



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 2, 2021 – 04:50 pm BST

PDB ID : 6I7V  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.1

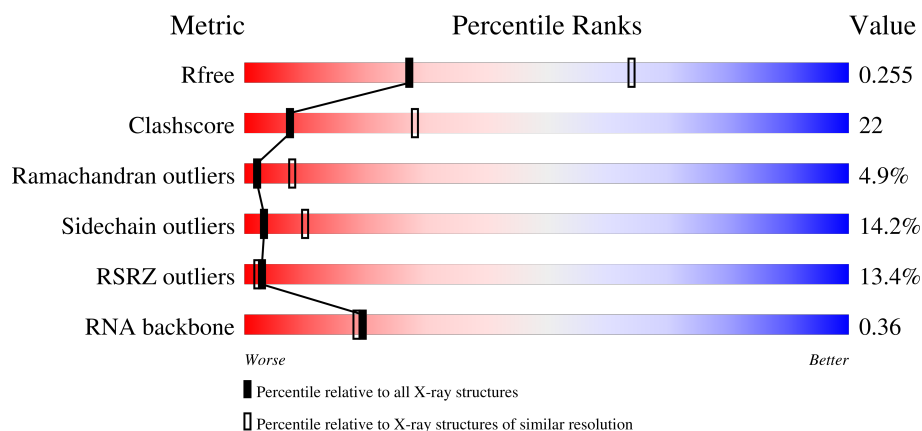
# 1 Overall quality at a glance ⓘ

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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>16%</div> <div>40%</div> <div>37%</div> <div>7%</div> </div>
2	BA	1533	<div> <div>19%</div> <div>45%</div> <div>30%</div> <div>6%</div> </div>
3	DA	2903	<div> <div>7%</div> <div>37%</div> <div>43%</div> <div>12%</div> </div>
4	CA	2904	<div> <div>20%</div> <div>48%</div> <div>27%</div> <div>.</div> </div>

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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	% 70% 26% .
32	CH	148	32% 55% 34% 10% .
32	DH	148	31% 61% 30% 8% .
33	CJ	141	85% 38% 41% 19% .
33	DJ	141	67% 30% 47% 21% .
34	CK	142	22% 61% 35% .
34	DK	142	% 57% 35% 6% .
35	CL	123	39% 67% 26% 6% .
35	DL	123	66% 30% .
36	CM	144	60% 53% 39% 6% ..
36	DM	144	% 68% 25% 6% .
37	CN	136	49% 72% 25% .
37	DN	136	63% 35% .
38	CO	120	42% 52% 38% 10% .
38	DO	120	52% 38% 8% .
39	CP	117	66% 62% 29% 9% .
39	DP	117	68% 26% 7% .
40	CQ	114	37% 54% 39% 6% .
40	DQ	114	70% 24% 5% .
41	CR	117	44% 68% 28% .
41	DR	117	55% 36% 9% .
42	CS	103	62% 47% 45% 9% .
42	DS	103	57% 32% 11% .
43	CT	110	50% 54% 36% 9% .
43	DT	110	53% 31% 15% .

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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	3049	-	-	-	X
58	MG	CA	3084	-	-	-	X
58	MG	CA	3102	-	-	-	X
58	MG	CA	3154	-	-	-	X
58	MG	CA	3159	-	-	-	X
58	MG	CA	3173	-	-	-	X
58	MG	D5	102	-	-	-	X
59	PGE	DD	301	-	-	-	X
59	PGE	DT	202	-	-	-	X
60	MPD	DA	3072	-	-	-	X
60	MPD	DE	301	-	-	-	X
60	MPD	DE	302	-	-	-	X
60	MPD	DT	201	-	-	-	X
61	PG4	DR	202	-	-	X	-
63	PUT	DA	3037	-	-	X	-
63	PUT	DA	3054	-	-	X	-
63	PUT	DP	202	-	-	X	-
65	ACY	DA	3064	-	-	X	-
66	PEG	D1	102	-	-	-	X
66	PEG	DA	3063	-	-	-	X
66	PEG	DP	201	-	-	-	X
66	PEG	DQ	201	-	-	-	X
67	EDO	DA	3059	-	-	X	-
67	EDO	DA	3060	-	-	X	-

## 2 Entry composition [i](#)

There are 69 unique types of molecules in this entry. The entry contains 484785 atoms, of which 191884 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

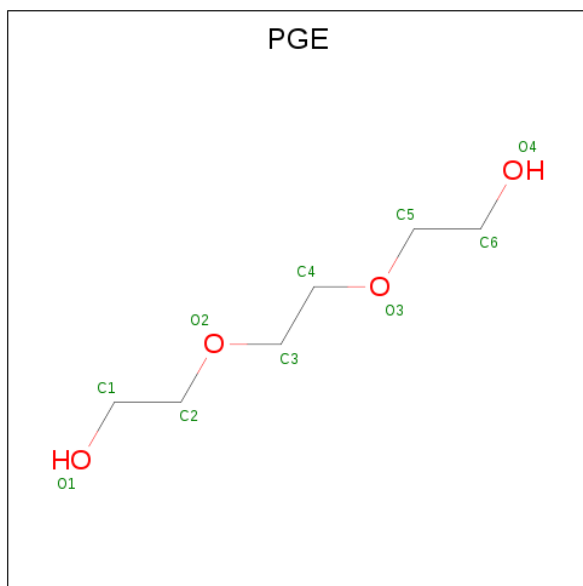
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	AA	57	Total	Mg	0	0
			57	57		
58	BA	49	Total	Mg	0	0
			49	49		
58	DA	156	Total	Mg	0	0
			156	156		
58	CA	176	Total	Mg	0	0
			176	176		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DB	4	Total	Mg	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 (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



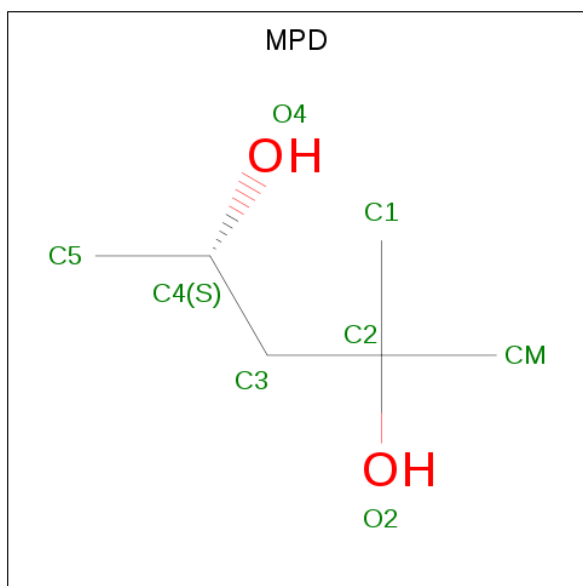
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	AA	1	Total	C	H	O	0	0
			24	6	14	4		
59	DA	1	Total	C	H	O	0	0
			24	6	14	4		

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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 (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



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 (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



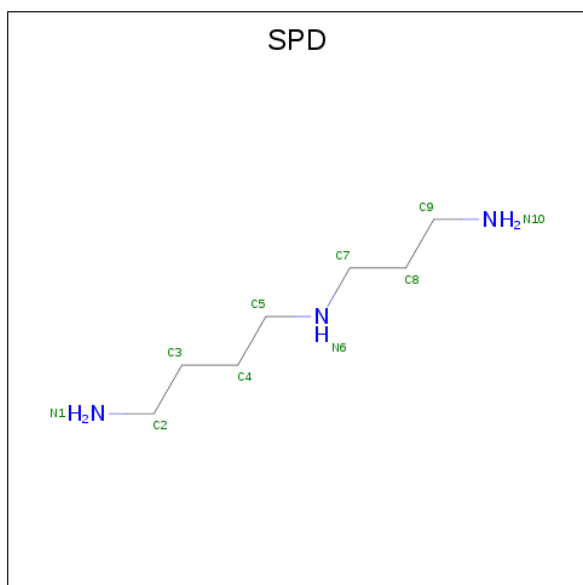
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	BA	1	Total	C	O	0	0
			13	8	5		
61	DA	1	Total	C	O	0	0
			13	8	5		
61	DQ	1	Total	C	O	0	0
			13	8	5		

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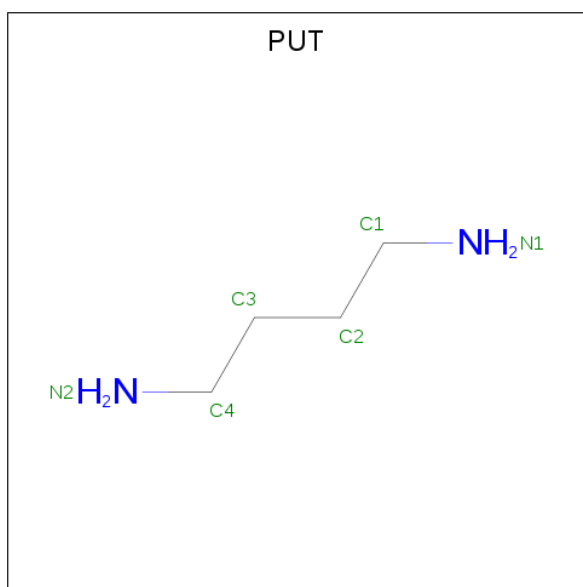
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	DR	1	Total	C	O	0	0
			13	8	5		
61	DS	1	Total	C	O	0	0
			13	8	5		

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



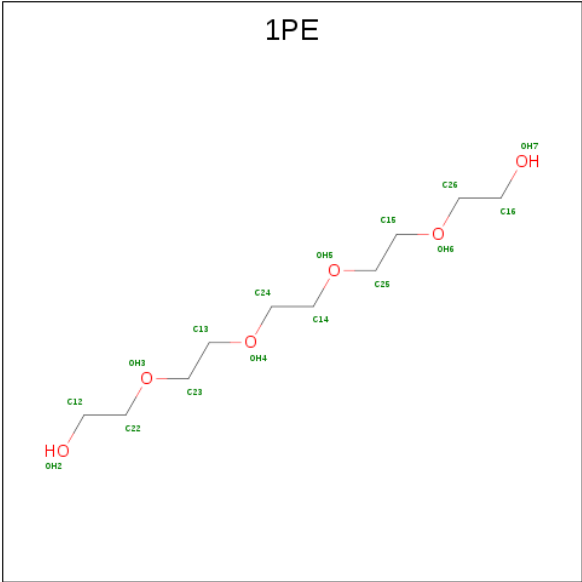
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	DA	1	Total	C	N	0	0
			10	7	3		
62	DA	1	Total	C	N	0	0
			10	7	3		
62	DA	1	Total	C	N	0	0
			10	7	3		

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



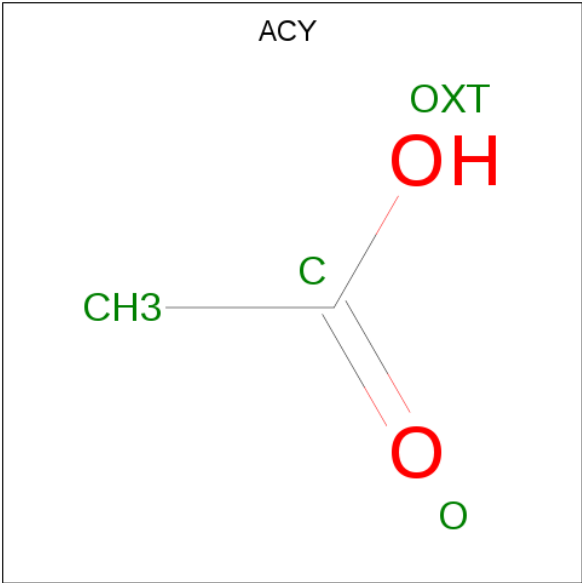
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	DA	1	Total	C	N	0	0
			6	4	2		
63	DA	1	Total	C	N	0	0
			6	4	2		
63	DA	1	Total	C	N	0	0
			6	4	2		
63	DA	1	Total	C	N	0	0
			6	4	2		
63	DM	1	Total	C	N	0	0
			6	4	2		
63	DP	1	Total	C	N	0	0
			6	4	2		
63	D5	1	Total	C	N	0	0
			6	4	2		

- Molecule 64 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



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

- Molecule 65 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

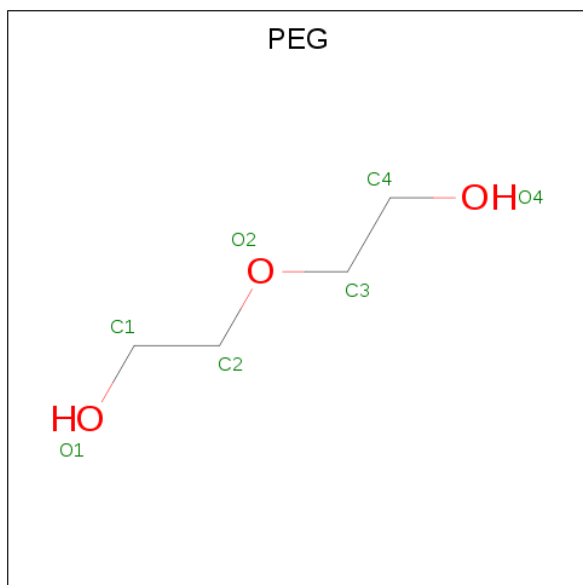
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
65	DA	1	Total	C	H	O	0	0
			7	2	3	2		

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



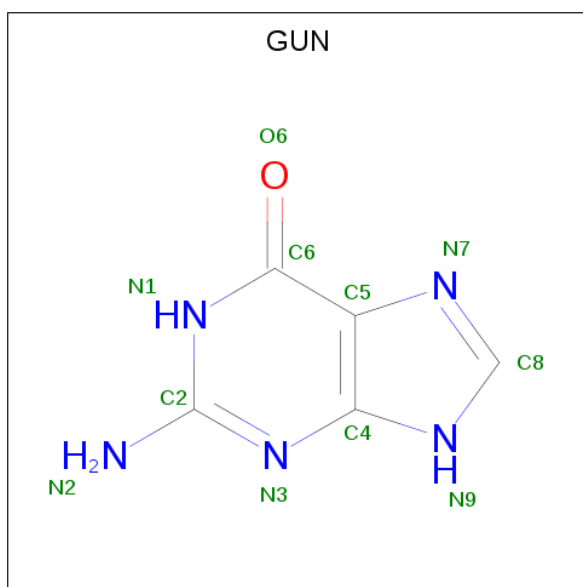
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			7	4	3		
66	DA	1	Total	C	O	0	0
			7	4	3		
66	DA	1	Total	C	O	0	0
			7	4	3		
66	DA	1	Total	C	O	0	0
			7	4	3		
66	DA	1	Total	C	O	0	0
			7	4	3		
66	DP	1	Total	C	O	0	0
			7	4	3		
66	DQ	1	Total	C	O	0	0
			7	4	3		
66	D1	1	Total	C	O	0	0
			7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

- Molecule 67 is 1,2-ETHANEDIOL (three-letter code: 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 (three-letter code: GUN) (formula: C<sub>5</sub>H<sub>5</sub>N<sub>5</sub>O).



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

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

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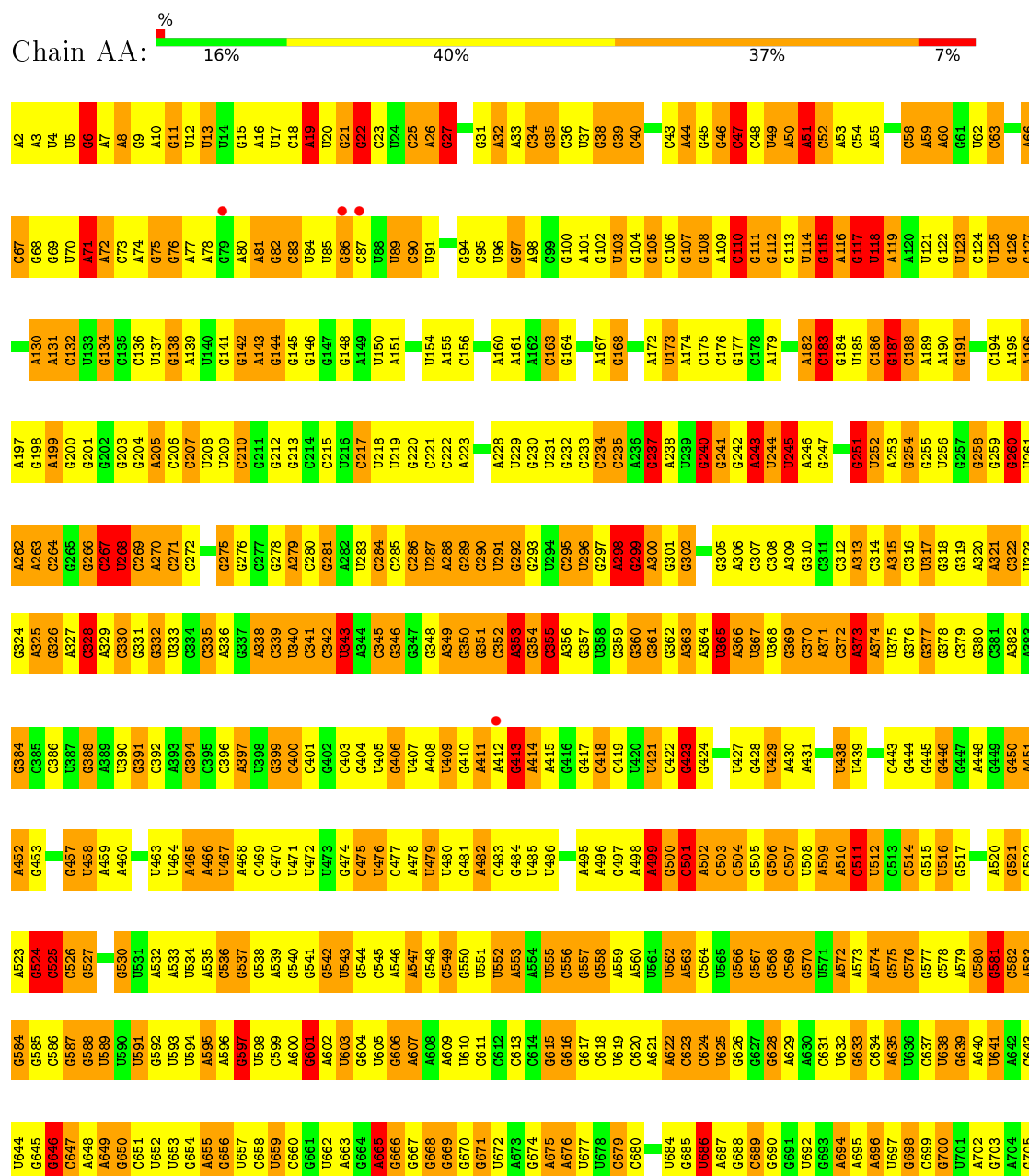
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	D2	4	Total 4	O 4	0	0
69	D3	24	Total 24	O 24	0	0
69	D4	27	Total 27	O 27	0	0
69	D5	9	Total 9	O 9	0	0

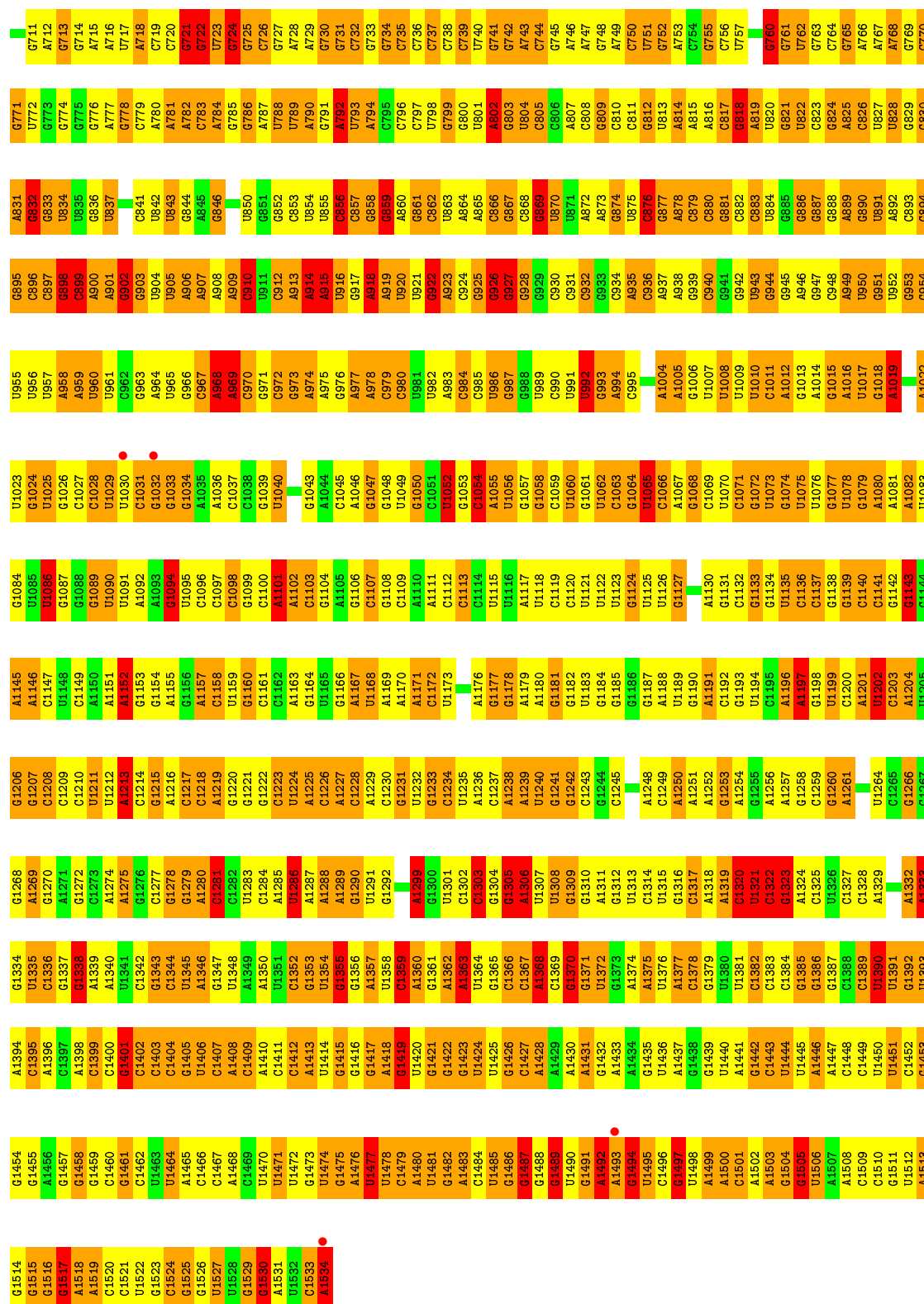


### 3 Residue-property plots

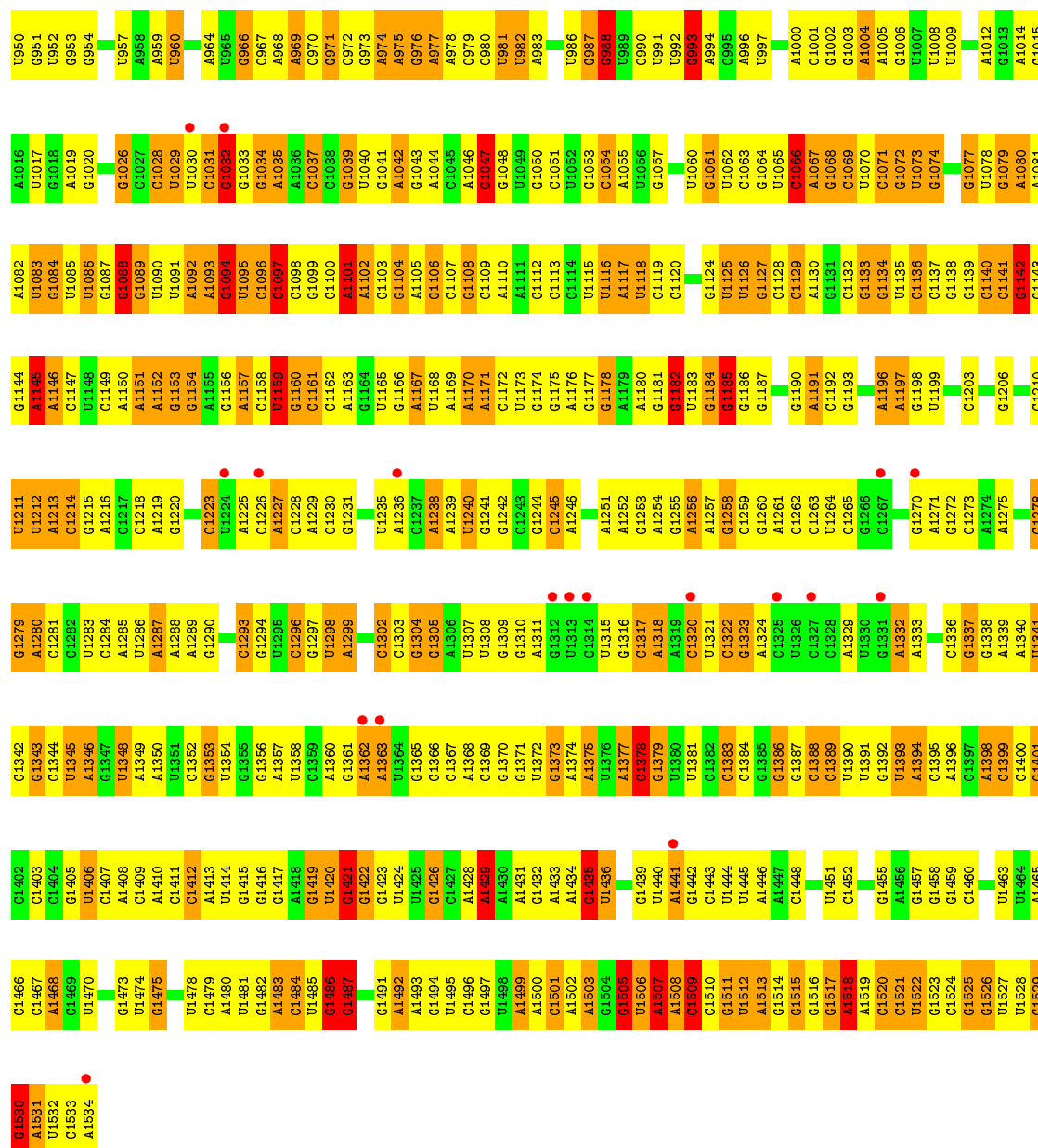
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

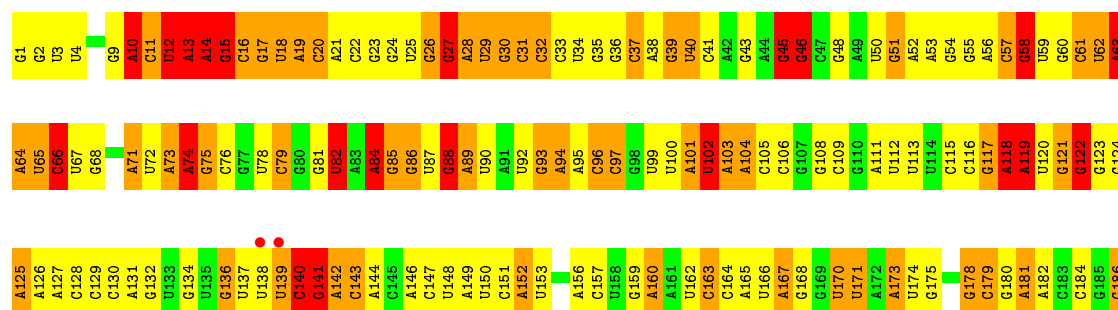




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A892	A893	C828	G765	A704	U641	A574	C513	G450	C386	U261	G198	U133	U5
C893	C894	G829	A766	G705	A642	G575	C514	A451	U387	U262	A199	G134	G6
G894	G895	G830	A767	A706	C643	G576	G515	A452	G388	A263	G200	C135	
C895	C896	G831	A768	U707	U644	G577	U516	A453	A389	C264	G201	C136	G8
G897	G898	C832	G769	C708	G645	C578	G517	G454	U390	G265	G202		A10
C898	C899	G833	C770	U709	A649	A579	C518	G455	G391	G266	G203	U140	G11
G900	G901	U834	U771	G710	G650	C580	C519	A456	C392	G267	G204	G141	U12
A901	A902	U835	G772	G711	A651	G581	A520	A457	A393	U268	G205	G142	U13
G903	G904		G773	A712	U653	C582	G521	U458	G394	C269	C206	A143	U14
A906	A907	C840	G774	G713	G654	A583	C522	A459	C395	A270	U203	G144	G15
G908	G909	C841	G775	G714	A655	G584	A523	A460	C396	C271	G207	G145	A16
U910	U911	U842	G776	A715	G656	C585	G524	A461	A397	C272	U209	G146	A17
A912	A913	U843	G777	A716	U657	C586	C525	G462	U398	U273	G210	G147	C18
C914	C915	G844	G778	U717	G658	G587	G526	U463	G399	A274	G211	G148	A19
A916	A917	U845	C779	A718	U659	G588	G527	U464	C400	G275	G212	A149	U20
G918	G919	A846	A780	C719	C660		C528	A465	C401	G276	G213	U150	G21
U920	U921	G847	A781	C720	G661	A595	G529	A466	G402	C277	C214	A151	G22
A922	A923	C848	A782	G721	U662	A596	G530	U467	C403	G278	C215	A152	C23
C924	C925	U849	C783	U722	U663	G597	U531	A468	G404	A279	U218	U154	U24
G926	G927	G850	A784	G723	A664	G598	A532	U469	U405	G280	U219	A155	U85
A928	A929	U851	G785	U724	G665	C599	A533	G470	U407	G281	G220	C156	C86
C930	C931	G852	A786	G725	U666	A600	U534	U473	A408	A282	C221	U157	C87
G932	G933		A787	C726	G667	U603	C536	G474	U409	C284	C222	U158	U88
A934	A935	C855	G788	G727	G668	G604	G537	U475	G410	G350	A223	G159	U91
C936	C937	U856	A789	A728	U669	U605	G538	C477	A411	G351	U224	A160	U92
G938	G939	G857	G790	G730	G670		A539	A478	A412	C352	G227	A161	G94
A940	A941	U858	A791	G731	G671	A608	G540	U479	G413	A162	U228	A162	C95
C942	C943	G859	C792	C732	U672	A609	G541	U480	A414	C163	A229	C163	C96
G944	G945	C860	G793	G733	A673	U610	G542	G481	A415	G164	G230	G164	C97
A946	A947	U861	C794	G734	G674	C611	U543	A482	G416	G165	U231	U166	C99
C948	C949	G862	G795	G735	U675	C612	G544	C483	G417	G292			
G950	G951	U863	C796	C736	A676	C613	C545	G484	C418	G293			
A952	A953	G864	A797	G737	U677	C614	C546	U485	C419	U294			
C954	C955	U865	G798	C738	U678	G615	A547	U486	G420	G295	C234	G168	G39
G956	G957	C866	U801	C739	C679	G616	G548	A487	U421	U296	C235	C169	C40
A958	A959	U867	A802	U740	C680	G617	C549	C488	C422	G297	A236	G104	G41
C960	C961	G868	G803	G741	A681	C618	G550		G423	A298	G237	U170	G42
G962	G963	U869	U804	G742	G682	U619	U551	G491	G424	A363	U238	A171	C43
A964	A965	C870	C805	G743	G683	C620	U552	C492		A364	G239	A172	A44
C966	C967	U871	A806	C744	U684	A621	A553	C493	U427	U365	G241	A174	G45
G968	G969	G872	G807	G745	G685	A622	G556	G494	G428	U367	G242	C175	G46
A970	A971	C873	C808	A746	U686	C623	C557	A495	U429	A243	G111	C176	C48
C972	C973	U874	G809	A747	A687	C624	G558	A496	A430	U244	G112	G177	C49
G974	G975	G875	C810	G748	G688	U625	G559	G497	A431	U245	U114	C178	A50
A976	A977	U876	C811	A749	C689	G626	A560	A498	A432	A246	G115	A179	A51
C978	C979	G877	G812	C750	G690	G627	U561	U499	G433	G247	U116	U180	C52
G980	G981	U878	U813	U751	G691	G628	U562	G500	U434	C248	G117	A181	A53
A982	A983	C880	A814		U692	A629	U563	C501	U435	U249	U118	A182	C54
C984	C985	U879	C815	C754	G693	A630	A564	A502	C436	A250	U119	C186	A55
G986	G987	G881	A816	G755	A694	C631	C564	C503	U437	G251	A120	G187	U56
A988	A989	U882	C817	C756	A695	U632	G565	C504	U438	U252	G121	G188	C58
C990	C991	G883	G818	U757	A696	G633	G566	G505	U439	A253	U122	A181	A59
G992	G993	U884	A819	C758	U697	C634	G567	G506	C440	G254	U123	A182	A60
A994	A995	G885	U820	C759	U698	A635	G568	C507	A441	G255	G128	A183	G61
C996	C997	G886	G821	A759	C699	U636	C569	U508		U256	U129		U62
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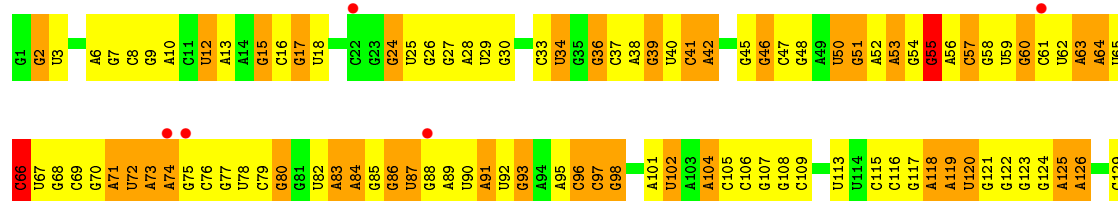


• Molecule 3: 23S ribosomal RNA



G1154	U1094	G1034	G974	G914	C854	A794	A734	G674	A614	G534	G493	G433	U373	G308	G247	G187
A1155	A1095	U1035	A975	C915	G855	C795	A735	A675	U615	U554	G494	U434	A374	A309	G248	G188
A1156	U1096	G1036	G976	G916	G856	C796	A736	A676	A616	G555	G495	U435	G375	A310	C249	G189
G1157	U1097	G1037	G977	G917	G857	C797	A737	A677	G617	G556	G496	C436	G376	A311	C250	A190
U1158	A1098	G1038	G978	A918	G858	C798	A738	G678	G618	C557	G497	U437	G377	G312	A251	A191
U1159	A1099	G1039	G979	A919	G859	C799	A739	G679	G619	C558	G498	U438	G378	G313	C252	C192
G1160	C1100	A1040	A980	A820	U860	A800	C740	C680	G620	C559	U499	U439	G379	C314	C253	U193
C1161	U1101	G1041	A981	C921	A861	G801	U741	G681	A621	C560	G500	C440	G380	G315	G254	G194
G1162	C1102	G1042	C982	C922	G862	A802	A742	G682	G622	G561	A501	U441	G381	C316	A255	A195
G1163	A1103	C1043	A983	G923	A863	U803	A743	U683	G623	U562	A502	U442	C382	G317	A256	A196
C1164	C1104	G1044	A984	G924	G864	A804	U744	G684	C624	A563	A503	U443	C383	C318	C257	A197
A1165	U1105	C1045	C985	A925	G865	G805	G745	A685	G625	C564	A504	U444	G319	G319	G258	C198
G1166	G1106	A1046	C986	G926	A866	C806	U746	U686	A626	C565	A505	U445	C385	A320	G259	A199
C1167	G1107	G1047	C987	A927	G867	U807	U747	C687	A627	U566	G506	U446	G386	U321	G260	U200
G1168	U1108	A1048	A988	A928	G868	G808	G748	U688	G628	U567	A507	U447	U387	A322	G261	C201
A1169	C1109	C1049	G989	U929	G869	G809	A749	A689	G629	U568	U508	U448	G388	C323	A262	U202
G1170	G1110	A1050	A990	G930	U870	U810	A750	G690	A630	U569	C509	U449	G389	A324	G263	A203
C1171	A1111	C1051	C991	U931	U871	U811	A751	G691	A631	U570	C510	U450	U390	G325	C264	A204
G1172	U1112	C1052	C992	U932	U872	C812	A752	G692	A632	U571	U511	U451	A391	G326	G265	G205
U1173	G1113	C1053	G993	A933	C873	U813	A753	A693	A633	U572	G512	U452	U392	G327	G266	U206
U1174	C1114	A1054	C994	U934	G874	C814	U754	A694	G634	U573	A513	U453	C393	U328	C267	A207
A1175	G1115	G1055	C995	G935	G875	C815	U755	G695	U635	A574	A514	U454	C394	G329	C268	C208
U1176	G1116	G1056	A996	A936	C876	C816	A756	G696	G636	A575	A515	U455	U395	A330	C269	C209
G1177	G1117	A1057	G997	G937	A877	C817	G757	G697	A637	U576	C516	U456	G396	C331	A270	C210
C1178	U1118	U1058	C998	G938	A878	G818	C758	U698	G638	U577	C517	U457	U397	A332	G271	C211
G1179	U1119	G1059	U999	G939	G879	A819	G759	A699	U639	G578	G518	U458	C398	G333	A272	G212
U1180	G1120	U1060	A1000	G940	G880	A820	G760	G700	G640	U579	U519	U459	U399	C334	G273	A213
C1181	C1121	U1061	A1001	A941	G881	A821	A761	G701	U641	U580	G520	U460	U400	C335	C274	G214
G1182	G1122	G1062	G1002	G942	G882	G822	U762	U702	U642	C581	U521	U461	A401	C336	C275	G215
U1183	C1123	G1063	G1003	A943	G883	G823	G763	U703	A643	A582	A522	U462	A402	C337	U276	A216
U1184	G1124	C1064	U1004	C944	U884	U824	A764	G704	G644	G583	C523	U463	U403	G338	G277	A217
G1185	G1125	U1065	C1005	A945	C885	A825	C765	A705	G645	C584	G524	U464	A404	U339	A218	A218
U1186	C1126	U1066	C1006	A946	A	U826	U766	A706	U646	G585	U525	U465	U405	A340	A219	A219
G1187	A1127	A1067	C1007	A947	U	U827	U767	G707	G647	A586	C526	U466	G406	C341	C281	G220
U1188	G1128	G1068	A1008	C948	C	U828	U768	G708	G648	C587	G527	U467	G407	A342	A282	A221
A1189	A1129	A1069	A1009	G949	C	A829	U769	U709	G649	U588	A528	G468	G408	C343	G283	A222
G1190	U1130	A1070	A1010	G950	C	G830	G770	U710	C650	U589	A529	U469	G409	G344	U284	A223
C1191	G1131	G1071	G1011	C951	G	G831	G771	G711	G651	A590	G530	U470	G410	A344	G285	U224
G1192	U1132	C1072	U1012	G952	A892	U832	G772	G712	U652	U591	C531	U471	A411	A345	U286	C225
C1193	A1133	A1073	C1013	G953	A893	A833	U773	G713	U653	A592	A532	U472	G412	A346	G287	A226
A1194	A1134	G1074	A1014	G954	U894	G834	G774	U714	A654	U593	G533	G473	C413	C351	U288	A227
G1195	C1135	C1075	U1015	U955	U895	C835	G775	A715	A655	U594	U534	U474	C414	A352	G289	C228
C1196	G1136	C1076	G1016	G956	A896	G836	G776	A716	G656	C595	G535	U475	A415	C353	U290	C229
G1197	G1137	A1077	G1017	C957	G897	C837	G777	G717	U657	U596	G536	U476	U416	G354	G291	G230
U1198	G1138	U1078	U1018	U958	C898	C838	G778	A718	U658	G597	G537	U477	C417	U355	U292	A231
U1199	G1139	C1079	U1019	A959	A899	U839	U779	U719	G659	U598	A538	U478	C418	G356	U293	G232
C1200	A1080	A1080	A1020	A960	A900	C840	G780	U720	C660	A599	G539	U479	U419	C357	A294	A233
U1201	U1141	U1081	A1021	C961	C901	G841	A781	A721	A661	G600	C540	U480	U420	U358	G295	U234
G1202	A1142	G1082	G1022	G962	C902	U842	A782	A722	G662	C601	A541	U481	C421	G359	U296	U235
U1203	A1143	U1083	U1023	U963	C903	G843	A783	C723	G663	A602	C542	U482	A422	U360	G297	C236
	A1144	A1084	G1024	C964	G904	A844	G784	U724	G664	A603	G543	U483	A423	G361	G298	C237
G1206	C1145	A1085	A1025	C965	A905	A845	G785	U725	U665	G604	C544	U484	G424	A362	A299	A238
C1207	C1146	A1086	G1026	G966	U906	U846	C786	G726	A666	G605	U546	U485	G425	G363	A300	C239
G1208	A1147	G1087	A1027	U967	G907	U847	C787	U727	U667		U547	U486	C426	G364	G301	C240
U1209	U1148	A1088	A1028	C968	C908	C848	A788	G728	A668	A608	G548	U487	U427	U365	G302	A241
G1210	G1149	A1089	A1029	G969	A909	A849	A789	G729	G669	A609	G549	U488	A428	G366	G303	G242
C1211	C1150	A1090	C1030	U970	A910	U850	U790	A730	A670	C610	G549	U489	A429	U369	U304	U243
G1212	A1151	G1091	G971	C971	A911	C851	C791	A731	C671	G611	C550	U490	A430	G370	A244	A243
A1213	C1092	C1092	A1032	A972	C912	U852	A792	C732	C672	G612	G551	U491	U431	A371	G245	C244
A1214	C1153	G1093	U1033	A973	U913	C853	A793	G733	C673	A613	U552	U492	A432	G372	C246	C245

C2123	C2063	A2003	C1942	A1877	G1817	A1757	G1697	A1637	C1577	G1455	A1395	C1335	A1275	G1215
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C2066	C2066	G2006	U1946	C1880	A1820	C1760	A1700	A1640	A1580	U1458	G1398	G1338	C1278	G1218
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U2068	U2068	G2008	G1948	U1883	C1822	A1762	G1702	G1642	G1582	U1460	U1400	U1340	G1280	U1220
G2068	G2068	A2009	G1949	U1884	G1823	A1763	G1703	C1643	A1583	C1461	G1401	G1341	G1281	C1221
A2070	A2070	G2010	U1950	U1885	G1824	C1764	A1704	C1644	U1584	C1462	A1402	A1342	U1282	U1222
A2071	A2071	U2011	U1951	U1886	U1825	U1765	A1705	C1645	C1585	C1463	A1403	G1343	G1283	G1223
C2072	C2072	G2012	A1952	G1887	G1826	C1766	G1706	A1646	A1586	G1464	C1404	U1344	A1284	U1224
C2073	C2073	A2013	A1953	G1888	U1827	C1767	G1707	G1647	G1587	G1465	A1405	U1345	A1285	G1225
U2074	U2074	A2014	G1954	A1889	G1828	C1768	G1708	G1648	G1588	U1466	U1406	G1346	A1286	U1226
G2075	G2075	A2015	U1955	A1890	A1829	U1769	U1709	U1649	U1589	U1467	G1407	A1347	A1287	G1227
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A2077	A2077	U2017	C1957	C1892	G1831	C1771	A1711	G1651	A1591	A1469	U1409	C1349	C1289	C1229
U2078	U2078	G2018	C1958	C1893	C1832	A1772	U1712	A1652	C1592	A1470	G1410	C1350	C1290	G1230
U2079	U2079	A2019	G1959	C1894	C1833	A1773	G1713	G1653	A1593	C1471	U1411	C1351	C1291	U1231
A2080	A2080	A2020	A1960	C1895	U1834	C1774	U1714	A1654	U1594	C1472	U1412	U1352	G1292	G1232
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A2082	A2082	U2022	C1962	G1897	C1836	C1776	U1716	C1656	A1596	U1474	A1414	A1354	U1294	U1234
G2083	G2083	C2023	U1963	C1898	C1837	U1777	A1717	U1657	A1597	G1475	U1415	G1355	C1295	G1235
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G2087	G2087	G2027	C1967	C1901	U1841	U1781	G1721	G1661	G1601	G1479	A1419	A1359	G1299	G1239
U2088	U2088	U2028	G1968	G1903	G1842	U1782	A1722	U1662	U1602	C1480	A1420	G1360	G1300	U1240
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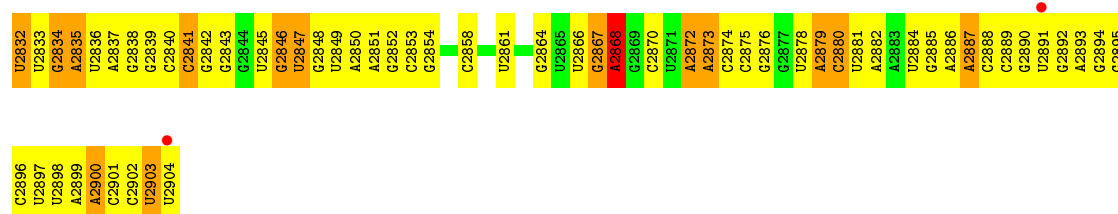


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A693	A694	G757	G758	G759	A693	A631	U569	G506	C444	G381	G318	C254	U194	G132
U694	U695	G757	G758	G759	U694	A632	U570	A507	C445	A382	G319	A255	A195	U135
G696	G697	G759	G760	G761	G696	A633	U571	A508	C446	C383	A320	A256	A196	G136
G698	G699	G760	G761	G762	G698	A634	U572	A509	C447	C384	A321	C257	A197	U137
A699	A700	G761	G762	G763	A699	A635	U573	A510	C448	C385	A322	C258	C198	U138
G700	G701	G762	G763	G764	G700	A636	U574	A511	C449	G386	A323	G259	A199	U139
U700	U701	G763	G764	G765	U700	A637	U575	A512	C450	U387	A324	G260	U200	C140
U702	U703	G764	G765	G766	U702	A638	U576	A513	C451	G388	G326	A261	C201	G141
U703	U704	G765	G766	G767	U703	A639	U577	A514	C452	G389	G327	A262	U202	A142
A704	A705	G766	G767	G768	A704	A640	U578	A515	C453	U390	G328	A263	A203	A143
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U707	U708	G768	G769	G770	U707	U642	U580	C517	C455	U392	G329	A265	G205	A144
G708	G709	G770	G771	G772	G708	A643	U581	A517	C456	C393	A330	G266	U206	C145
U709	U710	G771	G772	G773	U709	A644	U582	A518	C457	C394	C331	C267	A207	U148
U710	U711	G772	G773	G774	U710	A645	U583	A519	C458	U395	A332	C268	C208	U149
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U713	U714	G774	G775	G776	U713	U647	U585	A521	C460	U397	C334	A270	C210	C151
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U721	U722	G779	G780	G781	U720	U654	U590	A526	C465	U402	C341	A275	G215	A156
A723	A724	G780	G781	G782	U721	A655	U591	A527	C466	U403	C342	A276	A216	C157
G726	G727	G781	G782	G783	U722	A656	U592	A528	C467	U404	A343	A277	A217	U158
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G730	G731	G783	G784	G785	U724	U658	U594	A530	C469	G406	C345	U281	A219	A160
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U734	U735	G785	G786	G787	U726	U660	U596	A532	C471	G408	A347	U283	A221	G162
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G738	G739	G788	G789	G790	U729	U663	U599	A535	C474	U411	C350	U286	U224	A165
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C740	C741	G790	G791	G792	U731	U665	U601	A537	C476	U413	C352	U288	A226	A167
U741	U742	G791	G792	G793	U732	U666	U602	A538	C477	U414	A353	U289	G227	G168
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A751	A752	G798	G799	G800	U739	U673	U609	A545	C484	U421	C360	U295	U234	U174
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G818	G819	G802	G803	G804	U741	U675	U611	A547	C486	U423	C362	U297	U236	A176
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G821	G822	G805	G806	G807	U744	U678	U614	A550	C489	U426	C365	U300	C238	G179
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G825	G826	G811	G812	G813	U750	U684	U620	A556	C495	U432	A371	U306	U244	C184
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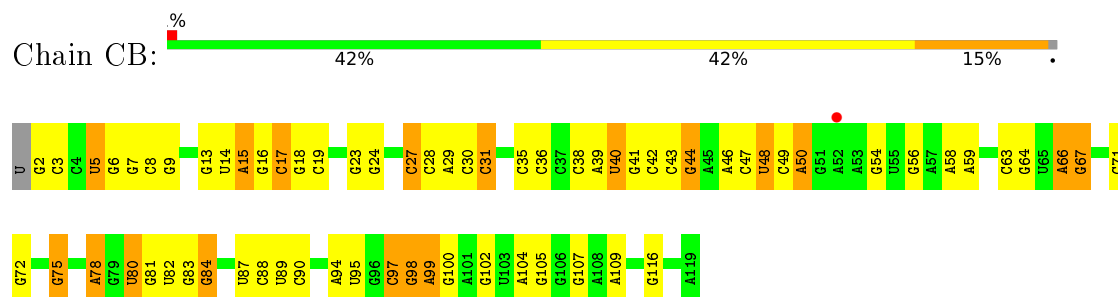
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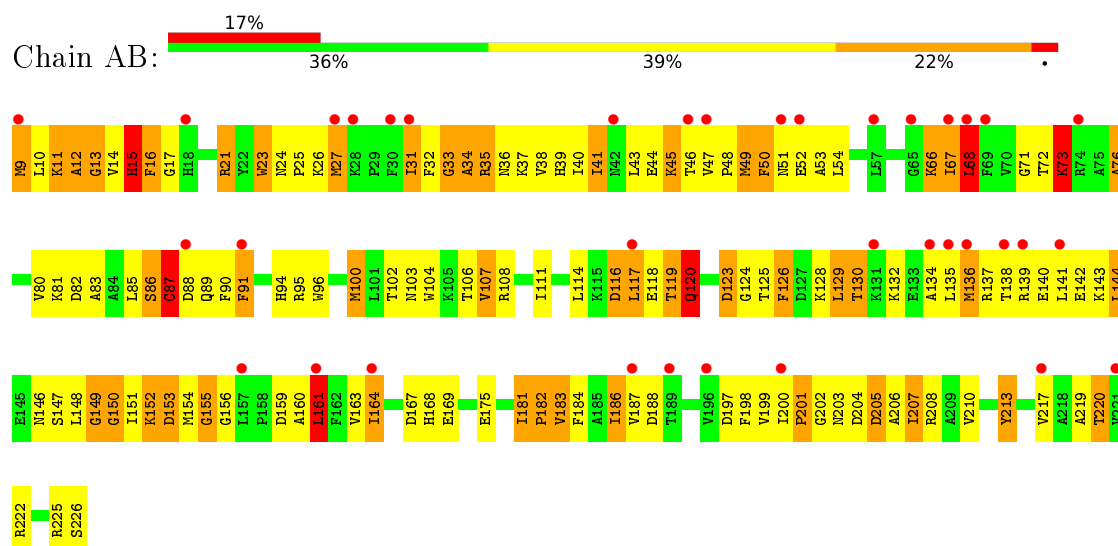
• Molecule 5: 5S ribosomal RNA



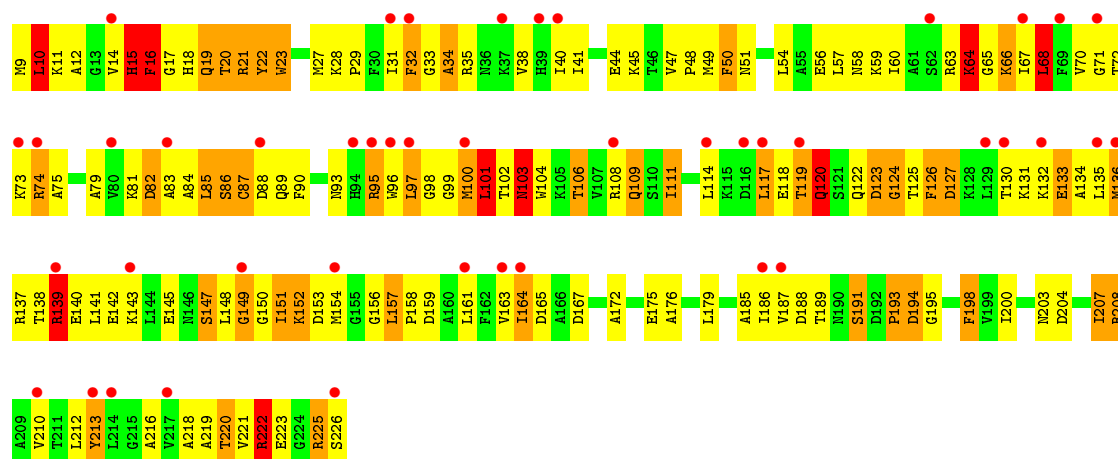
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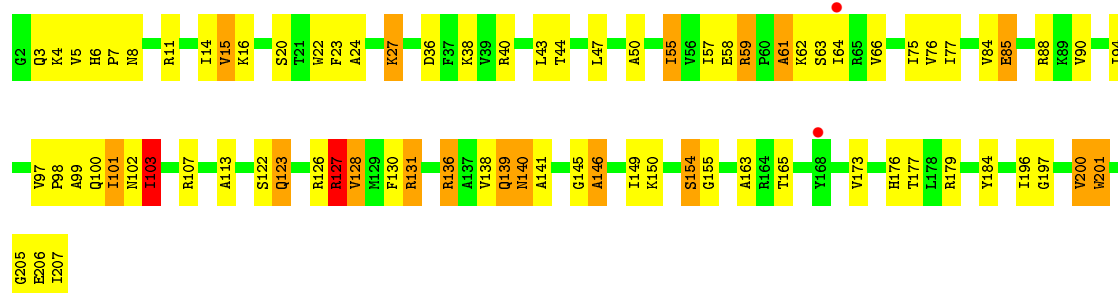
• Molecule 6: 30S ribosomal protein S2



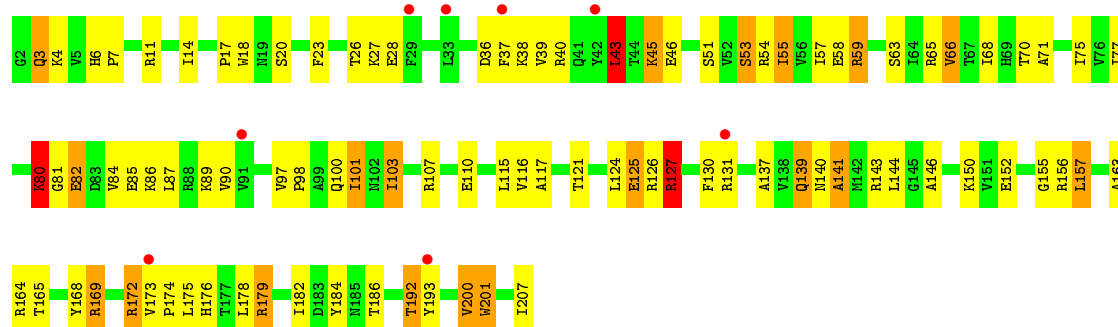
• Molecule 6: 30S ribosomal protein S2



• Molecule 7: 30S ribosomal protein S3

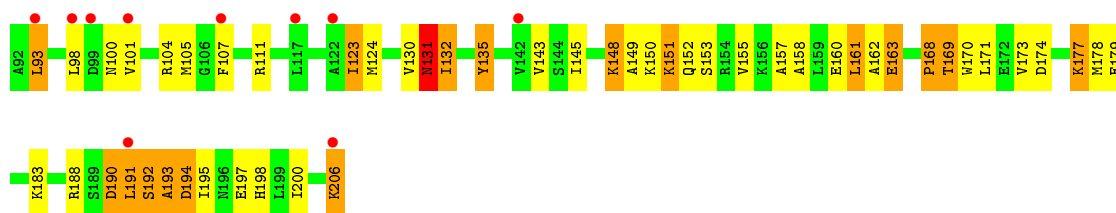


• Molecule 7: 30S ribosomal protein S3



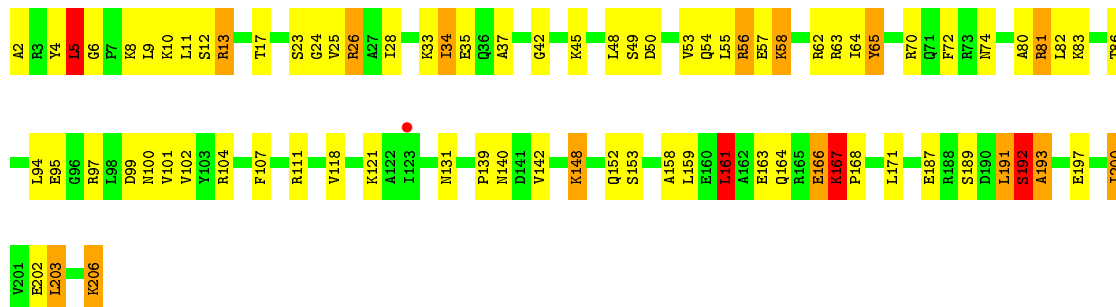
• Molecule 8: 30S ribosomal protein S4





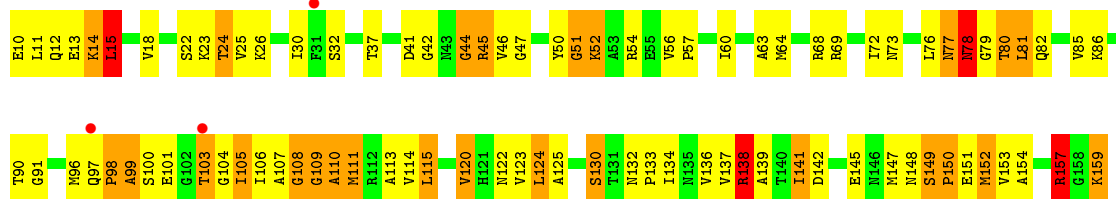
• Molecule 8: 30S ribosomal protein S4

Chain BD: 60% 31% 7% .



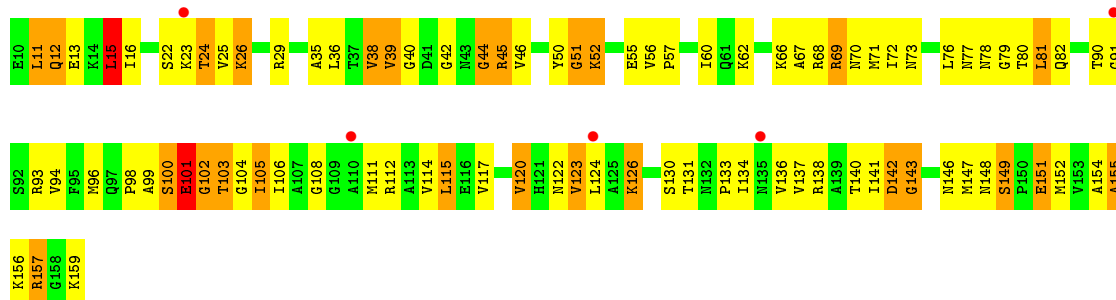
• Molecule 9: 30S ribosomal protein S5

Chain AE: 41% 39% 17% .



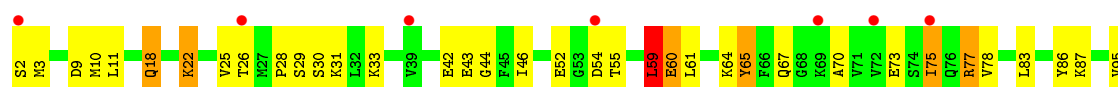
• Molecule 9: 30S ribosomal protein S5

Chain BE: 40% 41% 17% .



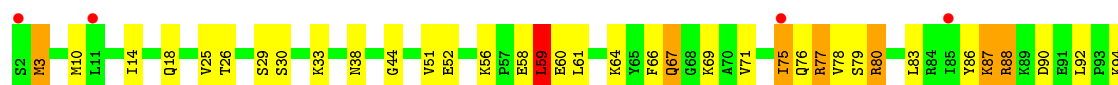
• Molecule 10: 30S ribosomal protein S6

Chain AF: 57% 34% 7% .

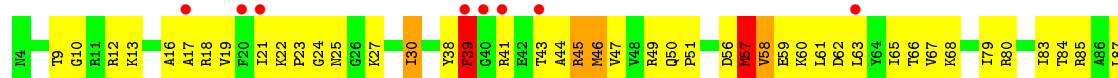




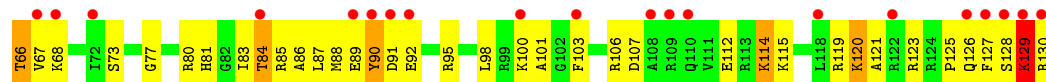
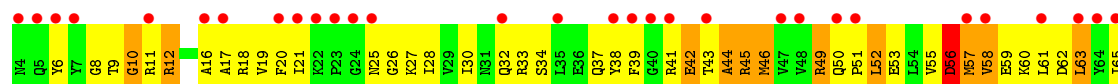
- Molecule 12: 30S ribosomal protein S8



- Molecule 13: 30S ribosomal protein S9



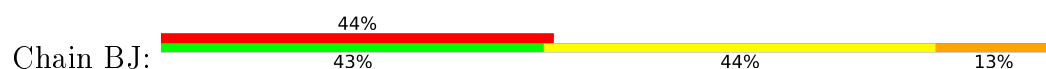
- Molecule 13: 30S ribosomal protein S9

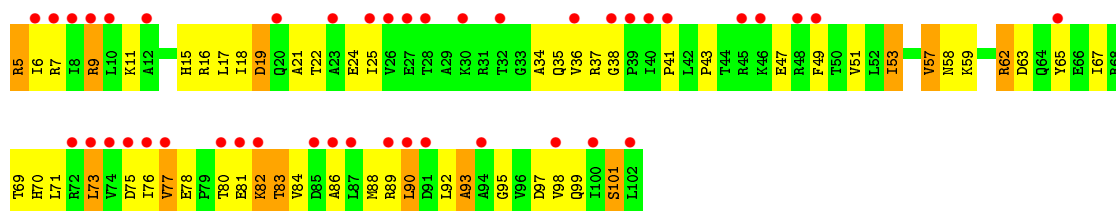


- Molecule 14: 30S ribosomal protein S10

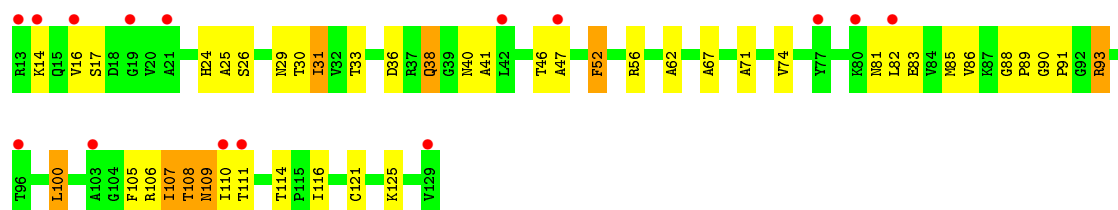


- Molecule 14: 30S ribosomal protein S10

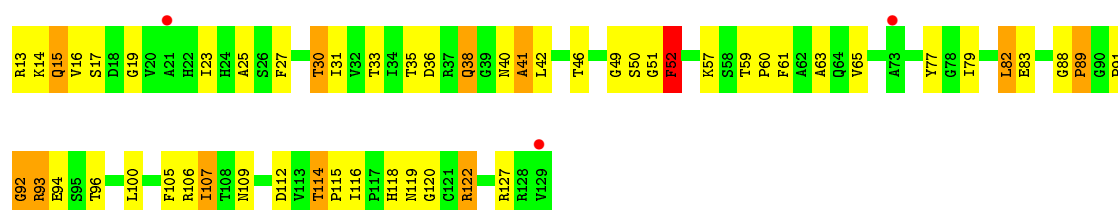




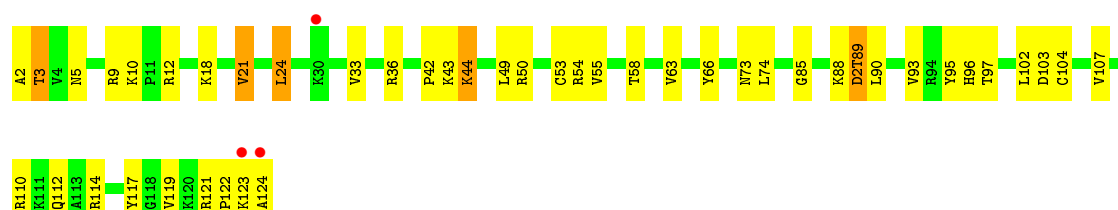
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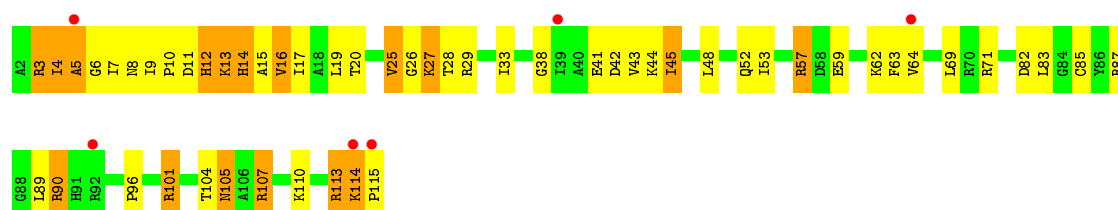
• Molecule 15: 30S ribosomal protein S11



• Molecule 16: 30S ribosomal protein S12

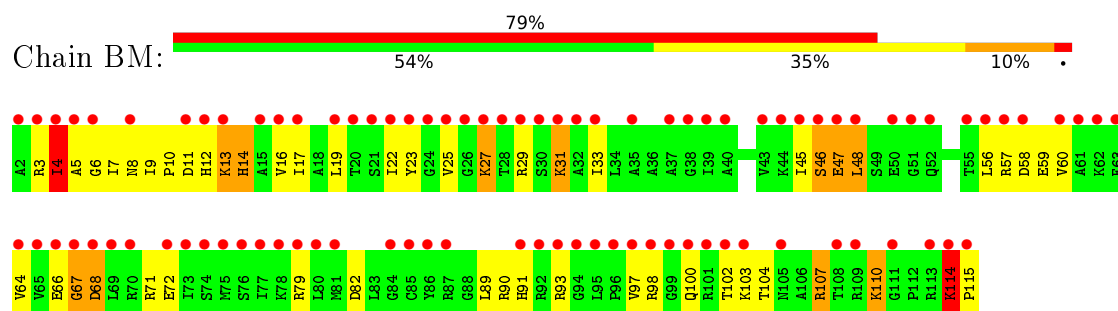


• Molecule 17: 30S ribosomal protein S13

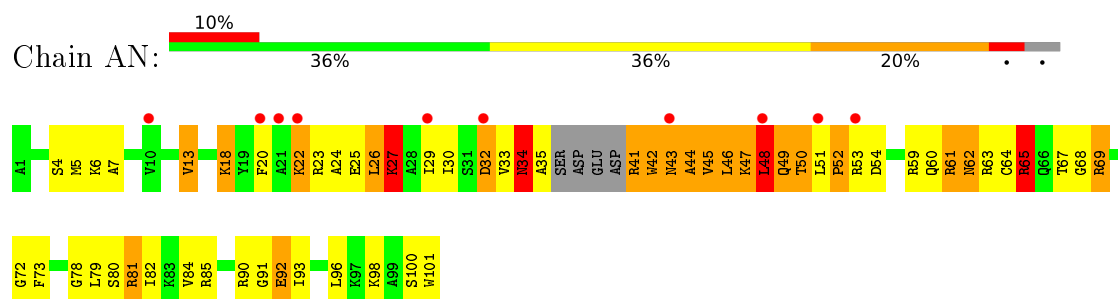




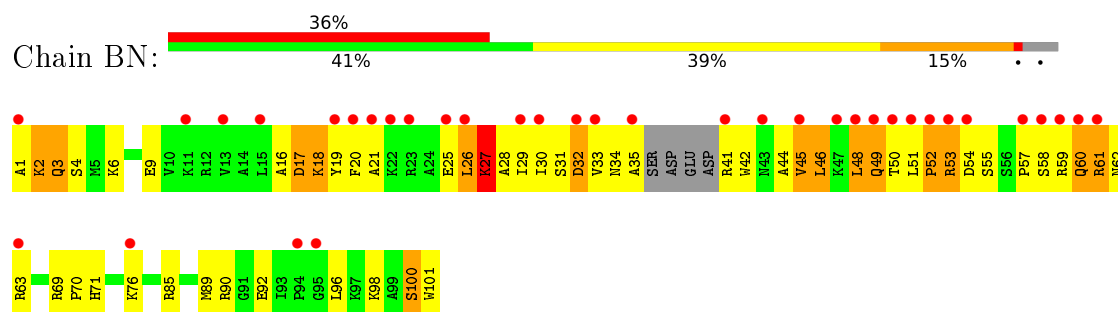
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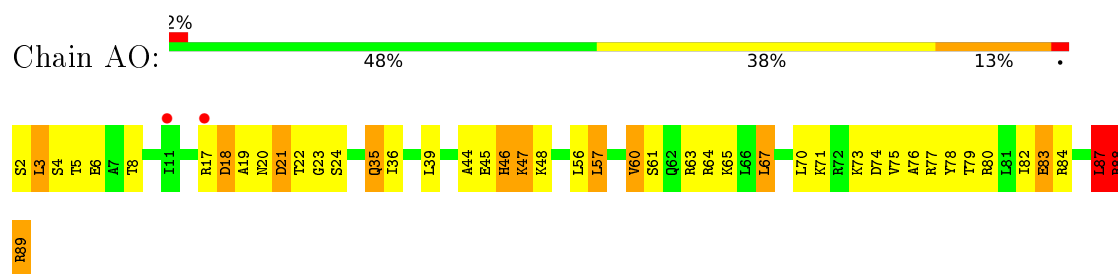
- Molecule 18: 30S ribosomal protein S14



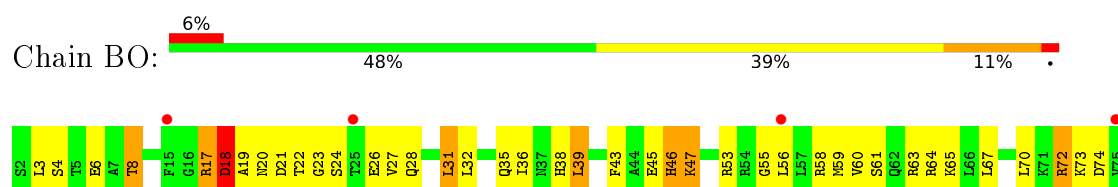
- Molecule 18: 30S ribosomal protein S14

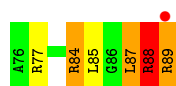


- Molecule 19: 30S ribosomal protein S15

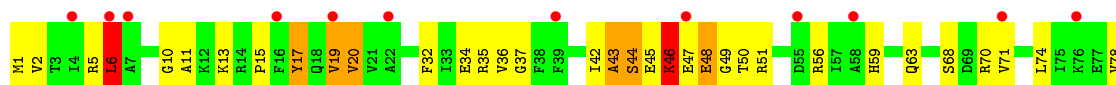


- Molecule 19: 30S ribosomal protein S15

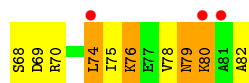
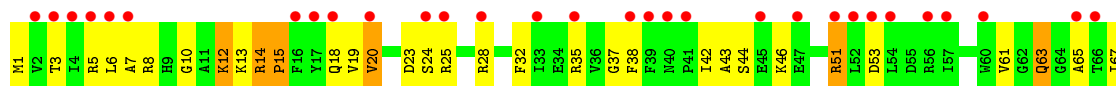
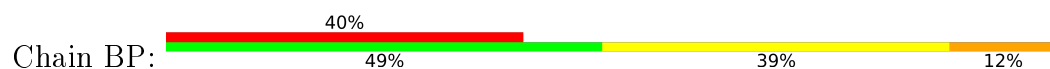




- Molecule 20: 30S ribosomal protein S16



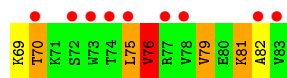
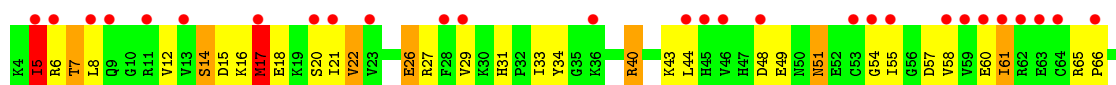
- Molecule 20: 30S ribosomal protein S16



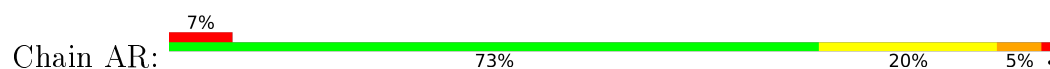
- Molecule 21: 30S ribosomal protein S17



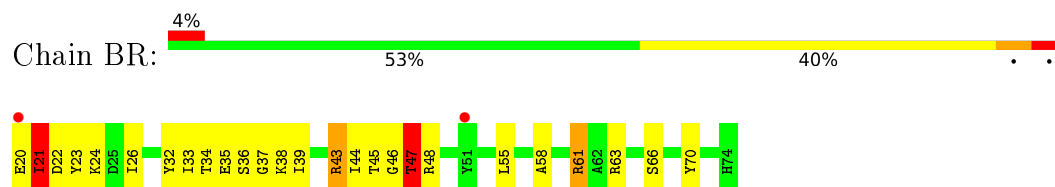
- Molecule 21: 30S ribosomal protein S17



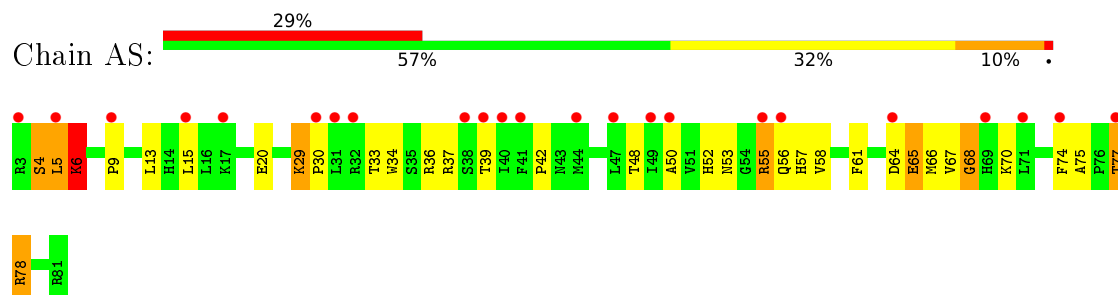
- Molecule 22: 30S ribosomal protein S18



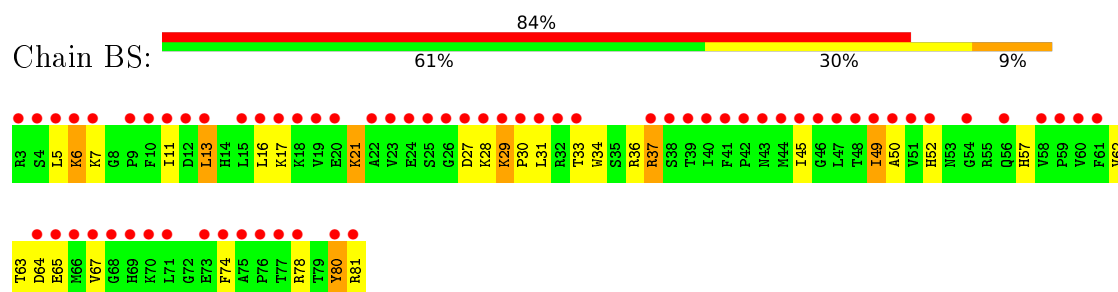
- Molecule 22: 30S ribosomal protein S18



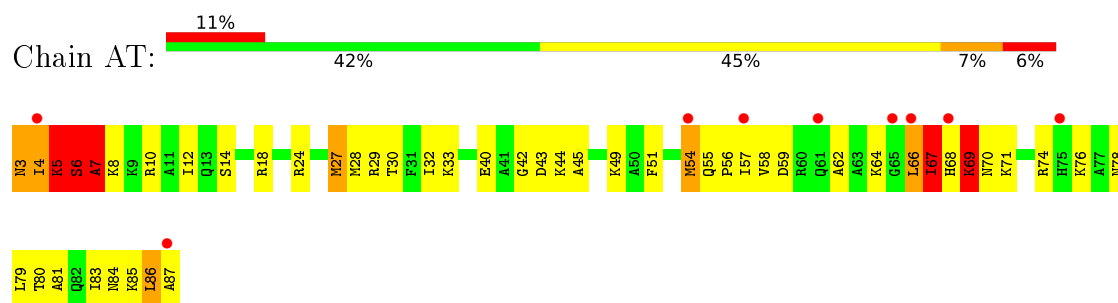
- Molecule 23: 30S ribosomal protein S19



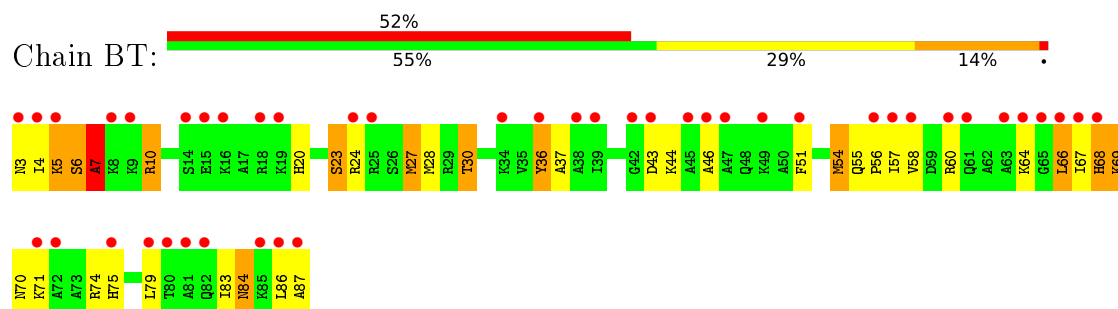
- Molecule 23: 30S ribosomal protein S19



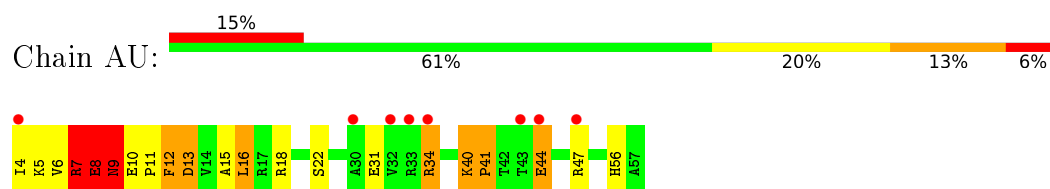
- Molecule 24: 30S ribosomal protein S20



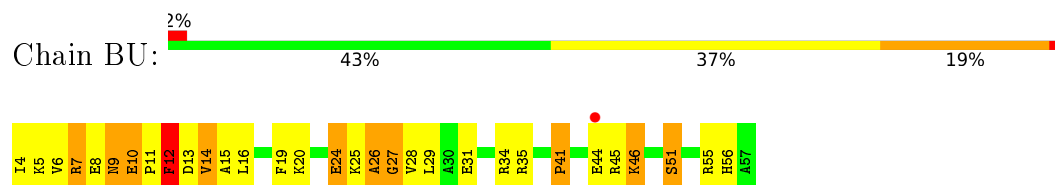
- Molecule 24: 30S ribosomal protein S20



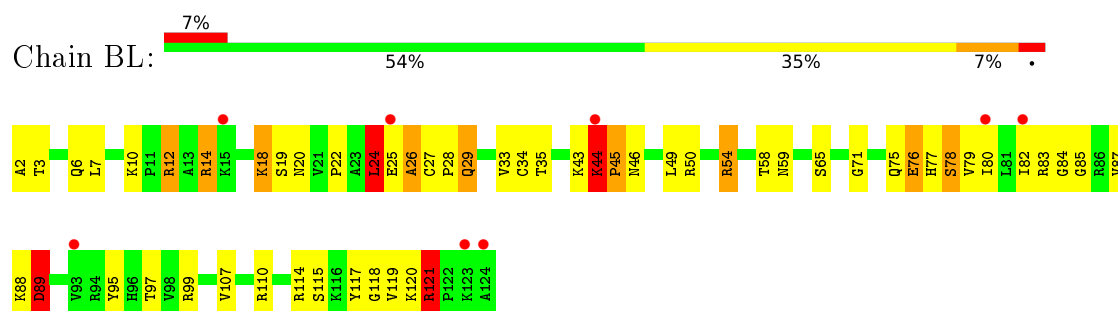
- Molecule 25: 30S ribosomal protein S21



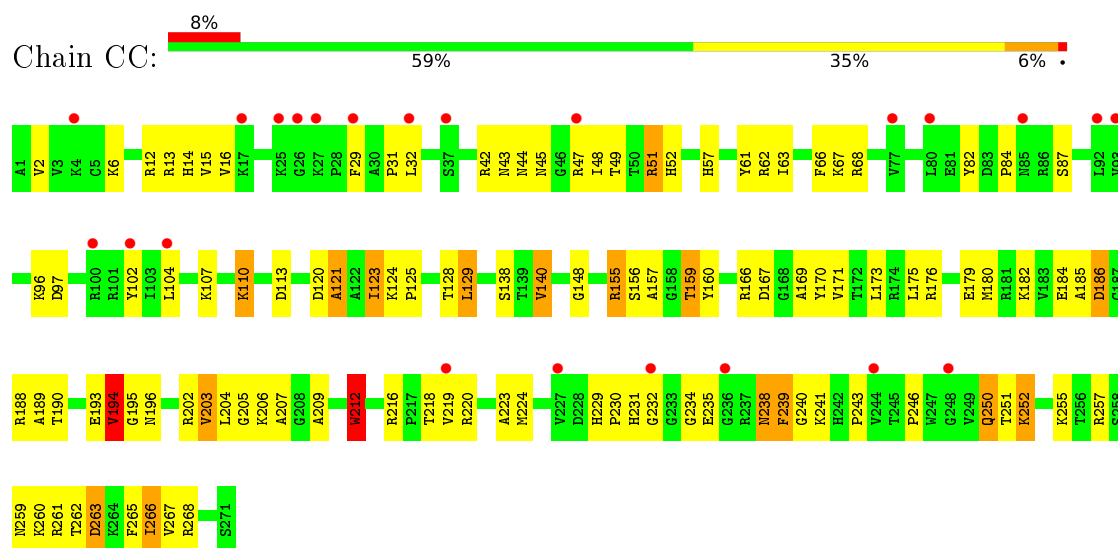
- Molecule 25: 30S ribosomal protein S21



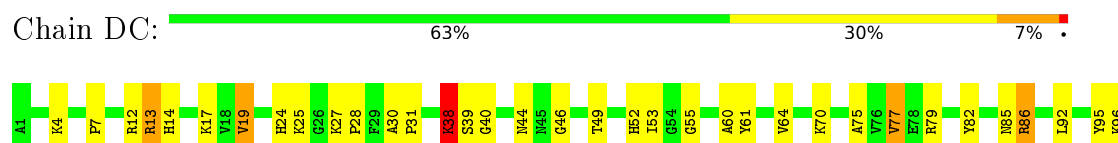
- Molecule 26: 30S ribosomal protein S12

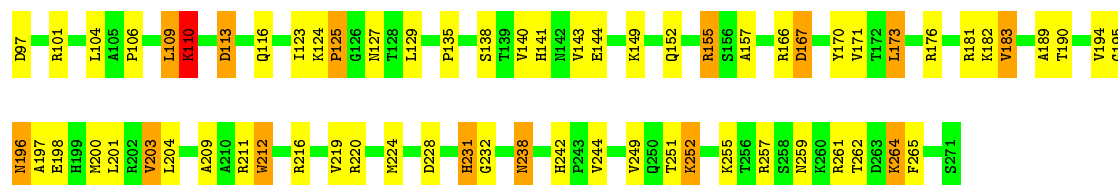


- Molecule 27: 50S ribosomal protein L2

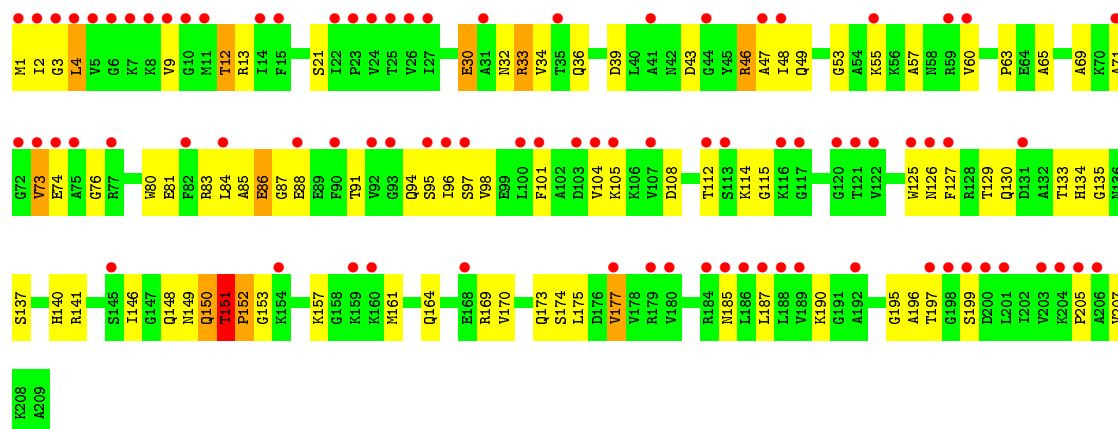
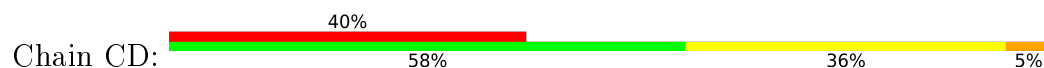


- Molecule 27: 50S ribosomal protein L2

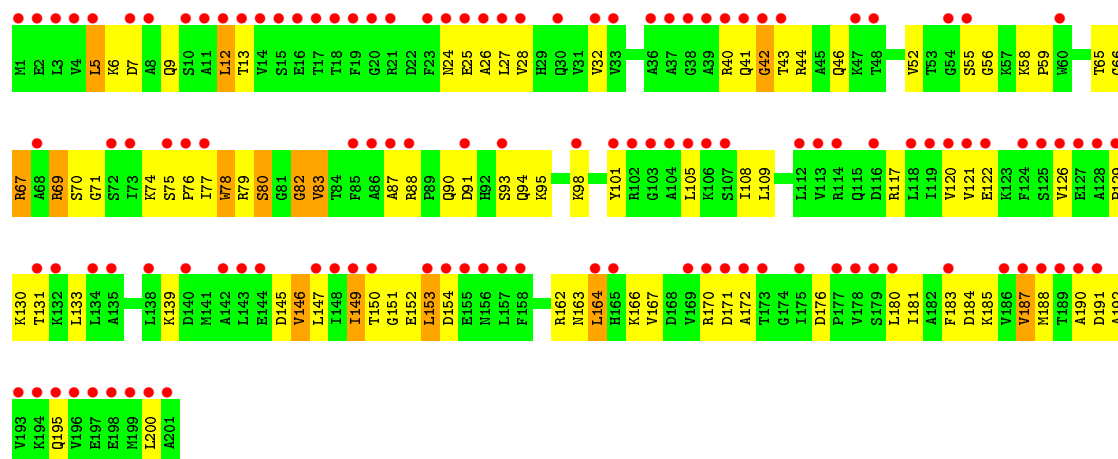




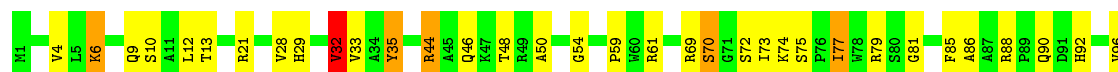
- Molecule 28: 50S ribosomal protein L3



- Molecule 29: 50S ribosomal protein L4

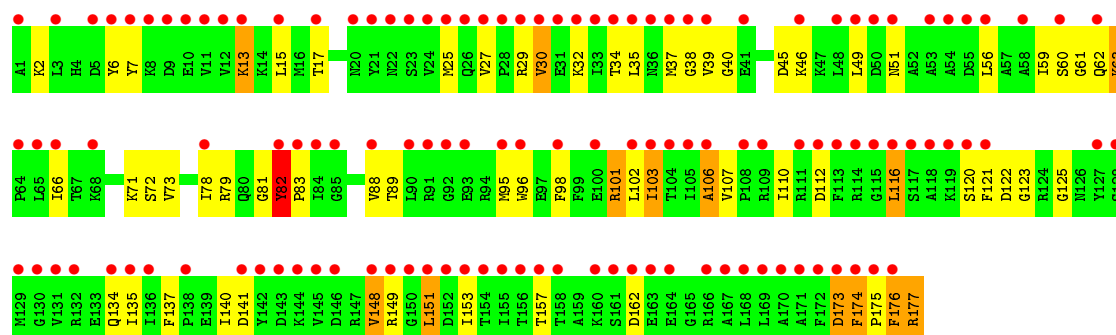
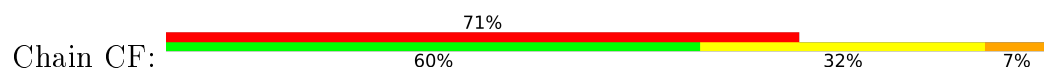


- Molecule 29: 50S ribosomal protein L4

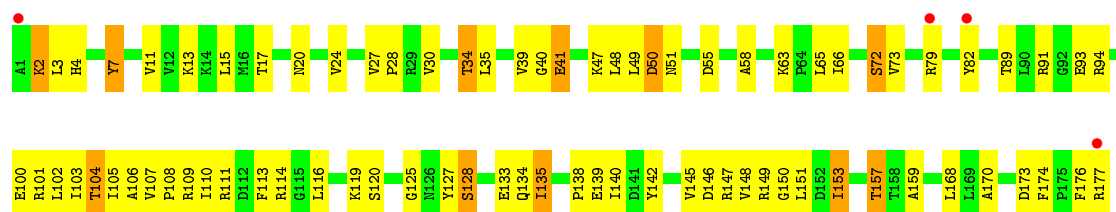




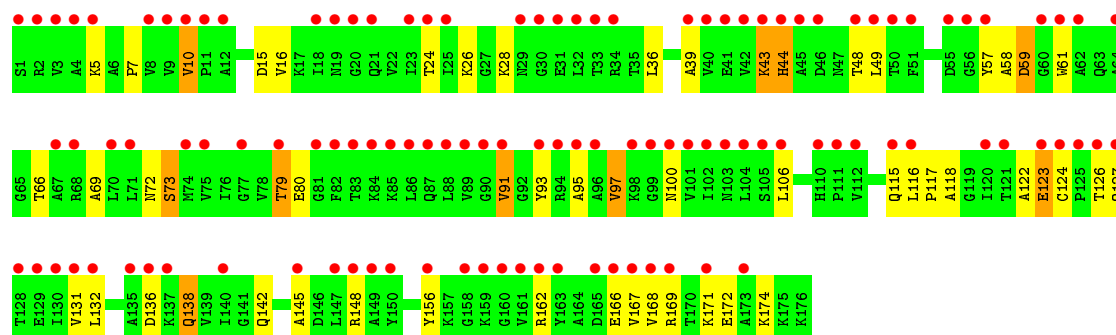
- Molecule 30: 50S ribosomal protein L5



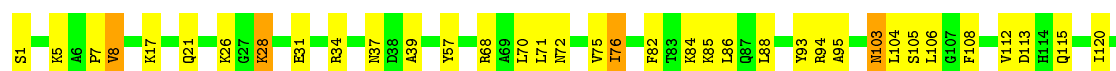
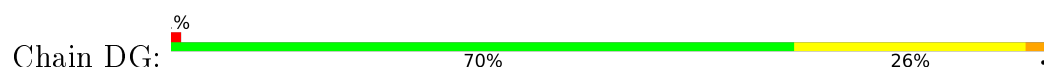
- Molecule 30: 50S ribosomal protein L5



- Molecule 31: 50S ribosomal protein L6

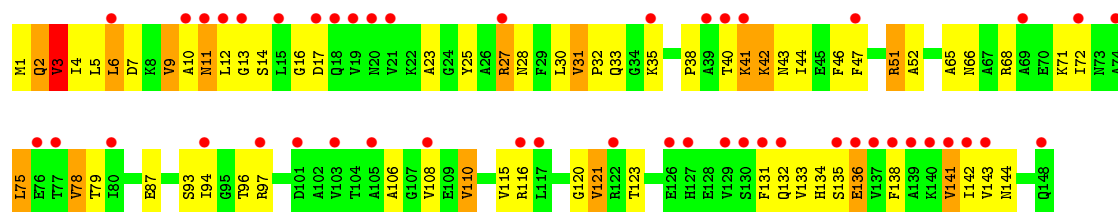


- Molecule 31: 50S ribosomal protein L6

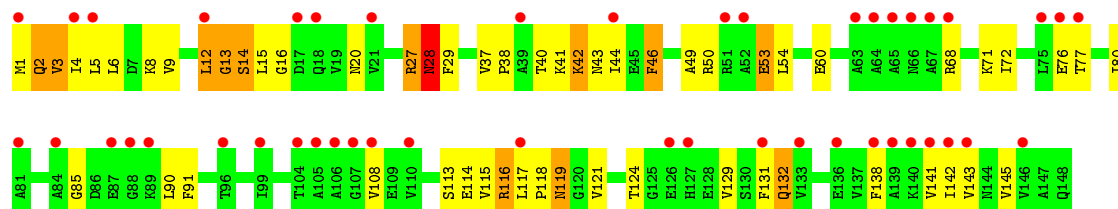




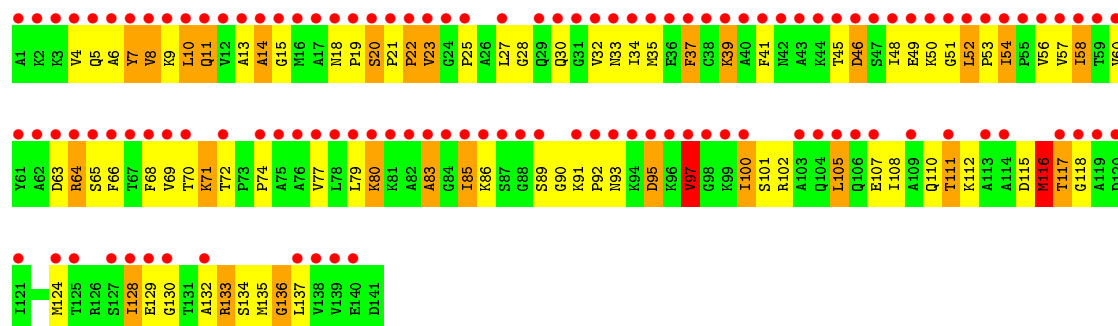
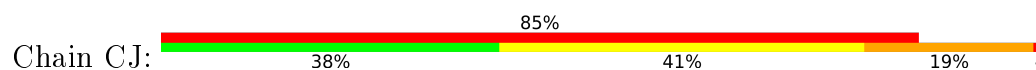
- Molecule 32: 50S ribosomal protein L9



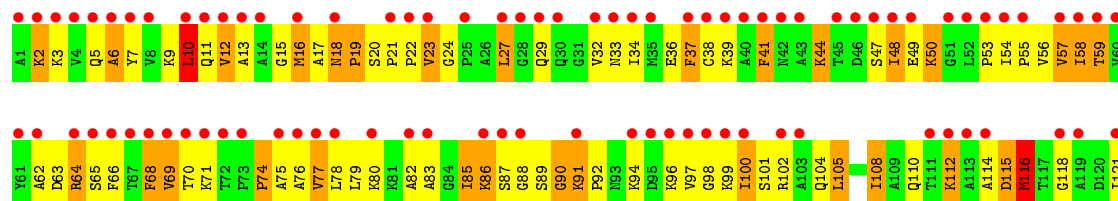
- Molecule 32: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L11

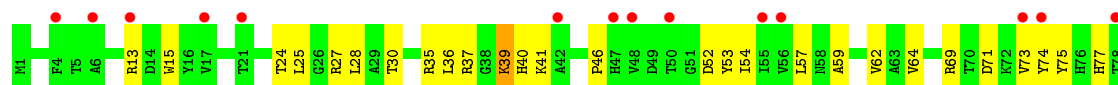


- Molecule 33: 50S ribosomal protein L11

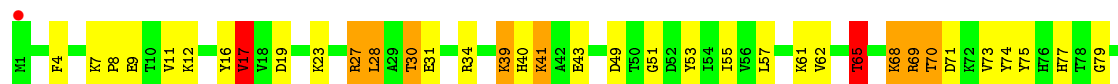




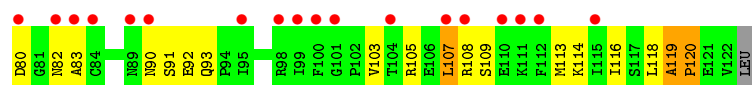
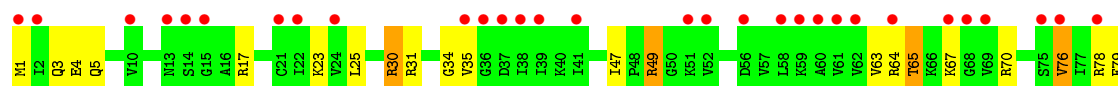
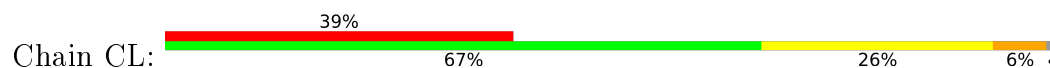
- Molecule 34: 50S ribosomal protein L13



- Molecule 34: 50S ribosomal protein L13



- Molecule 35: 50S ribosomal protein L14



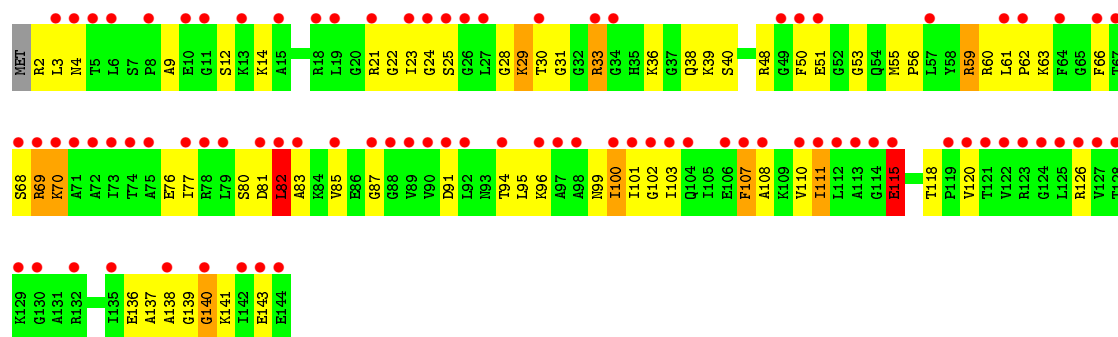
- Molecule 35: 50S ribosomal protein L14



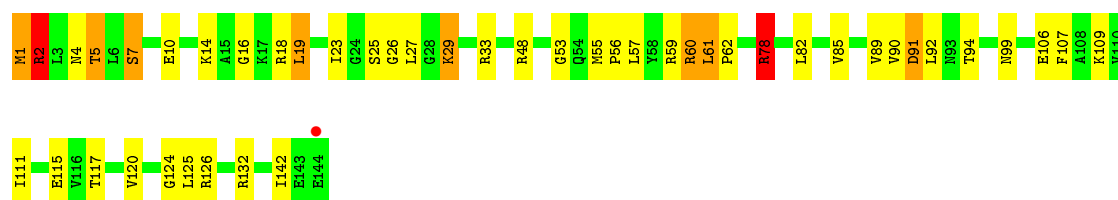
- Molecule 36: 50S ribosomal protein L15



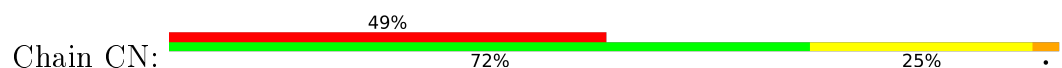




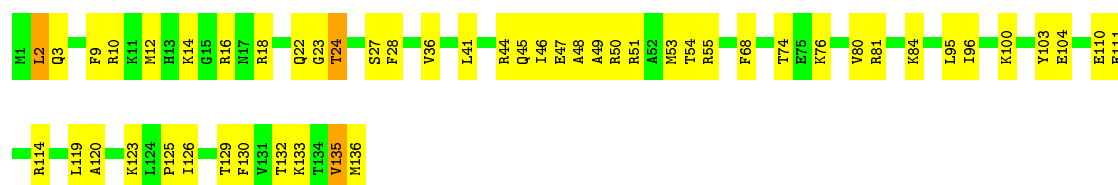
• Molecule 36: 50S ribosomal protein L15



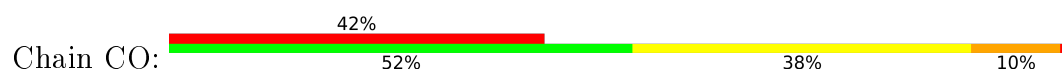
• Molecule 37: 50S ribosomal protein L16

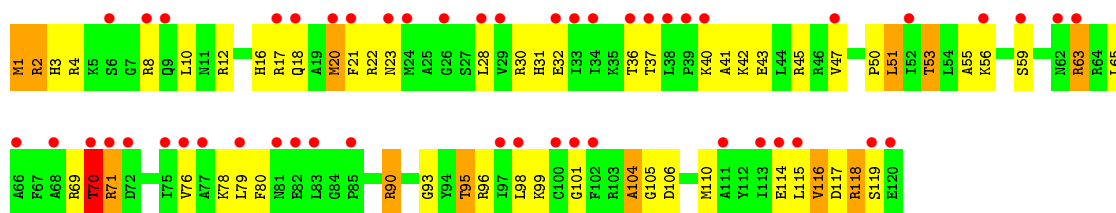


• Molecule 37: 50S ribosomal protein L16



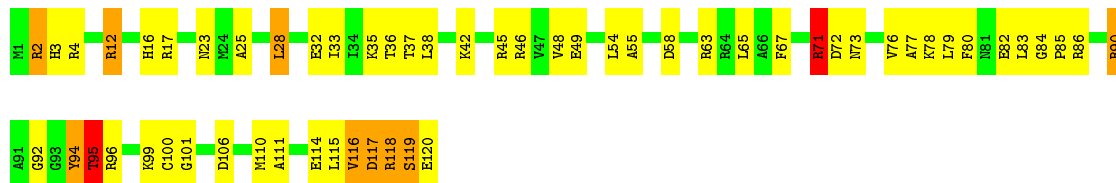
• Molecule 38: 50S ribosomal protein L17





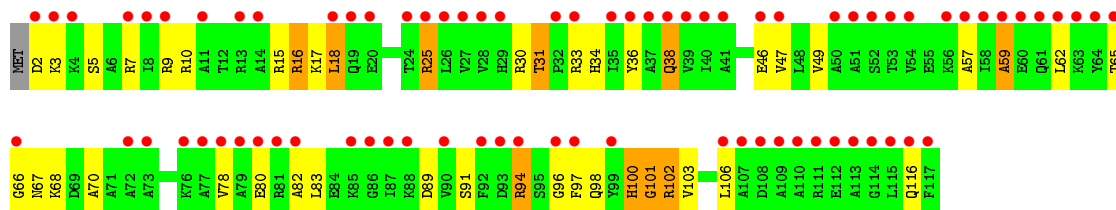
• Molecule 38: 50S ribosomal protein L17

Chain DO: 52% 38% 8% .



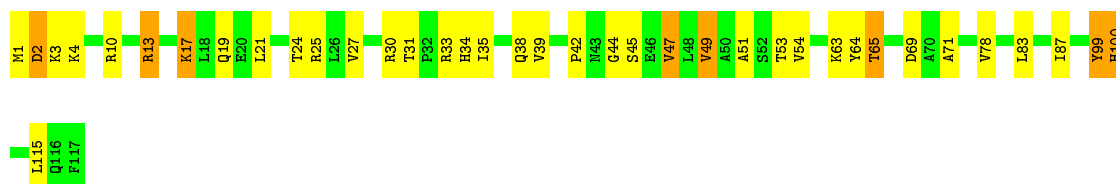
• Molecule 39: 50S ribosomal protein L18

Chain CP: 66% 62% 29% 9% .



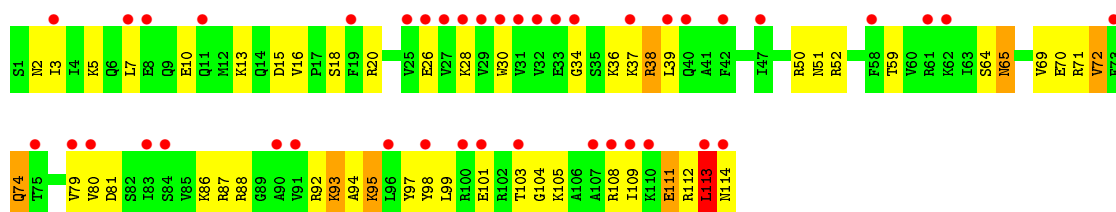
• Molecule 39: 50S ribosomal protein L18

Chain DP: 68% 26% 7%

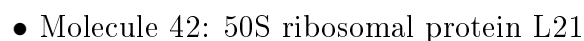
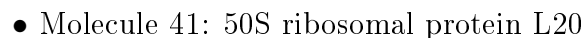
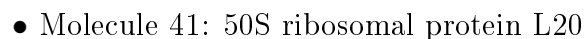


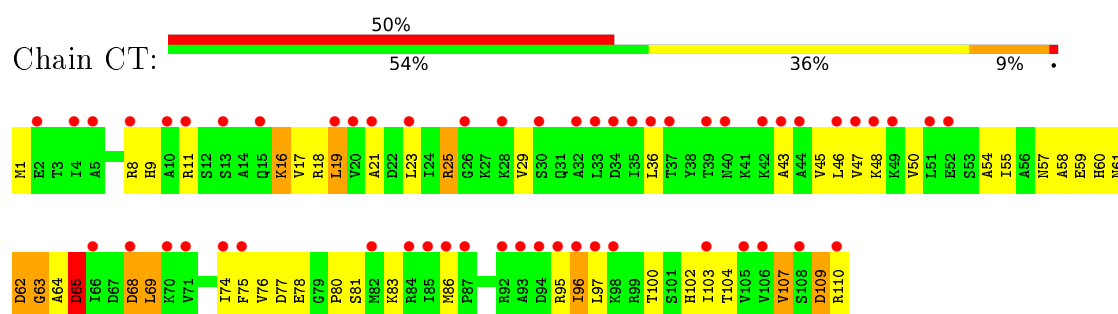
• Molecule 40: 50S ribosomal protein L19

Chain CQ: 37% 54% 39% 6% .

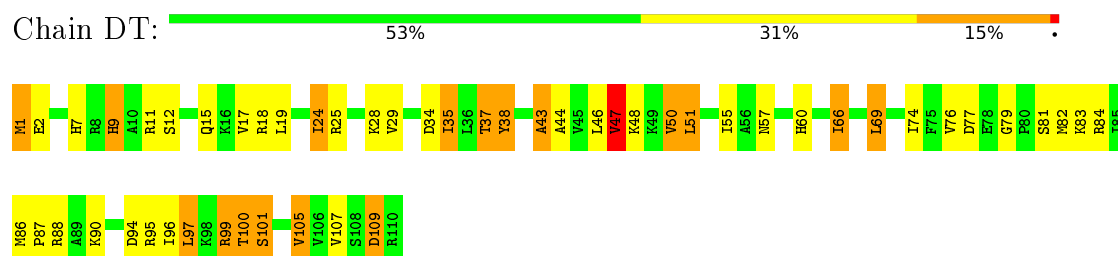


• Molecule 40: 50S ribosomal protein L19

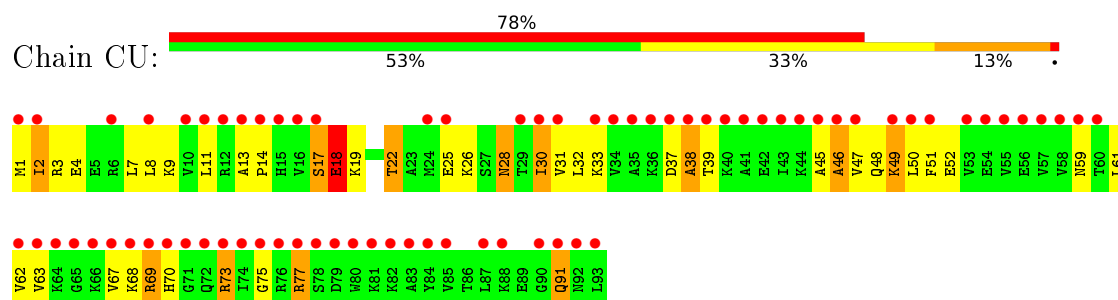




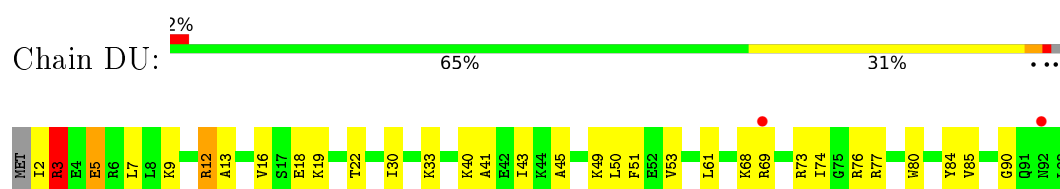
- Molecule 43: 50S ribosomal protein L22



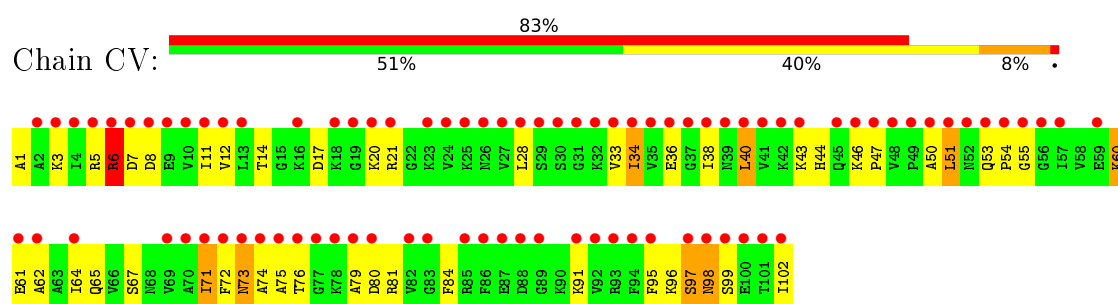
- Molecule 44: 50S ribosomal protein L23



- Molecule 44: 50S ribosomal protein L23



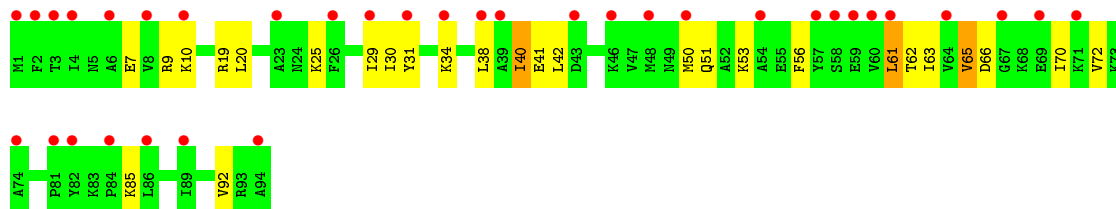
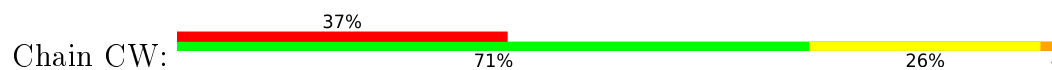
- Molecule 45: 50S ribosomal protein L24



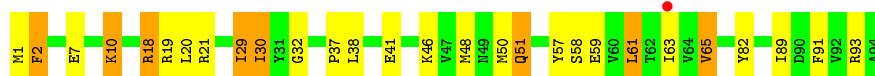
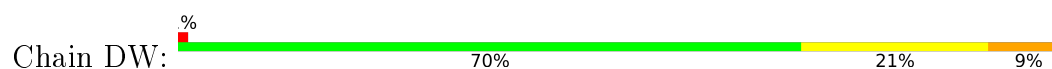
- Molecule 45: 50S ribosomal protein L24



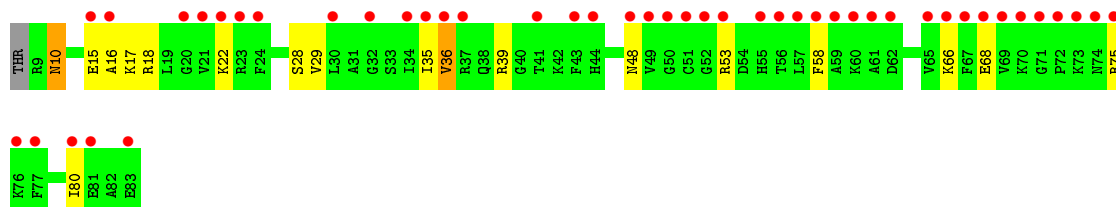
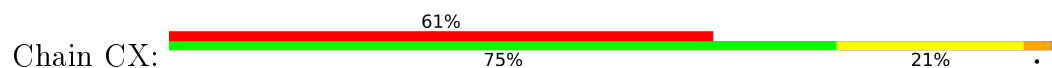
- Molecule 46: 50S ribosomal protein L25



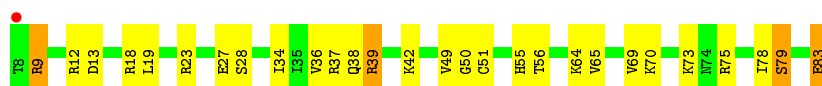
- Molecule 46: 50S ribosomal protein L25



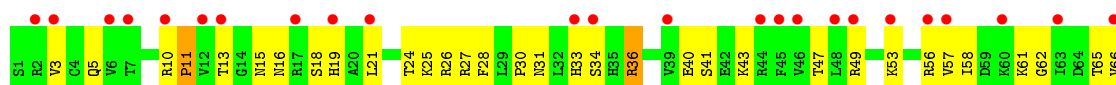
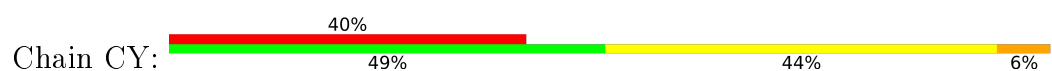
- Molecule 47: 50S ribosomal protein L27

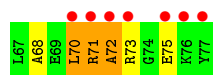


- Molecule 47: 50S ribosomal protein L27



- Molecule 48: 50S ribosomal protein L28





- Molecule 48: 50S ribosomal protein L28

Chain DY: 70% 26% .



- Molecule 49: 50S ribosomal protein L29

Chain CZ: 52% 60% 31% 8% .



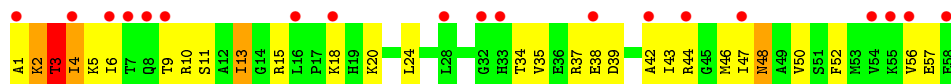
- Molecule 49: 50S ribosomal protein L29

Chain DZ: 2% 52% 35% 11% .



- Molecule 50: 50S ribosomal protein L30

Chain C0: 33% 50% 41% 7% .



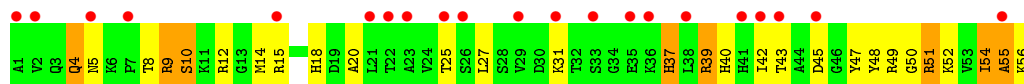
- Molecule 50: 50S ribosomal protein L30

Chain D0: 60% 31% 9%



- Molecule 51: 50S ribosomal protein L32

Chain C1: 38% 50% 36% 14%



- Molecule 51: 50S ribosomal protein L32

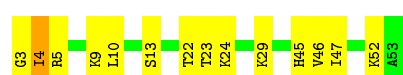
Chain D1: 57% 34% 5%



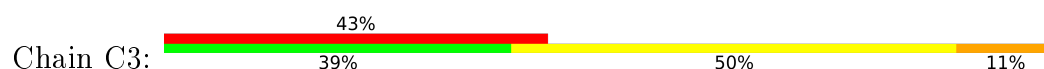
- Molecule 52: 50S ribosomal protein L33



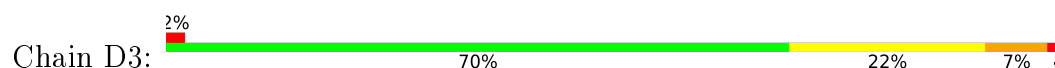
- Molecule 52: 50S ribosomal protein L33



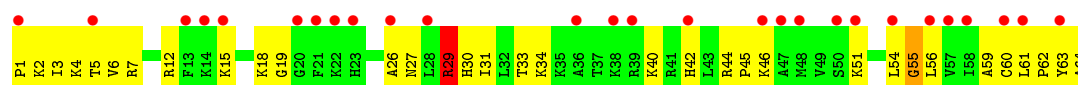
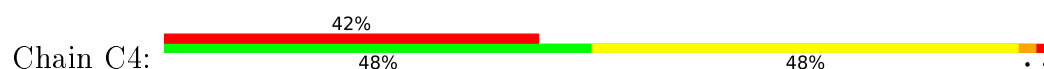
- Molecule 53: 50S ribosomal protein L34



- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35

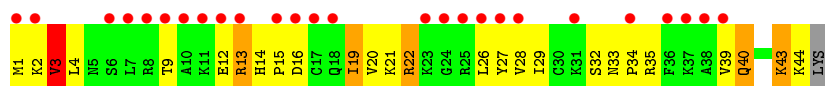


- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36 2

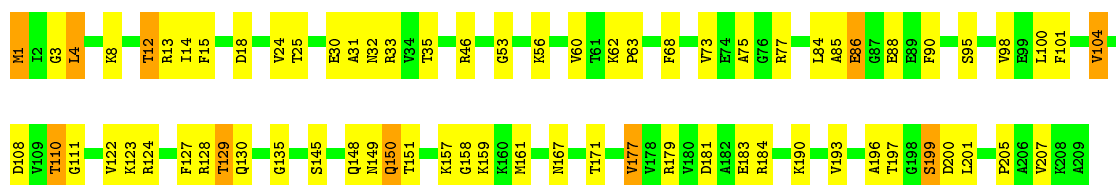




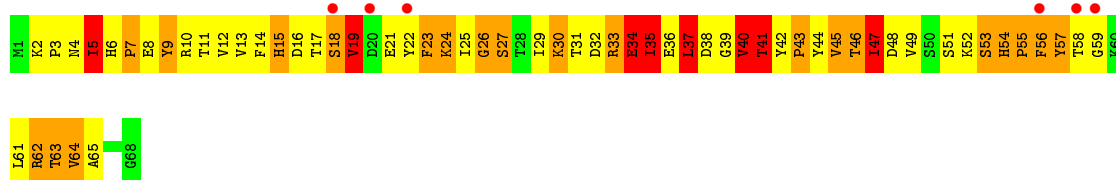
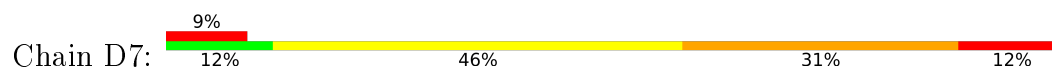
- Molecule 55: 50S ribosomal protein L36 2



- 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, $\alpha$ , $\beta$ , $\gamma$	212.02Å 434.57Å 623.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.32 – 2.90 69.32 – 2.83	Depositor EDS
% Data completeness (in resolution range)	85.2 (69.32-2.90) 79.8 (69.32-2.83)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.186 , 0.255 0.186 , 0.255	Depositor DCC
$R_{free}$ test set	5389 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 109.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	484785	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 3TD, G7M, D2T, MA6, UR3, PUT, 6MZ, 2MG, OMG, EDO, PGE, 1MG, PSU, GUN, ACY, MG, MEQ, OMC, 2MA, MPD, SPD, 5MU, OMU, PG4, 5MC, H2U, PEG, 1PE, 4OC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	AC	0	1
8	BD	0	1
10	BF	0	1

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

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

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

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

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

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

There are no chirality outliers.

5 of 85 planarity outliers are listed below:

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

## 5.2 Too-close contacts

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

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

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

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

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

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

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

The worst 5 of 10306 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DA:783:A:OP1	69:DA:3201:HOH:O	1.53	1.22

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

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:368:U:OP1	32:CH:93:SER:OG[4_455]	2.15	0.05
3:DA:2887:A:OP1	50:D0:1:ALA:N[4_545]	2.17	0.03

## 5.3 Torsion angles ⓘ

### 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%)	3	12
7	BC	204/206 (99%)	180 (88%)	14 (7%)	10 (5%)	2	8
8	AD	203/205 (99%)	184 (91%)	9 (4%)	10 (5%)	2	8
8	BD	203/205 (99%)	188 (93%)	8 (4%)	7 (3%)	3	15
9	AE	148/150 (99%)	123 (83%)	12 (8%)	13 (9%)	1	2
9	BE	148/150 (99%)	117 (79%)	18 (12%)	13 (9%)	1	2
10	AF	98/100 (98%)	85 (87%)	8 (8%)	5 (5%)	2	7
10	BF	98/100 (98%)	84 (86%)	9 (9%)	5 (5%)	2	7
11	AG	149/151 (99%)	131 (88%)	13 (9%)	5 (3%)	3	15
11	BG	149/151 (99%)	128 (86%)	18 (12%)	3 (2%)	7	27

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

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

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

5 of 550 Ramachandran outliers are listed below:

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

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

### 5.3.2 Protein sidechains ⓘ

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

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

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

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

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

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

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

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

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

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

### 5.3.3 RNA ⓘ

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

5 of 2427 RNA backbone outliers are listed below:

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

5 of 111 RNA pucker outliers are listed below:

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

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

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	PSU	DA	746	3,58	17,21,22	1.00	1 (5%)	20,30,33	2.94	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PSU	DA	2504	3	17,21,22	2.10	5 (29%)	20,30,33	3.70	6 (30%)
3	5MC	DA	1962	3	15,22,23	0.92	1 (6%)	19,32,35	1.46	3 (15%)
3	PSU	DA	1911	3	17,21,22	1.21	3 (17%)	20,30,33	3.11	6 (30%)
16	D2T	AL	89	16	4,9,10	0.94	0	3,11,13	2.09	1 (33%)
3	OMC	DA	2498	3,58	15,22,23	1.49	4 (26%)	17,31,34	1.69	2 (11%)
3	OMU	DA	2552	3	14,22,23	1.14	1 (7%)	14,31,34	1.15	2 (14%)
3	H2U	DA	2449	3	18,21,22	1.57	3 (16%)	21,30,33	2.15	3 (14%)
3	PSU	DA	2580	3	17,21,22	1.51	2 (11%)	20,30,33	3.69	4 (20%)
1	5MC	AA	1407	1	15,22,23	1.28	2 (13%)	19,32,35	1.99	3 (15%)
3	2MG	DA	2445	3	19,26,27	0.81	0	21,38,41	2.22	6 (28%)
3	2MA	DA	2503	3,58	17,25,26	1.16	2 (11%)	19,37,40	2.21	5 (26%)
1	5MC	AA	967	1	15,22,23	1.36	1 (6%)	19,32,35	1.57	4 (21%)
1	MA6	AA	1518	1	19,26,27	0.94	1 (5%)	18,38,41	1.67	3 (16%)
3	6MZ	DA	1618	3	18,25,26	1.09	0	16,36,39	3.51	5 (31%)
1	UR3	AA	1498	1	14,22,23	0.97	1 (7%)	15,32,35	0.94	1 (6%)
1	MA6	AA	1519	1	19,26,27	0.99	1 (5%)	18,38,41	1.44	3 (16%)
1	4OC	AA	1402	1	16,23,24	0.96	1 (6%)	17,32,35	2.51	2 (11%)
3	6MZ	DA	2030	3	18,25,26	1.33	2 (11%)	16,36,39	3.21	5 (31%)
3	G7M	DA	2069	3	20,26,27	1.55	3 (15%)	20,39,42	2.01	5 (25%)
3	5MU	DA	747	3	15,22,23	1.33	1 (6%)	16,32,35	1.75	1 (6%)
56	MEQ	DD	150	56	8,9,10	1.51	1 (12%)	5,10,12	1.52	1 (20%)
1	2MG	AA	1516	1	19,26,27	1.00	1 (5%)	21,38,41	2.50	8 (38%)
1	PSU	AA	516	1,58	17,21,22	1.03	1 (5%)	20,30,33	3.35	5 (25%)
3	PSU	DA	2457	3	17,21,22	1.40	2 (11%)	20,30,33	3.87	6 (30%)
3	PSU	DA	2605	3	17,21,22	1.38	3 (17%)	20,30,33	3.75	3 (15%)
3	1MG	DA	745	3	18,26,27	1.66	4 (22%)	19,39,42	1.66	3 (15%)
3	5MU	DA	1939	3	15,22,23	1.28	2 (13%)	16,32,35	1.29	2 (12%)
1	2MG	AA	1207	1	19,26,27	1.19	2 (10%)	21,38,41	2.14	6 (28%)
1	G7M	AA	527	1	20,26,27	1.40	2 (10%)	20,39,42	1.98	5 (25%)
3	PSU	DA	955	3	17,21,22	1.26	2 (11%)	20,30,33	2.76	5 (25%)
3	PSU	DA	2604	3	17,21,22	2.39	5 (29%)	20,30,33	3.92	6 (30%)
3	OMG	DA	2251	3	18,26,27	1.01	2 (11%)	20,38,41	1.92	6 (30%)
3	PSU	DA	1917	3	17,21,22	1.34	4 (23%)	20,30,33	3.54	7 (35%)
3	2MG	DA	1835	3	19,26,27	1.00	2 (10%)	21,38,41	2.46	8 (38%)
3	3TD	DA	1915	3	17,22,23	2.11	5 (29%)	19,32,35	2.41	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MG	AA	966	1	19,26,27	1.35	2 (10%)	21,38,41	2.06	4 (19%)

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	PSU	DA	746	3,58	-	3/7/25/26	0/2/2/2
3	PSU	DA	2504	3	-	2/7/25/26	0/2/2/2
3	5MC	DA	1962	3	-	2/5/25/26	0/2/2/2
3	PSU	DA	1911	3	-	0/7/25/26	0/2/2/2
16	D2T	AL	89	16	-	2/3/12/14	-
3	OMC	DA	2498	3,58	-	3/7/27/28	0/2/2/2
3	OMU	DA	2552	3	-	2/7/27/28	0/2/2/2
3	H2U	DA	2449	3	-	0/7/38/39	0/2/2/2
3	PSU	DA	2580	3	-	0/7/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/5/25/26	0/2/2/2
3	2MG	DA	2445	3	-	0/5/27/28	0/3/3/3
3	2MA	DA	2503	3,58	-	3/3/25/26	0/3/3/3
1	5MC	AA	967	1	-	0/5/25/26	0/2/2/2
1	MA6	AA	1518	1	-	2/7/29/30	0/3/3/3
3	6MZ	DA	1618	3	-	1/5/27/28	0/3/3/3
1	UR3	AA	1498	1	-	0/5/25/26	0/2/2/2
1	MA6	AA	1519	1	-	3/7/29/30	0/3/3/3
1	4OC	AA	1402	1	-	2/9/29/30	0/2/2/2
3	6MZ	DA	2030	3	-	1/5/27/28	0/3/3/3
3	G7M	DA	2069	3	-	2/3/25/26	0/3/3/3
3	5MU	DA	747	3	-	2/5/25/26	0/2/2/2
56	MEQ	DD	150	56	-	2/8/9/11	-
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	PSU	AA	516	1,58	-	0/7/25/26	0/2/2/2
3	PSU	DA	2457	3	-	1/7/25/26	0/2/2/2
3	PSU	DA	2605	3	-	0/7/25/26	0/2/2/2
3	1MG	DA	745	3	-	2/3/25/26	0/3/3/3
3	5MU	DA	1939	3	-	2/5/25/26	0/2/2/2
1	2MG	AA	1207	1	-	2/5/27/28	0/3/3/3
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	OMG	DA	2251	3	-	1/5/27/28	0/3/3/3
3	PSU	DA	1917	3	-	0/7/25/26	0/2/2/2
3	2MG	DA	1835	3	-	4/5/27/28	0/3/3/3
3	3TD	DA	1915	3	-	2/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3

The worst 5 of 75 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	DA	2604	PSU	C5-C1'	-7.49	1.45	1.52
3	DA	1915	3TD	C5-C1'	-6.29	1.46	1.52
3	DA	2504	PSU	C5-C1'	-5.77	1.47	1.52
1	AA	967	5MC	C5-C4	4.69	1.48	1.41
3	DA	745	1MG	C6-C5	4.40	1.48	1.41

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	DA	2605	PSU	N1-C2-N3	-14.71	116.73	128.43
3	DA	2604	PSU	N1-C2-N3	-13.66	117.57	128.43
3	DA	2580	PSU	N1-C2-N3	-13.51	117.69	128.43
3	DA	2457	PSU	N1-C2-N3	-13.07	118.04	128.43
3	DA	1917	PSU	N1-C2-N3	-11.98	118.91	128.43

There are no chirality outliers.

5 of 50 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	O4'-C1'-C5-C4

There are no ring outliers.

29 monomers are involved in 110 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	DA	2504	PSU	3	0
3	DA	1962	5MC	4	0
3	DA	1911	PSU	3	0
16	AL	89	D2T	4	0
3	DA	2498	OMC	8	0
3	DA	2552	OMU	6	0
3	DA	2449	H2U	1	0
1	AA	1407	5MC	4	0
3	DA	2445	2MG	2	0
3	DA	2503	2MA	4	0
1	AA	967	5MC	2	0
1	AA	1518	MA6	7	0
3	DA	1618	6MZ	2	0
1	AA	1519	MA6	12	0
1	AA	1402	4OC	3	0
3	DA	2030	6MZ	7	0
3	DA	2069	G7M	1	0
3	DA	747	5MU	8	0
56	DD	150	MEQ	3	0
1	AA	1516	2MG	2	0
1	AA	516	PSU	1	0
3	DA	2605	PSU	1	0
3	DA	745	1MG	5	0
3	DA	1939	5MU	4	0
1	AA	1207	2MG	2	0
3	DA	955	PSU	2	0
3	DA	2251	OMG	3	0
3	DA	1835	2MG	9	0
3	DA	1915	3TD	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
65	ACY	DA	3055	-	1,3,3	4.57	1 (100%)	0,3,3	0.00	-
60	MPD	DK	201	-	7,7,7	0.55	0	9,10,10	0.66	0
67	EDO	DA	3052	-	3,3,3	0.50	0	2,2,2	0.16	0
60	MPD	DN	201	-	7,7,7	0.49	0	9,10,10	0.84	1 (11%)
60	MPD	DA	3067	-	7,7,7	0.65	0	9,10,10	0.67	0
65	ACY	DA	3064	-	1,3,3	0.44	0	0,3,3	0.00	-
67	EDO	DA	3057	-	3,3,3	0.43	0	2,2,2	0.11	0
62	SPD	DA	3036	-	9,9,9	0.48	0	8,8,8	0.53	0
60	MPD	DA	3046	-	7,7,7	0.76	0	9,10,10	0.99	1 (11%)
60	MPD	DE	301	-	7,7,7	0.56	0	9,10,10	0.56	0
60	MPD	DT	201	-	7,7,7	0.55	0	9,10,10	1.02	1 (11%)
61	PG4	DS	202	-	12,12,12	0.74	0	11,11,11	0.73	0
61	PG4	DR	202	-	12,12,12	0.86	0	11,11,11	0.57	0
66	PEG	DP	201	-	6,6,6	1.16	0	5,5,5	0.64	0
67	EDO	DB	203	-	3,3,3	0.40	0	2,2,2	0.16	0
67	EDO	D1	101	-	3,3,3	0.38	0	2,2,2	0.15	0
60	MPD	DA	3045	-	7,7,7	0.34	0	9,10,10	1.38	2 (22%)
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
67	EDO	DA	3060	-	3,3,3	0.46	0	2,2,2	0.26	0
63	PUT	DA	3069	-	5,5,5	0.35	0	4,4,4	0.19	0
67	EDO	DA	3058	-	3,3,3	0.52	0	2,2,2	0.10	0
67	EDO	DB	201	-	3,3,3	0.42	0	2,2,2	0.38	0
60	MPD	DE	302	-	7,7,7	0.56	0	9,10,10	0.43	0
63	PUT	DA	3032	-	5,5,5	0.30	0	4,4,4	0.41	0
59	PGE	DA	3035	-	9,9,9	1.32	2 (22%)	8,8,8	1.12	1 (12%)
66	PEG	DA	3073	-	6,6,6	1.04	0	5,5,5	0.67	0
59	PGE	DA	3066	-	9,9,9	1.07	1 (11%)	8,8,8	0.93	0
64	1PE	DA	3034	-	15,15,15	0.74	0	14,14,14	1.04	1 (7%)
60	MPD	DA	3072	-	7,7,7	0.56	0	9,10,10	0.30	0
59	PGE	D3	101	-	9,9,9	0.92	0	8,8,8	0.43	0
62	SPD	DA	3031	-	9,9,9	0.62	0	8,8,8	0.31	0
67	EDO	DA	3059	-	3,3,3	0.52	0	2,2,2	0.61	0
59	PGE	AA	1613	-	9,9,9	1.13	1 (11%)	8,8,8	0.70	0
66	PEG	D3	102	-	6,6,6	0.92	0	5,5,5	0.27	0
67	EDO	DA	3076	-	3,3,3	0.53	0	2,2,2	0.06	0
61	PG4	DA	3048	-	12,12,12	0.89	0	11,11,11	0.67	0
67	EDO	DB	202	-	3,3,3	0.52	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
66	PEG	D1	102	-	6,6,6	1.50	1 (16%)	5,5,5	1.35	0
64	1PE	DA	3065	-	15,15,15	0.86	0	14,14,14	0.88	0
60	MPD	DA	3077	-	7,7,7	0.50	0	9,10,10	1.43	2 (22%)
66	PEG	DA	3063	-	6,6,6	1.06	0	5,5,5	0.42	0
67	EDO	DA	3075	-	3,3,3	0.35	0	2,2,2	0.18	0
66	PEG	DA	3062	-	6,6,6	1.17	1 (16%)	5,5,5	0.57	0
63	PUT	DA	3037	-	5,5,5	0.32	0	4,4,4	0.81	0
65	ACY	DA	3044	-	1,3,3	2.89	1 (100%)	0,3,3	0.00	-
63	PUT	DM	201	-	5,5,5	0.35	0	4,4,4	0.51	0
60	MPD	DA	3071	-	7,7,7	0.65	0	9,10,10	0.46	0
63	PUT	DP	202	-	5,5,5	0.36	0	4,4,4	0.16	0
68	GUN	DA	3078	-	9,12,12	2.14	2 (22%)	8,17,17	3.43	6 (75%)
63	PUT	DA	3054	-	5,5,5	0.47	0	4,4,4	0.81	0
61	PG4	BA	1607	-	12,12,12	0.89	0	11,11,11	0.57	0
59	PGE	DT	202	-	9,9,9	1.16	1 (11%)	8,8,8	0.71	0
66	PEG	DQ	201	-	6,6,6	1.01	0	5,5,5	0.26	0
59	PGE	DS	201	-	9,9,9	1.25	1 (11%)	8,8,8	1.03	0
59	PGE	DU	101	-	9,9,9	1.09	1 (11%)	8,8,8	0.58	0
60	MPD	AA	1615	-	7,7,7	0.54	0	9,10,10	0.67	0
60	MPD	DA	3043	-	7,7,7	0.58	0	9,10,10	0.70	0
63	PUT	D5	101	-	5,5,5	0.29	0	4,4,4	0.30	0
61	PG4	DQ	202	-	12,12,12	0.71	0	11,11,11	0.45	0
66	PEG	DA	3050	-	6,6,6	1.03	0	5,5,5	0.51	0
67	EDO	DR	204	-	3,3,3	0.55	0	2,2,2	0.28	0
59	PGE	DD	301	-	9,9,9	1.16	1 (11%)	8,8,8	0.77	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
60	MPD	DK	201	-	-	0/5/5/5	-
67	EDO	DA	3052	-	-	1/1/1/1	-
60	MPD	DN	201	-	-	3/5/5/5	-
60	MPD	DA	3067	-	-	1/5/5/5	-
67	EDO	DA	3057	-	-	0/1/1/1	-
62	SPD	DA	3036	-	-	3/7/7/7	-
60	MPD	DA	3046	-	-	0/5/5/5	-
60	MPD	DE	301	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	MPD	DT	201	-	-	0/5/5/5	-
61	PG4	DS	202	-	-	3/10/10/10	-
61	PG4	DR	202	-	-	5/10/10/10	-
66	PEG	DP	201	-	-	2/4/4/4	-
67	EDO	DB	203	-	-	0/1/1/1	-
67	EDO	D1	101	-	-	1/1/1/1	-
60	MPD	DA	3045	-	-	2/5/5/5	-
62	SPD	DA	3070	-	-	3/7/7/7	-
66	PEG	DA	3061	-	-	3/4/4/4	-
67	EDO	DA	3060	-	-	1/1/1/1	-
63	PUT	DA	3069	-	-	1/3/3/3	-
67	EDO	DA	3058	-	-	0/1/1/1	-
67	EDO	DB	201	-	-	1/1/1/1	-
60	MPD	DE	302	-	-	0/5/5/5	-
63	PUT	DA	3032	-	-	2/3/3/3	-
59	PGE	DA	3035	-	-	2/7/7/7	-
66	PEG	DA	3073	-	-	1/4/4/4	-
59	PGE	DA	3066	-	-	3/7/7/7	-
64	1PE	DA	3034	-	-	7/13/13/13	-
60	MPD	DA	3072	-	-	0/5/5/5	-
59	PGE	D3	101	-	-	4/7/7/7	-
62	SPD	DA	3031	-	-	6/7/7/7	-
67	EDO	DA	3059	-	-	0/1/1/1	-
59	PGE	AA	1613	-	-	5/7/7/7	-
66	PEG	D3	102	-	-	3/4/4/4	-
67	EDO	DA	3076	-	-	1/1/1/1	-
61	PG4	DA	3048	-	-	7/10/10/10	-
67	EDO	DB	202	-	-	1/1/1/1	-
66	PEG	D1	102	-	-	3/4/4/4	-
64	1PE	DA	3065	-	-	9/13/13/13	-
60	MPD	DA	3077	-	-	2/5/5/5	-
66	PEG	DA	3063	-	-	3/4/4/4	-
67	EDO	DA	3075	-	-	1/1/1/1	-
66	PEG	DA	3062	-	-	3/4/4/4	-
63	PUT	DA	3037	-	-	1/3/3/3	-
63	PUT	DM	201	-	-	2/3/3/3	-
60	MPD	DA	3071	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PUT	DP	202	-	-	0/3/3/3	-
68	GUN	DA	3078	-	-	-	0/2/2/2
63	PUT	DA	3054	-	-	0/3/3/3	-
61	PG4	BA	1607	-	-	1/10/10/10	-
59	PGE	DT	202	-	-	3/7/7/7	-
66	PEG	DQ	201	-	-	4/4/4/4	-
59	PGE	DS	201	-	-	2/7/7/7	-
59	PGE	DU	101	-	-	4/7/7/7	-
60	MPD	AA	1615	-	-	3/5/5/5	-
60	MPD	DA	3043	-	-	2/5/5/5	-
63	PUT	D5	101	-	-	1/3/3/3	-
61	PG4	DQ	202	-	-	5/10/10/10	-
66	PEG	DA	3050	-	-	1/4/4/4	-
67	EDO	DR	204	-	-	1/1/1/1	-
59	PGE	DD	301	-	-	1/7/7/7	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	DA	3078	GUN	C6-C5	5.51	1.50	1.41
65	DA	3055	ACY	CH3-C	4.57	1.54	1.48
65	DA	3044	ACY	CH3-C	2.89	1.52	1.48
68	DA	3078	GUN	C5-C4	2.85	1.48	1.40
66	D1	102	PEG	C2-C1	2.46	1.62	1.49

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	DA	3078	GUN	C2-N3-C4	5.70	121.86	115.36
68	DA	3078	GUN	C6-C5-C4	-4.33	116.66	120.80
68	DA	3078	GUN	C6-N1-C2	3.47	121.44	115.93
60	DA	3045	MPD	CM-C2-C1	-3.28	103.74	110.57
68	DA	3078	GUN	C4-C5-N7	-3.22	106.04	109.40

There are no chirality outliers.

5 of 127 torsion outliers are listed below:

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

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

There are no ring outliers.

39 monomers are involved in 100 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	DA	3052	EDO	1	0
60	DN	201	MPD	1	0
60	DA	3067	MPD	4	0
65	DA	3064	ACY	5	0
62	DA	3036	SPD	1	0
60	DA	3046	MPD	1	0
60	DE	301	MPD	1	0
61	DS	202	PG4	1	0
61	DR	202	PG4	8	0
66	DP	201	PEG	1	0
67	DB	203	EDO	1	0
60	DA	3045	MPD	1	0
67	DA	3060	EDO	5	0
63	DA	3069	PUT	2	0
59	DA	3066	PGE	2	0
64	DA	3034	1PE	5	0
60	DA	3072	MPD	2	0
62	DA	3031	SPD	3	0
67	DA	3059	EDO	4	0
66	D3	102	PEG	2	0
61	DA	3048	PG4	3	0
66	D1	102	PEG	3	0
64	DA	3065	1PE	2	0
60	DA	3077	MPD	1	0
66	DA	3063	PEG	1	0
66	DA	3062	PEG	2	0
63	DA	3037	PUT	7	0
65	DA	3044	ACY	1	0
63	DM	201	PUT	1	0
60	DA	3071	MPD	1	0
63	DP	202	PUT	10	0
68	DA	3078	GUN	2	0
63	DA	3054	PUT	4	0
59	DT	202	PGE	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
66	DQ	201	PEG	1	0
63	D5	101	PUT	2	0
61	DQ	202	PG4	3	0
66	DA	3050	PEG	2	0
67	DR	204	EDO	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1522/1533 (99%)	-0.45	8 (0%) 91 91	40, 89, 181, 376	0
2	BA	1533/1533 (100%)	-0.15	33 (2%) 62 59	52, 116, 235, 316	0
3	DA	2873/2903 (98%)	-0.40	30 (1%) 82 82	13, 44, 165, 340	0
4	CA	2898/2904 (99%)	0.24	97 (3%) 46 41	68, 150, 267, 488	0
5	CB	118/119 (99%)	-0.08	1 (0%) 86 86	112, 187, 233, 258	0
5	DB	119/119 (100%)	-0.62	0 100 100	21, 53, 81, 104	0
6	AB	218/218 (100%)	0.91	36 (16%) 1 1	56, 120, 185, 241	0
6	BB	218/218 (100%)	0.91	44 (20%) 1 0	75, 126, 188, 242	0
7	AC	206/206 (100%)	0.15	2 (0%) 82 82	54, 95, 145, 202	0
7	BC	206/206 (100%)	0.30	8 (3%) 39 35	68, 111, 159, 198	0
8	AD	205/205 (100%)	0.49	17 (8%) 11 8	60, 107, 155, 210	0
8	BD	205/205 (100%)	0.02	1 (0%) 91 91	53, 84, 126, 146	0
9	AE	150/150 (100%)	0.16	3 (2%) 65 63	52, 87, 148, 219	0
9	BE	150/150 (100%)	0.13	5 (3%) 46 41	55, 89, 151, 191	0
10	AF	100/100 (100%)	0.07	2 (2%) 65 63	60, 100, 136, 195	0
10	BF	100/100 (100%)	0.42	8 (8%) 12 9	79, 116, 156, 241	0
11	AG	151/151 (100%)	0.67	18 (11%) 4 3	83, 130, 170, 184	0
11	BG	151/151 (100%)	2.25	70 (46%) 0 0	102, 192, 268, 311	0
12	AH	129/129 (100%)	0.31	8 (6%) 20 16	59, 94, 138, 169	0
12	BH	129/129 (100%)	0.35	6 (4%) 31 28	76, 108, 153, 194	0
13	AI	127/127 (100%)	0.72	11 (8%) 10 7	75, 123, 185, 258	0
13	BI	127/127 (100%)	1.98	50 (39%) 0 0	102, 158, 232, 270	0
14	AJ	98/98 (100%)	0.48	9 (9%) 9 6	60, 102, 135, 146	0
14	BJ	98/98 (100%)	1.85	43 (43%) 0 0	75, 123, 150, 162	0

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

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

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

The worst 5 of 2751 RSRZ outliers are listed below:

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

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	0.96	0.09	59,91,109,122	0
1	G7M	AA	527	24/25	0.97	0.13	56,75,85,87	0
1	2MG	AA	966	24/25	0.97	0.15	48,77,86,88	0
1	5MC	AA	967	21/22	0.97	0.19	69,77,90,103	0
1	2MG	AA	1207	24/25	0.97	0.11	54,77,99,121	0
3	PSU	DA	1911	20/21	0.97	0.10	51,84,101,113	0
1	PSU	AA	516	20/21	0.97	0.09	53,86,108,117	0
1	UR3	AA	1498	21/22	0.98	0.13	32,52,68,74	0
1	MA6	AA	1519	24/25	0.98	0.17	37,65,78,84	0
1	4OC	AA	1402	22/23	0.98	0.15	44,63,81,91	0
1	5MC	AA	1407	21/22	0.98	0.12	45,56,73,104	0
3	PSU	DA	1917	20/21	0.98	0.09	42,78,92,94	0
3	5MU	DA	1939	21/22	0.98	0.16	9,38,57,72	0
16	D2T	AL	89	10/11	0.98	0.20	44,60,96,108	0
56	MEQ	DD	150	10/11	0.98	0.16	6,23,48,48	0
3	6MZ	DA	1618	23/24	0.99	0.17	7,32,46,47	0
3	2MG	DA	1835	24/25	0.99	0.13	27,50,59,62	0
1	MA6	AA	1518	24/25	0.99	0.13	21,41,61,72	0
1	2MG	AA	1516	24/25	0.99	0.12	33,63,70,86	0
3	1MG	DA	745	24/25	0.99	0.17	5,29,42,63	0
3	PSU	DA	746	20/21	0.99	0.14	3,21,34,43	0
3	5MC	DA	1962	21/22	0.99	0.13	35,51,64,84	0
3	6MZ	DA	2030	23/24	0.99	0.15	2,12,24,37	0
3	G7M	DA	2069	24/25	0.99	0.14	8,35,48,61	0
3	OMG	DA	2251	24/25	0.99	0.15	3,28,44,58	0
3	2MG	DA	2445	24/25	0.99	0.15	13,28,44,45	0
3	H2U	DA	2449	20/21	0.99	0.16	3,20,42,50	0
3	PSU	DA	2457	20/21	0.99	0.14	3,30,46,59	0
3	OMC	DA	2498	21/22	0.99	0.16	3,20,38,49	0
3	2MA	DA	2503	23/24	0.99	0.16	3,24,39,56	0
3	PSU	DA	2504	20/21	0.99	0.14	2,22,42,46	0
3	OMU	DA	2552	21/22	0.99	0.14	13,27,47,70	0
3	PSU	DA	2580	20/21	0.99	0.16	6,38,52,53	0
3	PSU	DA	2604	20/21	0.99	0.12	14,33,48,70	0
3	PSU	DA	2605	20/21	0.99	0.12	12,38,48,57	0
3	5MU	DA	747	21/22	0.99	0.15	3,19,31,42	0
3	PSU	DA	955	20/21	0.99	0.15	8,30,58,70	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
58	MG	CA	3154	1/1	-0.07	0.57	134,134,134,134	0
58	MG	CA	3129	1/1	0.10	0.31	176,176,176,176	0
58	MG	CA	3068	1/1	0.39	0.23	181,181,181,181	0
58	MG	BA	1643	1/1	0.45	0.15	171,171,171,171	0
58	MG	CA	3084	1/1	0.47	0.41	163,163,163,163	0
58	MG	CA	3159	1/1	0.55	1.10	202,202,202,202	0
58	MG	CA	3157	1/1	0.65	0.32	157,157,157,157	0
66	PEG	DP	201	7/7	0.66	0.65	78,92,105,106	0
60	MPD	DE	302	8/8	0.68	0.61	135,162,187,187	0
58	MG	CA	3135	1/1	0.68	0.14	158,158,158,158	0
58	MG	CA	3017	1/1	0.69	0.42	112,112,112,112	0
58	MG	D5	102	1/1	0.69	0.71	207,207,207,207	0
58	MG	CA	3050	1/1	0.71	0.19	181,181,181,181	0
58	MG	CA	3049	1/1	0.72	0.41	188,188,188,188	0
58	MG	CA	3144	1/1	0.72	0.40	143,143,143,143	0
66	PEG	DA	3063	7/7	0.73	0.75	82,120,134,137	0
63	PUT	DA	3054	6/6	0.73	0.39	38,81,86,88	0
66	PEG	DQ	201	7/7	0.74	0.91	109,111,119,123	0
58	MG	CA	3044	1/1	0.75	0.15	157,157,157,157	0
58	MG	CA	3140	1/1	0.75	0.32	161,161,161,161	0
59	PGE	DT	202	10/10	0.76	0.53	78,121,145,152	0
60	MPD	DT	201	8/8	0.76	0.55	115,144,166,166	0
59	PGE	DD	301	10/10	0.77	0.68	82,129,155,165	0
58	MG	CA	3176	1/1	0.78	0.10	128,128,128,128	0
58	MG	BA	1642	1/1	0.78	0.27	120,120,120,120	0
60	MPD	DA	3072	8/8	0.78	0.96	117,148,172,178	0
58	MG	BA	1612	1/1	0.79	0.07	135,135,135,135	0
60	MPD	DE	301	8/8	0.79	0.71	142,176,194,201	0
58	MG	CA	3173	1/1	0.79	0.73	201,201,201,201	0
58	MG	CA	3102	1/1	0.79	0.92	199,199,199,199	0
66	PEG	D1	102	7/7	0.80	0.41	57,70,83,89	0
58	MG	BA	1609	1/1	0.81	0.18	141,141,141,141	0
58	MG	BA	1637	1/1	0.81	0.14	143,143,143,143	0
63	PUT	DP	202	6/6	0.81	1.09	98,114,117,119	0
58	MG	BA	1638	1/1	0.81	0.10	156,156,156,156	0
58	MG	CA	3027	1/1	0.81	0.14	94,94,94,94	0

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

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

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

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

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

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

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

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

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

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

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

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

## 6.5 Other polymers [i](#)

There are no such residues in this entry.