wwPDB X-ray Structure Validation Summary Report (i)

Jan 14, 2024 – 10:26 am GMT

PDB ID	:	6I7V
Title	:	Ribosomal protein paralogs bL31 and bL36
Authors	:	Pulk, A.; Cate, J.H.D.; Remme, J.; Lilleorg, S.; Reier, K.; Peil, L.; Liiv, A.; Tammsalu, T.
Deposited on	:	2018-11-19
Resolution	:	2.90 Å(reported)

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

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

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

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

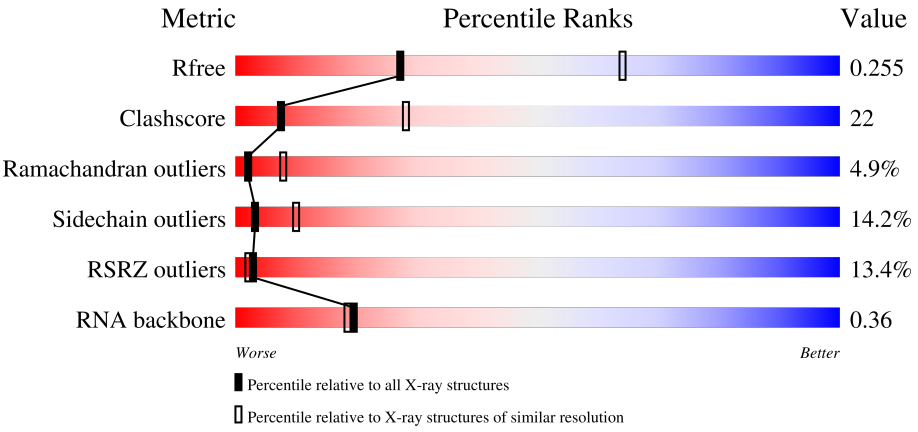
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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	1533	16% 40% 37% 7%
2	BA	1533	2% 19% 45% 30% 6%
3	DA	2903	7% 37% 43% 12%
4	CA	2904	3% 20% 48% 27%

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Mol	Chain	Length	Quality of chain
5	CB	119	42% 42% 15%
5	DB	119	9% 46% 41%
6	AB	218	17% 36% 39% 22%
6	BB	218	20% 31% 44% 20% 5%
7	AC	206	61% 30% 8%
7	BC	206	4% 54% 35% 9%
8	AD	205	8% 59% 28% 11%
8	BD	205	60% 31% 7%
9	AE	150	41% 39% 17%
9	BE	150	3% 40% 41% 17%
10	AF	100	57% 34% 7%
10	BF	100	8% 48% 36% 11% 5%
11	AG	151	12% 56% 38% 6%
11	BG	151	46% 42% 46% 11%
12	AH	129	6% 60% 32% 7%
12	BH	129	5% 59% 34% 6%
13	AI	127	9% 48% 39% 9%
13	BI	127	39% 36% 50% 13%
14	AJ	98	9% 26% 50% 22%
14	BJ	98	44% 43% 44% 13%
15	AK	117	13% 62% 31% 7%
15	BK	117	3% 54% 36% 9%
16	AL	123	63% 33%
17	AM	114	5% 53% 32% 15%
17	BM	114	79% 54% 35% 10%

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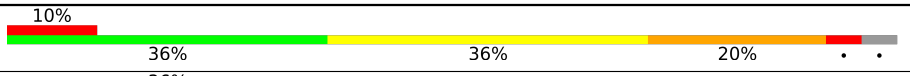
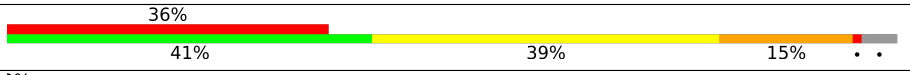
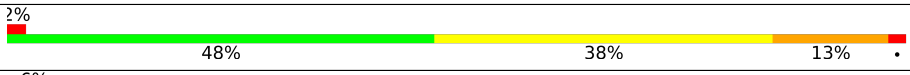
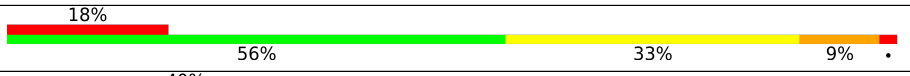
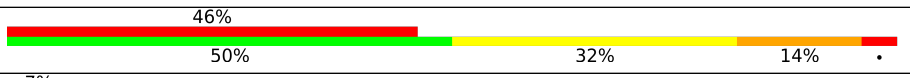
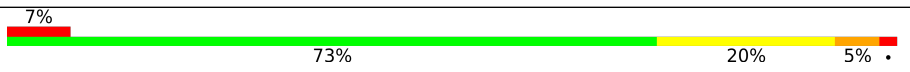
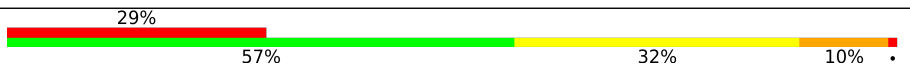
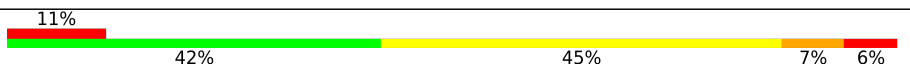
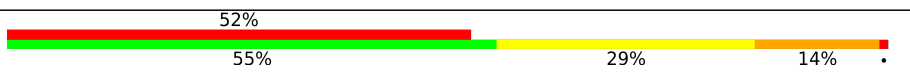
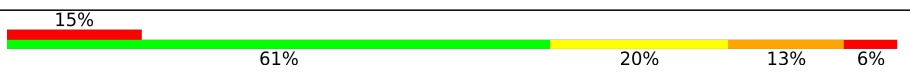
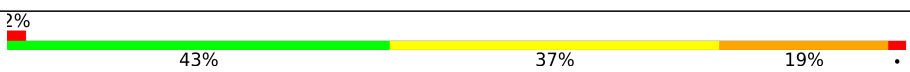
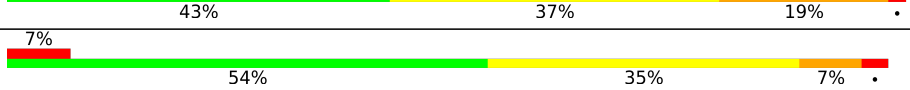
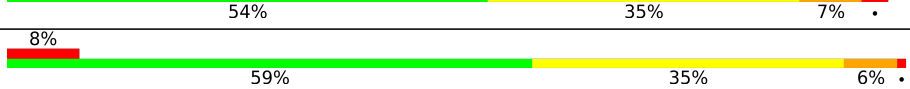
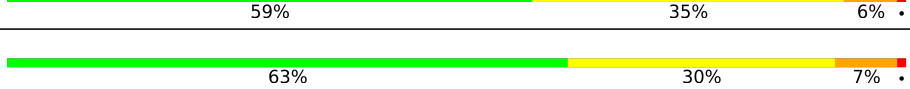
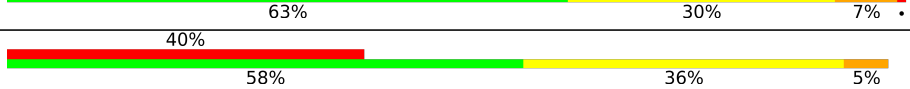
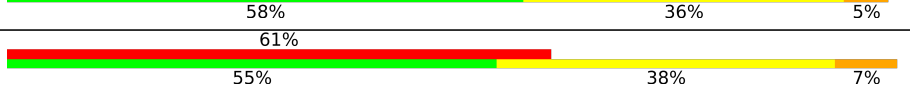
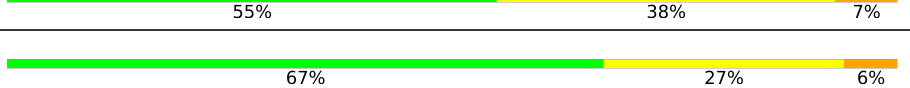
Mol	Chain	Length	Quality of chain
18	AN	100	
18	BN	100	
19	AO	88	
19	BO	88	
20	AP	82	
20	BP	82	
21	AQ	80	
21	BQ	80	
22	AR	55	
22	BR	55	
23	AS	79	
23	BS	79	
24	AT	85	
24	BT	85	
25	AU	54	
25	BU	54	
26	BL	123	
27	CC	271	
27	DC	271	
28	CD	209	
29	CE	201	
29	DE	201	
30	CF	177	
30	DF	177	
31	CG	176	

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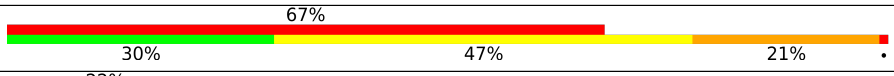
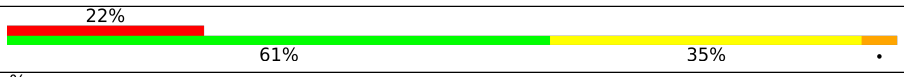
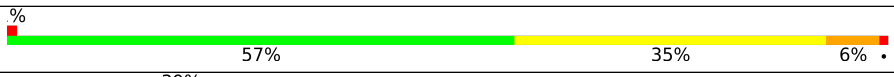
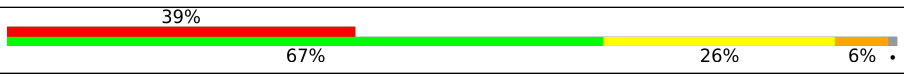
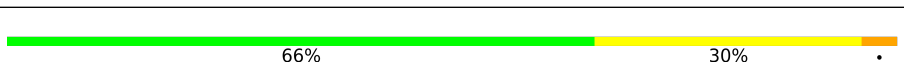
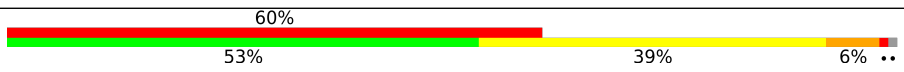
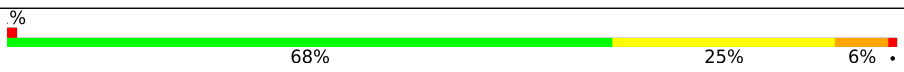
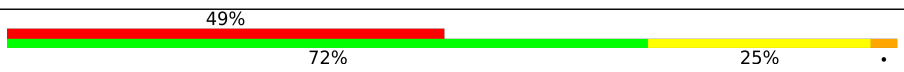
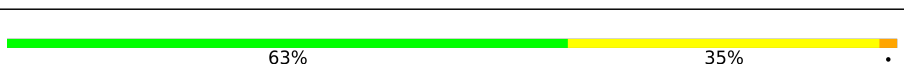
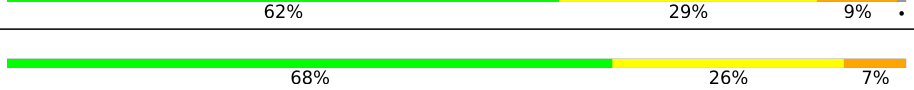
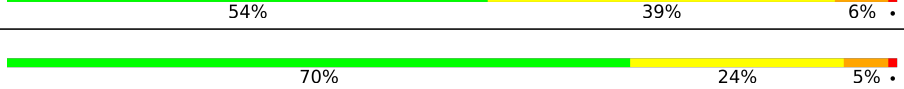
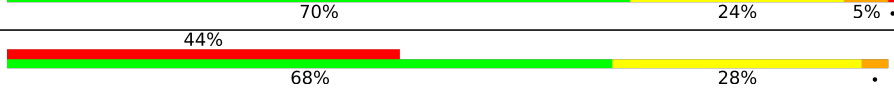
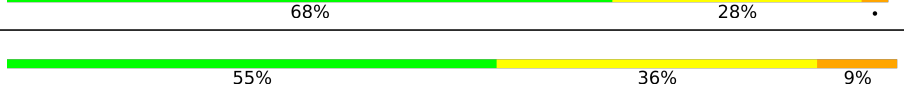
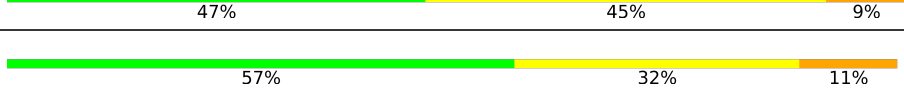
Mol	Chain	Length	Quality of chain
31	DG	176	
32	CH	148	
32	DH	148	
33	CJ	141	
33	DJ	141	
34	CK	142	
34	DK	142	
35	CL	123	
35	DL	123	
36	CM	144	
36	DM	144	
37	CN	136	
37	DN	136	
38	CO	120	
38	DO	120	
39	CP	117	
39	DP	117	
40	CQ	114	
40	DQ	114	
41	CR	117	
41	DR	117	
42	CS	103	
42	DS	103	
43	CT	110	
43	DT	110	

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Mol	Chain	Length	Quality of chain
44	CU	93	78% 53% 33% 13%
44	DU	93	2% 65% 31%
45	CV	102	83% 51% 40% 8%
45	DV	102	2% 68% 25% 5%
46	CW	94	37% 71% 26%
46	DW	94	% 70% 21% 9%
47	CX	76	61% 75% 21%
47	DX	76	% 63% 32% 5%
48	CY	77	40% 49% 44% 6%
48	DY	77	70% 26%
49	CZ	62	52% 60% 31% 8%
49	DZ	62	2% 52% 35% 11%
50	C0	58	33% 50% 41% 7%
50	D0	58	60% 31% 9%
51	C1	56	38% 50% 36% 14%
51	D1	56	57% 34% 5%
52	C2	51	57% 59% 39%
52	D2	51	73% 25%
53	C3	46	43% 39% 50% 11%
53	D3	46	2% 70% 22% 7%
54	C4	64	42% 48% 48%
54	D4	64	69% 22% 9%
55	C5	45	58% 40% 44% 11%
55	D5	45	36% 36% 29%
56	DD	209	66% 30% 5%

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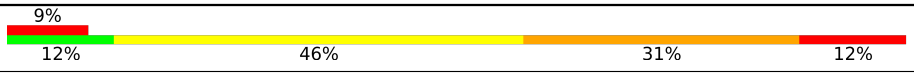
Mol	Chain	Length	Quality of chain
57	D7	68	

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
1	MA6	AA	1519	-	-	X	-
3	2MG	DA	1835	-	-	X	-
3	OMC	DA	2498	-	-	X	-
3	5MU	DA	747	-	-	X	-
58	MG	CA	3017	-	-	-	X
58	MG	CA	3049	-	-	-	X
58	MG	CA	3084	-	-	-	X
58	MG	CA	3102	-	-	-	X
58	MG	CA	3154	-	-	-	X
58	MG	CA	3159	-	-	-	X
58	MG	CA	3173	-	-	-	X
58	MG	D5	102	-	-	-	X
59	PGE	DD	301	-	-	-	X
59	PGE	DT	202	-	-	-	X
60	MPD	DA	3072	-	-	-	X
60	MPD	DE	301	-	-	-	X
60	MPD	DE	302	-	-	-	X
60	MPD	DT	201	-	-	-	X
61	PG4	DR	202	-	-	X	-
63	PUT	DA	3037	-	-	X	-
63	PUT	DA	3054	-	-	X	-
63	PUT	DP	202	-	-	X	-
65	ACY	DA	3064	-	-	X	-
66	PEG	D1	102	-	-	-	X
66	PEG	DA	3063	-	-	-	X
66	PEG	DP	201	-	-	-	X
66	PEG	DQ	201	-	-	-	X
67	EDO	DA	3059	-	-	X	-
67	EDO	DA	3060	-	-	X	-

2 Entry composition (i)

There are 69 unique types of molecules in this entry. The entry contains 484785 atoms, of which 191884 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	H	N	O	P			
1	AA	1533	49352	14684	16444	6036	10655	1533	0	0	0

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	BA	1533	49448	14671	16553	6036	10655	1533	0	0	0

- Molecule 3 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trac
			Total	C	H	N	O	P			
3	DA	2897	93383	27779	31129	11456	20120	2899	0	2	0

- Molecule 4 is a RNA chain called 23S ribsomal RNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trac
			Total	C	H	N	O	P			
4	CA	2898	93503	27754	31288	11448	20115	2898	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
5	DB	119	3840	1135	1291	466	829	119	0	0	0
5	CB	118	Total 3810	C 1126	H 1281	N 464	O 821	P 118	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	AB	218	Total	C	H	N	O	S	0	0	0
			3431	1081	1726	305	312	7			
6	BB	218	Total	C	H	N	O	S	0	0	0
			3431	1081	1726	305	312	7			

- Molecule 7 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	AC	206	Total	C	H	N	O	S	0	0	0
			3317	1028	1692	305	289	3			
7	BC	206	Total	C	H	N	O	S	0	0	0
			3317	1028	1692	305	289	3			

- Molecule 8 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	AD	205	Total	C	H	N	O	S	0	0	0
			3347	1026	1704	315	298	4			
8	BD	205	Total	C	H	N	O	S	0	0	0
			3347	1026	1704	315	298	4			

- Molecule 9 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	AE	150	Total	C	H	N	O	S	0	0	0
			2251	687	1145	211	202	6			
9	BE	150	Total	C	H	N	O	S	0	0	0
			2251	687	1145	211	202	6			

- Molecule 10 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
10	AF	100	Total	C	H	N	O	S	0	0	0
			1617	515	799	148	149	6			
10	BF	100	Total	C	H	N	O	S	0	0	0
			1617	515	799	148	149	6			

- Molecule 11 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	AG	151	Total	C	H	N	O	S	0	0	0
			2419	735	1237	227	216	4			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	BG	151	Total	C	H	N	O	S	0	0	0
			2419	735	1237	227	216	4			

- Molecule 12 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
12	AH	129	Total	C	H	N	O	S	0	0	0
			2010	616	1031	173	184	6			
12	BH	129	Total	C	H	N	O	S	0	0	0
			2010	616	1031	173	184	6			

- Molecule 13 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	AI	127	Total	C	H	N	O	S	0	0	0
			2091	634	1069	206	179	3			
13	BI	127	Total	C	H	N	O	S	0	0	0
			2091	634	1069	206	179	3			

- Molecule 14 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
14	AJ	98	Total	C	H	N	O	S	0	0	0
			1612	493	825	150	143	1			
14	BJ	98	Total	C	H	N	O	S	0	0	0
			1612	493	825	150	143	1			

- Molecule 15 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	AK	117	Total	C	H	N	O	S	0	0	0
			1761	540	884	174	160	3			
15	BK	117	Total	C	H	N	O	S	0	0	0
			1761	540	884	174	160	3			

- Molecule 16 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	AL	123	Total	C	H	N	O	S	0	0	0
			1966	591	1009	196	165	5			

- Molecule 17 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	AM	114	Total	C	H	N	O	S	0	0	0
			1822	546	938	178	157	3			
17	BM	114	Total	C	H	N	O	S	0	0	0
			1822	546	938	178	157	3			

- Molecule 18 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
18	AN	96	Total	C	H	N	O	S	0	0	0
			1597	483	823	160	128	3			
18	BN	96	Total	C	H	N	O	S	0	0	0
			1597	483	823	160	128	3			

- Molecule 19 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	AO	88	Total	C	H	N	O	S	0	0	0
			1450	440	734	146	129	1			
19	BO	88	Total	C	H	N	O	S	0	0	0
			1450	440	734	146	129	1			

- Molecule 20 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	AP	82	Total	C	H	N	O	S	0	0	0
			1310	406	661	128	114	1			
20	BP	82	Total	C	H	N	O	S	0	0	0
			1310	406	661	128	114	1			

- Molecule 21 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
21	AQ	80	Total	C	H	N	O	S	0	0	0
			1337	411	688	121	114	3			
21	BQ	80	Total	C	H	N	O	S	0	0	0
			1337	411	688	121	114	3			

- Molecule 22 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AR	55	Total	C	H	N	O	0	0	0
			933	288	477	86	82			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BR	55	Total	C	H	N	O	0	0	0
			933	288	477	86	82			

- Molecule 23 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	AS	79	Total	C	H	N	O	S	0	0	0
			1295	408	657	120	108	2			
23	BS	79	Total	C	H	N	O	S	0	0	0
			1299	408	661	120	108	2			

- Molecule 24 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	AT	85	Total	C	H	N	O	S	0	0	0
			1376	411	711	137	114	3			
24	BT	85	Total	C	H	N	O	S	0	0	0
			1376	411	711	137	114	3			

- Molecule 25 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
25	AU	54	Total	C	H	N	O	S	0	0	0
			924	280	473	94	76	1			
25	BU	54	Total	C	H	N	O	S	0	0	0
			924	280	473	94	76	1			

- Molecule 26 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
26	BL	123	Total	C	H	N	O	S	0	0	0
			1968	590	1013	196	165	4			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
27	CC	271	Total	C	H	N	O	S	0	0	0
			4231	1288	2148	423	365	7			
27	DC	271	Total	C	H	N	O	S	0	0	0
			4231	1288	2148	423	365	7			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
28	CD	209	Total	C	H	N	O	S	0	0	0
			3175	979	1610	288	294	4			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
29	CE	201	Total	C	H	N	O	S	0	0	0
			3165	974	1613	283	290	5			
29	DE	201	Total	C	H	N	O	S	0	0	0
			3165	974	1613	283	290	5			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
30	CF	177	Total	C	H	N	O	S	0	0	0
			2854	899	1443	249	257	6			
30	DF	177	Total	C	H	N	O	S	0	0	0
			2854	899	1443	249	257	6			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
31	CG	176	Total	C	H	N	O	S	0	0	0
			2691	832	1368	243	246	2			
31	DG	176	Total	C	H	N	O	S	0	0	0
			2691	832	1368	243	246	2			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
32	CH	148	Total	C	H	N	O	S	0	0	0
			2236	693	1134	197	211	1			
32	DH	148	Total	C	H	N	O	S	0	0	0
			2236	693	1134	197	211	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CH	?	-	LEU	deletion	UNP P0A7R1
CH	148	GLN	GLU	conflict	UNP P0A7R1
DH	?	-	LEU	deletion	UNP P0A7R1
DH	148	GLN	GLU	conflict	UNP P0A7R1

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
33	CJ	141	Total	C	H	N	O	S	0	0	0
			2117	651	1085	179	196	6			
33	DJ	141	Total	C	H	N	O	S	0	0	0
			2117	651	1085	179	196	6			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
34	CK	142	Total	C	H	N	O	S	0	0	0
			2281	714	1152	212	199	4			
34	DK	142	Total	C	H	N	O	S	0	0	0
			2281	714	1152	212	199	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
35	CL	122	Total	C	H	N	O	S	0	0	0
			1946	587	1008	180	165	6			
35	DL	123	Total	C	H	N	O	S	0	0	0
			1965	593	1019	181	166	6			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
36	CM	143	Total	C	H	N	O	S	0	0	0
			2161	649	1116	206	189	1			
36	DM	144	Total	C	H	N	O	S	0	0	0
			2178	654	1125	207	190	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
37	CN	136	Total	C	H	N	O	S	0	0	0
			2227	686	1153	205	177	6			
37	DN	136	Total	C	H	N	O	S	0	1	0
			2248	691	1166	208	177	6			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
38	CO	120	Total	C	H	N	O	S	0	0	0
			1955	593	994	196	167	5			
38	DO	120	Total	C	H	N	O	S	0	0	0
			1955	593	994	196	167	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
39	CP	116	Total	C	H	N	O		0	0	0
			1812	552	920	178	162				
39	DP	117	Total	C	H	N	O	S	0	0	0
			1829	557	929	179	163	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
40	CQ	114	Total	C	H	N	O	S	0	0	0
			1877	574	960	179	163	1			
40	DQ	114	Total	C	H	N	O	S	0	0	0
			1877	574	960	179	163	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CR	117	Total	C	H	N	O	0	0	0
			1965	604	1018	192	151			
41	DR	117	Total	C	H	N	O	0	0	0
			1965	604	1018	192	151			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
42	CS	103	Total	C	H	N	O	S	0	0	0
			1648	516	832	153	145	2			
42	DS	103	Total	C	H	N	O	S	0	0	0
			1648	516	832	153	145	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
43	CT	110	Total	C	H	N	O	S	0	0	0
			1772	532	915	166	156	3			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
43	DT	110	Total	C	H	N	O	S	0	0	0
			1772	532	915	166	156	3			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
44	CU	93	Total	C	H	N	O	S	0	0	0
			1541	466	802	139	132	2			
44	DU	92	Total	C	H	N	O	S	0	0	0
			1525	461	794	138	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	CV	102	Total	C	H	N	O	0	0	0
			1610	492	830	146	142			
45	DV	102	Total	C	H	N	O	0	0	0
			1610	492	830	146	142			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
46	CW	94	Total	C	H	N	O	S	0	0	0
			1527	479	774	137	134	3			
46	DW	94	Total	C	H	N	O	S	0	0	0
			1527	479	774	137	134	3			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
47	CX	75	Total	C	H	N	O	S	0	0	0
			1148	353	579	113	102	1			
47	DX	76	Total	C	H	N	O	S	0	2	0
			1197	365	606	121	104	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
48	CY	77	Total	C	H	N	O	S	0	0	0
			1274	388	649	129	106	2			
48	DY	77	Total	C	H	N	O	S	0	0	0
			1274	388	649	129	106	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
49	CZ	62	Total	C	H	N	O	S	0	0	0
			1031	308	530	98	94	1			
49	DZ	62	Total	C	H	N	O	S	0	0	0
			1031	308	530	98	94	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
50	C0	58	Total	C	H	N	O	S	0	0	0
			935	281	486	87	79	2			
50	D0	58	Total	C	H	N	O	S	0	1	0
			935	281	486	87	79	2			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
51	C1	56	Total	C	H	N	O	S	0	0	0
			898	269	454	94	80	1			
51	D1	56	Total	C	H	N	O	S	0	0	0
			898	269	454	94	80	1			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	C2	50	Total	C	H	N	O	0	0	0
			847	263	438	75	71			
52	D2	51	Total	C	H	N	O	0	0	0
			857	266	443	76	72			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C2	53	ALA	-	expression tag	UNP P0A7N9
D2	53	ALA	-	expression tag	UNP P0A7N9

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
53	C3	46	Total	C	H	N	O	S	0	0	0
			791	228	414	90	57	2			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
53	D3	46	Total	C	H	N	O	S	0	0	0
			791	228	414	90	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	C4	64	Total	C	H	N	O	S	0	0	0
			1072	323	568	105	74	2			
54	D4	64	Total	C	H	N	O	S	0	0	0
			1072	323	568	105	74	2			

- Molecule 55 is a protein called 50S ribosomal protein L36 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	C5	44	Total	C	H	N	O	S	0	0	0
			754	224	395	76	56	3			
55	D5	45	Total	C	H	N	O	S	0	0	0
			763	230	395	78	57	3			

- Molecule 56 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	DD	209	Total	C	H	N	O	S	0	0	0
			3178	980	1612	288	294	4			

- Molecule 57 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	D7	68	Total	C	H	N	O	S	0	0	0
			707	336	177	89	104	1			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	57	Total	Mg	0	0
			57	57		
58	BA	49	Total	Mg	0	0
			49	49		
58	DA	156	Total	Mg	0	0
			156	156		
58	CA	176	Total	Mg	0	0
			176	176		

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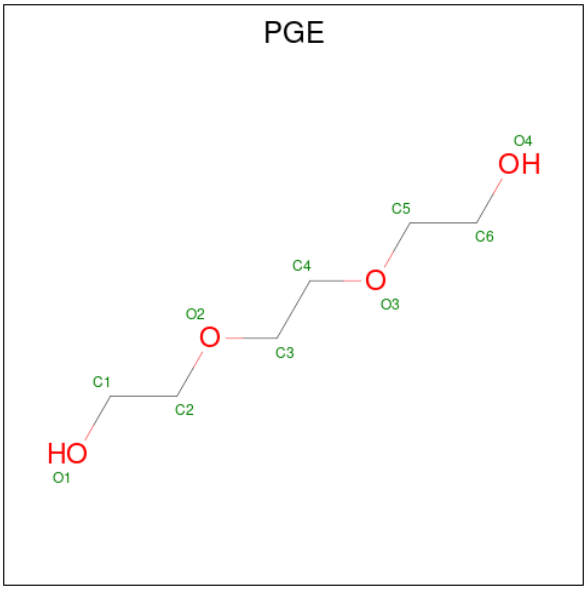
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	DB	4	Total Mg 4 4	0	0
58	CB	3	Total Mg 3 3	0	0
58	CM	1	Total Mg 1 1	0	0
58	CR	1	Total Mg 1 1	0	0
58	C3	1	Total Mg 1 1	0	0
58	DD	1	Total Mg 1 1	0	0
58	DM	1	Total Mg 1 1	0	0
58	DR	2	Total Mg 2 2	0	0
58	D5	1	Total Mg 1 1	0	0

- Molecule 59 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AA	1	Total C H O 24 6 14 4	0	0
59	DA	1	Total C H O 24 6 14 4	0	0

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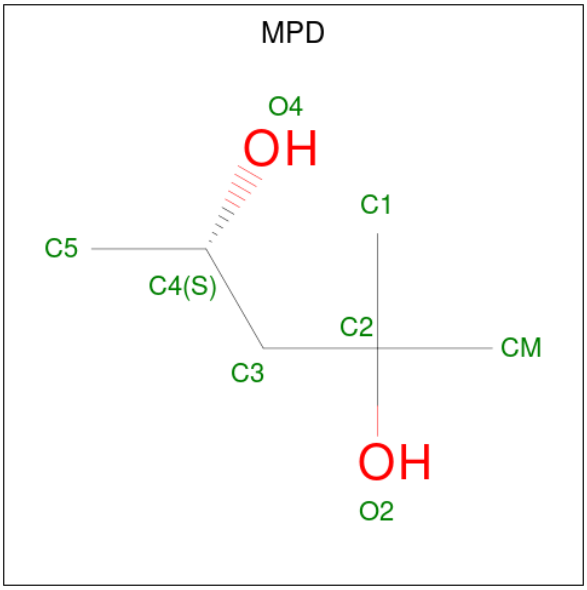
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	DA	1	Total	C	H	O	0	0
			24	6	14	4		
59	DD	1	Total	C	H	O	0	0
			24	6	14	4		
59	DS	1	Total	C	H	O	0	0
			24	6	14	4		
59	DT	1	Total	C	H	O	0	0
			24	6	14	4		
59	DU	1	Total	C	H	O	0	0
			24	6	14	4		
59	D3	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 60 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
60	AA	1	Total	C	H	O	0	0
			22	6	14	2		
60	DA	1	Total	C	H	O	0	0
			22	6	14	2		
60	DA	1	Total	C	H	O	0	0
			22	6	14	2		
60	DA	1	Total	C	H	O	0	0
			22	6	14	2		
60	DA	1	Total	C	H	O	0	0
			22	6	14	2		

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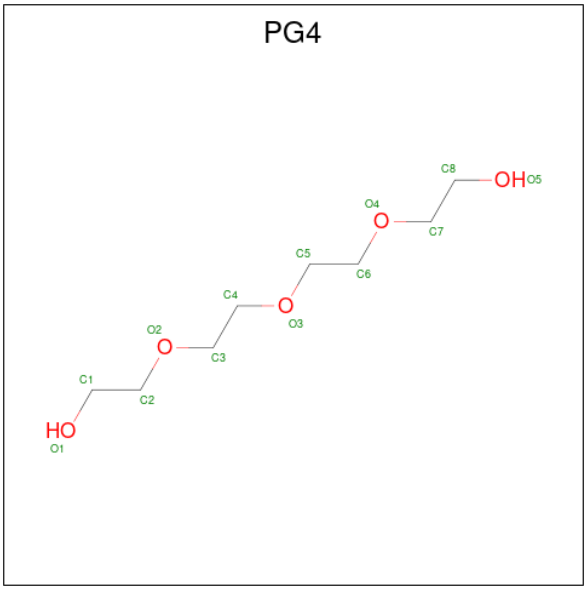
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	DA	1	Total C H O 22 6 14 2	0	0
60	DA	1	Total C H O 22 6 14 2	0	0
60	DA	1	Total C H O 22 6 14 2	0	0
60	DE	1	Total C H O 22 6 14 2	0	0
60	DE	1	Total C H O 22 6 14 2	0	0
60	DK	1	Total C H O 22 6 14 2	0	0
60	DN	1	Total C H O 22 6 14 2	0	0
60	DT	1	Total C H O 22 6 14 2	0	0

- Molecule 61 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	BA	1	Total C O 13 8 5	0	0
61	DA	1	Total C O 13 8 5	0	0
61	DQ	1	Total C O 13 8 5	0	0

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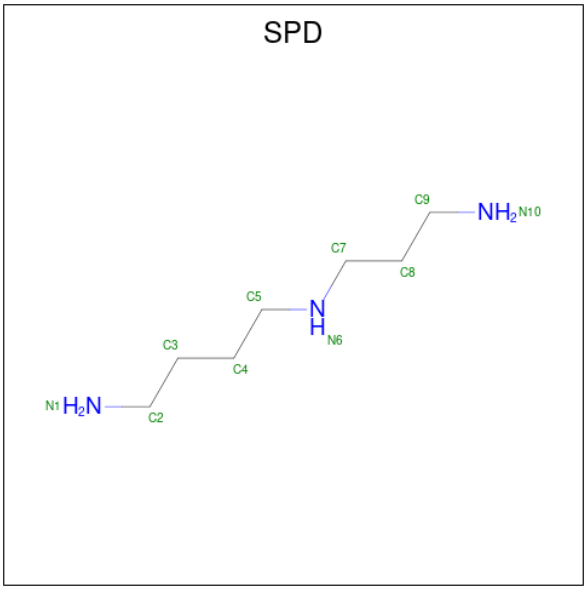
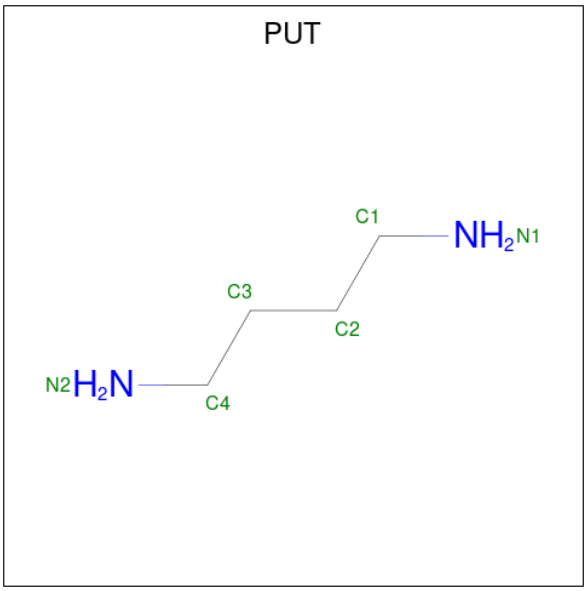
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	DR	1	Total C O 13 8 5	0	0
61	DS	1	Total C O 13 8 5	0	0

- Molecule 62 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



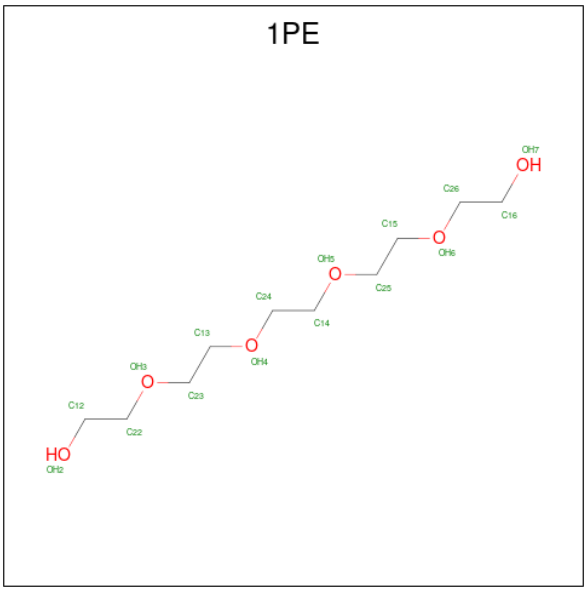
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	DA	1	Total C N 10 7 3	0	0
62	DA	1	Total C N 10 7 3	0	0
62	DA	1	Total C N 10 7 3	0	0

- Molecule 63 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



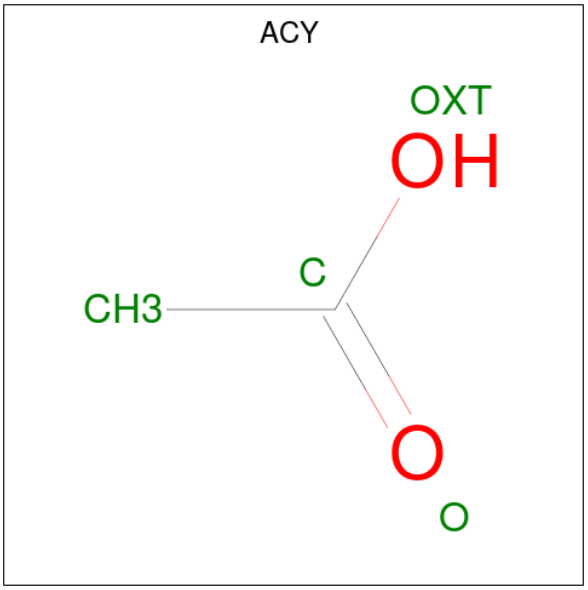
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	DA	1	Total C N 6 4 2	0	0
63	DA	1	Total C N 6 4 2	0	0
63	DA	1	Total C N 6 4 2	0	0
63	DA	1	Total C N 6 4 2	0	0
63	DM	1	Total C N 6 4 2	0	0
63	DP	1	Total C N 6 4 2	0	0
63	D5	1	Total C N 6 4 2	0	0

- Molecule 64 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	DA	1	Total C O 16 10 6	0	0
64	DA	1	Total C O 16 10 6	0	0

- Molecule 65 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
65	DA	1	Total C H O 7 2 3 2	0	0
65	DA	1	Total C H O 7 2 3 2	0	0

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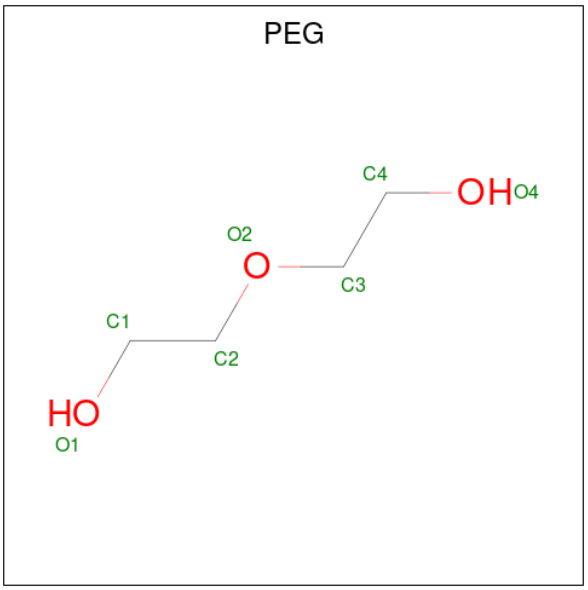
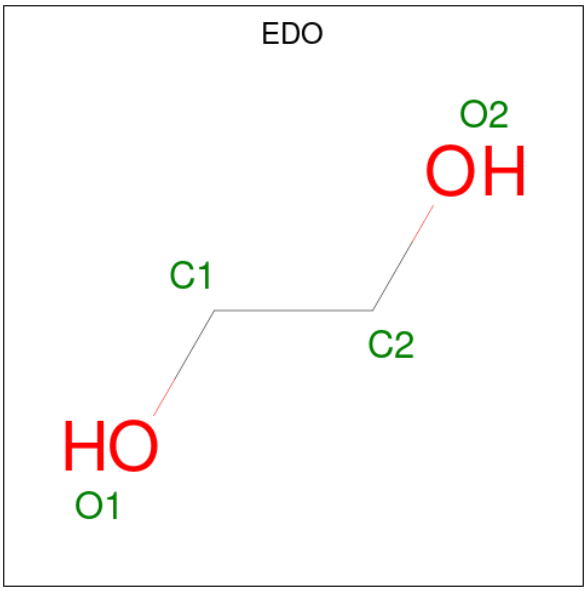
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
65	DA	1	Total C H O 7 2 3 2	0	0

- Molecule 66 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



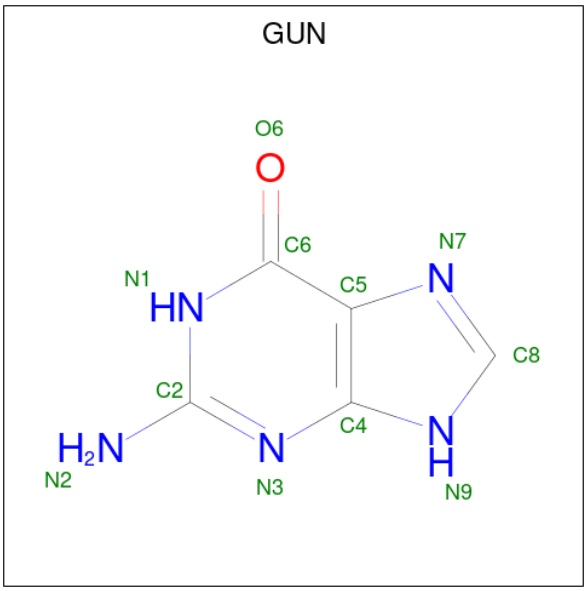
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
66	DA	1	Total C O 7 4 3	0	0
66	DA	1	Total C O 7 4 3	0	0
66	DA	1	Total C O 7 4 3	0	0
66	DA	1	Total C O 7 4 3	0	0
66	DA	1	Total C O 7 4 3	0	0
66	DP	1	Total C O 7 4 3	0	0
66	DQ	1	Total C O 7 4 3	0	0
66	D1	1	Total C O 7 4 3	0	0
66	D3	1	Total C O 7 4 3	0	0

- Molecule 67 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
67	DA	1	Total C O 4 2 2	0	0
67	DA	1	Total C O 4 2 2	0	0
67	DA	1	Total C O 4 2 2	0	0
67	DA	1	Total C O 4 2 2	0	0
67	DA	1	Total C O 4 2 2	0	0
67	DA	1	Total C O 4 2 2	0	0
67	DA	1	Total C O 4 2 2	0	0
67	DB	1	Total C O 4 2 2	0	0
67	DB	1	Total C O 4 2 2	0	0
67	DB	1	Total C O 4 2 2	0	0
67	DR	1	Total C O 4 2 2	0	0
67	D1	1	Total C O 4 2 2	0	0

- Molecule 68 is GUANINE (three-letter code: GUN) (formula: $C_5H_5N_5O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
68	DA	1	Total C N O 11 5 5 1	0	0

- Molecule 69 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	AA	371	Total O 371 371	0	0
69	BA	389	Total O 389 389	0	0
69	DA	3565	Total O 3565 3565	0	0
69	CA	1042	Total O 1042 1042	0	0
69	DB	90	Total O 90 90	0	0
69	CB	19	Total O 19 19	0	0
69	AB	11	Total O 11 11	0	0
69	AC	6	Total O 6 6	0	0
69	AD	3	Total O 3 3	0	0
69	AE	11	Total O 11 11	0	0
69	AF	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	AG	7	Total O 7 7	0	0
69	AH	2	Total O 2 2	0	0
69	AI	1	Total O 1 1	0	0
69	AJ	2	Total O 2 2	0	0
69	AK	8	Total O 8 8	0	0
69	AL	5	Total O 5 5	0	0
69	AM	7	Total O 7 7	0	0
69	AN	7	Total O 7 7	0	0
69	AO	1	Total O 1 1	0	0
69	AP	2	Total O 2 2	0	0
69	AQ	5	Total O 5 5	0	0
69	AS	3	Total O 3 3	0	0
69	AT	5	Total O 5 5	0	0
69	AU	2	Total O 2 2	0	0
69	BB	5	Total O 5 5	0	0
69	BC	3	Total O 3 3	0	0
69	BD	9	Total O 9 9	0	0
69	BE	5	Total O 5 5	0	0
69	BF	7	Total O 7 7	0	0
69	BG	7	Total O 7 7	0	0
69	BH	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	BI	4	Total O 4 4	0	0
69	BJ	1	Total O 1 1	0	0
69	BK	1	Total O 1 1	0	0
69	BL	3	Total O 3 3	0	0
69	BM	3	Total O 3 3	0	0
69	BN	8	Total O 8 8	0	0
69	BO	4	Total O 4 4	0	0
69	BP	4	Total O 4 4	0	0
69	BQ	1	Total O 1 1	0	0
69	BS	2	Total O 2 2	0	0
69	BT	5	Total O 5 5	0	0
69	BU	3	Total O 3 3	0	0
69	CC	8	Total O 8 8	0	0
69	CD	8	Total O 8 8	0	0
69	CE	7	Total O 7 7	0	0
69	CF	2	Total O 2 2	0	0
69	CG	4	Total O 4 4	0	0
69	CH	4	Total O 4 4	0	0
69	CK	5	Total O 5 5	0	0
69	CL	5	Total O 5 5	0	0
69	CM	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	CN	5	Total O 5 5	0	0
69	CO	5	Total O 5 5	0	0
69	CP	1	Total O 1 1	0	0
69	CQ	5	Total O 5 5	0	0
69	CR	3	Total O 3 3	0	0
69	CS	5	Total O 5 5	0	0
69	CT	3	Total O 3 3	0	0
69	CU	6	Total O 6 6	0	0
69	CV	7	Total O 7 7	0	0
69	CW	1	Total O 1 1	0	0
69	CZ	2	Total O 2 2	0	0
69	C0	3	Total O 3 3	0	0
69	C1	1	Total O 1 1	0	0
69	C2	1	Total O 1 1	0	0
69	C3	5	Total O 5 5	0	0
69	C4	3	Total O 3 3	0	0
69	C5	1	Total O 1 1	0	0
69	DC	59	Total O 59 59	0	0
69	DD	80	Total O 80 80	0	0
69	DE	51	Total O 51 51	0	0
69	DF	5	Total O 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	DG	5	Total O 5 5	0	0
69	DH	2	Total O 2 2	0	0
69	DJ	4	Total O 4 4	0	0
69	DK	37	Total O 37 37	0	0
69	DL	30	Total O 30 30	0	0
69	DM	52	Total O 52 52	0	0
69	DN	47	Total O 47 47	0	0
69	DO	33	Total O 33 33	0	0
69	DP	14	Total O 14 14	0	0
69	DQ	33	Total O 33 33	0	0
69	DR	52	Total O 52 52	0	0
69	DS	40	Total O 40 40	0	0
69	DT	57	Total O 57 57	0	0
69	DU	10	Total O 10 10	0	0
69	DV	14	Total O 14 14	0	0
69	DW	18	Total O 18 18	0	0
69	DX	15	Total O 15 15	0	0
69	DY	7	Total O 7 7	0	0
69	DZ	2	Total O 2 2	0	0
69	D0	14	Total O 14 14	0	0
69	D1	48	Total O 48 48	0	0

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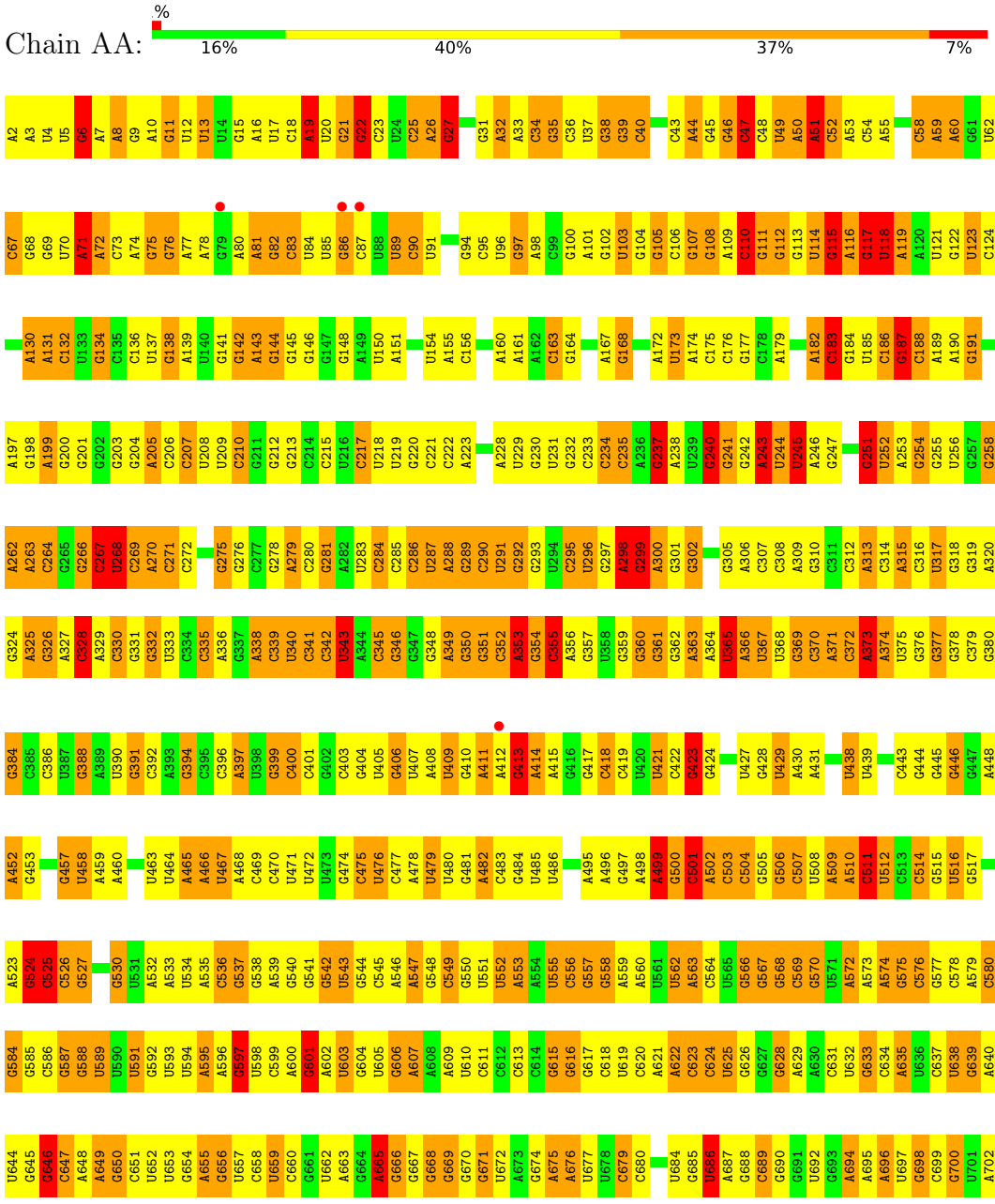
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
69	D2	4	Total O 4 4	0	0
69	D3	24	Total O 24 24	0	0
69	D4	27	Total O 27 27	0	0
69	D5	9	Total O 9 9	0	0

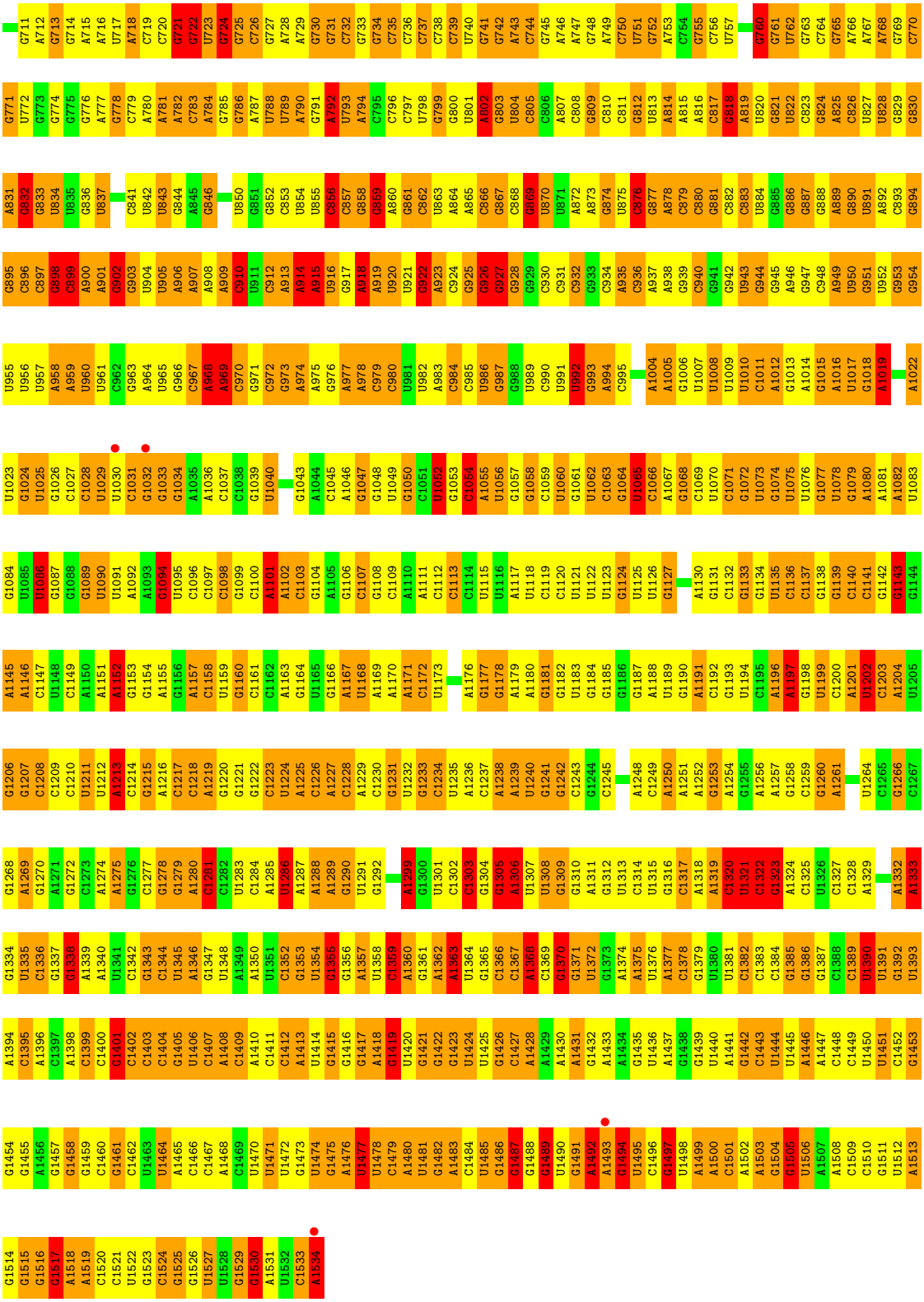
3 Residue-property plots (i)

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

- Molecule 1: 16S ribosomal RNA

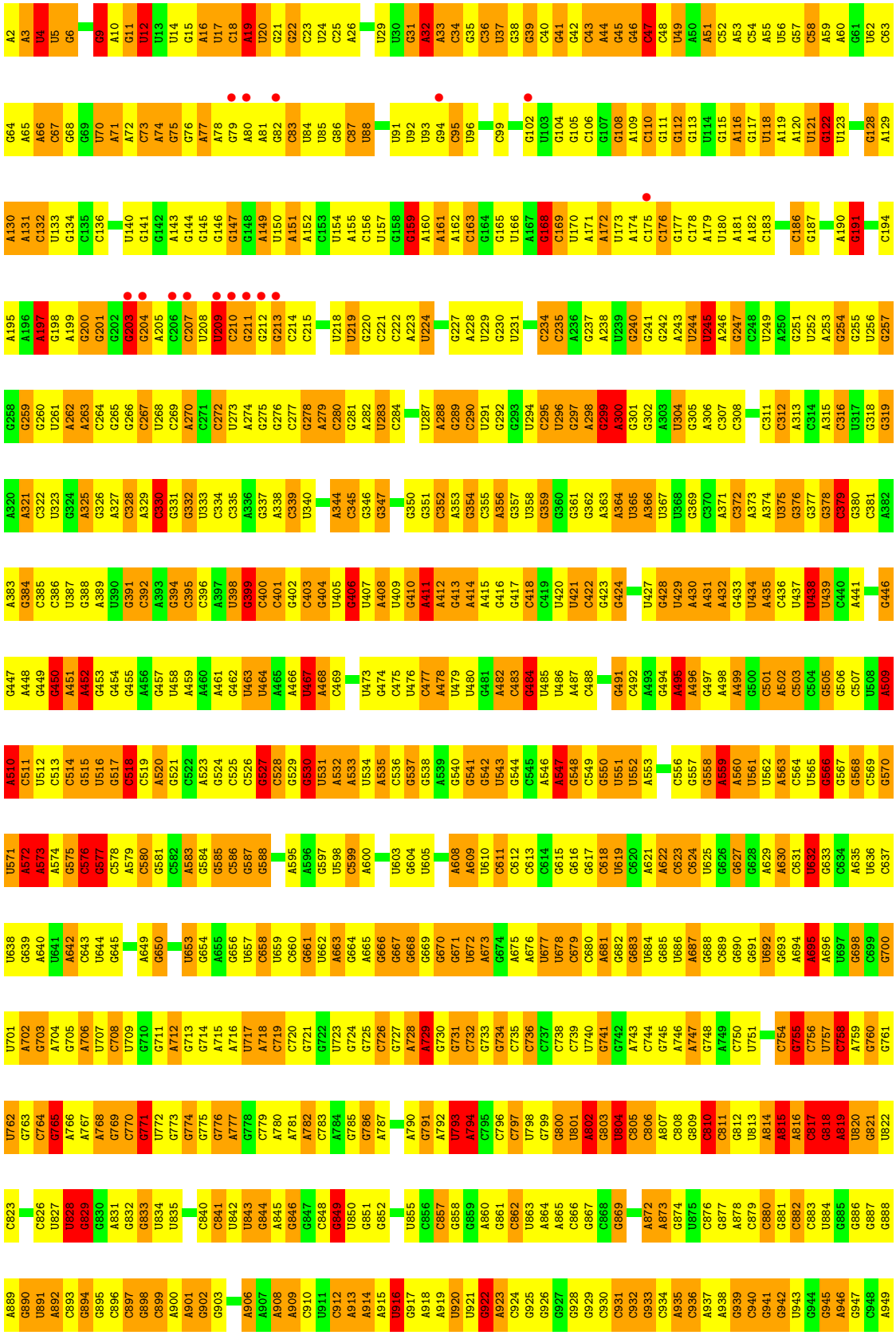
Chain AA:

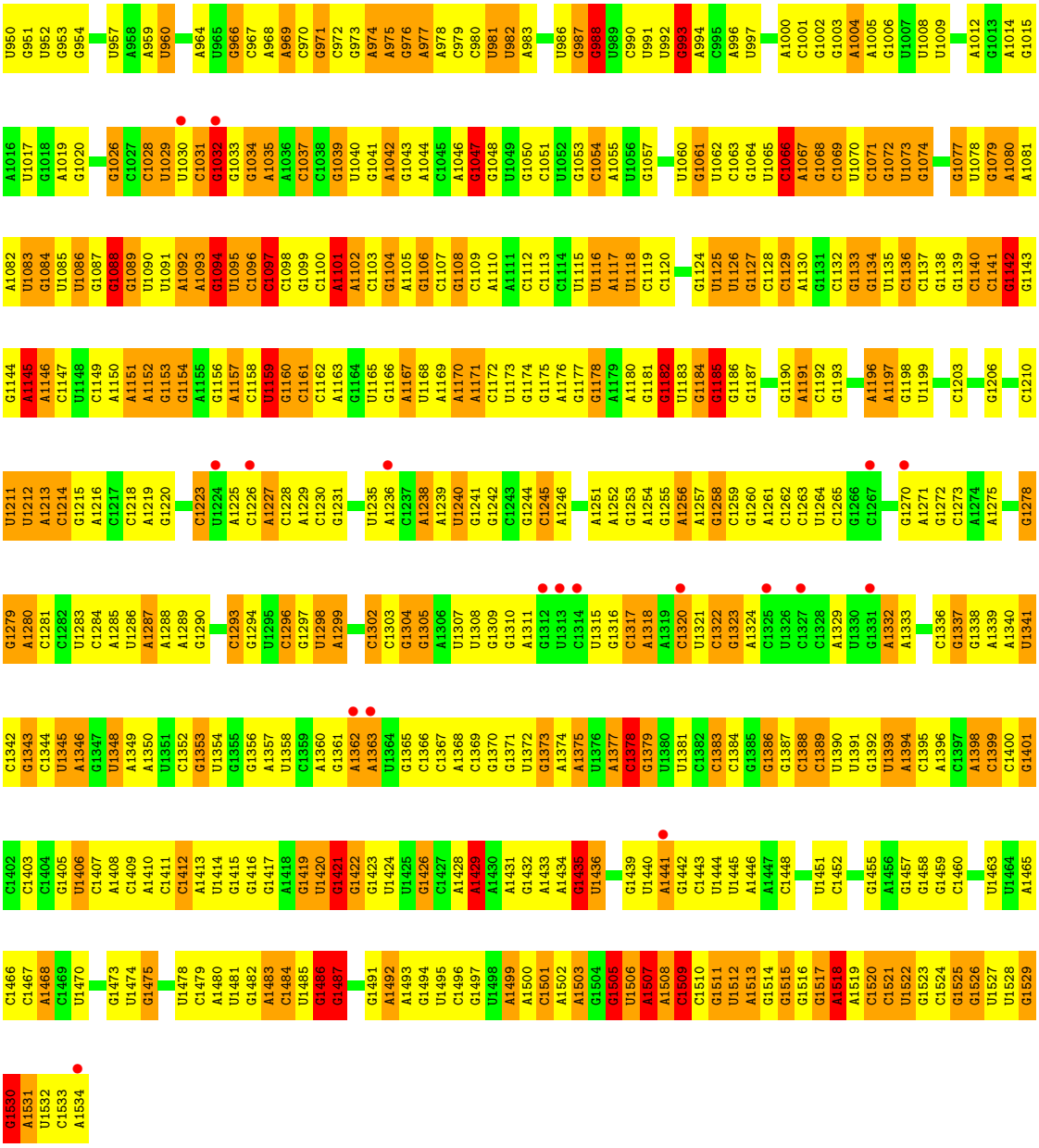




• Molecule 2: 16S ribosomal RNA

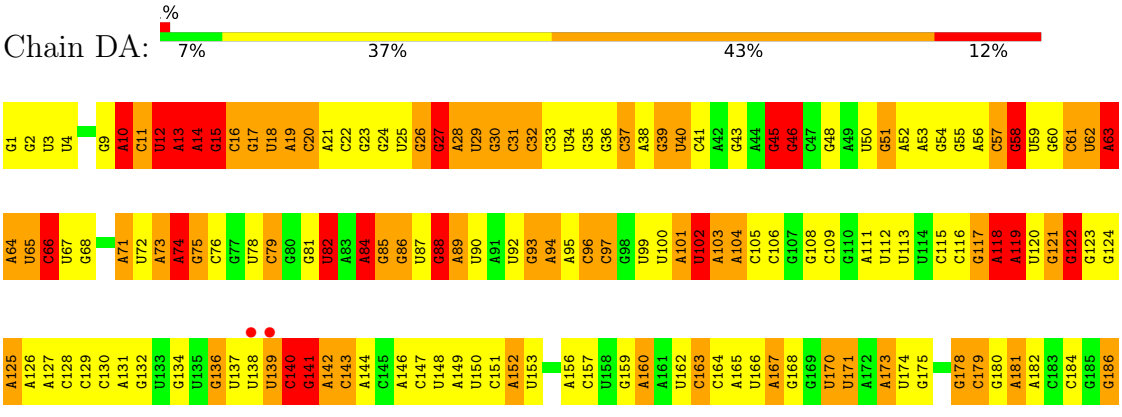
Chain BA:

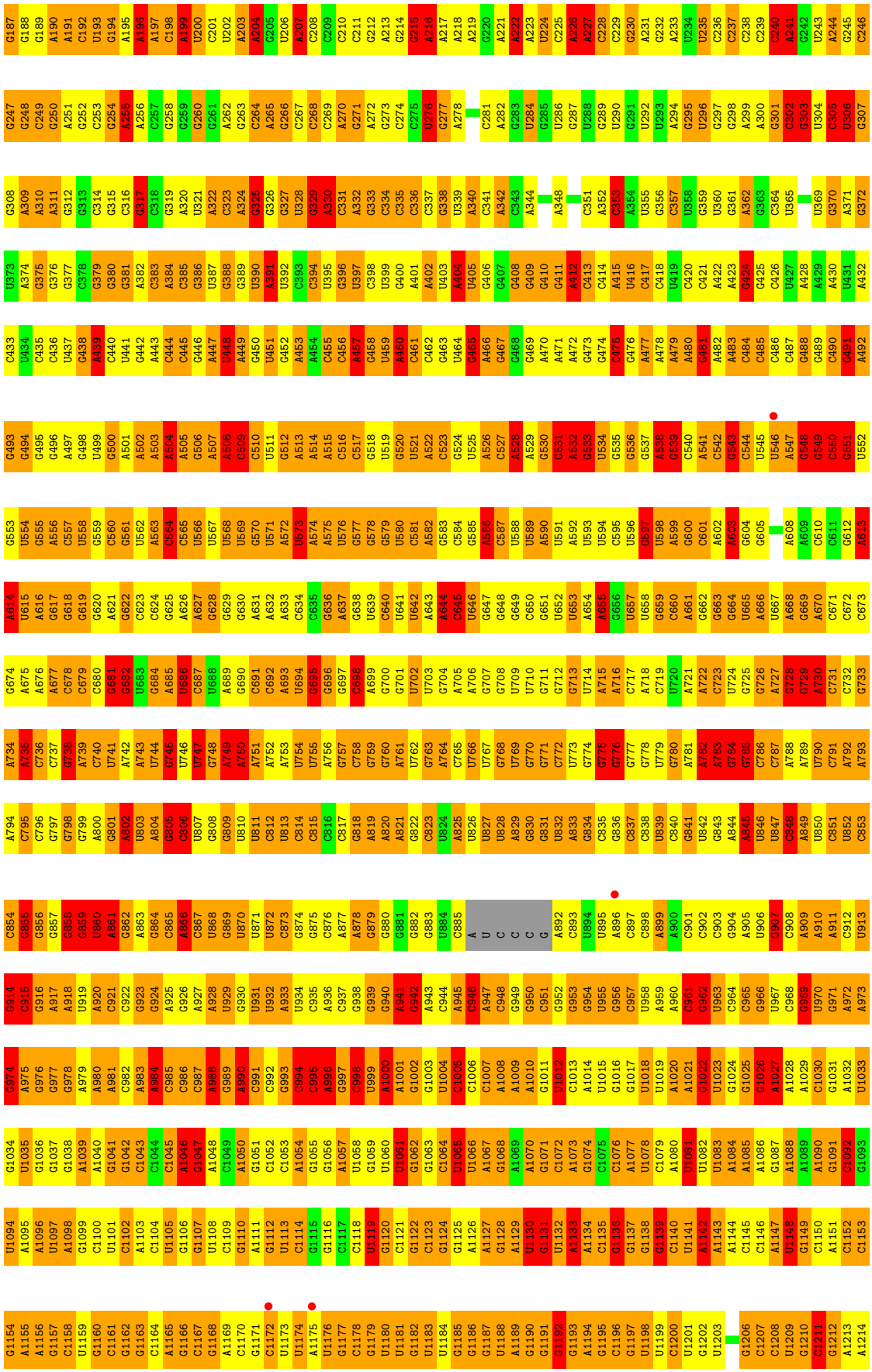


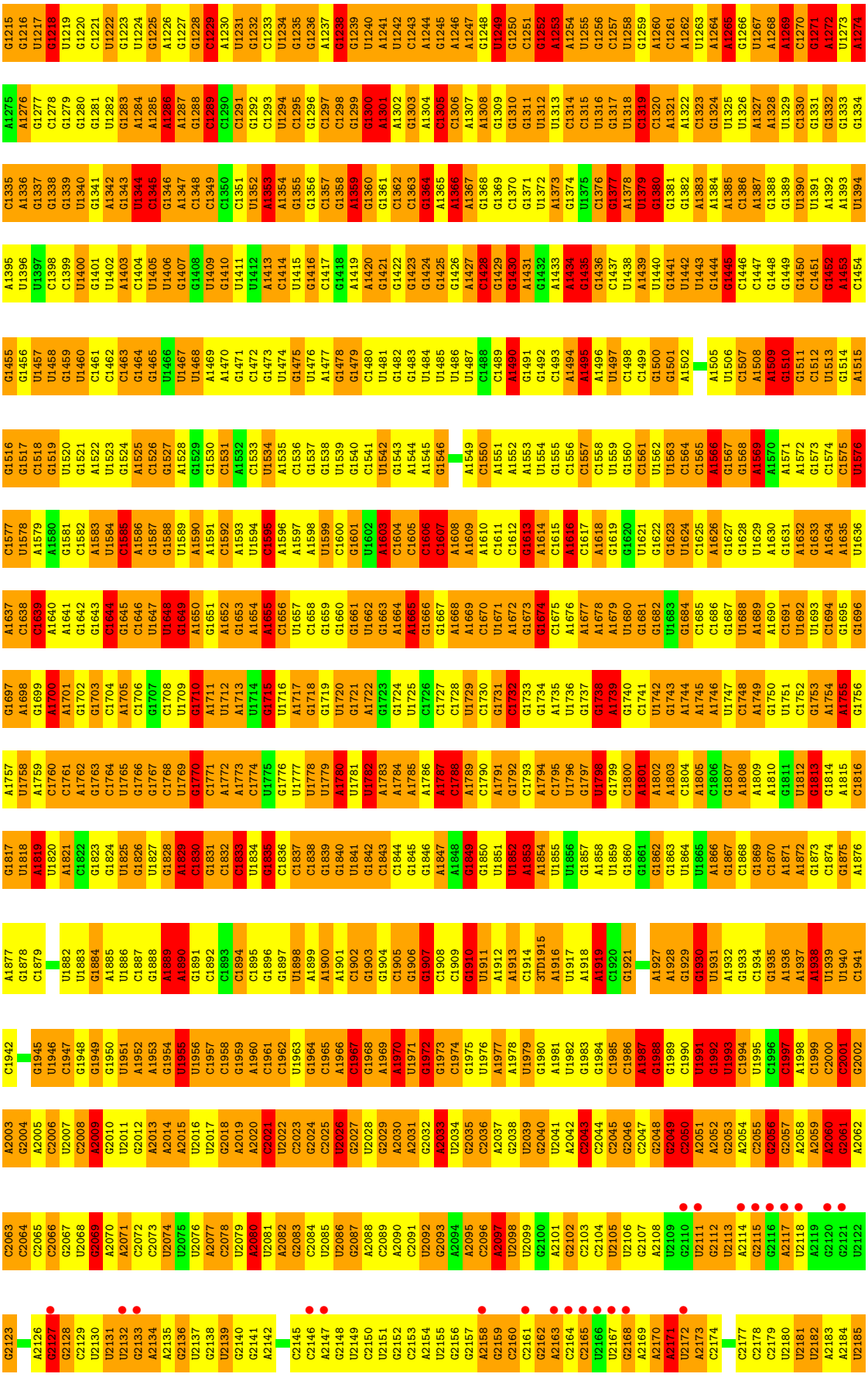


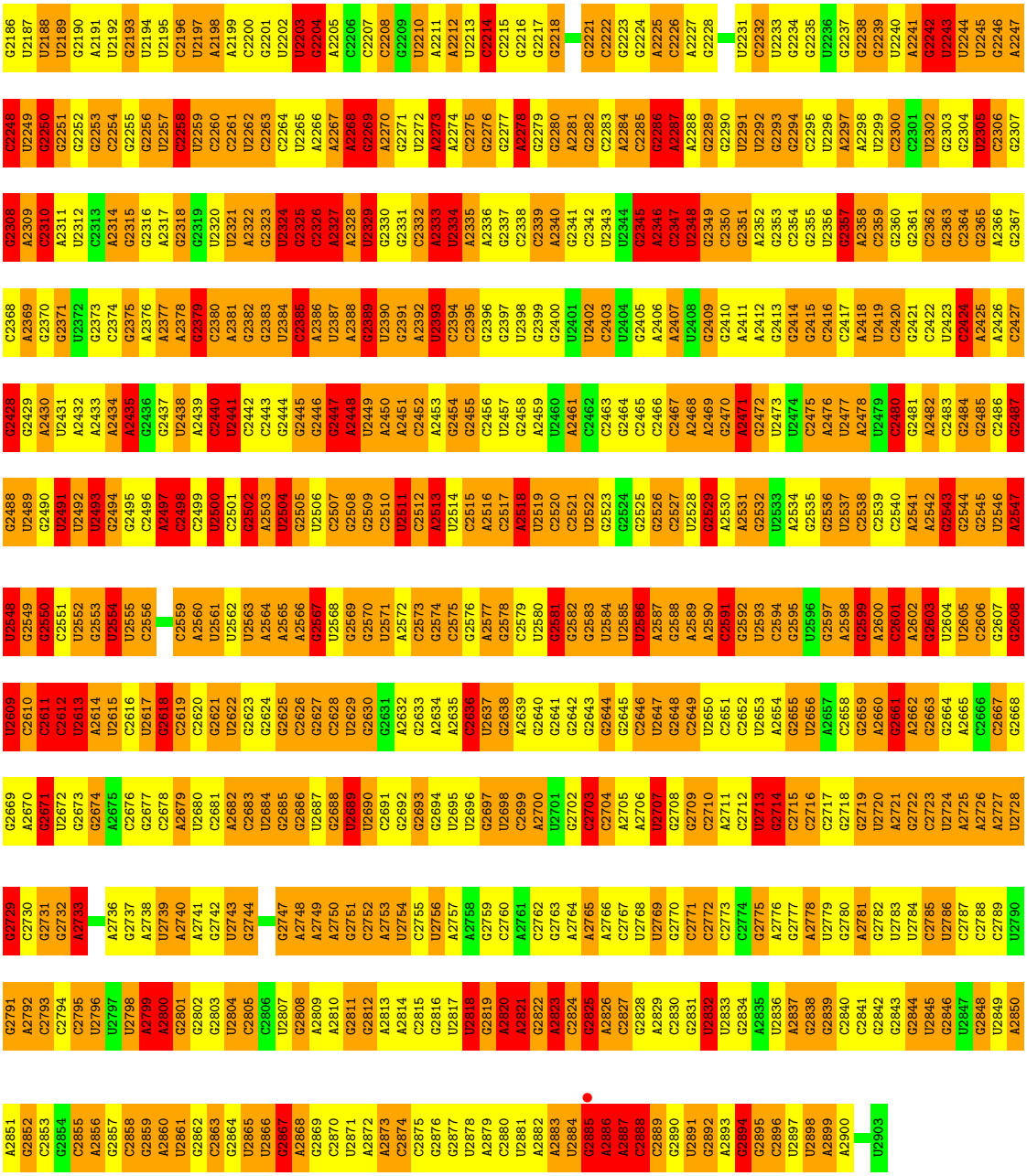
• Molecule 3: 23S ribosomal RNA

Chain DA:



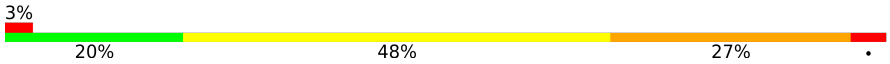


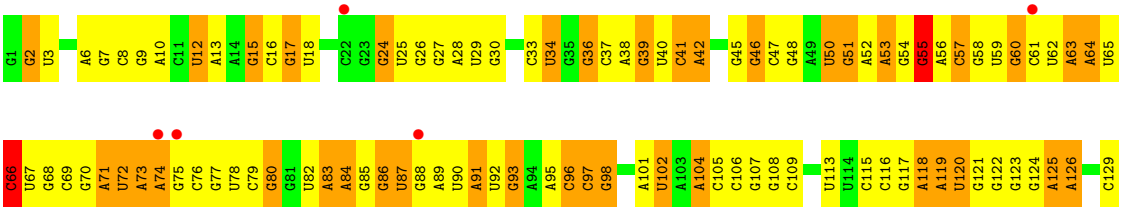


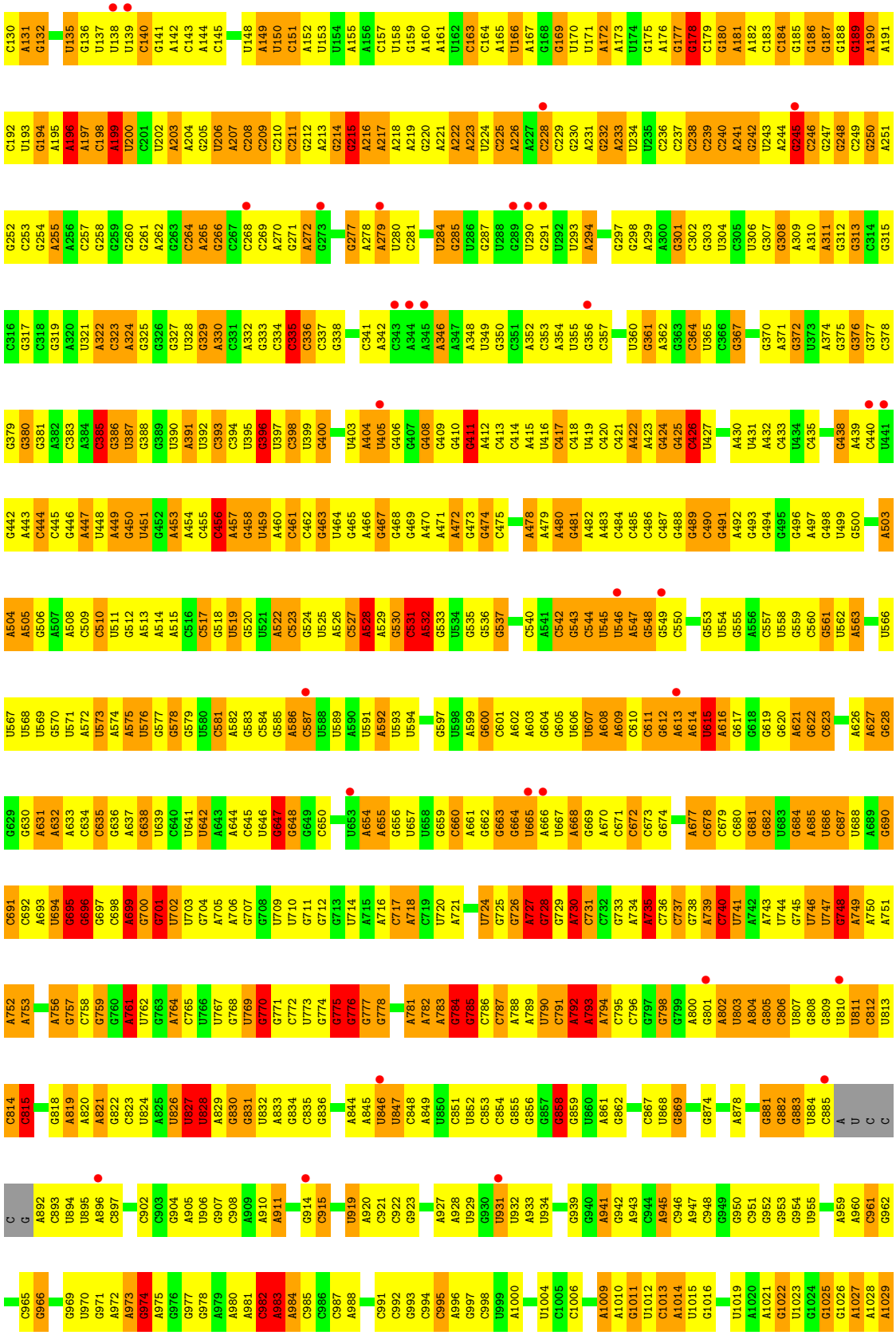


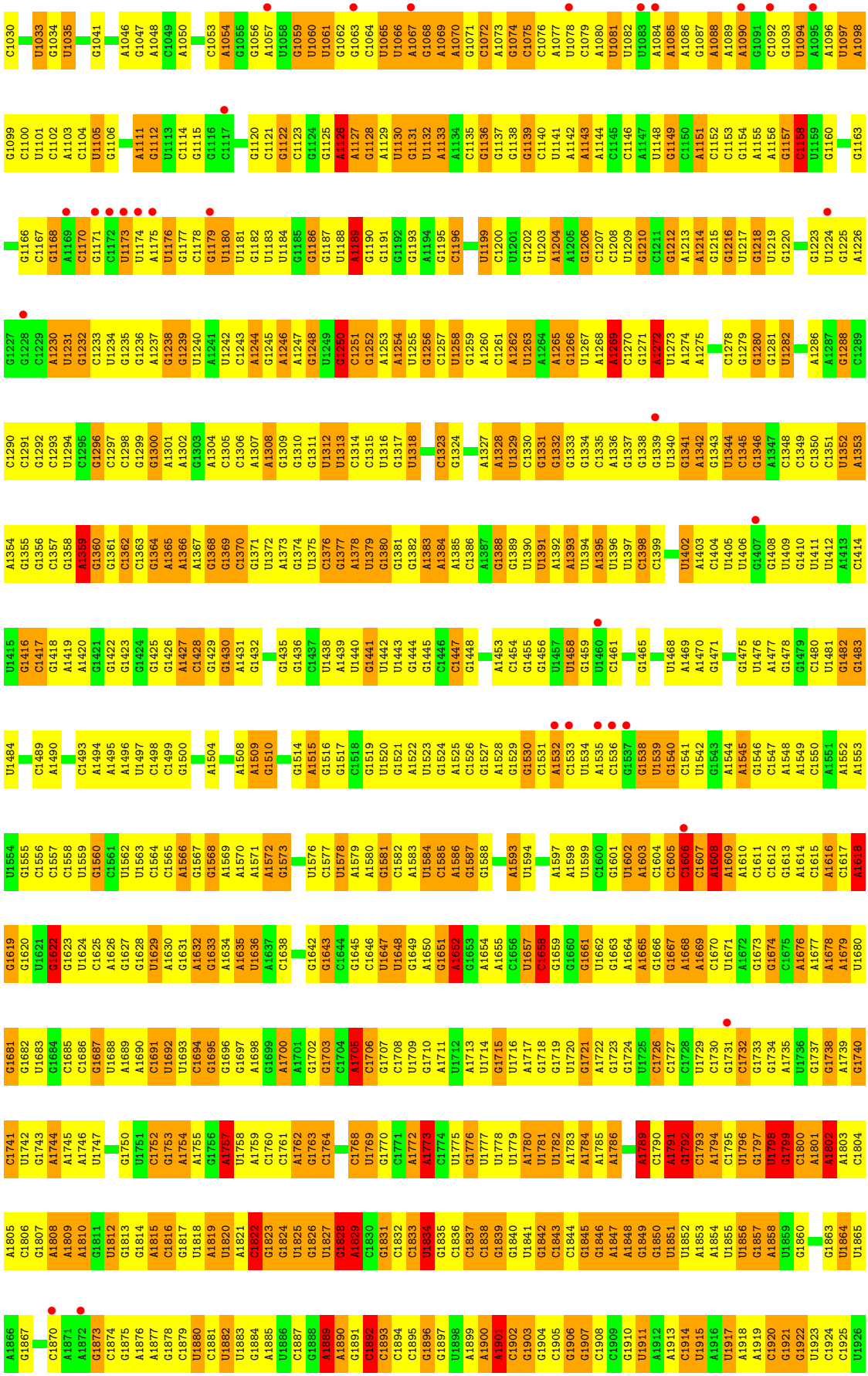
• Molecule 4: 23S ribsomal RNA

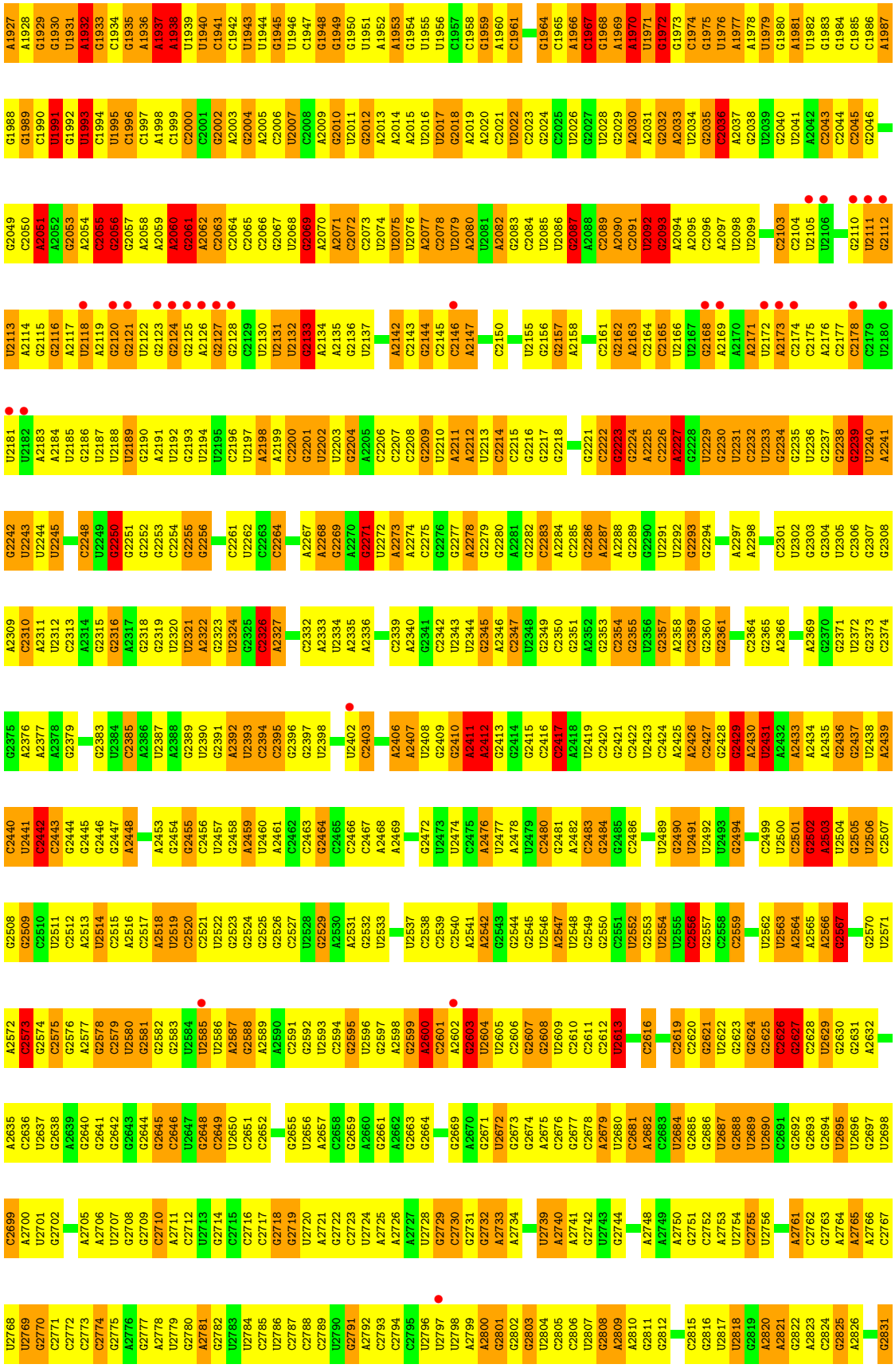
Chain CA:

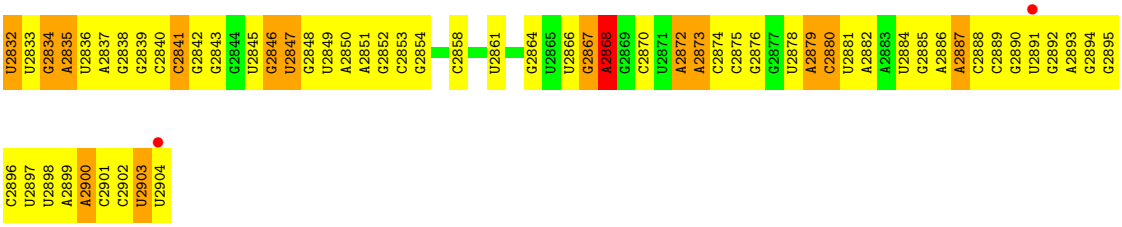






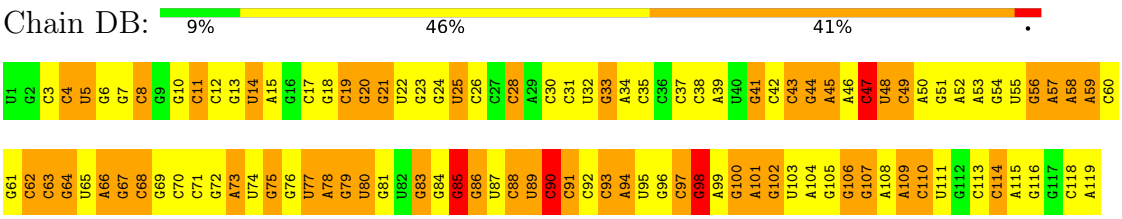






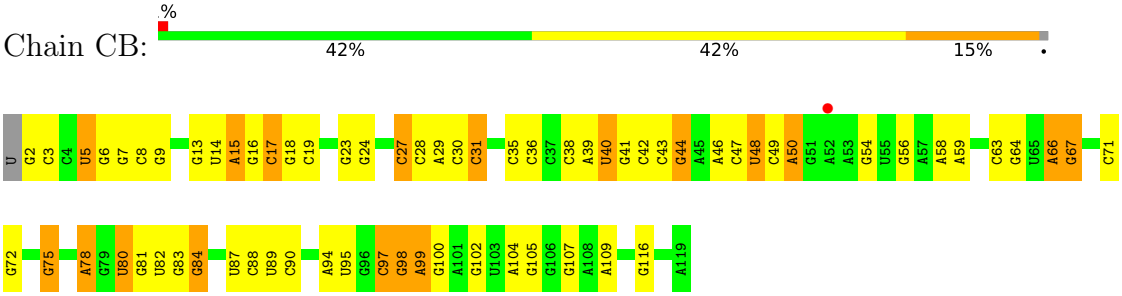
• Molecule 5: 5S ribosomal RNA

Chain DB:



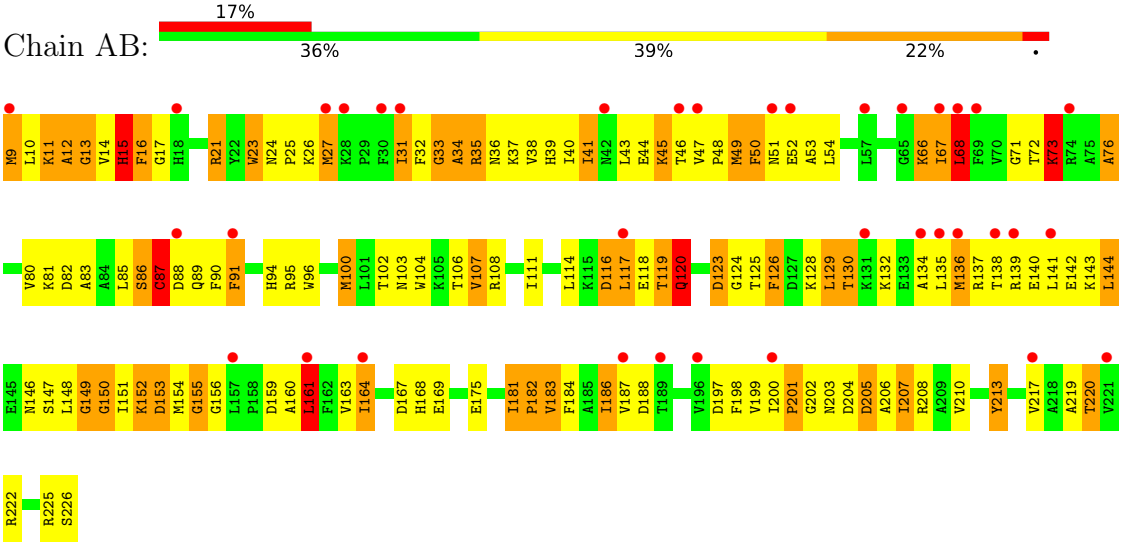
• Molecule 5: 5S ribosomal RNA

Chain CB:



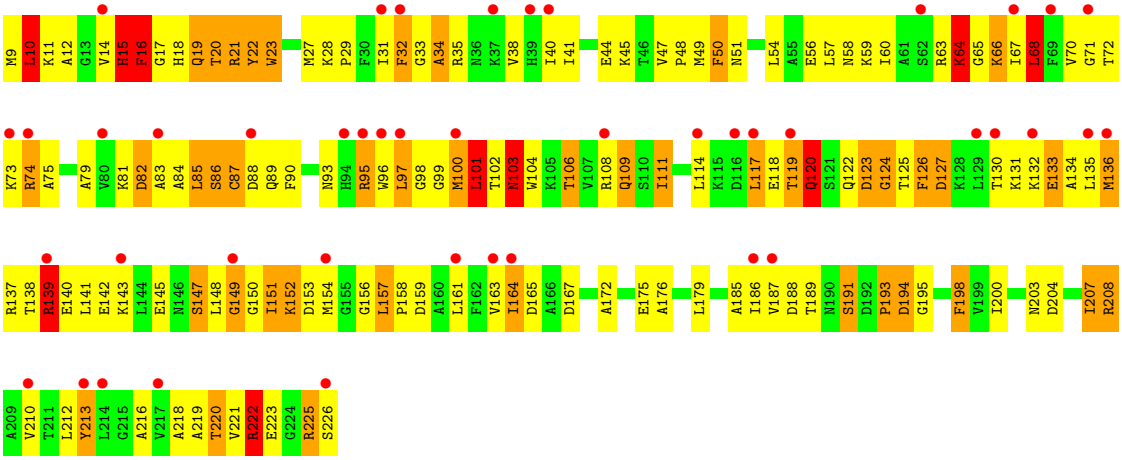
• Molecule 6: 30S ribosomal protein S2

Chain AB:



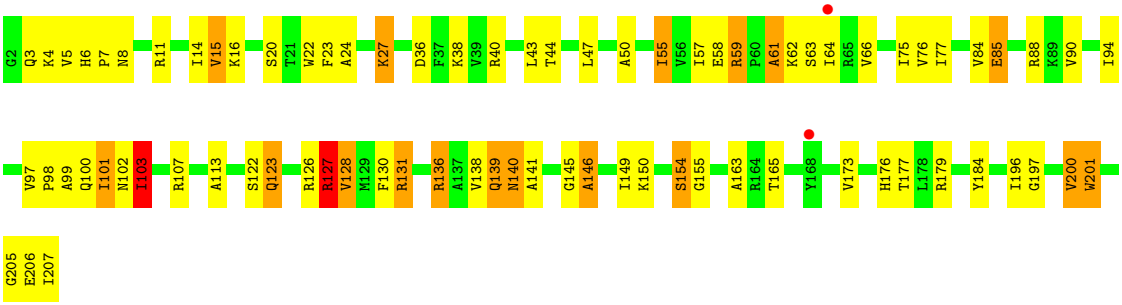
• Molecule 6: 30S ribosomal protein S2

Chain BB:



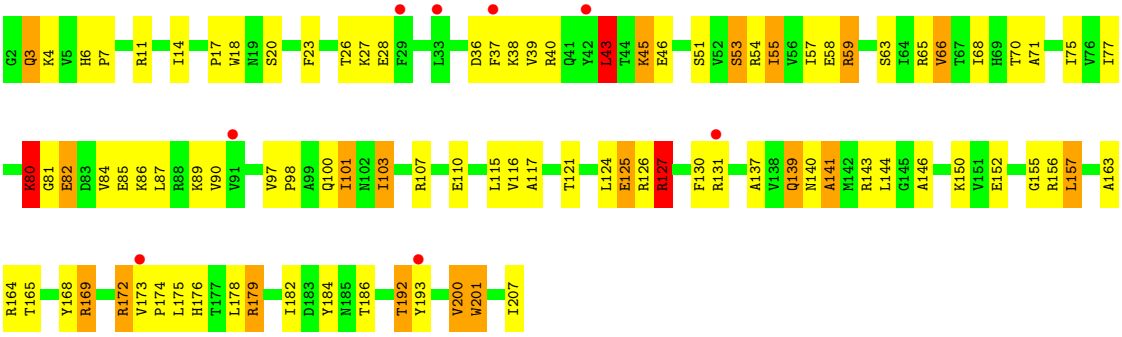
• Molecule 7: 30S ribosomal protein S3

Chain AC:



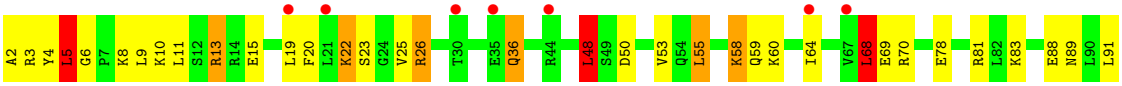
• Molecule 7: 30S ribosomal protein S3

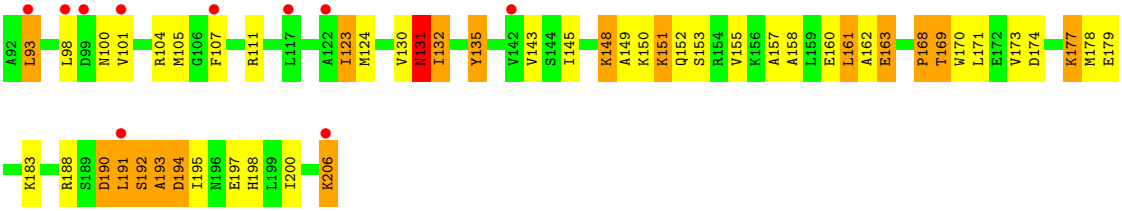
Chain BC:



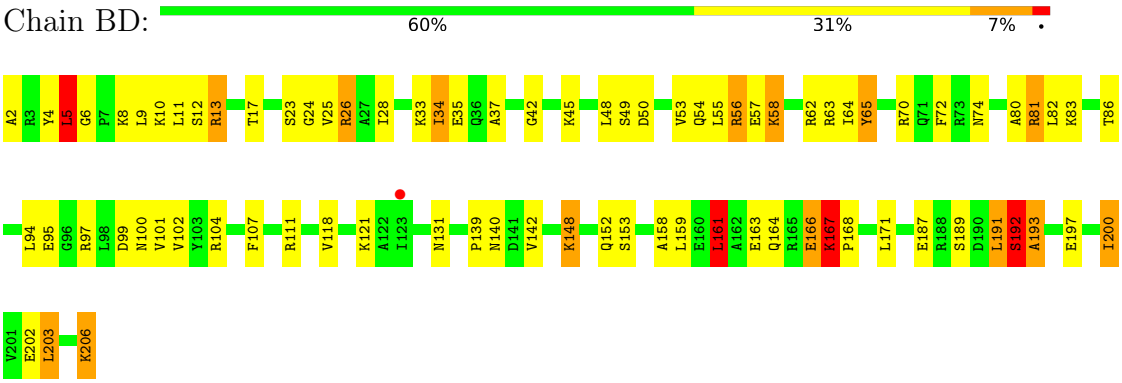
• Molecule 8: 30S ribosomal protein S4

Chain AD:

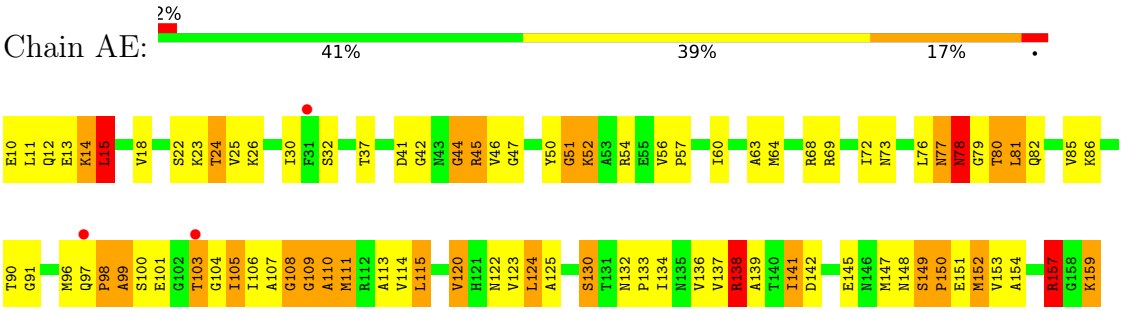




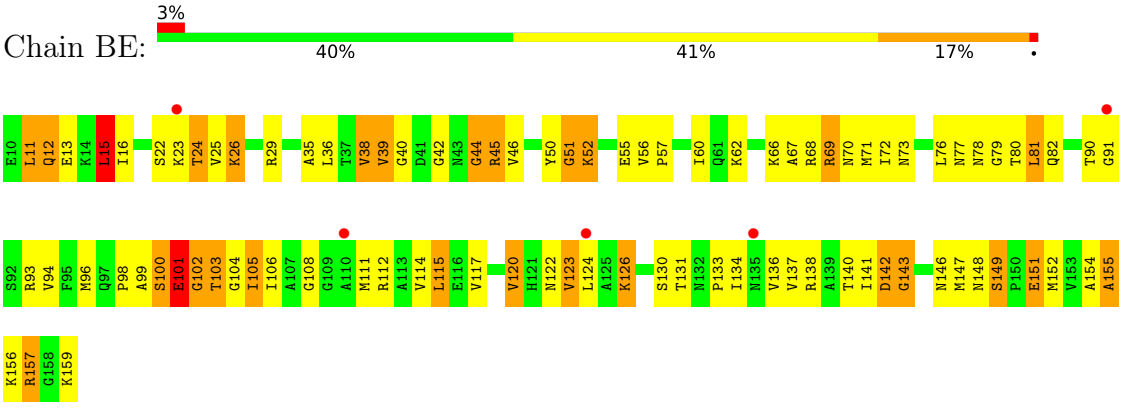
• Molecule 8: 30S ribosomal protein S4



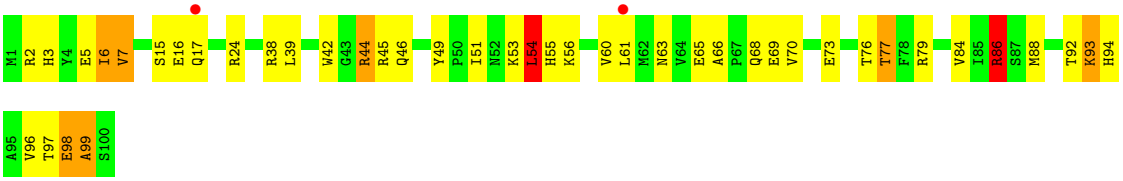
• Molecule 9: 30S ribosomal protein S5



• Molecule 9: 30S ribosomal protein S5

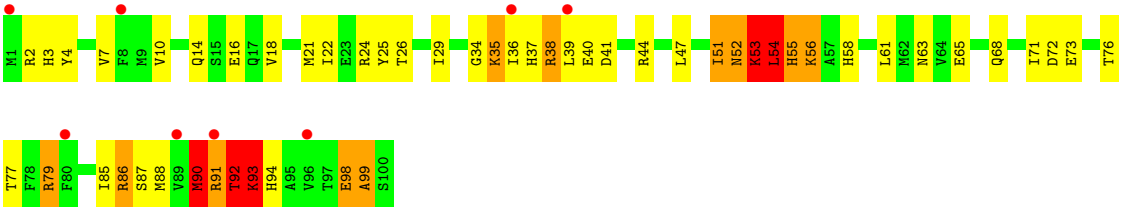


• Molecule 10: 30S ribosomal protein S6



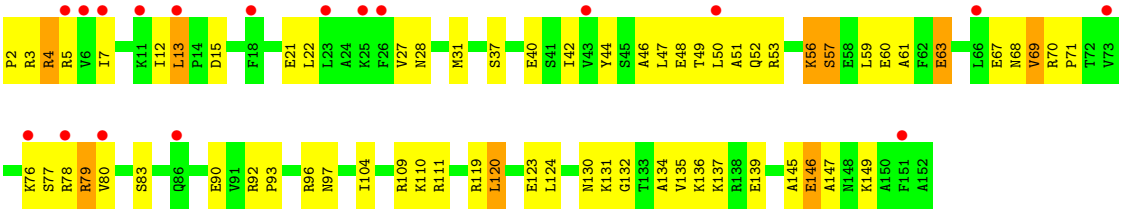
• Molecule 10: 30S ribosomal protein S6

Chain BF:



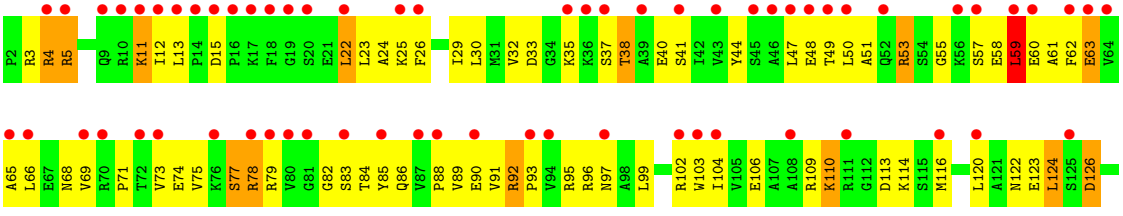
• Molecule 11: 30S ribosomal protein S7

Chain AG:



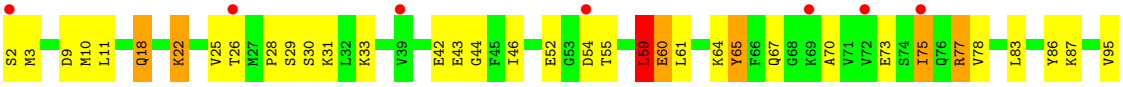
• Molecule 11: 30S ribosomal protein S7

Chain BG:



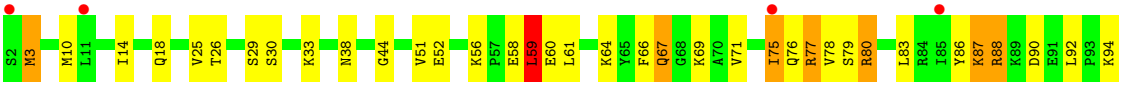
• Molecule 12: 30S ribosomal protein S8

Chain AH:



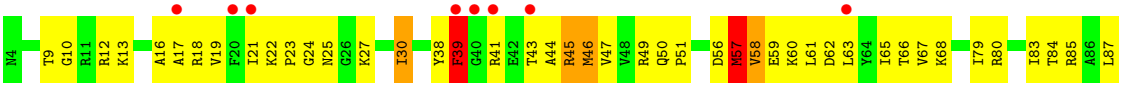
• Molecule 12: 30S ribosomal protein S8

Chain BH:



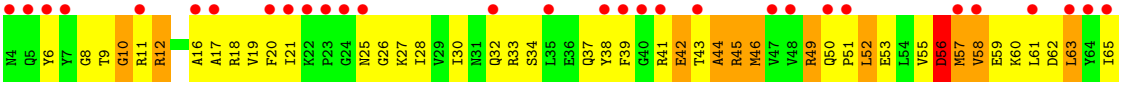
• Molecule 13: 30S ribosomal protein S9

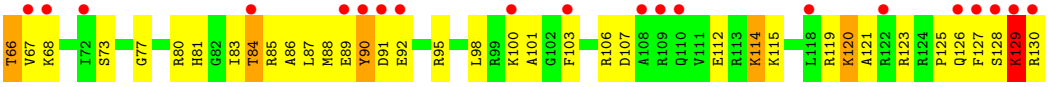
Chain AI:



• Molecule 13: 30S ribosomal protein S9

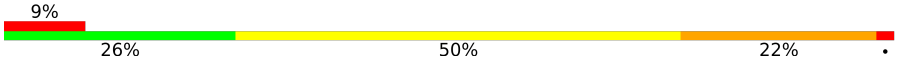
Chain BI:

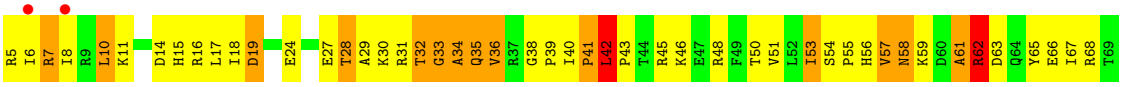


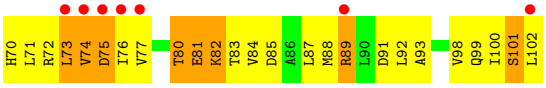


• Molecule 14: 30S ribosomal protein S10

Chain AJ:

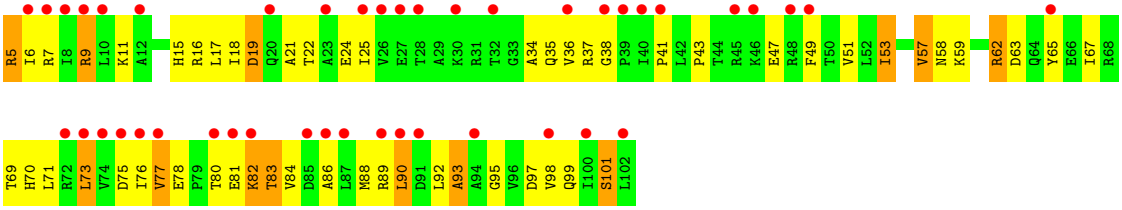




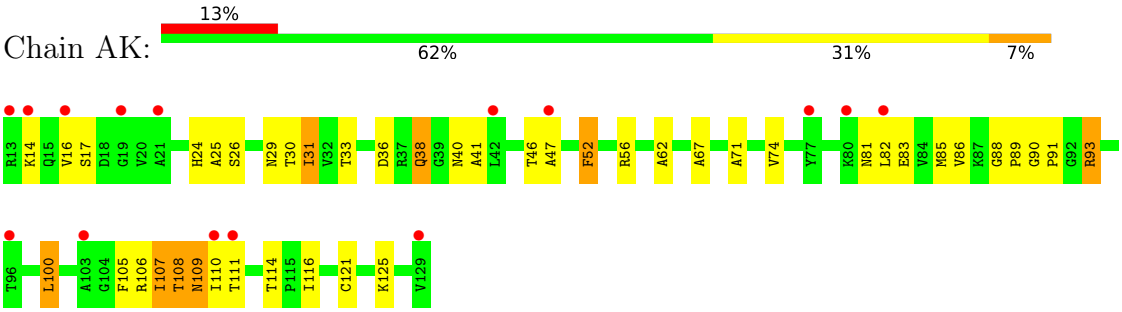


• Molecule 14: 30S ribosomal protein S10

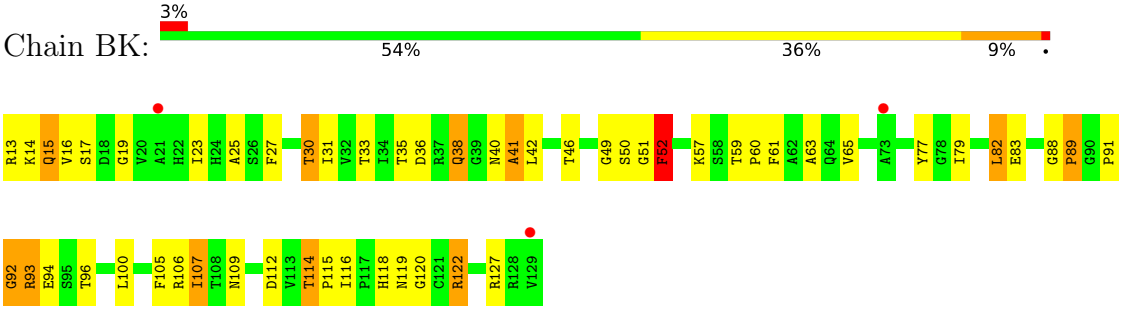
Chain BJ:



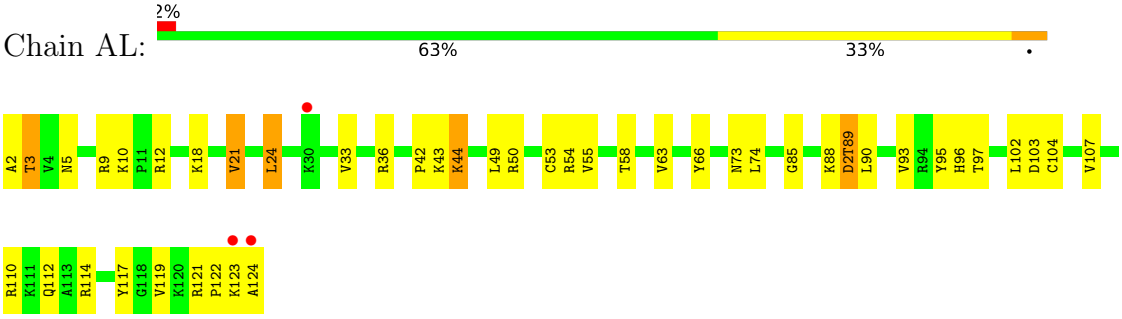
• Molecule 15: 30S ribosomal protein S11



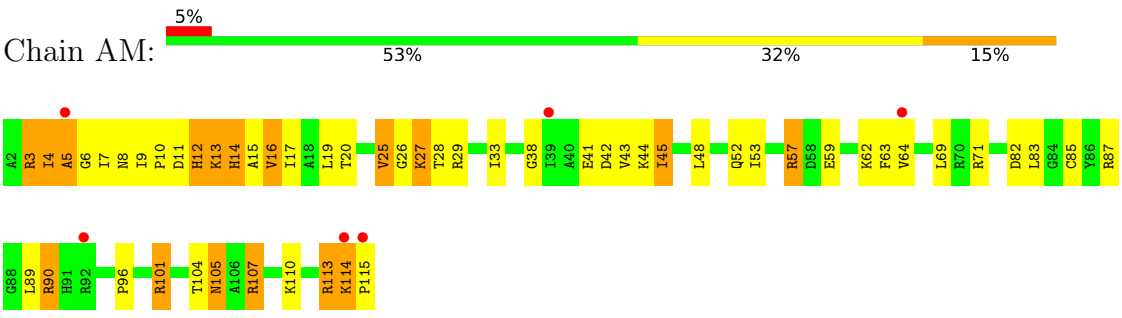
• Molecule 15: 30S ribosomal protein S11



• Molecule 16: 30S ribosomal protein S12

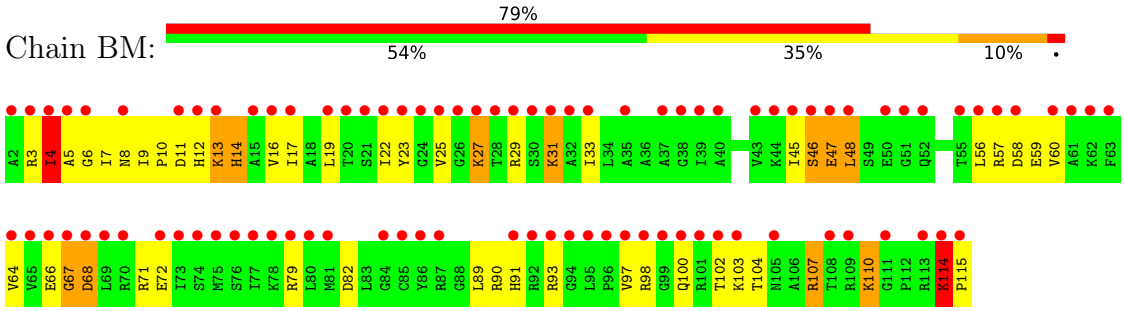


• Molecule 17: 30S ribosomal protein S13



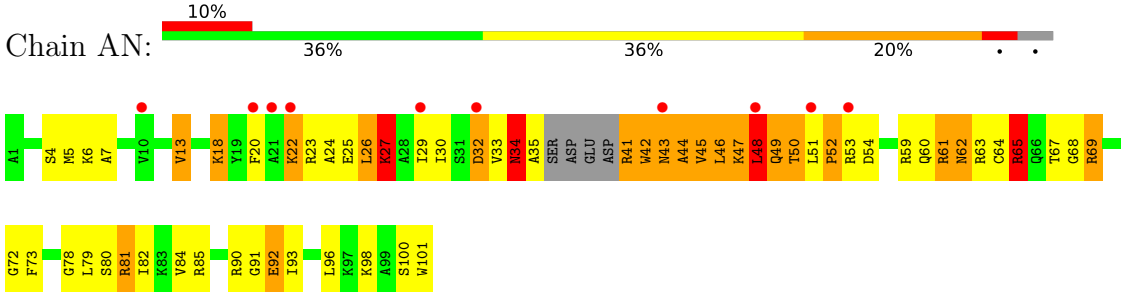
• Molecule 17: 30S ribosomal protein S13

Chain BM:



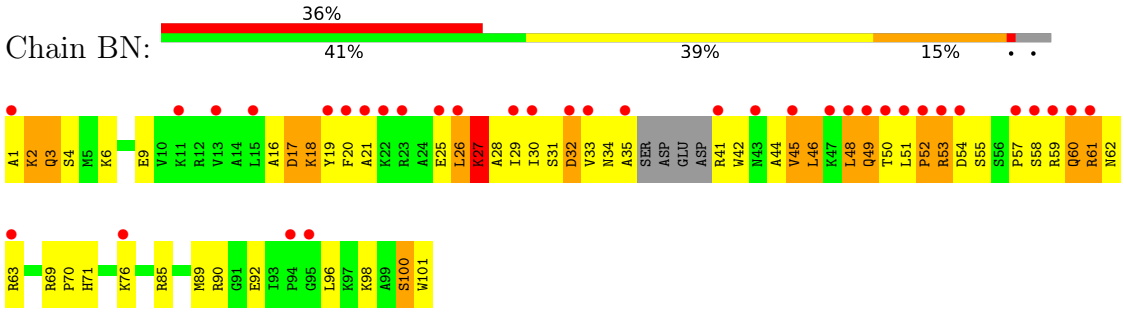
• Molecule 18: 30S ribosomal protein S14

Chain AN:



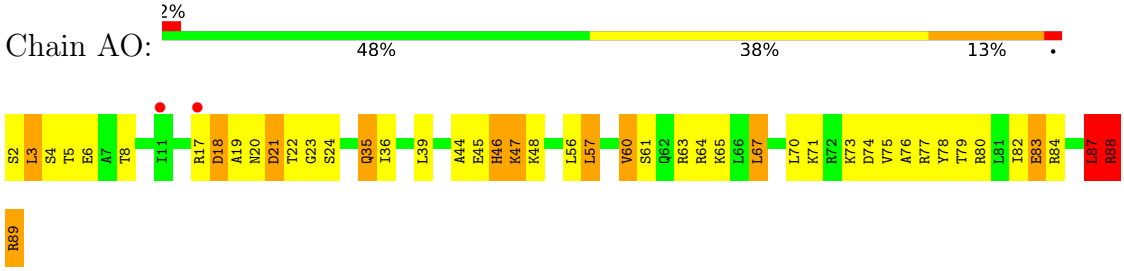
• Molecule 18: 30S ribosomal protein S14

Chain BN:



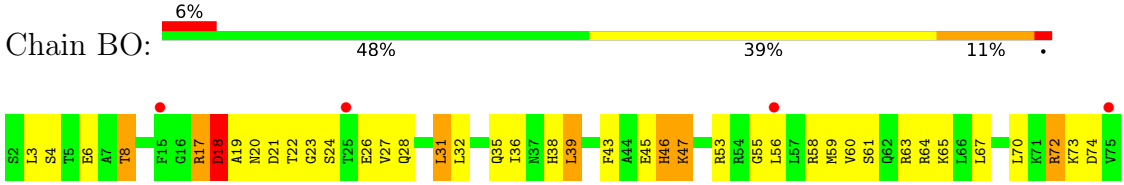
• Molecule 19: 30S ribosomal protein S15

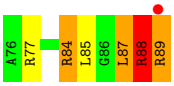
Chain AO:



• Molecule 19: 30S ribosomal protein S15

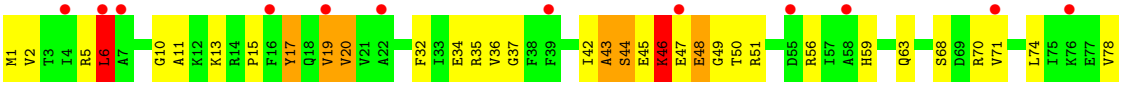
Chain BO:





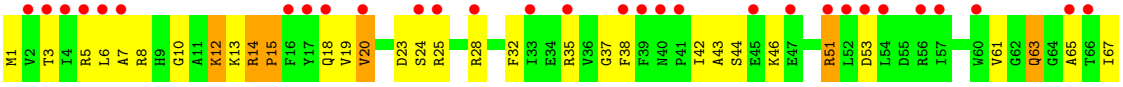
• Molecule 20: 30S ribosomal protein S16

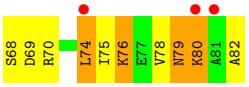
Chain AP:



• Molecule 20: 30S ribosomal protein S16

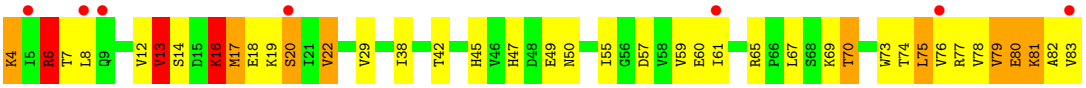
Chain BP:





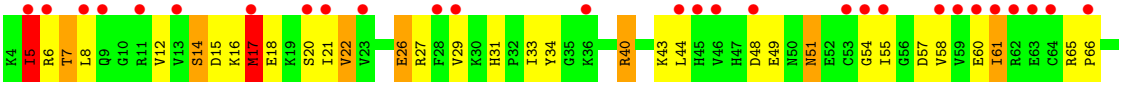
• Molecule 21: 30S ribosomal protein S17

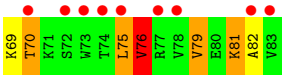
Chain AQ:



• Molecule 21: 30S ribosomal protein S17

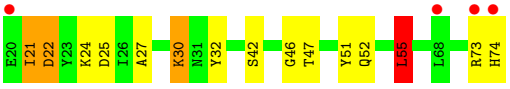
Chain BQ:





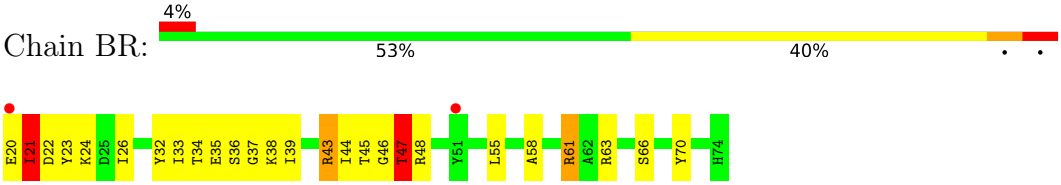
• Molecule 22: 30S ribosomal protein S18

Chain AR:



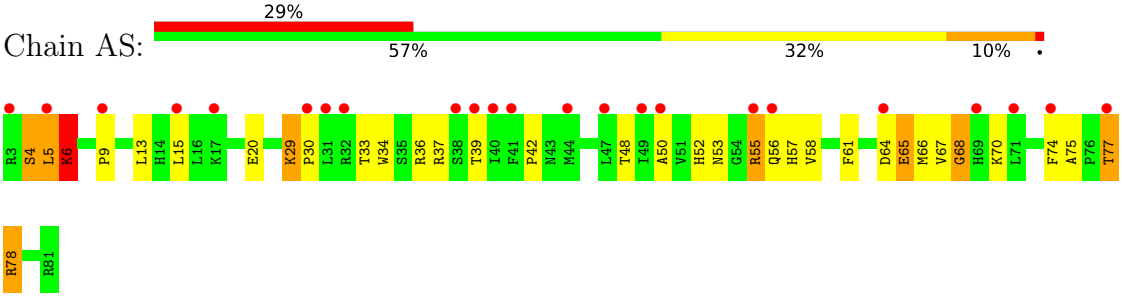
• Molecule 22: 30S ribosomal protein S18

Chain BR:



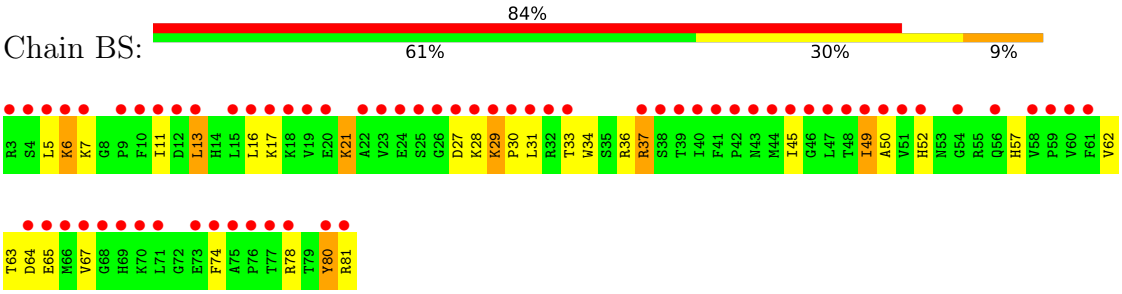
• Molecule 23: 30S ribosomal protein S19

Chain AS:



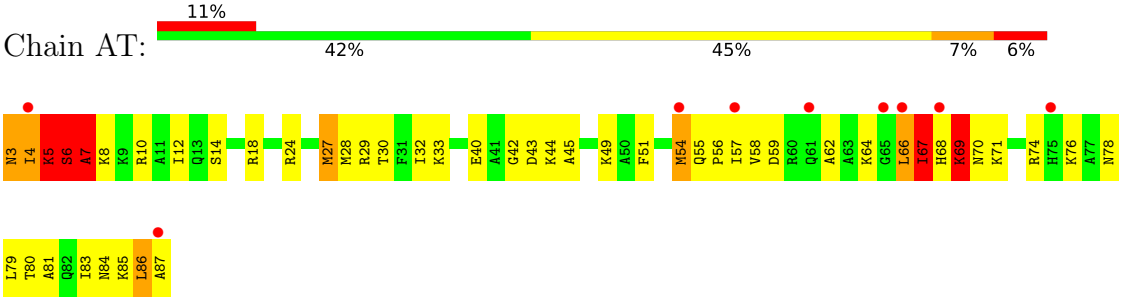
• Molecule 23: 30S ribosomal protein S19

Chain BS:



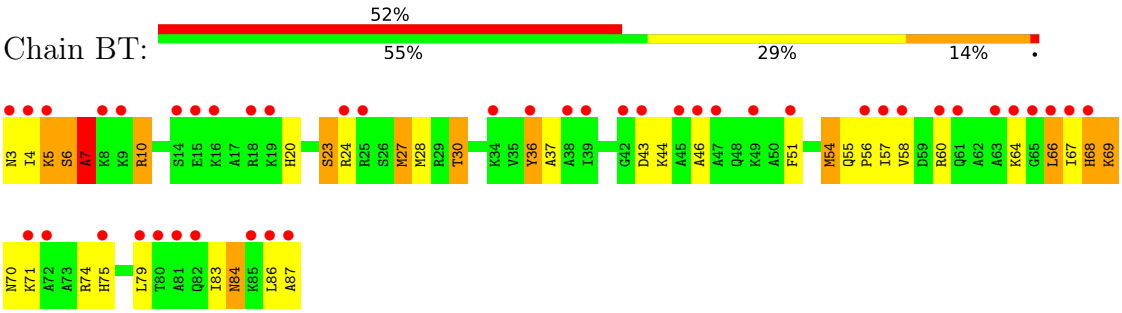
• Molecule 24: 30S ribosomal protein S20

Chain AT:



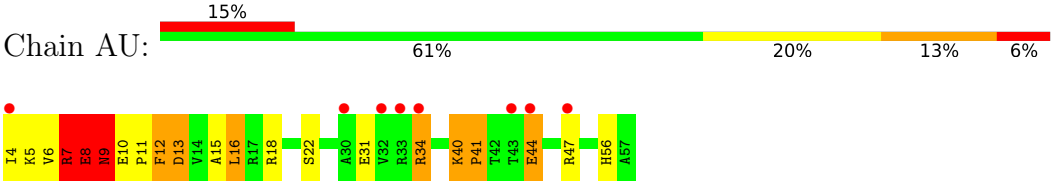
• Molecule 24: 30S ribosomal protein S20

Chain BT:



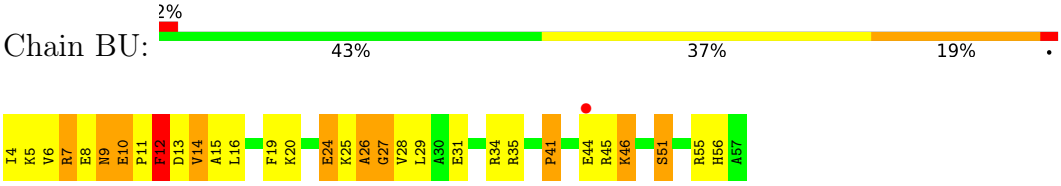
• Molecule 25: 30S ribosomal protein S21

Chain AU:



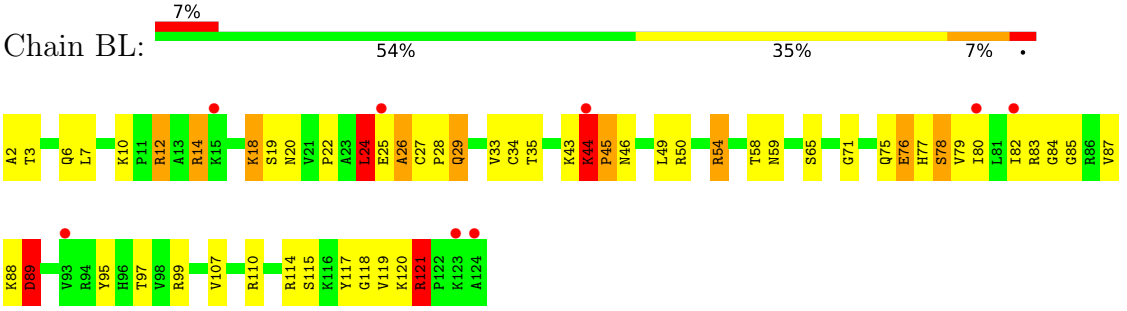
• Molecule 25: 30S ribosomal protein S21

Chain BU:



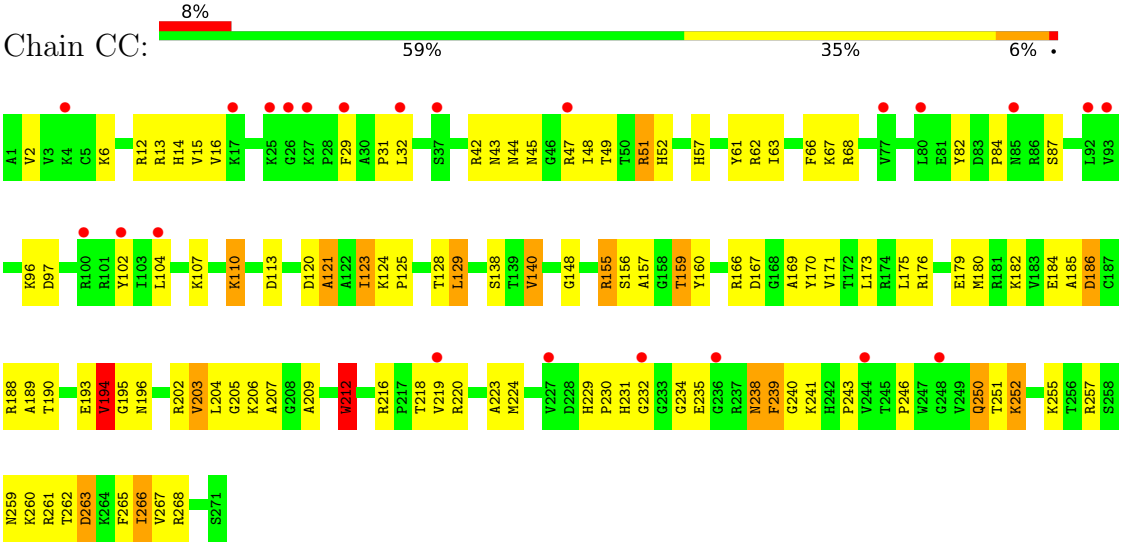
• Molecule 26: 30S ribosomal protein S12

Chain BL:



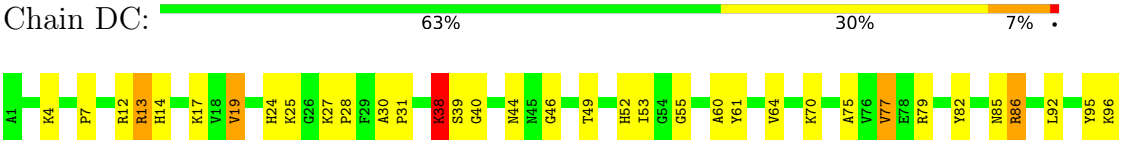
• Molecule 27: 50S ribosomal protein L2

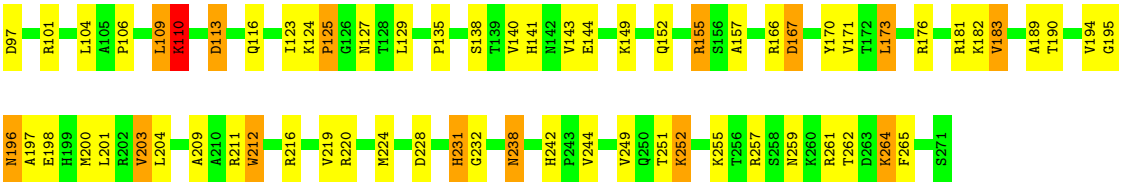
Chain CC:



• Molecule 27: 50S ribosomal protein L2

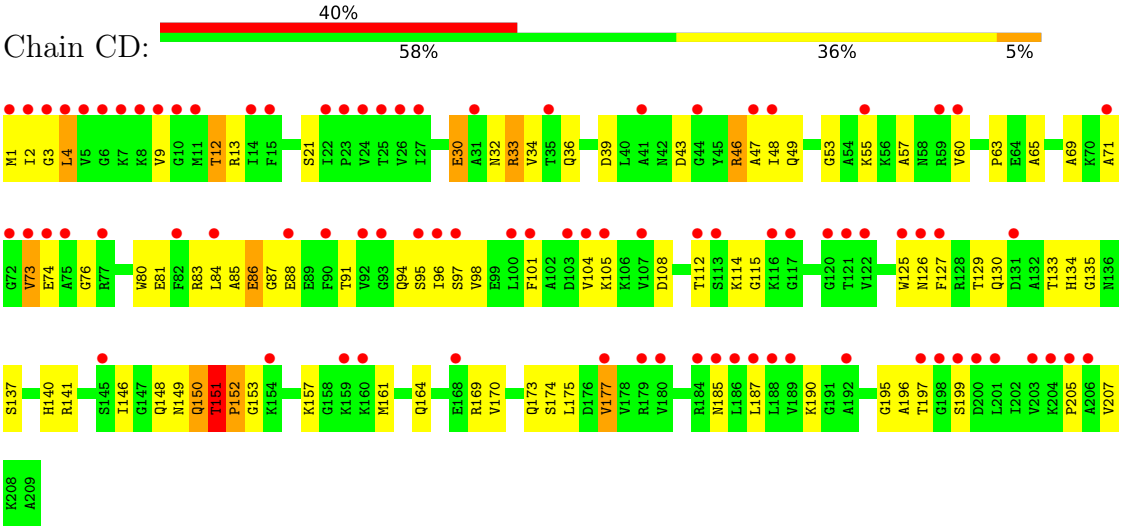
Chain DC:





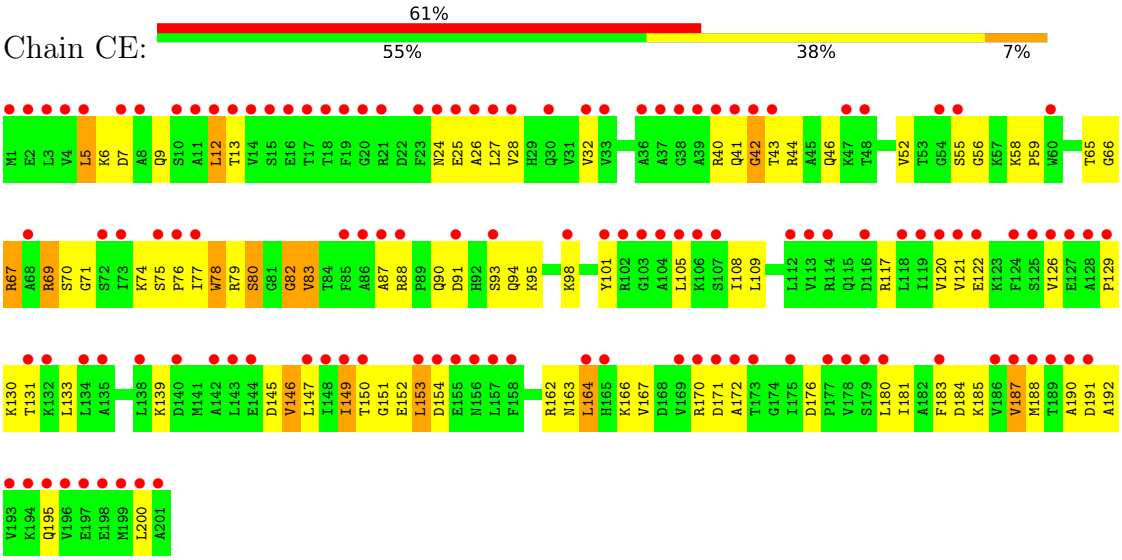
• Molecule 28: 50S ribosomal protein L3

Chain CD:



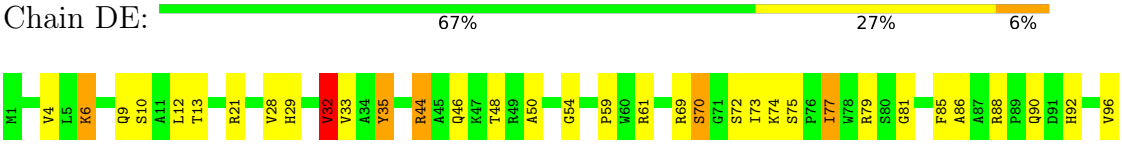
• Molecule 29: 50S ribosomal protein L4

Chain CE:



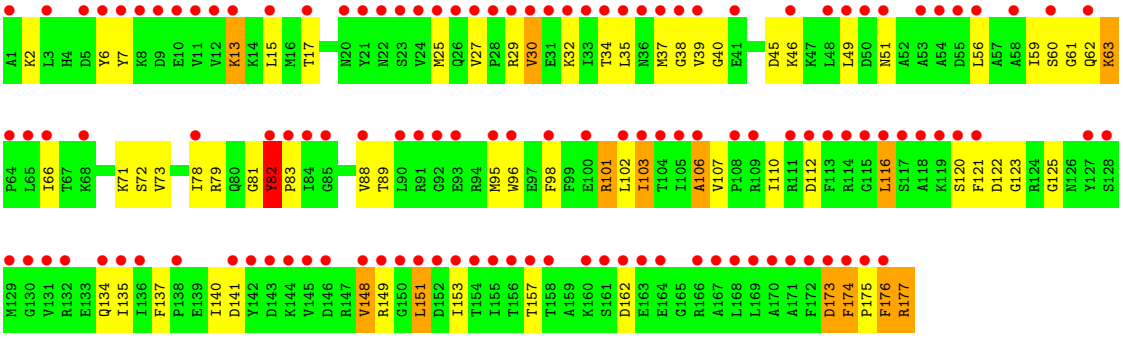
• Molecule 29: 50S ribosomal protein L4

Chain DE:



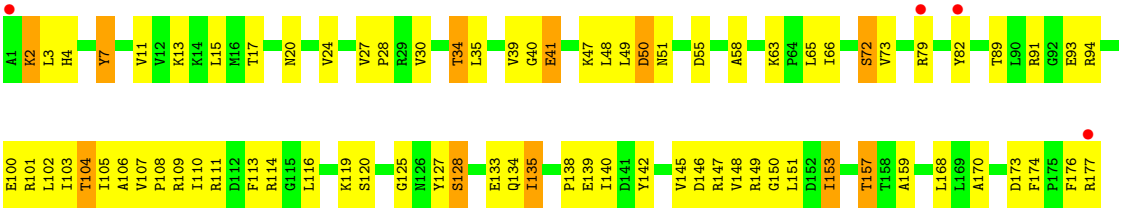
• Molecule 30: 50S ribosomal protein L5

Chain CF:



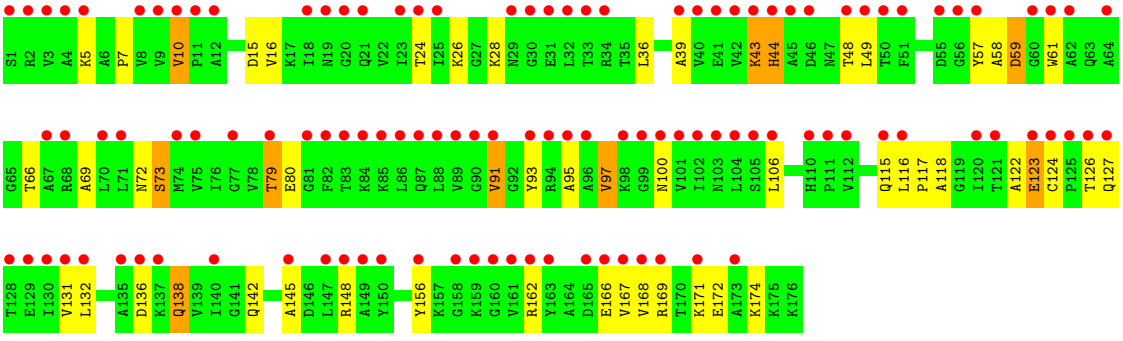
• Molecule 30: 50S ribosomal protein L5

Chain DF:



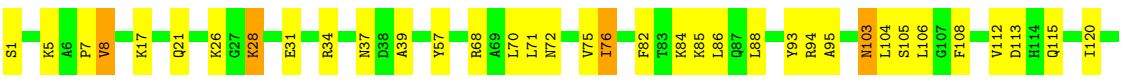
• Molecule 31: 50S ribosomal protein L6

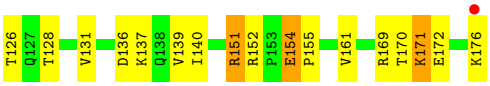
Chain CG:



• Molecule 31: 50S ribosomal protein L6

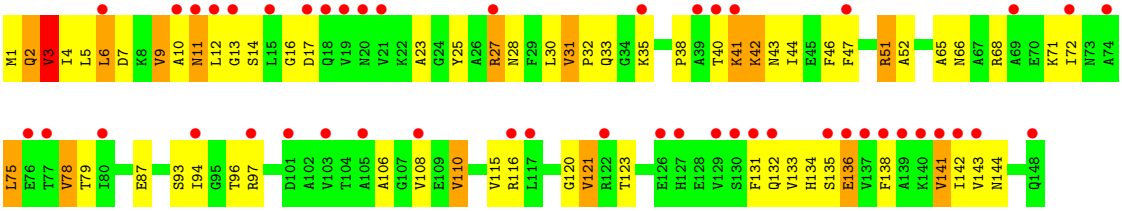
Chain DG:





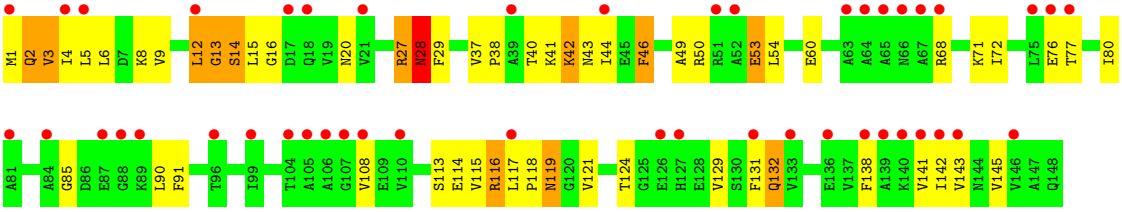
• Molecule 32: 50S ribosomal protein L9

Chain CH:



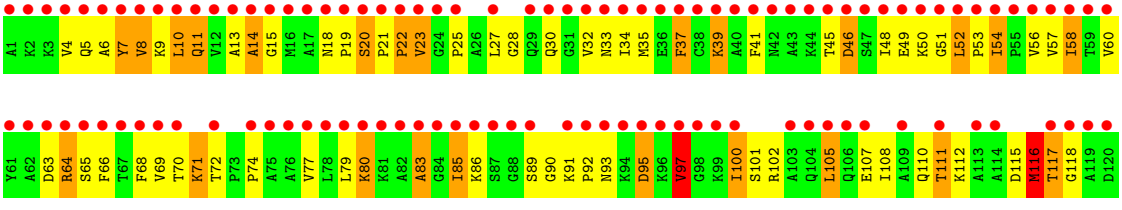
• Molecule 32: 50S ribosomal protein L9

Chain DH:



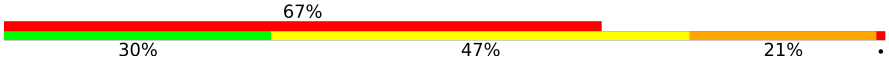
• Molecule 33: 50S ribosomal protein L11

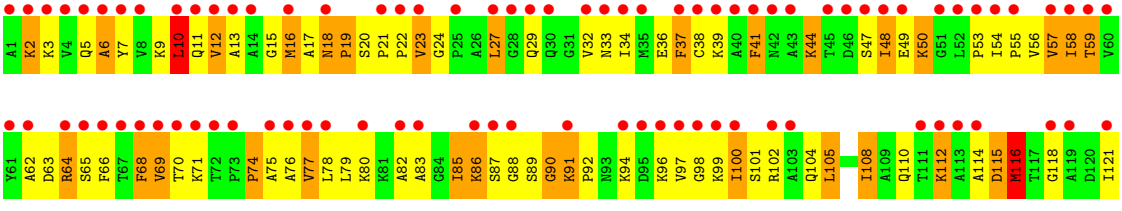
Chain CJ:

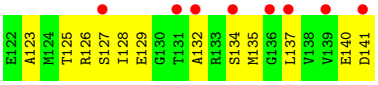


• Molecule 33: 50S ribosomal protein L11

Chain DJ:

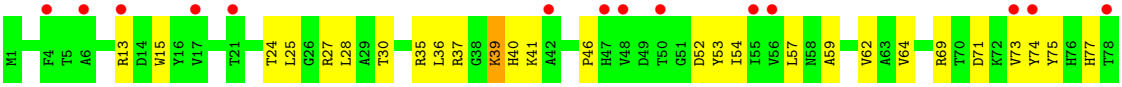


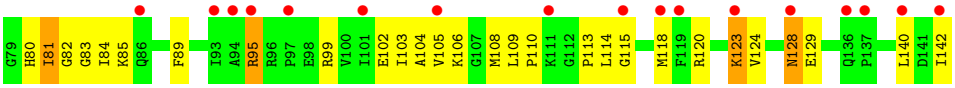




• Molecule 34: 50S ribosomal protein L13

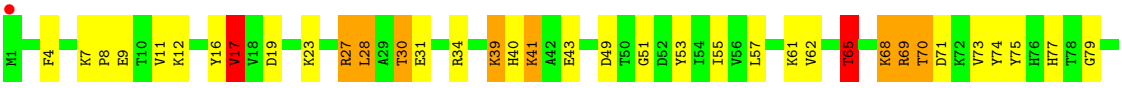
Chain CK:

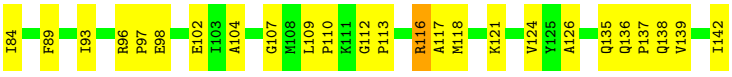




• Molecule 34: 50S ribosomal protein L13

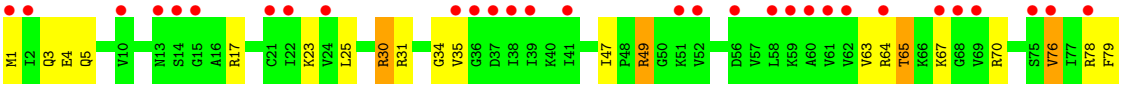
Chain DK:

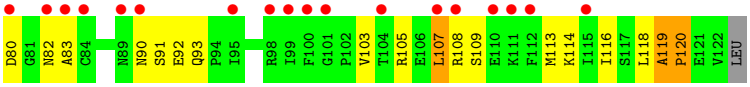




• Molecule 35: 50S ribosomal protein L14

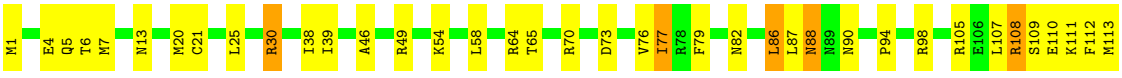
Chain CL:





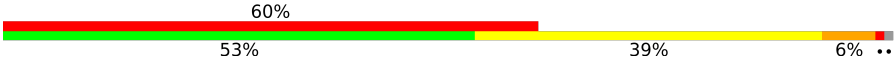
• Molecule 35: 50S ribosomal protein L14

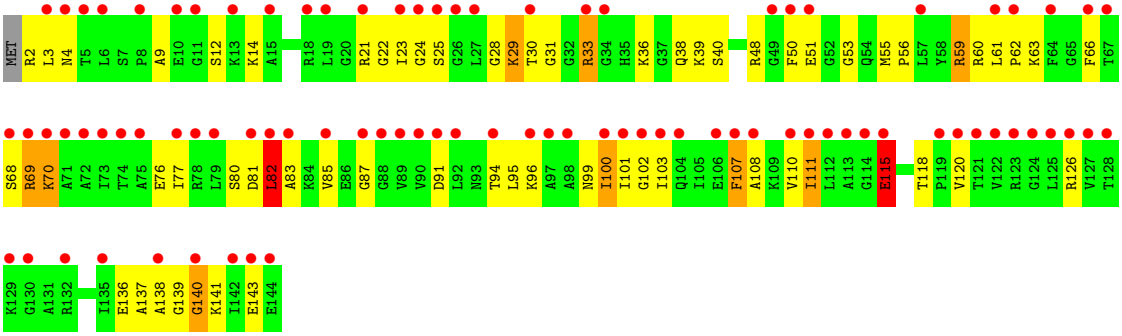
Chain DL:



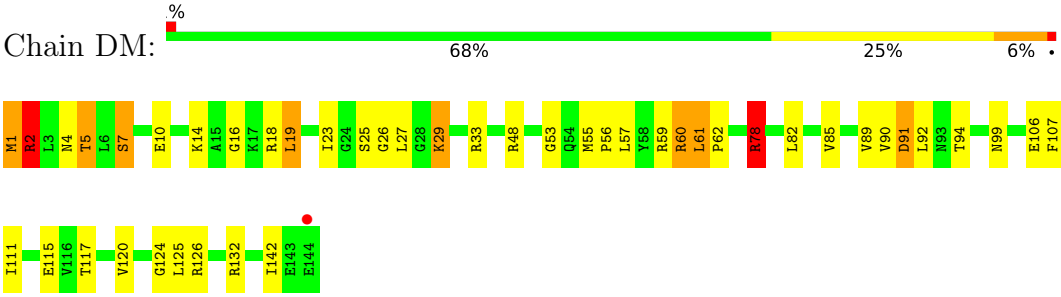
• Molecule 36: 50S ribosomal protein L15

Chain CM:

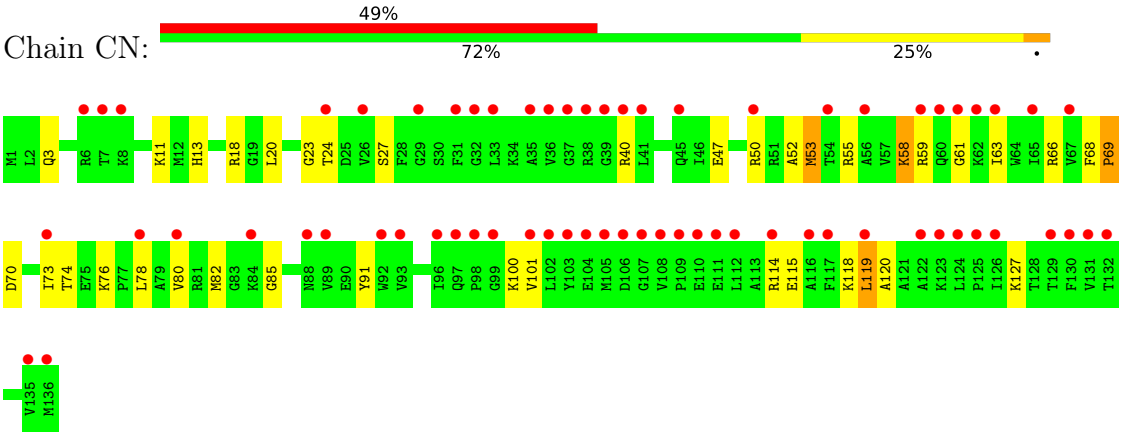




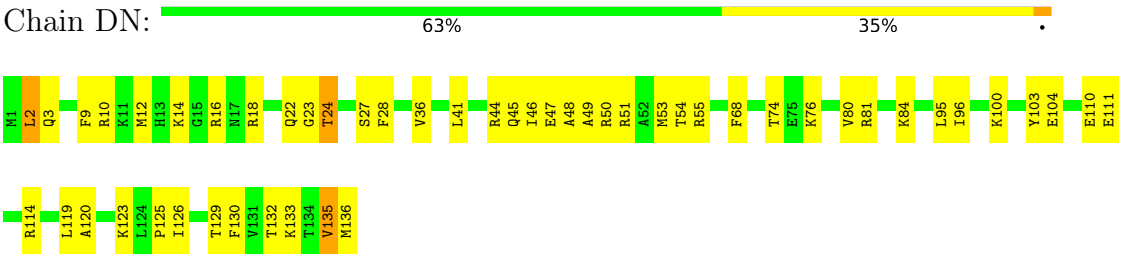
• Molecule 36: 50S ribosomal protein L15



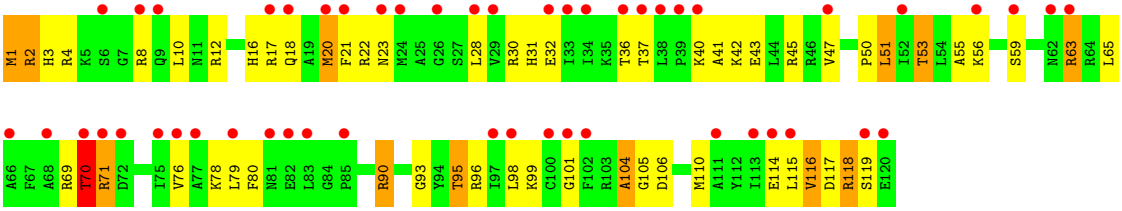
• Molecule 37: 50S ribosomal protein L16



• Molecule 37: 50S ribosomal protein L16

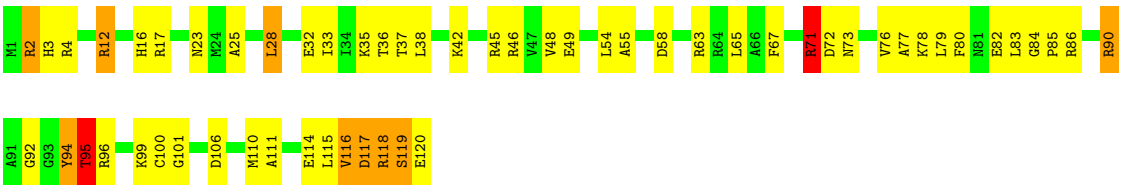


• Molecule 38: 50S ribosomal protein L17



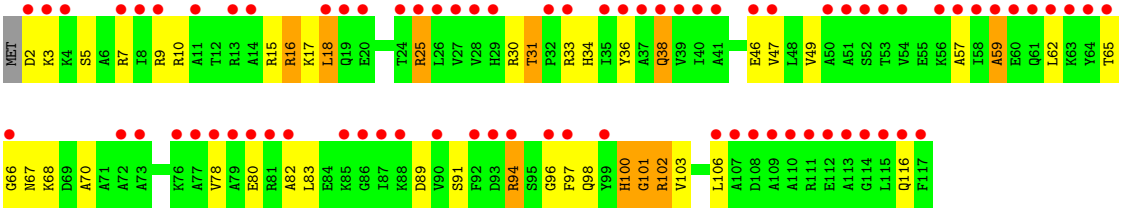
• Molecule 38: 50S ribosomal protein L17

Chain DO:



• Molecule 39: 50S ribosomal protein L18

Chain CP:

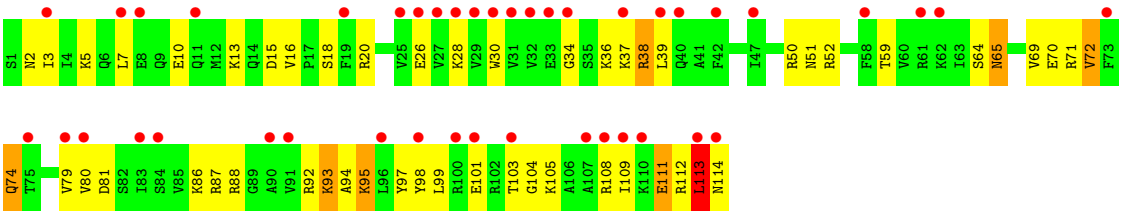


• Molecule 39: 50S ribosomal protein L18

Chain DP:

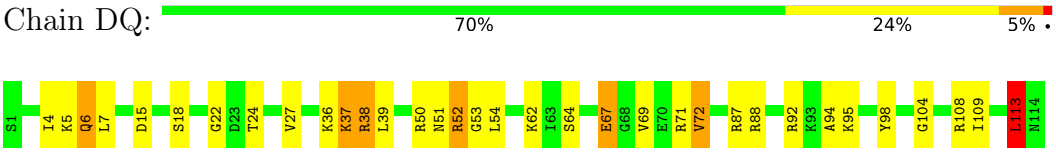
• Molecule 40: 50S ribosomal protein L19

Chain CQ:



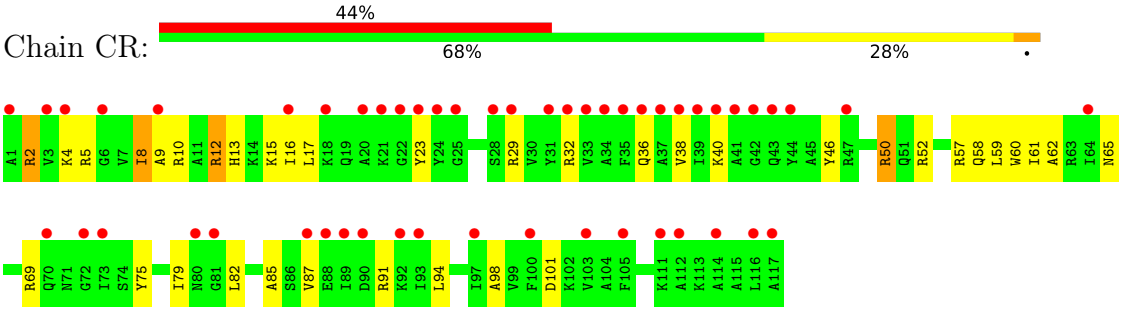
• Molecule 40: 50S ribosomal protein L19

Chain DQ:



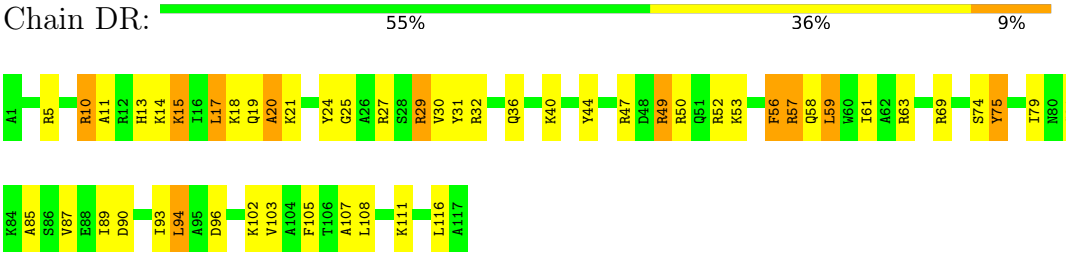
• Molecule 41: 50S ribosomal protein L20

Chain CR:



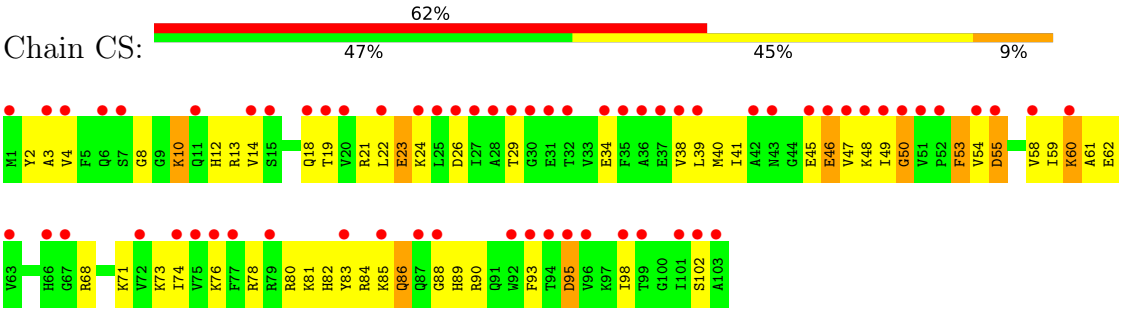
• Molecule 41: 50S ribosomal protein L20

Chain DR:



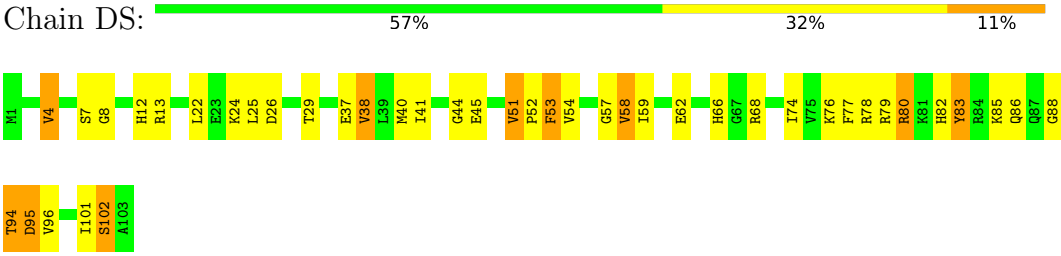
• Molecule 42: 50S ribosomal protein L21

Chain CS:



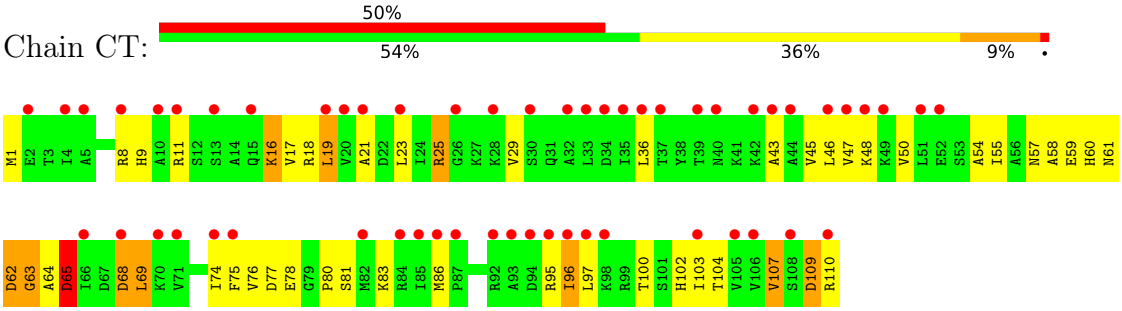
• Molecule 42: 50S ribosomal protein L21

Chain DS:



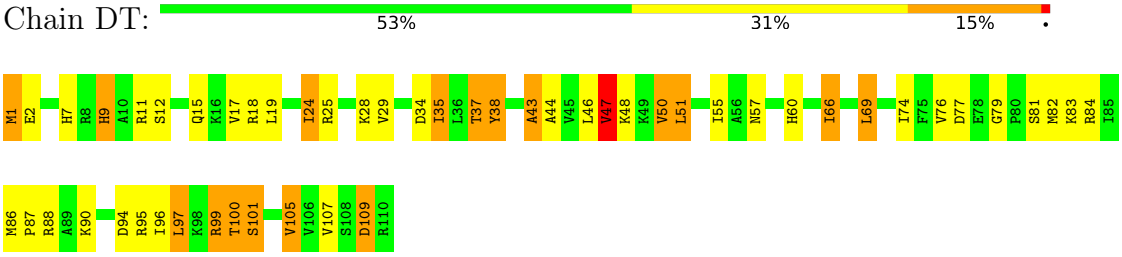
• Molecule 43: 50S ribosomal protein L22

Chain CT:



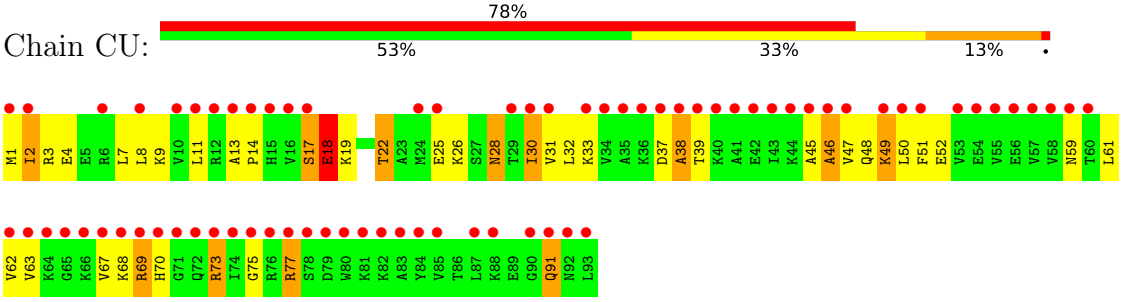
• Molecule 43: 50S ribosomal protein L22

Chain DT:



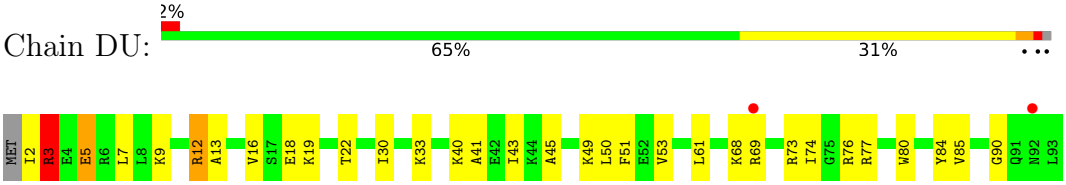
• Molecule 44: 50S ribosomal protein L23

Chain CU:



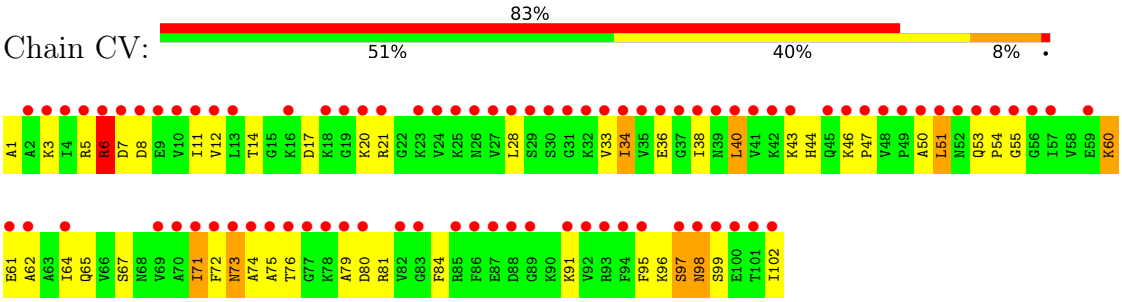
• Molecule 44: 50S ribosomal protein L23

Chain DU:



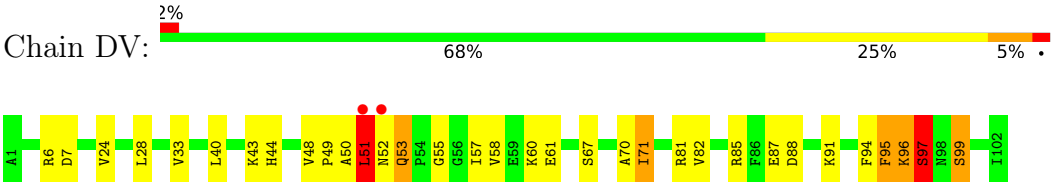
• Molecule 45: 50S ribosomal protein L24

Chain CV:



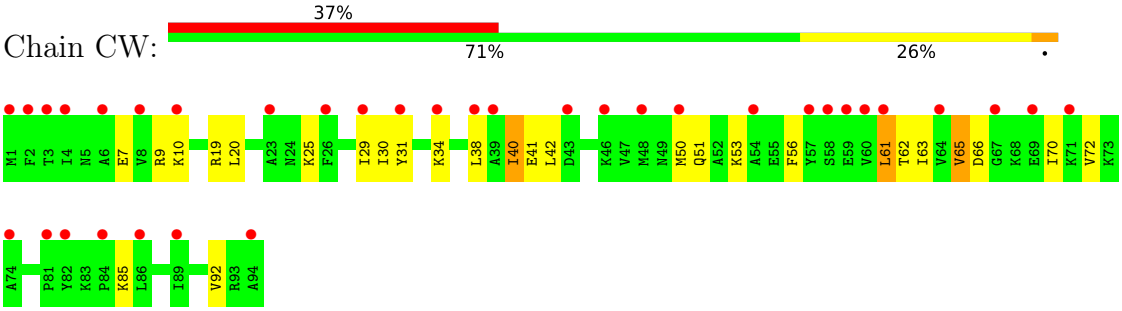
• Molecule 45: 50S ribosomal protein L24

Chain DV:



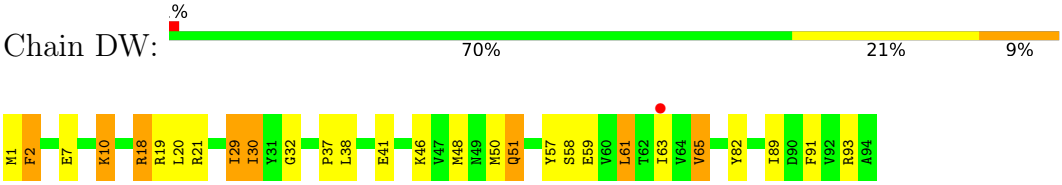
• Molecule 46: 50S ribosomal protein L25

Chain CW:



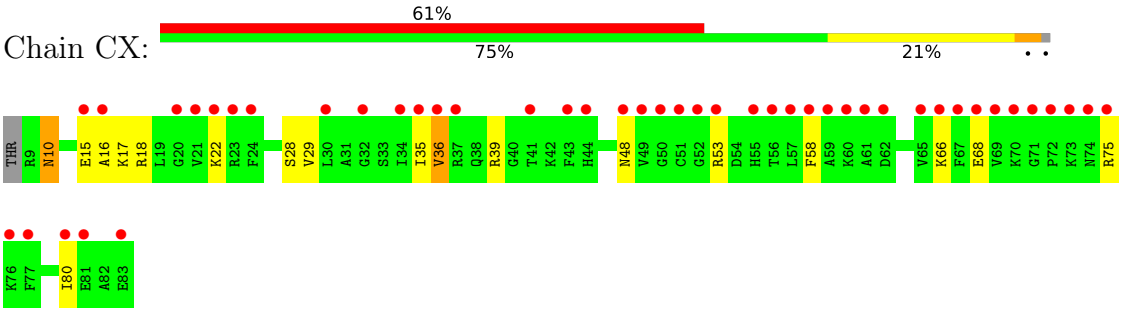
• Molecule 46: 50S ribosomal protein L25

Chain DW:



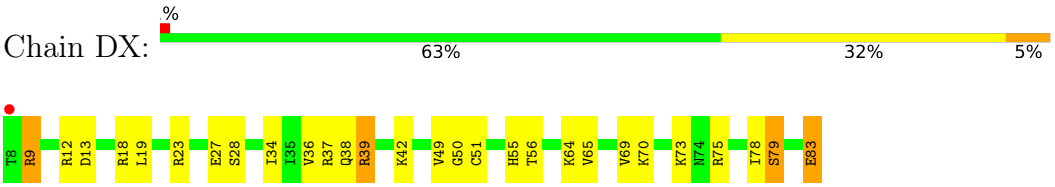
• Molecule 47: 50S ribosomal protein L27

Chain CX:



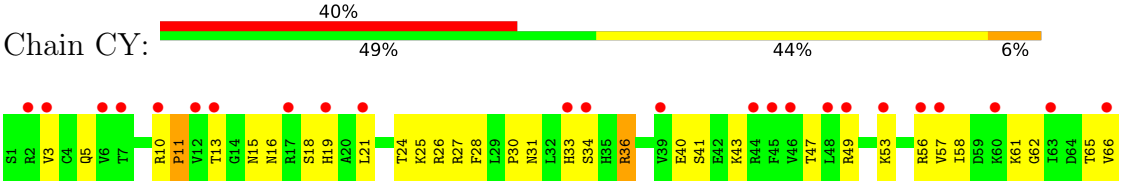
• Molecule 47: 50S ribosomal protein L27

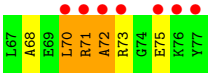
Chain DX:



• Molecule 48: 50S ribosomal protein L28

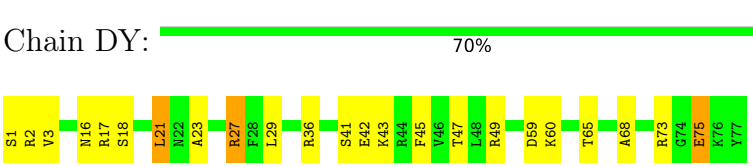
Chain CY:





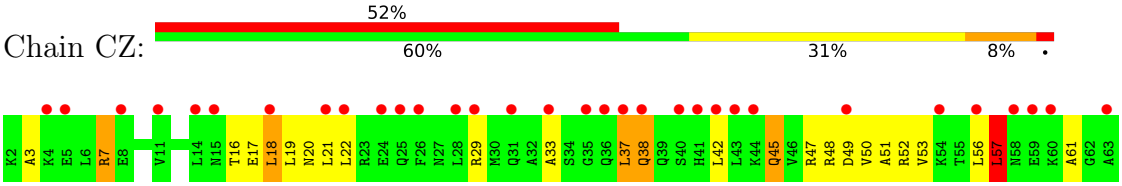
• Molecule 48: 50S ribosomal protein L28

Chain DY:



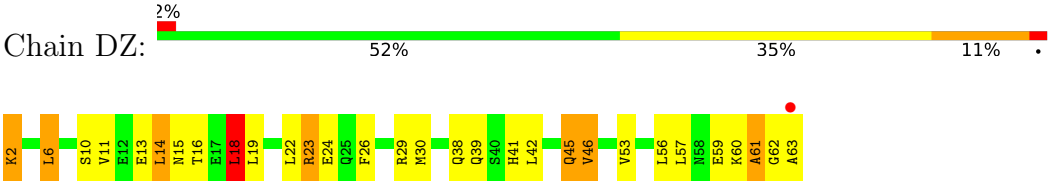
• Molecule 49: 50S ribosomal protein L29

Chain CZ:



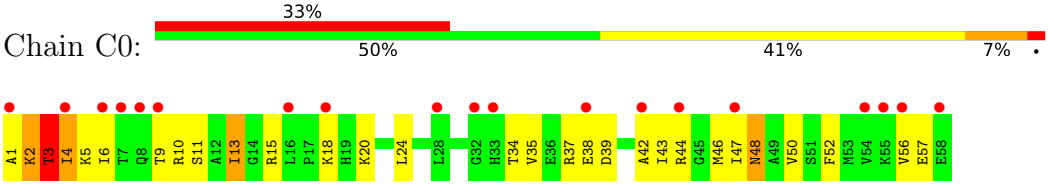
• Molecule 49: 50S ribosomal protein L29

Chain DZ:



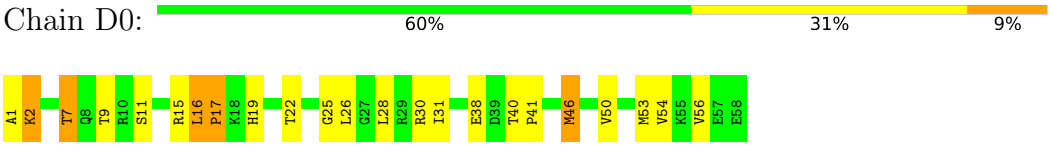
• Molecule 50: 50S ribosomal protein L30

Chain C0:



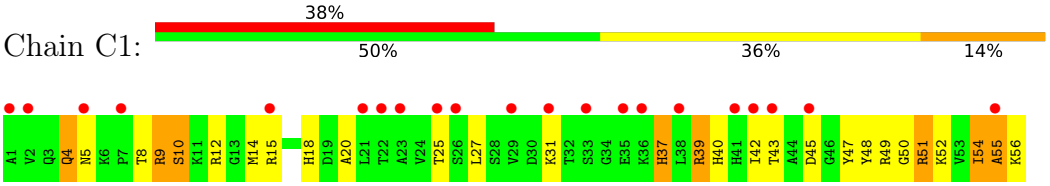
• Molecule 50: 50S ribosomal protein L30

Chain D0:



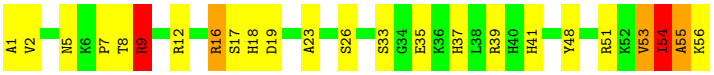
• Molecule 51: 50S ribosomal protein L32

Chain C1:



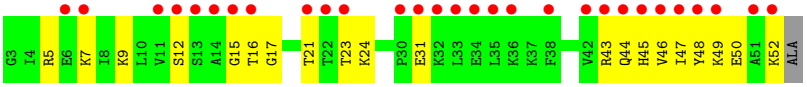
• Molecule 51: 50S ribosomal protein L32

Chain D1:



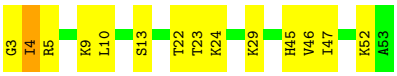
• Molecule 52: 50S ribosomal protein L33

Chain C2:



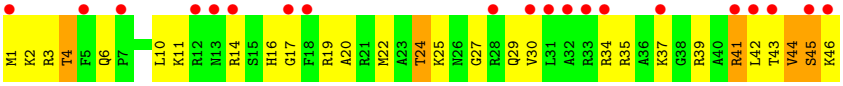
• Molecule 52: 50S ribosomal protein L33

Chain D2:



• Molecule 53: 50S ribosomal protein L34

Chain C3:

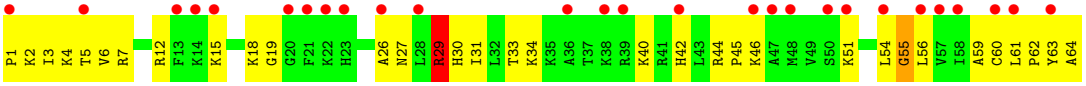


• Molecule 53: 50S ribosomal protein L34

Chain D3:

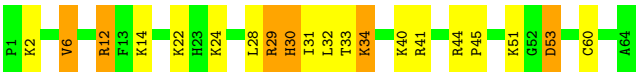
• Molecule 54: 50S ribosomal protein L35

Chain C4:



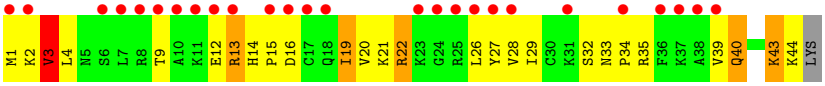
• Molecule 54: 50S ribosomal protein L35

Chain D4:



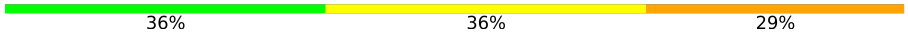
• Molecule 55: 50S ribosomal protein L36 2

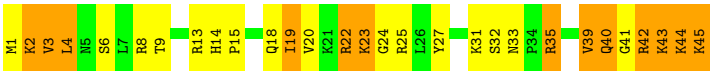
Chain C5:



• Molecule 55: 50S ribosomal protein L36 2

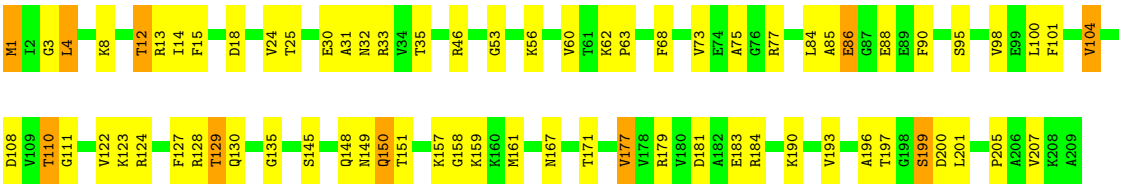
Chain D5:





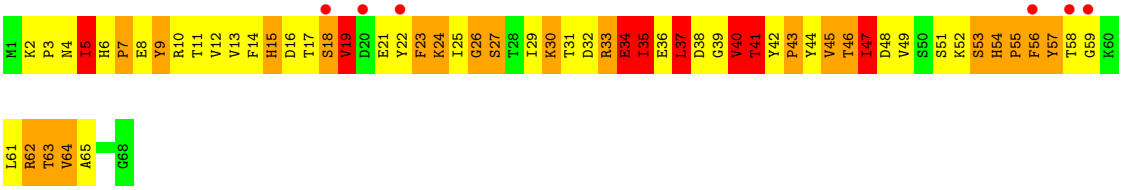
• Molecule 56: 50S ribosomal protein L3

Chain DD:



• Molecule 57: 50S ribosomal protein L31 type B

Chain D7:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	212.02Å 434.57Å 623.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.32 – 2.90 69.32 – 2.83	Depositor EDS
% Data completeness (in resolution range)	85.2 (69.32-2.90) 79.8 (69.32-2.83)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.186 , 0.255 0.186 , 0.255	Depositor DCC
R_{free} test set	5389 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å^2)	45.6	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 109.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	484785	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, PSU, 5MC, PUT, OMG, PEG, MEQ, 2MG, 2MA, 6MZ, D2T, MG, MPD, H2U, PG4, OMC, 3TD, EDO, G7M, PGE, UR3, 1MG, 5MU, 1PE, MA6, GUN, 4OC, SPD, ACY

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	1.13	110/36568 (0.3%)	1.87	1555/57042 (2.7%)
2	BA	0.95	49/36834 (0.1%)	1.61	852/57462 (1.5%)
3	DA	1.91	1848/69150 (2.7%)	2.50	6915/107874 (6.4%)
4	CA	0.77	39/69681 (0.1%)	1.45	1050/108706 (1.0%)
5	CB	0.53	0/2828	1.07	6/4410 (0.1%)
5	DB	1.79	68/2850 (2.4%)	2.47	288/4444 (6.5%)
6	AB	0.69	0/1736	1.12	6/2338 (0.3%)
6	BB	0.64	0/1736	1.11	8/2338 (0.3%)
7	AC	0.68	0/1652	0.97	2/2225 (0.1%)
7	BC	0.59	0/1652	0.97	5/2225 (0.2%)
8	AD	0.62	0/1665	0.97	4/2227 (0.2%)
8	BD	0.73	0/1665	1.05	7/2227 (0.3%)
9	AE	0.75	0/1119	1.21	5/1504 (0.3%)
9	BE	0.70	0/1119	1.13	4/1504 (0.3%)
10	AF	0.71	0/836	1.03	2/1128 (0.2%)
10	BF	0.65	0/836	1.09	3/1128 (0.3%)
11	AG	0.53	0/1196	0.83	0/1602
11	BG	0.50	0/1196	0.99	2/1602 (0.1%)
12	AH	0.71	0/989	1.07	4/1326 (0.3%)
12	BH	0.62	0/989	0.96	1/1326 (0.1%)
13	AI	0.58	0/1034	1.01	2/1375 (0.1%)
13	BI	0.54	0/1034	1.03	0/1375
14	AJ	0.73	1/797 (0.1%)	1.12	3/1077 (0.3%)
14	BJ	0.78	2/797 (0.3%)	1.02	0/1077
15	AK	0.53	0/893	0.90	0/1205
15	BK	0.63	0/893	1.05	2/1205 (0.2%)
16	AL	0.78	0/960	1.08	4/1286 (0.3%)
17	AM	0.56	0/893	0.98	1/1193 (0.1%)
17	BM	0.43	0/893	0.92	0/1193
18	AN	0.66	0/785	1.12	3/1043 (0.3%)
18	BN	0.51	0/785	0.95	0/1043

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
19	AO	0.63	0/724	1.07	3/966 (0.3%)
19	BO	0.58	0/724	1.03	2/966 (0.2%)
20	AP	0.66	0/659	1.03	1/884 (0.1%)
20	BP	0.67	0/659	1.11	2/884 (0.2%)
21	AQ	0.74	1/658 (0.2%)	0.99	2/881 (0.2%)
21	BQ	0.60	0/658	1.00	2/881 (0.2%)
22	AR	0.60	0/463	1.03	1/621 (0.2%)
22	BR	0.69	0/463	1.00	0/621
23	AS	0.72	1/653 (0.2%)	1.03	2/877 (0.2%)
23	BS	0.42	0/653	0.89	0/877
24	AT	0.70	0/671	0.94	2/888 (0.2%)
24	BT	0.54	0/671	1.01	2/888 (0.2%)
25	AU	0.69	0/457	1.12	2/606 (0.3%)
25	BU	0.76	0/457	1.22	2/606 (0.3%)
26	BL	0.74	0/969	1.23	8/1300 (0.6%)
27	CC	0.67	0/2122	1.02	4/2852 (0.1%)
27	DC	1.03	6/2122 (0.3%)	1.16	10/2852 (0.4%)
28	CD	0.52	0/1586	0.90	2/2134 (0.1%)
29	CE	0.47	0/1571	0.90	1/2113 (0.0%)
29	DE	0.93	3/1571 (0.2%)	1.15	6/2113 (0.3%)
30	CF	0.46	0/1435	0.98	4/1926 (0.2%)
30	DF	0.79	0/1435	1.10	7/1926 (0.4%)
31	CG	0.41	0/1343	0.71	0/1816
31	DG	0.83	1/1343 (0.1%)	1.02	4/1816 (0.2%)
32	CH	0.53	0/1113	0.82	1/1504 (0.1%)
32	DH	0.49	0/1113	0.91	2/1504 (0.1%)
33	CJ	0.45	0/1046	0.90	0/1410
33	DJ	0.47	0/1046	0.98	3/1410 (0.2%)
34	CK	0.51	0/1152	0.77	0/1551
34	DK	1.34	10/1152 (0.9%)	1.37	11/1551 (0.7%)
35	CL	0.59	0/947	0.96	1/1268 (0.1%)
35	DL	1.04	1/955 (0.1%)	1.23	4/1279 (0.3%)
36	CM	0.49	0/1054	0.99	3/1403 (0.2%)
36	DM	0.98	1/1062 (0.1%)	1.17	5/1413 (0.4%)
37	CN	0.55	0/1093	0.92	0/1460
37	DN	1.02	1/1104 (0.1%)	1.19	4/1474 (0.3%)
38	CO	0.54	0/974	0.98	1/1301 (0.1%)
38	DO	1.11	1/974 (0.1%)	1.43	9/1301 (0.7%)
39	CP	0.47	0/902	0.88	1/1209 (0.1%)
39	DP	0.93	1/910 (0.1%)	1.16	2/1219 (0.2%)
40	CQ	0.55	0/929	0.99	2/1242 (0.2%)
40	DQ	0.99	4/929 (0.4%)	1.13	5/1242 (0.4%)
41	CR	0.55	0/960	0.93	2/1278 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
41	DR	1.23	5/960 (0.5%)	1.37	11/1278 (0.9%)
42	CS	0.47	0/829	0.93	0/1107
42	DS	1.22	5/829 (0.6%)	1.25	6/1107 (0.5%)
43	CT	0.52	0/864	0.98	4/1156 (0.3%)
43	DT	1.12	2/864 (0.2%)	1.44	12/1156 (1.0%)
44	CU	0.46	0/745	0.92	0/994
44	DU	0.96	0/737	1.02	1/984 (0.1%)
45	CV	0.41	0/788	0.98	1/1051 (0.1%)
45	DV	1.06	4/788 (0.5%)	1.19	4/1051 (0.4%)
46	CW	0.40	0/766	0.77	0/1025
46	DW	0.98	2/766 (0.3%)	1.26	6/1025 (0.6%)
47	CX	0.59	0/576	0.82	0/762
47	DX	1.21	5/602 (0.8%)	1.24	0/795
48	CY	0.62	0/635	0.98	0/848
48	DY	0.92	1/635 (0.2%)	1.05	1/848 (0.1%)
49	CZ	0.42	0/502	0.92	0/667
49	DZ	0.79	1/502 (0.2%)	1.18	3/667 (0.4%)
50	C0	0.50	0/453	0.86	0/605
50	D0	1.09	1/460 (0.2%)	1.34	4/615 (0.7%)
51	C1	0.52	0/450	0.93	0/599
51	D1	1.02	1/450 (0.2%)	1.48	8/599 (1.3%)
52	C2	0.46	0/416	0.83	0/554
52	D2	0.93	0/421	1.09	1/561 (0.2%)
53	C3	0.72	0/380	1.02	1/498 (0.2%)
53	D3	1.01	0/380	1.43	8/498 (1.6%)
54	C4	0.57	0/513	1.02	0/676
54	D4	0.99	1/513 (0.2%)	1.18	2/676 (0.3%)
55	C5	0.54	0/363	0.68	0/479
55	D5	1.14	1/372 (0.3%)	1.19	1/490 (0.2%)
56	DD	1.09	4/1576 (0.3%)	1.20	5/2119 (0.2%)
57	D7	0.63	0/542	0.81	0/736
All	All	1.19	2181/309220 (0.7%)	1.75	10938/462249 (2.4%)

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
7	AC	0	1
8	BD	0	1
10	BF	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	AI	0	1
14	AJ	0	1
15	BK	0	1
19	AO	0	1
19	BO	0	1
21	AQ	0	1
23	AS	0	1
24	AT	0	2
24	BT	0	1
25	AU	0	1
27	CC	0	1
27	DC	0	5
28	CD	0	2
29	DE	0	6
30	DF	0	1
32	CH	0	1
33	CJ	0	1
33	DJ	0	1
34	DK	0	8
35	CL	0	1
35	DL	0	1
36	DM	0	3
38	DO	0	4
39	DP	0	1
40	DQ	0	1
41	DR	0	6
42	DS	0	1
43	DT	0	9
45	DV	0	1
46	DW	0	4
47	DX	0	4
49	DZ	0	2
50	D0	0	4
51	D1	0	2
57	D7	0	1
All	All	0	85

The worst 5 of 2181 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DA	2098	U	C4-O4	16.35	1.36	1.23
3	DA	2014	A	N7-C5	-15.31	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DA	2070	A	N9-C4	-13.38	1.29	1.37
3	DA	2886	A	N7-C5	13.28	1.47	1.39
3	DA	783	A	N9-C4	-13.27	1.29	1.37

The worst 5 of 10938 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	DA	2588	G	O5'-P-OP2	-20.85	85.68	110.70
3	DA	1658	C	C6-N1-C2	20.56	128.52	120.30
3	DA	783	A	C5-N7-C8	-19.61	94.09	103.90
3	DA	541	A	O5'-P-OP2	-19.15	87.72	110.70
3	DA	2868	A	O5'-P-OP2	-18.93	87.99	110.70

There are no chirality outliers.

5 of 85 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	AC	123	GLN	Sidechain
13	AI	57	MET	Peptide
14	AJ	58	ASN	Mainchain
19	AO	36	ILE	Mainchain
21	AQ	78	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32908	16444	16574	1167	1
2	BA	32895	16553	16553	1220	0
3	DA	62254	31129	31238	2187	1
4	CA	62215	31288	31289	2254	0
5	CB	2529	1281	1281	53	0
5	DB	2549	1291	1289	63	0
6	AB	1705	1726	1732	145	0
6	BB	1705	1726	1732	148	0
7	AC	1625	1692	1696	67	0
7	BC	1625	1692	1696	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AD	1643	1704	1707	87	0
8	BD	1643	1704	1707	65	0
9	AE	1106	1145	1148	81	0
9	BE	1106	1145	1148	97	0
10	AF	818	799	808	34	0
10	BF	818	799	808	39	0
11	AG	1182	1237	1238	50	0
11	BG	1182	1237	1238	60	0
12	AH	979	1031	1031	35	0
12	BH	979	1031	1031	41	0
13	AI	1022	1069	1070	55	0
13	BI	1022	1069	1070	69	0
14	AJ	787	825	828	81	0
14	BJ	787	825	828	30	0
15	AK	877	884	887	30	0
15	BK	877	884	887	52	0
16	AL	957	1009	1017	29	0
17	AM	884	938	941	49	0
17	BM	884	938	941	38	0
18	AN	774	823	827	65	0
18	BN	774	823	827	49	0
19	AO	716	734	739	39	0
19	BO	716	734	739	31	0
20	AP	649	661	666	26	0
20	BP	649	661	666	37	0
21	AQ	649	688	691	35	0
21	BQ	649	688	691	32	0
22	AR	456	477	478	9	0
22	BR	456	477	478	26	0
23	AS	638	657	665	29	0
23	BS	638	661	665	19	0
24	AT	665	711	714	38	0
24	BT	665	711	714	32	0
25	AU	451	473	474	16	0
25	BU	451	473	474	26	0
26	BL	955	1013	1016	46	0
27	CC	2083	2148	2157	92	0
27	DC	2083	2148	2157	71	0
28	CD	1565	1610	1616	73	0
29	CE	1552	1613	1619	73	0
29	DE	1552	1613	1619	40	0
30	CF	1411	1443	1447	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	DF	1411	1443	1447	62	0
31	CG	1323	1368	1374	29	0
31	DG	1323	1368	1374	29	0
32	CH	1102	1134	1139	40	1
32	DH	1102	1134	1139	42	0
33	CJ	1032	1085	1088	73	0
33	DJ	1032	1085	1088	83	0
34	CK	1129	1152	1162	37	0
34	DK	1129	1152	1162	39	0
35	CL	938	1008	1012	32	0
35	DL	946	1019	1023	34	0
36	CM	1045	1116	1117	73	0
36	DM	1053	1125	1129	41	0
37	CN	1074	1153	1157	26	0
37	DN	1082	1166	1170	44	0
38	CO	961	994	1000	56	0
38	DO	961	994	1000	48	0
39	CP	892	920	923	31	0
39	DP	900	929	935	37	0
40	CQ	917	960	965	39	0
40	DQ	917	960	965	24	0
41	CR	947	1018	1022	39	0
41	DR	947	1018	1022	45	0
42	CS	816	832	839	40	0
42	DS	816	832	839	35	0
43	CT	857	915	922	40	0
43	DT	857	915	922	35	0
44	CU	739	802	807	44	0
44	DU	731	794	795	22	0
45	CV	780	830	834	53	0
45	DV	780	830	834	20	0
46	CW	753	774	780	13	0
46	DW	753	774	780	19	0
47	CX	569	579	581	12	0
47	DX	591	606	604	18	0
48	CY	625	649	655	36	0
48	DY	625	649	655	16	0
49	CZ	501	530	531	22	0
49	DZ	501	530	531	21	0
50	C0	449	486	491	19	0
50	D0	449	486	484	15	1
51	C1	444	454	461	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	D1	444	454	461	28	0
52	C2	409	438	440	14	0
52	D2	414	443	445	9	0
53	C3	377	414	418	27	0
53	D3	377	414	418	8	0
54	C4	504	568	574	31	0
54	D4	504	568	574	22	0
55	C5	359	395	397	15	0
55	D5	368	395	410	34	0
56	DD	1566	1612	1618	55	0
57	D7	530	177	517	101	0
58	AA	57	0	0	0	0
58	BA	49	0	0	0	0
58	C3	1	0	0	0	0
58	CA	176	0	0	0	0
58	CB	3	0	0	0	0
58	CM	1	0	0	0	0
58	CR	1	0	0	0	0
58	D5	1	0	0	0	0
58	DA	156	0	0	0	0
58	DB	4	0	0	0	0
58	DD	1	0	0	0	0
58	DM	1	0	0	0	0
58	DR	2	0	0	0	0
59	AA	10	14	14	0	0
59	D3	10	14	14	0	0
59	DA	20	28	28	2	0
59	DD	10	14	14	0	0
59	DS	10	14	14	0	0
59	DT	10	14	14	2	0
59	DU	10	14	14	0	0
60	AA	8	14	14	0	0
60	DA	56	98	98	10	0
60	DE	16	28	28	1	0
60	DK	8	14	14	0	0
60	DN	8	14	14	1	0
60	DT	8	14	14	0	0
61	BA	13	0	18	0	0
61	DA	13	0	18	3	0
61	DQ	13	0	18	3	0
61	DR	13	0	18	8	0
61	DS	13	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	DA	30	0	57	4	0
63	D5	6	0	12	2	0
63	DA	24	0	48	13	0
63	DM	6	0	12	1	0
63	DP	6	0	12	10	0
64	DA	32	0	44	7	0
65	DA	12	9	9	6	0
66	D1	7	0	10	3	0
66	D3	7	0	10	2	0
66	DA	35	0	50	5	0
66	DP	7	0	10	1	0
66	DQ	7	0	10	1	0
67	D1	4	0	6	0	0
67	DA	28	0	42	10	0
67	DB	12	0	18	1	0
67	DR	4	0	6	2	0
68	DA	11	0	5	2	0
69	AA	371	0	0	95	0
69	AB	11	0	0	6	0
69	AC	6	0	0	1	0
69	AD	3	0	0	1	0
69	AE	11	0	0	9	0
69	AF	5	0	0	1	0
69	AG	7	0	0	6	0
69	AH	2	0	0	1	0
69	AI	1	0	0	0	0
69	AJ	2	0	0	0	0
69	AK	8	0	0	1	0
69	AL	5	0	0	1	0
69	AM	7	0	0	1	0
69	AN	7	0	0	4	0
69	AO	1	0	0	0	0
69	AP	2	0	0	0	0
69	AQ	5	0	0	0	0
69	AS	3	0	0	4	0
69	AT	5	0	0	2	0
69	AU	2	0	0	0	0
69	BA	389	0	0	119	0
69	BB	5	0	0	5	0
69	BC	3	0	0	3	0
69	BD	9	0	0	0	0
69	BE	5	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	BF	7	0	0	1	0
69	BG	7	0	0	1	0
69	BH	5	0	0	1	0
69	BI	4	0	0	2	0
69	BJ	1	0	0	0	0
69	BK	1	0	0	0	0
69	BL	3	0	0	0	0
69	BM	3	0	0	0	0
69	BN	8	0	0	3	0
69	BO	4	0	0	1	0
69	BP	4	0	0	5	0
69	BQ	1	0	0	0	0
69	BS	2	0	0	0	0
69	BT	5	0	0	2	0
69	BU	3	0	0	0	0
69	C0	3	0	0	1	0
69	C1	1	0	0	1	0
69	C2	1	0	0	0	0
69	C3	5	0	0	2	0
69	C4	3	0	0	1	0
69	C5	1	0	0	0	0
69	CA	1042	0	0	324	0
69	CB	19	0	0	2	0
69	CC	8	0	0	2	0
69	CD	8	0	0	2	0
69	CE	7	0	0	2	0
69	CF	2	0	0	1	0
69	CG	4	0	0	3	0
69	CH	4	0	0	3	0
69	CK	5	0	0	1	0
69	CL	5	0	0	1	0
69	CM	8	0	0	2	0
69	CN	5	0	0	0	0
69	CO	5	0	0	3	0
69	CP	1	0	0	0	0
69	CQ	5	0	0	3	0
69	CR	3	0	0	1	0
69	CS	5	0	0	4	0
69	CT	3	0	0	5	0
69	CU	6	0	0	2	0
69	CV	7	0	0	3	0
69	CW	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	CZ	2	0	0	2	0
69	D0	14	0	0	0	0
69	D1	48	0	0	11	0
69	D2	4	0	0	0	0
69	D3	24	0	0	3	0
69	D4	27	0	0	3	0
69	D5	9	0	0	6	0
69	DA	3565	0	0	603	0
69	DB	90	0	0	17	0
69	DC	59	0	0	10	0
69	DD	80	0	0	7	0
69	DE	51	0	0	7	0
69	DF	5	0	0	0	0
69	DG	5	0	0	1	0
69	DH	2	0	0	0	0
69	DJ	4	0	0	2	0
69	DK	37	0	0	4	0
69	DL	30	0	0	5	0
69	DM	52	0	0	6	0
69	DN	47	0	0	10	0
69	DO	33	0	0	10	0
69	DP	14	0	0	7	0
69	DQ	33	0	0	7	0
69	DR	52	0	0	7	0
69	DS	40	0	0	9	0
69	DT	57	0	0	10	0
69	DU	10	0	0	4	0
69	DV	14	0	0	1	0
69	DW	18	0	0	3	0
69	DX	15	0	0	6	0
69	DY	7	0	0	0	0
69	DZ	2	0	0	0	0
All	All	292901	191884	193327	10306	2

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 22.

The worst 5 of 10306 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)
3:DA:783:A:OP1	69:DA:3201:HOH:O	1.53	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DA:852:U:OP1	69:DA:3202:HOH:O	1.55	1.21
3:DA:1828:G:OP1	69:DA:3203:HOH:O	1.58	1.16
1:AA:411:A:OP2	8:AD:26:ARG:NH2	1.80	1.15
3:DA:576:U:OP1	69:DA:3205:HOH:O	1.64	1.15

All (2) 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)
1:AA:368:U:OP1	32:CH:93:SER:OG[4_455]	2.15	0.05
3:DA:2887:A:OP1	50:D0:1:ALA:N[4_545]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	AB	216/218 (99%)	165 (76%)	20 (9%)	31 (14%)	0 0
6	BB	216/218 (99%)	162 (75%)	22 (10%)	32 (15%)	0 0
7	AC	204/206 (99%)	177 (87%)	19 (9%)	8 (4%)	3 12
7	BC	204/206 (99%)	180 (88%)	14 (7%)	10 (5%)	2 8
8	AD	203/205 (99%)	184 (91%)	9 (4%)	10 (5%)	2 8
8	BD	203/205 (99%)	188 (93%)	8 (4%)	7 (3%)	3 15
9	AE	148/150 (99%)	123 (83%)	12 (8%)	13 (9%)	1 2
9	BE	148/150 (99%)	117 (79%)	18 (12%)	13 (9%)	1 2
10	AF	98/100 (98%)	85 (87%)	8 (8%)	5 (5%)	2 7
10	BF	98/100 (98%)	84 (86%)	9 (9%)	5 (5%)	2 7
11	AG	149/151 (99%)	131 (88%)	13 (9%)	5 (3%)	3 15
11	BG	149/151 (99%)	128 (86%)	18 (12%)	3 (2%)	7 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
12	AH	127/129 (98%)	116 (91%)	11 (9%)	0	100 100
12	BH	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	19 51
13	AI	125/127 (98%)	104 (83%)	17 (14%)	4 (3%)	4 16
13	BI	125/127 (98%)	96 (77%)	18 (14%)	11 (9%)	1 2
14	AJ	96/98 (98%)	68 (71%)	10 (10%)	18 (19%)	0 0
14	BJ	96/98 (98%)	65 (68%)	19 (20%)	12 (12%)	0 0
15	AK	115/117 (98%)	99 (86%)	12 (10%)	4 (4%)	3 14
15	BK	115/117 (98%)	98 (85%)	10 (9%)	7 (6%)	1 4
16	AL	120/123 (98%)	109 (91%)	8 (7%)	3 (2%)	5 21
17	AM	112/114 (98%)	93 (83%)	10 (9%)	9 (8%)	1 2
17	BM	112/114 (98%)	94 (84%)	10 (9%)	8 (7%)	1 3
18	AN	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0 0
18	BN	92/100 (92%)	64 (70%)	13 (14%)	15 (16%)	0 0
19	AO	86/88 (98%)	77 (90%)	3 (4%)	6 (7%)	1 3
19	BO	86/88 (98%)	78 (91%)	1 (1%)	7 (8%)	1 2
20	AP	80/82 (98%)	64 (80%)	8 (10%)	8 (10%)	0 1
20	BP	80/82 (98%)	60 (75%)	15 (19%)	5 (6%)	1 4
21	AQ	78/80 (98%)	66 (85%)	7 (9%)	5 (6%)	1 4
21	BQ	78/80 (98%)	60 (77%)	12 (15%)	6 (8%)	1 2
22	AR	53/55 (96%)	49 (92%)	2 (4%)	2 (4%)	3 13
22	BR	53/55 (96%)	46 (87%)	4 (8%)	3 (6%)	1 5
23	AS	77/79 (98%)	61 (79%)	11 (14%)	5 (6%)	1 3
23	BS	77/79 (98%)	59 (77%)	13 (17%)	5 (6%)	1 3
24	AT	83/85 (98%)	75 (90%)	1 (1%)	7 (8%)	1 2
24	BT	83/85 (98%)	75 (90%)	4 (5%)	4 (5%)	2 8
25	AU	52/54 (96%)	44 (85%)	5 (10%)	3 (6%)	1 5
25	BU	52/54 (96%)	43 (83%)	3 (6%)	6 (12%)	0 1
26	BL	121/123 (98%)	103 (85%)	9 (7%)	9 (7%)	1 2
27	CC	269/271 (99%)	247 (92%)	16 (6%)	6 (2%)	6 24
27	DC	269/271 (99%)	251 (93%)	15 (6%)	3 (1%)	14 42
28	CD	207/209 (99%)	189 (91%)	12 (6%)	6 (3%)	4 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	CE	199/201 (99%)	175 (88%)	17 (8%)	7 (4%)	3 14
29	DE	199/201 (99%)	187 (94%)	9 (4%)	3 (2%)	10 34
30	CF	175/177 (99%)	151 (86%)	15 (9%)	9 (5%)	2 7
30	DF	175/177 (99%)	161 (92%)	14 (8%)	0	100 100
31	CG	174/176 (99%)	138 (79%)	31 (18%)	5 (3%)	4 18
31	DG	174/176 (99%)	167 (96%)	7 (4%)	0	100 100
32	CH	146/148 (99%)	114 (78%)	24 (16%)	8 (6%)	2 5
32	DH	146/148 (99%)	117 (80%)	20 (14%)	9 (6%)	1 4
33	CJ	139/141 (99%)	89 (64%)	32 (23%)	18 (13%)	0 0
33	DJ	139/141 (99%)	87 (63%)	26 (19%)	26 (19%)	0 0
34	CK	140/142 (99%)	125 (89%)	12 (9%)	3 (2%)	7 26
34	DK	140/142 (99%)	137 (98%)	3 (2%)	0	100 100
35	CL	120/123 (98%)	104 (87%)	13 (11%)	3 (2%)	5 21
35	DL	121/123 (98%)	113 (93%)	5 (4%)	3 (2%)	5 21
36	CM	141/144 (98%)	113 (80%)	16 (11%)	12 (8%)	1 2
36	DM	142/144 (99%)	139 (98%)	2 (1%)	1 (1%)	22 54
37	CN	134/136 (98%)	120 (90%)	11 (8%)	3 (2%)	6 24
37	DN	135/136 (99%)	127 (94%)	8 (6%)	0	100 100
38	CO	118/120 (98%)	103 (87%)	11 (9%)	4 (3%)	3 15
38	DO	118/120 (98%)	108 (92%)	8 (7%)	2 (2%)	9 31
39	CP	114/117 (97%)	104 (91%)	5 (4%)	5 (4%)	2 10
39	DP	115/117 (98%)	110 (96%)	3 (3%)	2 (2%)	9 31
40	CQ	112/114 (98%)	101 (90%)	8 (7%)	3 (3%)	5 19
40	DQ	112/114 (98%)	106 (95%)	5 (4%)	1 (1%)	17 48
41	CR	115/117 (98%)	111 (96%)	3 (3%)	1 (1%)	17 48
41	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100 100
42	CS	101/103 (98%)	89 (88%)	7 (7%)	5 (5%)	2 7
42	DS	101/103 (98%)	95 (94%)	6 (6%)	0	100 100
43	CT	108/110 (98%)	97 (90%)	9 (8%)	2 (2%)	8 28
43	DT	108/110 (98%)	104 (96%)	4 (4%)	0	100 100
44	CU	91/93 (98%)	74 (81%)	13 (14%)	4 (4%)	2 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
44	DU	90/93 (97%)	82 (91%)	6 (7%)	2 (2%)	6 24
45	CV	100/102 (98%)	79 (79%)	15 (15%)	6 (6%)	1 4
45	DV	100/102 (98%)	91 (91%)	4 (4%)	5 (5%)	2 7
46	CW	92/94 (98%)	84 (91%)	8 (9%)	0	100 100
46	DW	92/94 (98%)	89 (97%)	3 (3%)	0	100 100
47	CX	73/76 (96%)	70 (96%)	3 (4%)	0	100 100
47	DX	76/76 (100%)	72 (95%)	3 (4%)	1 (1%)	12 37
48	CY	75/77 (97%)	69 (92%)	3 (4%)	3 (4%)	3 11
48	DY	75/77 (97%)	72 (96%)	3 (4%)	0	100 100
49	CZ	60/62 (97%)	51 (85%)	7 (12%)	2 (3%)	4 15
49	DZ	60/62 (97%)	55 (92%)	2 (3%)	3 (5%)	2 7
50	C0	56/58 (97%)	51 (91%)	3 (5%)	2 (4%)	3 14
50	D0	57/58 (98%)	56 (98%)	1 (2%)	0	100 100
51	C1	54/56 (96%)	41 (76%)	10 (18%)	3 (6%)	2 5
51	D1	54/56 (96%)	49 (91%)	3 (6%)	2 (4%)	3 13
52	C2	48/51 (94%)	41 (85%)	6 (12%)	1 (2%)	7 26
52	D2	49/51 (96%)	46 (94%)	2 (4%)	1 (2%)	7 27
53	C3	44/46 (96%)	40 (91%)	2 (4%)	2 (4%)	2 9
53	D3	44/46 (96%)	42 (96%)	2 (4%)	0	100 100
54	C4	62/64 (97%)	56 (90%)	4 (6%)	2 (3%)	4 16
54	D4	62/64 (97%)	59 (95%)	3 (5%)	0	100 100
55	C5	42/45 (93%)	26 (62%)	12 (29%)	4 (10%)	0 1
55	D5	43/45 (96%)	30 (70%)	6 (14%)	7 (16%)	0 0
56	DD	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	29 61
57	D7	66/68 (97%)	23 (35%)	22 (33%)	21 (32%)	0 0
All	All	11321/11536 (98%)	9810 (87%)	961 (8%)	550 (5%)	2 8

5 of 550 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	AB	10	LEU
6	AB	33	GLY
6	AB	88	ASP

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Mol	Chain	Res	Type
6	AB	126	PHE
6	AB	150	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	AB	180/180 (100%)	134 (74%)	46 (26%)	0 1
6	BB	180/180 (100%)	141 (78%)	39 (22%)	1 3
7	AC	170/170 (100%)	148 (87%)	22 (13%)	4 13
7	BC	170/170 (100%)	139 (82%)	31 (18%)	1 5
8	AD	172/172 (100%)	142 (83%)	30 (17%)	2 6
8	BD	172/172 (100%)	150 (87%)	22 (13%)	4 13
9	AE	113/113 (100%)	86 (76%)	27 (24%)	0 2
9	BE	113/113 (100%)	92 (81%)	21 (19%)	1 5
10	AF	87/87 (100%)	78 (90%)	9 (10%)	7 22
10	BF	87/87 (100%)	63 (72%)	24 (28%)	0 1
11	AG	124/124 (100%)	110 (89%)	14 (11%)	6 18
11	BG	124/124 (100%)	97 (78%)	27 (22%)	1 3
12	AH	104/104 (100%)	84 (81%)	20 (19%)	1 4
12	BH	104/104 (100%)	85 (82%)	19 (18%)	1 5
13	AI	105/105 (100%)	82 (78%)	23 (22%)	1 3
13	BI	105/105 (100%)	82 (78%)	23 (22%)	1 3
14	AJ	86/86 (100%)	70 (81%)	16 (19%)	1 5
14	BJ	86/86 (100%)	65 (76%)	21 (24%)	0 2
15	AK	90/90 (100%)	78 (87%)	12 (13%)	4 11
15	BK	90/90 (100%)	78 (87%)	12 (13%)	4 11
16	AL	102/102 (100%)	92 (90%)	10 (10%)	8 24
17	AM	92/92 (100%)	74 (80%)	18 (20%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	BM	92/92 (100%)	73 (79%)	19 (21%)	1 3
18	AN	79/83 (95%)	61 (77%)	18 (23%)	1 2
18	BN	79/83 (95%)	72 (91%)	7 (9%)	9 29
19	AO	76/76 (100%)	65 (86%)	11 (14%)	3 9
19	BO	76/76 (100%)	62 (82%)	14 (18%)	1 5
20	AP	65/65 (100%)	57 (88%)	8 (12%)	4 14
20	BP	65/65 (100%)	52 (80%)	13 (20%)	1 4
21	AQ	74/74 (100%)	59 (80%)	15 (20%)	1 3
21	BQ	74/74 (100%)	58 (78%)	16 (22%)	1 3
22	AR	48/48 (100%)	44 (92%)	4 (8%)	11 32
22	BR	48/48 (100%)	44 (92%)	4 (8%)	11 32
23	AS	70/70 (100%)	67 (96%)	3 (4%)	29 62
23	BS	70/70 (100%)	58 (83%)	12 (17%)	2 6
24	AT	65/65 (100%)	51 (78%)	14 (22%)	1 3
24	BT	65/65 (100%)	53 (82%)	12 (18%)	1 5
25	AU	46/46 (100%)	36 (78%)	10 (22%)	1 3
25	BU	46/46 (100%)	34 (74%)	12 (26%)	0 1
26	BL	103/103 (100%)	88 (85%)	15 (15%)	3 9
27	CC	216/216 (100%)	193 (89%)	23 (11%)	6 20
27	DC	216/216 (100%)	195 (90%)	21 (10%)	8 25
28	CD	164/164 (100%)	151 (92%)	13 (8%)	12 34
29	CE	165/165 (100%)	147 (89%)	18 (11%)	6 19
29	DE	165/165 (100%)	151 (92%)	14 (8%)	10 31
30	CF	148/148 (100%)	129 (87%)	19 (13%)	4 13
30	DF	148/148 (100%)	127 (86%)	21 (14%)	3 10
31	CG	137/137 (100%)	116 (85%)	21 (15%)	2 8
31	DG	137/137 (100%)	123 (90%)	14 (10%)	7 22
32	CH	113/113 (100%)	91 (80%)	22 (20%)	1 4
32	DH	113/113 (100%)	98 (87%)	15 (13%)	4 11
33	CJ	109/109 (100%)	83 (76%)	26 (24%)	0 2
33	DJ	109/109 (100%)	87 (80%)	22 (20%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
34	CK	116/116 (100%)	105 (90%)	11 (10%)	8 26
34	DK	116/116 (100%)	108 (93%)	8 (7%)	15 41
35	CL	103/104 (99%)	94 (91%)	9 (9%)	10 30
35	DL	104/104 (100%)	99 (95%)	5 (5%)	25 58
36	CM	102/103 (99%)	91 (89%)	11 (11%)	6 20
36	DM	103/103 (100%)	96 (93%)	7 (7%)	16 42
37	CN	109/109 (100%)	97 (89%)	12 (11%)	6 19
37	DN	110/109 (101%)	102 (93%)	8 (7%)	14 38
38	CO	100/100 (100%)	85 (85%)	15 (15%)	3 9
38	DO	100/100 (100%)	94 (94%)	6 (6%)	19 49
39	CP	86/87 (99%)	71 (83%)	15 (17%)	2 6
39	DP	87/87 (100%)	79 (91%)	8 (9%)	9 27
40	CQ	99/99 (100%)	83 (84%)	16 (16%)	2 7
40	DQ	99/99 (100%)	90 (91%)	9 (9%)	9 28
41	CR	89/89 (100%)	81 (91%)	8 (9%)	9 29
41	DR	89/89 (100%)	84 (94%)	5 (6%)	21 52
42	CS	84/84 (100%)	71 (84%)	13 (16%)	2 8
42	DS	84/84 (100%)	75 (89%)	9 (11%)	6 20
43	CT	93/93 (100%)	79 (85%)	14 (15%)	3 9
43	DT	93/93 (100%)	82 (88%)	11 (12%)	5 16
44	CU	80/80 (100%)	65 (81%)	15 (19%)	1 4
44	DU	79/80 (99%)	73 (92%)	6 (8%)	13 36
45	CV	83/83 (100%)	73 (88%)	10 (12%)	5 15
45	DV	83/83 (100%)	77 (93%)	6 (7%)	14 39
46	CW	78/78 (100%)	64 (82%)	14 (18%)	2 5
46	DW	78/78 (100%)	71 (91%)	7 (9%)	9 29
47	CX	56/58 (97%)	48 (86%)	8 (14%)	3 10
47	DX	58/58 (100%)	52 (90%)	6 (10%)	7 22
48	CY	67/67 (100%)	58 (87%)	9 (13%)	4 11
48	DY	67/67 (100%)	63 (94%)	4 (6%)	19 49
49	CZ	54/54 (100%)	46 (85%)	8 (15%)	3 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
49	DZ	54/54 (100%)	48 (89%)	6 (11%)	6 19
50	C0	48/48 (100%)	39 (81%)	9 (19%)	1 4
50	D0	49/48 (102%)	46 (94%)	3 (6%)	18 48
51	C1	47/47 (100%)	40 (85%)	7 (15%)	3 9
51	D1	47/47 (100%)	46 (98%)	1 (2%)	53 81
52	C2	45/45 (100%)	43 (96%)	2 (4%)	28 61
52	D2	45/45 (100%)	44 (98%)	1 (2%)	52 81
53	C3	38/38 (100%)	32 (84%)	6 (16%)	2 8
53	D3	38/38 (100%)	33 (87%)	5 (13%)	4 12
54	C4	51/51 (100%)	48 (94%)	3 (6%)	19 49
54	D4	51/51 (100%)	48 (94%)	3 (6%)	19 49
55	C5	39/41 (95%)	28 (72%)	11 (28%)	0 1
55	D5	40/41 (98%)	32 (80%)	8 (20%)	1 4
56	DD	163/163 (100%)	153 (94%)	10 (6%)	18 48
57	D7	60/63 (95%)	39 (65%)	21 (35%)	0 0
All	All	9401/9419 (100%)	8070 (86%)	1331 (14%)	3 10

5 of 1331 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	CR	10	ARG
32	DH	46	PHE
43	CT	81	SER
41	CR	8	ILE
52	C2	46	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
42	CS	66	HIS
55	C5	14	HIS
52	D2	18	HIS
42	CS	89	HIS
52	C2	45	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1533 (99%)	388 (25%)	18 (1%)
2	BA	1532/1533 (99%)	410 (26%)	13 (0%)
3	DA	2890/2903 (99%)	718 (24%)	42 (1%)
4	CA	2896/2904 (99%)	862 (29%)	38 (1%)
5	CB	117/119 (98%)	26 (22%)	0
5	DB	118/119 (99%)	23 (19%)	0
All	All	9082/9111 (99%)	2427 (26%)	111 (1%)

5 of 2427 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	19	A
1	AA	21	G

5 of 111 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	DA	1929	G
4	CA	2680	U
3	DA	2873	A
4	CA	2602	A
4	CA	1900	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	AA	1407	1	18,22,23	1.04	2 (11%)	26,32,35	1.63	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	5MU	DA	747	3	19,22,23	1.69	5 (26%)	28,32,35	2.54	10 (35%)
56	MEQ	DD	150	56	8,9,10	1.51	1 (12%)	5,10,12	1.52	1 (20%)
1	MA6	AA	1518	1	19,26,27	0.94	1 (5%)	18,38,41	1.67	3 (16%)
3	G7M	DA	2069	3	20,26,27	1.44	3 (15%)	17,39,42	1.43	2 (11%)
3	OMG	DA	2251	3	18,26,27	1.15	1 (5%)	19,38,41	1.44	4 (21%)
1	G7M	AA	527	1	20,26,27	1.16	1 (5%)	17,39,42	0.98	2 (11%)
3	3TD	DA	1915	3	18,22,23	1.56	4 (22%)	22,32,35	2.57	6 (27%)
3	2MG	DA	2445	3	18,26,27	1.19	2 (11%)	16,38,41	2.02	3 (18%)
1	2MG	AA	966	1	18,26,27	0.93	1 (5%)	16,38,41	1.36	3 (18%)
16	D2T	AL	89	16	7,9,10	1.00	0	6,11,13	2.31	3 (50%)
3	OMU	DA	2552	3	19,22,23	1.52	4 (21%)	26,31,34	2.78	7 (26%)
1	5MC	AA	967	1	18,22,23	1.03	1 (5%)	26,32,35	1.81	4 (15%)
3	2MG	DA	1835	3	18,26,27	1.10	1 (5%)	16,38,41	0.97	1 (6%)
3	PSU	DA	2504	3	18,21,22	1.74	4 (22%)	22,30,33	2.03	5 (22%)
3	PSU	DA	2604	3	18,21,22	1.21	1 (5%)	22,30,33	1.63	3 (13%)
3	2MA	DA	2503	3,58	17,25,26	1.20	1 (5%)	17,37,40	1.24	2 (11%)
3	PSU	DA	1917	3	18,21,22	1.21	2 (11%)	22,30,33	1.89	7 (31%)
1	4OC	AA	1402	1	20,23,24	0.99	1 (5%)	26,32,35	1.26	4 (15%)
3	1MG	DA	745	3	18,26,27	1.17	3 (16%)	19,39,42	2.53	6 (31%)
1	UR3	AA	1498	1	19,22,23	1.03	2 (10%)	26,32,35	1.94	4 (15%)
3	PSU	DA	2605	3	18,21,22	1.69	4 (22%)	22,30,33	1.90	4 (18%)
1	2MG	AA	1207	1	18,26,27	0.88	0	16,38,41	1.31	4 (25%)
3	6MZ	DA	2030	3	18,25,26	1.33	2 (11%)	16,36,39	3.21	5 (31%)
3	OMC	DA	2498	3,58	19,22,23	1.32	3 (15%)	26,31,34	1.24	4 (15%)
3	6MZ	DA	1618	3	18,25,26	1.09	0	16,36,39	3.51	5 (31%)
3	PSU	DA	2457	3	18,21,22	1.30	3 (16%)	22,30,33	1.48	4 (18%)
3	H2U	DA	2449	3	18,21,22	1.57	3 (16%)	21,30,33	2.15	3 (14%)
3	PSU	DA	746	3,58	18,21,22	1.18	2 (11%)	22,30,33	1.91	4 (18%)
3	PSU	DA	2580	3	18,21,22	1.03	2 (11%)	22,30,33	1.65	4 (18%)
1	2MG	AA	1516	1	18,26,27	0.98	1 (5%)	16,38,41	1.37	4 (25%)
3	5MC	DA	1962	3	18,22,23	0.89	1 (5%)	26,32,35	1.37	3 (11%)
1	PSU	AA	516	1,58	18,21,22	1.06	2 (11%)	22,30,33	1.65	3 (13%)
1	MA6	AA	1519	1	19,26,27	0.99	1 (5%)	18,38,41	1.44	3 (16%)
3	PSU	DA	955	3	18,21,22	1.13	0	22,30,33	2.18	4 (18%)
3	PSU	DA	1911	3	18,21,22	1.09	1 (5%)	22,30,33	1.74	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	5MU	DA	1939	3	19,22,23	1.46	2 (10%)	28,32,35	2.87	9 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
3	5MU	DA	747	3	-	2/7/25/26	0/2/2/2
56	MEQ	DD	150	56	-	2/8/9/11	-
1	MA6	AA	1518	1	-	2/7/29/30	0/3/3/3
3	G7M	DA	2069	3	-	2/3/25/26	0/3/3/3
3	OMG	DA	2251	3	-	1/5/27/28	0/3/3/3
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
3	3TD	DA	1915	3	-	2/7/25/26	0/2/2/2
3	2MG	DA	2445	3	-	0/5/27/28	0/3/3/3
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3
16	D2T	AL	89	16	-	2/7/12/14	-
3	OMU	DA	2552	3	-	2/9/27/28	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
3	2MG	DA	1835	3	-	4/5/27/28	0/3/3/3
3	PSU	DA	2504	3	-	2/7/25/26	0/2/2/2
3	PSU	DA	2604	3	-	0/7/25/26	0/2/2/2
3	2MA	DA	2503	3,58	-	3/3/25/26	0/3/3/3
3	PSU	DA	1917	3	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1	-	1/9/29/30	0/2/2/2
3	1MG	DA	745	3	-	2/3/25/26	0/3/3/3
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
3	PSU	DA	2605	3	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1	-	2/5/27/28	0/3/3/3
3	6MZ	DA	2030	3	-	1/5/27/28	0/3/3/3
3	OMC	DA	2498	3,58	-	3/9/27/28	0/2/2/2
3	6MZ	DA	1618	3	-	1/5/27/28	0/3/3/3
3	PSU	DA	2457	3	-	1/7/25/26	0/2/2/2
3	H2U	DA	2449	3	-	0/7/38/39	0/2/2/2
3	PSU	DA	746	3,58	-	3/7/25/26	0/2/2/2
3	PSU	DA	2580	3	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5MC	DA	1962	3	-	4/7/25/26	0/2/2/2
1	PSU	AA	516	1,58	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	3/7/29/30	0/3/3/3
3	PSU	DA	955	3	-	0/7/25/26	0/2/2/2
3	PSU	DA	1911	3	-	0/7/25/26	0/2/2/2
3	5MU	DA	1939	3	-	0/7/25/26	0/2/2/2

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DA	2504	PSU	C6-C5	4.79	1.40	1.35
3	DA	1939	5MU	C6-N1	-4.69	1.30	1.38
3	DA	2449	H2U	C2-N3	-4.27	1.30	1.38
3	DA	2605	PSU	C6-C5	3.89	1.39	1.35
3	DA	746	PSU	C6-C5	3.85	1.39	1.35

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	DA	1618	6MZ	C9-N6-C6	-11.88	112.64	122.87
3	DA	2030	6MZ	C9-N6-C6	-9.14	115.00	122.87
3	DA	1915	3TD	N1-C2-N3	9.04	123.27	116.14
3	DA	2449	H2U	C4-N3-C2	-7.62	119.47	125.79
3	DA	2552	OMU	O2-C2-N1	-7.22	113.19	122.79

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	AA	527	G7M	C3'-C4'-C5'-O5'
1	AA	1518	MA6	C5-C6-N6-C10
1	AA	1519	MA6	C5-C6-N6-C10
3	DA	746	PSU	C2'-C1'-C5-C4

There are no ring outliers.

29 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1407	5MC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	DA	747	5MU	8	0
56	DD	150	MEQ	3	0
1	AA	1518	MA6	7	0
3	DA	2069	G7M	1	0
3	DA	2251	OMG	3	0
3	DA	1915	3TD	1	0
3	DA	2445	2MG	2	0
16	AL	89	D2T	4	0
3	DA	2552	OMU	6	0
1	AA	967	5MC	2	0
3	DA	1835	2MG	9	0
3	DA	2504	PSU	3	0
3	DA	2503	2MA	4	0
1	AA	1402	4OC	3	0
3	DA	745	1MG	5	0
3	DA	2605	PSU	1	0
1	AA	1207	2MG	2	0
3	DA	2030	6MZ	7	0
3	DA	2498	OMC	8	0
3	DA	1618	6MZ	2	0
3	DA	2449	H2U	1	0
1	AA	1516	2MG	2	0
3	DA	1962	5MC	4	0
1	AA	516	PSU	1	0
1	AA	1519	MA6	12	0
3	DA	955	PSU	2	0
3	DA	1911	PSU	3	0
3	DA	1939	5MU	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 516 ligands modelled in this entry, 453 are monoatomic - leaving 63 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
66	PEG	DP	201	-	6,6,6	1.16	0	5,5,5	0.64	0
62	SPD	DA	3070	-	9,9,9	0.44	0	8,8,8	1.07	0
59	PGE	DA	3066	-	9,9,9	1.07	1 (11%)	8,8,8	0.93	0
67	EDO	DB	203	-	3,3,3	0.40	0	2,2,2	0.16	0
67	EDO	D1	101	-	3,3,3	0.38	0	2,2,2	0.15	0
62	SPD	DA	3031	-	9,9,9	0.62	0	8,8,8	0.31	0
67	EDO	DA	3059	-	3,3,3	0.52	0	2,2,2	0.61	0
68	GUN	DA	3078	-	7,12,12	1.58	1 (14%)	8,17,17	1.85	3 (37%)
59	PGE	DT	202	-	9,9,9	1.16	1 (11%)	8,8,8	0.71	0
62	SPD	DA	3036	-	9,9,9	0.48	0	8,8,8	0.53	0
65	ACY	DA	3055	-	3,3,3	1.03	0	3,3,3	1.30	0
67	EDO	DA	3075	-	3,3,3	0.35	0	2,2,2	0.18	0
60	MPD	DA	3043	-	7,7,7	0.58	0	9,10,10	0.70	0
67	EDO	DA	3052	-	3,3,3	0.50	0	2,2,2	0.16	0
59	PGE	DU	101	-	9,9,9	1.09	1 (11%)	8,8,8	0.58	0
60	MPD	DA	3045	-	7,7,7	0.34	0	9,10,10	1.38	2 (22%)
63	PUT	DA	3032	-	5,5,5	0.30	0	4,4,4	0.41	0
63	PUT	DM	201	-	5,5,5	0.35	0	4,4,4	0.51	0
66	PEG	DA	3073	-	6,6,6	1.04	0	5,5,5	0.67	0
60	MPD	DT	201	-	7,7,7	0.55	0	9,10,10	1.02	1 (11%)
61	PG4	DA	3048	-	12,12,12	0.89	0	11,11,11	0.67	0
66	PEG	DA	3061	-	6,6,6	1.08	0	5,5,5	0.32	0
67	EDO	DA	3060	-	3,3,3	0.46	0	2,2,2	0.26	0
63	PUT	DA	3054	-	5,5,5	0.47	0	4,4,4	0.81	0
60	MPD	DA	3071	-	7,7,7	0.65	0	9,10,10	0.46	0
61	PG4	BA	1607	-	12,12,12	0.89	0	11,11,11	0.57	0
60	MPD	DA	3046	-	7,7,7	0.76	0	9,10,10	0.99	1 (11%)
59	PGE	AA	1613	-	9,9,9	1.13	1 (11%)	8,8,8	0.70	0
60	MPD	DE	301	-	7,7,7	0.56	0	9,10,10	0.56	0
66	PEG	DA	3050	-	6,6,6	1.03	0	5,5,5	0.51	0
66	PEG	D3	102	-	6,6,6	0.92	0	5,5,5	0.27	0
66	PEG	DA	3063	-	6,6,6	1.06	0	5,5,5	0.42	0
65	ACY	DA	3044	-	3,3,3	0.87	0	3,3,3	1.23	0
63	PUT	DA	3069	-	5,5,5	0.35	0	4,4,4	0.19	0
65	ACY	DA	3064	-	3,3,3	0.61	0	3,3,3	1.12	0
66	PEG	DA	3062	-	6,6,6	1.17	1 (16%)	5,5,5	0.57	0
60	MPD	DA	3072	-	7,7,7	0.56	0	9,10,10	0.30	0
61	PG4	DS	202	-	12,12,12	0.74	0	11,11,11	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
61	PG4	DQ	202	-	12,12,12	0.71	0	11,11,11	0.45	0
67	EDO	DA	3076	-	3,3,3	0.53	0	2,2,2	0.06	0
59	PGE	DS	201	-	9,9,9	1.25	1 (11%)	8,8,8	1.03	0
64	1PE	DA	3034	-	15,15,15	0.74	0	14,14,14	1.04	1 (7%)
67	EDO	DR	204	-	3,3,3	0.55	0	2,2,2	0.28	0
60	MPD	AA	1615	-	7,7,7	0.54	0	9,10,10	0.67	0
67	EDO	DA	3057	-	3,3,3	0.43	0	2,2,2	0.11	0
60	MPD	DE	302	-	7,7,7	0.56	0	9,10,10	0.43	0
66	PEG	DQ	201	-	6,6,6	1.01	0	5,5,5	0.26	0
61	PG4	DR	202	-	12,12,12	0.86	0	11,11,11	0.57	0
59	PGE	DA	3035	-	9,9,9	1.32	2 (22%)	8,8,8	1.12	1 (12%)
59	PGE	DD	301	-	9,9,9	1.16	1 (11%)	8,8,8	0.77	0
60	MPD	DK	201	-	7,7,7	0.55	0	9,10,10	0.66	0
63	PUT	DP	202	-	5,5,5	0.36	0	4,4,4	0.16	0
67	EDO	DB	202	-	3,3,3	0.52	0	2,2,2	0.30	0
60	MPD	DA	3067	-	7,7,7	0.65	0	9,10,10	0.67	0
63	PUT	D5	101	-	5,5,5	0.29	0	4,4,4	0.30	0
67	EDO	DA	3058	-	3,3,3	0.52	0	2,2,2	0.10	0
67	EDO	DB	201	-	3,3,3	0.42	0	2,2,2	0.38	0
60	MPD	DN	201	-	7,7,7	0.49	0	9,10,10	0.84	1 (11%)
63	PUT	DA	3037	-	5,5,5	0.32	0	4,4,4	0.81	0
66	PEG	D1	102	-	6,6,6	1.50	1 (16%)	5,5,5	1.35	0
60	MPD	DA	3077	-	7,7,7	0.50	0	9,10,10	1.43	2 (22%)
64	1PE	DA	3065	-	15,15,15	0.86	0	14,14,14	0.88	0
59	PGE	D3	101	-	9,9,9	0.92	0	8,8,8	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
66	PEG	DP	201	-	-	2/4/4/4	-
62	SPD	DA	3070	-	-	3/7/7/7	-
59	PGE	DA	3066	-	-	3/7/7/7	-
67	EDO	DB	203	-	-	0/1/1/1	-
67	EDO	D1	101	-	-	1/1/1/1	-
62	SPD	DA	3031	-	-	6/7/7/7	-
67	EDO	DA	3059	-	-	0/1/1/1	-
68	GUN	DA	3078	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PGE	DT	202	-	-	3/7/7/7	-
62	SPD	DA	3036	-	-	3/7/7/7	-
67	EDO	DA	3075	-	-	1/1/1/1	-
60	MPD	DA	3043	-	-	2/5/5/5	-
67	EDO	DA	3052	-	-	1/1/1/1	-
59	PGE	DU	101	-	-	4/7/7/7	-
60	MPD	DA	3045	-	-	2/5/5/5	-
63	PUT	DA	3032	-	-	2/3/3/3	-
63	PUT	DM	201	-	-	2/3/3/3	-
66	PEG	DA	3073	-	-	1/4/4/4	-
60	MPD	DT	201	-	-	0/5/5/5	-
61	PG4	DA	3048	-	-	7/10/10/10	-
66	PEG	DA	3061	-	-	3/4/4/4	-
67	EDO	DA	3060	-	-	1/1/1/1	-
63	PUT	DA	3054	-	-	0/3/3/3	-
60	MPD	DA	3071	-	-	2/5/5/5	-
61	PG4	BA	1607	-	-	1/10/10/10	-
60	MPD	DA	3046	-	-	0/5/5/5	-
59	PGE	AA	1613	-	-	5/7/7/7	-
60	MPD	DE	301	-	-	1/5/5/5	-
66	PEG	DA	3050	-	-	1/4/4/4	-
66	PEG	D3	102	-	-	3/4/4/4	-
66	PEG	DA	3063	-	-	3/4/4/4	-
63	PUT	DA	3069	-	-	1/3/3/3	-
66	PEG	DA	3062	-	-	3/4/4/4	-
60	MPD	DA	3072	-	-	0/5/5/5	-
61	PG4	DS	202	-	-	3/10/10/10	-
61	PG4	DQ	202	-	-	5/10/10/10	-
67	EDO	DA	3076	-	-	1/1/1/1	-
59	PGE	DS	201	-	-	2/7/7/7	-
64	1PE	DA	3034	-	-	7/13/13/13	-
67	EDO	DR	204	-	-	1/1/1/1	-
60	MPD	AA	1615	-	-	3/5/5/5	-
67	EDO	DA	3057	-	-	0/1/1/1	-
60	MPD	DE	302	-	-	0/5/5/5	-
66	PEG	DQ	201	-	-	4/4/4/4	-
61	PG4	DR	202	-	-	5/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PGE	DA	3035	-	-	2/7/7/7	-
59	PGE	DD	301	-	-	1/7/7/7	-
60	MPD	DK	201	-	-	0/5/5/5	-
63	PUT	DP	202	-	-	0/3/3/3	-
67	EDO	DB	202	-	-	1/1/1/1	-
60	MPD	DA	3067	-	-	1/5/5/5	-
63	PUT	D5	101	-	-	1/3/3/3	-
67	EDO	DA	3058	-	-	0/1/1/1	-
67	EDO	DB	201	-	-	1/1/1/1	-
60	MPD	DN	201	-	-	3/5/5/5	-
63	PUT	DA	3037	-	-	1/3/3/3	-
66	PEG	D1	102	-	-	3/4/4/4	-
60	MPD	DA	3077	-	-	2/5/5/5	-
64	1PE	DA	3065	-	-	9/13/13/13	-
59	PGE	D3	101	-	-	4/7/7/7	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	DA	3078	GUN	C6-N1	-2.67	1.33	1.37
66	D1	102	PEG	C2-C1	2.46	1.62	1.49
59	DA	3035	PGE	C2-C1	2.30	1.61	1.49
59	DA	3066	PGE	C2-C1	2.28	1.61	1.49
59	DT	202	PGE	C2-C1	2.23	1.61	1.49

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	DA	3045	MPD	CM-C2-C1	-3.28	103.74	110.57
68	DA	3078	GUN	C5-C6-N1	3.00	119.25	113.95
64	DA	3034	1PE	OH3-C23-C13	-2.86	97.49	110.39
68	DA	3078	GUN	O6-C6-N1	-2.78	117.37	120.65
68	DA	3078	GUN	C8-N7-C5	2.54	107.83	102.99

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	DA	3067	MPD	C2-C3-C4-O4
60	DA	3077	MPD	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
60	DA	3077	MPD	O2-C2-C3-C4
60	DE	301	MPD	C2-C3-C4-O4
60	DN	201	MPD	O2-C2-C3-C4

There are no ring outliers.

39 monomers are involved in 100 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
66	DP	201	PEG	1	0
59	DA	3066	PGE	2	0
67	DB	203	EDO	1	0
62	DA	3031	SPD	3	0
67	DA	3059	EDO	4	0
68	DA	3078	GUN	2	0
59	DT	202	PGE	2	0
62	DA	3036	SPD	1	0
67	DA	3052	EDO	1	0
60	DA	3045	MPD	1	0
63	DM	201	PUT	1	0
61	DA	3048	PG4	3	0
67	DA	3060	EDO	5	0
63	DA	3054	PUT	4	0
60	DA	3071	MPD	1	0
60	DA	3046	MPD	1	0
60	DE	301	MPD	1	0
66	DA	3050	PEG	2	0
66	D3	102	PEG	2	0
66	DA	3063	PEG	1	0
65	DA	3044	ACY	1	0
63	DA	3069	PUT	2	0
65	DA	3064	ACY	5	0
66	DA	3062	PEG	2	0
60	DA	3072	MPD	2	0
61	DS	202	PG4	1	0
61	DQ	202	PG4	3	0
64	DA	3034	1PE	5	0
67	DR	204	EDO	2	0
66	DQ	201	PEG	1	0
61	DR	202	PG4	8	0
63	DP	202	PUT	10	0
60	DA	3067	MPD	4	0
63	D5	101	PUT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	DN	201	MPD	1	0
63	DA	3037	PUT	7	0
66	D1	102	PEG	3	0
60	DA	3077	MPD	1	0
64	DA	3065	1PE	2	0

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, 95^{th} 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	1522/1533 (99%)	-0.45	8 (0%) 91 91	40, 89, 181, 376	0
2	BA	1533/1533 (100%)	-0.15	33 (2%) 62 59	52, 116, 235, 316	0
3	DA	2873/2903 (98%)	-0.40	30 (1%) 82 82	13, 44, 165, 340	0
4	CA	2898/2904 (99%)	0.24	97 (3%) 46 41	68, 150, 267, 488	0
5	CB	118/119 (99%)	-0.08	1 (0%) 86 86	112, 187, 233, 258	0
5	DB	119/119 (100%)	-0.62	0 100 100	21, 53, 81, 104	0
6	AB	218/218 (100%)	0.91	36 (16%) 1 1	56, 120, 185, 241	0
6	BB	218/218 (100%)	0.91	44 (20%) 1 0	75, 126, 188, 242	0
7	AC	206/206 (100%)	0.15	2 (0%) 82 82	54, 95, 145, 202	0
7	BC	206/206 (100%)	0.30	8 (3%) 39 35	68, 111, 159, 198	0
8	AD	205/205 (100%)	0.49	17 (8%) 11 8	60, 107, 155, 210	0
8	BD	205/205 (100%)	0.02	1 (0%) 91 91	53, 84, 126, 146	0
9	AE	150/150 (100%)	0.16	3 (2%) 65 63	52, 87, 148, 219	0
9	BE	150/150 (100%)	0.13	5 (3%) 46 41	55, 89, 151, 191	0
10	AF	100/100 (100%)	0.07	2 (2%) 65 63	60, 100, 136, 195	0
10	BF	100/100 (100%)	0.42	8 (8%) 12 9	79, 116, 156, 241	0
11	AG	151/151 (100%)	0.67	18 (11%) 4 3	83, 130, 170, 184	0
11	BG	151/151 (100%)	2.25	70 (46%) 0 0	102, 192, 268, 311	0
12	AH	129/129 (100%)	0.31	8 (6%) 20 16	59, 94, 138, 169	0
12	BH	129/129 (100%)	0.35	6 (4%) 31 28	76, 108, 153, 194	0
13	AI	127/127 (100%)	0.72	11 (8%) 10 7	75, 123, 185, 258	0
13	BI	127/127 (100%)	1.98	50 (39%) 0 0	102, 158, 232, 270	0
14	AJ	98/98 (100%)	0.48	9 (9%) 9 6	60, 102, 135, 146	0
14	BJ	98/98 (100%)	1.85	43 (43%) 0 0	75, 123, 150, 162	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
15	AK	117/117 (100%)	0.75	15 (12%) 3 2	48, 106, 157, 184	0
15	BK	117/117 (100%)	0.34	3 (2%) 56 52	57, 106, 151, 177	0
16	AL	122/123 (99%)	0.13	3 (2%) 57 55	48, 73, 119, 184	0
17	AM	114/114 (100%)	0.48	6 (5%) 26 22	77, 121, 178, 234	0
17	BM	114/114 (100%)	3.83	90 (78%) 0 0	157, 261, 336, 381	0
18	AN	96/100 (96%)	0.61	10 (10%) 6 5	62, 110, 194, 228	0
18	BN	96/100 (96%)	1.83	36 (37%) 0 0	94, 160, 244, 307	0
19	AO	88/88 (100%)	0.13	2 (2%) 60 58	52, 90, 130, 169	0
19	BO	88/88 (100%)	0.31	5 (5%) 23 19	73, 108, 144, 217	0
20	AP	82/82 (100%)	0.90	15 (18%) 1 0	67, 92, 191, 230	0
20	BP	82/82 (100%)	2.23	33 (40%) 0 0	78, 122, 184, 281	0
21	AQ	80/80 (100%)	0.68	7 (8%) 10 7	61, 93, 139, 255	0
21	BQ	80/80 (100%)	2.15	37 (46%) 0 0	81, 138, 200, 249	0
22	AR	55/55 (100%)	0.37	4 (7%) 15 11	69, 98, 148, 204	0
22	BR	55/55 (100%)	-0.22	2 (3%) 42 37	60, 88, 137, 161	0
23	AS	79/79 (100%)	1.35	23 (29%) 0 0	86, 122, 173, 208	0
23	BS	79/79 (100%)	5.42	66 (83%) 0 0	158, 244, 332, 391	0
24	AT	85/85 (100%)	0.66	9 (10%) 6 4	70, 94, 138, 181	0
24	BT	85/85 (100%)	2.26	44 (51%) 0 0	95, 145, 195, 224	0
25	AU	54/54 (100%)	1.02	8 (14%) 2 1	74, 118, 185, 235	0
25	BU	54/54 (100%)	0.32	1 (1%) 66 65	59, 103, 157, 187	0
26	BL	123/123 (100%)	0.40	8 (6%) 18 14	63, 92, 137, 187	0
27	CC	271/271 (100%)	0.58	23 (8%) 10 8	67, 107, 141, 188	0
27	DC	271/271 (100%)	-0.36	0 100 100	24, 55, 84, 115	0
28	CD	209/209 (100%)	2.20	84 (40%) 0 0	86, 143, 237, 384	0
29	CE	201/201 (100%)	2.92	123 (61%) 0 0	92, 220, 455, 650	0
29	DE	201/201 (100%)	-0.37	0 100 100	17, 56, 108, 211	0
30	CF	177/177 (100%)	3.73	125 (70%) 0 0	142, 213, 268, 324	0
30	DF	177/177 (100%)	-0.08	4 (2%) 60 58	43, 73, 121, 163	0
31	CG	176/176 (100%)	3.29	114 (64%) 0 0	131, 203, 310, 435	0
31	DG	176/176 (100%)	-0.11	1 (0%) 89 89	40, 74, 104, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
32	CH	148/148 (100%)	1.49	48 (32%) 0 0	82, 147, 207, 323	0
32	DH	148/148 (100%)	1.47	46 (31%) 0 0	60, 153, 228, 323	0
33	CJ	141/141 (100%)	4.98	120 (85%) 0 0	170, 248, 330, 407	0
33	DJ	141/141 (100%)	4.41	95 (67%) 0 0	137, 217, 299, 345	0
34	CK	142/142 (100%)	1.18	31 (21%) 0 0	86, 140, 201, 269	0
34	DK	142/142 (100%)	-0.59	1 (0%) 87 87	16, 34, 62, 119	0
35	CL	122/123 (99%)	1.86	48 (39%) 0 0	88, 127, 175, 245	0
35	DL	123/123 (100%)	-0.49	0 100 100	26, 47, 78, 135	0
36	CM	143/144 (99%)	3.01	87 (60%) 0 0	99, 187, 295, 413	0
36	DM	144/144 (100%)	-0.38	1 (0%) 87 87	16, 55, 85, 124	0
37	CN	136/136 (100%)	2.03	66 (48%) 0 0	84, 131, 174, 197	0
37	DN	136/136 (100%)	-0.59	0 100 100	19, 42, 73, 126	0
38	CO	120/120 (100%)	1.90	50 (41%) 0 0	101, 155, 266, 459	0
38	DO	120/120 (100%)	-0.49	0 100 100	16, 37, 58, 172	0
39	CP	116/117 (99%)	2.96	77 (66%) 0 0	141, 186, 251, 276	0
39	DP	117/117 (100%)	-0.24	0 100 100	34, 57, 94, 117	0
40	CQ	114/114 (100%)	1.82	42 (36%) 0 0	94, 148, 198, 298	0
40	DQ	114/114 (100%)	-0.42	0 100 100	33, 56, 97, 126	0
41	CR	117/117 (100%)	2.02	51 (43%) 0 0	102, 148, 210, 243	0
41	DR	117/117 (100%)	-0.66	0 100 100	8, 29, 56, 116	0
42	CS	103/103 (100%)	3.30	64 (62%) 0 0	104, 176, 281, 363	0
42	DS	103/103 (100%)	-0.63	0 100 100	14, 40, 78, 150	0
43	CT	110/110 (100%)	2.50	55 (50%) 0 0	99, 165, 276, 367	0
43	DT	110/110 (100%)	-0.56	0 100 100	11, 33, 63, 104	0
44	CU	93/93 (100%)	4.03	73 (78%) 0 0	130, 230, 437, 563	0
44	DU	92/93 (98%)	0.01	2 (2%) 62 59	26, 60, 116, 158	0
45	CV	102/102 (100%)	6.48	85 (83%) 0 0	141, 375, 591, 635	0
45	DV	102/102 (100%)	-0.38	2 (1%) 65 63	32, 59, 96, 202	0
46	CW	94/94 (100%)	1.64	35 (37%) 0 0	128, 172, 231, 275	0
46	DW	94/94 (100%)	-0.28	1 (1%) 80 80	24, 49, 86, 108	0
47	CX	75/76 (98%)	2.79	46 (61%) 0 0	94, 149, 187, 210	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
47	DX	76/76 (100%)	-0.44	1 (1%) 77 77	21, 43, 67, 110	0
48	CY	77/77 (100%)	2.08	31 (40%) 0 0	90, 137, 205, 223	0
48	DY	77/77 (100%)	-0.20	0 100 100	29, 62, 98, 128	0
49	CZ	62/62 (100%)	2.55	32 (51%) 0 0	130, 327, 506, 577	0
49	DZ	62/62 (100%)	0.04	1 (1%) 72 71	46, 72, 114, 228	0
50	C0	58/58 (100%)	1.53	19 (32%) 0 0	109, 144, 193, 216	0
50	D0	58/58 (100%)	-0.50	0 100 100	19, 34, 64, 121	0
51	C1	56/56 (100%)	1.81	21 (37%) 0 0	103, 175, 307, 370	0
51	D1	56/56 (100%)	-0.63	0 100 100	9, 39, 67, 147	0
52	C2	50/51 (98%)	2.70	29 (58%) 0 0	129, 173, 229, 244	0
52	D2	51/51 (100%)	-0.10	0 100 100	47, 64, 98, 145	0
53	C3	46/46 (100%)	1.89	20 (43%) 0 0	101, 130, 206, 237	0
53	D3	46/46 (100%)	-0.32	1 (2%) 62 59	27, 44, 67, 231	0
54	C4	64/64 (100%)	2.14	27 (42%) 0 0	103, 139, 181, 213	0
54	D4	64/64 (100%)	-0.37	0 100 100	27, 42, 58, 70	0
55	C5	44/45 (97%)	3.07	26 (59%) 0 0	102, 147, 198, 254	0
55	D5	45/45 (100%)	-0.38	0 100 100	28, 52, 77, 103	0
56	DD	208/209 (99%)	-0.49	0 100 100	14, 41, 71, 152	0
57	D7	68/68 (100%)	0.39	6 (8%) 10 7	58, 116, 185, 264	0
All	All	20582/20647 (99%)	0.53	2751 (13%) 3 2	8, 107, 246, 650	0

The worst 5 of 2751 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	DJ	52	LEU	37.8
23	BS	39	THR	31.4
33	DJ	1	ALA	24.3
23	BS	74	PHE	23.8
33	DJ	113	ALA	22.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	3TD	DA	1915	21/22	0.96	0.09	59,91,109,122	0
1	G7M	AA	527	24/25	0.97	0.13	56,75,85,87	0
1	2MG	AA	966	24/25	0.97	0.15	48,77,86,88	0
1	5MC	AA	967	21/22	0.97	0.19	69,77,90,103	0
1	2MG	AA	1207	24/25	0.97	0.11	54,77,99,121	0
3	PSU	DA	1911	20/21	0.97	0.10	51,84,101,113	0
1	PSU	AA	516	20/21	0.97	0.09	53,86,108,117	0
1	UR3	AA	1498	21/22	0.98	0.13	32,52,68,74	0
1	MA6	AA	1519	24/25	0.98	0.17	37,65,78,84	0
1	4OC	AA	1402	22/23	0.98	0.15	44,63,81,91	0
1	5MC	AA	1407	21/22	0.98	0.12	45,56,73,104	0
3	PSU	DA	1917	20/21	0.98	0.09	42,78,92,94	0
3	5MU	DA	1939	21/22	0.98	0.16	9,38,57,72	0
16	D2T	AL	89	10/11	0.98	0.20	44,60,96,108	0
56	MEQ	DD	150	10/11	0.98	0.16	6,23,48,48	0
3	6MZ	DA	1618	23/24	0.99	0.17	7,32,46,47	0
3	2MG	DA	1835	24/25	0.99	0.13	27,50,59,62	0
1	MA6	AA	1518	24/25	0.99	0.13	21,41,61,72	0
1	2MG	AA	1516	24/25	0.99	0.12	33,63,70,86	0
3	1MG	DA	745	24/25	0.99	0.17	5,29,42,63	0
3	PSU	DA	746	20/21	0.99	0.14	3,21,34,43	0
3	5MC	DA	1962	21/22	0.99	0.13	35,51,64,84	0
3	6MZ	DA	2030	23/24	0.99	0.15	2,12,24,37	0
3	G7M	DA	2069	24/25	0.99	0.14	8,35,48,61	0
3	OMG	DA	2251	24/25	0.99	0.15	3,28,44,58	0
3	2MG	DA	2445	24/25	0.99	0.15	13,28,44,45	0
3	H2U	DA	2449	20/21	0.99	0.16	3,20,42,50	0
3	PSU	DA	2457	20/21	0.99	0.14	3,30,46,59	0
3	OMC	DA	2498	21/22	0.99	0.16	3,20,38,49	0
3	2MA	DA	2503	23/24	0.99	0.16	3,24,39,56	0
3	PSU	DA	2504	20/21	0.99	0.14	2,22,42,46	0
3	OMU	DA	2552	21/22	0.99	0.14	13,27,47,70	0
3	PSU	DA	2580	20/21	0.99	0.16	6,38,52,53	0
3	PSU	DA	2604	20/21	0.99	0.12	14,33,48,70	0
3	PSU	DA	2605	20/21	0.99	0.12	12,38,48,57	0
3	5MU	DA	747	21/22	0.99	0.15	3,19,31,42	0
3	PSU	DA	955	20/21	0.99	0.15	8,30,58,70	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
58	MG	CA	3154	1/1	-0.07	0.57	134,134,134,134	0
58	MG	CA	3129	1/1	0.10	0.31	176,176,176,176	0
58	MG	CA	3068	1/1	0.39	0.23	181,181,181,181	0
58	MG	BA	1643	1/1	0.45	0.15	171,171,171,171	0
58	MG	CA	3084	1/1	0.47	0.41	163,163,163,163	0
58	MG	CA	3159	1/1	0.55	1.10	202,202,202,202	0
58	MG	CA	3157	1/1	0.65	0.32	157,157,157,157	0
66	PEG	DP	201	7/7	0.66	0.65	78,92,105,106	0
60	MPD	DE	302	8/8	0.68	0.61	135,162,187,187	0
58	MG	CA	3135	1/1	0.68	0.14	158,158,158,158	0
58	MG	CA	3017	1/1	0.69	0.42	112,112,112,112	0
58	MG	D5	102	1/1	0.69	0.71	207,207,207,207	0
58	MG	CA	3050	1/1	0.71	0.19	181,181,181,181	0
58	MG	CA	3049	1/1	0.72	0.41	188,188,188,188	0
58	MG	CA	3144	1/1	0.72	0.40	143,143,143,143	0
66	PEG	DA	3063	7/7	0.73	0.75	82,120,134,137	0
63	PUT	DA	3054	6/6	0.73	0.39	38,81,86,88	0
66	PEG	DQ	201	7/7	0.74	0.91	109,111,119,123	0
58	MG	CA	3044	1/1	0.75	0.15	157,157,157,157	0
58	MG	CA	3140	1/1	0.75	0.32	161,161,161,161	0
59	PGE	DT	202	10/10	0.76	0.53	78,121,145,152	0
60	MPD	DT	201	8/8	0.76	0.55	115,144,166,166	0
59	PGE	DD	301	10/10	0.77	0.68	82,129,155,165	0
58	MG	CA	3176	1/1	0.78	0.10	128,128,128,128	0
58	MG	BA	1642	1/1	0.78	0.27	120,120,120,120	0
60	MPD	DA	3072	8/8	0.78	0.96	117,148,172,178	0
58	MG	BA	1612	1/1	0.79	0.07	135,135,135,135	0
60	MPD	DE	301	8/8	0.79	0.71	142,176,194,201	0
58	MG	CA	3173	1/1	0.79	0.73	201,201,201,201	0
58	MG	CA	3102	1/1	0.79	0.92	199,199,199,199	0
66	PEG	D1	102	7/7	0.80	0.41	57,70,83,89	0
58	MG	BA	1609	1/1	0.81	0.18	141,141,141,141	0
58	MG	BA	1637	1/1	0.81	0.14	143,143,143,143	0
63	PUT	DP	202	6/6	0.81	1.09	98,114,117,119	0
58	MG	BA	1638	1/1	0.81	0.10	156,156,156,156	0
58	MG	CA	3027	1/1	0.81	0.14	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3036	1/1	0.81	0.20	67,67,67,67	0
58	MG	CB	201	1/1	0.81	0.04	131,131,131,131	0
63	PUT	DA	3069	6/6	0.83	0.38	53,86,95,96	0
58	MG	CA	3133	1/1	0.83	0.41	163,163,163,163	0
58	MG	AA	1606	1/1	0.84	0.23	77,77,77,77	0
58	MG	CA	3052	1/1	0.85	0.14	136,136,136,136	0
59	PGE	D3	101	10/10	0.85	0.64	97,121,145,145	0
58	MG	CA	3118	1/1	0.85	0.20	207,207,207,207	0
58	MG	BA	1602	1/1	0.85	0.21	74,74,74,74	0
58	MG	CA	3075	1/1	0.85	0.10	107,107,107,107	0
60	MPD	DK	201	8/8	0.85	0.31	113,136,162,162	0
58	MG	CA	3008	1/1	0.85	0.24	97,97,97,97	0
60	MPD	AA	1615	8/8	0.86	0.62	83,114,154,154	0
58	MG	CA	3047	1/1	0.86	0.25	170,170,170,170	0
58	MG	CA	3021	1/1	0.86	0.38	83,83,83,83	0
58	MG	CA	3043	1/1	0.86	0.26	69,69,69,69	0
58	MG	CA	3014	1/1	0.86	0.13	82,82,82,82	0
58	MG	CA	3053	1/1	0.86	0.16	123,123,123,123	0
61	PG4	BA	1607	13/13	0.86	0.28	77,89,111,117	0
67	EDO	DB	202	4/4	0.86	0.21	74,84,88,90	0
58	MG	CA	3045	1/1	0.87	0.08	133,133,133,133	0
58	MG	CA	3155	1/1	0.87	0.13	110,110,110,110	0
58	MG	CA	3145	1/1	0.87	0.04	119,119,119,119	0
63	PUT	DA	3032	6/6	0.87	0.28	50,68,76,81	0
58	MG	CA	3048	1/1	0.88	0.09	172,172,172,172	0
58	MG	CA	3096	1/1	0.88	0.14	111,111,111,111	0
59	PGE	DU	101	10/10	0.88	0.34	59,92,160,162	0
67	EDO	DA	3076	4/4	0.88	0.34	74,92,96,101	0
58	MG	CA	3083	1/1	0.88	0.36	135,135,135,135	0
58	MG	CA	3109	1/1	0.89	0.11	112,112,112,112	0
58	MG	CA	3113	1/1	0.89	0.10	106,106,106,106	0
58	MG	CA	3164	1/1	0.89	0.10	117,117,117,117	0
58	MG	CA	3117	1/1	0.89	0.28	143,143,143,143	0
61	PG4	DR	202	13/13	0.89	0.47	93,108,117,118	0
58	MG	CA	3066	1/1	0.89	0.44	141,141,141,141	0
58	MG	CA	3026	1/1	0.89	0.30	89,89,89,89	0
58	MG	CA	3131	1/1	0.89	0.08	142,142,142,142	0
58	MG	CA	3070	1/1	0.89	0.32	199,199,199,199	0
58	MG	BA	1604	1/1	0.89	0.35	70,70,70,70	0
58	MG	BA	1605	1/1	0.89	0.10	107,107,107,107	0
58	MG	AA	1612	1/1	0.89	0.35	71,71,71,71	0
58	MG	CA	3086	1/1	0.89	0.11	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
67	EDO	DA	3060	4/4	0.89	0.44	55,57,80,84	0
58	MG	CA	3019	1/1	0.89	0.33	84,84,84,84	0
58	MG	AA	1609	1/1	0.89	0.13	69,69,69,69	0
58	MG	CA	3059	1/1	0.90	0.30	167,167,167,167	0
58	MG	CA	3119	1/1	0.90	0.04	112,112,112,112	0
63	PUT	D5	101	6/6	0.90	0.33	82,99,108,108	0
65	ACY	DA	3055	4/4	0.90	0.21	43,67,78,78	0
58	MG	CA	3098	1/1	0.90	0.54	171,171,171,171	0
58	MG	AA	1610	1/1	0.90	0.13	82,82,82,82	0
58	MG	AA	1611	1/1	0.90	0.30	65,65,65,65	0
58	MG	CA	3158	1/1	0.90	0.08	132,132,132,132	0
58	MG	BA	1615	1/1	0.90	0.07	124,124,124,124	0
58	MG	CA	3090	1/1	0.90	0.08	134,134,134,134	0
58	MG	CA	3170	1/1	0.90	0.10	111,111,111,111	0
58	MG	BA	1618	1/1	0.91	0.05	107,107,107,107	0
58	MG	BA	1606	1/1	0.91	0.13	60,60,60,60	0
58	MG	DA	3051	1/1	0.91	0.24	57,57,57,57	0
58	MG	DA	3056	1/1	0.91	0.22	69,69,69,69	0
58	MG	CA	3168	1/1	0.91	0.12	93,93,93,93	0
58	MG	CA	3120	1/1	0.91	0.10	143,143,143,143	0
58	MG	CA	3079	1/1	0.91	0.10	156,156,156,156	0
58	MG	CA	3022	1/1	0.91	0.18	89,89,89,89	0
58	MG	CA	3002	1/1	0.91	0.38	70,70,70,70	0
58	MG	CR	201	1/1	0.91	0.31	75,75,75,75	0
58	MG	CA	3005	1/1	0.91	0.09	81,81,81,81	0
58	MG	CA	3032	1/1	0.91	0.28	79,79,79,79	0
59	PGE	DS	201	10/10	0.91	0.28	38,84,110,122	0
66	PEG	DA	3062	7/7	0.91	0.37	56,86,100,103	0
58	MG	BA	1611	1/1	0.91	0.07	136,136,136,136	0
58	MG	CA	3037	1/1	0.91	0.26	63,63,63,63	0
58	MG	CA	3061	1/1	0.91	0.13	139,139,139,139	0
58	MG	CA	3065	1/1	0.91	0.11	115,115,115,115	0
67	EDO	DA	3059	4/4	0.91	0.33	50,62,77,77	0
60	MPD	DA	3045	8/8	0.91	0.62	69,120,140,144	0
60	MPD	DA	3046	8/8	0.91	0.26	56,87,103,110	0
60	MPD	DA	3071	8/8	0.91	0.37	52,97,138,149	0
67	EDO	DR	204	4/4	0.91	0.41	49,74,82,89	0
61	PG4	DA	3048	13/13	0.92	0.47	48,76,98,100	0
58	MG	CA	3025	1/1	0.92	0.12	84,84,84,84	0
59	PGE	DA	3066	10/10	0.92	0.32	52,88,126,129	0
58	MG	AA	1616	1/1	0.92	0.34	91,91,91,91	0
58	MG	CA	3148	1/1	0.92	0.15	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	DA	3039	1/1	0.92	0.27	82,82,82,82	0
58	MG	CA	3030	1/1	0.92	0.10	67,67,67,67	0
58	MG	CA	3015	1/1	0.92	0.15	91,91,91,91	0
66	PEG	DA	3061	7/7	0.92	0.32	52,94,106,108	0
58	MG	BA	1634	1/1	0.92	0.16	114,114,114,114	0
58	MG	CA	3122	1/1	0.92	0.28	109,109,109,109	0
66	PEG	DA	3073	7/7	0.92	0.41	53,58,93,101	0
58	MG	CA	3125	1/1	0.92	0.14	115,115,115,115	0
58	MG	CA	3056	1/1	0.92	0.11	130,130,130,130	0
58	MG	AA	1623	1/1	0.92	0.35	107,107,107,107	0
66	PEG	D3	102	7/7	0.92	0.55	82,87,94,100	0
58	MG	AA	1631	1/1	0.92	0.10	100,100,100,100	0
58	MG	CA	3134	1/1	0.92	0.12	145,145,145,145	0
58	MG	AA	1636	1/1	0.92	0.07	101,101,101,101	0
58	MG	CM	201	1/1	0.92	0.24	135,135,135,135	0
58	MG	CA	3023	1/1	0.92	0.30	82,82,82,82	0
58	MG	CA	3035	1/1	0.93	0.34	66,66,66,66	0
58	MG	CA	3004	1/1	0.93	0.25	80,80,80,80	0
62	SPD	DA	3070	10/10	0.93	0.27	59,83,96,97	0
58	MG	CA	3136	1/1	0.93	0.18	143,143,143,143	0
58	MG	BA	1635	1/1	0.93	0.07	112,112,112,112	0
58	MG	CA	3110	1/1	0.93	0.06	136,136,136,136	0
58	MG	CA	3071	1/1	0.93	0.16	118,118,118,118	0
58	MG	CA	3072	1/1	0.93	0.08	95,95,95,95	0
58	MG	CA	3018	1/1	0.93	0.13	75,75,75,75	0
58	MG	CA	3054	1/1	0.93	0.06	98,98,98,98	0
58	MG	CA	3156	1/1	0.93	0.09	142,142,142,142	0
58	MG	CA	3082	1/1	0.93	0.18	137,137,137,137	0
58	MG	DA	3038	1/1	0.93	0.28	56,56,56,56	0
60	MPD	DA	3067	8/8	0.93	0.52	79,113,125,135	0
58	MG	CA	3123	1/1	0.93	0.05	103,103,103,103	0
58	MG	CA	3009	1/1	0.93	0.18	85,85,85,85	0
58	MG	CA	3126	1/1	0.93	0.31	183,183,183,183	0
67	EDO	DA	3058	4/4	0.93	0.30	62,73,84,87	0
58	MG	CA	3060	1/1	0.93	0.13	114,114,114,114	0
58	MG	CA	3130	1/1	0.93	0.10	149,149,149,149	0
60	MPD	DN	201	8/8	0.93	0.38	51,89,115,115	0
58	MG	CA	3031	1/1	0.93	0.10	64,64,64,64	0
58	MG	AA	1618	1/1	0.93	0.10	105,105,105,105	0
67	EDO	D1	101	4/4	0.93	0.19	47,52,68,74	0
58	MG	CA	3175	1/1	0.94	0.07	107,107,107,107	0
65	ACY	DA	3044	4/4	0.94	0.18	60,73,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3141	1/1	0.94	0.20	129,129,129,129	0
58	MG	CA	3012	1/1	0.94	0.17	82,82,82,82	0
58	MG	AA	1608	1/1	0.94	0.15	64,64,64,64	0
58	MG	CA	3091	1/1	0.94	0.15	153,153,153,153	0
58	MG	BA	1610	1/1	0.94	0.13	78,78,78,78	0
58	MG	CA	3034	1/1	0.94	0.11	60,60,60,60	0
58	MG	CA	3058	1/1	0.94	0.15	124,124,124,124	0
58	MG	CA	3103	1/1	0.94	0.19	98,98,98,98	0
58	MG	AA	1648	1/1	0.94	0.13	96,96,96,96	0
58	MG	CA	3077	1/1	0.94	0.10	139,139,139,139	0
62	SPD	DA	3031	10/10	0.94	0.25	27,70,87,89	0
58	MG	BA	1649	1/1	0.94	0.12	107,107,107,107	0
58	MG	DA	3139	1/1	0.94	0.05	85,85,85,85	0
60	MPD	DA	3043	8/8	0.94	0.16	75,104,118,125	0
58	MG	CA	3062	1/1	0.94	0.10	102,102,102,102	0
58	MG	CA	3051	1/1	0.94	0.04	129,129,129,129	0
58	MG	BA	1645	1/1	0.95	0.06	94,94,94,94	0
58	MG	BA	1636	1/1	0.95	0.16	131,131,131,131	0
63	PUT	DM	201	6/6	0.95	0.23	25,58,65,71	0
58	MG	DA	3026	1/1	0.95	0.26	52,52,52,52	0
58	MG	DA	3033	1/1	0.95	0.18	52,52,52,52	0
64	1PE	DA	3065	16/16	0.95	0.23	40,72,82,90	0
58	MG	CA	3007	1/1	0.95	0.33	83,83,83,83	0
58	MG	CA	3039	1/1	0.95	0.26	74,74,74,74	0
58	MG	CA	3163	1/1	0.95	0.15	113,113,113,113	0
58	MG	CA	3132	1/1	0.95	0.32	177,177,177,177	0
58	MG	BA	1603	1/1	0.95	0.15	65,65,65,65	0
58	MG	BA	1627	1/1	0.95	0.06	81,81,81,81	0
58	MG	CA	3112	1/1	0.95	0.12	102,102,102,102	0
58	MG	CA	3080	1/1	0.95	0.25	111,111,111,111	0
58	MG	CA	3138	1/1	0.95	0.06	117,117,117,117	0
58	MG	CA	3010	1/1	0.95	0.15	89,89,89,89	0
58	MG	AA	1655	1/1	0.95	0.09	148,148,148,148	0
58	MG	AA	1602	1/1	0.95	0.10	73,73,73,73	0
58	MG	DA	3074	1/1	0.95	0.30	75,75,75,75	0
59	PGE	AA	1613	10/10	0.95	0.16	41,88,109,113	0
67	EDO	DB	201	4/4	0.95	0.19	62,69,70,77	0
58	MG	CA	3087	1/1	0.95	0.10	139,139,139,139	0
67	EDO	DB	203	4/4	0.95	0.15	61,72,76,79	0
58	MG	CA	3151	1/1	0.95	0.21	92,92,92,92	0
58	MG	CA	3152	1/1	0.95	0.09	138,138,138,138	0
68	GUN	DA	3078	11/11	0.95	0.20	77,96,105,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
63	PUT	DA	3037	6/6	0.96	0.12	28,40,58,59	0
58	MG	CA	3115	1/1	0.96	0.08	109,109,109,109	0
58	MG	DA	3053	1/1	0.96	0.23	44,44,44,44	0
58	MG	DA	3020	1/1	0.96	0.06	46,46,46,46	0
58	MG	BA	1644	1/1	0.96	0.04	94,94,94,94	0
58	MG	DA	3089	1/1	0.96	0.16	46,46,46,46	0
58	MG	CA	3153	1/1	0.96	0.11	96,96,96,96	0
58	MG	AA	1656	1/1	0.96	0.05	94,94,94,94	0
58	MG	CA	3033	1/1	0.96	0.34	60,60,60,60	0
58	MG	CA	3124	1/1	0.96	0.09	115,115,115,115	0
58	MG	AA	1637	1/1	0.96	0.16	92,92,92,92	0
58	MG	CA	3092	1/1	0.96	0.12	93,93,93,93	0
58	MG	CA	3127	1/1	0.96	0.03	106,106,106,106	0
58	MG	CA	3094	1/1	0.96	0.06	118,118,118,118	0
58	MG	DA	3009	1/1	0.96	0.17	54,54,54,54	0
60	MPD	DA	3077	8/8	0.96	0.30	44,97,123,123	0
58	MG	CA	3166	1/1	0.96	0.10	123,123,123,123	0
58	MG	DA	3041	1/1	0.96	0.34	52,52,52,52	0
58	MG	CA	3100	1/1	0.96	0.24	149,149,149,149	0
58	MG	CA	3171	1/1	0.96	0.12	113,113,113,113	0
67	EDO	DA	3075	4/4	0.96	0.23	68,83,95,95	0
58	MG	CA	3073	1/1	0.96	0.12	109,109,109,109	0
58	MG	CA	3074	1/1	0.96	0.45	159,159,159,159	0
58	MG	CA	3107	1/1	0.96	0.18	92,92,92,92	0
58	MG	DA	3047	1/1	0.96	0.17	52,52,52,52	0
58	MG	CA	3038	1/1	0.96	0.09	61,61,61,61	0
58	MG	DA	3049	1/1	0.96	0.13	56,56,56,56	0
58	MG	DA	3017	1/1	0.96	0.15	60,60,60,60	0
58	MG	CA	3089	1/1	0.97	0.25	148,148,148,148	0
58	MG	CA	3028	1/1	0.97	0.10	73,73,73,73	0
58	MG	CA	3029	1/1	0.97	0.15	59,59,59,59	0
58	MG	AA	1630	1/1	0.97	0.16	89,89,89,89	0
58	MG	BA	1648	1/1	0.97	0.07	91,91,91,91	0
58	MG	AA	1645	1/1	0.97	0.09	93,93,93,93	0
58	MG	CA	3142	1/1	0.97	0.06	103,103,103,103	0
58	MG	CA	3097	1/1	0.97	0.21	115,115,115,115	0
58	MG	AA	1605	1/1	0.97	0.33	54,54,54,54	0
58	MG	CA	3011	1/1	0.97	0.14	87,87,87,87	0
58	MG	CA	3149	1/1	0.97	0.13	111,111,111,111	0
58	MG	CA	3101	1/1	0.97	0.24	147,147,147,147	0
58	MG	CA	3063	1/1	0.97	0.11	92,92,92,92	0
58	MG	BA	1613	1/1	0.97	0.04	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3106	1/1	0.97	0.12	106,106,106,106	0
58	MG	DA	3018	1/1	0.97	0.19	49,49,49,49	0
61	PG4	DQ	202	13/13	0.97	0.12	42,58,66,70	0
58	MG	CA	3067	1/1	0.97	0.17	117,117,117,117	0
61	PG4	DS	202	13/13	0.97	0.19	29,44,81,89	0
58	MG	AA	1632	1/1	0.97	0.08	63,63,63,63	0
58	MG	CA	3111	1/1	0.97	0.25	55,55,55,55	0
58	MG	CA	3069	1/1	0.97	0.09	96,96,96,96	0
58	MG	CA	3160	1/1	0.97	0.11	157,157,157,157	0
58	MG	CA	3161	1/1	0.97	0.08	78,78,78,78	0
58	MG	CA	3016	1/1	0.97	0.16	100,100,100,100	0
58	MG	AA	1601	1/1	0.97	0.21	54,54,54,54	0
58	MG	CA	3165	1/1	0.97	0.15	84,84,84,84	0
58	MG	CA	3116	1/1	0.97	0.06	106,106,106,106	0
58	MG	CA	3041	1/1	0.97	0.14	75,75,75,75	0
58	MG	DA	3027	1/1	0.97	0.13	77,77,77,77	0
58	MG	DA	3029	1/1	0.97	0.22	57,57,57,57	0
58	MG	CA	3172	1/1	0.97	0.07	94,94,94,94	0
58	MG	CA	3020	1/1	0.97	0.13	71,71,71,71	0
58	MG	CA	3174	1/1	0.97	0.09	123,123,123,123	0
58	MG	CA	3121	1/1	0.97	0.06	88,88,88,88	0
58	MG	CA	3076	1/1	0.97	0.17	105,105,105,105	0
58	MG	CA	3046	1/1	0.97	0.17	107,107,107,107	0
58	MG	CB	203	1/1	0.97	0.07	123,123,123,123	0
58	MG	CA	3078	1/1	0.97	0.15	73,73,73,73	0
67	EDO	DA	3052	4/4	0.97	0.20	48,48,57,58	0
67	EDO	DA	3057	4/4	0.97	0.24	47,57,58,71	0
58	MG	DA	3166	1/1	0.97	0.18	12,12,12,12	0
58	MG	C3	101	1/1	0.97	0.20	168,168,168,168	0
58	MG	DR	201	1/1	0.97	0.29	27,27,27,27	0
58	MG	DA	3188	1/1	0.97	0.12	36,36,36,36	0
58	MG	DA	3030	1/1	0.97	0.14	37,37,37,37	0
59	PGE	DA	3035	10/10	0.97	0.17	38,81,109,119	0
58	MG	CA	3024	1/1	0.97	0.09	61,61,61,61	0
58	MG	CA	3003	1/1	0.97	0.34	61,61,61,61	0
58	MG	AA	1657	1/1	0.97	0.08	95,95,95,95	0
58	MG	BA	1628	1/1	0.97	0.06	95,95,95,95	0
58	MG	CA	3088	1/1	0.97	0.15	127,127,127,127	0
58	MG	AA	1620	1/1	0.98	0.06	84,84,84,84	0
58	MG	CA	3139	1/1	0.98	0.11	124,124,124,124	0
58	MG	AA	1622	1/1	0.98	0.12	73,73,73,73	0
58	MG	BA	1631	1/1	0.98	0.12	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	CA	3013	1/1	0.98	0.10	66,66,66,66	0
58	MG	CA	3095	1/1	0.98	0.10	82,82,82,82	0
58	MG	BA	1633	1/1	0.98	0.08	66,66,66,66	0
58	MG	CA	3146	1/1	0.98	0.08	106,106,106,106	0
58	MG	CA	3147	1/1	0.98	0.12	95,95,95,95	0
58	MG	AA	1639	1/1	0.98	0.13	50,50,50,50	0
58	MG	AA	1604	1/1	0.98	0.28	51,51,51,51	0
58	MG	CA	3150	1/1	0.98	0.21	84,84,84,84	0
58	MG	CA	3099	1/1	0.98	0.10	77,77,77,77	0
58	MG	AA	1617	1/1	0.98	0.06	61,61,61,61	0
58	MG	CA	3057	1/1	0.98	0.17	90,90,90,90	0
58	MG	AA	1650	1/1	0.98	0.13	65,65,65,65	0
58	MG	DA	3042	1/1	0.98	0.15	60,60,60,60	0
58	MG	CA	3104	1/1	0.98	0.12	80,80,80,80	0
58	MG	CA	3105	1/1	0.98	0.09	83,83,83,83	0
58	MG	AA	1652	1/1	0.98	0.08	80,80,80,80	0
62	SPD	DA	3036	10/10	0.98	0.17	33,53,66,69	0
58	MG	AA	1603	1/1	0.98	0.15	45,45,45,45	0
58	MG	AA	1619	1/1	0.98	0.05	80,80,80,80	0
58	MG	AA	1633	1/1	0.98	0.08	84,84,84,84	0
58	MG	CA	3162	1/1	0.98	0.18	94,94,94,94	0
58	MG	CA	3064	1/1	0.98	0.08	104,104,104,104	0
58	MG	BA	1616	1/1	0.98	0.12	96,96,96,96	0
58	MG	BA	1617	1/1	0.98	0.12	73,73,73,73	0
58	MG	CA	3114	1/1	0.98	0.14	116,116,116,116	0
64	1PE	DA	3034	16/16	0.98	0.15	21,51,96,96	0
58	MG	CA	3167	1/1	0.98	0.14	93,93,93,93	0
58	MG	DA	3085	1/1	0.98	0.05	75,75,75,75	0
58	MG	AA	1635	1/1	0.98	0.05	89,89,89,89	0
66	PEG	DA	3050	7/7	0.98	0.20	51,62,68,78	0
58	MG	DA	3118	1/1	0.98	0.13	80,80,80,80	0
58	MG	DA	3120	1/1	0.98	0.18	31,31,31,31	0
58	MG	DA	3125	1/1	0.98	0.15	48,48,48,48	0
58	MG	DA	3002	1/1	0.98	0.14	10,10,10,10	0
58	MG	DA	3147	1/1	0.98	0.08	104,104,104,104	0
58	MG	DA	3156	1/1	0.98	0.03	58,58,58,58	0
58	MG	DA	3157	1/1	0.98	0.07	75,75,75,75	0
58	MG	CB	202	1/1	0.98	0.09	116,116,116,116	0
58	MG	DA	3005	1/1	0.98	0.24	35,35,35,35	0
58	MG	BA	1619	1/1	0.98	0.05	81,81,81,81	0
58	MG	CA	3001	1/1	0.98	0.35	68,68,68,68	0
58	MG	DA	3012	1/1	0.98	0.18	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	DA	3013	1/1	0.98	0.27	44,44,44,44	0
58	MG	BA	1620	1/1	0.98	0.15	87,87,87,87	0
58	MG	CA	3042	1/1	0.98	0.20	57,57,57,57	0
58	MG	BA	1622	1/1	0.98	0.08	89,89,89,89	0
58	MG	CA	3006	1/1	0.98	0.21	49,49,49,49	0
58	MG	BA	1626	1/1	0.98	0.11	62,62,62,62	0
58	MG	DA	3022	1/1	0.98	0.09	51,51,51,51	0
58	MG	DA	3023	1/1	0.98	0.28	36,36,36,36	0
58	MG	CA	3137	1/1	0.98	0.07	95,95,95,95	0
58	MG	AA	1607	1/1	0.99	0.14	46,46,46,46	0
58	MG	DA	3019	1/1	0.99	0.19	34,34,34,34	0
58	MG	BA	1621	1/1	0.99	0.10	69,69,69,69	0
58	MG	DA	3021	1/1	0.99	0.26	37,37,37,37	0
58	MG	AA	1653	1/1	0.99	0.09	70,70,70,70	0
58	MG	BA	1623	1/1	0.99	0.13	68,68,68,68	0
58	MG	DA	3024	1/1	0.99	0.14	60,60,60,60	0
58	MG	DA	3025	1/1	0.99	0.20	25,25,25,25	0
58	MG	BA	1624	1/1	0.99	0.14	70,70,70,70	0
58	MG	BA	1625	1/1	0.99	0.21	107,107,107,107	0
58	MG	DA	3028	1/1	0.99	0.14	36,36,36,36	0
58	MG	AA	1654	1/1	0.99	0.10	63,63,63,63	0
58	MG	CA	3143	1/1	0.99	0.32	117,117,117,117	0
58	MG	AA	1624	1/1	0.99	0.20	65,65,65,65	0
58	MG	AA	1625	1/1	0.99	0.06	77,77,77,77	0
58	MG	BA	1629	1/1	0.99	0.08	65,65,65,65	0
58	MG	BA	1630	1/1	0.99	0.07	74,74,74,74	0
58	MG	AA	1626	1/1	0.99	0.06	69,69,69,69	0
58	MG	BA	1632	1/1	0.99	0.09	59,59,59,59	0
58	MG	AA	1658	1/1	0.99	0.15	59,59,59,59	0
58	MG	BA	1601	1/1	0.99	0.25	67,67,67,67	0
58	MG	AA	1627	1/1	0.99	0.17	55,55,55,55	0
58	MG	AA	1638	1/1	0.99	0.05	51,51,51,51	0
58	MG	AA	1628	1/1	0.99	0.09	70,70,70,70	0
58	MG	CA	3040	1/1	0.99	0.30	60,60,60,60	0
58	MG	DA	3068	1/1	0.99	0.22	47,47,47,47	0
58	MG	AA	1640	1/1	0.99	0.04	71,71,71,71	0
58	MG	DA	3080	1/1	0.99	0.10	29,29,29,29	0
58	MG	DA	3081	1/1	0.99	0.15	63,63,63,63	0
58	MG	DA	3083	1/1	0.99	0.04	74,74,74,74	0
58	MG	DA	3084	1/1	0.99	0.07	46,46,46,46	0
58	MG	BA	1639	1/1	0.99	0.15	91,91,91,91	0
58	MG	BA	1640	1/1	0.99	0.08	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	DA	3092	1/1	0.99	0.16	24,24,24,24	0
58	MG	DA	3093	1/1	0.99	0.12	22,22,22,22	0
58	MG	DA	3095	1/1	0.99	0.09	35,35,35,35	0
58	MG	DA	3096	1/1	0.99	0.13	35,35,35,35	0
58	MG	DA	3097	1/1	0.99	0.12	31,31,31,31	0
58	MG	CA	3169	1/1	0.99	0.22	80,80,80,80	0
58	MG	DA	3098	1/1	0.99	0.12	27,27,27,27	0
58	MG	CA	3055	1/1	0.99	0.19	82,82,82,82	0
58	MG	DA	3101	1/1	0.99	0.19	50,50,50,50	0
58	MG	DA	3104	1/1	0.99	0.15	20,20,20,20	0
58	MG	DA	3105	1/1	0.99	0.12	32,32,32,32	0
58	MG	DA	3106	1/1	0.99	0.20	40,40,40,40	0
58	MG	DA	3107	1/1	0.99	0.19	41,41,41,41	0
58	MG	DB	204	1/1	0.99	0.12	62,62,62,62	0
58	MG	DB	205	1/1	0.99	0.07	38,38,38,38	0
58	MG	DB	206	1/1	0.99	0.08	41,41,41,41	0
58	MG	DA	3108	1/1	0.99	0.15	28,28,28,28	0
58	MG	DA	3109	1/1	0.99	0.16	7,7,7,7	0
58	MG	DA	3111	1/1	0.99	0.17	15,15,15,15	0
58	MG	DA	3112	1/1	0.99	0.22	25,25,25,25	0
58	MG	BA	1641	1/1	0.99	0.12	62,62,62,62	0
58	MG	DA	3119	1/1	0.99	0.13	51,51,51,51	0
58	MG	DD	302	1/1	0.99	0.21	49,49,49,49	0
58	MG	DM	202	1/1	0.99	0.11	47,47,47,47	0
58	MG	AA	1641	1/1	0.99	0.06	70,70,70,70	0
58	MG	DR	203	1/1	0.99	0.18	38,38,38,38	0
58	MG	DA	3121	1/1	0.99	0.05	68,68,68,68	0
58	MG	BA	1608	1/1	0.99	0.11	82,82,82,82	0
58	MG	DA	3126	1/1	0.99	0.19	44,44,44,44	0
58	MG	DA	3129	1/1	0.99	0.07	19,19,19,19	0
58	MG	DA	3130	1/1	0.99	0.11	52,52,52,52	0
58	MG	DA	3131	1/1	0.99	0.17	34,34,34,34	0
58	MG	DA	3133	1/1	0.99	0.15	24,24,24,24	0
58	MG	DA	3134	1/1	0.99	0.15	38,38,38,38	0
58	MG	AA	1642	1/1	0.99	0.16	73,73,73,73	0
58	MG	DA	3142	1/1	0.99	0.14	20,20,20,20	0
58	MG	DA	3143	1/1	0.99	0.17	15,15,15,15	0
58	MG	DA	3145	1/1	0.99	0.17	38,38,38,38	0
58	MG	DA	3146	1/1	0.99	0.06	55,55,55,55	0
58	MG	CA	3081	1/1	0.99	0.21	102,102,102,102	0
58	MG	AA	1643	1/1	0.99	0.07	78,78,78,78	0
58	MG	DA	3148	1/1	0.99	0.13	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	DA	3149	1/1	0.99	0.17	55,55,55,55	0
58	MG	CA	3085	1/1	0.99	0.09	91,91,91,91	0
58	MG	DA	3150	1/1	0.99	0.18	18,18,18,18	0
58	MG	DA	3153	1/1	0.99	0.18	26,26,26,26	0
58	MG	BA	1646	1/1	0.99	0.11	59,59,59,59	0
58	MG	BA	1647	1/1	0.99	0.11	68,68,68,68	0
58	MG	DA	3158	1/1	0.99	0.05	27,27,27,27	0
58	MG	DA	3159	1/1	0.99	0.04	56,56,56,56	0
58	MG	DA	3162	1/1	0.99	0.16	42,42,42,42	0
58	MG	CA	3093	1/1	0.99	0.09	65,65,65,65	0
58	MG	DA	3165	1/1	0.99	0.23	22,22,22,22	0
58	MG	AA	1644	1/1	0.99	0.07	83,83,83,83	0
58	MG	DA	3168	1/1	0.99	0.17	51,51,51,51	0
58	MG	DA	3169	1/1	0.99	0.16	8,8,8,8	0
58	MG	DA	3171	1/1	0.99	0.11	60,60,60,60	0
58	MG	DA	3172	1/1	0.99	0.20	46,46,46,46	0
58	MG	DA	3173	1/1	0.99	0.10	50,50,50,50	0
58	MG	DA	3174	1/1	0.99	0.10	67,67,67,67	0
58	MG	DA	3175	1/1	0.99	0.15	22,22,22,22	0
58	MG	DA	3177	1/1	0.99	0.13	31,31,31,31	0
58	MG	DA	3179	1/1	0.99	0.10	36,36,36,36	0
58	MG	DA	3180	1/1	0.99	0.18	19,19,19,19	0
58	MG	DA	3183	1/1	0.99	0.11	38,38,38,38	0
58	MG	DA	3185	1/1	0.99	0.12	28,28,28,28	0
58	MG	CA	3108	1/1	0.99	0.09	92,92,92,92	0
65	ACY	DA	3064	4/4	0.99	0.22	12,15,38,45	0
58	MG	DA	3186	1/1	0.99	0.16	36,36,36,36	0
58	MG	DA	3187	1/1	0.99	0.10	18,18,18,18	0
58	MG	AA	1629	1/1	0.99	0.07	30,30,30,30	0
58	MG	DA	3189	1/1	0.99	0.14	47,47,47,47	0
58	MG	DA	3191	1/1	0.99	0.19	16,16,16,16	0
58	MG	BA	1650	1/1	0.99	0.09	96,96,96,96	0
58	MG	AA	1646	1/1	0.99	0.12	99,99,99,99	0
58	MG	DA	3003	1/1	0.99	0.17	53,53,53,53	0
58	MG	DA	3004	1/1	0.99	0.15	30,30,30,30	0
58	MG	AA	1647	1/1	0.99	0.20	100,100,100,100	0
58	MG	DA	3006	1/1	0.99	0.21	31,31,31,31	0
58	MG	DA	3007	1/1	0.99	0.15	48,48,48,48	0
58	MG	DA	3008	1/1	0.99	0.27	27,27,27,27	0
58	MG	AA	1621	1/1	0.99	0.14	63,63,63,63	0
58	MG	DA	3010	1/1	0.99	0.14	40,40,40,40	0
58	MG	AA	1649	1/1	0.99	0.04	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	AA	1614	1/1	0.99	0.12	39,39,39,39	0
58	MG	DA	3014	1/1	0.99	0.17	36,36,36,36	0
58	MG	DA	3015	1/1	0.99	0.31	48,48,48,48	0
58	MG	CA	3128	1/1	0.99	0.07	104,104,104,104	0
58	MG	DA	3016	1/1	0.99	0.27	41,41,41,41	0
58	MG	AA	1651	1/1	0.99	0.12	74,74,74,74	0
58	MG	AA	1634	1/1	1.00	0.10	64,64,64,64	0
58	MG	DA	3102	1/1	1.00	0.14	35,35,35,35	0
58	MG	DA	3181	1/1	1.00	0.16	47,47,47,47	0
58	MG	DA	3182	1/1	1.00	0.19	73,73,73,73	0
58	MG	DA	3132	1/1	1.00	0.16	12,12,12,12	0
58	MG	DA	3184	1/1	1.00	0.16	60,60,60,60	0
58	MG	DA	3103	1/1	1.00	0.10	37,37,37,37	0
58	MG	DA	3086	1/1	1.00	0.12	15,15,15,15	0
58	MG	DA	3135	1/1	1.00	0.08	25,25,25,25	0
58	MG	DA	3136	1/1	1.00	0.12	9,9,9,9	0
58	MG	DA	3137	1/1	1.00	0.18	52,52,52,52	0
58	MG	DA	3190	1/1	1.00	0.09	29,29,29,29	0
58	MG	DA	3138	1/1	1.00	0.13	30,30,30,30	0
58	MG	DA	3087	1/1	1.00	0.13	21,21,21,21	0
58	MG	DA	3140	1/1	1.00	0.11	38,38,38,38	0
58	MG	DA	3141	1/1	1.00	0.10	12,12,12,12	0
58	MG	DA	3088	1/1	1.00	0.15	25,25,25,25	0
58	MG	DA	3011	1/1	1.00	0.17	27,27,27,27	0
58	MG	DA	3144	1/1	1.00	0.13	52,52,52,52	0
58	MG	DA	3090	1/1	1.00	0.14	4,4,4,4	0
58	MG	DA	3091	1/1	1.00	0.14	30,30,30,30	0
58	MG	DA	3110	1/1	1.00	0.13	19,19,19,19	0
58	MG	DA	3079	1/1	1.00	0.10	25,25,25,25	0
58	MG	AA	1659	1/1	1.00	0.10	55,55,55,55	0
58	MG	DA	3113	1/1	1.00	0.20	75,75,75,75	0
58	MG	DA	3151	1/1	1.00	0.10	61,61,61,61	0
58	MG	DA	3152	1/1	1.00	0.19	38,38,38,38	0
58	MG	DA	3114	1/1	1.00	0.24	17,17,17,17	0
58	MG	DA	3154	1/1	1.00	0.10	38,38,38,38	0
58	MG	DA	3155	1/1	1.00	0.11	65,65,65,65	0
58	MG	DA	3115	1/1	1.00	0.12	28,28,28,28	0
58	MG	DA	3116	1/1	1.00	0.12	23,23,23,23	0
58	MG	DA	3117	1/1	1.00	0.06	16,16,16,16	0
58	MG	DB	207	1/1	1.00	0.12	36,36,36,36	0
58	MG	DA	3094	1/1	1.00	0.15	10,10,10,10	0
58	MG	DA	3160	1/1	1.00	0.08	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	DA	3161	1/1	1.00	0.10	29,29,29,29	0
58	MG	BA	1614	1/1	1.00	0.15	96,96,96,96	0
58	MG	DA	3163	1/1	1.00	0.10	27,27,27,27	0
58	MG	DA	3164	1/1	1.00	0.17	27,27,27,27	0
58	MG	DA	3082	1/1	1.00	0.13	61,61,61,61	0
58	MG	DA	3040	1/1	1.00	0.16	38,38,38,38	0
58	MG	DA	3167	1/1	1.00	0.15	21,21,21,21	0
58	MG	DA	3122	1/1	1.00	0.13	27,27,27,27	0
58	MG	DA	3123	1/1	1.00	0.12	19,19,19,19	0
58	MG	DA	3170	1/1	1.00	0.18	64,64,64,64	0
58	MG	DA	3124	1/1	1.00	0.09	19,19,19,19	0
58	MG	DA	3001	1/1	1.00	0.12	12,12,12,12	0
58	MG	DA	3099	1/1	1.00	0.24	177,177,177,177	0
58	MG	DA	3127	1/1	1.00	0.13	19,19,19,19	0
58	MG	DA	3128	1/1	1.00	0.12	34,34,34,34	0
58	MG	DA	3176	1/1	1.00	0.12	27,27,27,27	0
58	MG	DA	3100	1/1	1.00	0.14	29,29,29,29	0
58	MG	DA	3178	1/1	1.00	0.13	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.