



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 21, 2026 – 04:03 pm BST

PDB ID : 6I7V / pdb_00006i7v
Title : Ribosomal protein paralogs bL31 and bL36
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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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

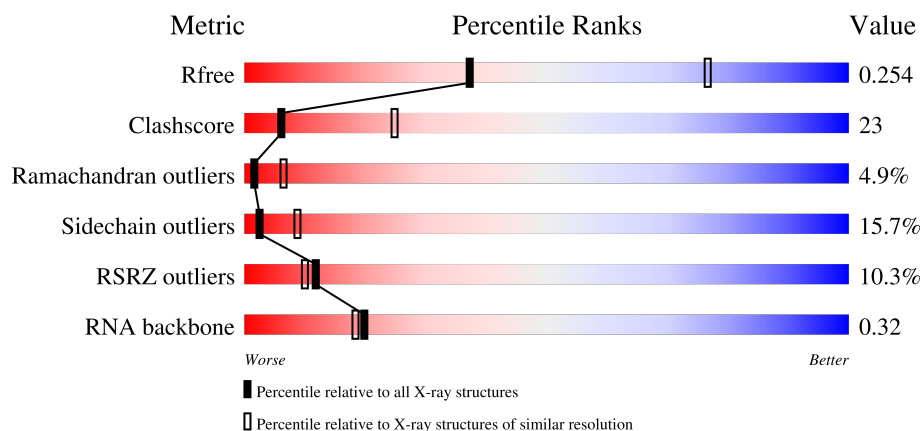
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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 $\leq 5\%$. 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	26% 55% 18%
2	BA	1533	3% 26% 55% 19%
3	DA	2903	31% 49% 19%
4	CA	2904	10% 23% 56% 20%

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Mol	Chain	Length	Quality of chain
5	CB	119	
5	DB	119	
6	AB	218	
6	BB	218	
7	AC	206	
7	BC	206	
8	AD	205	
8	BD	205	
9	AE	150	
9	BE	150	
10	AF	100	
10	BF	100	
11	AG	151	
11	BG	151	
12	AH	129	
12	BH	129	
13	AI	127	
13	BI	127	
14	AJ	98	
14	BJ	98	
15	AK	117	
15	BK	117	
16	AL	123	
17	AM	114	
17	BM	114	

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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	
44	DU	93	
45	CV	102	
45	DV	102	
46	CW	94	
46	DW	94	
47	CX	76	
47	DX	76	
48	CY	77	
48	DY	77	
49	CZ	62	
49	DZ	62	
50	C0	58	
50	D0	58	
51	C1	56	
51	D1	56	
52	C2	51	
52	D2	51	
53	C3	46	
53	D3	46	
54	C4	64	
54	D4	64	
55	C5	45	
55	D5	45	
56	DD	209	

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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	3083	-	-	-	X
58	MG	CA	3154	-	-	-	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	-
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
1	AA	1533	Total	C	H	N	O	P	0	0	0
			49352	14684	16444	6036	10655	1533			

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

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

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

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

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

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

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

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

- 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 924	C 280	H 473	N 94	O 76	S 1	0	0	0
25	BU	54	Total 924	C 280	H 473	N 94	O 76	S 1	0	0	0

- 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 (CCD ID: MG) (formula: Mg).

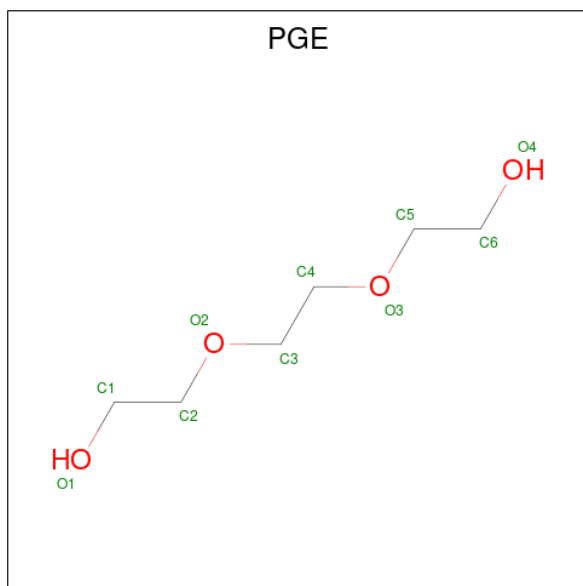
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	57	Total	Mg	0	0
			57	57		
58	BA	49	Total	Mg	0	0
			49	49		
58	DA	156	Total	Mg	0	0
			156	156		
58	CA	176	Total	Mg	0	0
			176	176		

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

- Molecule 59 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



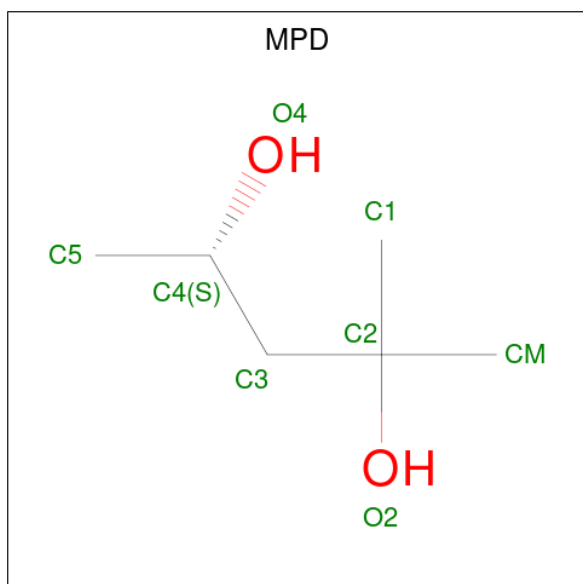
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	AA	1	Total	C	H	O	0	0
			24	6	14	4		
59	DA	1	Total	C	H	O	0	0
			24	6	14	4		

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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 (CCD ID: MPD) (formula: C₆H₁₄O₂).



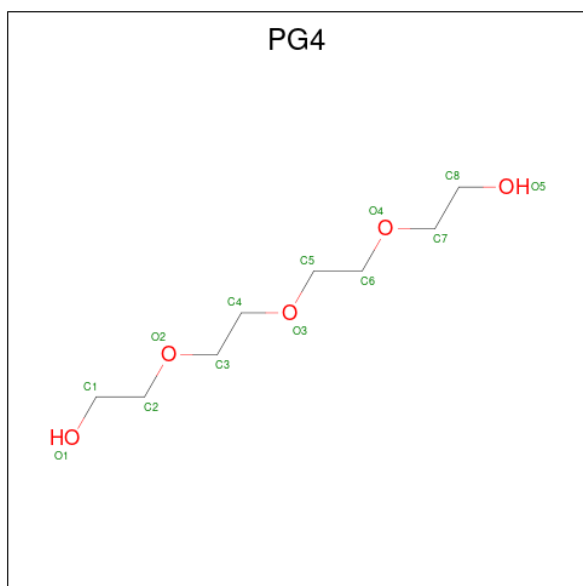
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
60	AA	1	Total	C	H	O	0	0
			22	6	14	2		
60	DA	1	Total	C	H	O	0	0
			22	6	14	2		
60	DA	1	Total	C	H	O	0	0
			22	6	14	2		
60	DA	1	Total	C	H	O	0	0
			22	6	14	2		
60	DA	1	Total	C	H	O	0	0
			22	6	14	2		

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

- Molecule 61 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



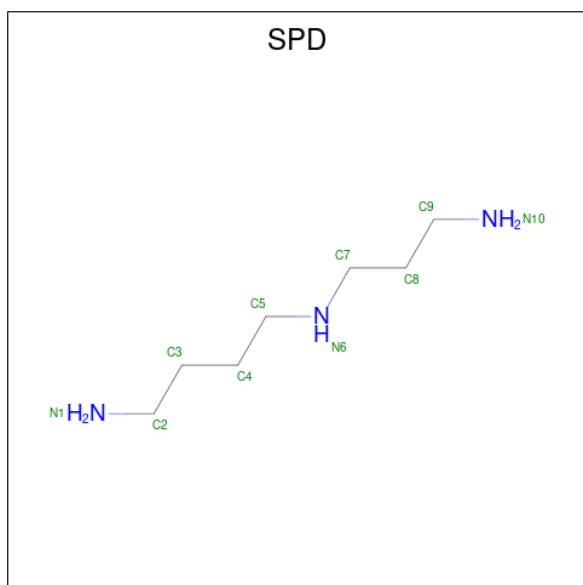
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	BA	1	Total	C	O	0	0
			13	8	5		
61	DA	1	Total	C	O	0	0
			13	8	5		
61	DQ	1	Total	C	O	0	0
			13	8	5		

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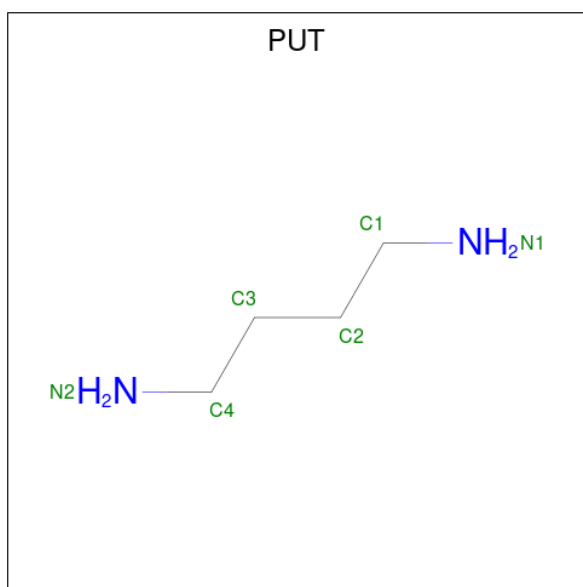
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	DR	1	Total	C	O	0	0
			13	8	5		
61	DS	1	Total	C	O	0	0
			13	8	5		

- Molecule 62 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



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

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



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

- Molecule 64 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



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

- Molecule 65 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



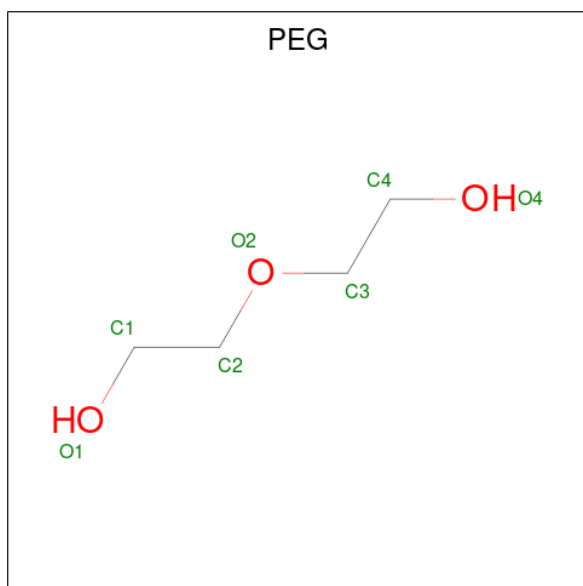
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
65	DA	1	Total 7	C 2	H 3	O 2	0	0
65	DA	1	Total 7	C 2	H 3	O 2	0	0

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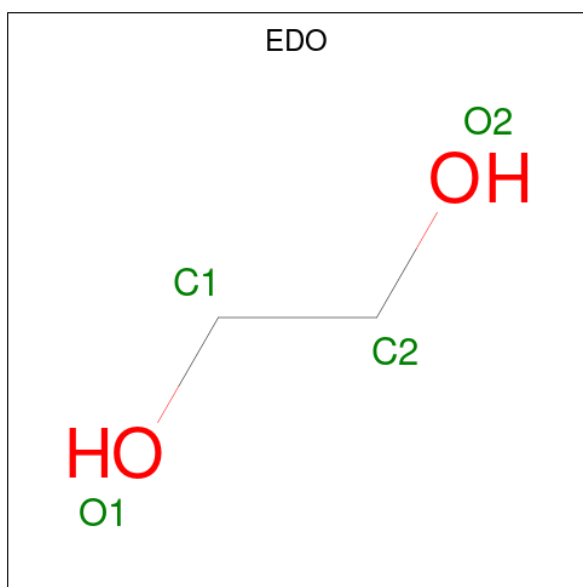
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
65	DA	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 66 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



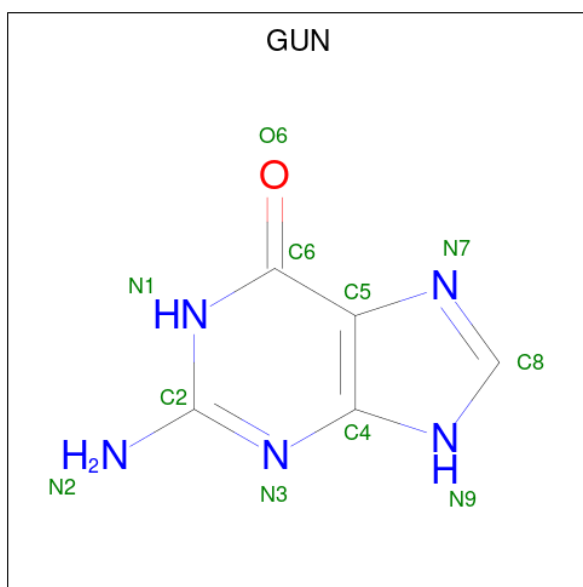
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			7	4	3		
66	DA	1	Total	C	O	0	0
			7	4	3		
66	DA	1	Total	C	O	0	0
			7	4	3		
66	DA	1	Total	C	O	0	0
			7	4	3		
66	DA	1	Total	C	O	0	0
			7	4	3		
66	DP	1	Total	C	O	0	0
			7	4	3		
66	DQ	1	Total	C	O	0	0
			7	4	3		
66	D1	1	Total	C	O	0	0
			7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

- Molecule 67 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 68 is GUANINE (CCD ID: GUN) (formula: C₅H₅N₅O).



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

- Molecule 69 is water.

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

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

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

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

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

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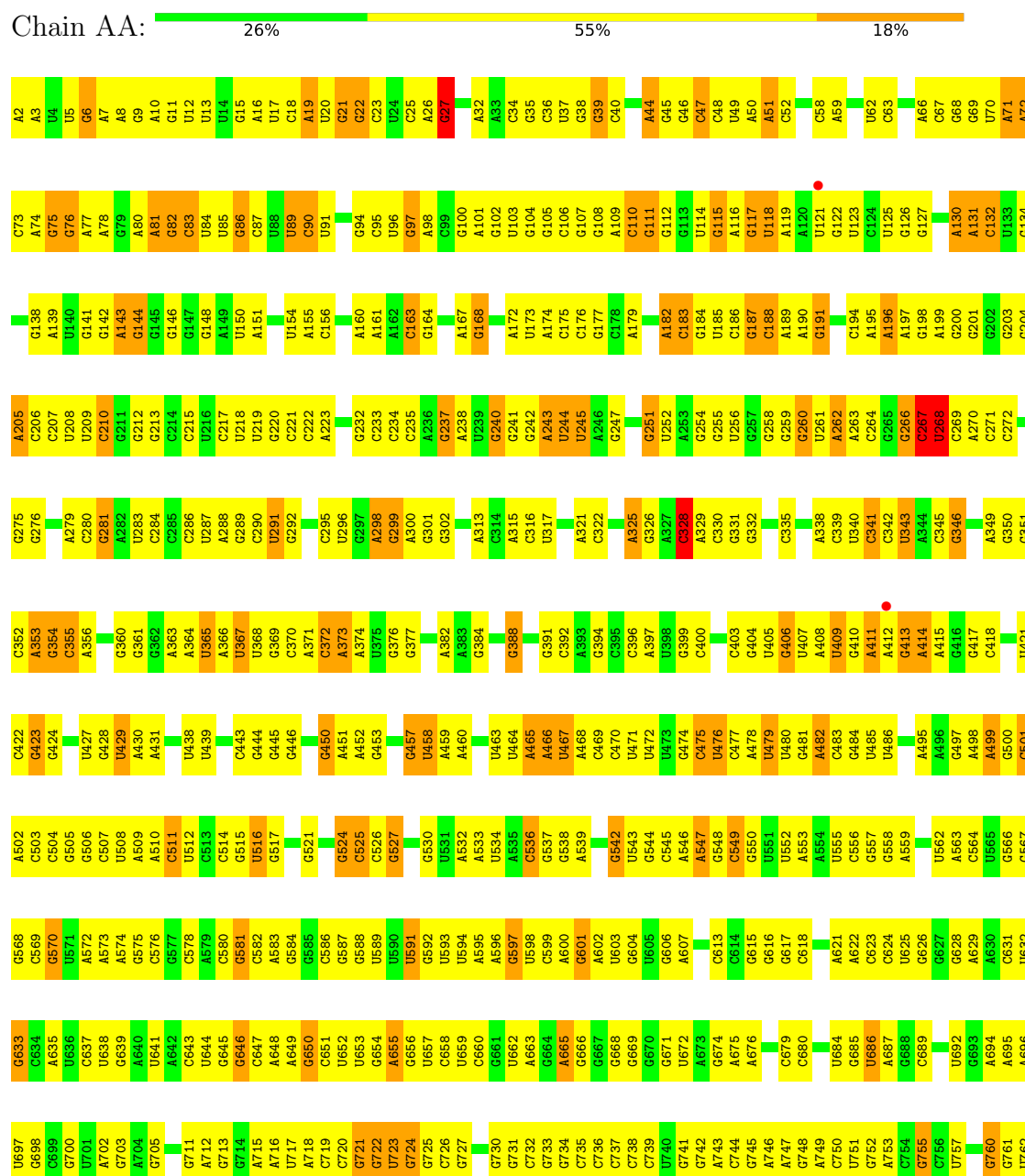
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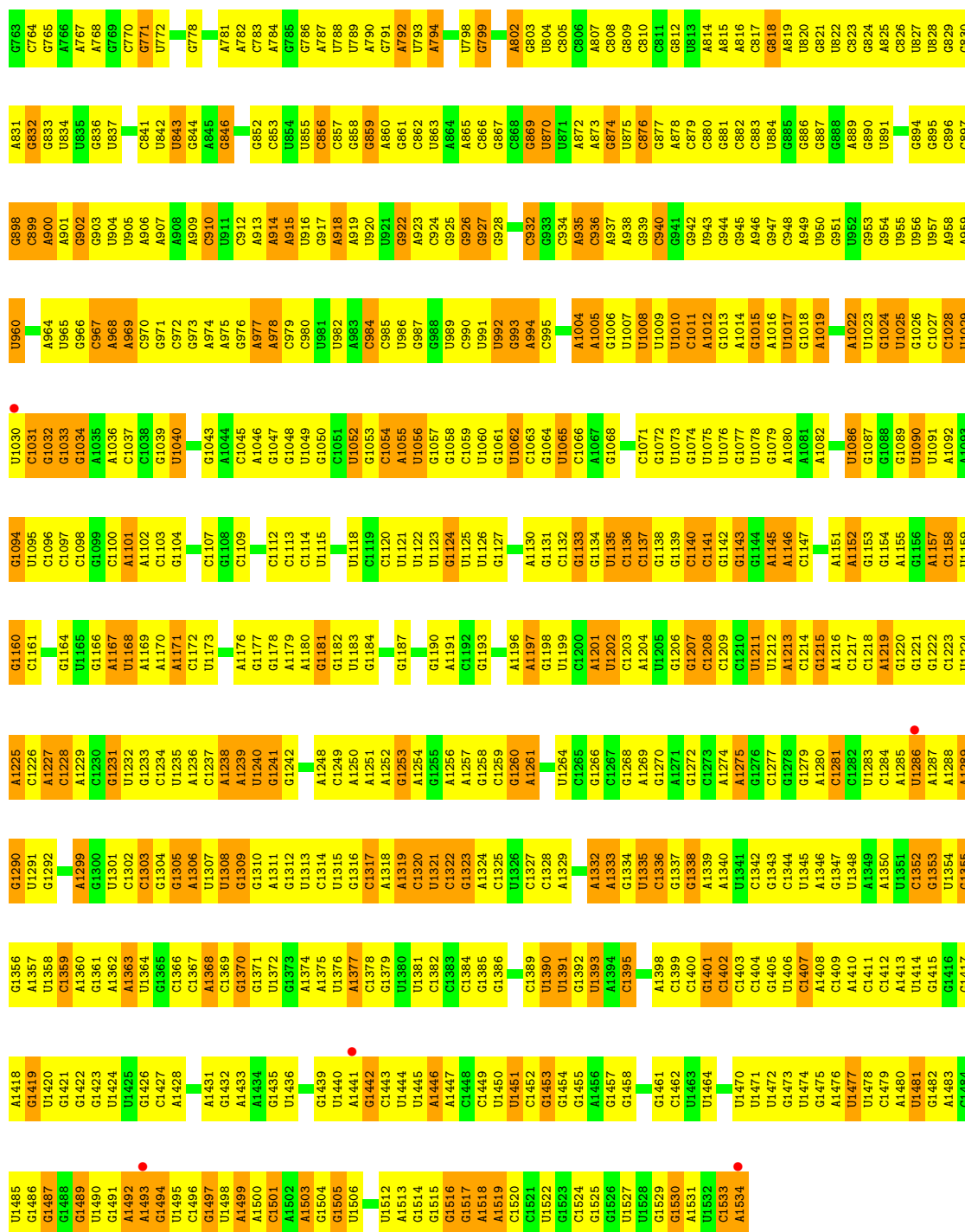
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	D2	4	Total 4	O 4	0	0
69	D3	24	Total 24	O 24	0	0
69	D4	27	Total 27	O 27	0	0
69	D5	9	Total 9	O 9	0	0

3 Residue-property plots

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

• Molecule 1: 16S ribosomal RNA

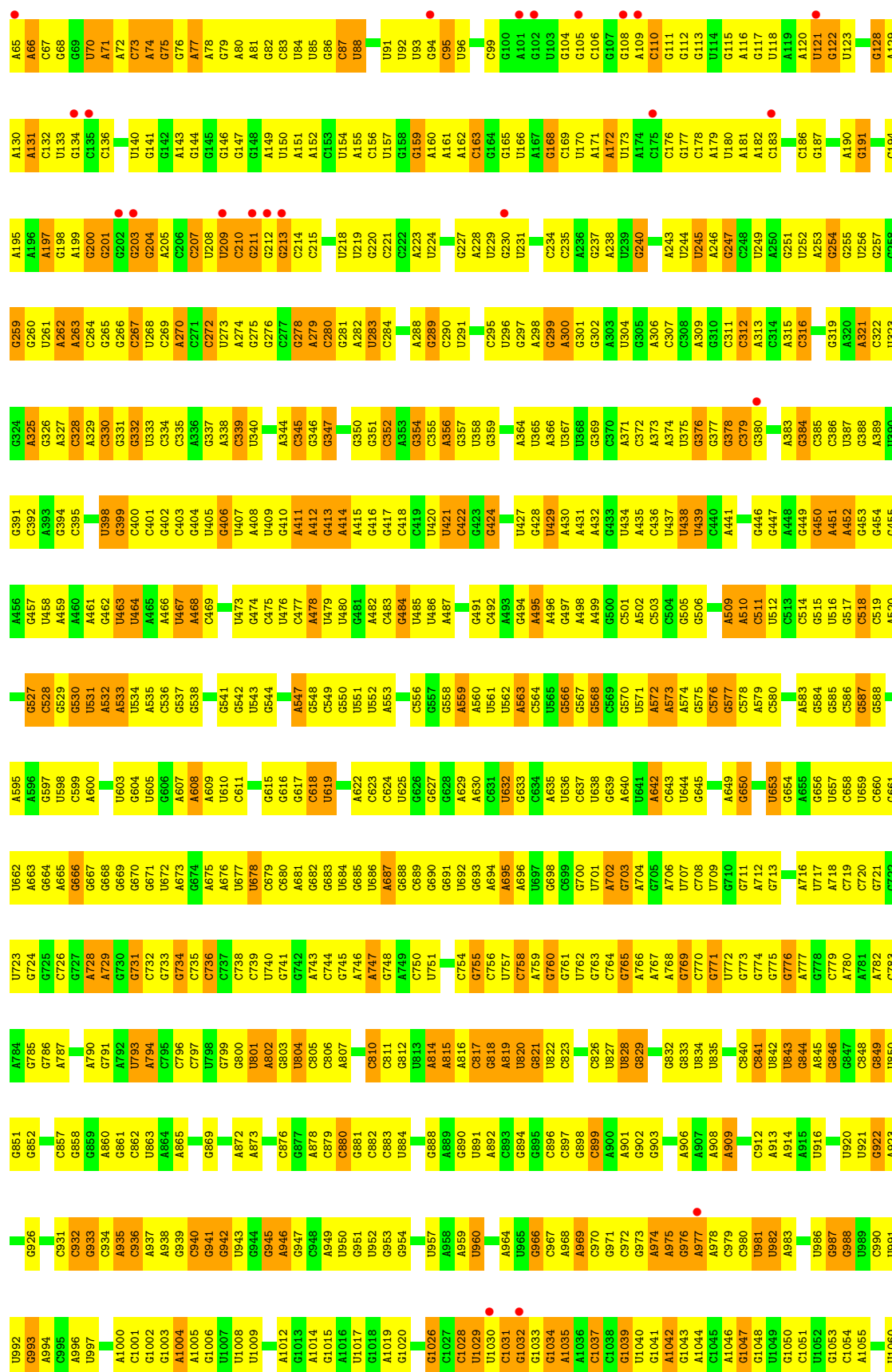




• Molecule 2: 16S ribosomal RNA

Chain BA: 3% 26% 55% 19%

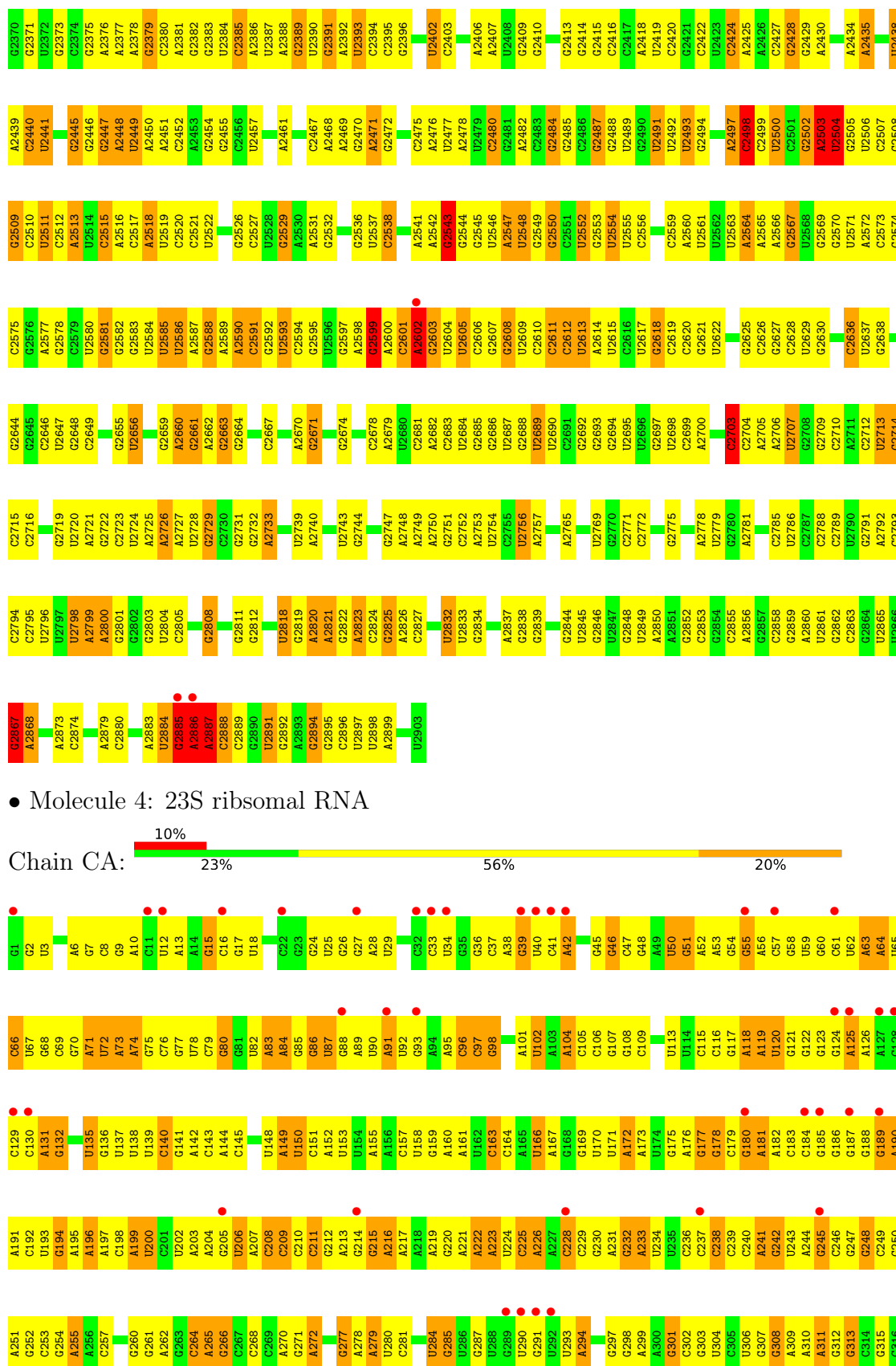


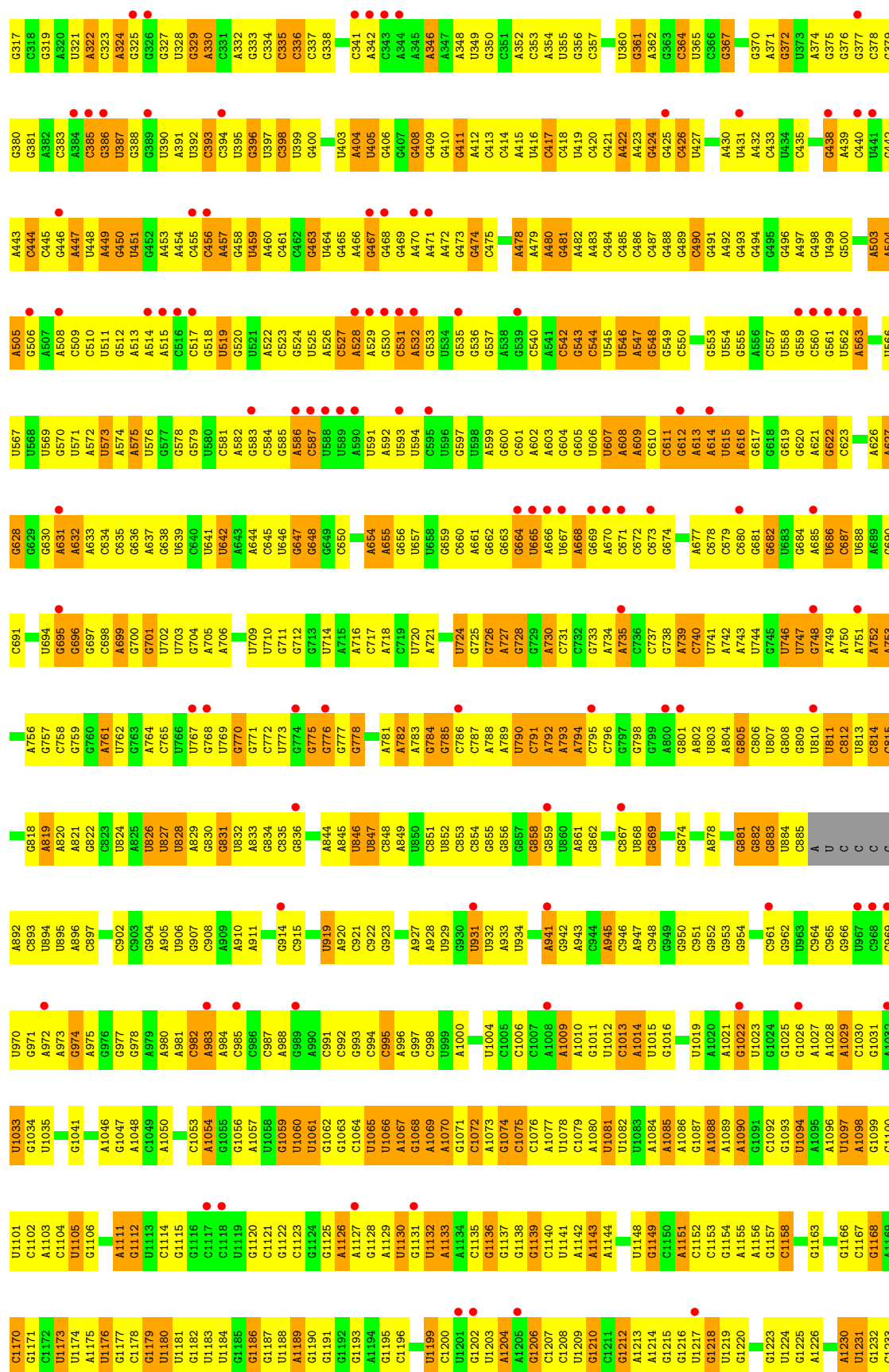




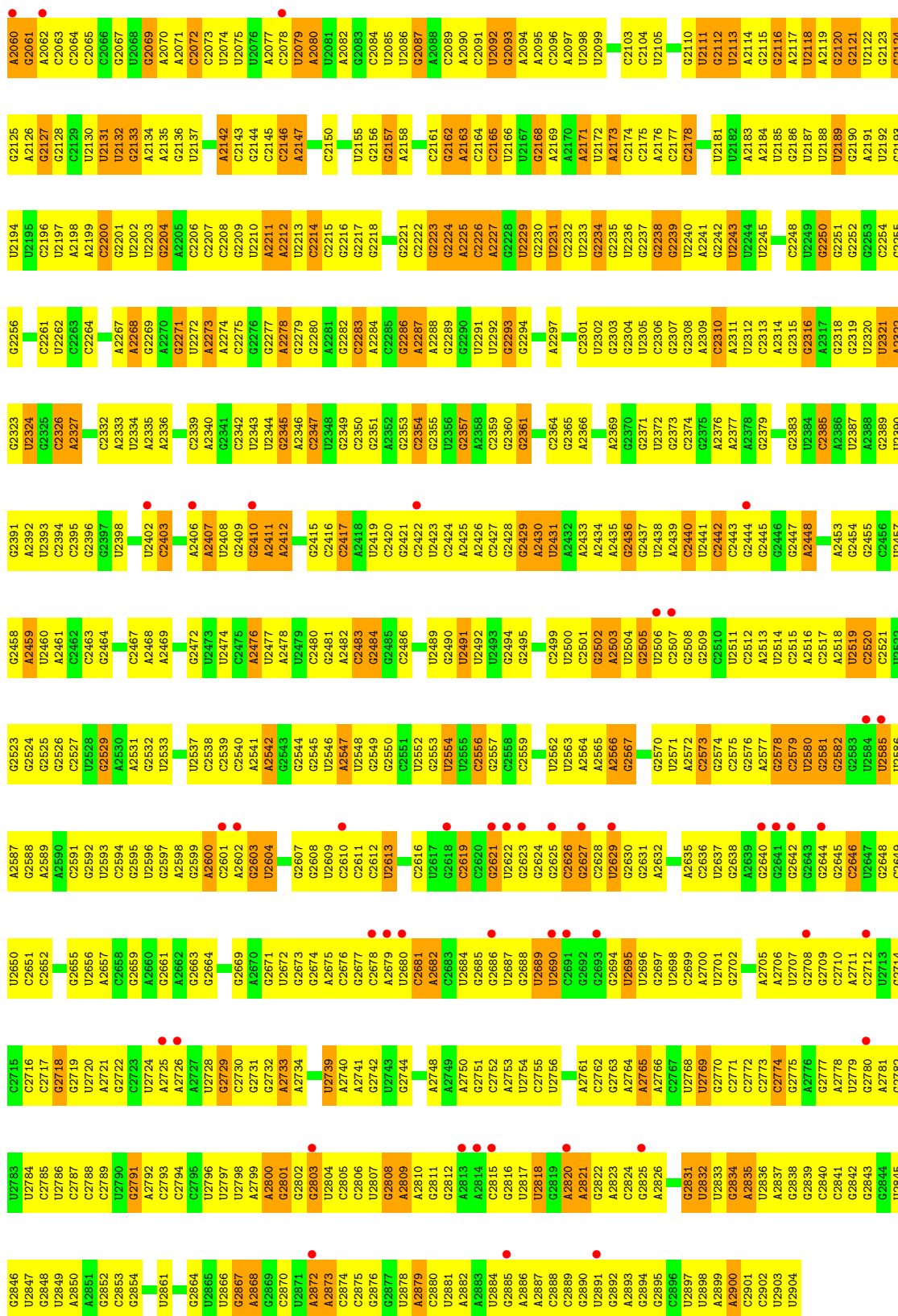
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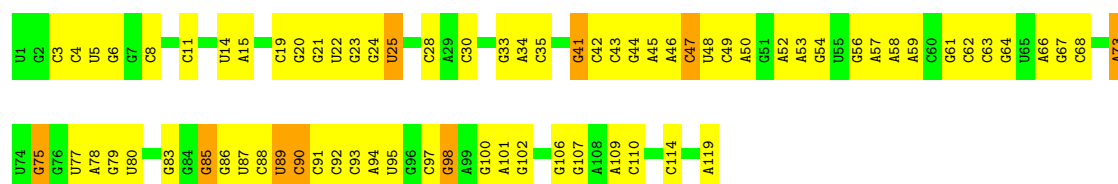
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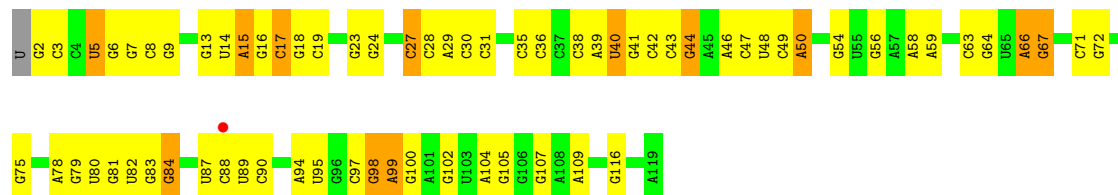




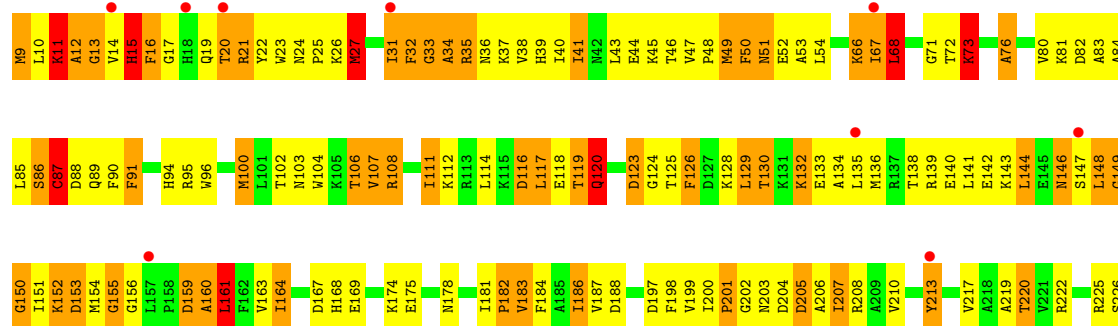




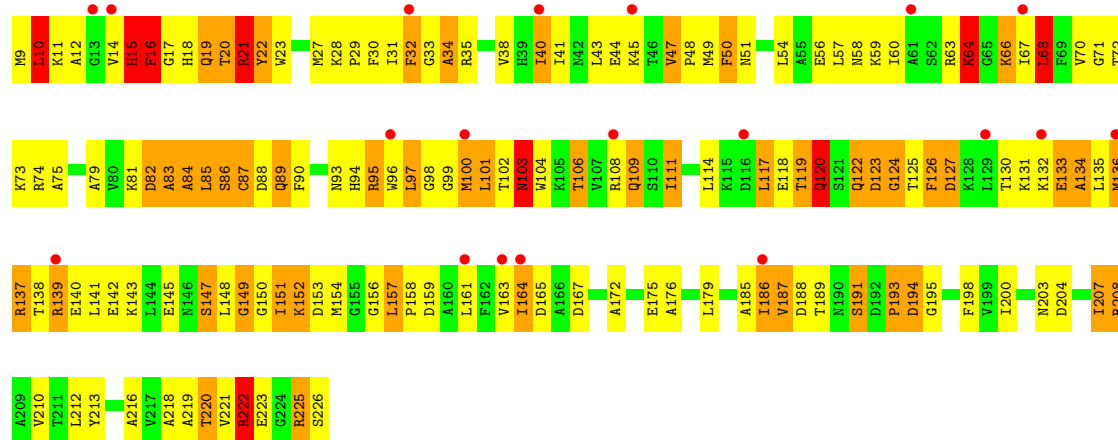
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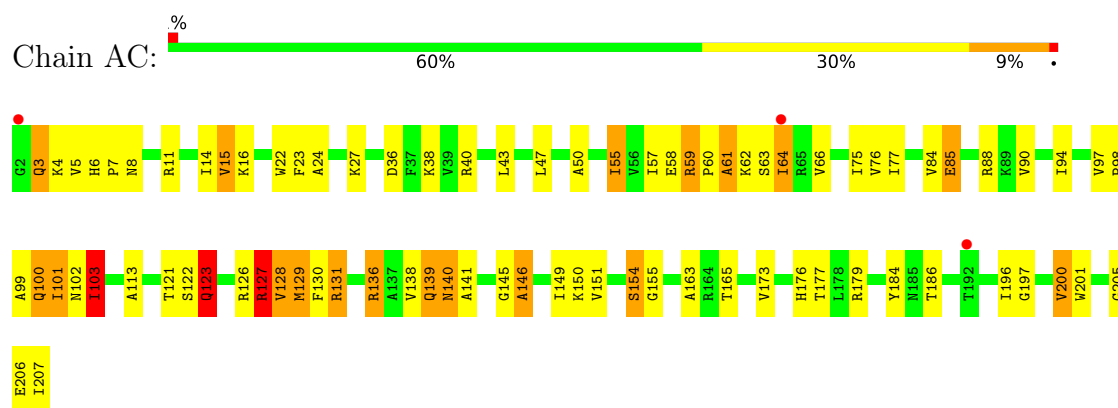
• Molecule 6: 30S ribosomal protein S2



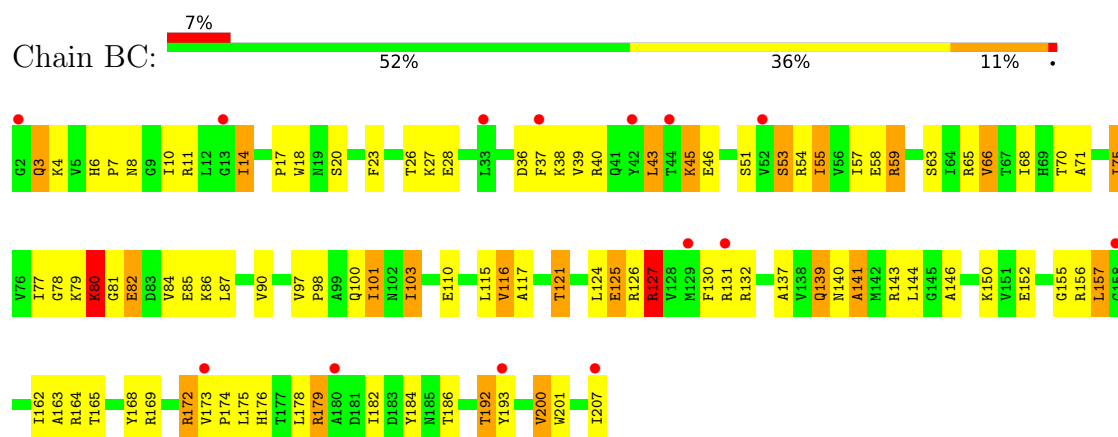
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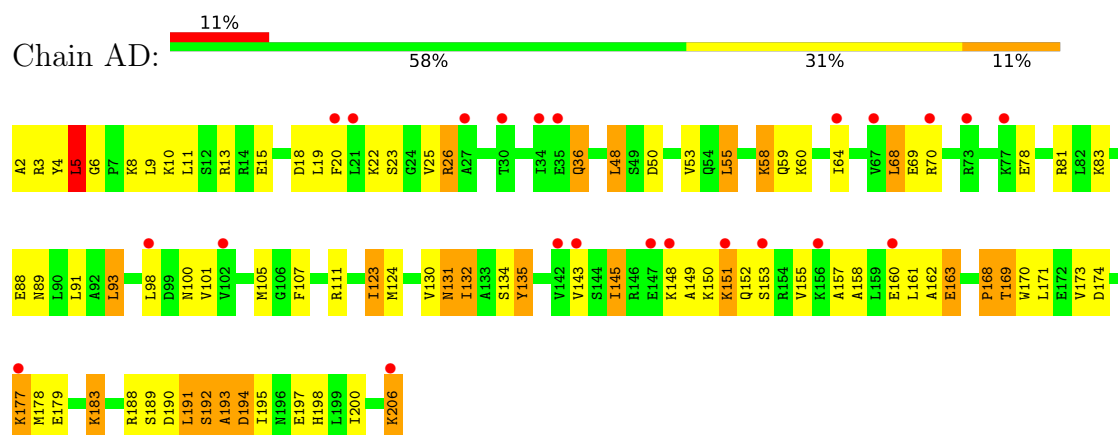
• Molecule 7: 30S ribosomal protein S3



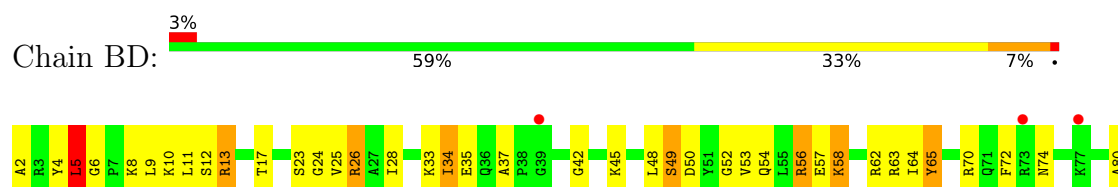
• Molecule 7: 30S ribosomal protein S3

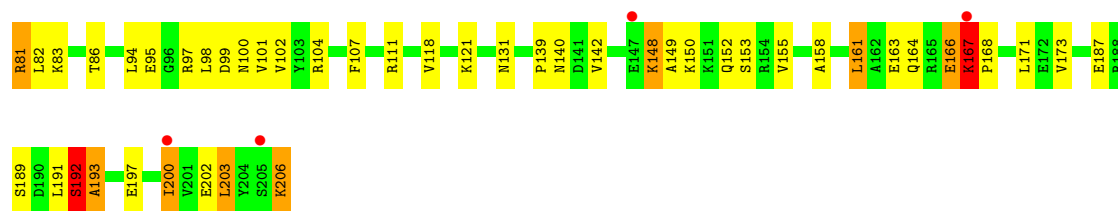


• Molecule 8: 30S ribosomal protein S4

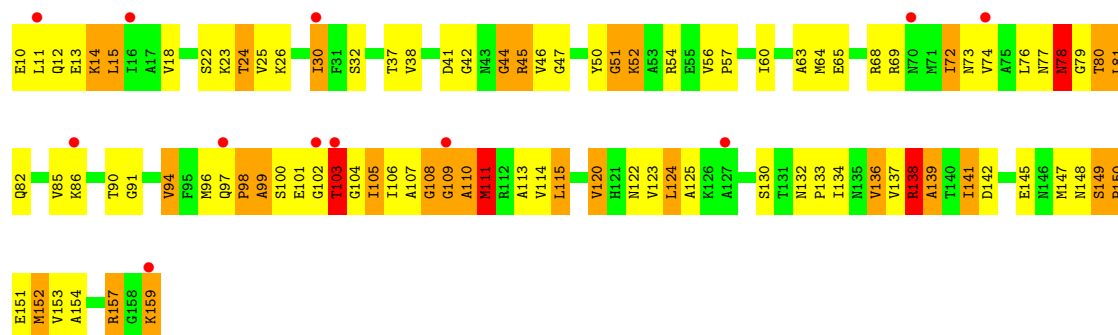


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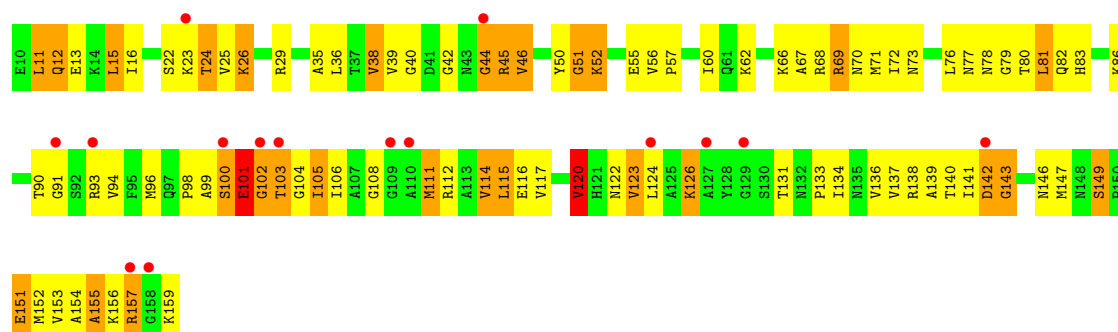




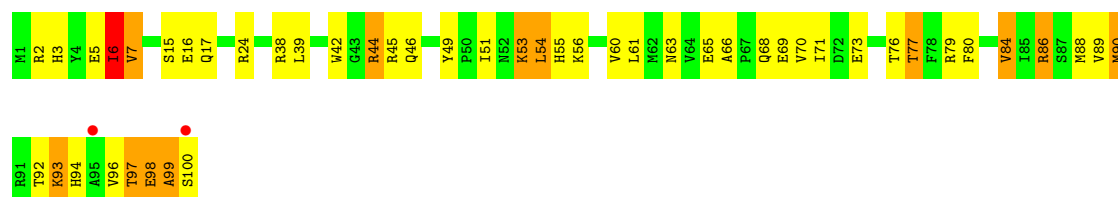
• Molecule 9: 30S ribosomal protein S5



• Molecule 9: 30S ribosomal protein S5

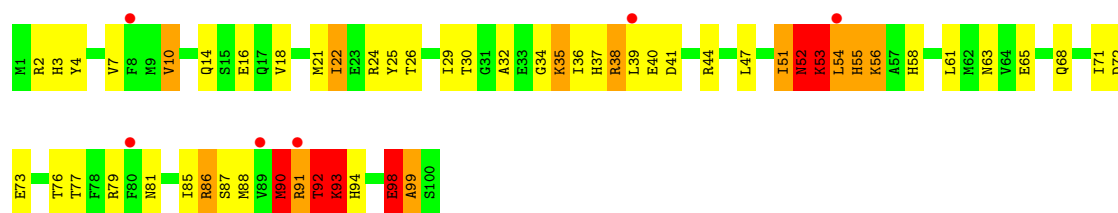


• Molecule 10: 30S ribosomal protein S6

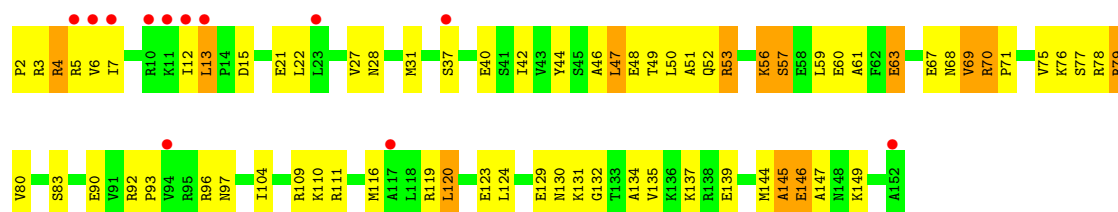


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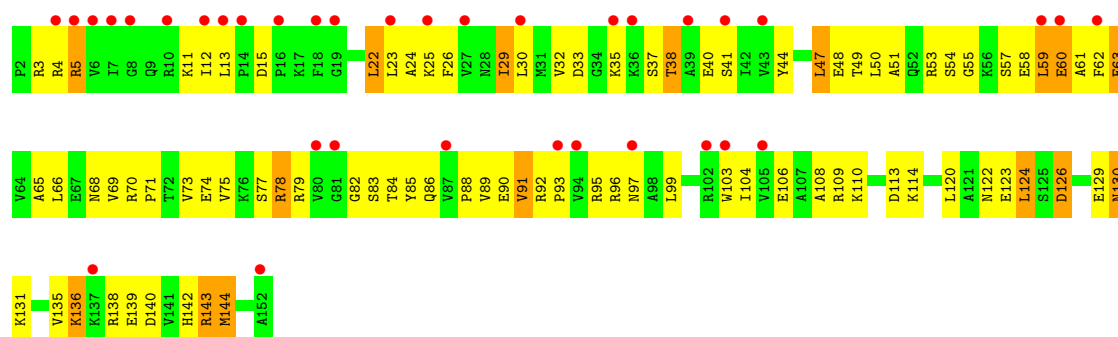
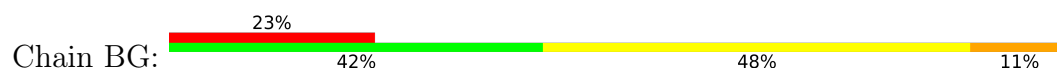




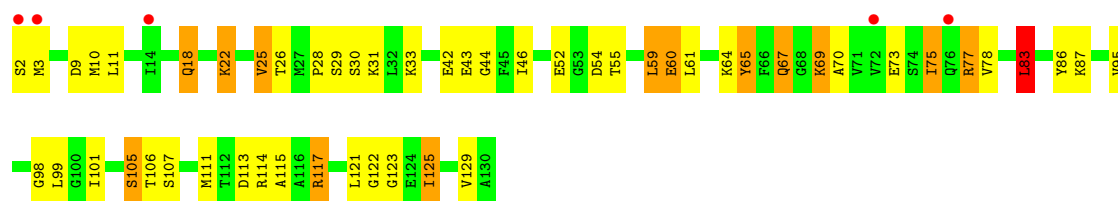
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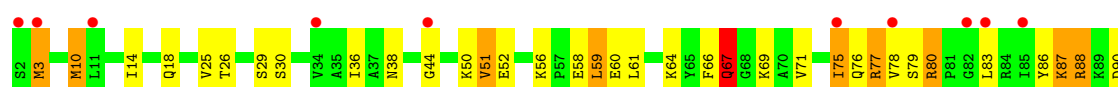
• Molecule 11: 30S ribosomal protein S7



• Molecule 12: 30S ribosomal protein S8

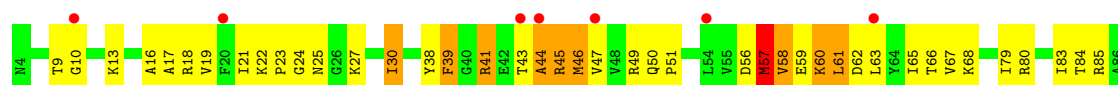


• Molecule 12: 30S ribosomal protein S8

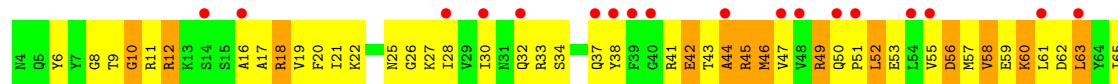




• Molecule 13: 30S ribosomal protein S9



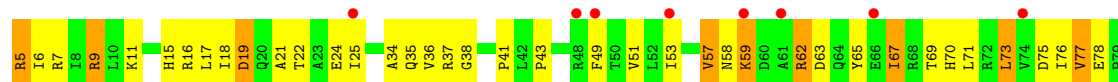
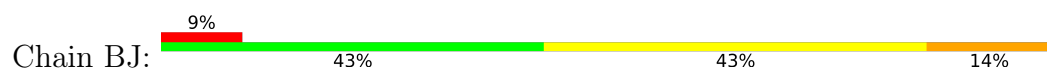
• Molecule 13: 30S ribosomal protein S9



• Molecule 14: 30S ribosomal protein S10

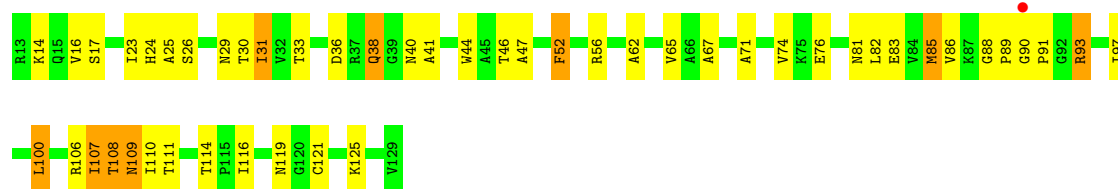


• Molecule 14: 30S ribosomal protein S10

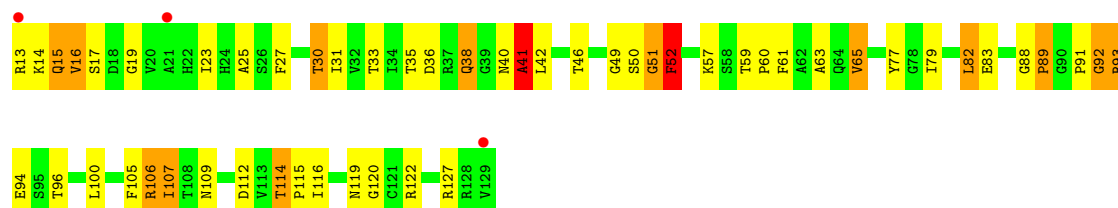


• Molecule 15: 30S ribosomal protein S11

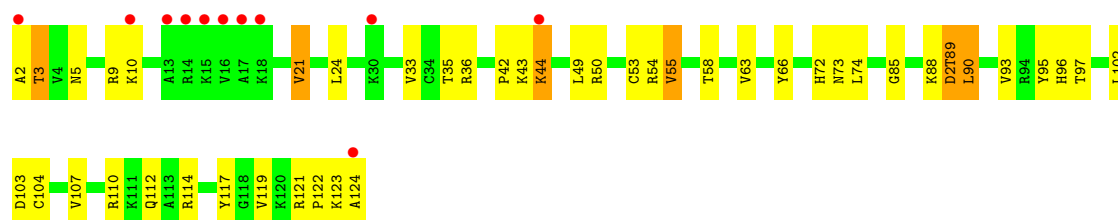




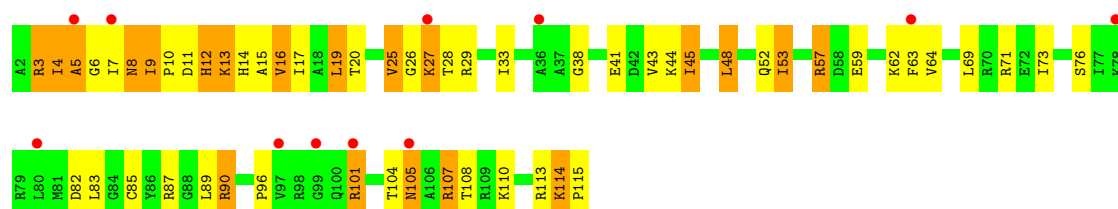
• Molecule 15: 30S ribosomal protein S11



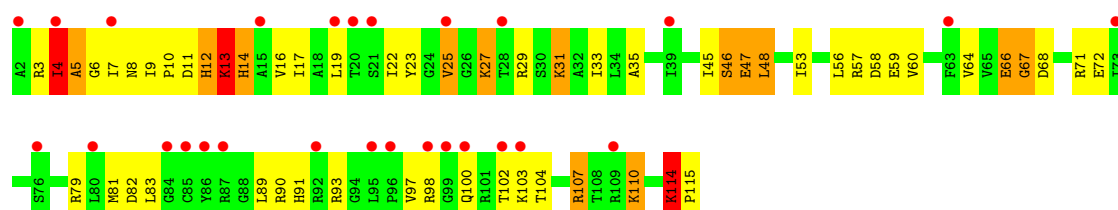
• Molecule 16: 30S ribosomal protein S12



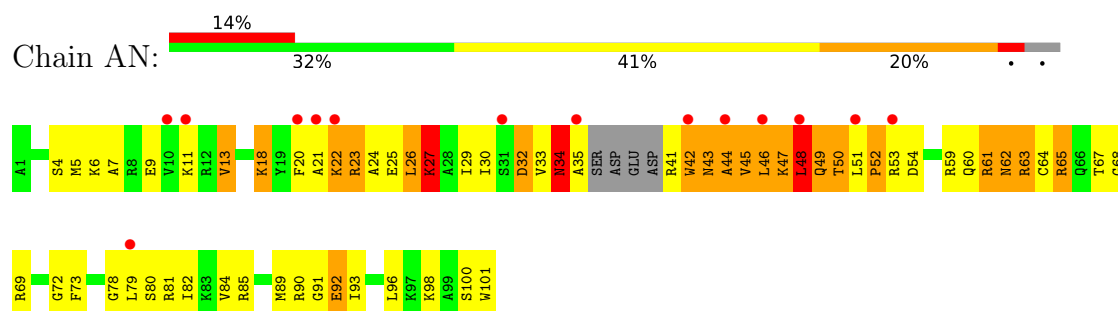
• Molecule 17: 30S ribosomal protein S13



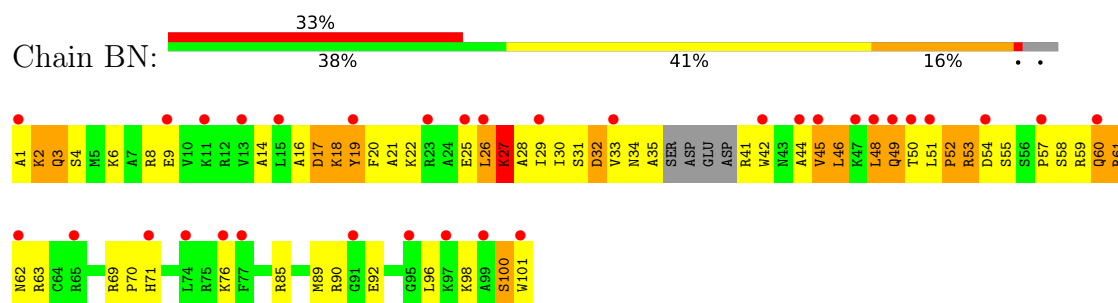
• Molecule 17: 30S ribosomal protein S13



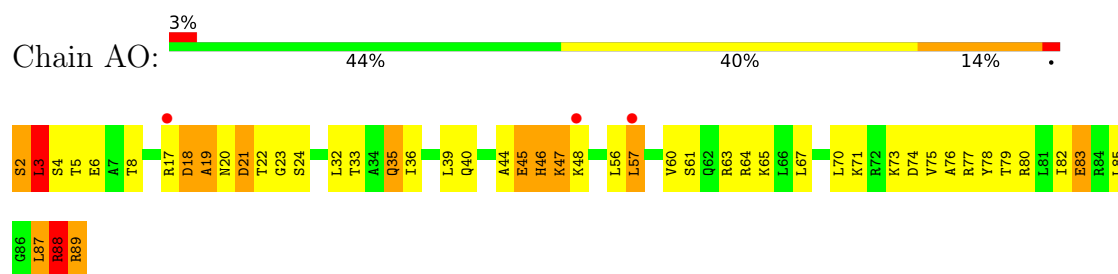
- Molecule 18: 30S ribosomal protein S14



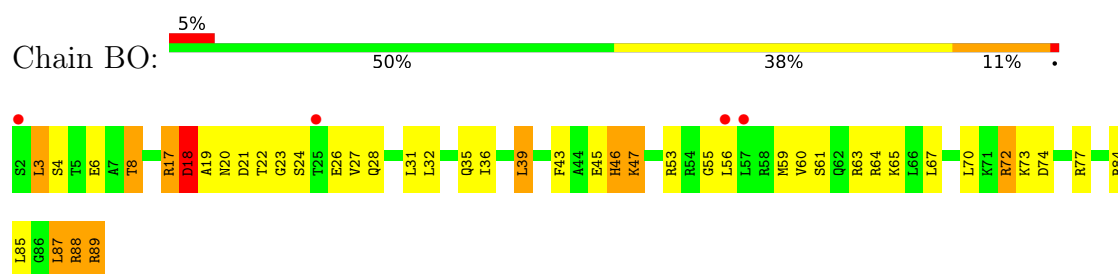
- Molecule 18: 30S ribosomal protein S14



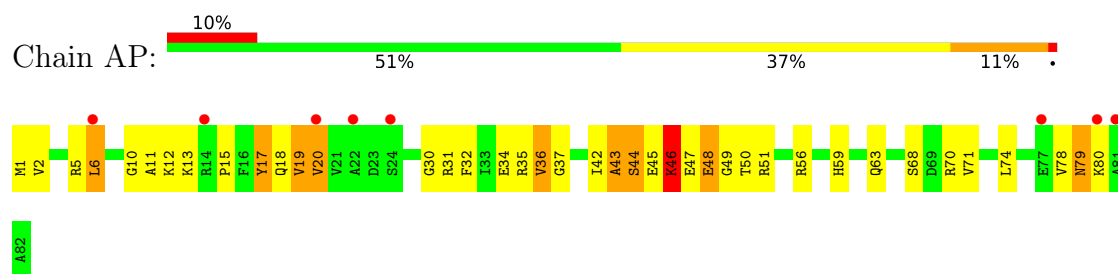
- Molecule 19: 30S ribosomal protein S15



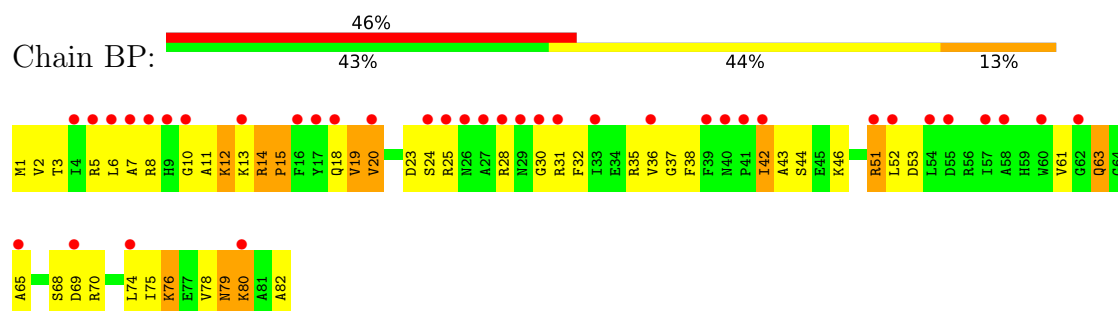
- Molecule 19: 30S ribosomal protein S15



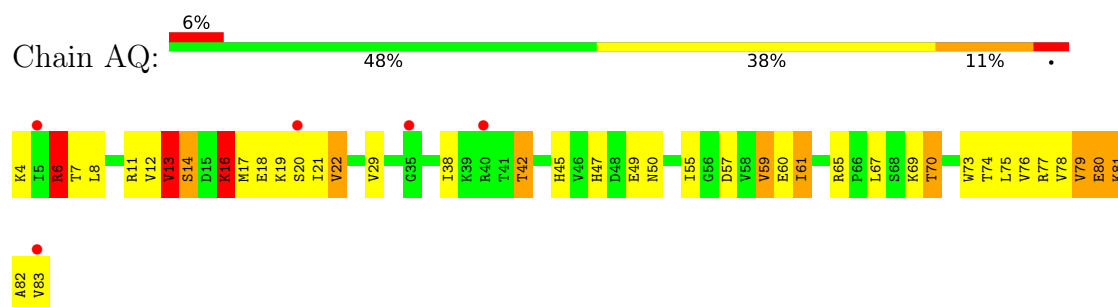
- Molecule 20: 30S ribosomal protein S16



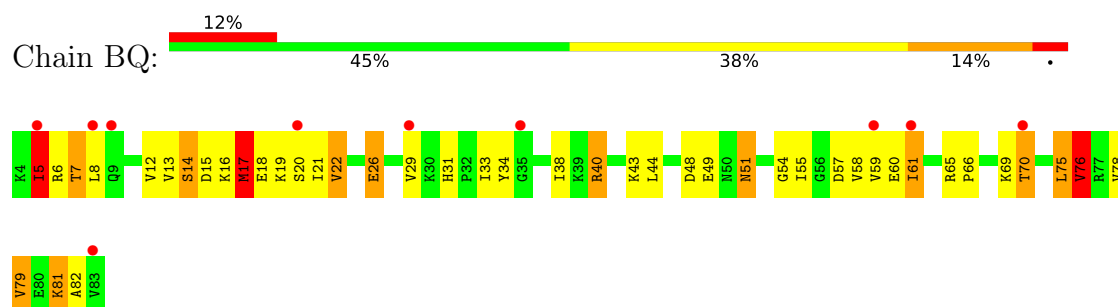
- Molecule 20: 30S ribosomal protein S16



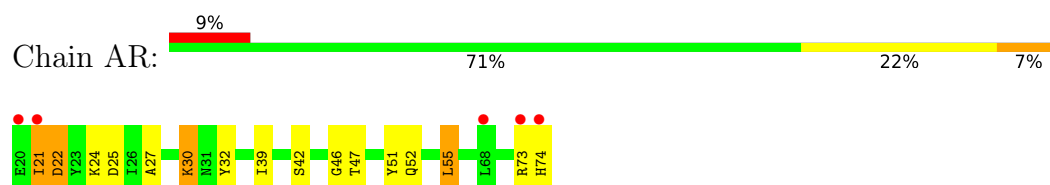
- Molecule 21: 30S ribosomal protein S17



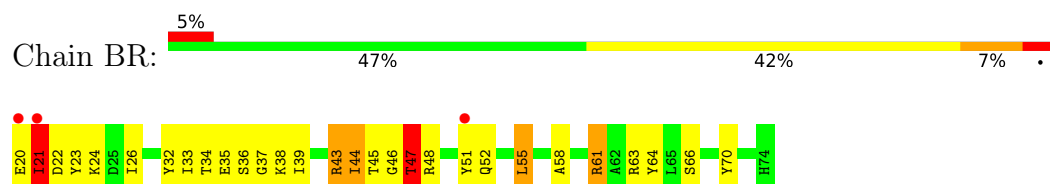
- Molecule 21: 30S ribosomal protein S17



- Molecule 22: 30S ribosomal protein S18



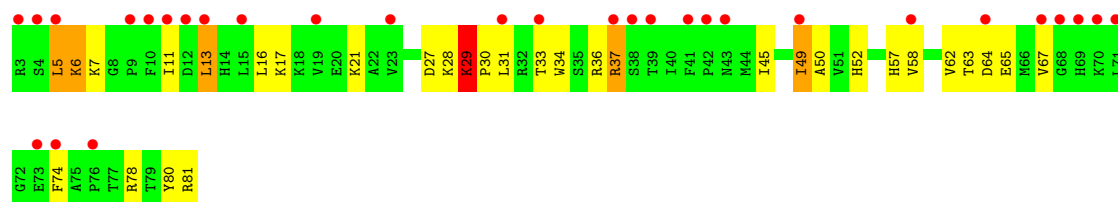
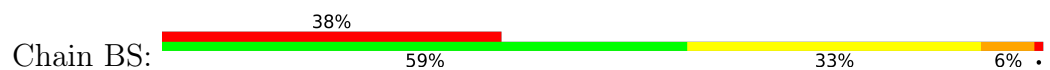
- Molecule 22: 30S ribosomal protein S18



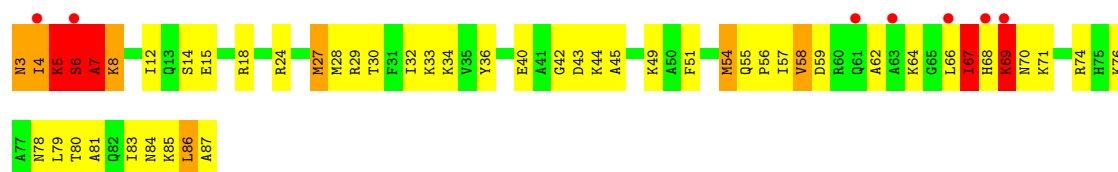
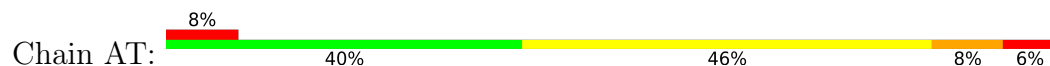
- Molecule 23: 30S ribosomal protein S19



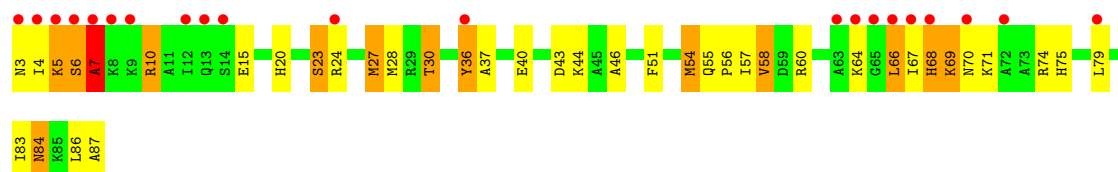
• Molecule 23: 30S ribosomal protein S19



• Molecule 24: 30S ribosomal protein S20



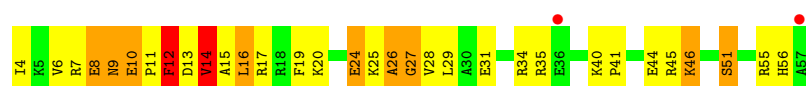
• Molecule 24: 30S ribosomal protein S20



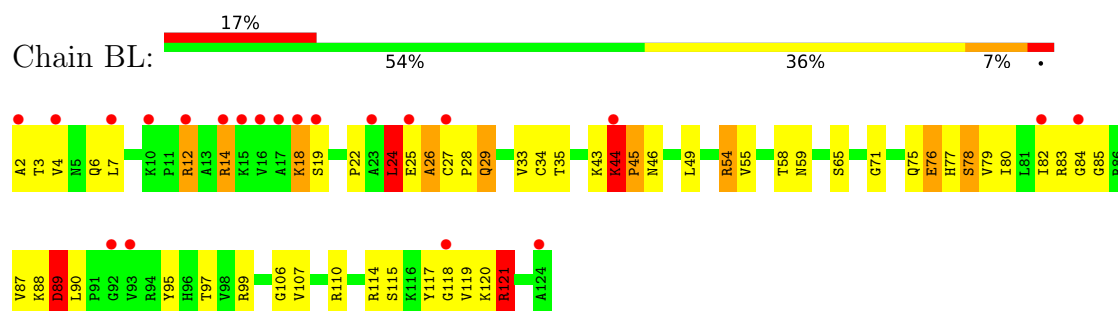
• Molecule 25: 30S ribosomal protein S21



• Molecule 25: 30S ribosomal protein S21



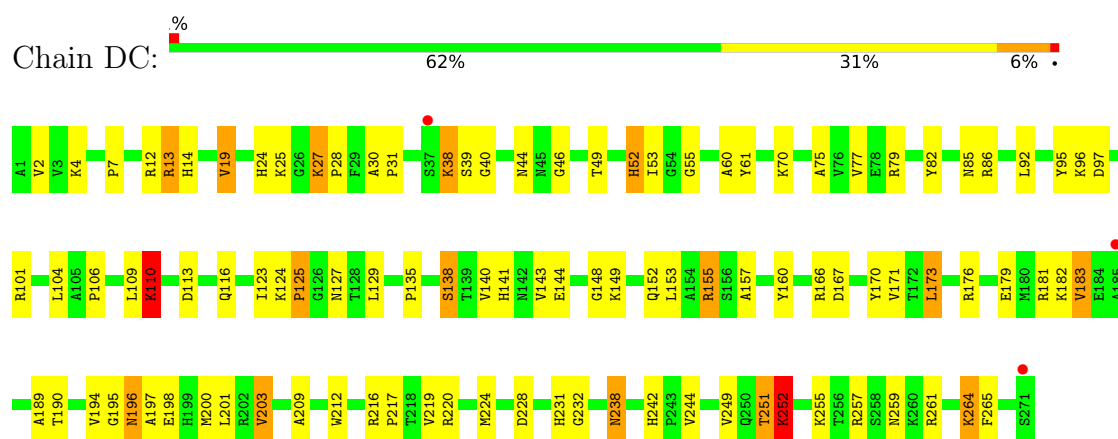
- Molecule 26: 30S ribosomal protein S12



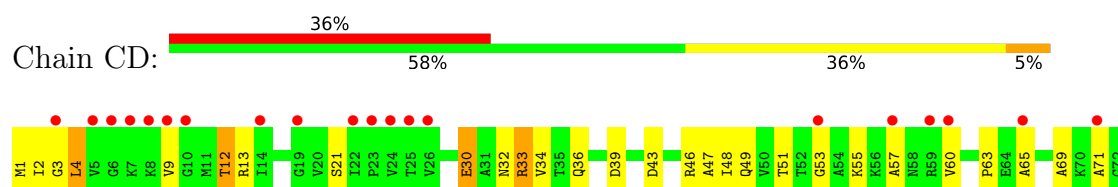
- Molecule 27: 50S ribosomal protein L2

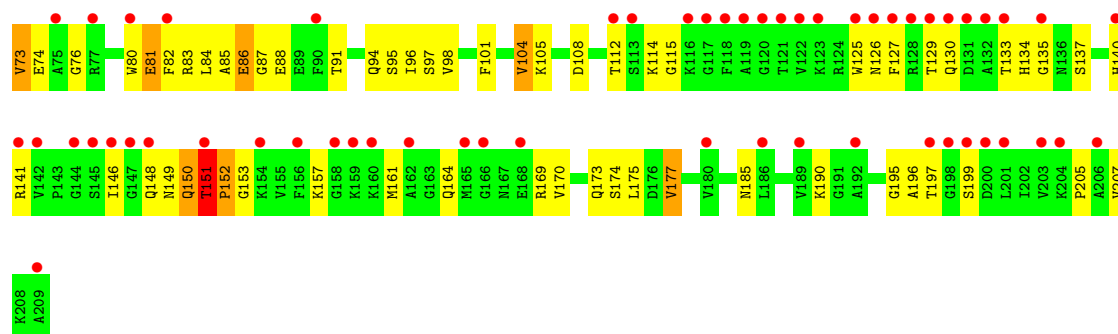


- Molecule 27: 50S ribosomal protein L2

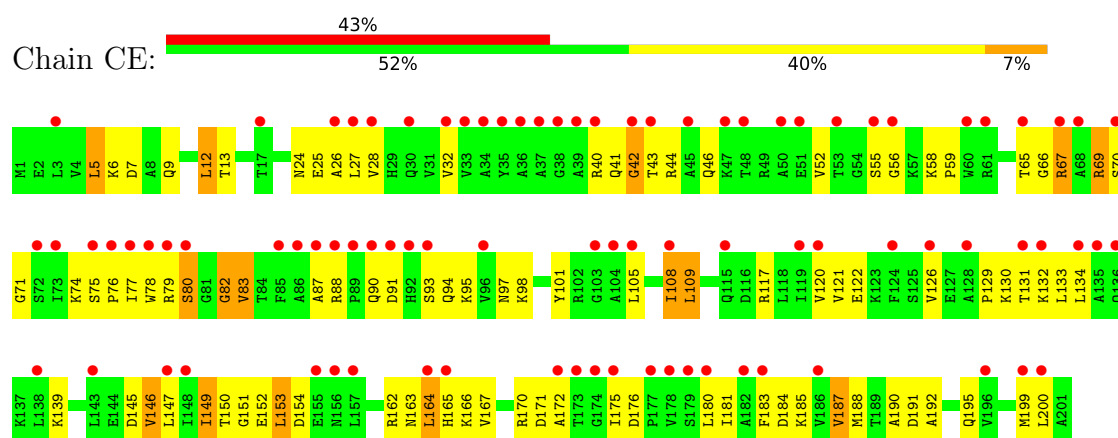


- Molecule 28: 50S ribosomal protein L3

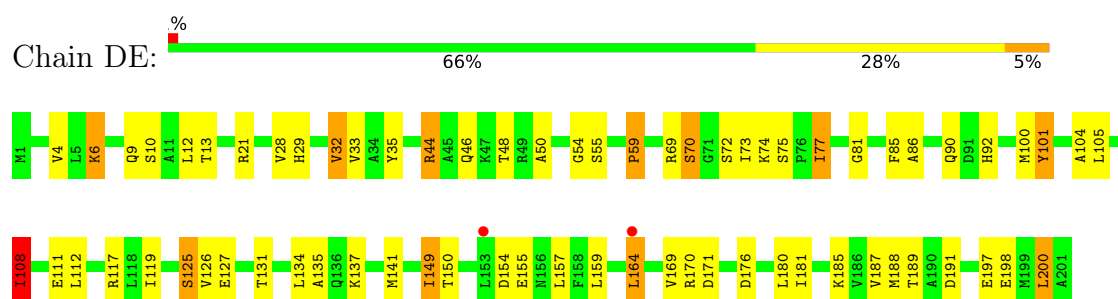




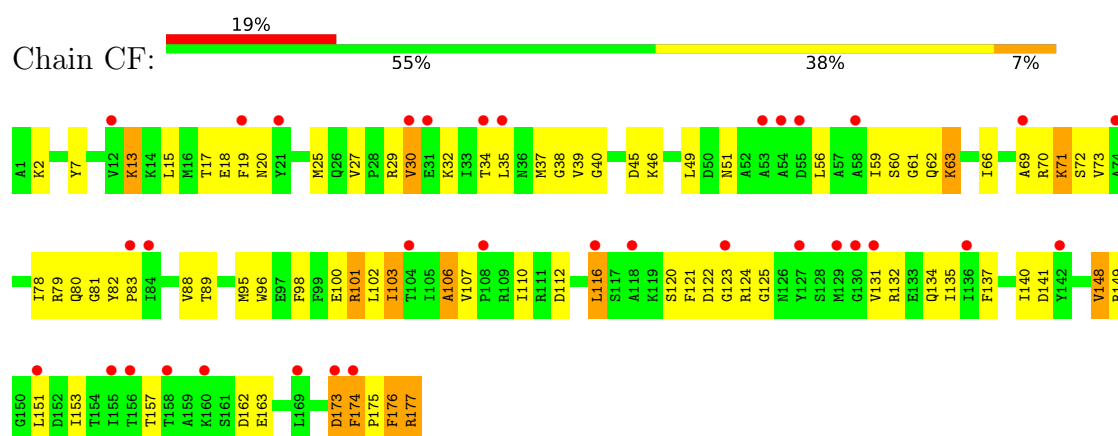
• Molecule 29: 50S ribosomal protein L4



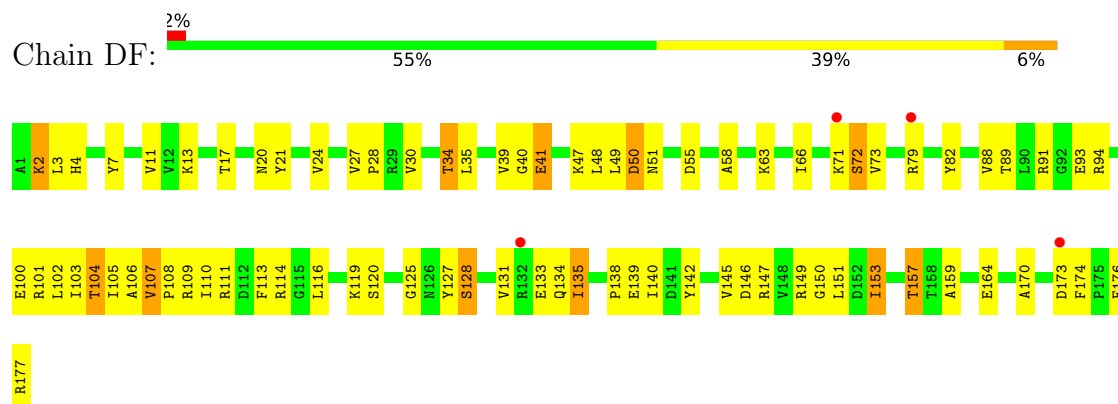
• Molecule 29: 50S ribosomal protein L4



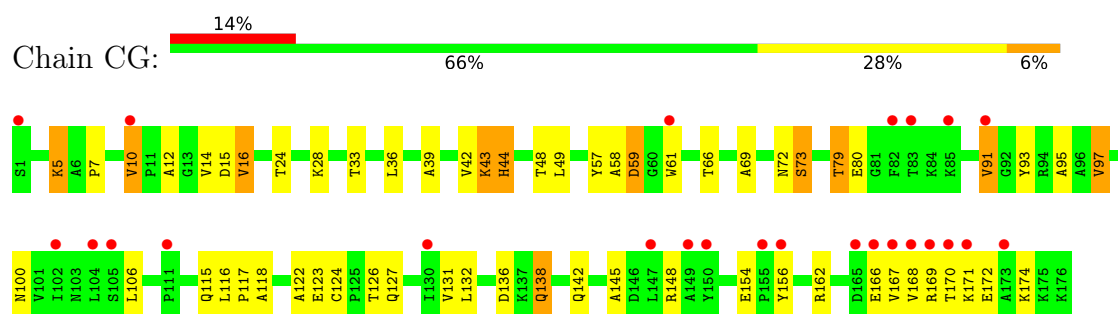
• Molecule 30: 50S ribosomal protein L5



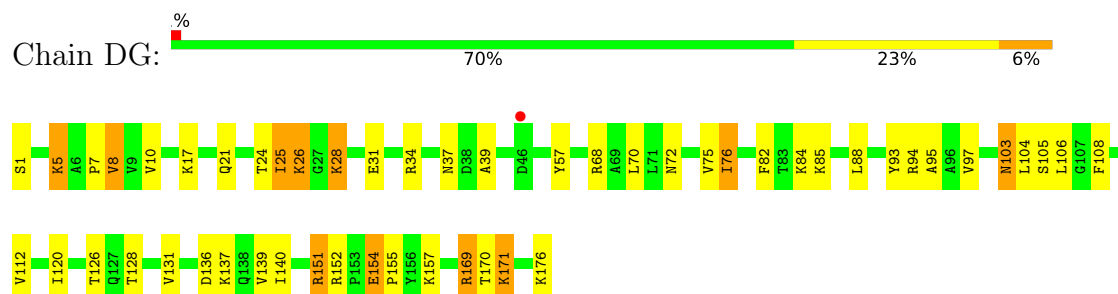
• Molecule 30: 50S ribosomal protein L5



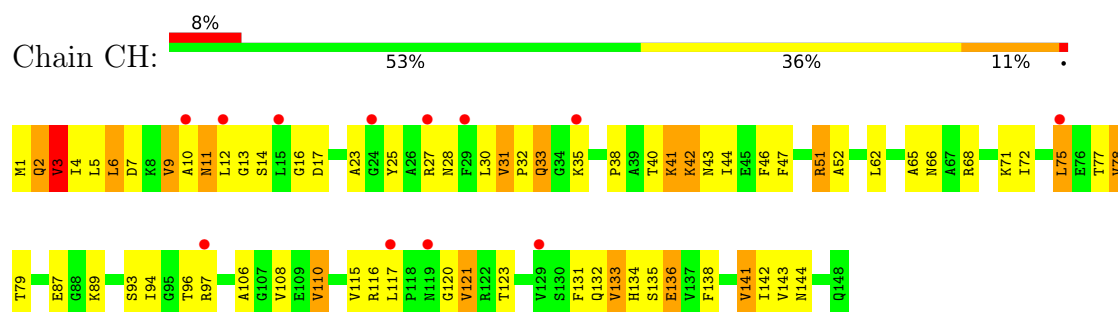
• Molecule 31: 50S ribosomal protein L6



• Molecule 31: 50S ribosomal protein L6

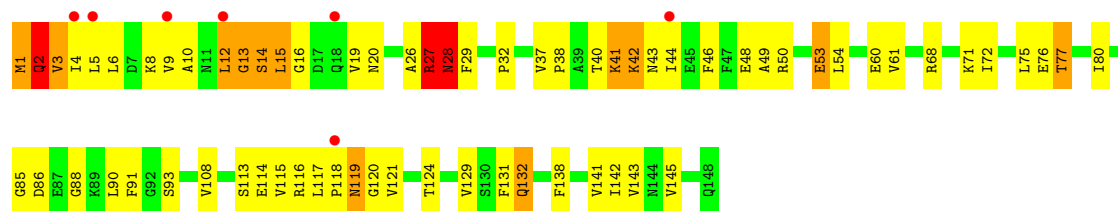


• Molecule 32: 50S ribosomal protein L9

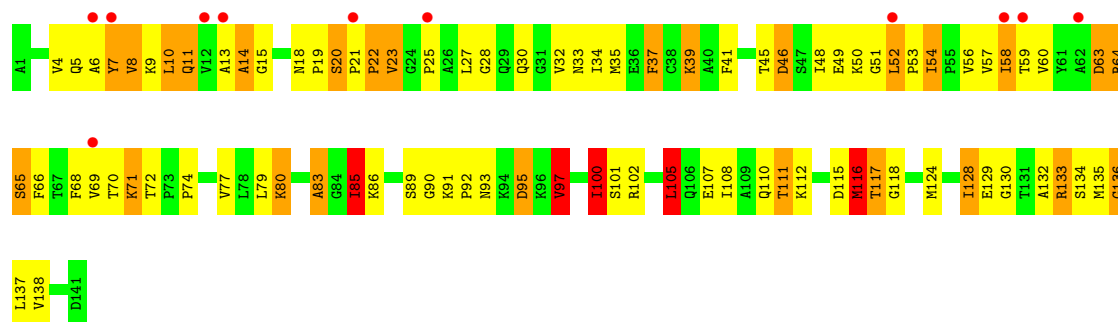


• Molecule 32: 50S ribosomal protein L9

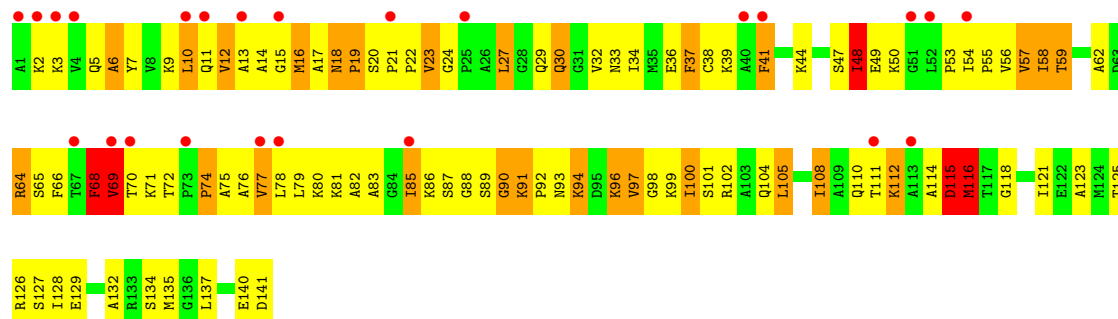




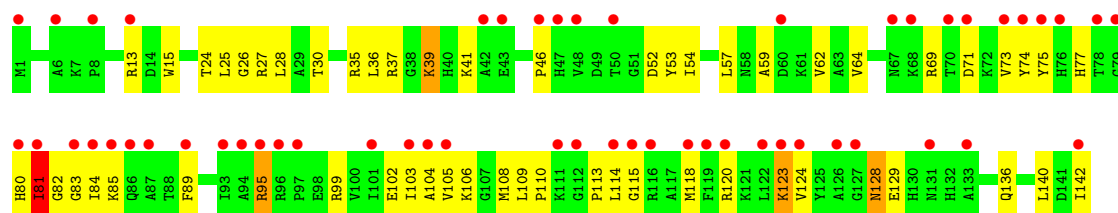
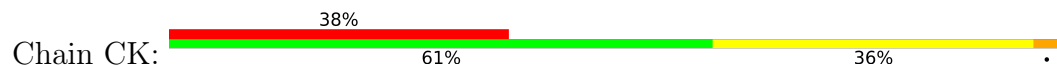
• Molecule 33: 50S ribosomal protein L11



• Molecule 33: 50S ribosomal protein L11

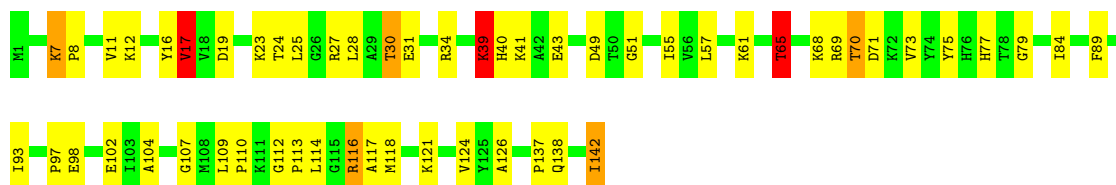


• Molecule 34: 50S ribosomal protein L13

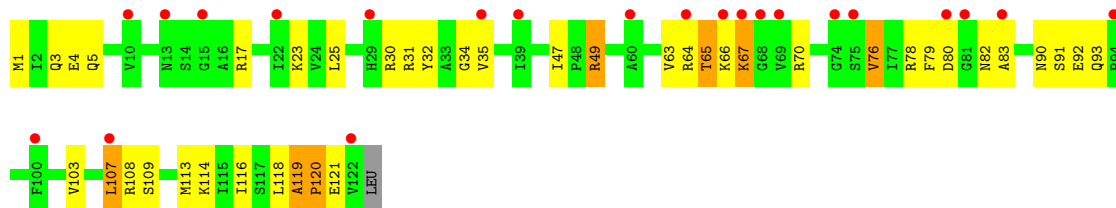


• Molecule 34: 50S ribosomal protein L13

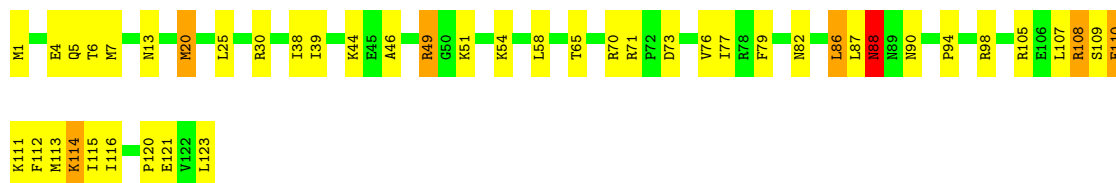




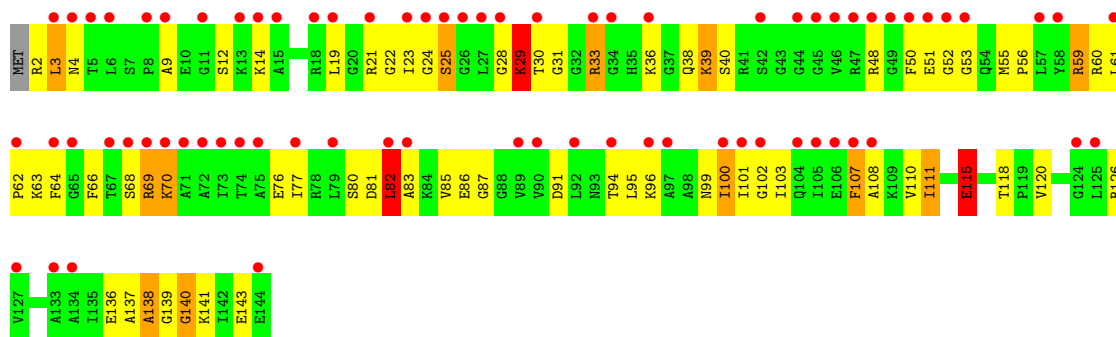
• Molecule 35: 50S ribosomal protein L14



• Molecule 35: 50S ribosomal protein L14

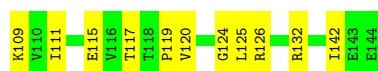


• Molecule 36: 50S ribosomal protein L15



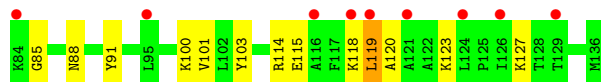
• Molecule 36: 50S ribosomal protein L15





• Molecule 37: 50S ribosomal protein L16

Chain CN: 15% 71% 25% .



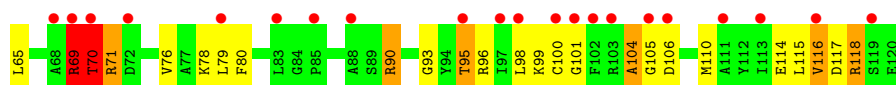
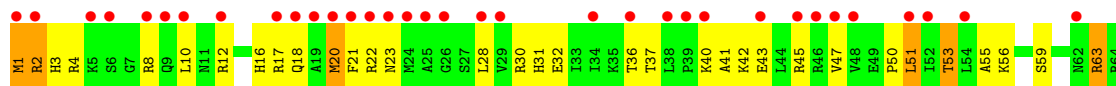
• Molecule 37: 50S ribosomal protein L16

Chain DN: 63% 32% .



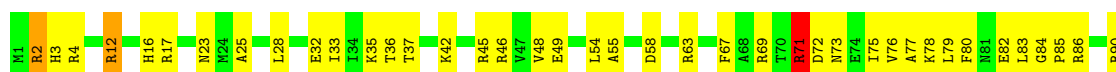
• Molecule 38: 50S ribosomal protein L17

Chain CO: 46% 52% 37% 10% .



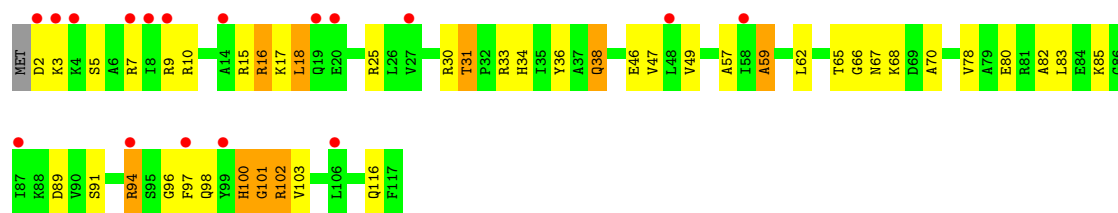
• Molecule 38: 50S ribosomal protein L17

Chain DO: 52% 41% 5% .

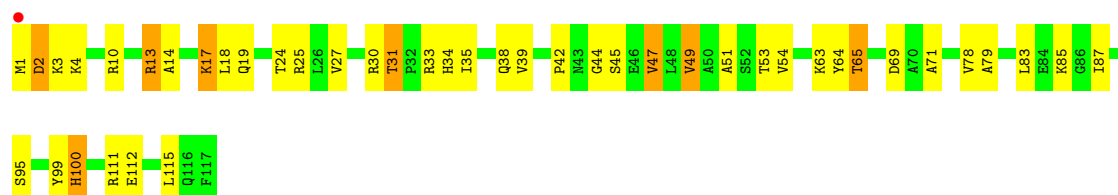


• Molecule 39: 50S ribosomal protein L18

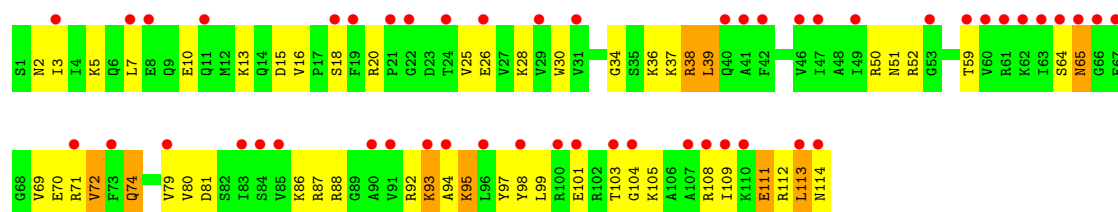
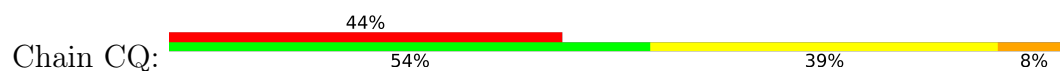
Chain CP: 15% 62% 30% 8% .



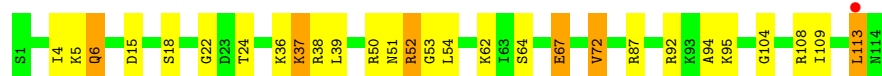
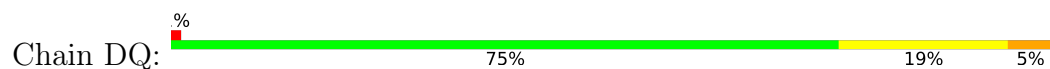
• Molecule 39: 50S ribosomal protein L18



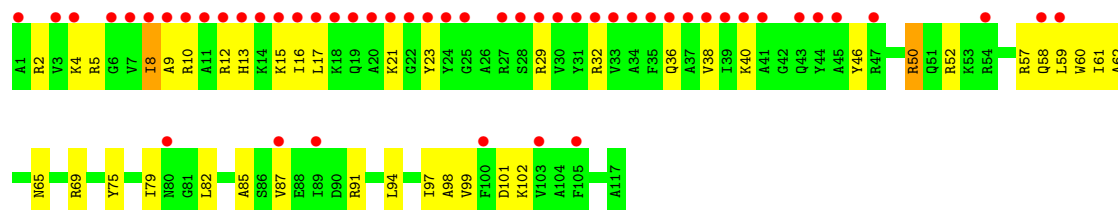
• Molecule 40: 50S ribosomal protein L19



• Molecule 40: 50S ribosomal protein L19

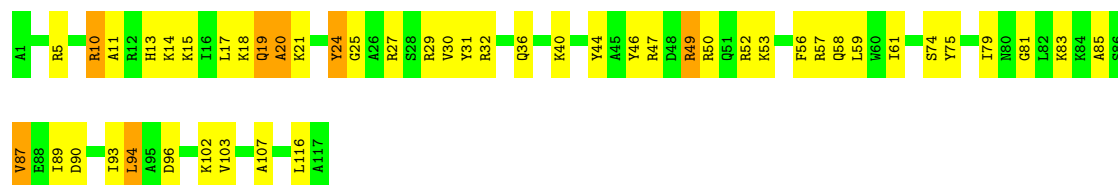


• Molecule 41: 50S ribosomal protein L20

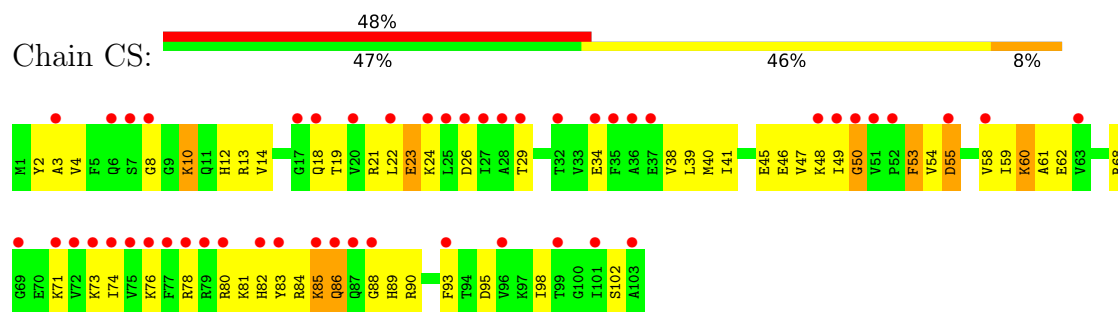


• Molecule 41: 50S ribosomal protein L20

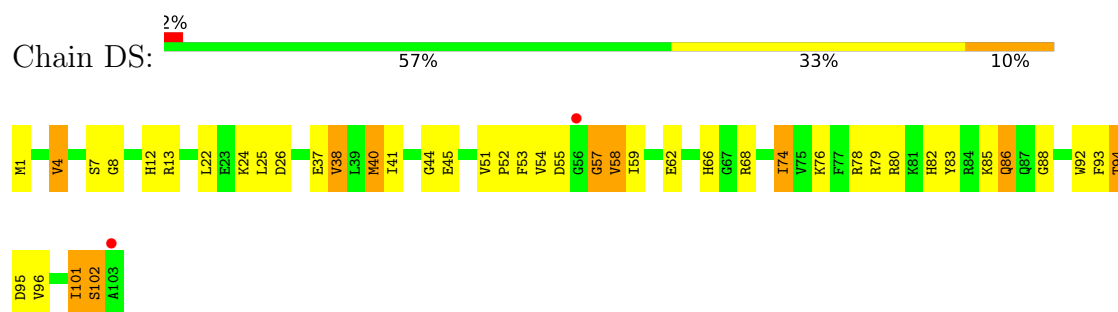




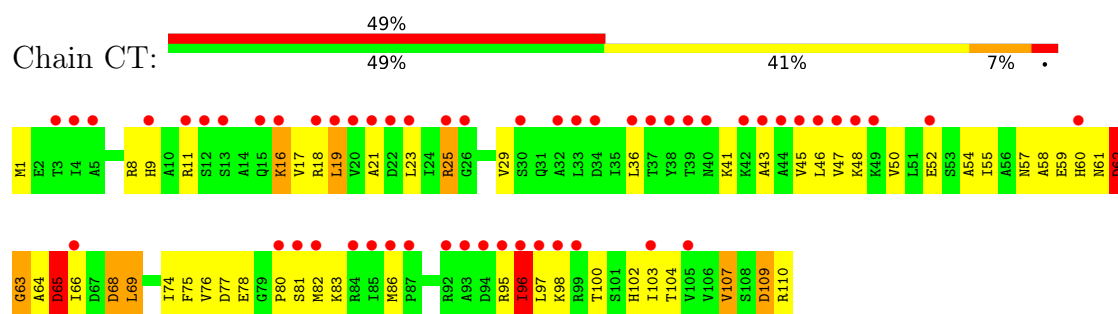
• Molecule 42: 50S ribosomal protein L21



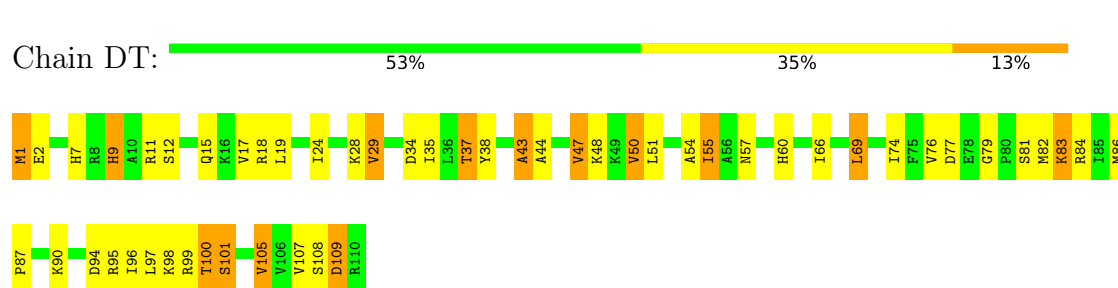
• Molecule 42: 50S ribosomal protein L21



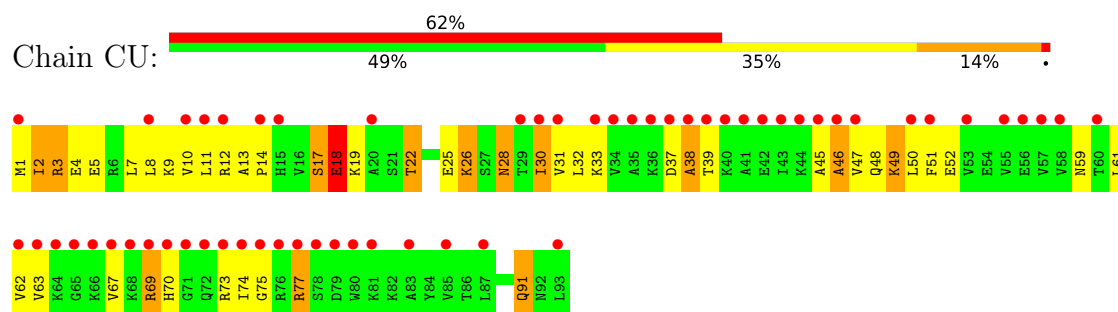
• Molecule 43: 50S ribosomal protein L22



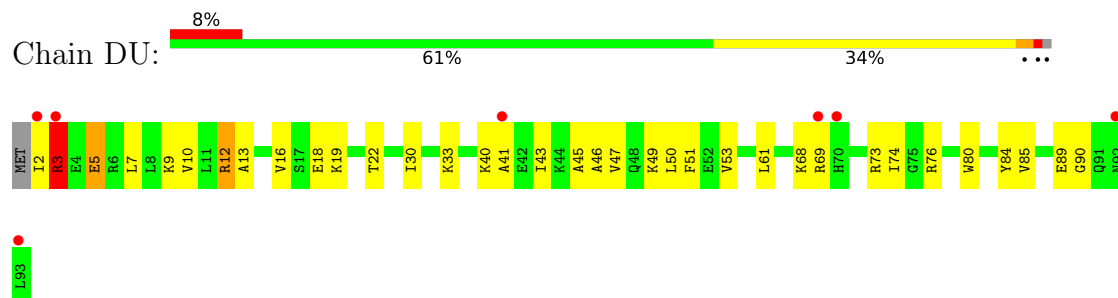
• Molecule 43: 50S ribosomal protein L22



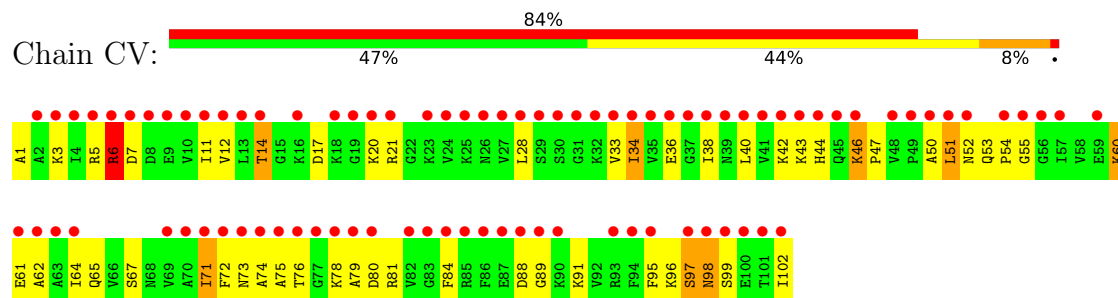
• Molecule 44: 50S ribosomal protein L23



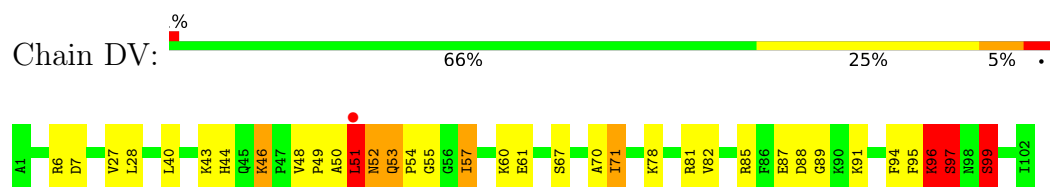
- Molecule 44: 50S ribosomal protein L23



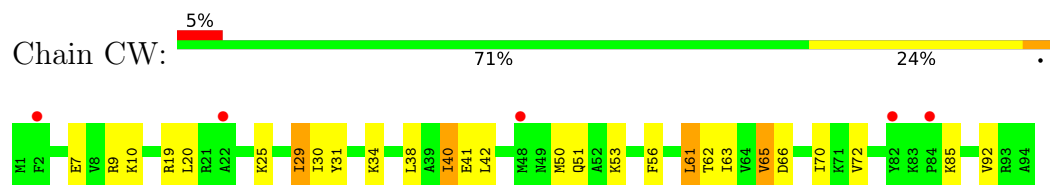
- Molecule 45: 50S ribosomal protein L24



- Molecule 45: 50S ribosomal protein L24

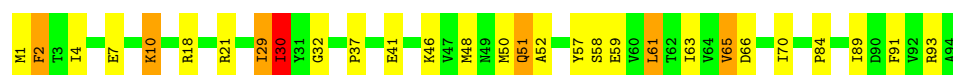


- Molecule 46: 50S ribosomal protein L25

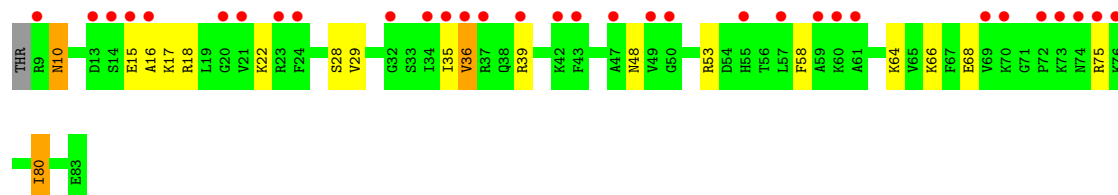
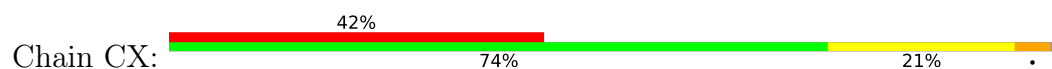


- Molecule 46: 50S ribosomal protein L25

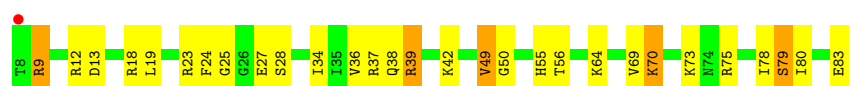




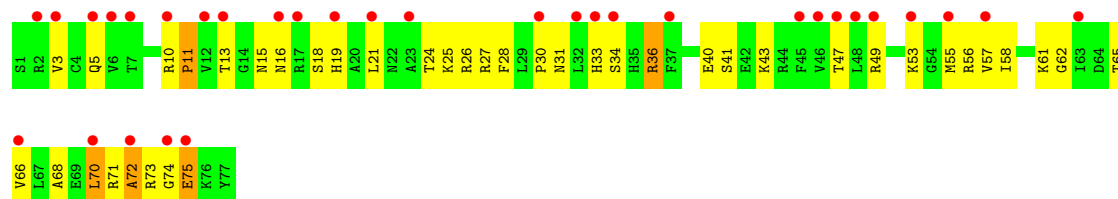
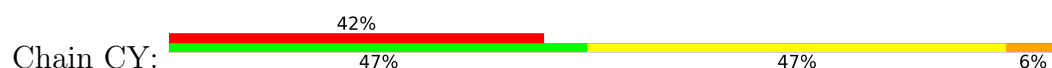
- Molecule 47: 50S ribosomal protein L27



- Molecule 47: 50S ribosomal protein L27



- Molecule 48: 50S ribosomal protein L28



- Molecule 48: 50S ribosomal protein L28



- Molecule 49: 50S ribosomal protein L29



- Molecule 49: 50S ribosomal protein L29





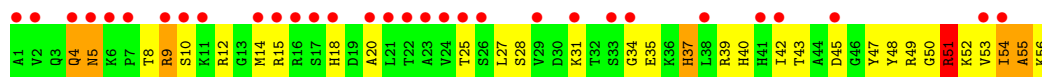
- Molecule 50: 50S ribosomal protein L30



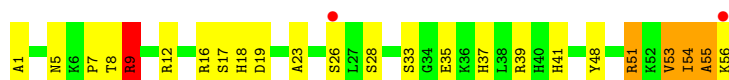
- Molecule 50: 50S ribosomal protein L30



- Molecule 51: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L32



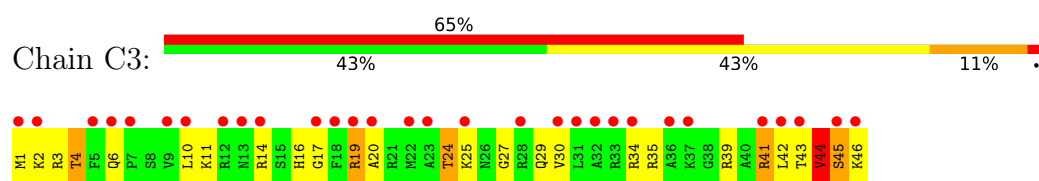
- Molecule 52: 50S ribosomal protein L33



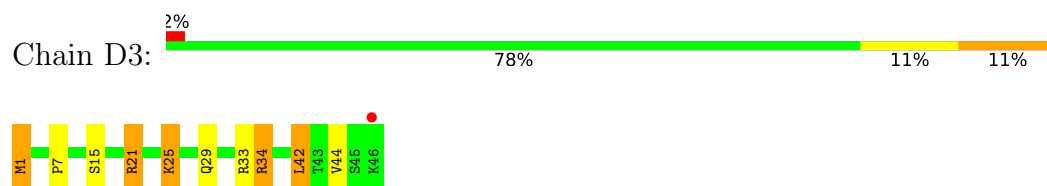
- Molecule 52: 50S ribosomal protein L33



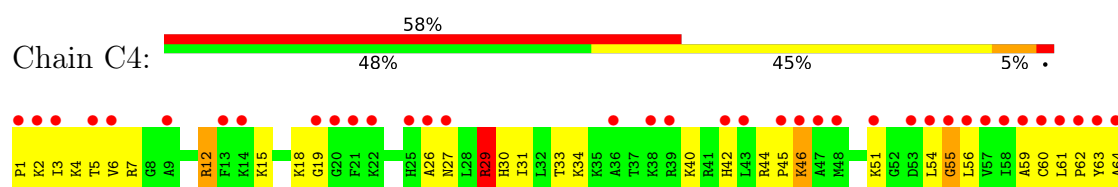
- Molecule 53: 50S ribosomal protein L34



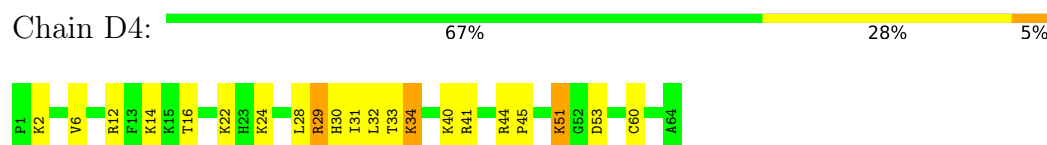
- Molecule 53: 50S ribosomal protein L34



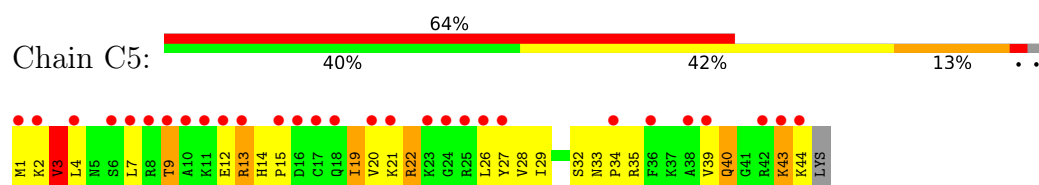
- Molecule 54: 50S ribosomal protein L35



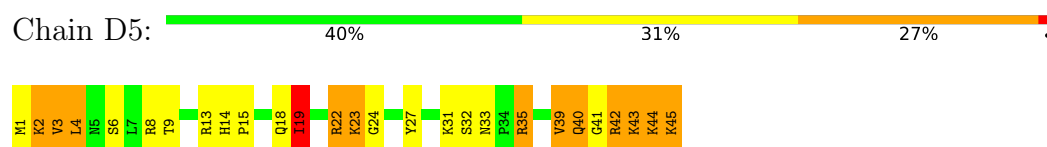
- Molecule 54: 50S ribosomal protein L35



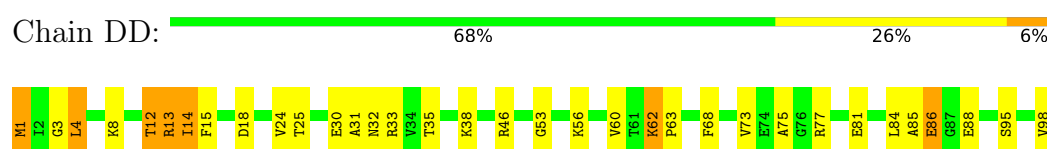
- Molecule 55: 50S ribosomal protein L36 2



- Molecule 55: 50S ribosomal protein L36 2

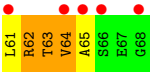


- Molecule 56: 50S ribosomal protein L3





● Molecule 57: 50S ribosomal protein L31 type B



4 Data and refinement statistics

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 – 2.90	Depositor EDS
% Data completeness (in resolution range)	85.2 (69.32-2.90) 85.2 (69.32-2.90)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.186 , 0.255 0.186 , 0.254	Depositor DCC
R_{free} test set	5389 reflections (0.43%)	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)	0.30 , 107.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MEQ, MG, 4OC, PEG, D2T, PSU, SPD, 1MG, H2U, EDO, MA6, PUT, PGE, 2MA, 2MG, 3TD, OMC, 1PE, GUN, 5MC, 6MZ, OMU, UR3, G7M, MPD, PG4, OMG, 5MU, 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	0.60	0/36568	0.86	21/57042 (0.0%)
2	BA	0.51	0/36834	0.75	5/57462 (0.0%)
3	DA	0.96	14/69150 (0.0%)	1.10	121/107874 (0.1%)
4	CA	0.43	0/69681	0.65	1/108706 (0.0%)
5	CB	0.30	0/2828	0.48	0/4410
5	DB	0.89	0/2850	1.08	6/4444 (0.1%)
6	AB	0.69	0/1736	1.37	12/2338 (0.5%)
6	BB	0.62	0/1736	1.30	10/2338 (0.4%)
7	AC	0.65	0/1652	1.09	3/2225 (0.1%)
7	BC	0.58	0/1652	1.12	5/2225 (0.2%)
8	AD	0.60	0/1665	1.06	2/2227 (0.1%)
8	BD	0.71	0/1665	1.14	3/2227 (0.1%)
9	AE	0.76	0/1119	1.36	8/1504 (0.5%)
9	BE	0.73	0/1119	1.32	6/1504 (0.4%)
10	AF	0.69	0/836	1.15	4/1128 (0.4%)
10	BF	0.67	0/836	1.27	8/1128 (0.7%)
11	AG	0.51	0/1196	1.00	1/1602 (0.1%)
11	BG	0.50	0/1196	1.13	1/1602 (0.1%)
12	AH	0.68	0/989	1.18	6/1326 (0.5%)
12	BH	0.60	0/989	1.12	1/1326 (0.1%)
13	AI	0.57	0/1034	1.15	2/1375 (0.1%)
13	BI	0.53	0/1034	1.20	3/1375 (0.2%)
14	AJ	0.73	0/797	1.24	5/1077 (0.5%)
14	BJ	0.76	0/797	1.12	1/1077 (0.1%)
15	AK	0.54	0/893	1.07	0/1205
15	BK	0.62	0/893	1.27	7/1205 (0.6%)
16	AL	0.74	0/960	1.13	1/1286 (0.1%)
17	AM	0.57	0/893	1.13	1/1193 (0.1%)
17	BM	0.47	0/893	1.18	5/1193 (0.4%)
18	AN	0.68	0/785	1.24	3/1043 (0.3%)
18	BN	0.49	0/785	1.08	1/1043 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	AO	0.67	0/724	1.15	4/966 (0.4%)
19	BO	0.61	0/724	1.11	0/966
20	AP	0.65	0/659	1.17	0/884
20	BP	0.66	0/659	1.22	1/884 (0.1%)
21	AQ	0.66	0/658	1.17	1/881 (0.1%)
21	BQ	0.58	0/658	1.09	1/881 (0.1%)
22	AR	0.61	0/463	1.10	0/621
22	BR	0.71	0/463	1.16	0/621
23	AS	0.70	0/653	1.11	0/877
23	BS	0.44	0/653	1.12	0/877
24	AT	0.72	0/671	1.16	3/888 (0.3%)
24	BT	0.57	0/671	1.15	2/888 (0.2%)
25	AU	0.64	0/457	1.27	6/606 (1.0%)
25	BU	0.75	0/457	1.53	8/606 (1.3%)
26	BL	0.72	0/969	1.28	4/1300 (0.3%)
27	CC	0.65	0/2122	1.17	6/2852 (0.2%)
27	DC	1.03	1/2122 (0.0%)	1.29	6/2852 (0.2%)
28	CD	0.51	0/1586	1.02	0/2134
29	CE	0.46	0/1571	1.08	3/2113 (0.1%)
29	DE	0.99	1/1571 (0.1%)	1.26	3/2113 (0.1%)
30	CF	0.47	0/1435	1.12	2/1926 (0.1%)
30	DF	0.80	0/1435	1.19	2/1926 (0.1%)
31	CG	0.36	0/1343	0.77	0/1816
31	DG	0.81	0/1343	1.11	2/1816 (0.1%)
32	CH	0.50	0/1113	0.93	0/1504
32	DH	0.50	0/1113	1.06	6/1504 (0.4%)
33	CJ	0.46	0/1046	1.17	8/1410 (0.6%)
33	DJ	0.52	0/1046	1.25	10/1410 (0.7%)
34	CK	0.60	1/1152 (0.1%)	0.90	1/1551 (0.1%)
34	DK	1.31	2/1152 (0.2%)	1.40	5/1551 (0.3%)
35	CL	0.57	0/947	1.00	0/1268
35	DL	1.03	0/955	1.29	4/1279 (0.3%)
36	CM	0.50	0/1054	1.15	4/1403 (0.3%)
36	DM	1.05	0/1062	1.28	2/1413 (0.1%)
37	CN	0.52	0/1093	0.99	0/1460
37	DN	1.08	0/1104	1.33	5/1474 (0.3%)
38	CO	0.54	0/974	1.12	3/1301 (0.2%)
38	DO	1.17	1/974 (0.1%)	1.52	7/1301 (0.5%)
39	CP	0.47	0/902	1.06	0/1209
39	DP	0.94	0/910	1.27	3/1219 (0.2%)
40	CQ	0.52	0/929	1.07	2/1242 (0.2%)
40	DQ	0.94	0/929	1.18	0/1242
41	CR	0.51	0/960	1.05	1/1278 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
41	DR	1.25	0/960	1.55	8/1278 (0.6%)
42	CS	0.45	0/829	1.08	1/1107 (0.1%)
42	DS	1.20	1/829 (0.1%)	1.37	3/1107 (0.3%)
43	CT	0.49	0/864	1.05	4/1156 (0.3%)
43	DT	1.21	0/864	1.52	1/1156 (0.1%)
44	CU	0.47	0/745	1.07	1/994 (0.1%)
44	DU	0.94	0/737	1.16	0/984
45	CV	0.42	0/788	1.18	1/1051 (0.1%)
45	DV	0.99	0/788	1.35	10/1051 (1.0%)
46	CW	0.37	0/766	0.85	0/1025
46	DW	1.01	0/766	1.36	2/1025 (0.2%)
47	CX	0.52	0/576	0.96	0/762
47	DX	1.15	2/602 (0.3%)	1.37	0/795
48	CY	0.60	0/635	1.13	1/848 (0.1%)
48	DY	0.91	0/635	1.13	0/848
49	CZ	0.40	0/502	1.03	0/667
49	DZ	0.81	0/502	1.30	2/667 (0.3%)
50	C0	0.51	0/453	1.02	0/605
50	D0	1.25	0/460	1.44	1/615 (0.2%)
51	C1	0.51	0/450	1.05	1/599 (0.2%)
51	D1	1.11	0/450	1.59	3/599 (0.5%)
52	C2	0.47	0/416	0.95	0/554
52	D2	0.91	0/421	1.21	0/561
53	C3	0.68	0/380	1.16	1/498 (0.2%)
53	D3	1.10	0/380	1.40	1/498 (0.2%)
54	C4	0.59	0/513	1.16	1/676 (0.1%)
54	D4	1.04	0/513	1.32	2/676 (0.3%)
55	C5	0.49	0/363	0.62	0/479
55	D5	1.07	0/372	1.17	0/490
56	DD	1.10	0/1576	1.34	2/2119 (0.1%)
57	D7	0.60	0/542	0.95	0/736
All	All	0.70	23/309220 (0.0%)	0.96	414/462249 (0.1%)

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 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	CK	136	GLN	C-O	11.23	1.29	1.23
3	DA	2886	A	P-OP1	10.24	1.69	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DA	2886	A	P-OP2	8.61	1.66	1.49
3	DA	2884	U	O3'-P	7.05	1.71	1.61
3	DA	2098	U	C4-O4	6.54	1.36	1.23

The worst 5 of 414 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	DC	27	LYS	CA-C-N	11.27	133.93	119.84
27	DC	27	LYS	C-N-CA	11.27	133.93	119.84
46	DW	18	ARG	CA-CB-CG	10.00	134.11	114.10
49	DZ	45	GLN	N-CA-C	-9.68	94.90	110.20
9	AE	44	GLY	N-CA-C	-9.66	99.29	112.52

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	1169	1
2	BA	32895	16553	16553	1228	0
3	DA	62254	31129	31238	2190	1
4	CA	62215	31288	31289	2251	0
5	CB	2529	1281	1281	54	0
5	DB	2549	1291	1289	63	0
6	AB	1705	1726	1732	155	0
6	BB	1705	1726	1732	163	0
7	AC	1625	1692	1696	68	0
7	BC	1625	1692	1696	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AD	1643	1704	1707	90	0
8	BD	1643	1704	1707	70	0
9	AE	1106	1145	1148	86	0
9	BE	1106	1145	1148	105	0
10	AF	818	799	808	35	0
10	BF	818	799	808	46	0
11	AG	1182	1237	1238	54	0
11	BG	1182	1237	1238	62	0
12	AH	979	1031	1031	38	0
12	BH	979	1031	1031	43	0
13	AI	1022	1069	1070	56	0
13	BI	1022	1069	1070	73	0
14	AJ	787	825	828	85	0
14	BJ	787	825	828	29	0
15	AK	877	884	887	35	0
15	BK	877	884	887	53	0
16	AL	957	1009	1017	31	0
17	AM	884	938	941	53	0
17	BM	884	938	941	45	0
18	AN	774	823	827	70	0
18	BN	774	823	827	52	0
19	AO	716	734	739	40	0
19	BO	716	734	739	32	0
20	AP	649	661	666	29	0
20	BP	649	661	666	40	0
21	AQ	649	688	691	35	0
21	BQ	649	688	691	32	0
22	AR	456	477	478	10	0
22	BR	456	477	478	29	0
23	AS	638	657	665	30	0
23	BS	638	661	665	19	0
24	AT	665	711	714	41	0
24	BT	665	711	714	33	0
25	AU	451	473	474	16	0
25	BU	451	473	474	28	0
26	BL	955	1013	1016	47	0
27	CC	2083	2148	2157	96	0
27	DC	2083	2148	2157	77	0
28	CD	1565	1610	1616	74	0
29	CE	1552	1613	1619	77	0
29	DE	1552	1613	1619	45	0
30	CF	1411	1443	1447	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	DF	1411	1443	1447	63	0
31	CG	1323	1368	1374	31	0
31	DG	1323	1368	1374	32	0
32	CH	1102	1134	1139	43	1
32	DH	1102	1134	1139	51	0
33	CJ	1032	1085	1088	76	0
33	DJ	1032	1085	1088	89	0
34	CK	1129	1152	1162	38	0
34	DK	1129	1152	1162	41	0
35	CL	938	1008	1012	33	0
35	DL	946	1019	1023	38	0
36	CM	1045	1116	1117	77	0
36	DM	1053	1125	1129	43	0
37	CN	1074	1153	1157	28	0
37	DN	1082	1166	1170	46	0
38	CO	961	994	1000	57	0
38	DO	961	994	1000	48	0
39	CP	892	920	923	31	0
39	DP	900	929	935	40	0
40	CQ	917	960	965	39	0
40	DQ	917	960	965	25	0
41	CR	947	1018	1022	40	0
41	DR	947	1018	1022	49	0
42	CS	816	832	839	40	0
42	DS	816	832	839	38	0
43	CT	857	915	922	41	0
43	DT	857	915	922	38	0
44	CU	739	802	807	47	0
44	DU	731	794	795	24	0
45	CV	780	830	834	54	0
45	DV	780	830	834	22	0
46	CW	753	774	780	13	0
46	DW	753	774	780	22	0
47	CX	569	579	581	12	0
47	DX	591	606	604	19	0
48	CY	625	649	655	38	0
48	DY	625	649	655	16	0
49	CZ	501	530	531	23	0
49	DZ	501	530	531	23	0
50	C0	449	486	491	19	0
50	D0	449	486	484	14	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	16	0
52	D2	414	443	445	9	0
53	C3	377	414	418	27	0
53	D3	377	414	418	9	0
54	C4	504	568	574	32	0
54	D4	504	568	574	23	0
55	C5	359	395	397	17	0
55	D5	368	395	410	35	0
56	DD	1566	1612	1618	59	0
57	D7	530	177	517	104	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	1	0
60	DA	56	98	98	9	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	4	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	9	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	2	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	2	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	5	0
69	AT	5	0	0	2	0
69	AU	2	0	0	0	0
69	BA	389	0	0	122	0
69	BB	5	0	0	6	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	325	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	4	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	604	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	8	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	11	0
69	DU	10	0	0	5	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	10550	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 23.

The worst 5 of 10550 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

5.3.1 Protein backbone

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

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

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

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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%)	16	44
13	AI	125/127 (98%)	104 (83%)	17 (14%)	4 (3%)	3	13
13	BI	125/127 (98%)	96 (77%)	18 (14%)	11 (9%)	0	1
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	12
15	BK	115/117 (98%)	98 (85%)	10 (9%)	7 (6%)	1	4
16	AL	120/123 (98%)	109 (91%)	8 (7%)	3 (2%)	4	17
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	2
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	2
19	BO	86/88 (98%)	78 (91%)	1 (1%)	7 (8%)	1	1
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	3
21	AQ	78/80 (98%)	66 (85%)	7 (9%)	5 (6%)	1	3
21	BQ	78/80 (98%)	60 (77%)	12 (15%)	6 (8%)	1	2
22	AR	53/55 (96%)	49 (92%)	2 (4%)	2 (4%)	2	10
22	BR	53/55 (96%)	46 (87%)	4 (8%)	3 (6%)	1	4
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%)	0	1
24	BT	83/85 (98%)	75 (90%)	4 (5%)	4 (5%)	2	7
25	AU	52/54 (96%)	44 (85%)	5 (10%)	3 (6%)	1	4
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%)	5	20
27	DC	269/271 (99%)	251 (93%)	15 (6%)	3 (1%)	11	36
28	CD	207/209 (99%)	189 (91%)	12 (6%)	6 (3%)	3	15

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	DU	90/93 (97%)	82 (91%)	6 (7%)	2 (2%)	5	20
45	CV	100/102 (98%)	79 (79%)	15 (15%)	6 (6%)	1	4
45	DV	100/102 (98%)	91 (91%)	4 (4%)	5 (5%)	1	6
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%)	9	32
48	CY	75/77 (97%)	69 (92%)	3 (4%)	3 (4%)	2	9
48	DY	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
49	CZ	60/62 (97%)	51 (85%)	7 (12%)	2 (3%)	3	13
49	DZ	60/62 (97%)	55 (92%)	2 (3%)	3 (5%)	1	6
50	C0	56/58 (97%)	51 (91%)	3 (5%)	2 (4%)	2	11
50	D0	57/58 (98%)	56 (98%)	1 (2%)	0	100	100
51	C1	54/56 (96%)	41 (76%)	10 (18%)	3 (6%)	1	4
51	D1	54/56 (96%)	49 (91%)	3 (6%)	2 (4%)	2	11
52	C2	48/51 (94%)	41 (85%)	6 (12%)	1 (2%)	5	21
52	D2	49/51 (96%)	46 (94%)	2 (4%)	1 (2%)	6	22
53	C3	44/46 (96%)	40 (91%)	2 (4%)	2 (4%)	2	8
53	D3	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
54	C4	62/64 (97%)	56 (90%)	4 (6%)	2 (3%)	3	13
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%)	24	54
57	D7	66/68 (97%)	23 (35%)	22 (33%)	21 (32%)	0	0
All	All	11321/11536 (98%)	9810 (87%)	961 (8%)	550 (5%)	1	6

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 ⓘ

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%)	131 (73%)	49 (27%)	0	1
6	BB	180/180 (100%)	138 (77%)	42 (23%)	1	3
7	AC	170/170 (100%)	145 (85%)	25 (15%)	3	10
7	BC	170/170 (100%)	138 (81%)	32 (19%)	1	5
8	AD	172/172 (100%)	145 (84%)	27 (16%)	2	9
8	BD	172/172 (100%)	148 (86%)	24 (14%)	3	11
9	AE	113/113 (100%)	81 (72%)	32 (28%)	0	1
9	BE	113/113 (100%)	88 (78%)	25 (22%)	1	3
10	AF	87/87 (100%)	73 (84%)	14 (16%)	2	8
10	BF	87/87 (100%)	62 (71%)	25 (29%)	0	1
11	AG	124/124 (100%)	106 (86%)	18 (14%)	3	10
11	BG	124/124 (100%)	98 (79%)	26 (21%)	1	4
12	AH	104/104 (100%)	83 (80%)	21 (20%)	1	4
12	BH	104/104 (100%)	79 (76%)	25 (24%)	1	2
13	AI	105/105 (100%)	84 (80%)	21 (20%)	1	4
13	BI	105/105 (100%)	83 (79%)	22 (21%)	1	4
14	AJ	86/86 (100%)	69 (80%)	17 (20%)	1	5
14	BJ	86/86 (100%)	63 (73%)	23 (27%)	0	1
15	AK	90/90 (100%)	74 (82%)	16 (18%)	2	6
15	BK	90/90 (100%)	79 (88%)	11 (12%)	5	16
16	AL	102/102 (100%)	89 (87%)	13 (13%)	4	14
17	AM	92/92 (100%)	71 (77%)	21 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	BM	92/92 (100%)	73 (79%)	19 (21%)	1	4
18	AN	79/83 (95%)	59 (75%)	20 (25%)	0	2
18	BN	79/83 (95%)	70 (89%)	9 (11%)	5	18
19	AO	76/76 (100%)	63 (83%)	13 (17%)	2	7
19	BO	76/76 (100%)	65 (86%)	11 (14%)	3	10
20	AP	65/65 (100%)	55 (85%)	10 (15%)	2	9
20	BP	65/65 (100%)	49 (75%)	16 (25%)	1	2
21	AQ	74/74 (100%)	56 (76%)	18 (24%)	1	2
21	BQ	74/74 (100%)	55 (74%)	19 (26%)	0	2
22	AR	48/48 (100%)	44 (92%)	4 (8%)	10	32
22	BR	48/48 (100%)	42 (88%)	6 (12%)	4	15
23	AS	70/70 (100%)	66 (94%)	4 (6%)	18	49
23	BS	70/70 (100%)	57 (81%)	13 (19%)	1	5
24	AT	65/65 (100%)	50 (77%)	15 (23%)	1	3
24	BT	65/65 (100%)	50 (77%)	15 (23%)	1	3
25	AU	46/46 (100%)	36 (78%)	10 (22%)	1	3
25	BU	46/46 (100%)	36 (78%)	10 (22%)	1	3
26	BL	103/103 (100%)	86 (84%)	17 (16%)	2	8
27	CC	216/216 (100%)	189 (88%)	27 (12%)	4	15
27	DC	216/216 (100%)	195 (90%)	21 (10%)	8	25
28	CD	164/164 (100%)	150 (92%)	14 (8%)	10	31
29	CE	165/165 (100%)	146 (88%)	19 (12%)	5	18
29	DE	165/165 (100%)	150 (91%)	15 (9%)	9	28
30	CF	148/148 (100%)	126 (85%)	22 (15%)	3	10
30	DF	148/148 (100%)	124 (84%)	24 (16%)	2	8
31	CG	137/137 (100%)	112 (82%)	25 (18%)	2	6
31	DG	137/137 (100%)	121 (88%)	16 (12%)	5	17
32	CH	113/113 (100%)	87 (77%)	26 (23%)	1	3
32	DH	113/113 (100%)	96 (85%)	17 (15%)	3	10
33	CJ	109/109 (100%)	82 (75%)	27 (25%)	1	2
33	DJ	109/109 (100%)	88 (81%)	21 (19%)	1	5

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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%)	107 (92%)	9 (8%)	11	35
35	CL	103/104 (99%)	92 (89%)	11 (11%)	6	22
35	DL	104/104 (100%)	96 (92%)	8 (8%)	12	35
36	CM	102/103 (99%)	88 (86%)	14 (14%)	3	12
36	DM	103/103 (100%)	96 (93%)	7 (7%)	14	42
37	CN	109/109 (100%)	97 (89%)	12 (11%)	6	20
37	DN	110/109 (101%)	100 (91%)	10 (9%)	9	28
38	CO	100/100 (100%)	85 (85%)	15 (15%)	3	10
38	DO	100/100 (100%)	92 (92%)	8 (8%)	11	34
39	CP	86/87 (99%)	71 (83%)	15 (17%)	2	7
39	DP	87/87 (100%)	77 (88%)	10 (12%)	5	18
40	CQ	99/99 (100%)	82 (83%)	17 (17%)	2	7
40	DQ	99/99 (100%)	90 (91%)	9 (9%)	9	28
41	CR	89/89 (100%)	80 (90%)	9 (10%)	7	24
41	DR	89/89 (100%)	86 (97%)	3 (3%)	32	66
42	CS	84/84 (100%)	73 (87%)	11 (13%)	4	13
42	DS	84/84 (100%)	73 (87%)	11 (13%)	4	13
43	CT	93/93 (100%)	75 (81%)	18 (19%)	1	5
43	DT	93/93 (100%)	78 (84%)	15 (16%)	2	8
44	CU	80/80 (100%)	65 (81%)	15 (19%)	1	5
44	DU	79/80 (99%)	71 (90%)	8 (10%)	7	24
45	CV	83/83 (100%)	71 (86%)	12 (14%)	3	10
45	DV	83/83 (100%)	73 (88%)	10 (12%)	5	16
46	CW	78/78 (100%)	63 (81%)	15 (19%)	1	5
46	DW	78/78 (100%)	69 (88%)	9 (12%)	5	18
47	CX	56/58 (97%)	46 (82%)	10 (18%)	2	6
47	DX	58/58 (100%)	49 (84%)	9 (16%)	2	9
48	CY	67/67 (100%)	58 (87%)	9 (13%)	4	12
48	DY	67/67 (100%)	62 (92%)	5 (8%)	12	37
49	CZ	54/54 (100%)	45 (83%)	9 (17%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	DZ	54/54 (100%)	47 (87%)	7 (13%)	4	13
50	C0	48/48 (100%)	39 (81%)	9 (19%)	1	5
50	D0	49/48 (102%)	44 (90%)	5 (10%)	7	23
51	C1	47/47 (100%)	38 (81%)	9 (19%)	1	5
51	D1	47/47 (100%)	44 (94%)	3 (6%)	16	44
52	C2	45/45 (100%)	42 (93%)	3 (7%)	15	43
52	D2	45/45 (100%)	44 (98%)	1 (2%)	45	77
53	C3	38/38 (100%)	31 (82%)	7 (18%)	1	6
53	D3	38/38 (100%)	33 (87%)	5 (13%)	4	13
54	C4	51/51 (100%)	47 (92%)	4 (8%)	11	35
54	D4	51/51 (100%)	49 (96%)	2 (4%)	28	63
55	C5	39/41 (95%)	28 (72%)	11 (28%)	0	1
55	D5	40/41 (98%)	31 (78%)	9 (22%)	1	3
56	DD	163/163 (100%)	150 (92%)	13 (8%)	11	34
57	D7	60/63 (95%)	37 (62%)	23 (38%)	0	0
All	All	9401/9419 (100%)	7924 (84%)	1477 (16%)	2	9

5 of 1477 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	CK	128	ASN
53	C3	41	ARG
36	CM	120	VAL
34	CK	124	VAL
43	CT	66	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
40	CQ	14	GLN
27	DC	141	HIS
50	D0	48	ASN
41	CR	51	GLN
48	CY	35	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1533 (99%)	388 (25%)	18 (1%)
2	BA	1532/1533 (99%)	410 (26%)	13 (0%)
3	DA	2894/2903 (99%)	725 (25%)	42 (1%)
4	CA	2896/2904 (99%)	866 (29%)	38 (1%)
5	CB	117/119 (98%)	26 (22%)	0
5	DB	118/119 (99%)	23 (19%)	0
All	All	9089/9111 (99%)	2438 (26%)	111 (1%)

5 of 2438 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 ⓘ

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	$\# Z > 2$
3	2MA	DA	2503	58,3	22,25,26	1.56	4 (18%)	33,37,40	2.77	13 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	AA	1518	1	23,26,27	1.49	5 (21%)	34,38,41	2.30	12 (35%)
3	G7M	DA	2069	3	23,26,27	1.70	3 (13%)	35,39,42	2.13	7 (20%)
3	PSU	DA	746	58,3	18,21,22	1.18	2 (11%)	22,30,33	1.91	4 (18%)
3	2MG	DA	1835	3	23,26,27	1.31	3 (13%)	32,38,41	2.08	5 (15%)
1	5MC	AA	967	1	18,22,23	1.03	1 (5%)	26,32,35	1.81	4 (15%)
3	6MZ	DA	1618	3	22,25,26	1.53	5 (22%)	30,36,39	3.06	10 (33%)
1	2MG	AA	1207	1	23,26,27	1.33	5 (21%)	32,38,41	2.12	7 (21%)
3	PSU	DA	955	3	18,21,22	1.13	0	22,30,33	2.18	4 (18%)
3	PSU	DA	2604	3	18,21,22	1.21	1 (5%)	22,30,33	1.63	3 (13%)
3	2MG	DA	2445	3	23,26,27	1.35	4 (17%)	32,38,41	2.48	8 (25%)
1	UR3	AA	1498	1	19,22,23	1.03	2 (10%)	26,32,35	1.94	4 (15%)
3	PSU	DA	1911	3	18,21,22	1.09	1 (5%)	22,30,33	1.74	4 (18%)
1	2MG	AA	1516	1	23,26,27	1.25	4 (17%)	32,38,41	2.11	7 (21%)
3	5MC	DA	1962	3	18,22,23	0.89	1 (5%)	26,32,35	1.37	3 (11%)
3	5MU	DA	1939	3	19,22,23	1.46	2 (10%)	28,32,35	2.87	9 (32%)
1	4OC	AA	1402	1	20,23,24	0.99	1 (5%)	26,32,35	1.26	4 (15%)
3	3TD	DA	1915	3	18,22,23	1.56	4 (22%)	22,32,35	2.57	6 (27%)
3	5MU	DA	747	3	19,22,23	1.69	5 (26%)	28,32,35	2.54	10 (35%)
3	6MZ	DA	2030	3	22,25,26	1.81	5 (22%)	30,36,39	2.65	8 (26%)
3	OMU	DA	2552	3	19,22,23	1.52	4 (21%)	26,31,34	2.78	7 (26%)
3	PSU	DA	2605	3	18,21,22	1.69	4 (22%)	22,30,33	1.90	4 (18%)
1	G7M	AA	527	1	23,26,27	1.42	4 (17%)	35,39,42	2.04	8 (22%)
1	PSU	AA	516	58,1	18,21,22	1.06	2 (11%)	22,30,33	1.65	3 (13%)
3	OMG	DA	2251	3	23,26,27	1.29	3 (13%)	33,38,41	2.32	10 (30%)
3	PSU	DA	1917	3	18,21,22	1.21	2 (11%)	22,30,33	1.89	7 (31%)
3	OMC	DA	2498	58,3	19,22,23	1.32	3 (15%)	26,31,34	1.24	4 (15%)
56	MEQ	DD	150	56	8,9,10	1.51	1 (12%)	5,10,12	1.52	1 (20%)
3	PSU	DA	2504	3	18,21,22	1.74	4 (22%)	22,30,33	2.03	5 (22%)
16	D2T	AL	89	16	7,9,10	1.00	0	6,11,13	2.31	3 (50%)
1	2MG	AA	966	1	23,26,27	1.44	3 (13%)	32,38,41	2.01	6 (18%)
3	PSU	DA	2457	3	18,21,22	1.30	3 (16%)	22,30,33	1.48	4 (18%)
3	1MG	DA	745	3	22,26,27	1.27	4 (18%)	33,39,42	2.36	13 (39%)
1	MA6	AA	1519	1	23,26,27	1.45	4 (17%)	34,38,41	2.05	10 (29%)
1	5MC	AA	1407	1	18,22,23	1.04	2 (11%)	26,32,35	1.63	4 (15%)
3	PSU	DA	2580	3	18,21,22	1.03	2 (11%)	22,30,33	1.65	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H2U	DA	2449	3	18,21,22	1.57	3 (16%)	21,30,33	2.15	3 (14%)

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
3	2MA	DA	2503	58,3	-	3/7/25/26	0/3/3/3
1	MA6	AA	1518	1	-	2/11/29/30	0/3/3/3
3	G7M	DA	2069	3	-	2/7/25/26	0/3/3/3
3	PSU	DA	746	58,3	-	3/7/25/26	0/2/2/2
3	2MG	DA	1835	3	-	4/9/27/28	0/3/3/3
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
3	6MZ	DA	1618	3	-	1/9/27/28	0/3/3/3
1	2MG	AA	1207	1	-	2/9/27/28	0/3/3/3
3	PSU	DA	955	3	-	0/7/25/26	0/2/2/2
3	PSU	DA	2604	3	-	0/7/25/26	0/2/2/2
3	2MG	DA	2445	3	-	0/9/27/28	0/3/3/3
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
3	PSU	DA	1911	3	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/9/27/28	0/3/3/3
3	5MC	DA	1962	3	-	4/7/25/26	0/2/2/2
3	5MU	DA	1939	3	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1	-	1/9/29/30	0/2/2/2
3	3TD	DA	1915	3	-	2/7/25/26	0/2/2/2
3	5MU	DA	747	3	-	2/7/25/26	0/2/2/2
3	6MZ	DA	2030	3	-	1/9/27/28	0/3/3/3
3	OMU	DA	2552	3	-	2/9/27/28	0/2/2/2
3	PSU	DA	2605	3	-	0/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	2/7/25/26	0/3/3/3
1	PSU	AA	516	58,1	-	0/7/25/26	0/2/2/2
3	OMG	DA	2251	3	-	1/9/27/28	0/3/3/3
3	PSU	DA	1917	3	-	0/7/25/26	0/2/2/2
3	OMC	DA	2498	58,3	-	3/9/27/28	0/2/2/2
56	MEQ	DD	150	56	-	2/8/9/11	-
3	PSU	DA	2504	3	-	2/7/25/26	0/2/2/2
16	D2T	AL	89	16	-	2/7/12/14	-
1	2MG	AA	966	1	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	DA	2457	3	-	1/7/25/26	0/2/2/2
3	1MG	DA	745	3	-	2/7/25/26	0/3/3/3
1	MA6	AA	1519	1	-	3/11/29/30	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
3	PSU	DA	2580	3	-	0/7/25/26	0/2/2/2
3	H2U	DA	2449	3	-	0/7/38/39	0/2/2/2

The worst 5 of 106 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DA	2069	G7M	C5-N7	-5.68	1.32	1.39
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
1	AA	1519	MA6	C5-C4	4.21	1.46	1.39

The worst 5 of 228 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	2503	2MA	C5-C4-N3	-8.77	117.33	127.19
3	DA	2445	2MG	C2-N3-C4	8.26	122.28	112.04

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.

28 monomers are involved in 105 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	DA	2503	2MA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1518	MA6	7	0
3	DA	1835	2MG	9	0
1	AA	967	5MC	2	0
3	DA	1618	6MZ	2	0
1	AA	1207	2MG	2	0
3	DA	955	PSU	2	0
3	DA	2445	2MG	2	0
3	DA	1911	PSU	3	0
1	AA	1516	2MG	2	0
3	DA	1962	5MC	3	0
3	DA	1939	5MU	3	0
1	AA	1402	4OC	3	0
3	DA	1915	3TD	1	0
3	DA	747	5MU	7	0
3	DA	2030	6MZ	7	0
3	DA	2552	OMU	6	0
3	DA	2605	PSU	1	0
1	AA	516	PSU	1	0
3	DA	2251	OMG	3	0
3	DA	2498	OMC	8	0
56	DD	150	MEQ	4	0
3	DA	2504	PSU	3	0
16	AL	89	D2T	4	0
3	DA	745	1MG	4	0
1	AA	1519	MA6	12	0
1	AA	1407	5MC	4	0
3	DA	2449	H2U	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
59	PGE	D3	101	-	9,9,9	0.92	0	8,8,8	0.43	0
59	PGE	AA	1613	-	9,9,9	1.13	1 (11%)	8,8,8	0.70	0
67	EDO	DB	202	-	3,3,3	0.52	0	2,2,2	0.30	0
60	MPD	DA	3077	-	7,7,7	0.50	0	9,10,10	1.43	2 (22%)
63	PUT	DA	3054	-	5,5,5	0.47	0	4,4,4	0.81	0
61	PG4	DR	202	-	12,12,12	0.86	0	11,11,11	0.57	0
65	ACY	DA	3055	-	3,3,3	1.03	0	3,3,3	1.30	0
62	SPD	DA	3031	-	9,9,9	0.62	0	8,8,8	0.31	0
67	EDO	DA	3060	-	3,3,3	0.46	0	2,2,2	0.26	0
59	PGE	DD	301	-	9,9,9	1.16	1 (11%)	8,8,8	0.77	0
67	EDO	DA	3075	-	3,3,3	0.35	0	2,2,2	0.18	0
59	PGE	DS	201	-	9,9,9	1.25	1 (11%)	8,8,8	1.03	0
63	PUT	DA	3037	-	5,5,5	0.32	0	4,4,4	0.81	0
67	EDO	DA	3076	-	3,3,3	0.53	0	2,2,2	0.06	0
66	PEG	D3	102	-	6,6,6	0.92	0	5,5,5	0.27	0
64	1PE	DA	3034	-	15,15,15	0.74	0	14,14,14	1.04	1 (7%)
67	EDO	DB	201	-	3,3,3	0.42	0	2,2,2	0.38	0
66	PEG	DA	3063	-	6,6,6	1.06	0	5,5,5	0.42	0
60	MPD	DA	3067	-	7,7,7	0.65	0	9,10,10	0.67	0
67	EDO	DA	3057	-	3,3,3	0.43	0	2,2,2	0.11	0
59	PGE	DA	3035	-	9,9,9	1.32	2 (22%)	8,8,8	1.12	1 (12%)
60	MPD	DE	302	-	7,7,7	0.56	0	9,10,10	0.43	0
61	PG4	DS	202	-	12,12,12	0.74	0	11,11,11	0.73	0
61	PG4	DA	3048	-	12,12,12	0.89	0	11,11,11	0.67	0
66	PEG	DA	3073	-	6,6,6	1.04	0	5,5,5	0.67	0
59	PGE	DT	202	-	9,9,9	1.16	1 (11%)	8,8,8	0.71	0
60	MPD	DE	301	-	7,7,7	0.56	0	9,10,10	0.56	0
60	MPD	AA	1615	-	7,7,7	0.54	0	9,10,10	0.67	0
67	EDO	D1	101	-	3,3,3	0.38	0	2,2,2	0.15	0
62	SPD	DA	3070	-	9,9,9	0.44	0	8,8,8	1.07	0
66	PEG	DA	3061	-	6,6,6	1.08	0	5,5,5	0.32	0
61	PG4	DQ	202	-	12,12,12	0.71	0	11,11,11	0.45	0
63	PUT	D5	101	-	5,5,5	0.29	0	4,4,4	0.30	0
64	1PE	DA	3065	-	15,15,15	0.86	0	14,14,14	0.88	0
66	PEG	DP	201	-	6,6,6	1.16	0	5,5,5	0.64	0
59	PGE	DA	3066	-	9,9,9	1.07	1 (11%)	8,8,8	0.93	0
60	MPD	DT	201	-	7,7,7	0.55	0	9,10,10	1.02	1 (11%)
60	MPD	DA	3043	-	7,7,7	0.58	0	9,10,10	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	MPD	DA	3072	-	7,7,7	0.56	0	9,10,10	0.30	0
60	MPD	DN	201	-	7,7,7	0.49	0	9,10,10	0.84	1 (11%)
66	PEG	D1	102	-	6,6,6	1.50	1 (16%)	5,5,5	1.35	0
67	EDO	DA	3052	-	3,3,3	0.50	0	2,2,2	0.16	0
60	MPD	DA	3045	-	7,7,7	0.34	0	9,10,10	1.38	2 (22%)
59	PGE	DU	101	-	9,9,9	1.09	1 (11%)	8,8,8	0.58	0
63	PUT	DP	202	-	5,5,5	0.36	0	4,4,4	0.16	0
60	MPD	DA	3046	-	7,7,7	0.76	0	9,10,10	0.99	1 (11%)
67	EDO	DR	204	-	3,3,3	0.55	0	2,2,2	0.28	0
67	EDO	DB	203	-	3,3,3	0.40	0	2,2,2	0.16	0
61	PG4	BA	1607	-	12,12,12	0.89	0	11,11,11	0.57	0
62	SPD	DA	3036	-	9,9,9	0.48	0	8,8,8	0.53	0
63	PUT	DA	3032	-	5,5,5	0.30	0	4,4,4	0.41	0
60	MPD	DA	3071	-	7,7,7	0.65	0	9,10,10	0.46	0
66	PEG	DQ	201	-	6,6,6	1.01	0	5,5,5	0.26	0
66	PEG	DA	3050	-	6,6,6	1.03	0	5,5,5	0.51	0
67	EDO	DA	3059	-	3,3,3	0.52	0	2,2,2	0.61	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
63	PUT	DM	201	-	5,5,5	0.35	0	4,4,4	0.51	0
68	GUN	DA	3078	-	12,12,12	1.91	2 (16%)	16,17,17	2.77	7 (43%)
60	MPD	DK	201	-	7,7,7	0.55	0	9,10,10	0.66	0
67	EDO	DA	3058	-	3,3,3	0.52	0	2,2,2	0.10	0
66	PEG	DA	3062	-	6,6,6	1.17	1 (16%)	5,5,5	0.57	0
65	ACY	DA	3044	-	3,3,3	0.87	0	3,3,3	1.23	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
59	PGE	D3	101	-	-	4/7/7/7	-
59	PGE	AA	1613	-	-	5/7/7/7	-
67	EDO	DB	202	-	-	1/1/1/1	-
60	MPD	DA	3077	-	-	2/5/5/5	-
63	PUT	DA	3054	-	-	0/3/3/3	-
61	PG4	DR	202	-	-	5/10/10/10	-
62	SPD	DA	3031	-	-	6/7/7/7	-
67	EDO	DA	3060	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PGE	DD	301	-	-	1/7/7/7	-
67	EDO	DA	3075	-	-	1/1/1/1	-
59	PGE	DS	201	-	-	2/7/7/7	-
63	PUT	DA	3037	-	-	1/3/3/3	-
67	EDO	DA	3076	-	-	1/1/1/1	-
66	PEG	D3	102	-	-	3/4/4/4	-
64	1PE	DA	3034	-	-	7/13/13/13	-
67	EDO	DB	201	-	-	1/1/1/1	-
66	PEG	DA	3063	-	-	3/4/4/4	-
60	MPD	DA	3067	-	-	1/5/5/5	-
67	EDO	DA	3057	-	-	0/1/1/1	-
59	PGE	DA	3035	-	-	2/7/7/7	-
60	MPD	DE	302	-	-	0/5/5/5	-
61	PG4	DS	202	-	-	3/10/10/10	-
61	PG4	DA	3048	-	-	7/10/10/10	-
66	PEG	DA	3073	-	-	1/4/4/4	-
59	PGE	DT	202	-	-	3/7/7/7	-
60	MPD	DE	301	-	-	1/5/5/5	-
60	MPD	AA	1615	-	-	3/5/5/5	-
67	EDO	D1	101	-	-	1/1/1/1	-
62	SPD	DA	3070	-	-	3/7/7/7	-
66	PEG	DA	3061	-	-	3/4/4/4	-
61	PG4	DQ	202	-	-	5/10/10/10	-
63	PUT	D5	101	-	-	1/3/3/3	-
64	1PE	DA	3065	-	-	9/13/13/13	-
66	PEG	DP	201	-	-	2/4/4/4	-
59	PGE	DA	3066	-	-	3/7/7/7	-
60	MPD	DT	201	-	-	0/5/5/5	-
60	MPD	DA	3043	-	-	2/5/5/5	-
60	MPD	DA	3072	-	-	0/5/5/5	-
60	MPD	DN	201	-	-	3/5/5/5	-
66	PEG	D1	102	-	-	3/4/4/4	-
67	EDO	DA	3052	-	-	1/1/1/1	-
60	MPD	DA	3045	-	-	2/5/5/5	-
59	PGE	DU	101	-	-	4/7/7/7	-
63	PUT	DP	202	-	-	0/3/3/3	-
60	MPD	DA	3046	-	-	0/5/5/5	-
67	EDO	DR	204	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
67	EDO	DB	203	-	-	0/1/1/1	-
61	PG4	BA	1607	-	-	1/10/10/10	-
62	SPD	DA	3036	-	-	3/7/7/7	-
63	PUT	DA	3032	-	-	2/3/3/3	-
60	MPD	DA	3071	-	-	2/5/5/5	-
66	PEG	DQ	201	-	-	4/4/4/4	-
66	PEG	DA	3050	-	-	1/4/4/4	-
67	EDO	DA	3059	-	-	0/1/1/1	-
63	PUT	DA	3069	-	-	1/3/3/3	-
63	PUT	DM	201	-	-	2/3/3/3	-
68	GUN	DA	3078	-	-	-	0/2/2/2
60	MPD	DK	201	-	-	0/5/5/5	-
67	EDO	DA	3058	-	-	0/1/1/1	-
66	PEG	DA	3062	-	-	3/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	DA	3078	GUN	C5-C4	4.54	1.48	1.39
68	DA	3078	GUN	C6-N1	-2.66	1.33	1.38
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

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	DA	3078	GUN	N9-C4-N3	7.07	135.60	126.05
68	DA	3078	GUN	C2-N3-C4	4.67	121.86	113.43
68	DA	3078	GUN	C6-C5-N7	3.79	137.30	130.25
60	DA	3045	MPD	CM-C2-C1	-3.28	103.74	110.57
64	DA	3034	1PE	OH3-C23-C13	-2.86	97.49	110.39

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
60	DA	3077	MPD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
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
60	DA	3077	MPD	1	0
63	DA	3054	PUT	4	0
61	DR	202	PG4	8	0
62	DA	3031	SPD	3	0
67	DA	3060	EDO	5	0
63	DA	3037	PUT	7	0
66	D3	102	PEG	2	0
64	DA	3034	1PE	5	0
66	DA	3063	PEG	1	0
60	DA	3067	MPD	4	0
61	DS	202	PG4	1	0
61	DA	3048	PG4	3	0
59	DT	202	PGE	2	0
60	DE	301	MPD	1	0
60	AA	1615	MPD	1	0
61	DQ	202	PG4	4	0
63	D5	101	PUT	2	0
64	DA	3065	1PE	2	0
66	DP	201	PEG	1	0
59	DA	3066	PGE	2	0
60	DA	3072	MPD	1	0
60	DN	201	MPD	1	0
66	D1	102	PEG	3	0
60	DA	3045	MPD	1	0
63	DP	202	PUT	10	0
60	DA	3046	MPD	1	0
67	DR	204	EDO	2	0
67	DB	203	EDO	1	0
62	DA	3036	SPD	1	0
60	DA	3071	MPD	1	0
66	DQ	201	PEG	1	0
66	DA	3050	PEG	2	0
67	DA	3059	EDO	4	0
63	DA	3069	PUT	2	0
65	DA	3064	ACY	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	DM	201	PUT	1	0
68	DA	3078	GUN	2	0
66	DA	3062	PEG	2	0
65	DA	3044	ACY	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1522/1533 (99%)	-0.30	7 (0%) 87 83	41, 95, 192, 402	0
2	BA	1533/1533 (100%)	0.17	44 (2%) 53 45	55, 124, 251, 339	0
3	DA	2873/2903 (98%)	-1.05	14 (0%) 87 83	13, 48, 176, 361	2 (0%)
4	CA	2898/2904 (99%)	0.83	285 (9%) 13 11	71, 161, 284, 521	0
5	CB	118/119 (99%)	0.20	1 (0%) 82 77	117, 200, 250, 277	0
5	DB	119/119 (100%)	-1.12	0 100 100	22, 56, 88, 107	0
6	AB	218/218 (100%)	0.45	9 (4%) 41 33	62, 132, 203, 272	0
6	BB	218/218 (100%)	0.66	19 (8%) 16 13	80, 140, 208, 274	0
7	AC	206/206 (100%)	0.35	3 (1%) 72 64	56, 106, 160, 230	0
7	BC	206/206 (100%)	0.67	14 (6%) 23 18	74, 120, 178, 212	0
8	AD	205/205 (100%)	0.88	23 (11%) 10 9	59, 120, 174, 227	0
8	BD	205/205 (100%)	0.42	7 (3%) 48 39	54, 93, 136, 166	0
9	AE	150/150 (100%)	0.65	12 (8%) 18 15	54, 98, 161, 235	0
9	BE	150/150 (100%)	0.73	15 (10%) 12 10	57, 99, 164, 209	0
10	AF	100/100 (100%)	0.39	2 (2%) 65 56	66, 110, 156, 219	0
10	BF	100/100 (100%)	0.54	6 (6%) 27 21	82, 126, 170, 263	0
11	AG	151/151 (100%)	0.69	12 (7%) 18 15	91, 145, 189, 203	0
11	BG	151/151 (100%)	1.32	35 (23%) 2 2	110, 212, 293, 336	0
12	AH	129/129 (100%)	0.56	5 (3%) 43 35	62, 104, 155, 192	0
12	BH	129/129 (100%)	0.67	12 (9%) 14 12	78, 121, 172, 209	0
13	AI	127/127 (100%)	1.06	22 (17%) 4 3	87, 136, 208, 278	0
13	BI	127/127 (100%)	1.51	41 (32%) 1 1	106, 173, 255, 309	0
14	AJ	98/98 (100%)	0.69	8 (8%) 17 14	65, 114, 148, 162	0
14	BJ	98/98 (100%)	0.93	9 (9%) 14 12	79, 136, 164, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
15	AK	117/117 (100%)	0.29	1 (0%)	81	75	50, 118, 172, 211	0
15	BK	117/117 (100%)	0.26	3 (2%)	57	48	60, 116, 169, 196	0
16	AL	122/123 (99%)	0.22	11 (9%)	15	13	53, 82, 135, 200	0
17	AM	114/114 (100%)	0.85	11 (9%)	13	11	80, 134, 199, 264	0
17	BM	114/114 (100%)	1.38	27 (23%)	2	2	166, 282, 369, 424	0
18	AN	96/100 (96%)	1.16	14 (14%)	6	4	65, 119, 213, 248	0
18	BN	96/100 (96%)	1.67	33 (34%)	1	1	101, 177, 271, 348	0
19	AO	88/88 (100%)	0.21	3 (3%)	48	39	52, 101, 142, 188	0
19	BO	88/88 (100%)	0.44	4 (4%)	38	30	77, 120, 158, 239	0
20	AP	82/82 (100%)	0.98	8 (9%)	13	11	70, 102, 210, 261	0
20	BP	82/82 (100%)	2.03	38 (46%)	0	0	83, 135, 210, 311	0
21	AQ	80/80 (100%)	0.48	5 (6%)	26	20	68, 106, 160, 291	0
21	BQ	80/80 (100%)	1.00	10 (12%)	8	7	88, 152, 220, 278	0
22	AR	55/55 (100%)	0.33	5 (9%)	15	12	75, 110, 169, 218	0
22	BR	55/55 (100%)	0.29	3 (5%)	30	24	67, 98, 161, 179	0
23	AS	79/79 (100%)	1.22	14 (17%)	4	3	93, 137, 192, 239	0
23	BS	79/79 (100%)	1.66	30 (37%)	1	0	169, 266, 365, 433	0
24	AT	85/85 (100%)	0.96	7 (8%)	17	14	80, 106, 155, 214	0
24	BT	85/85 (100%)	1.50	21 (24%)	2	1	96, 160, 216, 241	0
25	AU	54/54 (100%)	1.00	9 (16%)	4	3	80, 128, 214, 252	0
25	BU	54/54 (100%)	0.57	2 (3%)	45	37	64, 111, 175, 203	0
26	BL	123/123 (100%)	0.78	21 (17%)	4	3	64, 101, 154, 211	0
27	CC	271/271 (100%)	1.42	64 (23%)	2	2	73, 119, 159, 204	0
27	DC	271/271 (100%)	-0.08	3 (1%)	78	71	24, 61, 95, 128	0
28	CD	209/209 (100%)	1.80	76 (36%)	1	0	95, 156, 264, 431	0
29	CE	201/201 (100%)	2.01	87 (43%)	0	0	98, 238, 501, 716	0
29	DE	201/201 (100%)	-0.38	2 (0%)	79	73	19, 62, 113, 223	0
30	CF	177/177 (100%)	1.19	34 (19%)	3	2	155, 235, 294, 367	0
30	DF	177/177 (100%)	0.14	4 (2%)	61	52	49, 81, 139, 182	0
31	CG	176/176 (100%)	1.06	25 (14%)	6	5	139, 226, 348, 489	0
31	DG	176/176 (100%)	-0.01	1 (0%)	85	81	46, 82, 119, 204	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
32	CH	148/148 (100%)	0.74	12 (8%) 18 15	92, 161, 230, 348	0
32	DH	148/148 (100%)	0.56	7 (4%) 36 28	62, 167, 251, 346	0
33	CJ	141/141 (100%)	0.85	11 (7%) 19 16	186, 269, 360, 457	0
33	DJ	141/141 (100%)	1.22	24 (17%) 4 3	147, 236, 329, 386	0
34	CK	142/142 (100%)	1.77	54 (38%) 1 0	92, 155, 221, 296	0
34	DK	142/142 (100%)	-0.66	0 100 100	18, 39, 73, 141	0
35	CL	122/123 (99%)	1.21	22 (18%) 3 3	95, 139, 192, 270	0
35	DL	123/123 (100%)	-0.49	0 100 100	27, 49, 85, 150	0
36	CM	143/144 (99%)	2.34	73 (51%) 0 0	109, 204, 327, 455	0
36	DM	144/144 (100%)	-0.37	0 100 100	18, 60, 97, 151	0
37	CN	136/136 (100%)	1.00	20 (14%) 6 4	86, 147, 195, 220	0
37	DN	136/136 (100%)	-0.61	0 100 100	13, 46, 82, 141	1 (0%)
38	CO	120/120 (100%)	2.12	55 (45%) 0 0	102, 168, 292, 503	0
38	DO	120/120 (100%)	-0.66	1 (0%) 82 77	15, 42, 65, 186	0
39	CP	116/117 (99%)	1.09	17 (14%) 6 4	151, 205, 272, 305	0
39	DP	117/117 (100%)	-0.21	1 (0%) 81 75	36, 64, 103, 128	0
40	CQ	114/114 (100%)	2.03	50 (43%) 0 0	104, 165, 218, 317	0
40	DQ	114/114 (100%)	-0.22	1 (0%) 81 75	35, 60, 111, 139	0
41	CR	117/117 (100%)	2.09	51 (43%) 0 0	120, 164, 236, 276	0
41	DR	117/117 (100%)	-0.81	0 100 100	7, 33, 61, 123	0
42	CS	103/103 (100%)	2.08	49 (47%) 0 0	106, 195, 307, 404	0
42	DS	103/103 (100%)	-0.50	2 (1%) 66 58	16, 46, 84, 162	0
43	CT	110/110 (100%)	2.23	54 (49%) 0 0	108, 181, 300, 414	0
43	DT	110/110 (100%)	-0.68	0 100 100	13, 36, 75, 120	0
44	CU	93/93 (100%)	2.72	58 (62%) 0 0	132, 254, 491, 644	0
44	DU	92/93 (98%)	-0.01	7 (7%) 20 16	31, 67, 130, 180	0
45	CV	102/102 (100%)	3.79	86 (84%) 0 0	148, 404, 655, 701	0
45	DV	102/102 (100%)	-0.31	1 (0%) 79 73	38, 65, 110, 226	0
46	CW	94/94 (100%)	0.57	5 (5%) 32 25	138, 187, 255, 306	0
46	DW	94/94 (100%)	-0.32	0 100 100	27, 55, 97, 125	0
47	CX	75/76 (98%)	1.79	32 (42%) 0 0	101, 163, 209, 232	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
47	DX	76/76 (100%)	-0.37	1 (1%) 75 67	20, 47, 82, 127	1 (1%)
48	CY	77/77 (100%)	1.99	32 (41%) 0 0	94, 151, 225, 254	0
48	DY	77/77 (100%)	-0.13	0 100 100	34, 69, 114, 147	0
49	CZ	62/62 (100%)	2.15	33 (53%) 0 0	139, 374, 567, 650	0
49	DZ	62/62 (100%)	-0.08	1 (1%) 70 62	48, 81, 122, 246	0
50	C0	58/58 (100%)	1.10	8 (13%) 6 5	117, 160, 212, 242	0
50	D0	58/58 (100%)	-0.54	1 (1%) 69 61	22, 39, 75, 137	0
51	C1	56/56 (100%)	2.35	31 (55%) 0 0	108, 190, 336, 404	0
51	D1	56/56 (100%)	-0.68	2 (3%) 46 38	10, 42, 77, 173	0
52	C2	50/51 (98%)	0.99	6 (12%) 9 7	135, 193, 256, 268	0
52	D2	51/51 (100%)	-0.18	3 (5%) 28 22	45, 71, 113, 165	0
53	C3	46/46 (100%)	2.91	30 (65%) 0 0	110, 145, 226, 259	0
53	D3	46/46 (100%)	-0.14	1 (2%) 62 53	29, 52, 72, 254	0
54	C4	64/64 (100%)	2.77	37 (57%) 0 0	108, 153, 194, 244	0
54	D4	64/64 (100%)	-0.39	0 100 100	27, 49, 71, 86	0
55	C5	44/45 (97%)	3.12	29 (65%) 0 0	111, 162, 226, 282	0
55	D5	45/45 (100%)	-0.37	0 100 100	32, 56, 90, 120	0
56	DD	208/209 (99%)	-0.61	1 (0%) 87 83	12, 44, 81, 162	0
57	D7	68/68 (100%)	1.77	24 (35%) 1 1	66, 116, 186, 289	0
All	All	20582/20647 (99%)	0.38	2114 (10%) 12 10	7, 117, 268, 716	4 (0%)

The worst 5 of 2114 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	CM	26	GLY	13.5
36	CM	15	ALA	11.3
36	CM	27	LEU	11.1
44	CU	62	VAL	11.0
45	CV	35	VAL	10.9

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($\text{\AA}^2$)	Q<0.9
3	3TD	DA	1915	21/22	0.93	0.07	59,91,109,122	0
3	PSU	DA	1917	20/21	0.93	0.07	42,78,92,94	0
1	2MG	AA	966	24/25	0.94	0.10	48,77,86,88	0
3	PSU	DA	1911	20/21	0.95	0.06	51,84,101,113	0
1	G7M	AA	527	24/25	0.95	0.10	56,75,85,87	0
1	2MG	AA	1207	24/25	0.95	0.07	54,77,99,121	0
1	5MC	AA	967	21/22	0.96	0.11	69,77,90,103	0
1	PSU	AA	516	20/21	0.96	0.06	53,86,108,117	0
1	UR3	AA	1498	21/22	0.96	0.08	32,52,68,74	0
1	4OC	AA	1402	22/23	0.97	0.08	44,63,81,91	0
1	5MC	AA	1407	21/22	0.97	0.07	45,56,73,104	0
16	D2T	AL	89	10/11	0.97	0.09	44,60,96,108	0
1	2MG	AA	1516	24/25	0.98	0.07	33,63,70,86	0
1	MA6	AA	1518	24/25	0.98	0.06	21,41,61,72	0
1	MA6	AA	1519	24/25	0.98	0.07	37,65,78,84	0
3	5MU	DA	1939	21/22	0.98	0.07	9,38,57,72	0
3	5MC	DA	1962	21/22	0.98	0.06	35,51,64,84	0
3	G7M	DA	2069	24/25	0.98	0.06	8,35,48,61	0
3	2MG	DA	1835	24/25	0.98	0.06	27,50,59,62	0
56	MEQ	DD	150	10/11	0.98	0.07	6,23,48,48	0
3	6MZ	DA	1618	23/24	0.99	0.06	7,32,46,47	0
3	1MG	DA	745	24/25	0.99	0.05	5,29,42,63	0
3	6MZ	DA	2030	23/24	0.99	0.04	2,12,24,37	0
3	PSU	DA	746	20/21	0.99	0.04	3,21,34,43	0
3	OMG	DA	2251	24/25	0.99	0.05	3,28,44,58	0
3	2MG	DA	2445	24/25	0.99	0.05	13,28,44,45	0
3	H2U	DA	2449	20/21	0.99	0.04	3,20,42,50	0
3	PSU	DA	2457	20/21	0.99	0.04	3,30,46,59	0
3	OMC	DA	2498	21/22	0.99	0.04	3,20,38,49	0
3	2MA	DA	2503	23/24	0.99	0.05	3,24,39,56	0
3	PSU	DA	2504	20/21	0.99	0.04	2,22,42,46	0
3	OMU	DA	2552	21/22	0.99	0.04	13,27,47,70	0
3	PSU	DA	2580	20/21	0.99	0.05	6,38,52,53	0
3	PSU	DA	2604	20/21	0.99	0.04	14,33,48,70	0
3	PSU	DA	2605	20/21	0.99	0.06	12,38,48,57	0
3	5MU	DA	747	21/22	0.99	0.05	3,19,31,42	0
3	PSU	DA	955	20/21	0.99	0.05	8,30,58,70	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	BA	1642	1/1	0.44	0.19	120,120,120,120	0
58	MG	CA	3148	1/1	0.47	0.26	126,126,126,126	0
58	MG	CA	3067	1/1	0.58	0.32	117,117,117,117	0
58	MG	CA	3154	1/1	0.59	0.49	134,134,134,134	0
58	MG	CA	3017	1/1	0.60	0.42	112,112,112,112	0
58	MG	CA	3133	1/1	0.60	0.11	163,163,163,163	0
58	MG	CA	3083	1/1	0.61	0.43	135,135,135,135	0
58	MG	CA	3049	1/1	0.67	0.09	188,188,188,188	0
58	MG	CA	3084	1/1	0.68	0.14	163,163,163,163	0
58	MG	CA	3129	1/1	0.69	0.17	176,176,176,176	0
58	MG	BA	1643	1/1	0.69	0.08	171,171,171,171	0
58	MG	CA	3159	1/1	0.70	0.22	202,202,202,202	0
58	MG	CA	3118	1/1	0.72	0.10	207,207,207,207	0
58	MG	BA	1605	1/1	0.73	0.16	107,107,107,107	0
58	MG	D5	102	1/1	0.73	0.24	207,207,207,207	0
58	MG	AA	1606	1/1	0.74	0.30	77,77,77,77	0
58	MG	CA	3157	1/1	0.74	0.19	157,157,157,157	0
60	MPD	DK	201	8/8	0.75	0.17	113,136,162,162	0
58	MG	AA	1623	1/1	0.76	0.28	107,107,107,107	0
58	MG	CA	3102	1/1	0.77	0.24	199,199,199,199	0
58	MG	CA	3050	1/1	0.77	0.10	181,181,181,181	0
58	MG	CA	3059	1/1	0.78	0.20	167,167,167,167	0
58	MG	CA	3173	1/1	0.78	0.17	201,201,201,201	0
58	MG	CA	3019	1/1	0.79	0.27	84,84,84,84	0
63	PUT	DP	202	6/6	0.79	0.37	98,114,117,119	0
60	MPD	DE	301	8/8	0.80	0.19	142,176,194,201	0
58	MG	CA	3027	1/1	0.81	0.14	94,94,94,94	0
58	MG	CA	3043	1/1	0.81	0.16	69,69,69,69	0
58	MG	CA	3070	1/1	0.81	0.23	199,199,199,199	0
58	MG	CA	3008	1/1	0.82	0.10	97,97,97,97	0
60	MPD	DA	3072	8/8	0.83	0.36	117,148,172,178	0
58	MG	CA	3068	1/1	0.83	0.18	181,181,181,181	0
58	MG	CA	3047	1/1	0.84	0.12	170,170,170,170	0
58	MG	CA	3144	1/1	0.84	0.18	143,143,143,143	0
58	MG	CA	3022	1/1	0.84	0.12	89,89,89,89	0
60	MPD	DN	201	8/8	0.84	0.16	51,89,115,115	0
58	MG	CA	3131	1/1	0.84	0.10	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	1602	1/1	0.85	0.19	74,74,74,74	0
58	MG	BA	1636	1/1	0.86	0.11	131,131,131,131	0
58	MG	CA	3044	1/1	0.86	0.10	157,157,157,157	0
58	MG	CA	3009	1/1	0.86	0.08	85,85,85,85	0
58	MG	AA	1612	1/1	0.86	0.17	71,71,71,71	0
58	MG	AA	1610	1/1	0.86	0.21	82,82,82,82	0
58	MG	CA	3053	1/1	0.86	0.10	123,123,123,123	0
58	MG	CA	3002	1/1	0.86	0.20	70,70,70,70	0
58	MG	CA	3061	1/1	0.86	0.08	139,139,139,139	0
58	MG	CA	3005	1/1	0.86	0.09	81,81,81,81	0
58	MG	CA	3032	1/1	0.86	0.20	79,79,79,79	0
65	ACY	DA	3055	4/4	0.86	0.17	43,67,78,78	0
58	MG	DA	3027	1/1	0.87	0.15	77,77,77,77	0
58	MG	CA	3048	1/1	0.87	0.13	172,172,172,172	0
63	PUT	DA	3054	6/6	0.87	0.24	38,81,86,88	0
58	MG	CA	3140	1/1	0.87	0.15	161,161,161,161	0
58	MG	BA	1604	1/1	0.87	0.23	70,70,70,70	0
67	EDO	DB	202	4/4	0.87	0.17	74,84,88,90	0
58	MG	C3	101	1/1	0.88	0.16	168,168,168,168	0
58	MG	CA	3023	1/1	0.88	0.15	82,82,82,82	0
58	MG	CA	3120	1/1	0.88	0.11	143,143,143,143	0
58	MG	CA	3166	1/1	0.88	0.13	123,123,123,123	0
66	PEG	DQ	201	7/7	0.88	0.21	109,111,119,123	0
58	MG	CA	3015	1/1	0.88	0.10	91,91,91,91	0
59	PGE	D3	101	10/10	0.89	0.27	97,121,145,145	0
60	MPD	DA	3067	8/8	0.89	0.15	79,113,125,135	0
58	MG	CA	3130	1/1	0.89	0.12	149,149,149,149	0
58	MG	BA	1611	1/1	0.89	0.08	136,136,136,136	0
58	MG	CA	3132	1/1	0.89	0.22	177,177,177,177	0
58	MG	CA	3103	1/1	0.89	0.16	98,98,98,98	0
58	MG	CA	3037	1/1	0.89	0.10	63,63,63,63	0
58	MG	CR	201	1/1	0.89	0.13	75,75,75,75	0
58	MG	CA	3026	1/1	0.89	0.14	89,89,89,89	0
66	PEG	DP	201	7/7	0.89	0.14	78,92,105,106	0
58	MG	CA	3001	1/1	0.89	0.23	68,68,68,68	0
66	PEG	D1	102	7/7	0.89	0.27	57,70,83,89	0
59	PGE	DT	202	10/10	0.89	0.22	78,121,145,152	0
58	MG	CA	3110	1/1	0.90	0.07	136,136,136,136	0
58	MG	CA	3147	1/1	0.90	0.12	95,95,95,95	0
58	MG	CA	3010	1/1	0.90	0.13	89,89,89,89	0
58	MG	CA	3153	1/1	0.90	0.07	96,96,96,96	0
60	MPD	DE	302	8/8	0.90	0.32	135,162,187,187	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	1637	1/1	0.90	0.07	143,143,143,143	0
58	MG	CA	3126	1/1	0.90	0.17	183,183,183,183	0
61	PG4	BA	1607	13/13	0.90	0.24	77,89,111,117	0
58	MG	AA	1611	1/1	0.90	0.13	65,65,65,65	0
58	MG	CA	3036	1/1	0.90	0.16	67,67,67,67	0
58	MG	BA	1634	1/1	0.90	0.09	114,114,114,114	0
58	MG	CA	3090	1/1	0.90	0.06	134,134,134,134	0
58	MG	BA	1606	1/1	0.90	0.10	60,60,60,60	0
58	MG	CA	3135	1/1	0.90	0.09	158,158,158,158	0
67	EDO	DA	3060	4/4	0.90	0.19	55,57,80,84	0
67	EDO	DB	201	4/4	0.90	0.20	62,69,70,77	0
58	MG	DA	3038	1/1	0.90	0.17	56,56,56,56	0
58	MG	CA	3136	1/1	0.91	0.08	143,143,143,143	0
58	MG	AA	1602	1/1	0.91	0.10	73,73,73,73	0
58	MG	CM	201	1/1	0.91	0.10	135,135,135,135	0
58	MG	CA	3089	1/1	0.91	0.14	148,148,148,148	0
58	MG	CA	3062	1/1	0.91	0.11	102,102,102,102	0
63	PUT	DA	3069	6/6	0.91	0.26	53,86,95,96	0
58	MG	CA	3098	1/1	0.91	0.25	171,171,171,171	0
58	MG	CA	3151	1/1	0.91	0.16	92,92,92,92	0
58	MG	CA	3011	1/1	0.91	0.11	87,87,87,87	0
60	MPD	AA	1615	8/8	0.91	0.17	83,114,154,154	0
60	MPD	DA	3046	8/8	0.91	0.18	56,87,103,110	0
58	MG	CA	3007	1/1	0.91	0.16	83,83,83,83	0
58	MG	BA	1638	1/1	0.91	0.08	156,156,156,156	0
58	MG	CA	3004	1/1	0.91	0.18	80,80,80,80	0
58	MG	BA	1615	1/1	0.92	0.09	124,124,124,124	0
58	MG	CA	3074	1/1	0.92	0.31	159,159,159,159	0
58	MG	CA	3082	1/1	0.92	0.08	137,137,137,137	0
60	MPD	DT	201	8/8	0.92	0.27	115,144,166,166	0
59	PGE	DS	201	10/10	0.92	0.13	38,84,110,122	0
61	PG4	DR	202	13/13	0.92	0.23	93,108,117,118	0
58	MG	CA	3035	1/1	0.92	0.18	66,66,66,66	0
59	PGE	DU	101	10/10	0.92	0.15	59,92,160,162	0
58	MG	CA	3066	1/1	0.92	0.30	141,141,141,141	0
65	ACY	DA	3044	4/4	0.92	0.14	60,73,98,98	0
58	MG	CA	3086	1/1	0.92	0.07	136,136,136,136	0
60	MPD	DA	3045	8/8	0.92	0.22	69,120,140,144	0
58	MG	CA	3122	1/1	0.92	0.15	109,109,109,109	0
58	MG	CA	3028	1/1	0.92	0.07	73,73,73,73	0
60	MPD	DA	3071	8/8	0.92	0.14	52,97,138,149	0
58	MG	CA	3176	1/1	0.92	0.07	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3030	1/1	0.92	0.08	67,67,67,67	0
68	GUN	DA	3078	11/11	0.92	0.16	77,96,105,107	0
58	MG	CA	3164	1/1	0.93	0.13	117,117,117,117	0
58	MG	BA	1609	1/1	0.93	0.21	141,141,141,141	0
58	MG	CA	3168	1/1	0.93	0.10	93,93,93,93	0
58	MG	CA	3021	1/1	0.93	0.16	83,83,83,83	0
58	MG	CA	3134	1/1	0.93	0.06	145,145,145,145	0
58	MG	DA	3047	1/1	0.93	0.14	52,52,52,52	0
58	MG	DA	3051	1/1	0.93	0.12	57,57,57,57	0
61	PG4	DA	3048	13/13	0.93	0.18	48,76,98,100	0
58	MG	CA	3024	1/1	0.93	0.08	61,61,61,61	0
58	MG	CA	3143	1/1	0.93	0.19	117,117,117,117	0
59	PGE	DD	301	10/10	0.93	0.21	82,129,155,165	0
58	MG	CA	3045	1/1	0.93	0.08	133,133,133,133	0
58	MG	AA	1601	1/1	0.93	0.16	54,54,54,54	0
58	MG	AA	1616	1/1	0.93	0.15	91,91,91,91	0
66	PEG	DA	3062	7/7	0.93	0.27	56,86,100,103	0
66	PEG	DA	3063	7/7	0.93	0.22	82,120,134,137	0
58	MG	CA	3079	1/1	0.93	0.11	156,156,156,156	0
58	MG	CA	3012	1/1	0.93	0.08	82,82,82,82	0
60	MPD	DA	3043	8/8	0.93	0.13	75,104,118,125	0
58	MG	AA	1608	1/1	0.93	0.14	64,64,64,64	0
58	MG	CA	3051	1/1	0.93	0.08	129,129,129,129	0
58	MG	CA	3158	1/1	0.93	0.08	132,132,132,132	0
67	EDO	DB	203	4/4	0.93	0.17	61,72,76,79	0
58	MG	AA	1655	1/1	0.93	0.11	148,148,148,148	0
58	MG	CA	3033	1/1	0.94	0.11	60,60,60,60	0
59	PGE	AA	1613	10/10	0.94	0.11	41,88,109,113	0
59	PGE	DA	3066	10/10	0.94	0.17	52,88,126,129	0
58	MG	CA	3149	1/1	0.94	0.15	111,111,111,111	0
62	SPD	DA	3070	10/10	0.94	0.19	59,83,96,97	0
63	PUT	DA	3032	6/6	0.94	0.20	50,68,76,81	0
63	PUT	DA	3037	6/6	0.94	0.10	28,40,58,59	0
58	MG	BA	1603	1/1	0.94	0.19	65,65,65,65	0
58	MG	CA	3018	1/1	0.94	0.10	75,75,75,75	0
58	MG	CA	3029	1/1	0.94	0.09	59,59,59,59	0
58	MG	CA	3038	1/1	0.94	0.11	61,61,61,61	0
58	MG	CA	3091	1/1	0.94	0.07	153,153,153,153	0
66	PEG	DA	3061	7/7	0.94	0.17	52,94,106,108	0
58	MG	CA	3039	1/1	0.94	0.09	74,74,74,74	0
58	MG	CA	3160	1/1	0.94	0.14	157,157,157,157	0
58	MG	CA	3100	1/1	0.94	0.14	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3071	1/1	0.94	0.11	118,118,118,118	0
58	MG	CA	3052	1/1	0.94	0.10	136,136,136,136	0
66	PEG	D3	102	7/7	0.94	0.18	82,87,94,100	0
58	MG	CA	3077	1/1	0.94	0.10	139,139,139,139	0
58	MG	CA	3141	1/1	0.94	0.09	129,129,129,129	0
58	MG	CA	3117	1/1	0.94	0.07	143,143,143,143	0
58	MG	BA	1622	1/1	0.94	0.08	89,89,89,89	0
58	MG	DA	3007	1/1	0.94	0.13	48,48,48,48	0
58	MG	CA	3119	1/1	0.95	0.06	112,112,112,112	0
58	MG	AA	1605	1/1	0.95	0.26	54,54,54,54	0
58	MG	DA	3056	1/1	0.95	0.10	69,69,69,69	0
58	MG	CA	3124	1/1	0.95	0.07	115,115,115,115	0
58	MG	BA	1618	1/1	0.95	0.07	107,107,107,107	0
58	MG	CA	3171	1/1	0.95	0.08	113,113,113,113	0
58	MG	CA	3014	1/1	0.95	0.12	82,82,82,82	0
58	MG	DA	3009	1/1	0.95	0.17	54,54,54,54	0
61	PG4	DS	202	13/13	0.95	0.09	29,44,81,89	0
62	SPD	DA	3031	10/10	0.95	0.17	27,70,87,89	0
58	MG	CB	203	1/1	0.95	0.12	123,123,123,123	0
58	MG	CA	3031	1/1	0.95	0.06	64,64,64,64	0
58	MG	CA	3003	1/1	0.95	0.14	61,61,61,61	0
58	MG	DA	3017	1/1	0.95	0.11	60,60,60,60	0
58	MG	CA	3087	1/1	0.95	0.07	139,139,139,139	0
58	MG	DA	3026	1/1	0.95	0.20	52,52,52,52	0
58	MG	CA	3056	1/1	0.95	0.12	130,130,130,130	0
58	MG	CA	3058	1/1	0.95	0.08	124,124,124,124	0
58	MG	CA	3006	1/1	0.95	0.11	49,49,49,49	0
58	MG	BA	1601	1/1	0.95	0.14	67,67,67,67	0
58	MG	CA	3101	1/1	0.95	0.14	147,147,147,147	0
66	PEG	DA	3073	7/7	0.95	0.18	53,58,93,101	0
58	MG	BA	1640	1/1	0.95	0.10	85,85,85,85	0
58	MG	AA	1604	1/1	0.95	0.22	51,51,51,51	0
58	MG	CA	3109	1/1	0.95	0.09	112,112,112,112	0
58	MG	CA	3040	1/1	0.95	0.29	60,60,60,60	0
67	EDO	DA	3059	4/4	0.95	0.21	50,62,77,77	0
58	MG	CA	3113	1/1	0.95	0.08	106,106,106,106	0
58	MG	CA	3115	1/1	0.95	0.12	109,109,109,109	0
58	MG	CA	3041	1/1	0.95	0.11	75,75,75,75	0
58	MG	CA	3025	1/1	0.95	0.06	84,84,84,84	0
60	MPD	DA	3077	8/8	0.95	0.15	44,97,123,123	0
58	MG	AA	1636	1/1	0.96	0.06	101,101,101,101	0
58	MG	CA	3060	1/1	0.96	0.07	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	MG	CA	3123	1/1	0.96	0.05	103,103,103,103	0
58	MG	CA	3042	1/1	0.96	0.11	57,57,57,57	0
58	MG	CA	3163	1/1	0.96	0.07	113,113,113,113	0
58	MG	CA	3125	1/1	0.96	0.08	115,115,115,115	0
58	MG	AA	1609	1/1	0.96	0.08	69,69,69,69	0
58	MG	DA	3033	1/1	0.96	0.07	52,52,52,52	0
58	MG	CA	3170	1/1	0.96	0.07	111,111,111,111	0
58	MG	CA	3094	1/1	0.96	0.06	118,118,118,118	0
58	MG	CA	3097	1/1	0.96	0.15	115,115,115,115	0
58	MG	DA	3010	1/1	0.96	0.09	40,40,40,40	0
58	MG	DA	3039	1/1	0.96	0.19	82,82,82,82	0
58	MG	DA	3041	1/1	0.96	0.22	52,52,52,52	0
58	MG	CA	3034	1/1	0.96	0.07	60,60,60,60	0
58	MG	CA	3072	1/1	0.96	0.10	95,95,95,95	0
58	MG	DR	201	1/1	0.96	0.07	27,27,27,27	0
58	MG	CA	3137	1/1	0.96	0.06	95,95,95,95	0
58	MG	CA	3106	1/1	0.96	0.15	106,106,106,106	0
65	ACY	DA	3064	4/4	0.96	0.10	12,15,38,45	0
59	PGE	DA	3035	10/10	0.96	0.10	38,81,109,119	0
58	MG	CA	3107	1/1	0.96	0.13	92,92,92,92	0
58	MG	DA	3015	1/1	0.96	0.20	48,48,48,48	0
58	MG	CA	3076	1/1	0.96	0.09	105,105,105,105	0
58	MG	CA	3146	1/1	0.96	0.17	106,106,106,106	0
58	MG	BA	1635	1/1	0.96	0.07	112,112,112,112	0
58	MG	DA	3018	1/1	0.96	0.16	49,49,49,49	0
58	MG	CA	3116	1/1	0.96	0.10	106,106,106,106	0
67	EDO	DA	3057	4/4	0.96	0.11	47,57,58,71	0
58	MG	CA	3150	1/1	0.96	0.15	84,84,84,84	0
58	MG	DA	3074	1/1	0.96	0.19	75,75,75,75	0
58	MG	DA	3022	1/1	0.96	0.07	51,51,51,51	0
58	MG	CA	3013	1/1	0.96	0.15	66,66,66,66	0
58	MG	CA	3155	1/1	0.96	0.07	110,110,110,110	0
67	EDO	DR	204	4/4	0.96	0.16	49,74,82,89	0
67	EDO	D1	101	4/4	0.96	0.10	47,52,68,74	0
58	MG	CA	3156	1/1	0.96	0.10	142,142,142,142	0
58	MG	BA	1620	1/1	0.97	0.08	87,87,87,87	0
58	MG	AA	1603	1/1	0.97	0.05	45,45,45,45	0
58	MG	BA	1625	1/1	0.97	0.10	107,107,107,107	0
58	MG	DA	3099	1/1	0.97	0.19	177,177,177,177	0
58	MG	CA	3080	1/1	0.97	0.14	111,111,111,111	0
58	MG	CA	3081	1/1	0.97	0.08	102,102,102,102	0
58	MG	DA	3118	1/1	0.97	0.09	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3165	1/1	0.97	0.06	84,84,84,84	0
61	PG4	DQ	202	13/13	0.97	0.06	42,58,66,70	0
58	MG	DA	3182	1/1	0.97	0.13	73,73,73,73	0
58	MG	CA	3167	1/1	0.97	0.09	93,93,93,93	0
58	MG	DA	3013	1/1	0.97	0.15	44,44,44,44	0
62	SPD	DA	3036	10/10	0.97	0.14	33,53,66,69	0
58	MG	AA	1645	1/1	0.97	0.08	93,93,93,93	0
58	MG	AA	1648	1/1	0.97	0.09	96,96,96,96	0
58	MG	AA	1614	1/1	0.97	0.04	39,39,39,39	0
58	MG	CA	3175	1/1	0.97	0.05	107,107,107,107	0
58	MG	DA	3019	1/1	0.97	0.05	34,34,34,34	0
63	PUT	DM	201	6/6	0.97	0.12	25,58,65,71	0
58	MG	CA	3054	1/1	0.97	0.08	98,98,98,98	0
63	PUT	D5	101	6/6	0.97	0.21	82,99,108,108	0
64	1PE	DA	3065	16/16	0.97	0.13	40,72,82,90	0
58	MG	DA	3020	1/1	0.97	0.06	46,46,46,46	0
58	MG	CA	3096	1/1	0.97	0.09	111,111,111,111	0
58	MG	AA	1656	1/1	0.97	0.07	94,94,94,94	0
66	PEG	DA	3050	7/7	0.97	0.13	51,62,68,78	0
58	MG	DA	3024	1/1	0.97	0.16	60,60,60,60	0
58	MG	CA	3139	1/1	0.97	0.07	124,124,124,124	0
58	MG	AA	1657	1/1	0.97	0.08	95,95,95,95	0
58	MG	BA	1612	1/1	0.97	0.05	135,135,135,135	0
58	MG	DA	3028	1/1	0.97	0.06	36,36,36,36	0
58	MG	CA	3063	1/1	0.97	0.08	92,92,92,92	0
58	MG	CA	3145	1/1	0.97	0.04	119,119,119,119	0
58	MG	CA	3065	1/1	0.97	0.06	115,115,115,115	0
58	MG	AA	1631	1/1	0.97	0.05	100,100,100,100	0
67	EDO	DA	3058	4/4	0.97	0.14	62,73,84,87	0
58	MG	AA	1634	1/1	0.97	0.06	64,64,64,64	0
58	MG	BA	1645	1/1	0.97	0.09	94,94,94,94	0
67	EDO	DA	3076	4/4	0.97	0.18	74,92,96,101	0
58	MG	CA	3111	1/1	0.97	0.30	55,55,55,55	0
58	MG	CA	3112	1/1	0.97	0.10	102,102,102,102	0
58	MG	CA	3152	1/1	0.97	0.05	138,138,138,138	0
58	MG	BA	1648	1/1	0.97	0.06	91,91,91,91	0
58	MG	CA	3016	1/1	0.97	0.07	100,100,100,100	0
58	MG	DA	3003	1/1	0.97	0.18	53,53,53,53	0
58	MG	AA	1625	1/1	0.98	0.04	77,77,77,77	0
58	MG	AA	1630	1/1	0.98	0.05	89,89,89,89	0
58	MG	DA	3023	1/1	0.98	0.20	36,36,36,36	0
58	MG	AA	1637	1/1	0.98	0.06	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3069	1/1	0.98	0.05	96,96,96,96	0
58	MG	CA	3114	1/1	0.98	0.04	116,116,116,116	0
58	MG	BA	1628	1/1	0.98	0.04	95,95,95,95	0
58	MG	BA	1650	1/1	0.98	0.06	96,96,96,96	0
58	MG	BA	1633	1/1	0.98	0.04	66,66,66,66	0
58	MG	CA	3161	1/1	0.98	0.04	78,78,78,78	0
58	MG	CA	3162	1/1	0.98	0.10	94,94,94,94	0
58	MG	DA	3030	1/1	0.98	0.06	37,37,37,37	0
58	MG	CA	3075	1/1	0.98	0.06	107,107,107,107	0
58	MG	DA	3005	1/1	0.98	0.06	35,35,35,35	0
58	MG	DA	3006	1/1	0.98	0.10	31,31,31,31	0
58	MG	BA	1610	1/1	0.98	0.09	78,78,78,78	0
58	MG	AA	1624	1/1	0.98	0.09	65,65,65,65	0
58	MG	CA	3169	1/1	0.98	0.10	80,80,80,80	0
58	MG	DA	3042	1/1	0.98	0.13	60,60,60,60	0
58	MG	AA	1646	1/1	0.98	0.07	99,99,99,99	0
58	MG	CA	3046	1/1	0.98	0.10	107,107,107,107	0
58	MG	CA	3174	1/1	0.98	0.07	123,123,123,123	0
64	1PE	DA	3034	16/16	0.98	0.09	21,51,96,96	0
58	MG	DA	3049	1/1	0.98	0.14	56,56,56,56	0
58	MG	DA	3012	1/1	0.98	0.09	33,33,33,33	0
58	MG	CB	202	1/1	0.98	0.05	116,116,116,116	0
58	MG	AA	1647	1/1	0.98	0.13	100,100,100,100	0
58	MG	CA	3088	1/1	0.98	0.12	127,127,127,127	0
58	MG	CA	3020	1/1	0.98	0.06	71,71,71,71	0
58	MG	DA	3068	1/1	0.98	0.16	47,47,47,47	0
58	MG	DA	3014	1/1	0.98	0.12	36,36,36,36	0
58	MG	DR	203	1/1	0.98	0.06	38,38,38,38	0
58	MG	CA	3092	1/1	0.98	0.05	93,93,93,93	0
58	MG	CA	3138	1/1	0.98	0.07	117,117,117,117	0
58	MG	DA	3096	1/1	0.98	0.05	35,35,35,35	0
58	MG	BA	1617	1/1	0.98	0.09	73,73,73,73	0
67	EDO	DA	3052	4/4	0.98	0.12	48,48,57,58	0
58	MG	DA	3016	1/1	0.98	0.16	41,41,41,41	0
58	MG	CA	3142	1/1	0.98	0.06	103,103,103,103	0
58	MG	DA	3120	1/1	0.98	0.09	31,31,31,31	0
58	MG	DA	3148	1/1	0.98	0.10	65,65,65,65	0
67	EDO	DA	3075	4/4	0.98	0.15	68,83,95,95	0
58	MG	DA	3174	1/1	0.98	0.09	67,67,67,67	0
58	MG	BA	1639	1/1	0.98	0.09	91,91,91,91	0
58	MG	AA	1633	1/1	0.98	0.06	84,84,84,84	0
58	MG	CA	3104	1/1	0.98	0.07	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	BA	1641	1/1	0.98	0.04	62,62,62,62	0
58	MG	CA	3064	1/1	0.98	0.06	104,104,104,104	0
58	MG	CA	3108	1/1	0.98	0.04	92,92,92,92	0
58	MG	BA	1626	1/1	0.99	0.04	62,62,62,62	0
58	MG	BA	1627	1/1	0.99	0.04	81,81,81,81	0
58	MG	CA	3085	1/1	0.99	0.05	91,91,91,91	0
58	MG	AA	1607	1/1	0.99	0.05	46,46,46,46	0
58	MG	BA	1630	1/1	0.99	0.04	74,74,74,74	0
58	MG	BA	1631	1/1	0.99	0.03	76,76,76,76	0
58	MG	DA	3021	1/1	0.99	0.12	37,37,37,37	0
58	MG	CA	3172	1/1	0.99	0.04	94,94,94,94	0
58	MG	BA	1632	1/1	0.99	0.04	59,59,59,59	0
58	MG	AA	1658	1/1	0.99	0.07	59,59,59,59	0
58	MG	AA	1639	1/1	0.99	0.08	50,50,50,50	0
58	MG	CA	3093	1/1	0.99	0.03	65,65,65,65	0
58	MG	DB	204	1/1	0.99	0.08	62,62,62,62	0
58	MG	DB	206	1/1	0.99	0.02	41,41,41,41	0
58	MG	CB	201	1/1	0.99	0.04	131,131,131,131	0
58	MG	DA	3025	1/1	0.99	0.06	25,25,25,25	0
58	MG	CA	3095	1/1	0.99	0.03	82,82,82,82	0
58	MG	AA	1641	1/1	0.99	0.03	70,70,70,70	0
58	MG	AA	1642	1/1	0.99	0.03	73,73,73,73	0
58	MG	AA	1643	1/1	0.99	0.03	78,78,78,78	0
58	MG	CA	3099	1/1	0.99	0.06	77,77,77,77	0
58	MG	DA	3029	1/1	0.99	0.07	57,57,57,57	0
58	MG	AA	1644	1/1	0.99	0.05	83,83,83,83	0
58	MG	AA	1618	1/1	0.99	0.06	105,105,105,105	0
58	MG	BA	1608	1/1	0.99	0.03	82,82,82,82	0
58	MG	AA	1632	1/1	0.99	0.03	63,63,63,63	0
58	MG	CA	3105	1/1	0.99	0.04	83,83,83,83	0
58	MG	DA	3040	1/1	0.99	0.04	38,38,38,38	0
58	MG	AA	1620	1/1	0.99	0.02	84,84,84,84	0
58	MG	AA	1626	1/1	0.99	0.03	69,69,69,69	0
58	MG	BA	1644	1/1	0.99	0.05	94,94,94,94	0
58	MG	AA	1649	1/1	0.99	0.02	66,66,66,66	0
58	MG	BA	1646	1/1	0.99	0.04	59,59,59,59	0
58	MG	DA	3053	1/1	0.99	0.15	44,44,44,44	0
58	MG	BA	1647	1/1	0.99	0.07	68,68,68,68	0
58	MG	BA	1613	1/1	0.99	0.04	96,96,96,96	0
58	MG	BA	1649	1/1	0.99	0.12	107,107,107,107	0
58	MG	DA	3081	1/1	0.99	0.10	63,63,63,63	0
58	MG	DA	3082	1/1	0.99	0.08	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	DA	3083	1/1	0.99	0.03	74,74,74,74	0
58	MG	DA	3089	1/1	0.99	0.03	46,46,46,46	0
58	MG	BA	1614	1/1	0.99	0.06	96,96,96,96	0
58	MG	CA	3121	1/1	0.99	0.03	88,88,88,88	0
58	MG	DA	3001	1/1	0.99	0.03	12,12,12,12	0
58	MG	DA	3101	1/1	0.99	0.09	50,50,50,50	0
58	MG	DA	3102	1/1	0.99	0.03	35,35,35,35	0
58	MG	DA	3106	1/1	0.99	0.09	40,40,40,40	0
58	MG	DA	3107	1/1	0.99	0.04	41,41,41,41	0
58	MG	CA	3127	1/1	0.99	0.05	106,106,106,106	0
58	MG	CA	3128	1/1	0.99	0.04	104,104,104,104	0
58	MG	DA	3002	1/1	0.99	0.04	10,10,10,10	0
58	MG	DA	3119	1/1	0.99	0.06	51,51,51,51	0
58	MG	AA	1651	1/1	0.99	0.04	74,74,74,74	0
58	MG	DA	3121	1/1	0.99	0.04	68,68,68,68	0
58	MG	DA	3125	1/1	0.99	0.04	48,48,48,48	0
58	MG	DA	3133	1/1	0.99	0.03	24,24,24,24	0
58	MG	DA	3139	1/1	0.99	0.03	85,85,85,85	0
58	MG	DA	3146	1/1	0.99	0.04	55,55,55,55	0
58	MG	CA	3055	1/1	0.99	0.10	82,82,82,82	0
58	MG	DA	3147	1/1	0.99	0.08	104,104,104,104	0
58	MG	CA	3057	1/1	0.99	0.06	90,90,90,90	0
58	MG	DA	3004	1/1	0.99	0.04	30,30,30,30	0
58	MG	DA	3155	1/1	0.99	0.04	65,65,65,65	0
58	MG	DA	3156	1/1	0.99	0.02	58,58,58,58	0
58	MG	DA	3157	1/1	0.99	0.04	75,75,75,75	0
58	MG	DA	3159	1/1	0.99	0.03	56,56,56,56	0
58	MG	DA	3165	1/1	0.99	0.10	22,22,22,22	0
58	MG	DA	3166	1/1	0.99	0.04	12,12,12,12	0
58	MG	DA	3168	1/1	0.99	0.09	51,51,51,51	0
58	MG	DA	3170	1/1	0.99	0.10	64,64,64,64	0
58	MG	DA	3172	1/1	0.99	0.07	46,46,46,46	0
58	MG	BA	1616	1/1	0.99	0.06	96,96,96,96	0
58	MG	AA	1652	1/1	0.99	0.03	80,80,80,80	0
58	MG	DA	3184	1/1	0.99	0.07	60,60,60,60	0
58	MG	DA	3186	1/1	0.99	0.06	36,36,36,36	0
58	MG	DA	3188	1/1	0.99	0.03	36,36,36,36	0
58	MG	CA	3073	1/1	0.99	0.05	109,109,109,109	0
58	MG	AA	1653	1/1	0.99	0.04	70,70,70,70	0
58	MG	DA	3008	1/1	0.99	0.05	27,27,27,27	0
58	MG	BA	1619	1/1	0.99	0.03	81,81,81,81	0
58	MG	AA	1654	1/1	0.99	0.05	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	CA	3078	1/1	0.99	0.06	73,73,73,73	0
58	MG	BA	1621	1/1	0.99	0.04	69,69,69,69	0
58	MG	AA	1635	1/1	0.99	0.03	89,89,89,89	0
58	MG	BA	1624	1/1	0.99	0.05	70,70,70,70	0
58	MG	AA	1628	1/1	0.99	0.03	70,70,70,70	0
58	MG	DA	3091	1/1	1.00	0.02	30,30,30,30	0
58	MG	DA	3167	1/1	1.00	0.02	21,21,21,21	0
58	MG	DA	3092	1/1	1.00	0.03	24,24,24,24	0
58	MG	DA	3169	1/1	1.00	0.02	8,8,8,8	0
58	MG	DA	3093	1/1	1.00	0.01	22,22,22,22	0
58	MG	DA	3171	1/1	1.00	0.02	60,60,60,60	0
58	MG	DA	3094	1/1	1.00	0.03	10,10,10,10	0
58	MG	DA	3173	1/1	1.00	0.03	50,50,50,50	0
58	MG	DA	3095	1/1	1.00	0.02	35,35,35,35	0
58	MG	DA	3175	1/1	1.00	0.03	22,22,22,22	0
58	MG	DA	3176	1/1	1.00	0.03	27,27,27,27	0
58	MG	DA	3177	1/1	1.00	0.04	31,31,31,31	0
58	MG	DA	3178	1/1	1.00	0.02	36,36,36,36	0
58	MG	DA	3179	1/1	1.00	0.02	36,36,36,36	0
58	MG	DA	3180	1/1	1.00	0.02	19,19,19,19	0
58	MG	DA	3181	1/1	1.00	0.03	47,47,47,47	0
58	MG	BA	1623	1/1	1.00	0.04	68,68,68,68	0
58	MG	DA	3183	1/1	1.00	0.01	38,38,38,38	0
58	MG	DA	3097	1/1	1.00	0.01	31,31,31,31	0
58	MG	DB	205	1/1	1.00	0.02	38,38,38,38	0
58	MG	DA	3185	1/1	1.00	0.03	28,28,28,28	0
58	MG	DB	207	1/1	1.00	0.03	36,36,36,36	0
58	MG	DA	3098	1/1	1.00	0.02	27,27,27,27	0
58	MG	DA	3187	1/1	1.00	0.02	18,18,18,18	0
58	MG	AA	1619	1/1	1.00	0.04	80,80,80,80	0
58	MG	DA	3189	1/1	1.00	0.02	47,47,47,47	0
58	MG	DA	3190	1/1	1.00	0.01	29,29,29,29	0
58	MG	DA	3191	1/1	1.00	0.03	16,16,16,16	0
58	MG	DD	302	1/1	1.00	0.06	49,49,49,49	0
58	MG	DM	202	1/1	1.00	0.03	47,47,47,47	0
58	MG	DA	3100	1/1	1.00	0.04	29,29,29,29	0
58	MG	DA	3011	1/1	1.00	0.02	27,27,27,27	0
58	MG	AA	1629	1/1	1.00	0.04	30,30,30,30	0
58	MG	DA	3103	1/1	1.00	0.02	37,37,37,37	0
58	MG	DA	3104	1/1	1.00	0.02	20,20,20,20	0
58	MG	DA	3105	1/1	1.00	0.01	32,32,32,32	0
58	MG	AA	1617	1/1	1.00	0.03	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	AA	1621	1/1	1.00	0.05	63,63,63,63	0
58	MG	DA	3108	1/1	1.00	0.01	28,28,28,28	0
58	MG	DA	3109	1/1	1.00	0.03	7,7,7,7	0
58	MG	DA	3110	1/1	1.00	0.01	19,19,19,19	0
58	MG	DA	3111	1/1	1.00	0.02	15,15,15,15	0
58	MG	DA	3112	1/1	1.00	0.02	25,25,25,25	0
58	MG	DA	3113	1/1	1.00	0.05	75,75,75,75	0
58	MG	DA	3114	1/1	1.00	0.08	17,17,17,17	0
58	MG	DA	3115	1/1	1.00	0.02	28,28,28,28	0
58	MG	DA	3116	1/1	1.00	0.02	23,23,23,23	0
58	MG	DA	3117	1/1	1.00	0.04	16,16,16,16	0
58	MG	AA	1638	1/1	1.00	0.01	51,51,51,51	0
58	MG	BA	1629	1/1	1.00	0.03	65,65,65,65	0
58	MG	AA	1622	1/1	1.00	0.03	73,73,73,73	0
58	MG	DA	3079	1/1	1.00	0.01	25,25,25,25	0
58	MG	DA	3122	1/1	1.00	0.02	27,27,27,27	0
58	MG	DA	3123	1/1	1.00	0.02	19,19,19,19	0
58	MG	DA	3124	1/1	1.00	0.01	19,19,19,19	0
58	MG	DA	3080	1/1	1.00	0.02	29,29,29,29	0
58	MG	DA	3126	1/1	1.00	0.05	44,44,44,44	0
58	MG	DA	3127	1/1	1.00	0.02	19,19,19,19	0
58	MG	DA	3128	1/1	1.00	0.01	34,34,34,34	0
58	MG	DA	3129	1/1	1.00	0.02	19,19,19,19	0
58	MG	DA	3130	1/1	1.00	0.04	52,52,52,52	0
58	MG	DA	3131	1/1	1.00	0.03	34,34,34,34	0
58	MG	DA	3132	1/1	1.00	0.02	12,12,12,12	0
58	MG	AA	1640	1/1	1.00	0.02	71,71,71,71	0
58	MG	DA	3134	1/1	1.00	0.01	38,38,38,38	0
58	MG	DA	3135	1/1	1.00	0.02	25,25,25,25	0
58	MG	DA	3136	1/1	1.00	0.01	9,9,9,9	0
58	MG	DA	3137	1/1	1.00	0.06	52,52,52,52	0
58	MG	DA	3138	1/1	1.00	0.02	30,30,30,30	0
58	MG	AA	1627	1/1	1.00	0.05	55,55,55,55	0
58	MG	DA	3140	1/1	1.00	0.02	38,38,38,38	0
58	MG	DA	3141	1/1	1.00	0.03	12,12,12,12	0
58	MG	DA	3142	1/1	1.00	0.04	20,20,20,20	0
58	MG	DA	3143	1/1	1.00	0.02	15,15,15,15	0
58	MG	DA	3144	1/1	1.00	0.03	52,52,52,52	0
58	MG	DA	3145	1/1	1.00	0.03	38,38,38,38	0
58	MG	AA	1659	1/1	1.00	0.02	55,55,55,55	0
58	MG	DA	3084	1/1	1.00	0.02	46,46,46,46	0
58	MG	DA	3085	1/1	1.00	0.03	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	DA	3149	1/1	1.00	0.04	55,55,55,55	0
58	MG	DA	3150	1/1	1.00	0.02	18,18,18,18	0
58	MG	DA	3151	1/1	1.00	0.03	61,61,61,61	0
58	MG	DA	3152	1/1	1.00	0.04	38,38,38,38	0
58	MG	DA	3153	1/1	1.00	0.04	26,26,26,26	0
58	MG	DA	3154	1/1	1.00	0.01	38,38,38,38	0
58	MG	DA	3086	1/1	1.00	0.01	15,15,15,15	0
58	MG	DA	3087	1/1	1.00	0.02	21,21,21,21	0
58	MG	DA	3088	1/1	1.00	0.02	25,25,25,25	0
58	MG	DA	3158	1/1	1.00	0.02	27,27,27,27	0
58	MG	AA	1650	1/1	1.00	0.06	65,65,65,65	0
58	MG	DA	3160	1/1	1.00	0.04	31,31,31,31	0
58	MG	DA	3161	1/1	1.00	0.01	29,29,29,29	0
58	MG	DA	3162	1/1	1.00	0.02	42,42,42,42	0
58	MG	DA	3163	1/1	1.00	0.02	27,27,27,27	0
58	MG	DA	3164	1/1	1.00	0.02	27,27,27,27	0
58	MG	DA	3090	1/1	1.00	0.02	4,4,4,4	0

6.5 Other polymers [i](#)

There are no such residues in this entry.