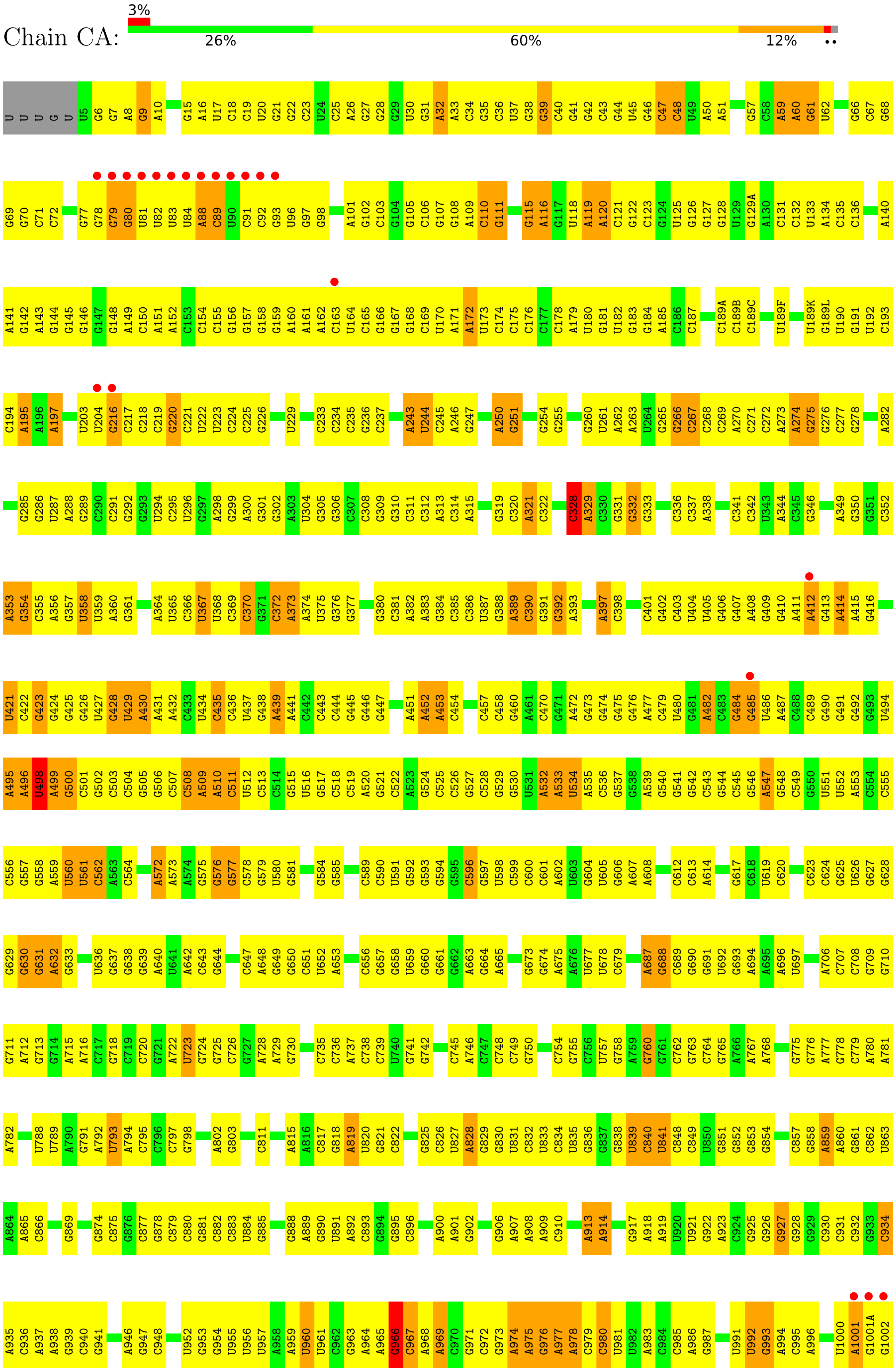
Chain AA:

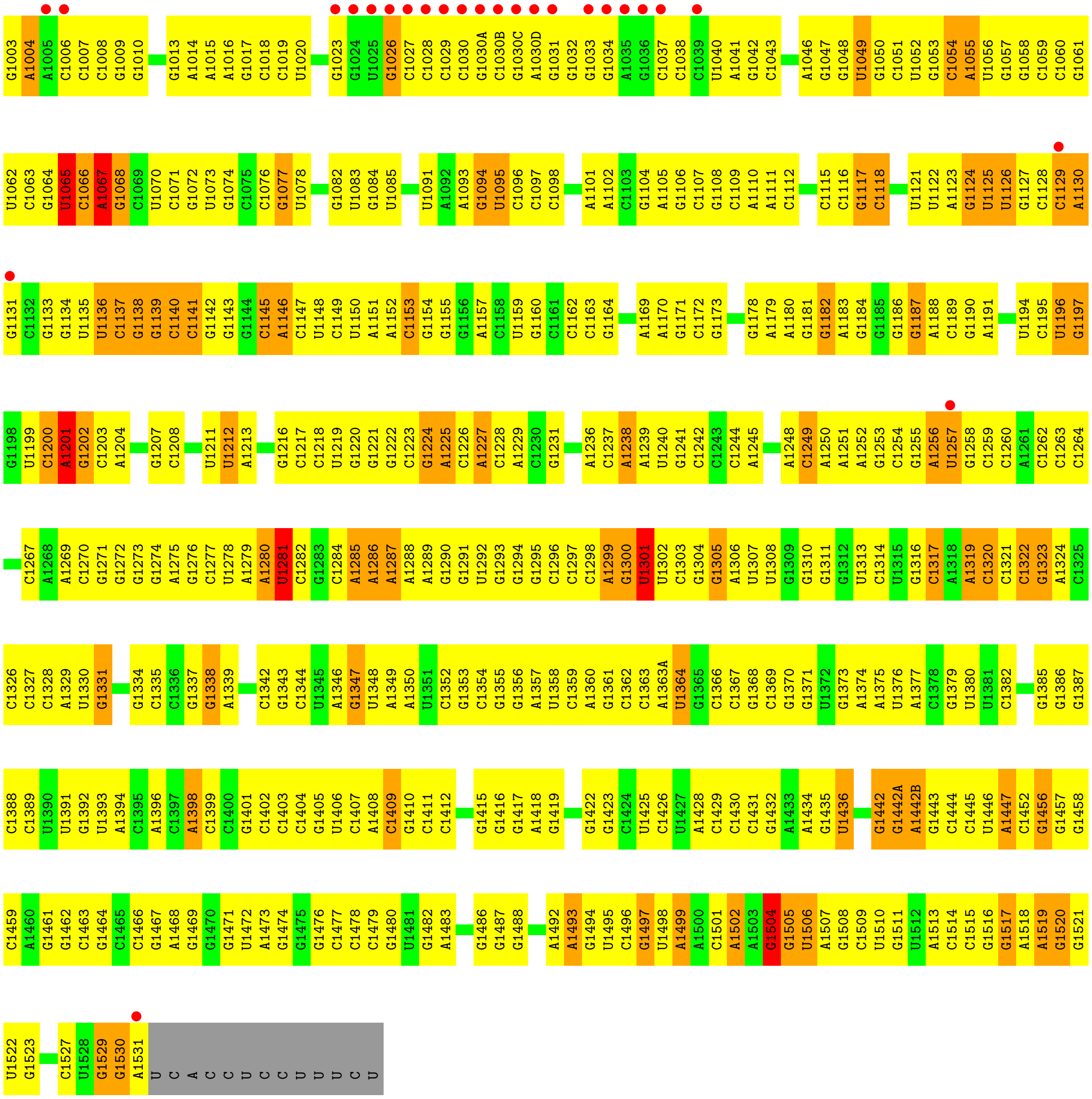




- Molecule 1: 16S ribosomal RNA

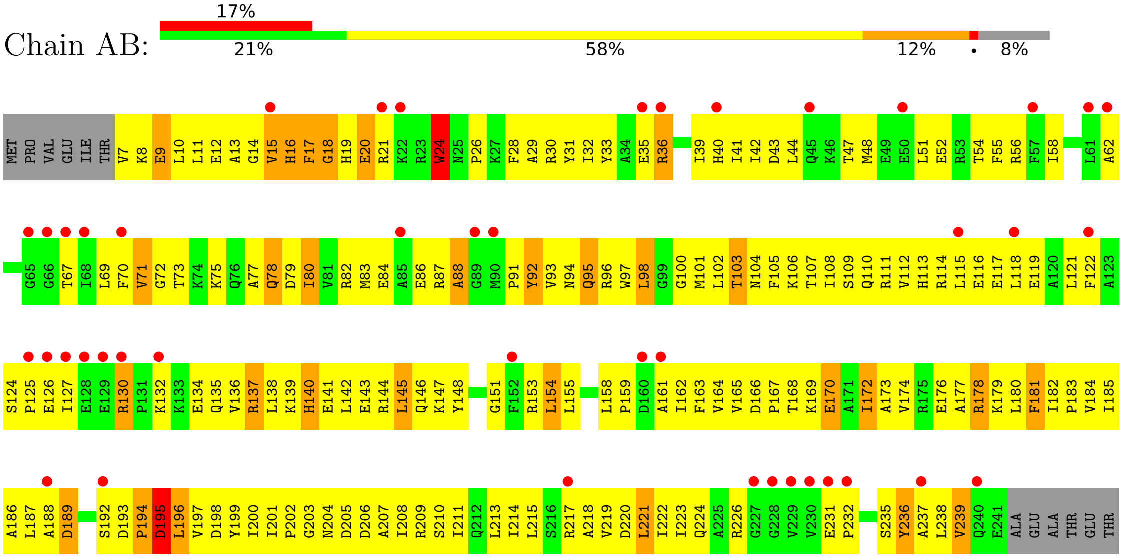
Chain CA:


3%
26%
60%
12%
••
U U U G U U5 G6 G7 A8 G9 A10 G15 A16 U17 C18 C19 U20 G21 G22 C23 U24 C25 A26 G27 G28 G29 U30 G31 A32 A33 C34 G35 C36 U37 G38 G39 C40 G41 G42 C43 G44 U45 G46 C47 C48 U49 A50 A51 G57 C58 A59 A60 G61 U62 G66 C67 G68
G69 G70 C71 C72 G77 G78 G79 G80 U81 U82 U83 U84 A88 C89 U90 C91 C92 G93 U96 G97 G98 A101 G102 C103 G104 G105 C106 G107 G108 A109 C110 G111 G115 A116 G117 U118 A119 A120 C121 G122 C123 G124 U125 G126 G127 G128 U129 G129A A130 C131 U132 U133 A134 C135 C136 A140
A141 G142 A143 G144 G145 G146 G147 G148 A149 C150 A151 A152 C153 C154 C155 G156 G157 G158 G159 A160 A161 A162 C163 U164 C165 G166 G167 G168 C169 U170 A171 A172 U173 C174 C175 C176 C177 C178 A179 U180 G181 U182 G183 G184 A185 C186 C187 C189A C189B C189C U189F U189K G189L U190 G191 U192 C193
C194 A195 A196 A197 U203 U204 G216 C217 C218 C219 G220 C221 U222 U223 C224 C225 G226 U229 C233 C234 C235 G236 C237 A243 U244 C245 A246 G247 A250 G251 G254 G255 G260 U261 A262 A263 U264 G265 G266 C267 C268 C269 A270 C271 C272 A273 A274 G275 G276 C277 G278 A282
G285 G286 U287 A288 G289 C290 C291 G292 G293 U294 C295 U296 G297 A298 G299 A300 G301 G302 A303 U304 G305 G306 C307 C308 G309 G310 C311 C312 A313 C314 A315 G319 C320 A321 C322 C328 A329 C330 G331 G332 G333 C336 C337 A338 C341 C342 U343 A344 C345 G346 A349 G350 G351 C352
A353 G354 C355 A356 G357 U358 U359 A360 G361 A364 U365 C366 U367 U368 C369 C370 G371 C372 A373 A374 U375 G376 G377 G380 C381 A382 A383 G384 C385 C386 U387 G388 A389 C390 G391 G392 A393 A397 C398 C401 G402 C403 U404 U405 G406 G407 A408 G409 G410 A411 A412 G413 A414 A415 G416
U421 C422 G423 G424 G425 G426 U427 G428 U429 A430 A431 A432 C433 U434 C435 C436 U437 G438 A439 A441 C442 C443 C444 G445 G446 G447 A451 A452 A453 C454 C457 C458 G460 A461 C470 G471 A472 G473 G474 G475 G476 A477 C479 U480 G481 A482 C483 G484 G485 U486 A487 C488 C489 G490 G491 G492 G493 U494
A495 A496 U498 A499 G500 C501 G502 C503 G504 G505 G506 C507 C508 A509 A510 C511 U512 C513 C514 G515 U516 G517 C518 C519 A520 G521 C522 A523 G524 C525 G526 C527 G528 G529 G530 U531 A532 A533 U534 A535 C536 G537 G538 A539 G540 G541 C542 G543 G544 C545 G546 A547 G548 C549 G550 U551 U552 A553 C554 C555
C556 G557 G558 A559 U560 U561 C562 A563 C564 A572 A573 A574 G575 G576 G577 C578 G579 U580 G581 G584 G585 C589 C590 U591 G592 G593 G594 G595 C596 G597 U598 C599 C600 C601 A602 U603 G604 U605 G606 A607 A608 C612 C613 A614 G617 C618 U619 C620 C623 C624 G625 U626 G627 G628
G629 G630 G631 A632 G633 U636 G637 G638 G639 A640 U641 A642 C643 G644 C647 A648 G649 G650 C651 U652 A653 C656 G657 G658 U659 G660 G661 G662 A663 G664 A665 G673 G674 A675 A676 U677 U678 C679 A687 G688 C689 G690 G691 U692 G693 A694 A695 A696 U697 A706 C707 C708 G709 G710
G711 A712 G713 G714 A715 A716 C717 G718 C719 C720 G721 A722 U723 G724 G725 C726 G727 A728 A729 C730 C735 C736 A737 C738 C739 U740 G741 G742 C745 A746 C747 C748 C749 G750 C754 G755 C756 U757 G758 A759 G760 G761 C762 G763 C764 G765 A766 A767 A768 G775 C776 A777 G778 C779 A780 A781
A782 U788 U789 A790 G791 A792 U793 A794 C795 C796 C797 G798 A802 G803 C811 A815 A816 C817 G818 A819 U820 G821 C822 G825 C826 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 G837 C838 U839 C840 U841 C848 C849 U850 G851 G852 G853 G854 C857 G858 A859 A860 G861 C862 U863
A864 A865 C866 G869 G874 C875 G876 C877 G878 C879 C880 G881 C882 C883 U884 G885 G888 A889 G890 U891 A892 C893 G894 G895 C896 A900 A901 G902 G906 A907 A908 A909 C910 A913 A914 G917 A918 A919 U920 U921 G922 A923 C924 G925 G926 G927 G928 G929 C930 C931 C932 G933 C934
A935 C936 A937 A938 G939 C940 G941 A946 G947 C948 U952 G953 G954 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 G987 U991 U992 G993 A994 C995 A996 U1000 A1001 G1001A G1002

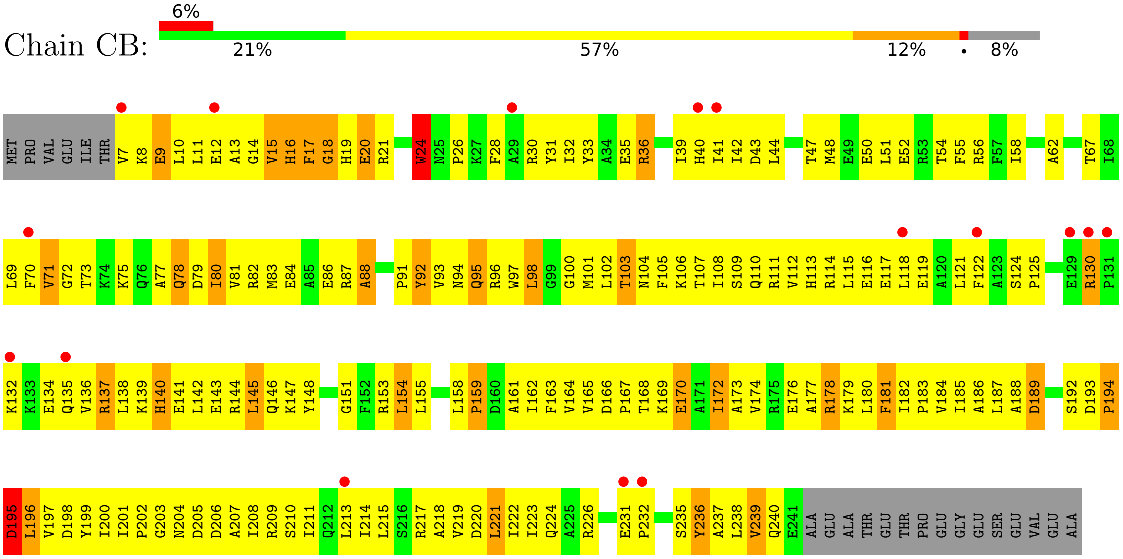


- Molecule 2: 30S RIBOSOMAL PROTEIN S2

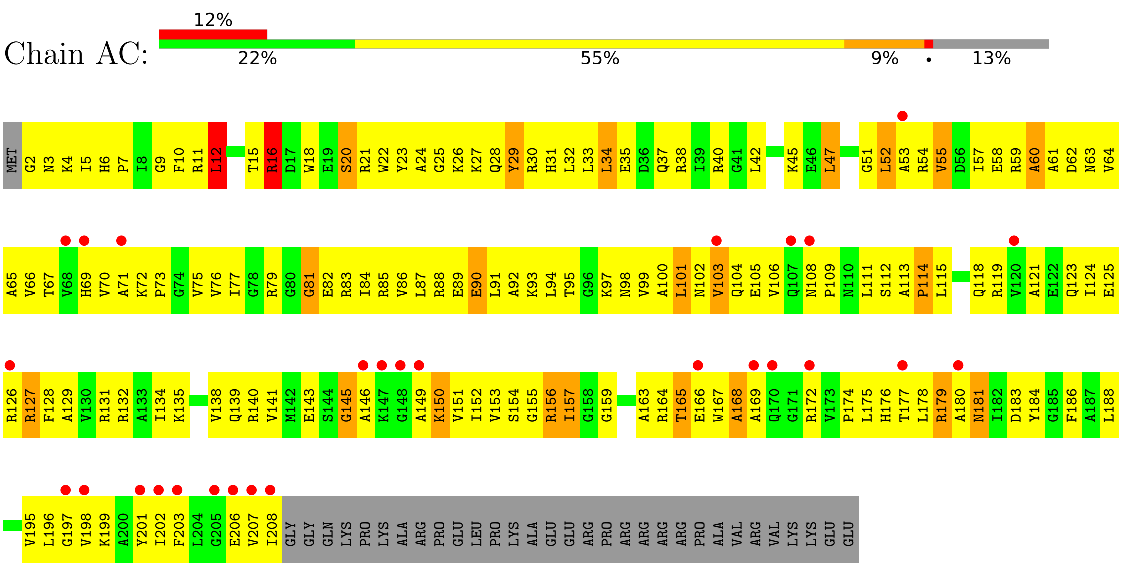
Chain AB:



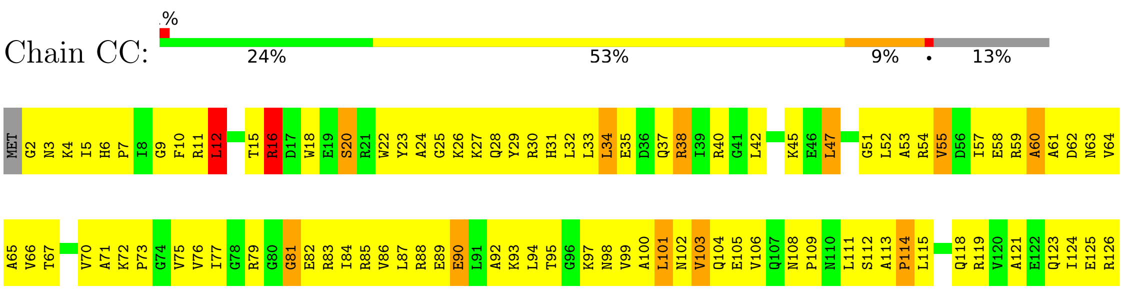
- Molecule 2: 30S RIBOSOMAL PROTEIN S2

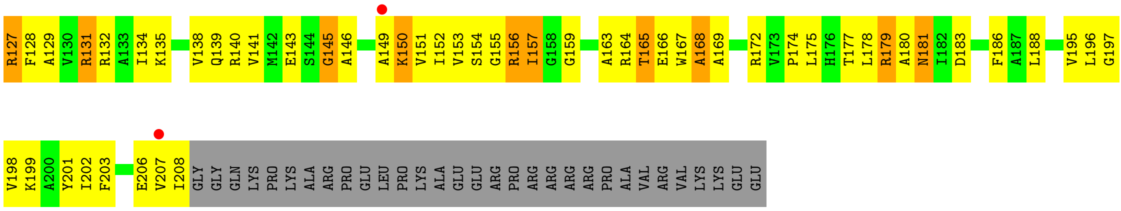


- Molecule 3: 30S RIBOSOMAL PROTEIN S3



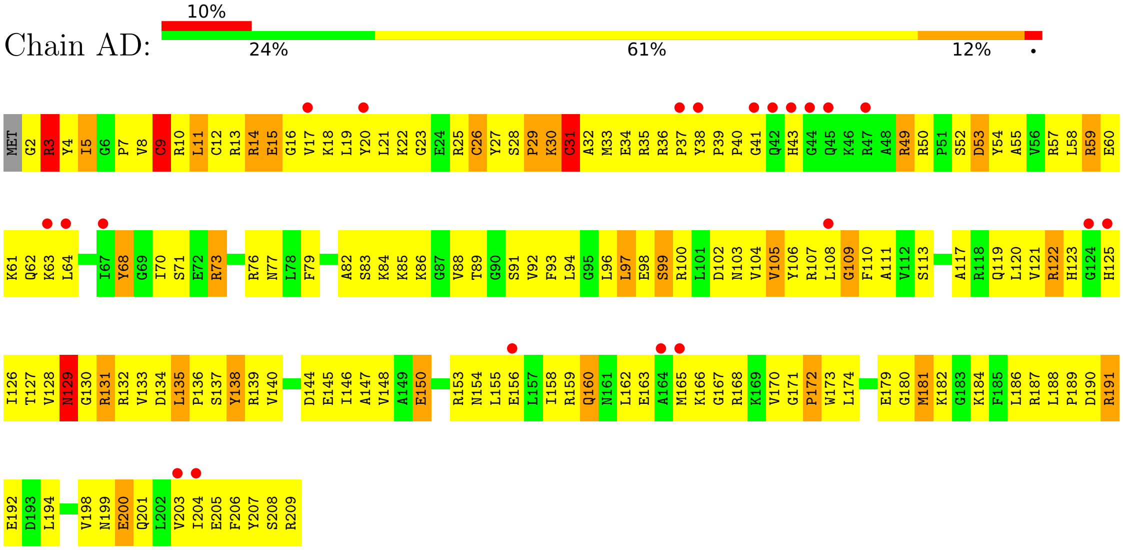
- Molecule 3: 30S RIBOSOMAL PROTEIN S3





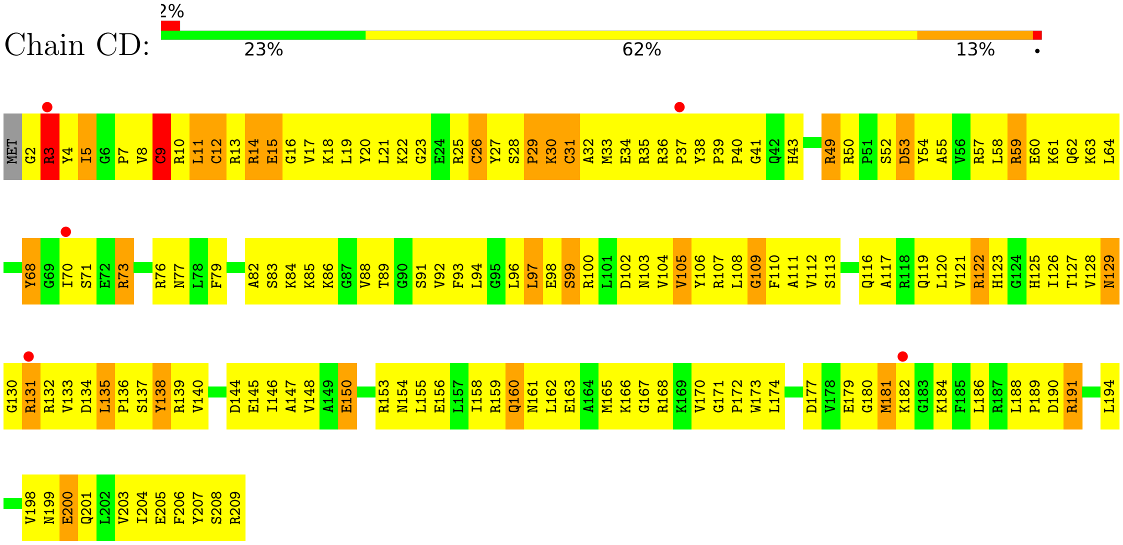
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



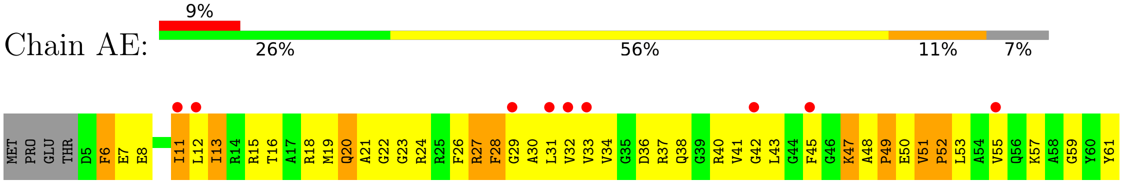
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

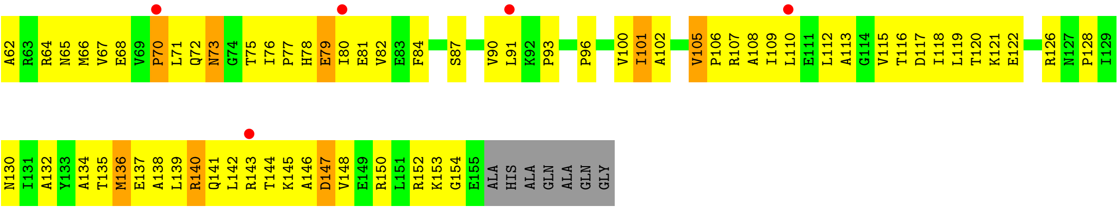
Chain CD:



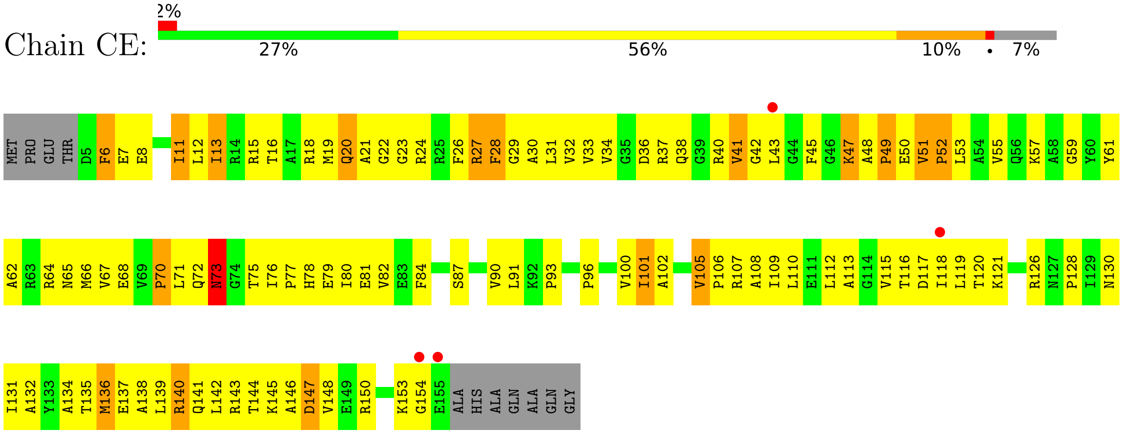
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:

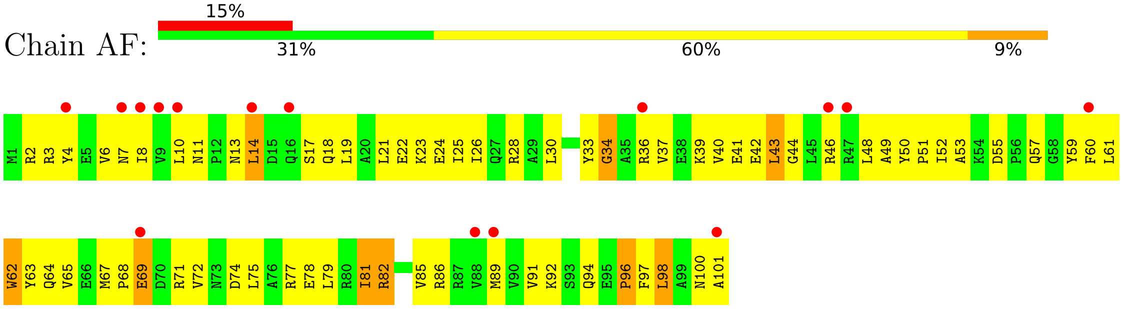




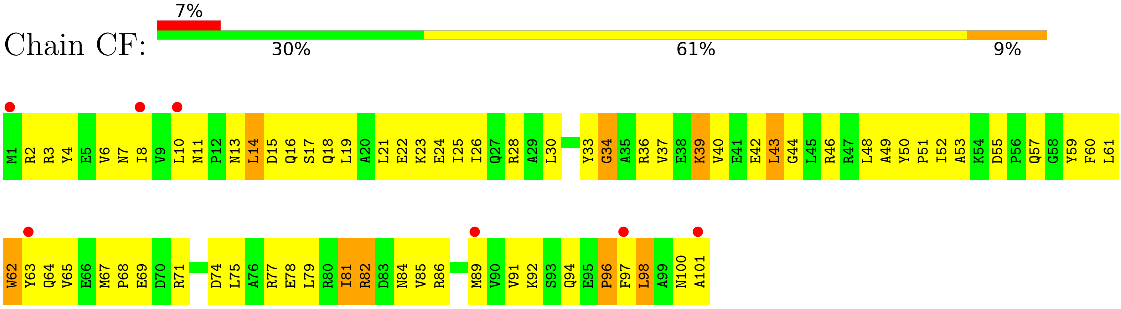
- Molecule 5: 30S RIBOSOMAL PROTEIN S5



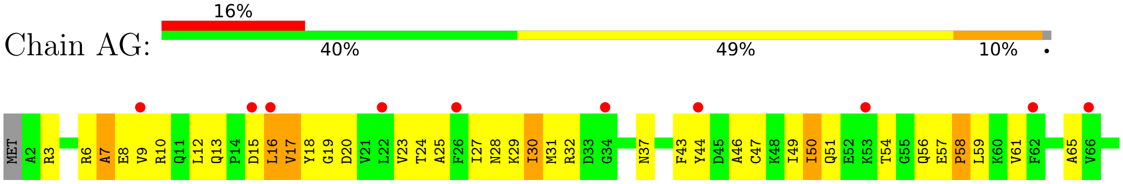
- Molecule 6: 30S RIBOSOMAL PROTEIN S6

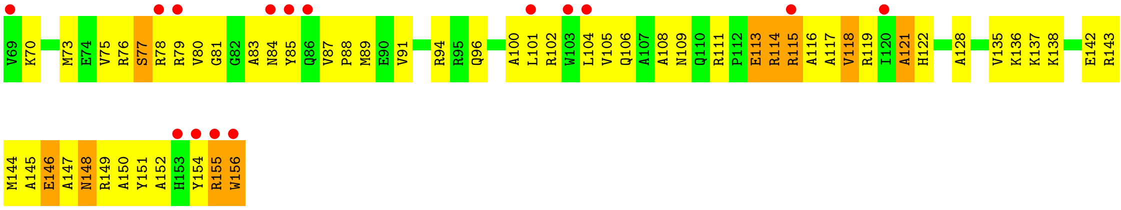


- Molecule 6: 30S RIBOSOMAL PROTEIN S6



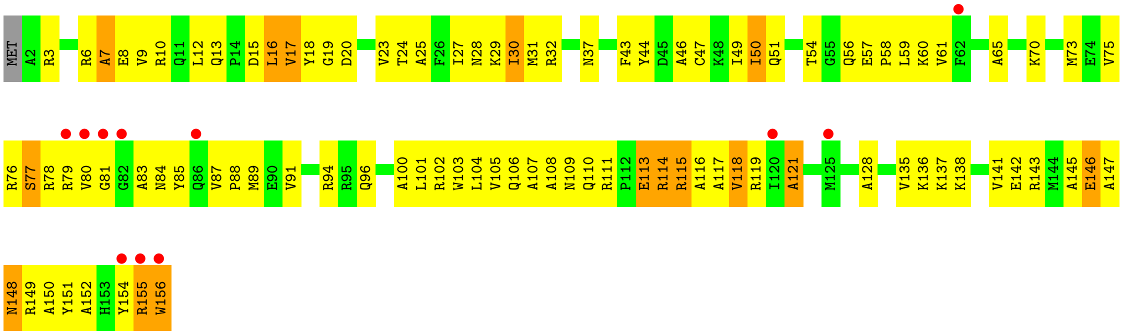
- Molecule 7: 30S RIBOSOMAL PROTEIN S7





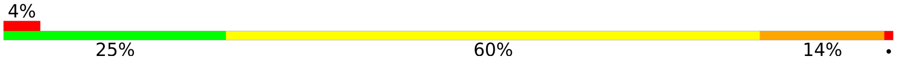
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

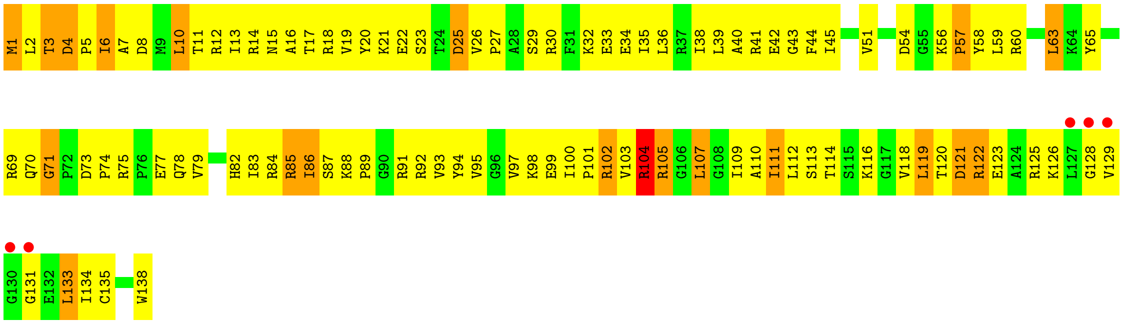
Chain CG:



- Molecule 8: 30S RIBOSOMAL PROTEIN S8

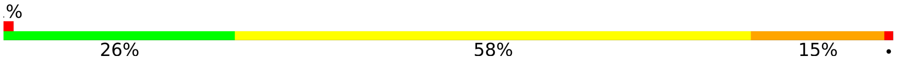
Chain AH:

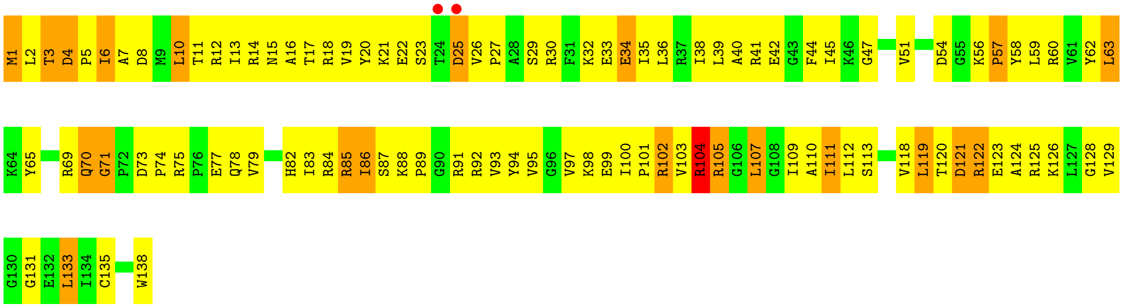




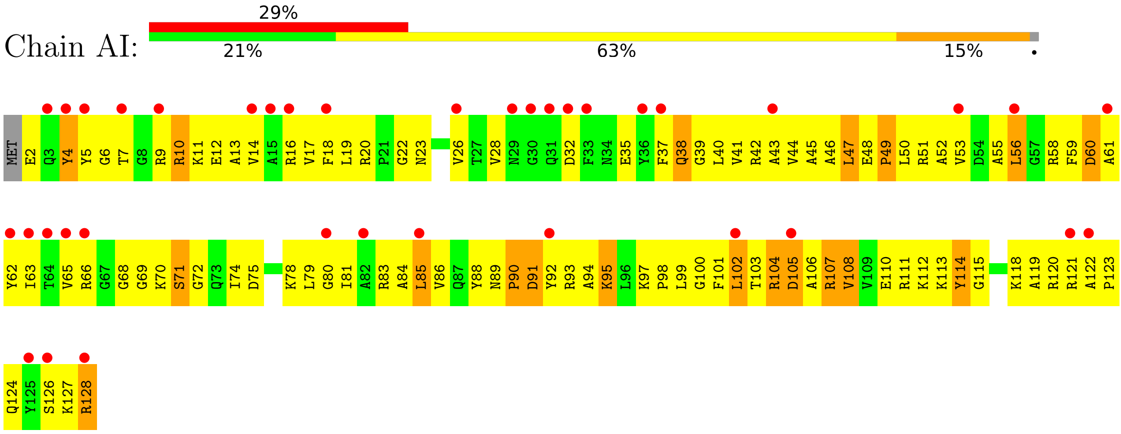
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH:

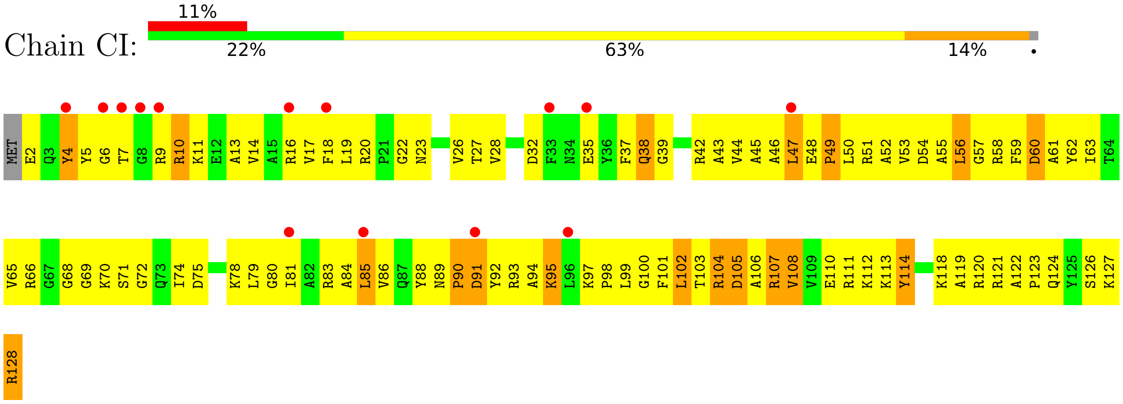




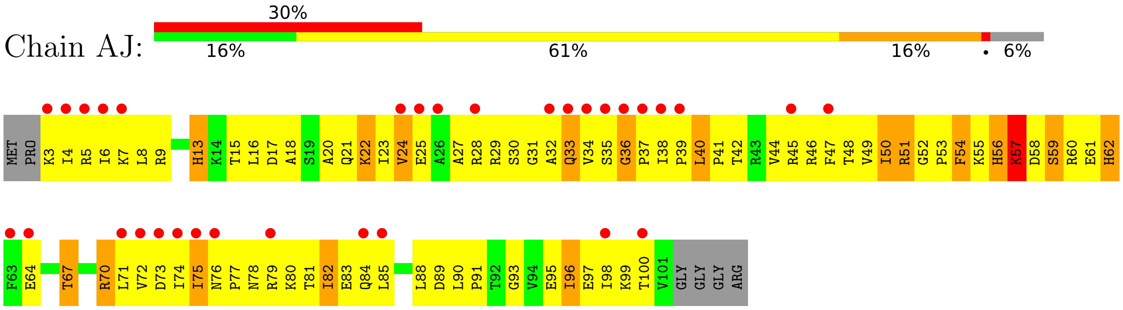
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



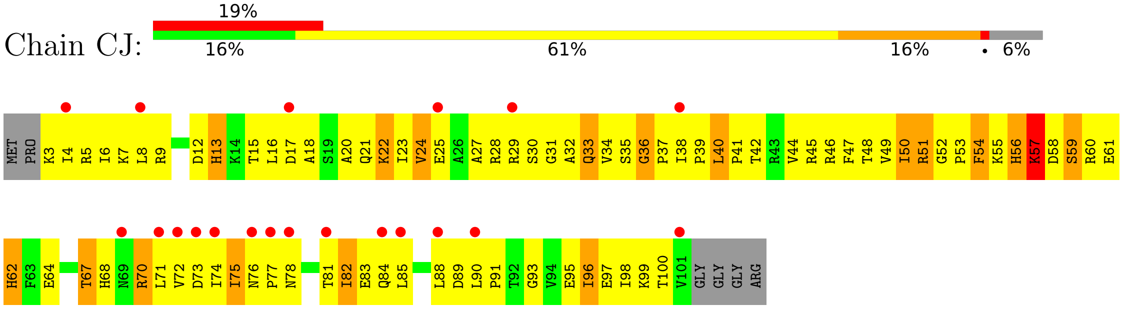
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

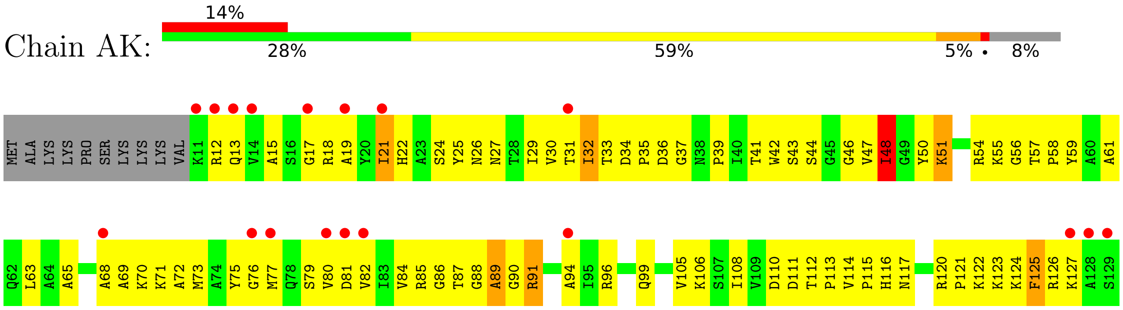


- Molecule 10: 30S RIBOSOMAL PROTEIN S10



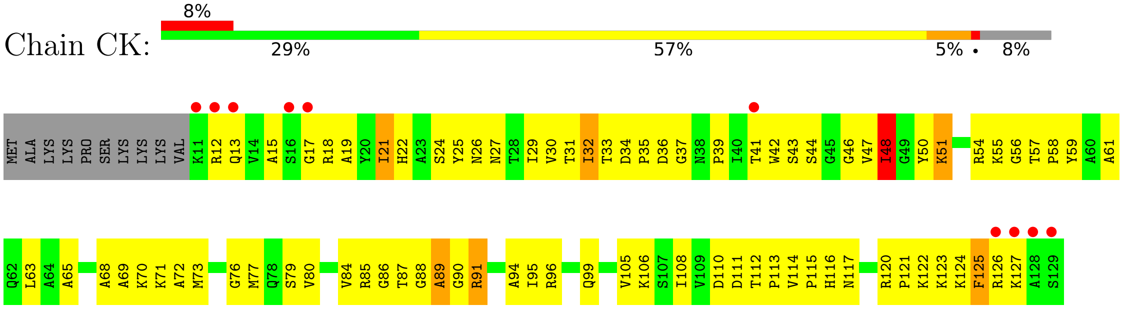
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



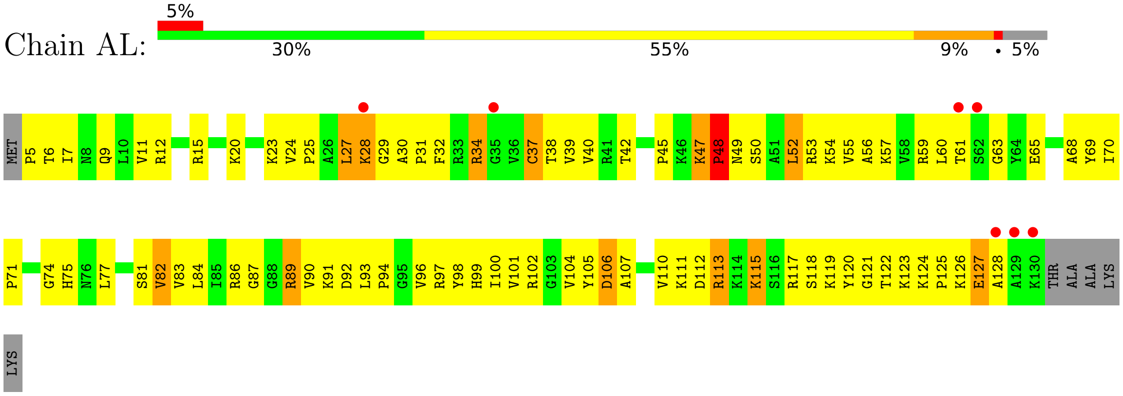
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



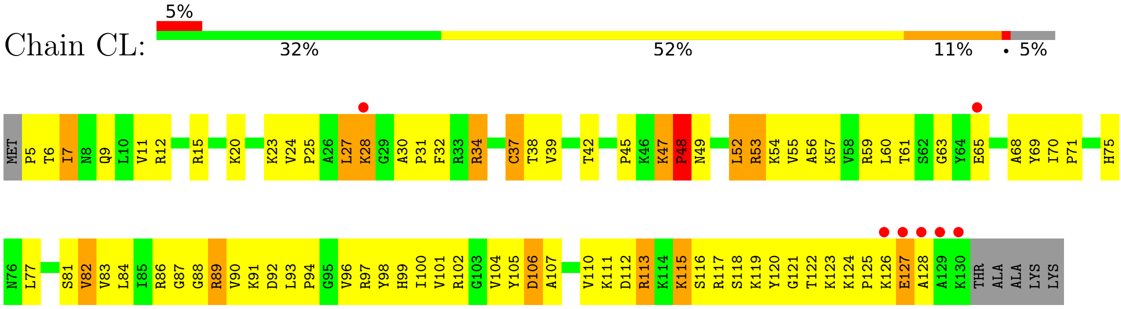
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



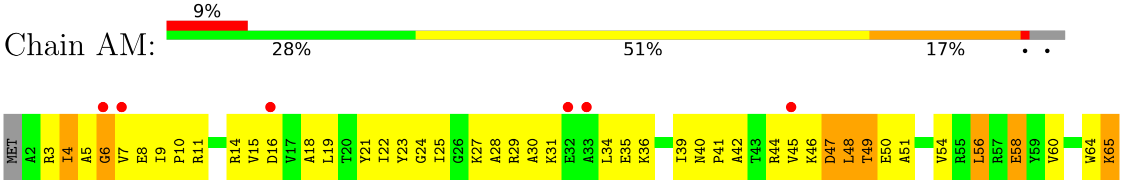
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

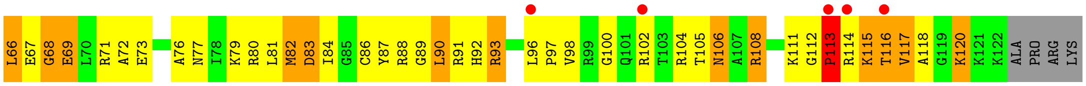
Chain CL:



- Molecule 13: 30S RIBOSOMAL PROTEIN S13

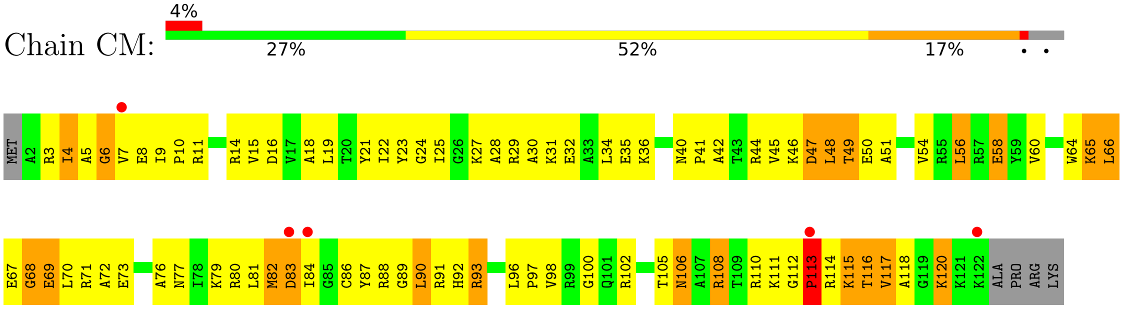
Chain AM:





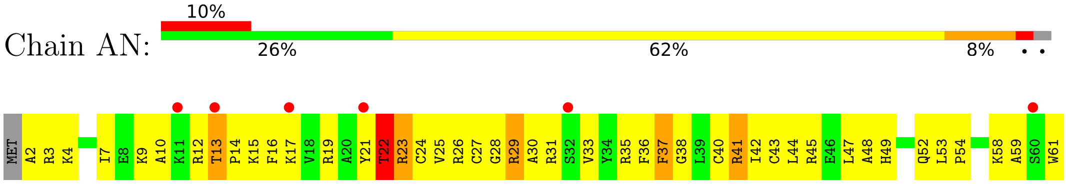
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



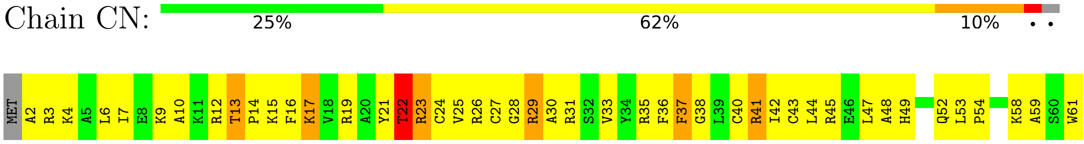
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:



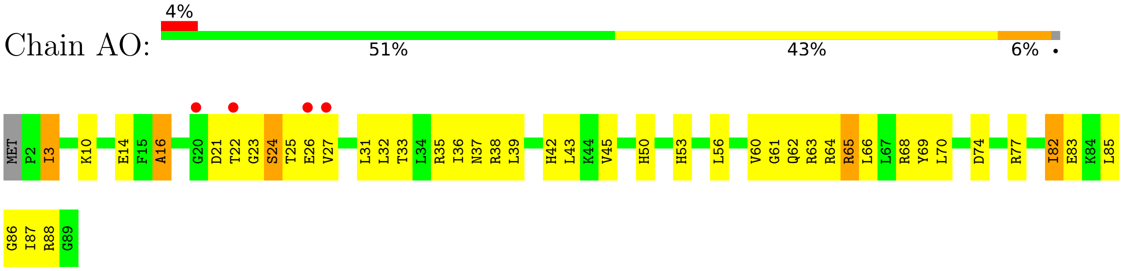
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN:



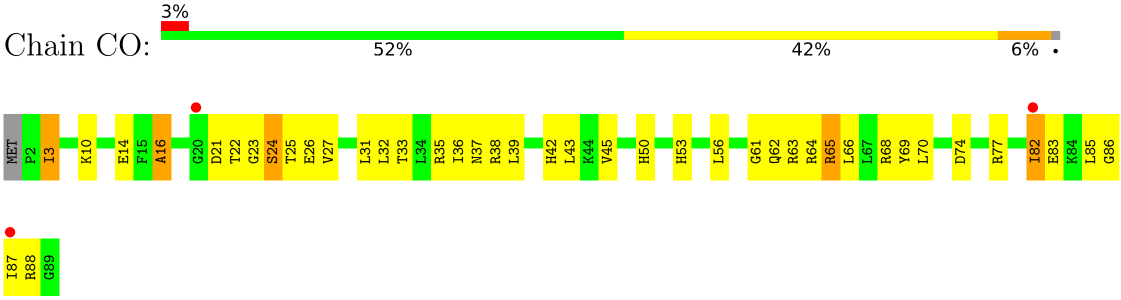
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



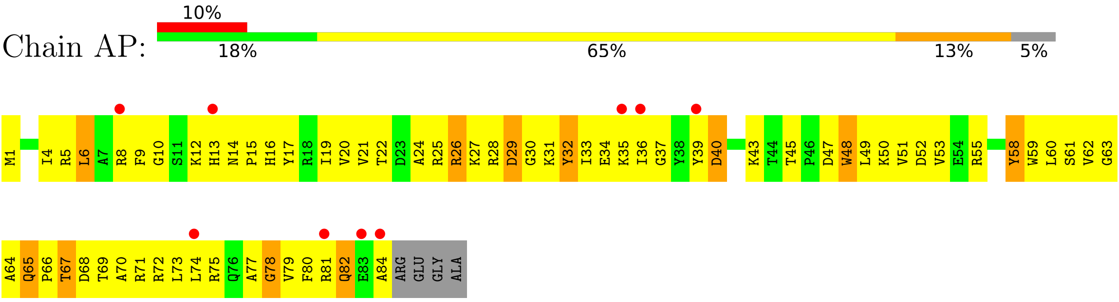
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



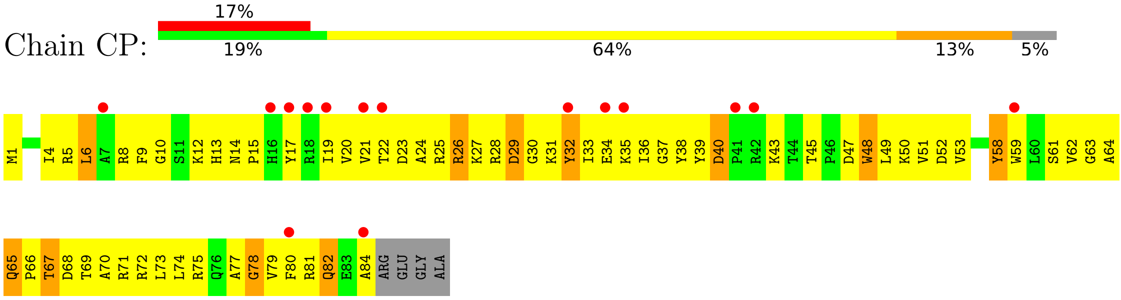
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



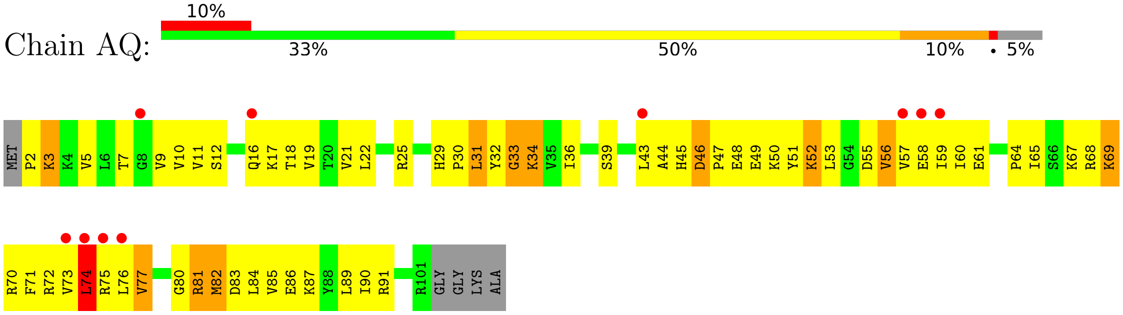
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



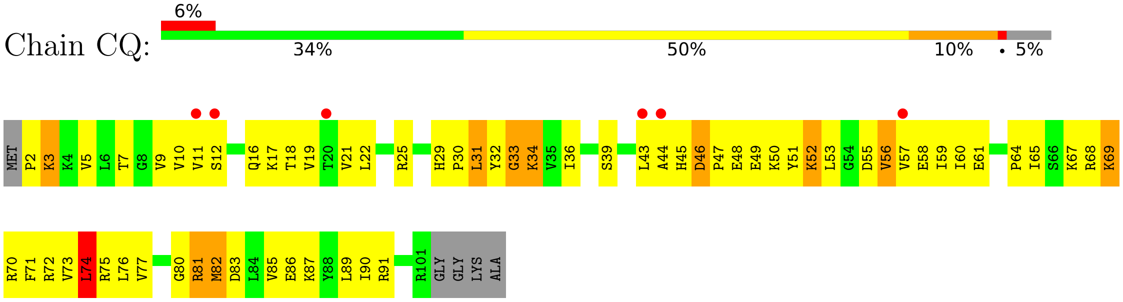
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



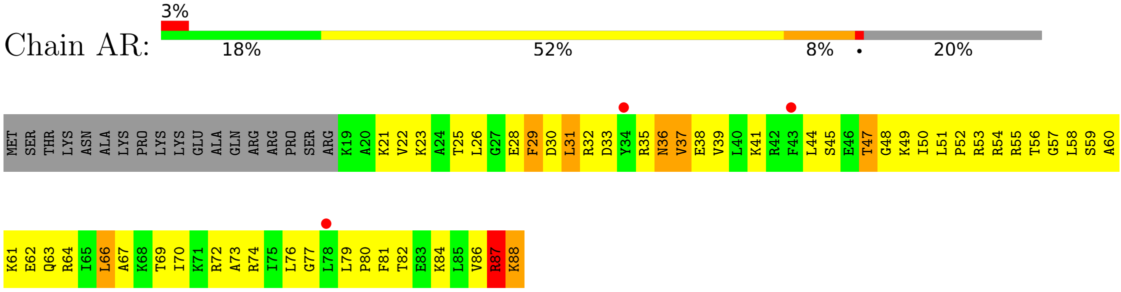
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



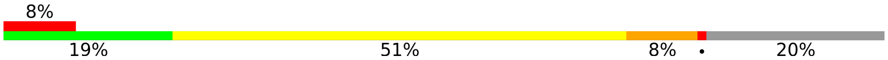
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

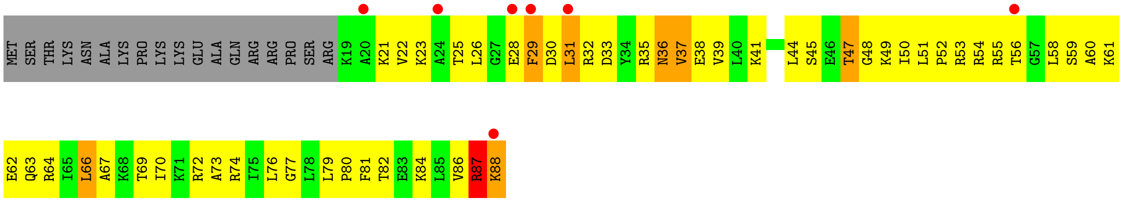
Chain AR:



- Molecule 18: 30S RIBOSOMAL PROTEIN S18

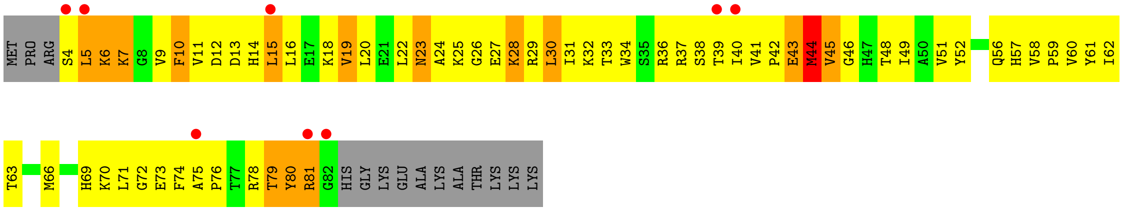
Chain CR:





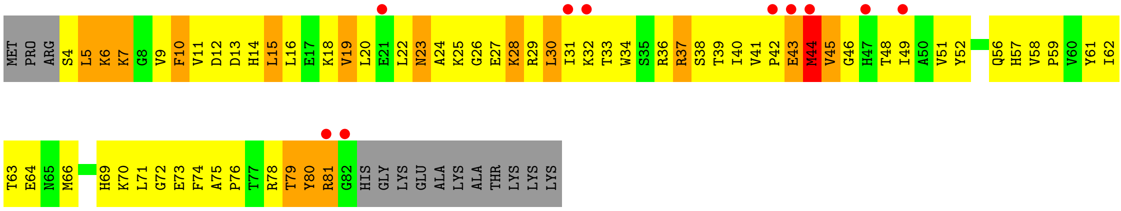
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



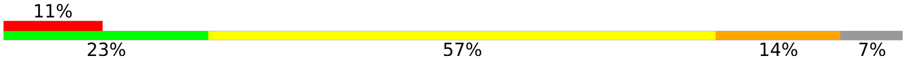
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

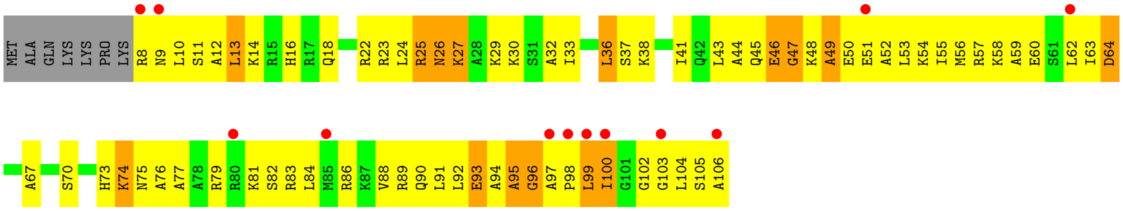
Chain CS:



- Molecule 20: 30S RIBOSOMAL PROTEIN S20

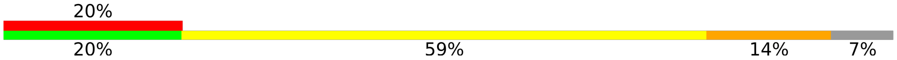
Chain AT:

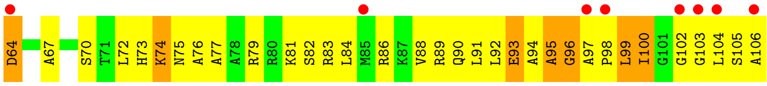




- Molecule 20: 30S RIBOSOMAL PROTEIN S20

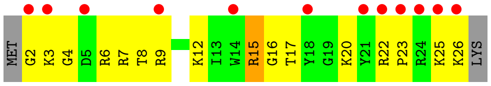
Chain CT:





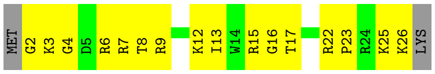
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



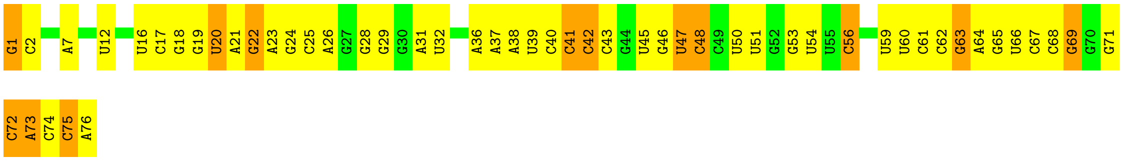
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:



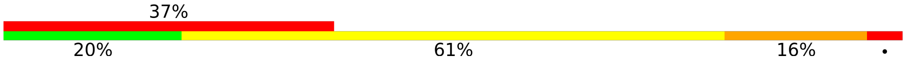
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

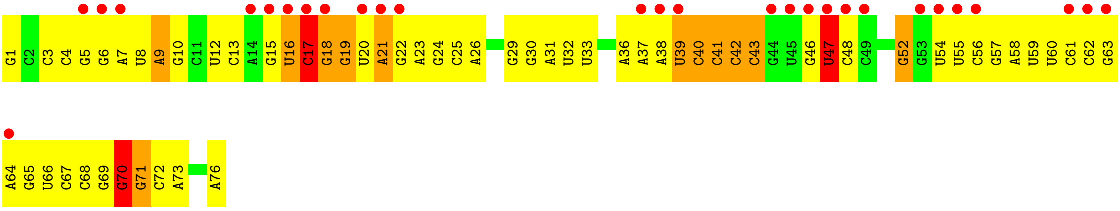
Chain AV:



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

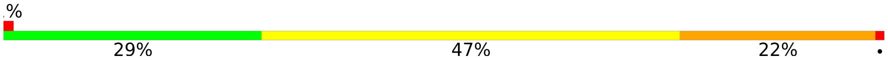
Chain AW:

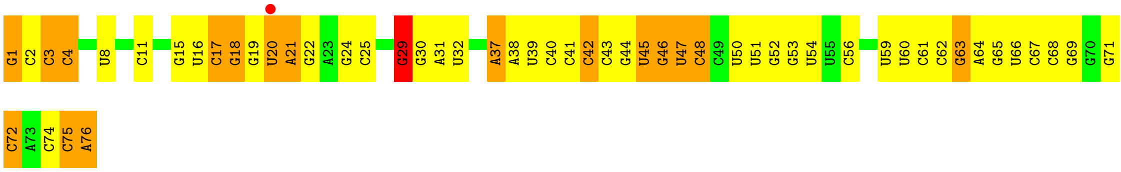




- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

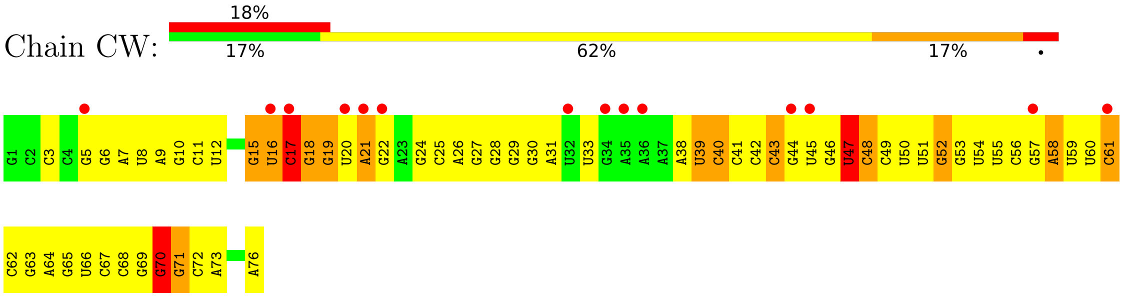
Chain CV:





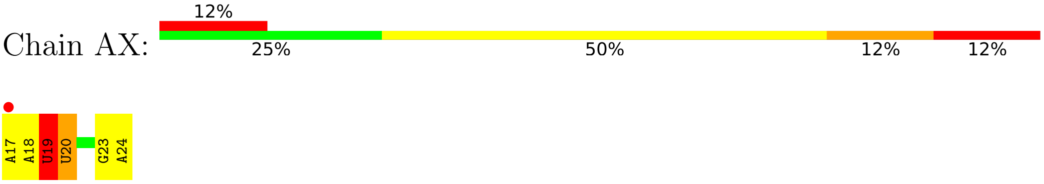
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

Chain CW:



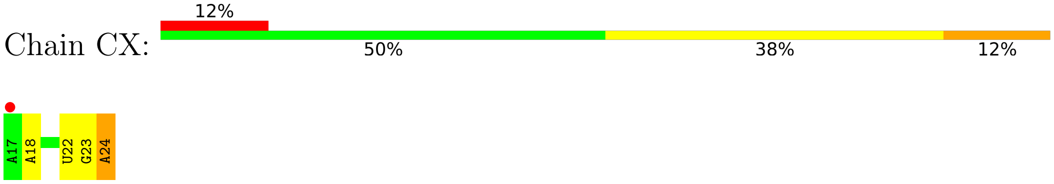
- Molecule 23: MRNA

Chain AX:



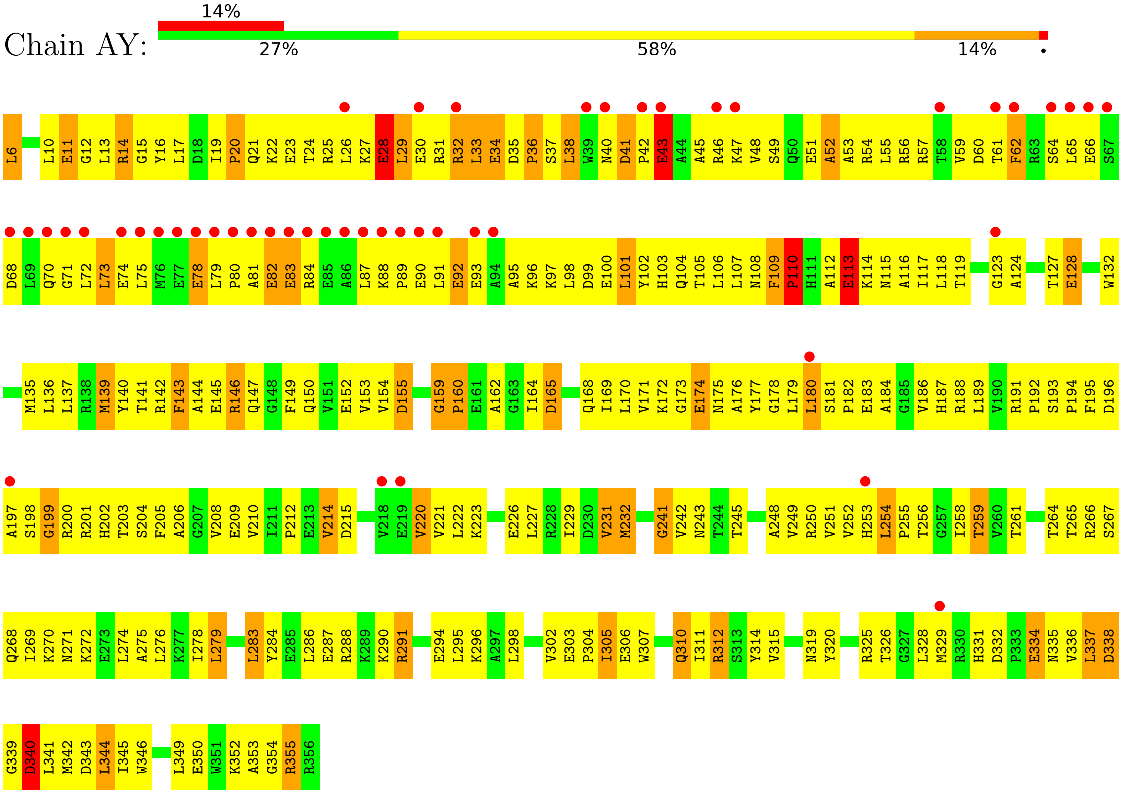
- Molecule 23: MRNA

Chain CX:

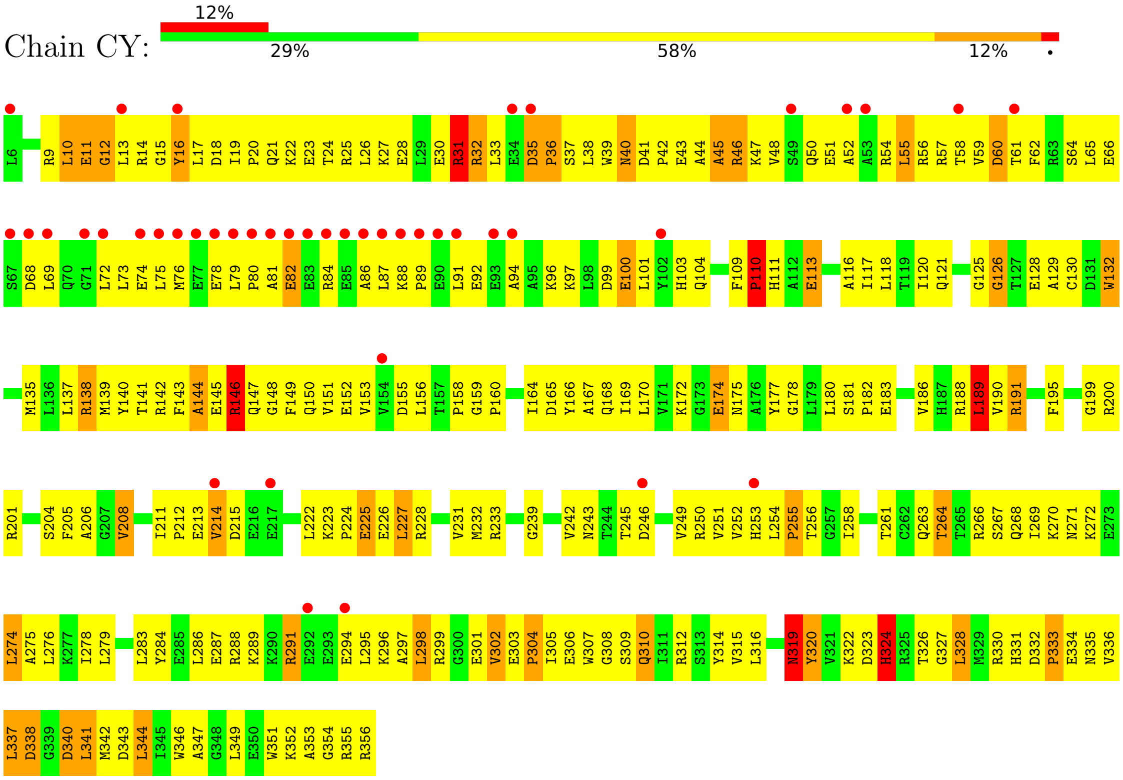


- Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2

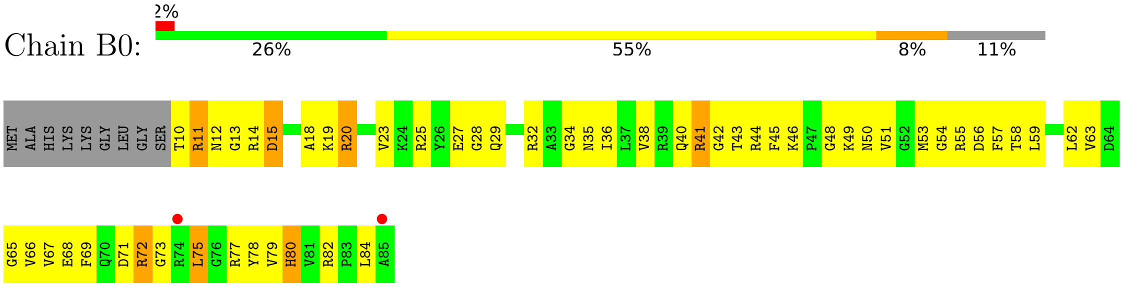
Chain AY:



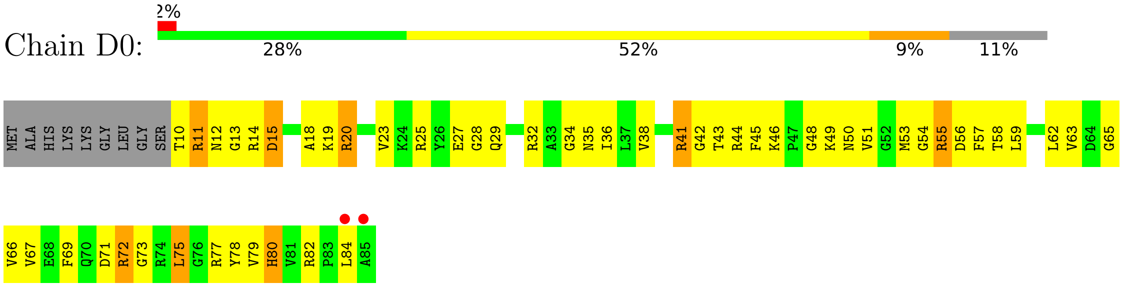
- Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2



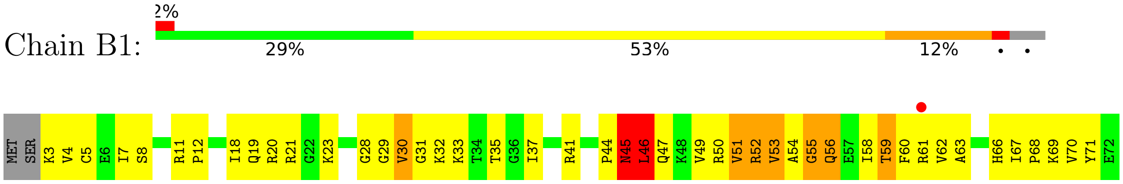
- Molecule 25: 50S RIBOSOMAL PROTEIN L27

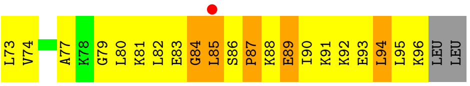


- Molecule 25: 50S RIBOSOMAL PROTEIN L27



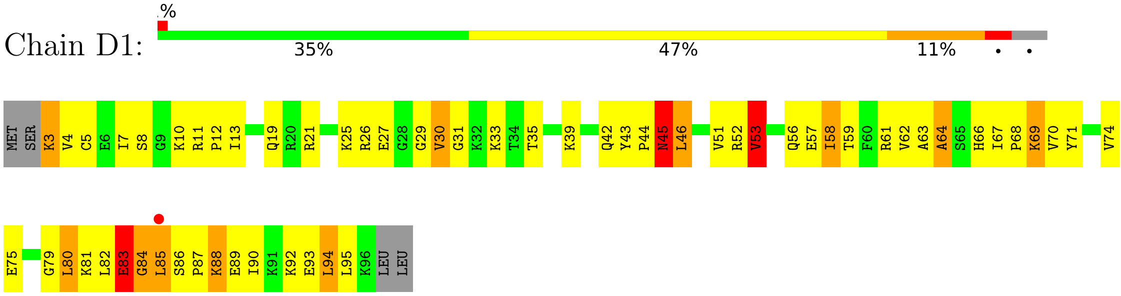
- Molecule 26: 50S RIBOSOMAL PROTEIN L28





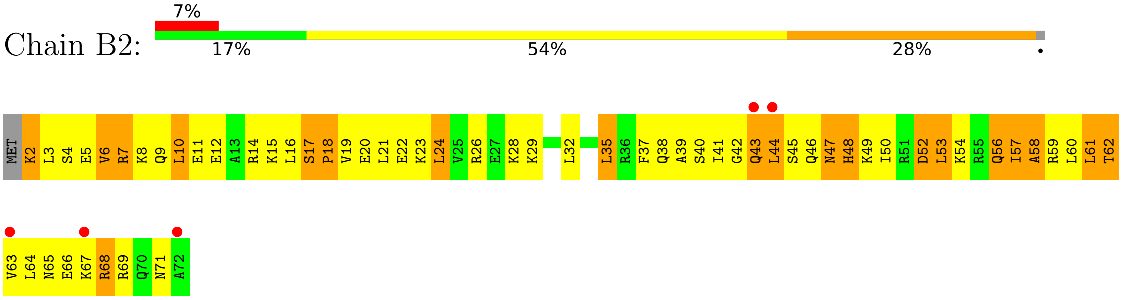
- Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain D1:



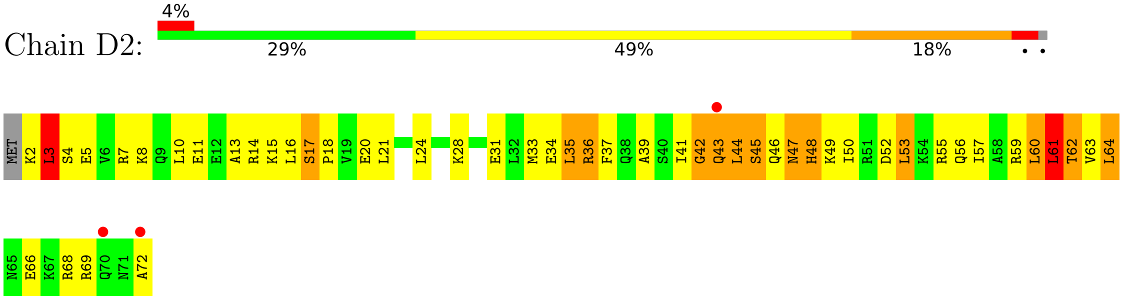
- Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain B2:



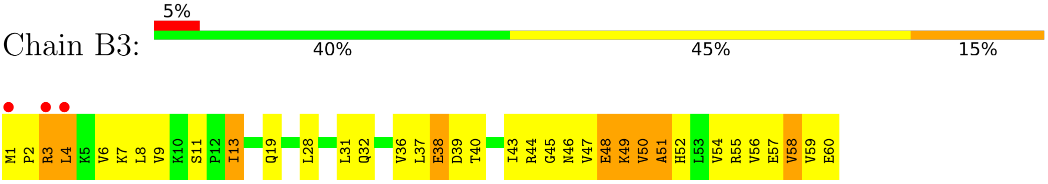
- Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain D2:



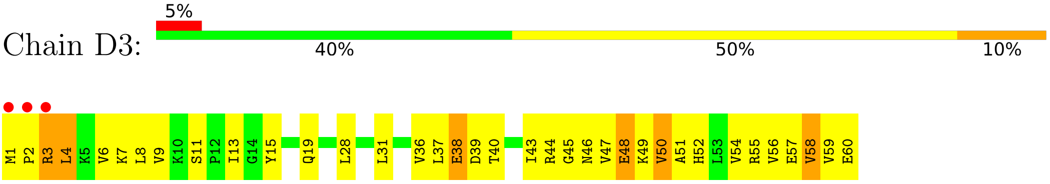
- Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain B3:



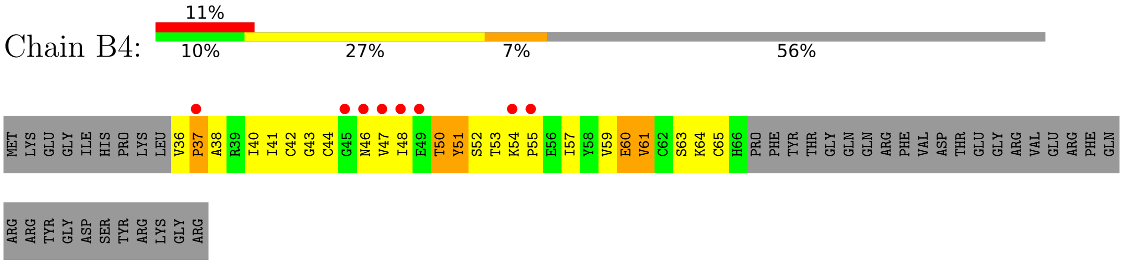
- Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain D3:



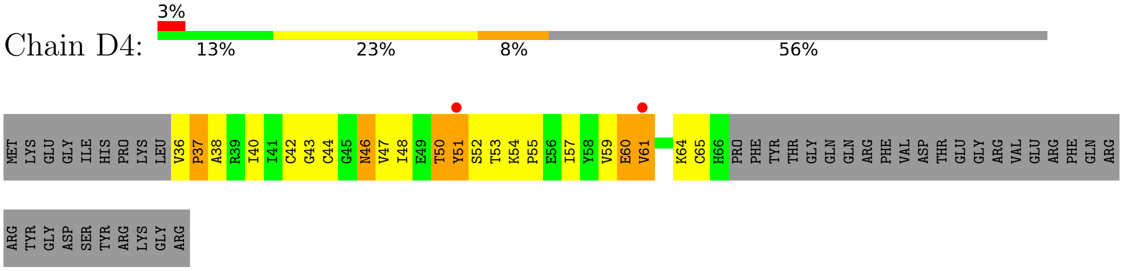
- Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain B4:



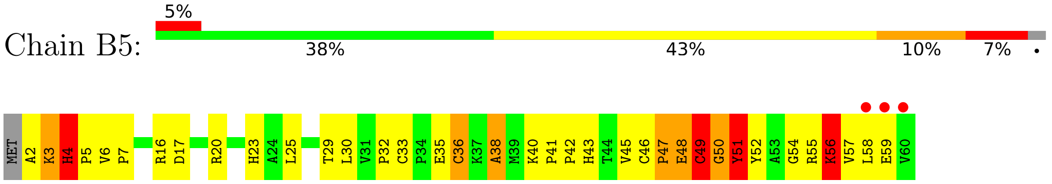
- Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain D4:



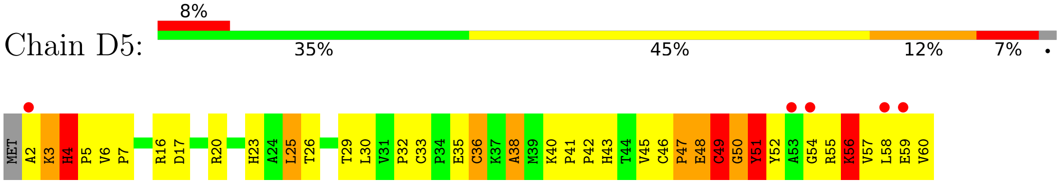
- Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain B5:



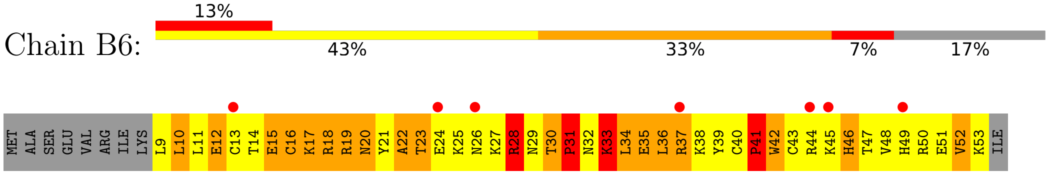
- Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain D5:



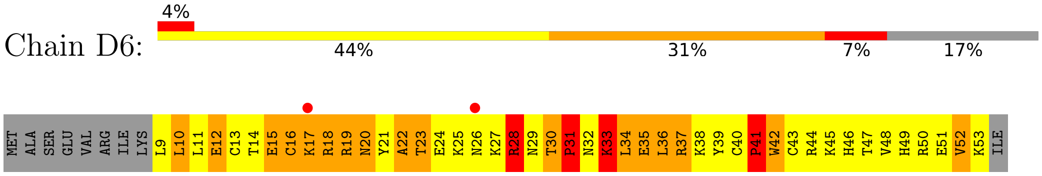
- Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain B6:



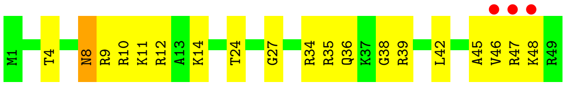
- Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain D6:



- Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain B7:

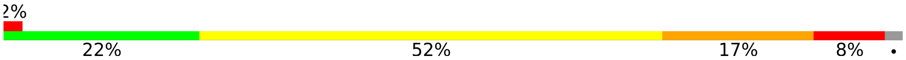


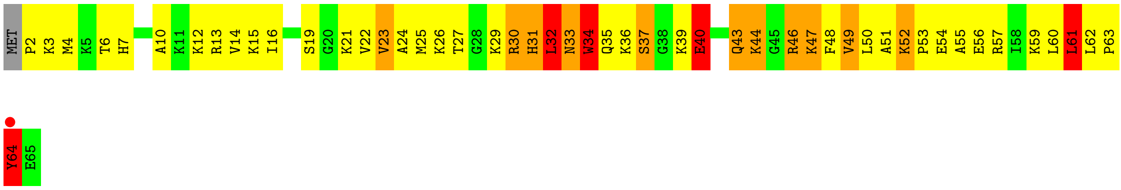
- Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain D7:

- Molecule 33: 50S RIBOSOMAL PROTEIN L35

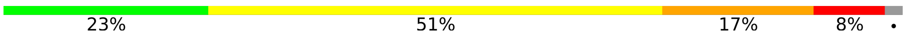
Chain B8:

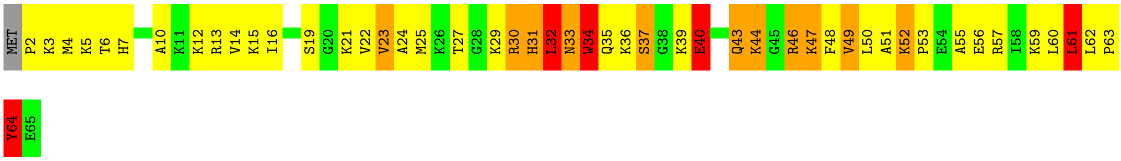




- Molecule 33: 50S RIBOSOMAL PROTEIN L35

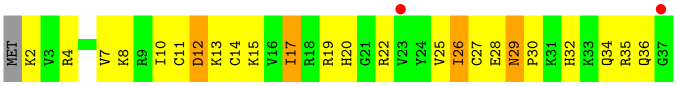
Chain D8:





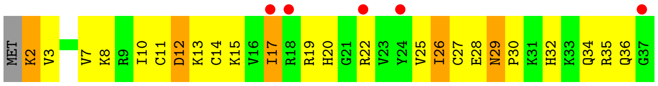
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain B9:



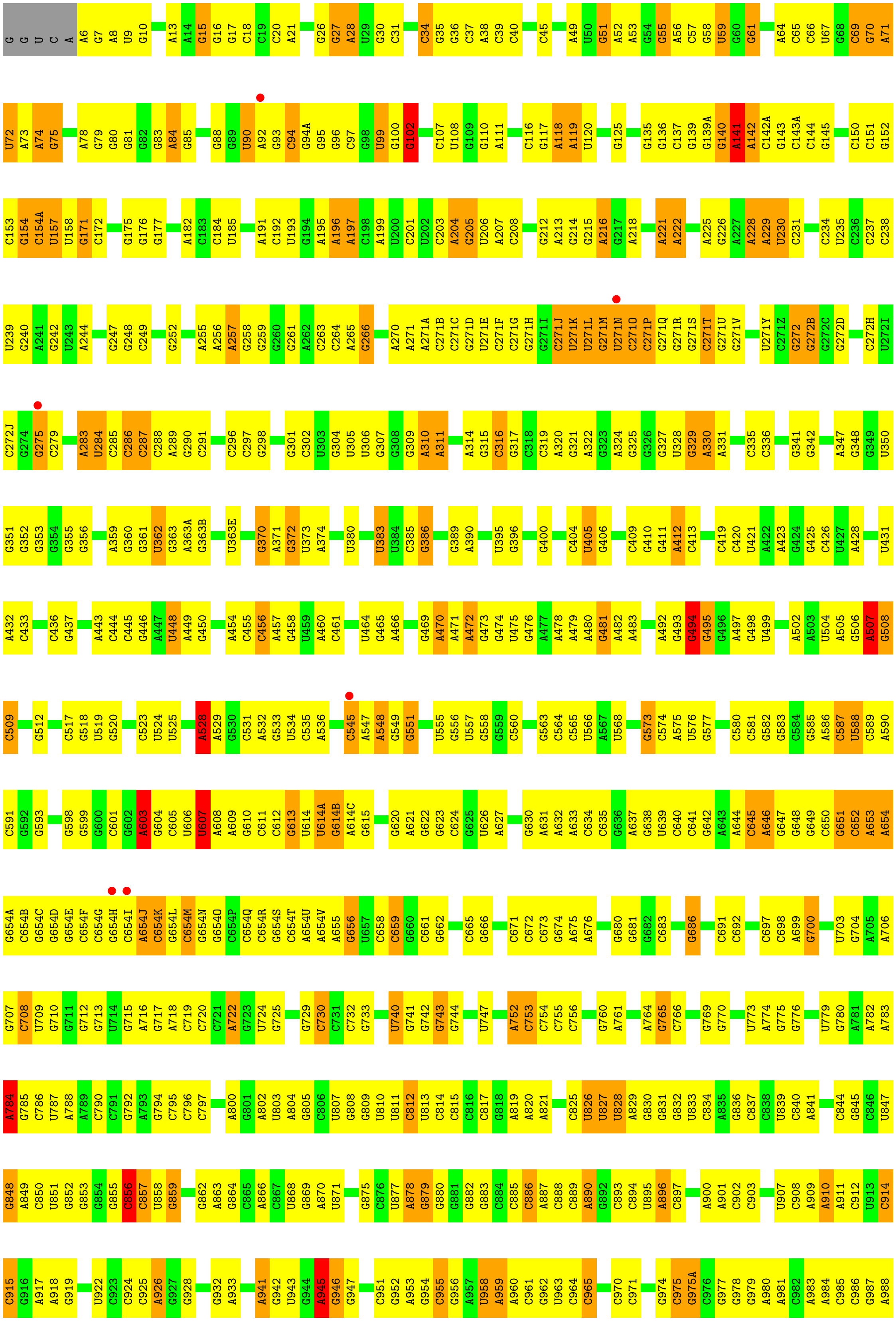
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain D9:



- Molecule 35: 23S RIBOSOMAL RNA

Chain BA: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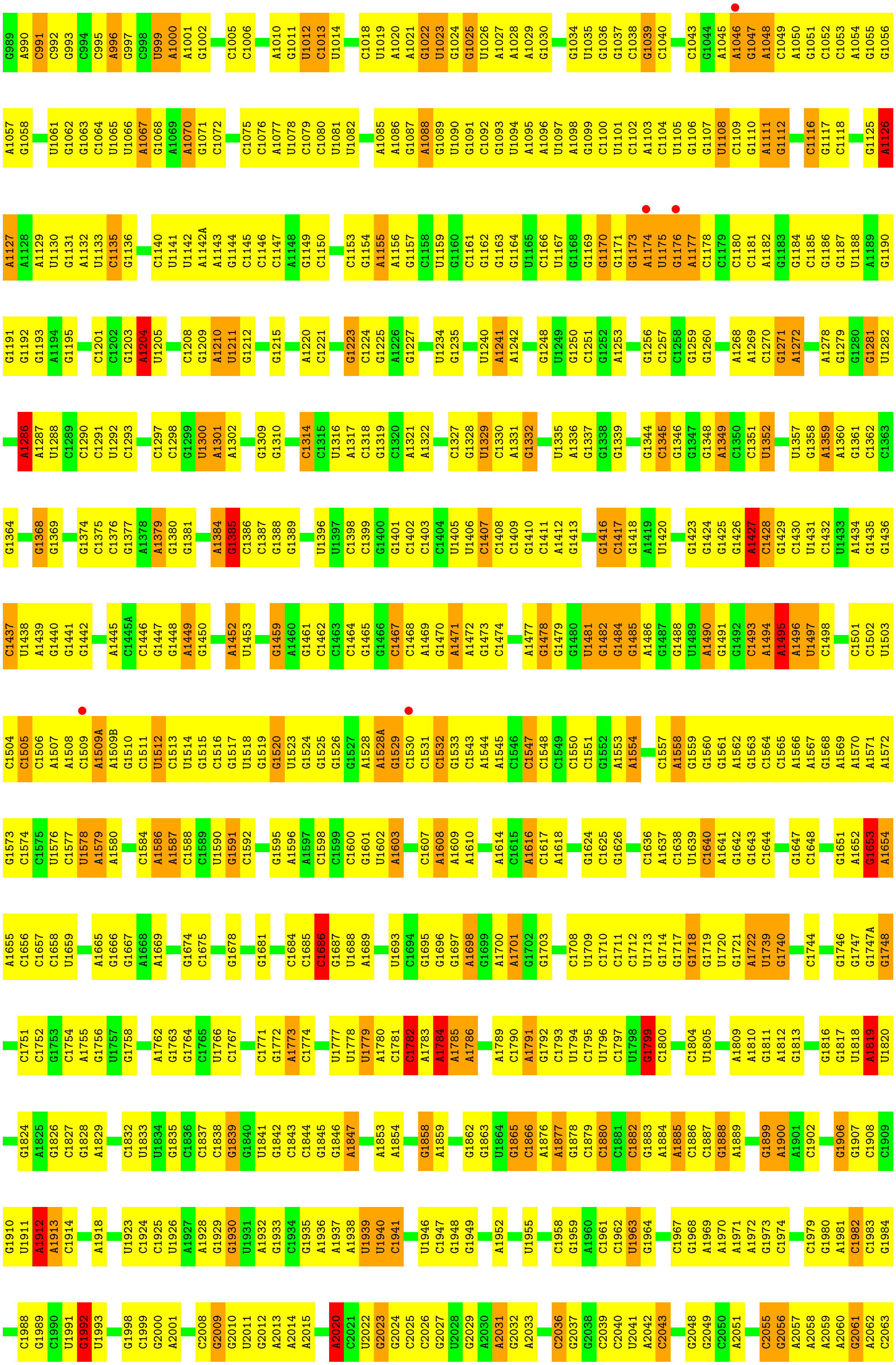
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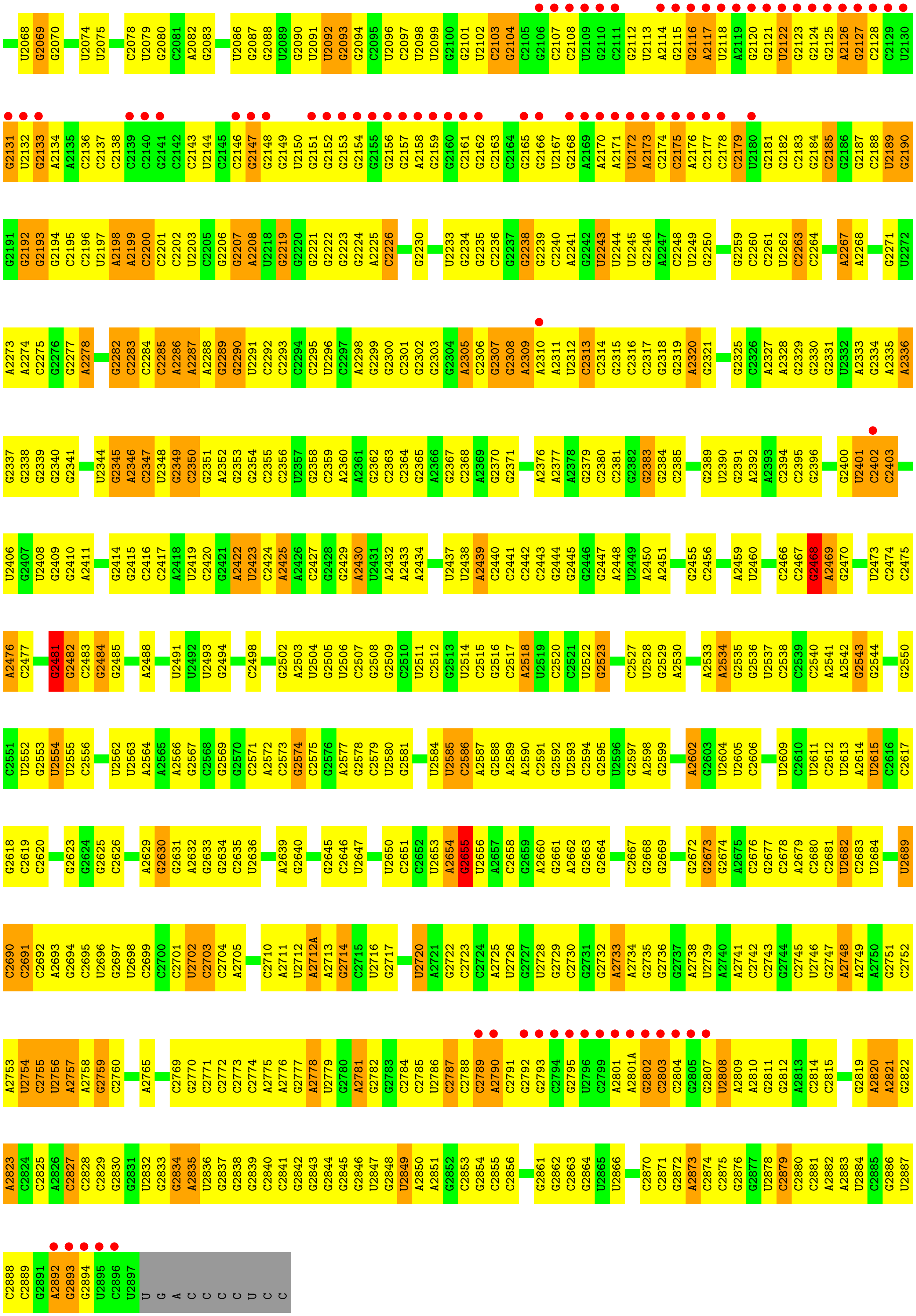
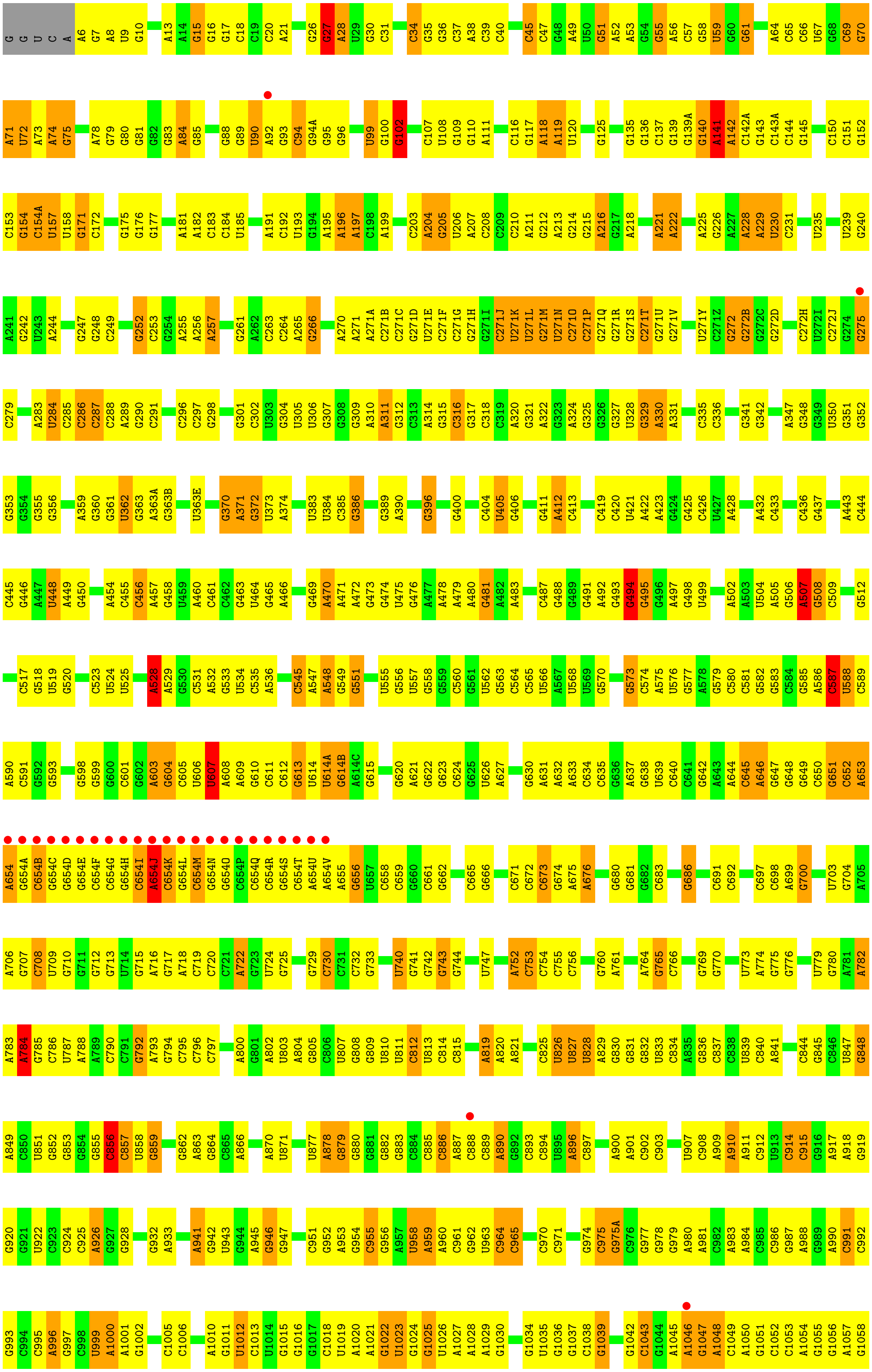


- Molecule 35: 23S RIBOSOMAL RNA

Chain DA: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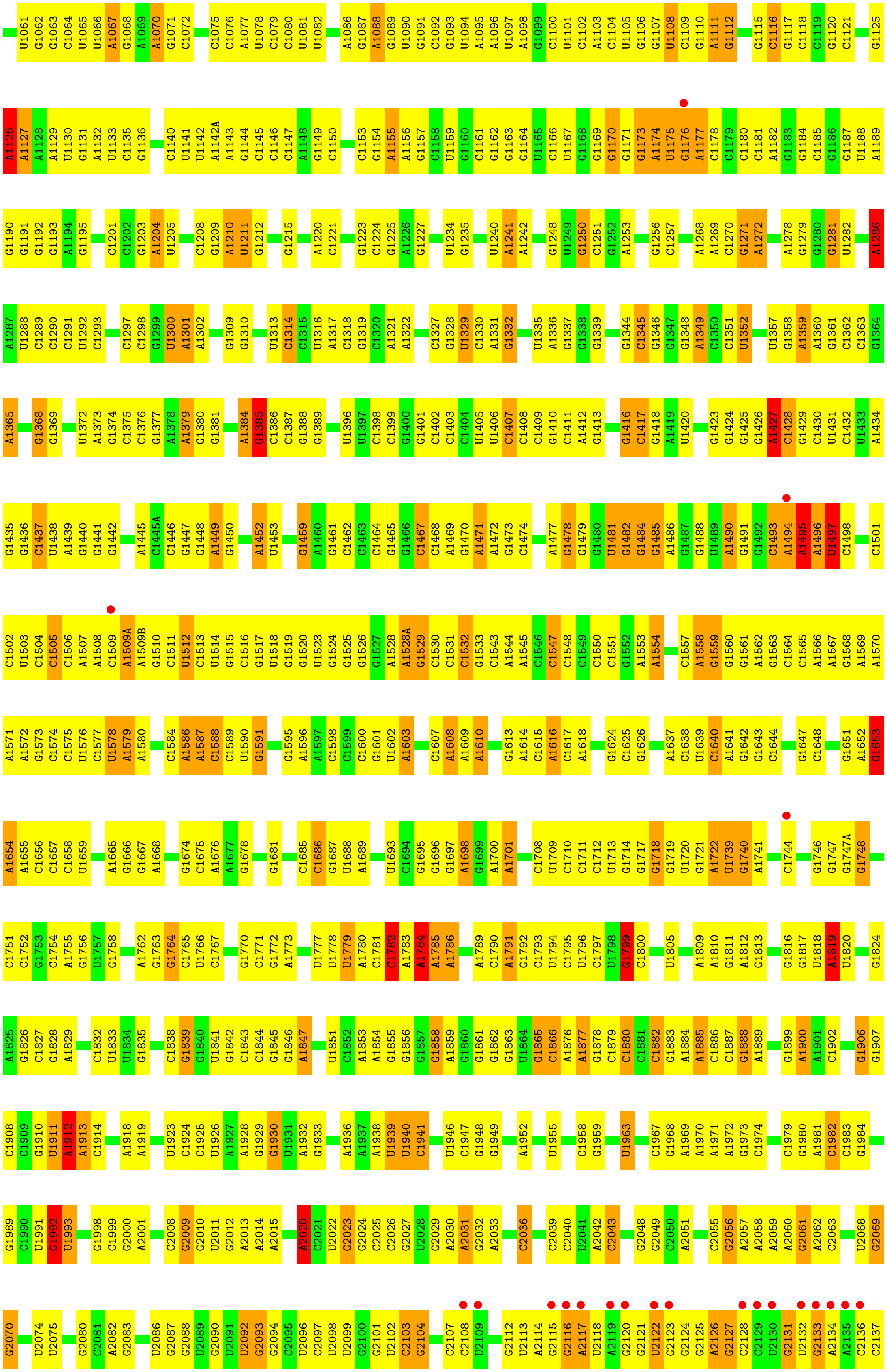
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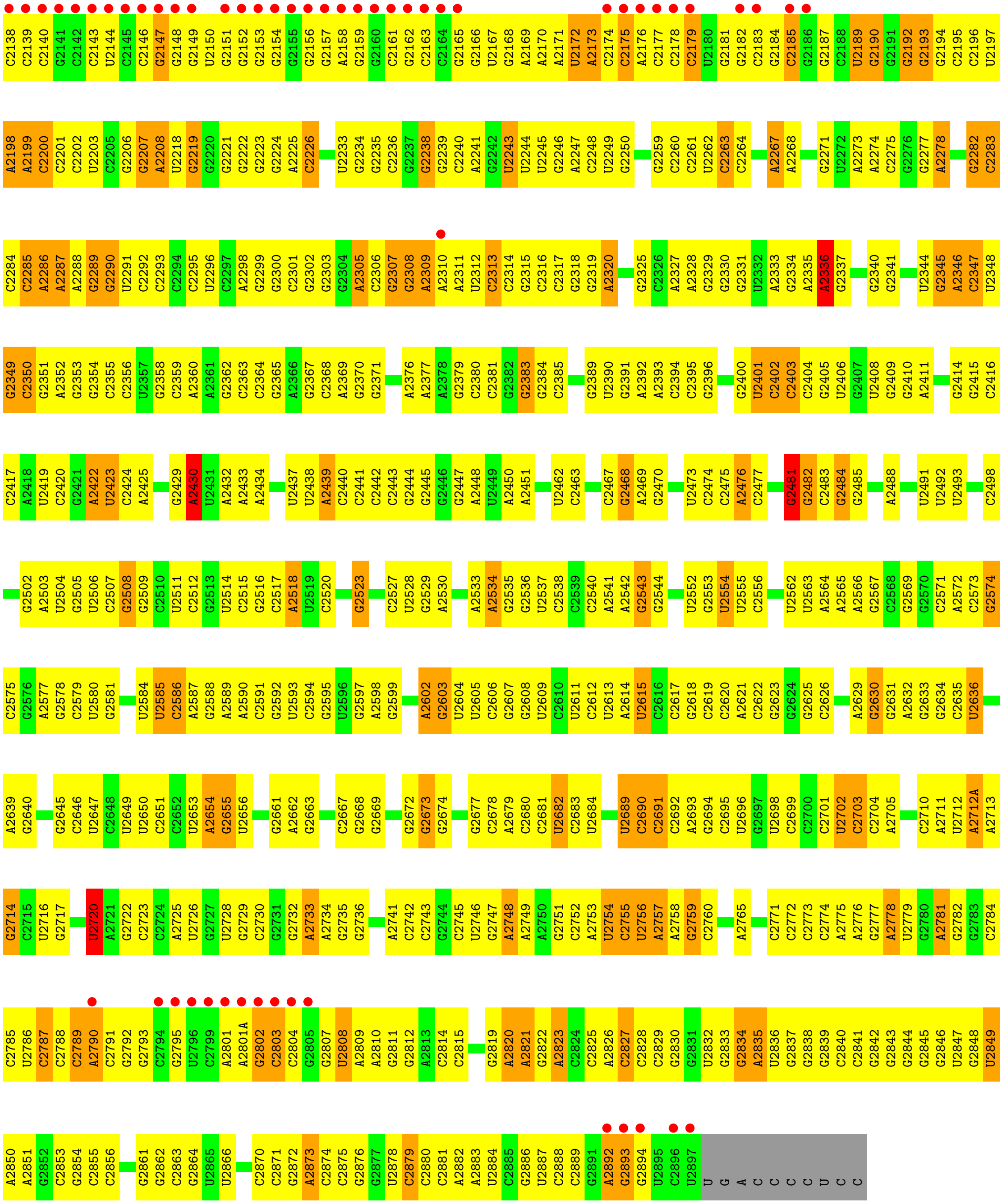
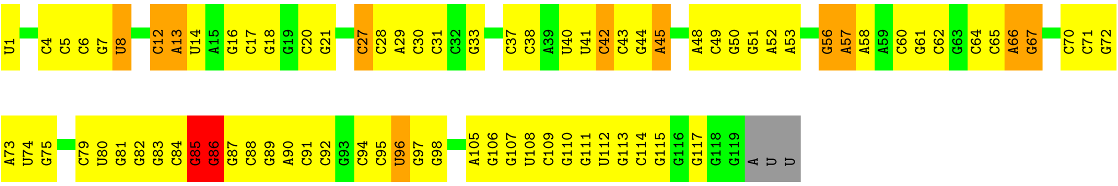
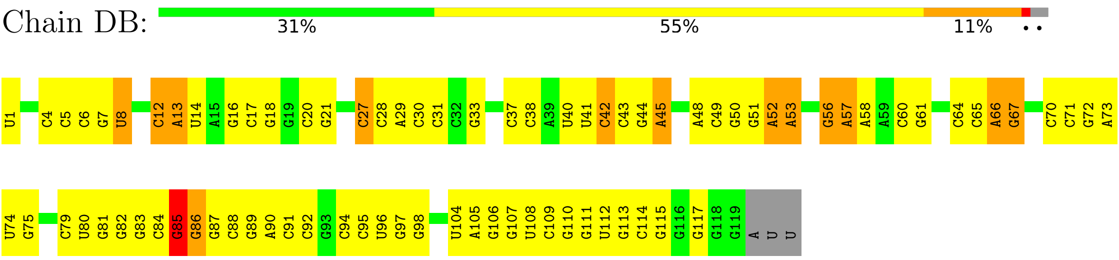


- Molecule 36: 5S RIBOSOMAL RNA

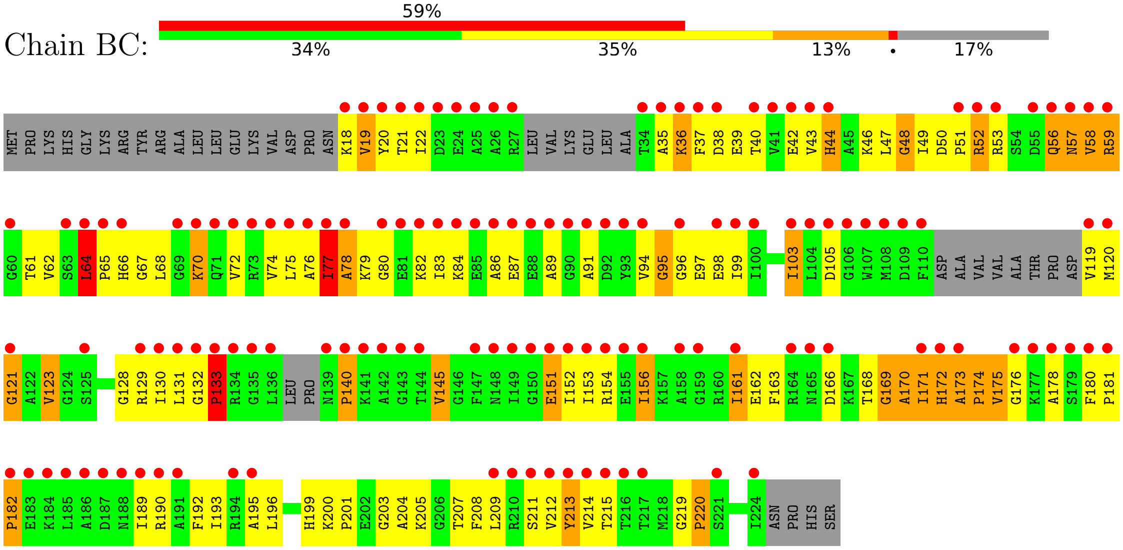
Chain BB:



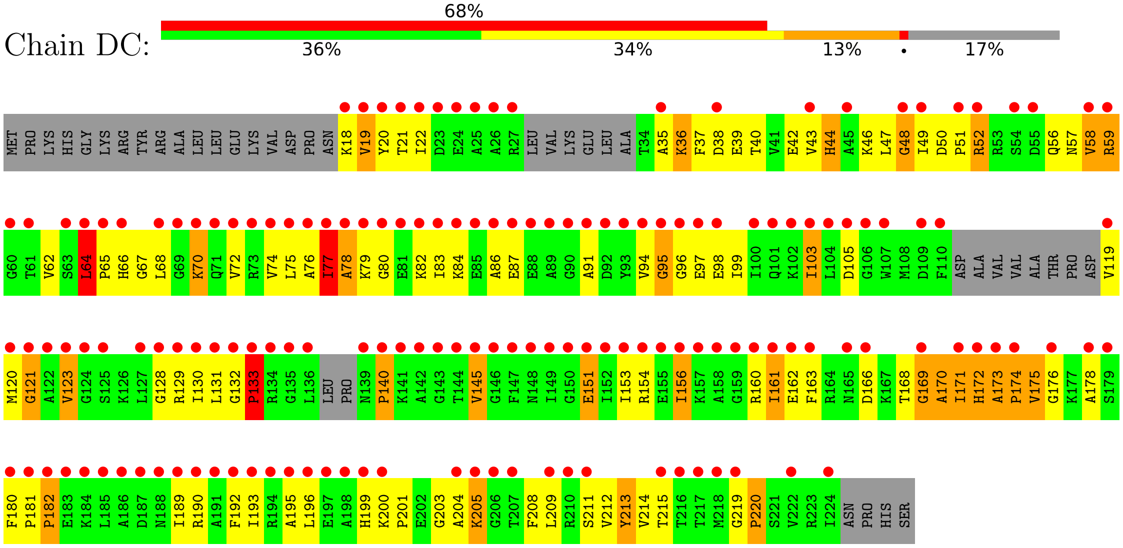
- Molecule 36: 5S RIBOSOMAL RNA



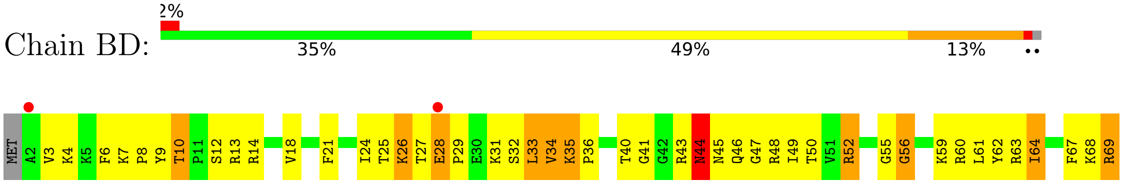
- Molecule 37: 50S RIBOSOMAL PROTEIN L1

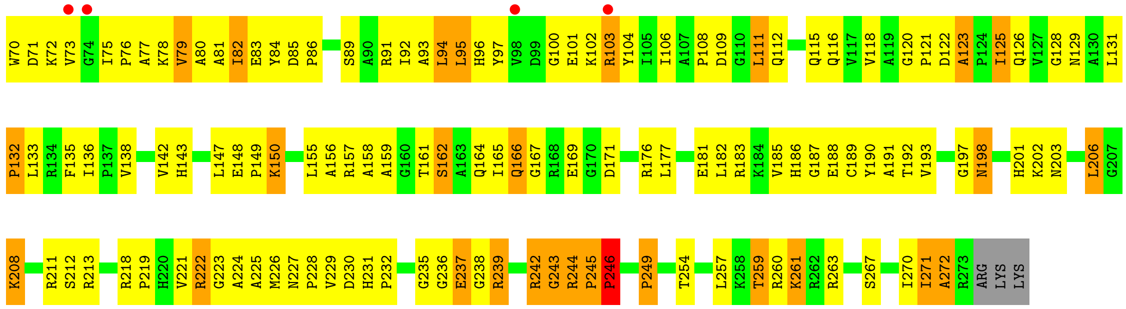


- Molecule 37: 50S RIBOSOMAL PROTEIN L1



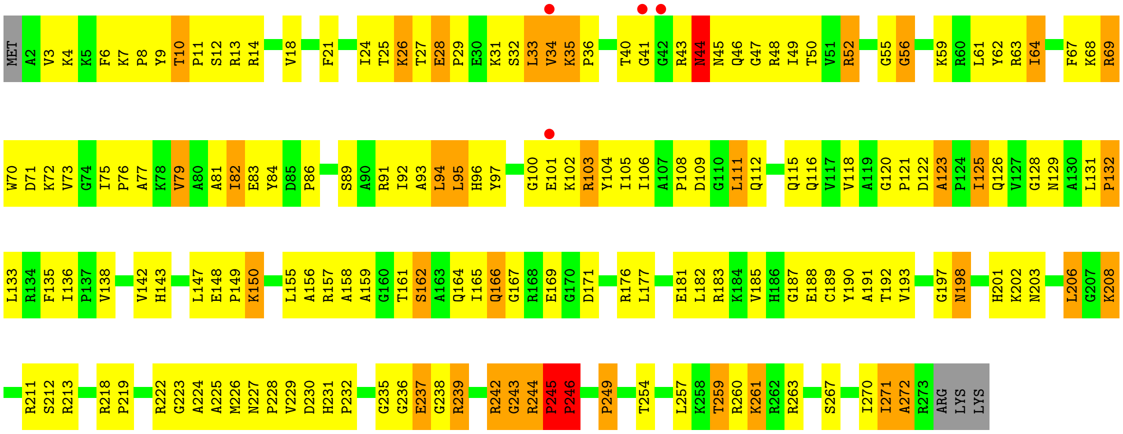
- Molecule 38: 50S RIBOSOMAL PROTEIN L2





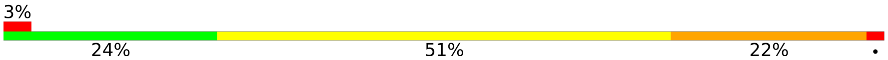
- Molecule 38: 50S RIBOSOMAL PROTEIN L2

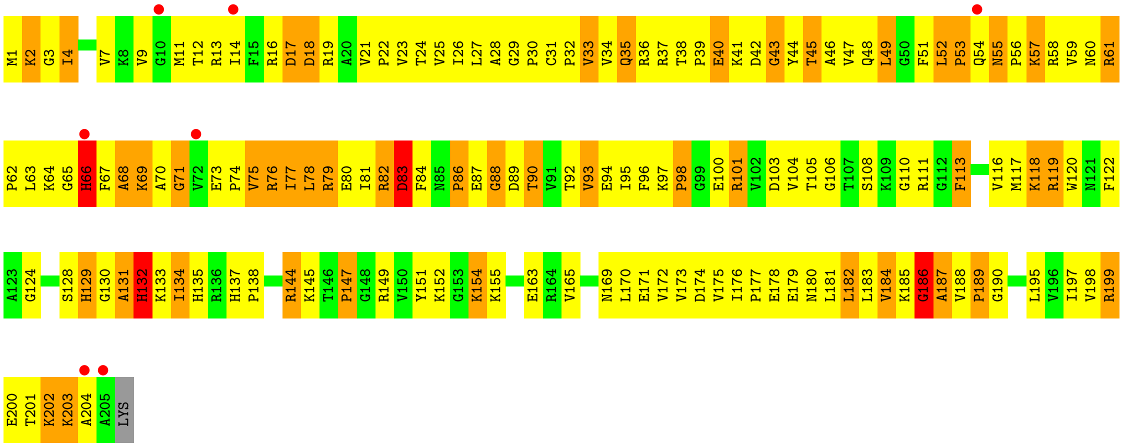
Chain DD:



- Molecule 39: 50S RIBOSOMAL PROTEIN L3

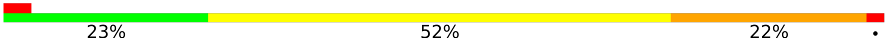
Chain BE:

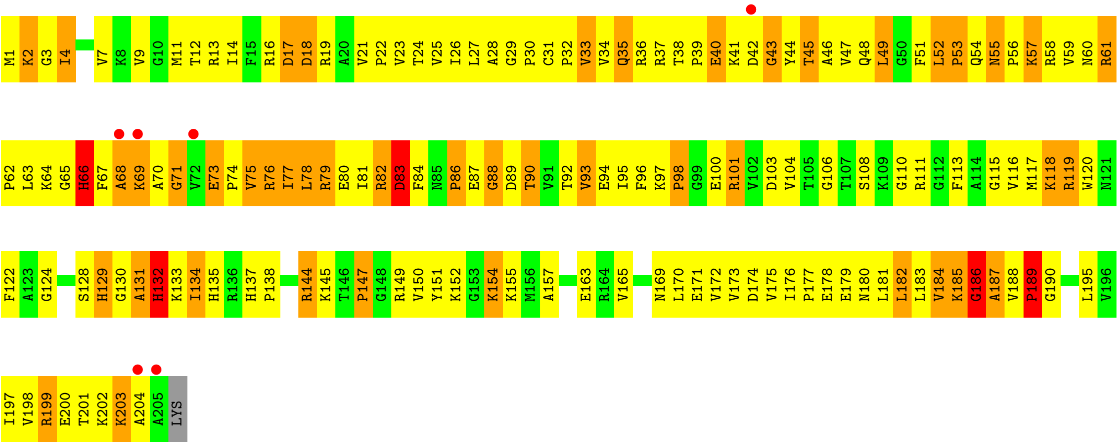




- Molecule 39: 50S RIBOSOMAL PROTEIN L3

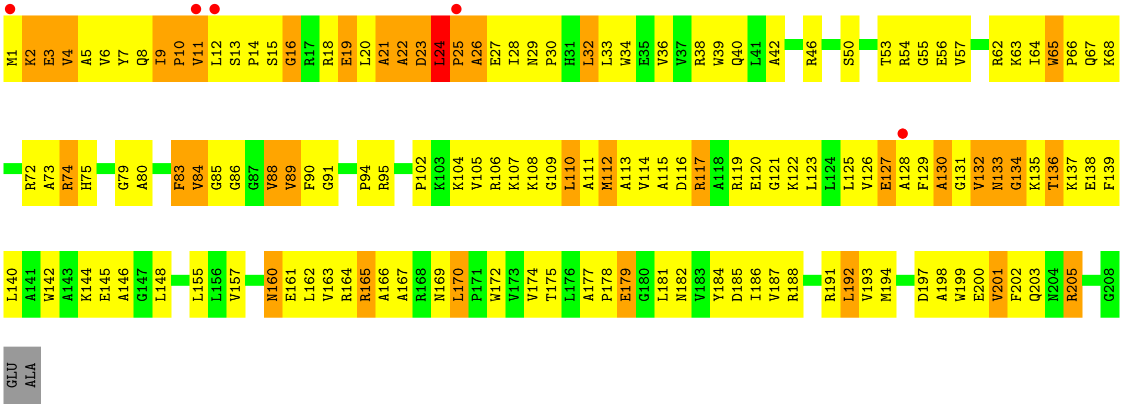
Chain DE:





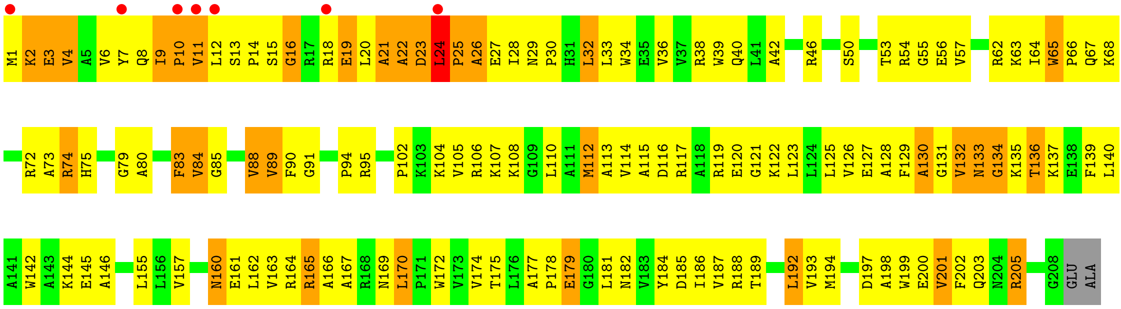
- Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain BF:



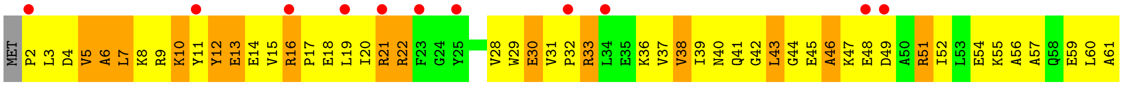
- Molecule 40: 50S RIBOSOMAL PROTEIN L4

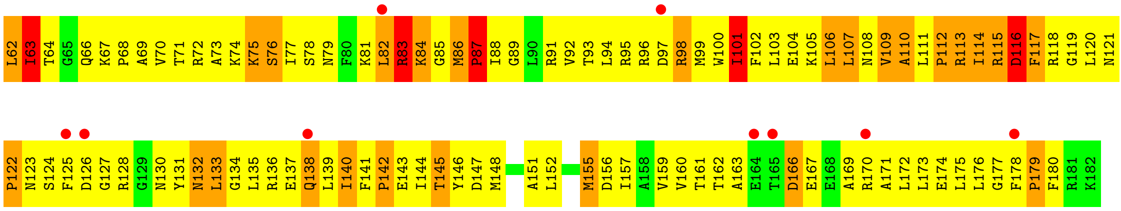
Chain DF:



- Molecule 41: 50S RIBOSOMAL PROTEIN L5

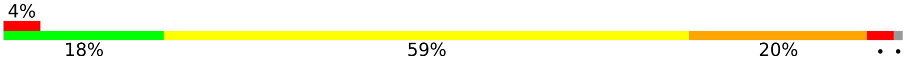
Chain BG:

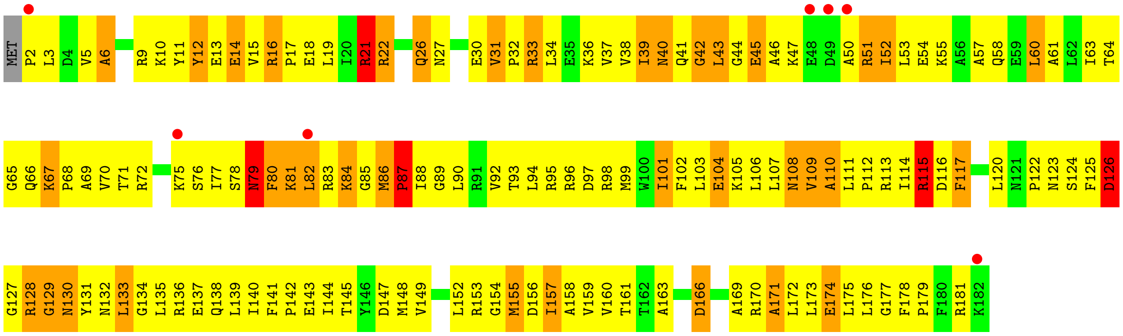




- Molecule 41: 50S RIBOSOMAL PROTEIN L5

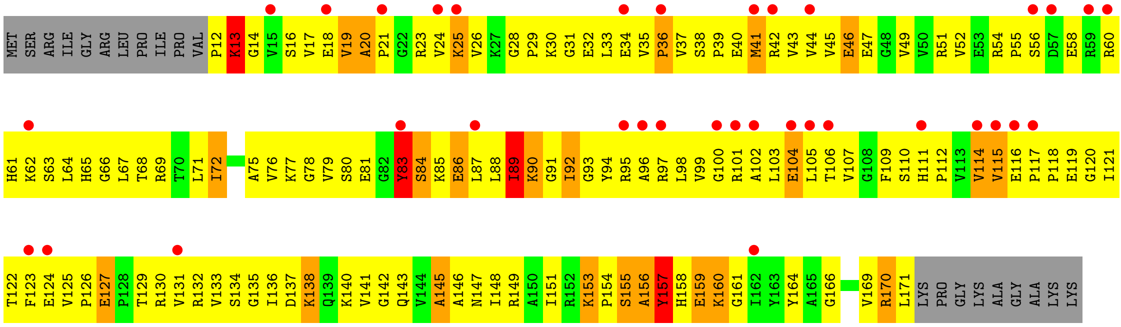
Chain DG:





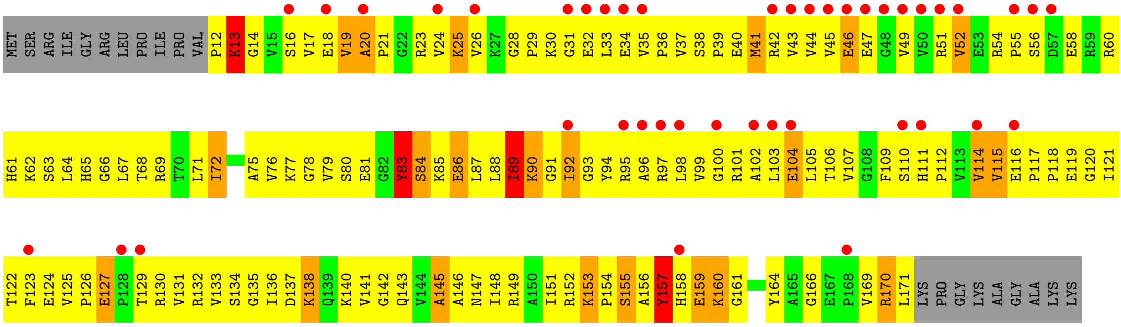
- Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain BH:

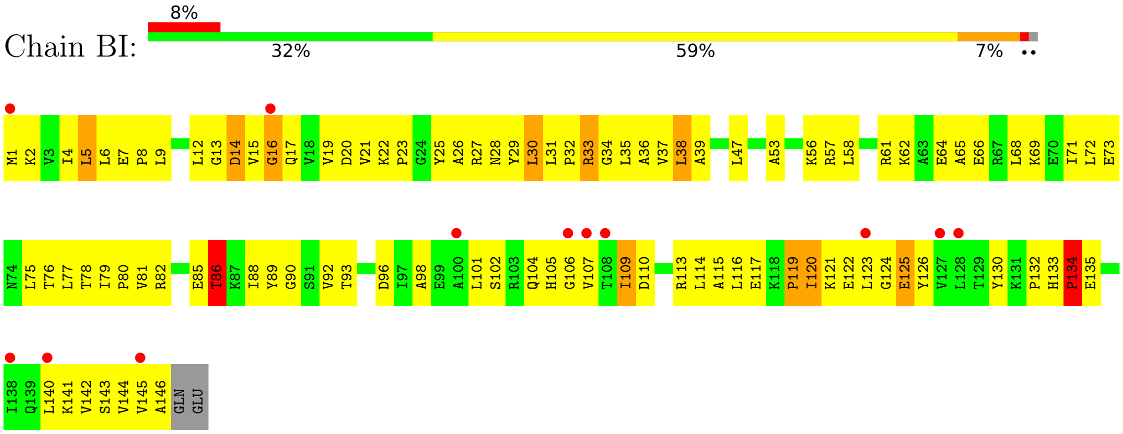


- Molecule 42: 50S RIBOSOMAL PROTEIN L6

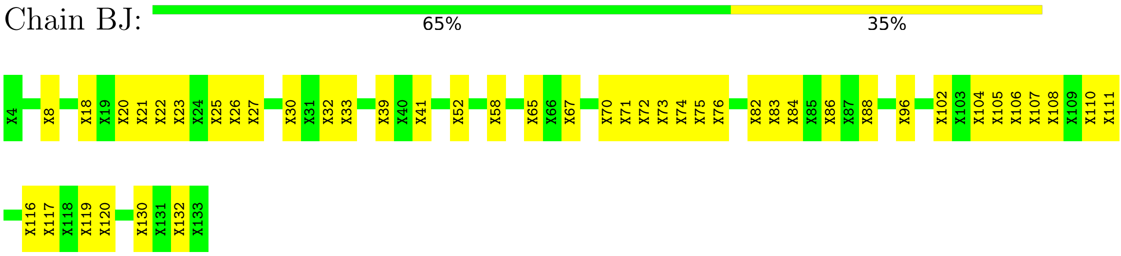
Chain DH:



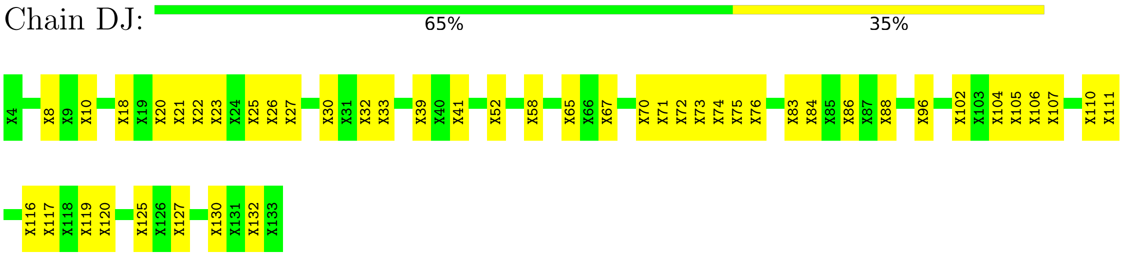
- Molecule 43: 50S RIBOSOMAL PROTEIN L9



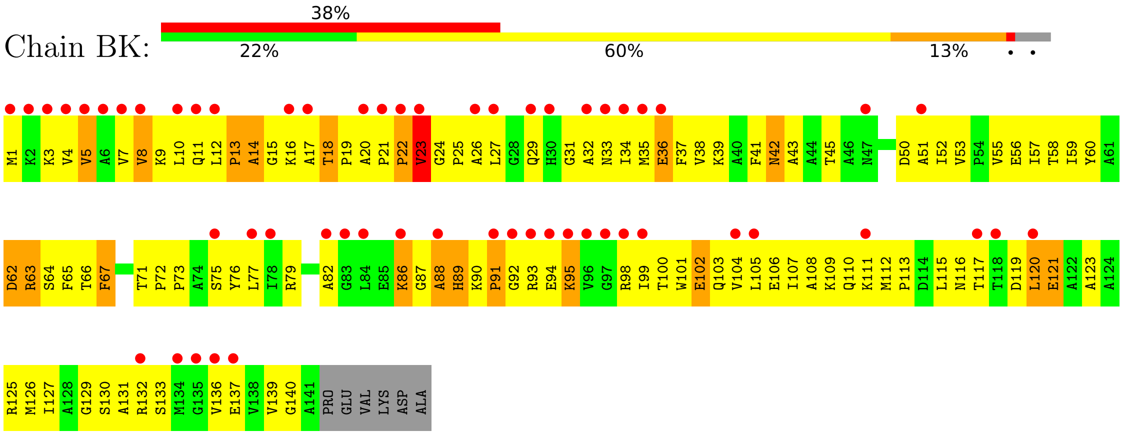
- Molecule 44: 50S RIBOSOMAL PROTEIN L10



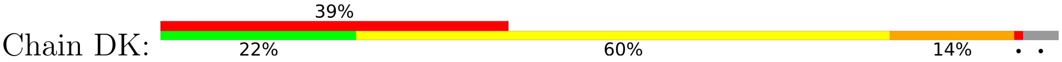
- Molecule 44: 50S RIBOSOMAL PROTEIN L10

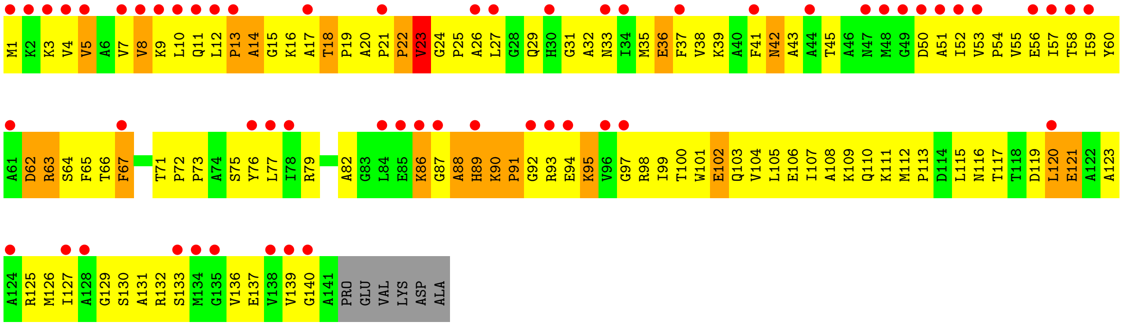


- Molecule 45: 50S RIBOSOMAL PROTEIN L11



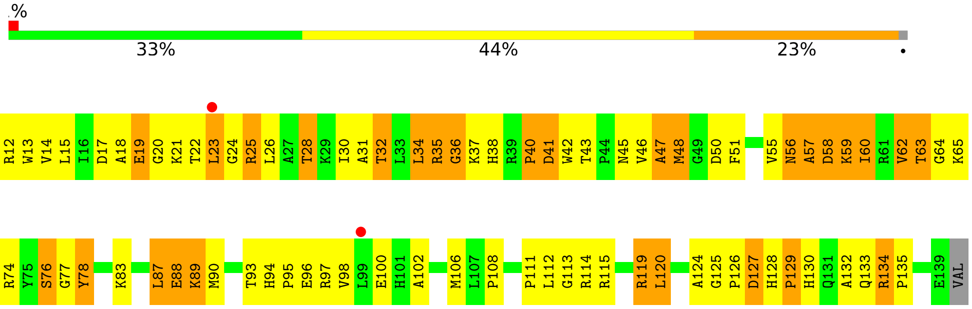
- Molecule 45: 50S RIBOSOMAL PROTEIN L11





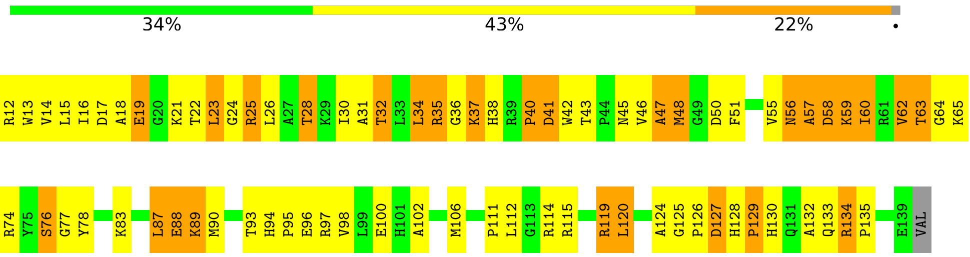
- Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:



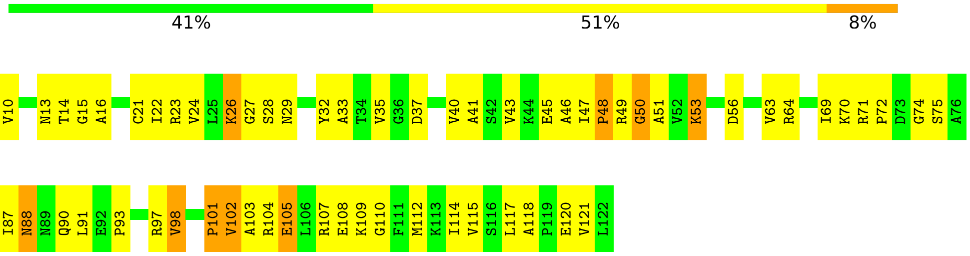
- Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN:



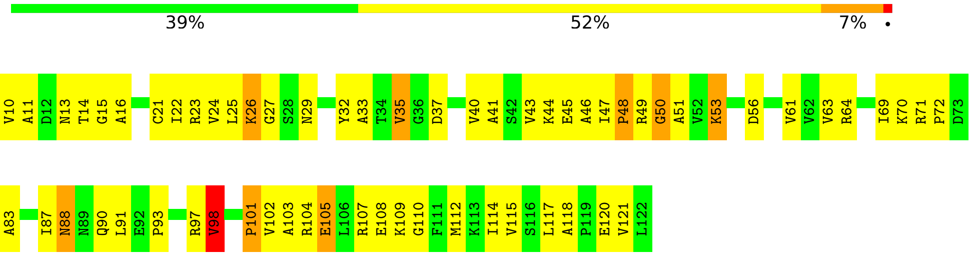
- Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:



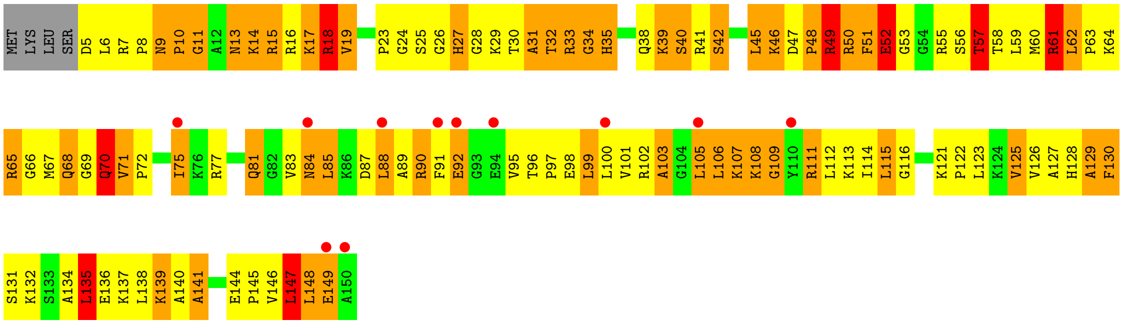
- Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO:



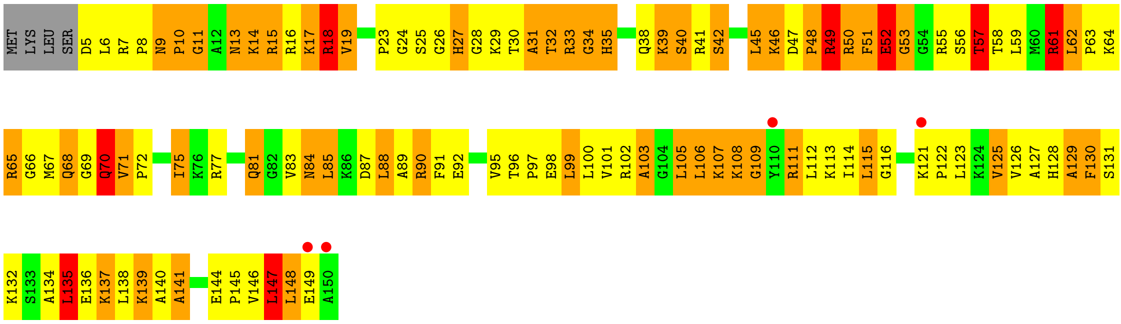
- Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP:



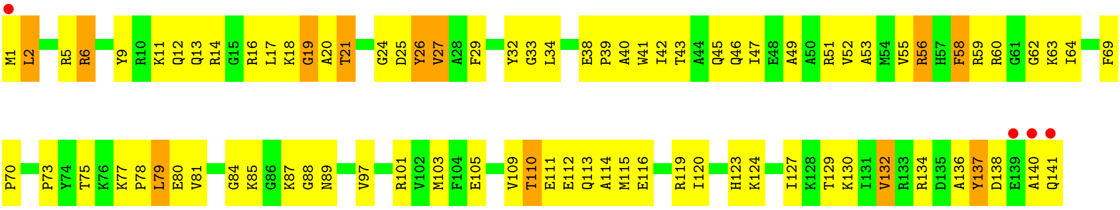
- Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP:



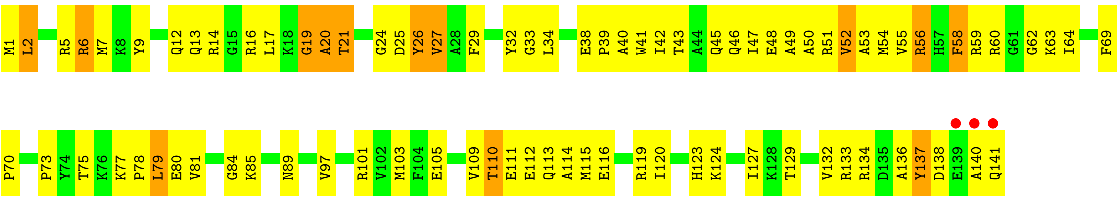
- Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:

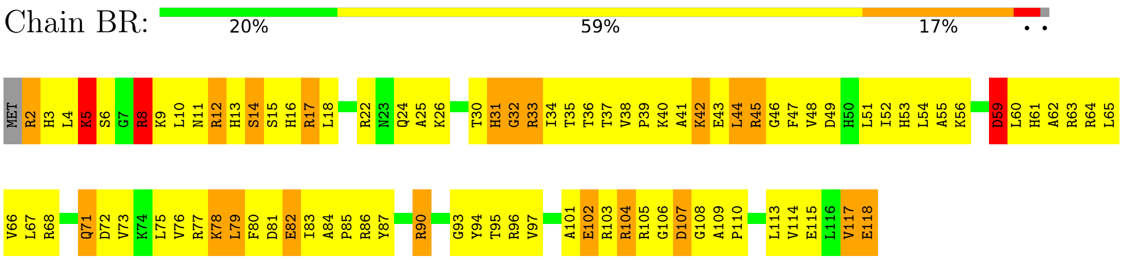


- Molecule 49: 50S RIBOSOMAL PROTEIN L16

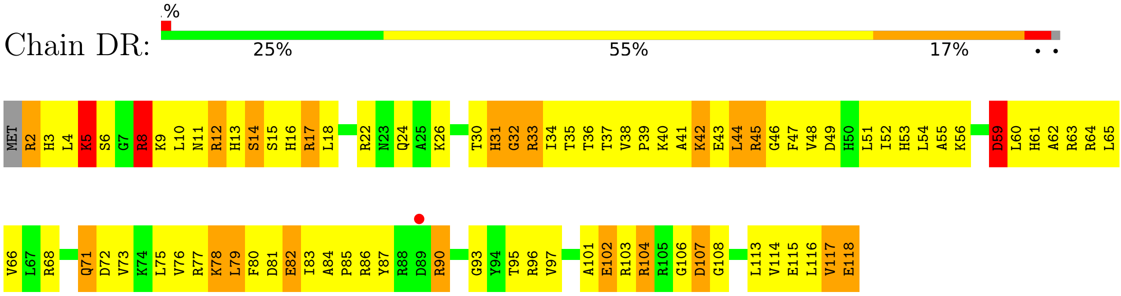
Chain DQ:



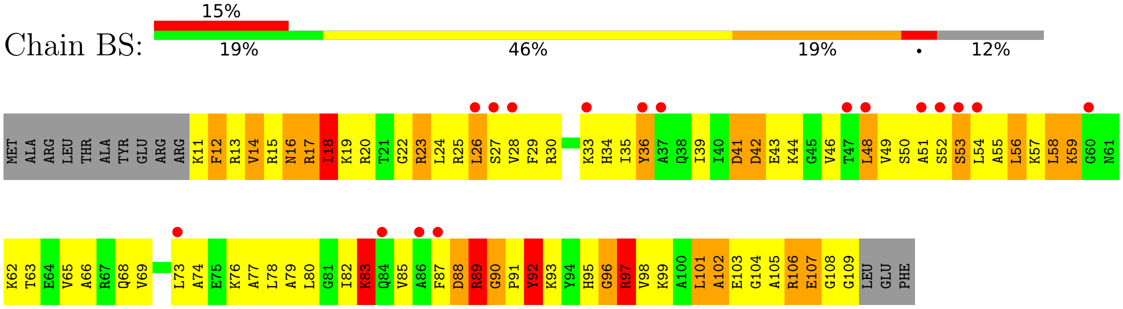
- Molecule 50: 50S RIBOSOMAL PROTEIN L17



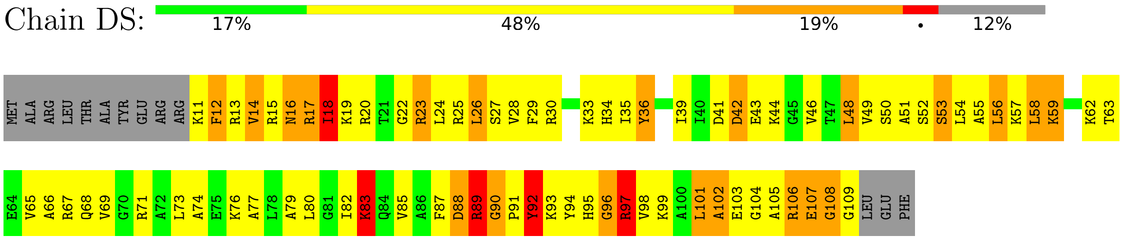
- Molecule 50: 50S RIBOSOMAL PROTEIN L17



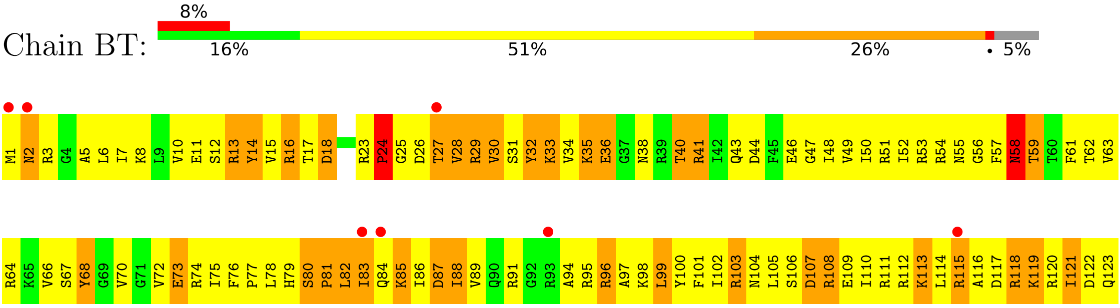
- Molecule 51: 50S RIBOSOMAL PROTEIN L18

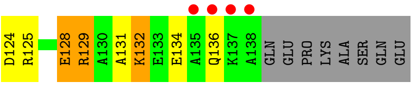


- Molecule 51: 50S RIBOSOMAL PROTEIN L18



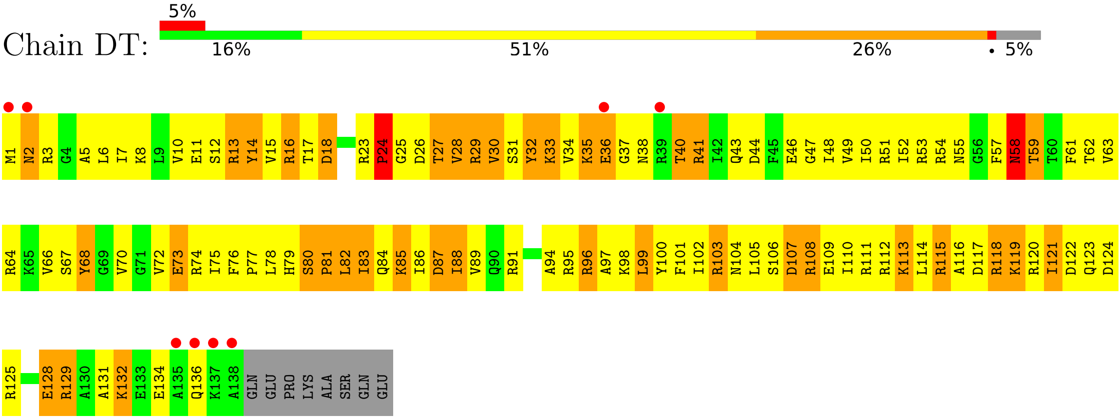
- Molecule 52: 50S RIBOSOMAL PROTEIN L19





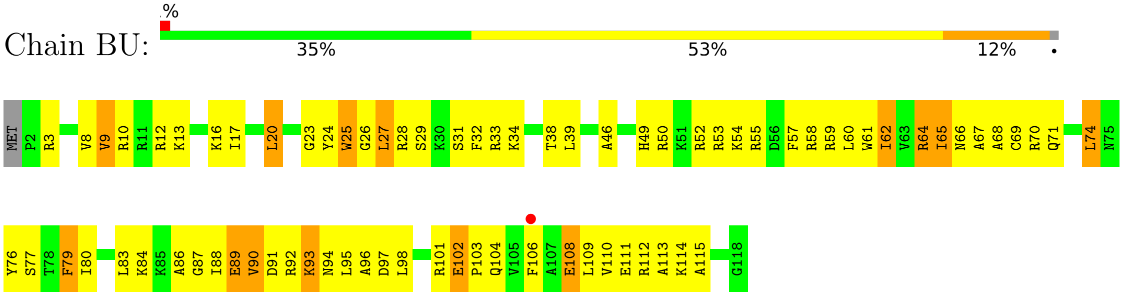
- Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain DT:



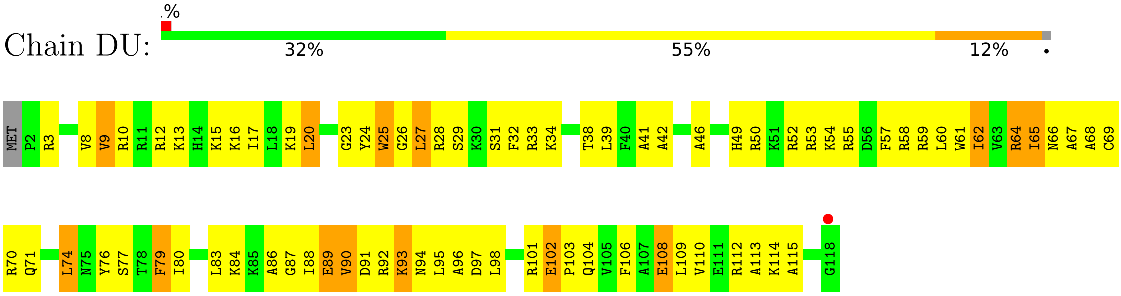
- Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU:



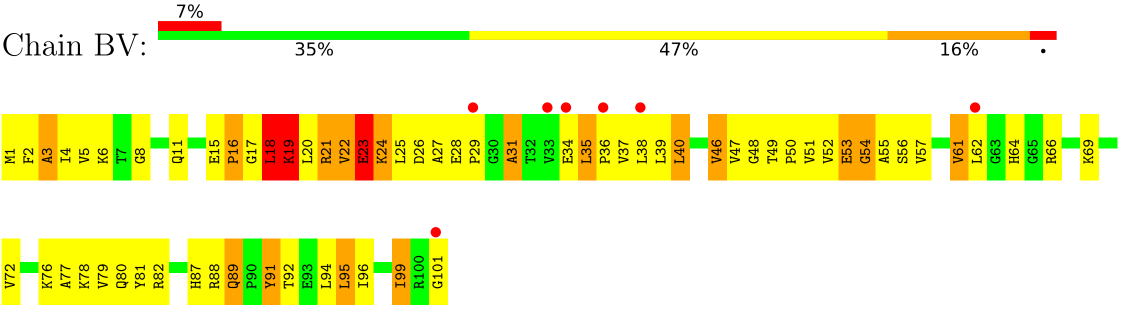
- Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain DU:



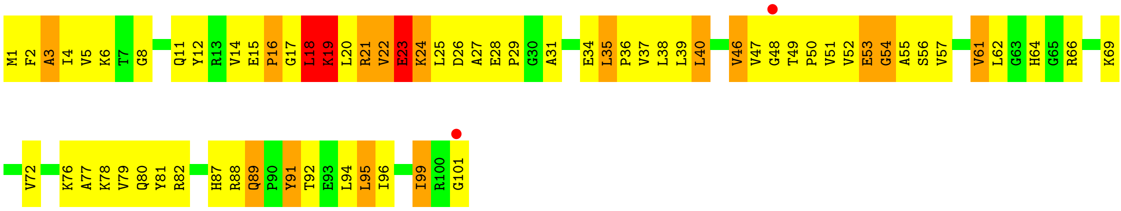
- Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain BV:



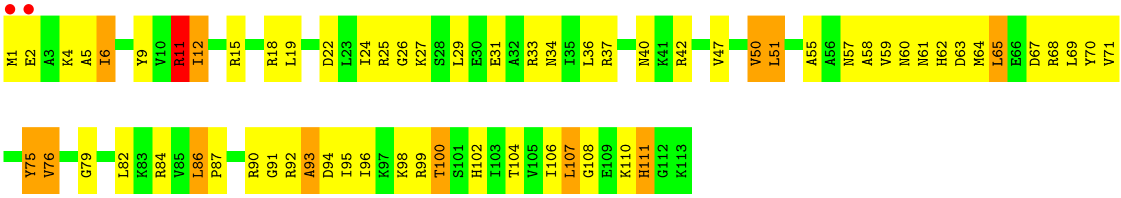
- Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain DV:



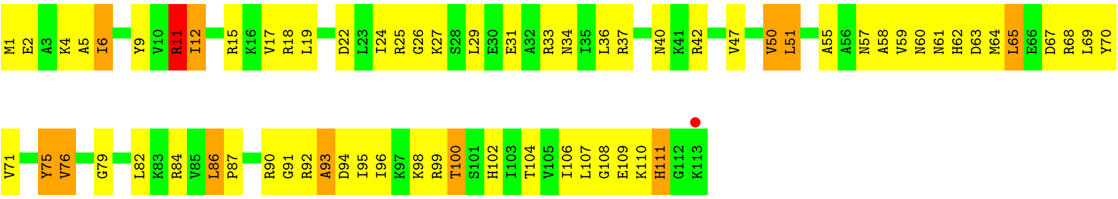
- Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain BW:



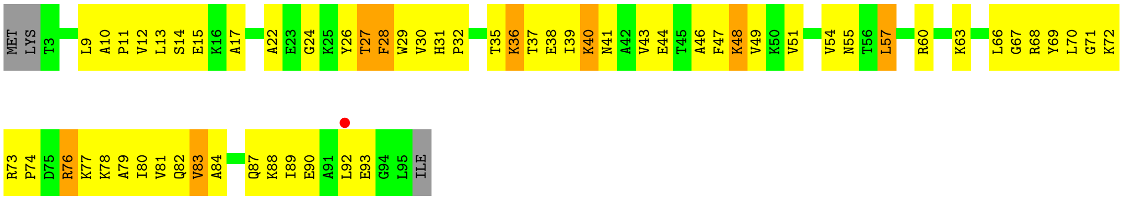
- Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain DW:



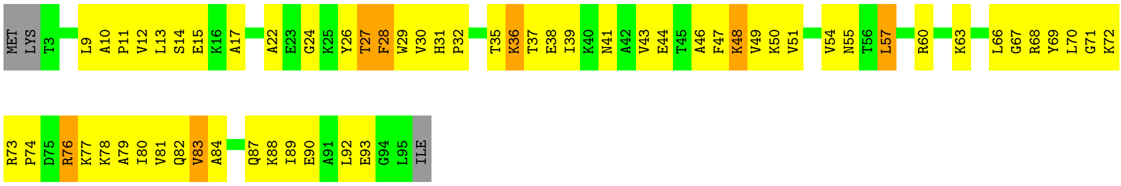
- Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



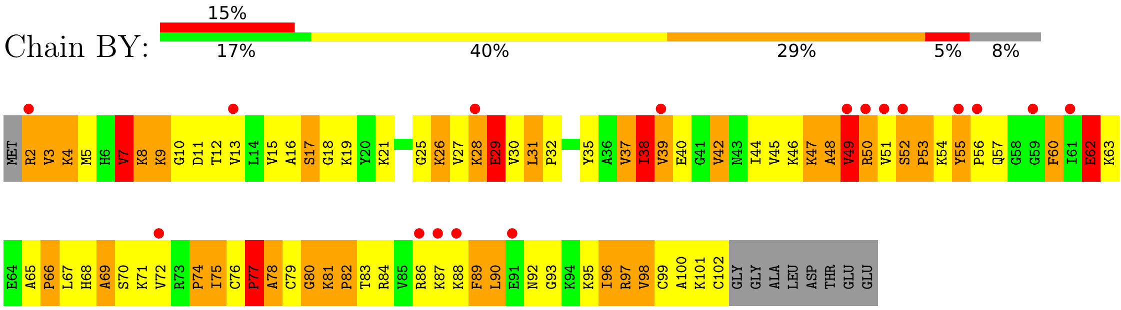
- Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain DX:



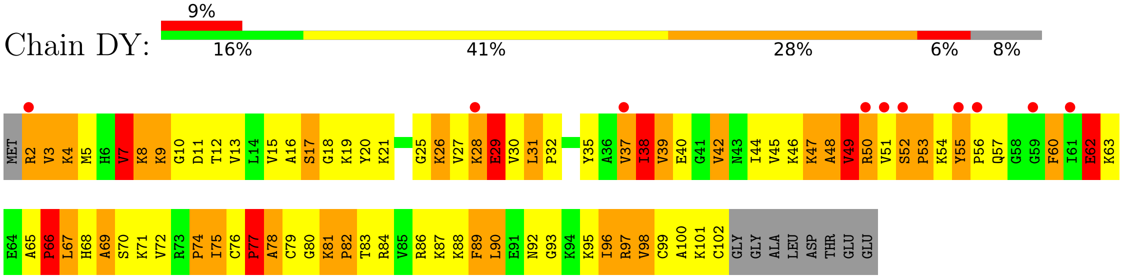
- Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY:



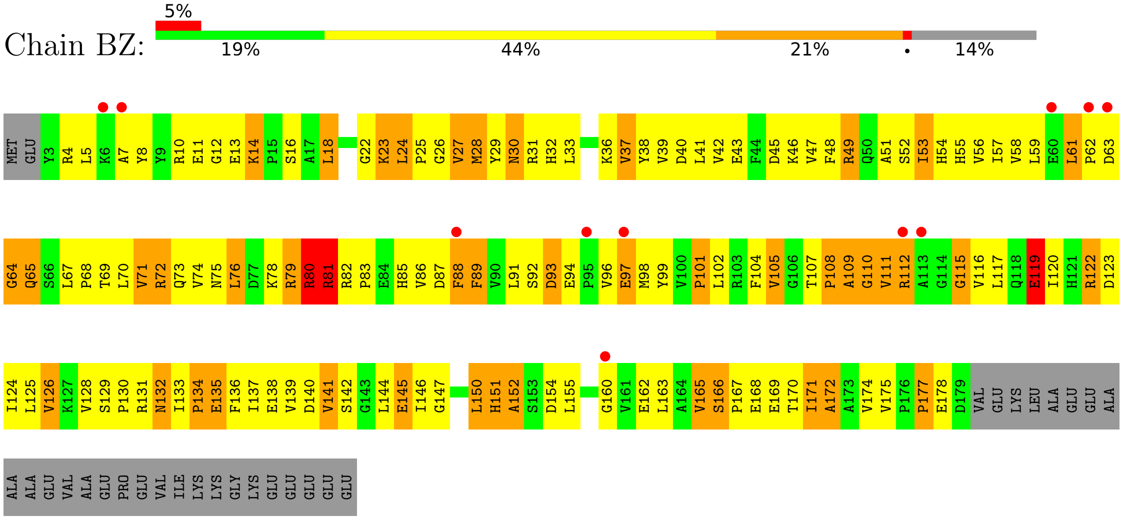
- Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain DY:



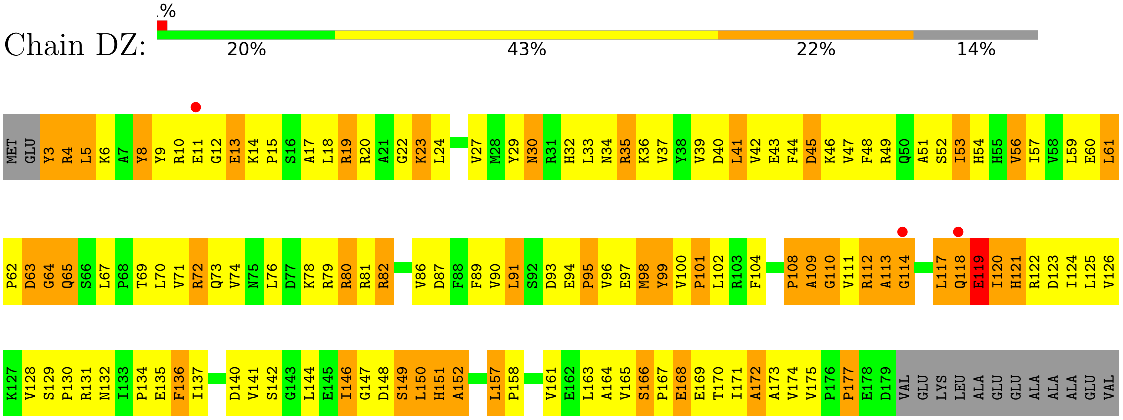
- Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain BZ:

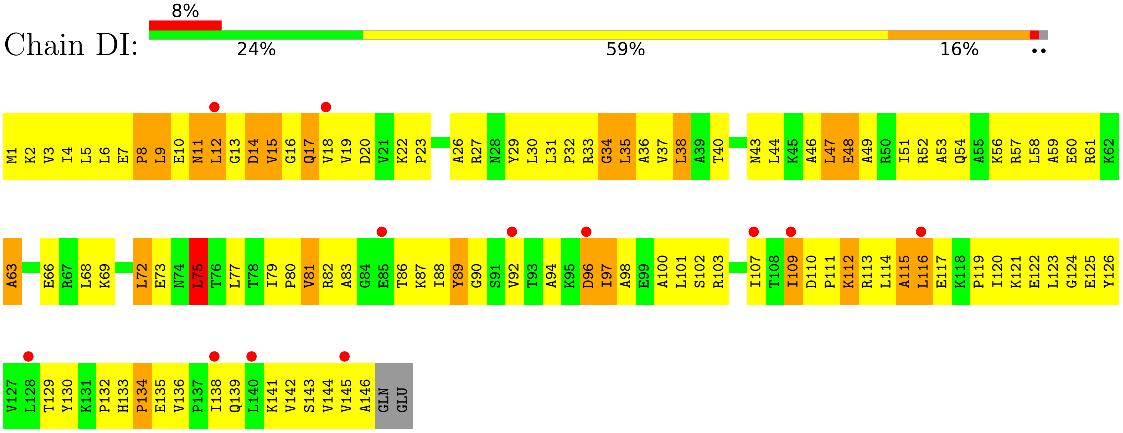


- Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain DZ:



- Molecule 59: 50S RIBOSOMAL PROTEIN L9



4 Data and refinement statistics

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.*

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[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 ⓘ

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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	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 ⓘ

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 ⓘ

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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

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

There are no such residues in this entry.