



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 4, 2025 – 04:31 AM EST

PDB ID : 5J5B  
Title : Structure of the WT E coli ribosome bound to tetracycline  
Authors : Cocozaki, A.; Ferguson, A.  
Deposited on : 2016-04-01  
Resolution : 2.80 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

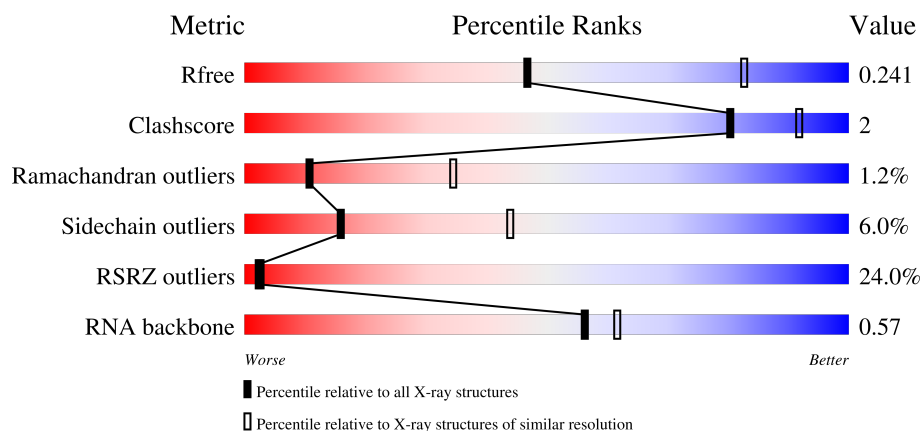
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)
RNA backbone	3690	1037 (3.00-2.60)

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	1534	<div> <div>8%</div> <div>78%</div> <div>20%</div> </div>
1	BA	1534	<div> <div>27%</div> <div>77%</div> <div>20%</div> </div>
2	AB	224	<div> <div>17%</div> <div>88%</div> <div>11%</div> </div>
2	BB	224	<div> <div>21%</div> <div>86%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	155	
5	BE	155	
6	AF	106	
6	BF	106	
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	99	
10	BJ	99	
11	AK	117	
11	BK	117	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	

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Mol	Chain	Length	Quality of chain
15	BO	88	<div> <div>9%</div> <div>88%</div> <div>11%</div> </div>
16	AP	82	<div> <div>12%</div> <div>94%</div> <div>6%</div> </div>
16	BP	82	<div> <div>73%</div> <div>89%</div> <div>10%</div> </div>
17	AQ	80	<div> <div>9%</div> <div>78%</div> <div>22%</div> </div>
17	BQ	80	<div> <div>35%</div> <div>75%</div> <div>24%</div> </div>
18	AR	55	<div> <div>9%</div> <div>85%</div> <div>13%</div> </div>
18	BR	55	<div> <div>9%</div> <div>89%</div> <div>11%</div> </div>
19	AS	79	<div> <div>27%</div> <div>82%</div> <div>14%</div> </div>
19	BS	79	<div> <div>46%</div> <div>82%</div> <div>11%</div> <div>5%</div> </div>
20	AT	86	<div> <div>17%</div> <div>91%</div> <div>8%</div> </div>
20	BT	86	<div> <div>52%</div> <div>74%</div> <div>20%</div> <div>5%</div> </div>
21	AU	56	<div> <div>25%</div> <div>88%</div> <div>12%</div> </div>
21	BU	56	<div> <div>20%</div> <div>88%</div> <div>12%</div> </div>
22	C1	56	<div> <div>62%</div> <div>64%</div> <div>30%</div> <div>5%</div> </div>
22	D1	56	<div> <div>4%</div> <div>73%</div> <div>27%</div> </div>
23	C2	51	<div> <div>41%</div> <div>76%</div> <div>22%</div> </div>
23	D2	51	<div> <div>6%</div> <div>80%</div> <div>18%</div> </div>
24	C3	46	<div> <div>80%</div> <div>76%</div> <div>24%</div> </div>
24	D3	46	<div> <div>7%</div> <div>89%</div> <div>11%</div> </div>
25	C4	64	<div> <div>91%</div> <div>86%</div> <div>12%</div> </div>
25	D4	64	<div> <div>2%</div> <div>83%</div> <div>16%</div> </div>
26	C5	38	<div> <div>66%</div> <div>76%</div> <div>21%</div> </div>
26	D5	38	<div> <div>3%</div> <div>95%</div> <div>5%</div> </div>
27	C0	58	<div> <div>47%</div> <div>88%</div> <div>10%</div> </div>
27	D0	58	<div> <div>2%</div> <div>91%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
28	CB	120	
28	DB	120	
29	CC	271	
29	DC	271	
30	CD	209	
30	DD	209	
31	CA	2904	
32	CE	201	
32	DE	201	
33	CF	177	
33	DF	177	
34	CG	176	
34	DG	176	
35	CH	149	
35	DH	149	
36	CJ	134	
36	DJ	134	
37	CK	142	
37	DK	142	
38	CL	123	
38	DL	123	
39	CM	144	
39	DM	144	
40	CN	136	
40	DN	136	

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Mol	Chain	Length	Quality of chain
41	CO	125	<div> <div>56%</div> <div>84%</div> <div>10%</div> <div>• •</div> </div>
41	DO	125	<div> <div>93%</div> <div>7%</div> </div>
42	CP	117	<div> <div>17%</div> <div>88%</div> <div>9%</div> <div>• •</div> </div>
42	DP	117	<div> <div>2%</div> <div>90%</div> <div>8%</div> <div>•</div> </div>
43	CQ	114	<div> <div>29%</div> <div>89%</div> <div>11%</div> <div>•</div> </div>
43	DQ	114	<div> <div>3%</div> <div>90%</div> <div>10%</div> </div>
44	CR	117	<div> <div>59%</div> <div>88%</div> <div>12%</div> </div>
44	DR	117	<div> <div>0%</div> <div>93%</div> <div>6%</div> <div>•</div> </div>
45	CS	103	<div> <div>50%</div> <div>85%</div> <div>13%</div> <div>• •</div> </div>
45	DS	103	<div> <div>2%</div> <div>92%</div> <div>7%</div> <div>•</div> </div>
46	CT	110	<div> <div>69%</div> <div>78%</div> <div>20%</div> <div>•</div> </div>
46	DT	110	<div> <div>2%</div> <div>86%</div> <div>14%</div> </div>
47	CU	93	<div> <div>67%</div> <div>75%</div> <div>22%</div> <div>•</div> </div>
47	DU	93	<div> <div>10%</div> <div>90%</div> <div>10%</div> </div>
48	CV	102	<div> <div>68%</div> <div>83%</div> <div>16%</div> <div>•</div> </div>
48	DV	102	<div> <div>5%</div> <div>91%</div> <div>8%</div> <div>•</div> </div>
49	CW	94	<div> <div>22%</div> <div>89%</div> <div>11%</div> </div>
49	DW	94	<div> <div>0%</div> <div>91%</div> <div>9%</div> </div>
50	CX	76	<div> <div>42%</div> <div>95%</div> <div>• •</div> </div>
50	DX	76	<div> <div>0%</div> <div>91%</div> <div>9%</div> </div>
51	CY	77	<div> <div>61%</div> <div>83%</div> <div>17%</div> </div>
51	DY	77	<div> <div>0%</div> <div>90%</div> <div>10%</div> </div>
52	CZ	62	<div> <div>63%</div> <div>92%</div> <div>8%</div> </div>
52	DZ	62	<div> <div>5%</div> <div>94%</div> <div>6%</div> </div>
53	DI	135	<div> <div>38%</div> <div>71%</div> <div>27%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
54	DA	2904	

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
55	MG	AA	1601	-	-	-	X
55	MG	AA	1603	-	-	-	X
55	MG	AA	1605	-	-	-	X
55	MG	AA	1606	-	-	-	X
55	MG	AA	1616	-	-	-	X
55	MG	BA	1638	-	-	-	X
55	MG	BA	1640	-	-	-	X
55	MG	BA	1642	-	-	-	X
55	MG	CA	3055	-	-	-	X
55	MG	CA	3116	-	-	-	X
55	MG	CA	3118	-	-	-	X
55	MG	CA	3121	-	-	-	X
55	MG	CA	3124	-	-	-	X
55	MG	CA	3138	-	-	-	X
55	MG	CA	3140	-	-	-	X
55	MG	CA	3146	-	-	-	X
55	MG	CA	3147	-	-	-	X
55	MG	DA	3124	-	-	-	X
55	MG	DA	3139	-	-	-	X
55	MG	DA	3153	-	-	-	X
55	MG	DA	3172	-	-	-	X
57	MPD	AA	1676	-	-	-	X
58	PUT	AA	1672	-	-	-	X
66	ACY	DA	3196	-	X	-	-

## 2 Entry composition

There are 69 unique types of molecules in this entry. The entry contains 295188 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0	0
			32930	14694	6041	10661	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32908	14684	6036	10655	1533			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	224	Total	C	N	O	S	0	0	0
			1753	1109	315	321	8			
2	BB	224	Total	C	N	O	S	0	0	0
			1753	1109	315	321	8			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	BC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
4	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	155	Total	C	N	O	S	0	0	0
			1144	711	216	211	6			
5	BE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	106	Total	C	N	O	S	0	0	0
			862	545	156	154	7			
6	BF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	BG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
9	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	0
			796	498	152	145	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	BJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
11	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			957	591	196	165	5			
12	BL	123	Total	C	N	O	S	0	0	0
			957	591	196	165	5			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	BM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	100	Total	C	N	O	S	0	0	0
			805	499	164	139	3			
14	BN	100	Total	C	N	O	S	0	0	0
			805	499	164	139	3			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	BQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	BR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	BS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0	0
			670	414	138	115	3			
20	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			
21	BU	56	Total	C	N	O	S	0	0	0
			465	290	96	78	1			

- Molecule 22 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	C1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
22	D1	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 23 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	C2	50	Total	C	N	O	0	0	0
			409	263	75	71			
23	D2	51	Total	C	N	O	0	0	0
			414	266	76	72			

- Molecule 24 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	C3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
24	D3	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 25 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	C4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
25	D4	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 26 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	C5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	D5	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	C0	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
27	D0	58	Total	C	N	O	S	0	2	0
			463	290	90	81	2			

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
28	DB	120	Total	C	N	O	P	0	0	0
			2569	1144	468	837	120			

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
29	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
30	DD	209	Total	C	N	O	S	0	1	0
			1576	986	290	296	4			

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CA	2898	Total	C	N	O	P	0	0	0
			62229	27768	11448	20115	2898			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	1723	G	A	conflict	GB 939731527
CA	1725	U	C	conflict	GB 939731527
CA	1726	C	G	conflict	GB 939731527
CA	1727	C	A	conflict	GB 939731527
CA	1730	C	U	conflict	GB 939731527
CA	1733	G	U	conflict	GB 939731527
CA	1734	G	C	conflict	GB 939731527
CA	1735	A	G	conflict	GB 939731527

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
32	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 33 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			
33	DF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
34	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
35	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 36 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			
36	DJ	134	Total	C	N	O	S	0	0	0
			979	619	169	185	6			

- Molecule 37 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
37	DK	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 38 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CL	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
38	DL	123	Total	C	N	O	S	0	0	0
			946	593	181	166	6			

- Molecule 39 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	CM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
39	DM	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 40 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	CN	136	Total	C	N	O	S	0	0	0
			1075	686	205	178	6			
40	DN	136	Total	C	N	O	S	0	2	0
			1092	696	211	179	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CN	81	4D4	ARG	modified residue	UNP P0ADY7
DN	81	4D4	ARG	modified residue	UNP P0ADY7

- Molecule 41 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CO	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
41	DO	125	Total	C	N	O	S	0	0	0
			993	613	202	173	5			

- Molecule 42 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CP	116	Total	C	N	O		0	0	0
			892	552	178	162				
42	DP	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 43 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CQ	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
43	DQ	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 44 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	CR	117	Total	C	N	O	0	0	0
			947	604	192	151			
44	DR	117	Total	C	N	O	0	0	0
			947	604	192	151			

- Molecule 45 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	CS	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
45	DS	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 46 is a protein called 50S ribosomal protein L22.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CT	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
46	DT	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CU	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
47	DU	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 48 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	CV	102	Total	C	N	O	0	0	0
			780	492	146	142			
48	DV	102	Total	C	N	O	0	0	0
			780	492	146	142			

- Molecule 49 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
49	DW	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	CX	75	Total	C	N	O	S	0	0	0
			569	353	113	102	1			
50	DX	76	Total	C	N	O	S	0	1	0
			591	365	121	104	1			

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	CY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	DY	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 52 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	CZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			
52	DZ	62	Total	C	N	O	S	0	0	0
			501	308	98	94	1			

- Molecule 53 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	DI	135	Total	C	N	O	S	0	0	0
			1023	649	179	192	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DI	85	VAL	SER	conflict	UNP P0A7J3
DI	86	THR	MET	conflict	UNP P0A7J3

- Molecule 54 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	DA	2897	Total	C	N	O	P	0	11	0
			62423	27855	11485	20176	2907			

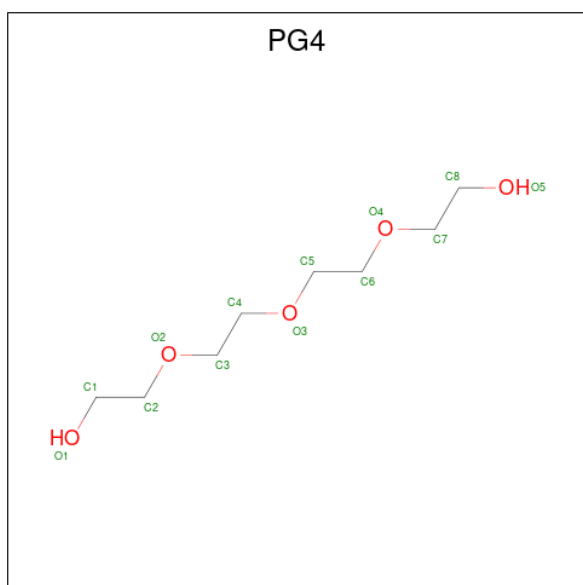
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	1723	G	A	conflict	GB 939731527
DA	1725	U	C	conflict	GB 939731527
DA	1726	C	G	conflict	GB 939731527
DA	1727	C	A	conflict	GB 939731527
DA	1730	C	U	conflict	GB 939731527
DA	1733	G	U	conflict	GB 939731527
DA	1734	G	C	conflict	GB 939731527
DA	1735	A	G	conflict	GB 939731527

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	AA	71	Total	Mg	0	0
			71	71		
55	C3	1	Total	Mg	0	0
			1	1		
55	BA	43	Total	Mg	0	0
			43	43		
55	CB	3	Total	Mg	0	0
			3	3		
55	CA	155	Total	Mg	0	0
			155	155		
55	DD	2	Total	Mg	0	0
			2	2		
55	DM	1	Total	Mg	0	0
			1	1		
55	DR	2	Total	Mg	0	0
			2	2		
55	DB	9	Total	Mg	0	0
			9	9		
55	DA	182	Total	Mg	0	0
			182	182		

- Molecule 56 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



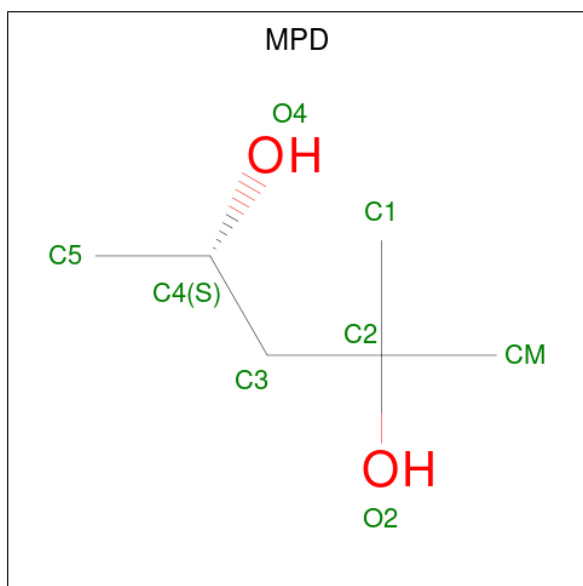
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
56	AA	1	Total	C	O	0	0
			13	8	5		
56	BA	1	Total	C	O	0	0
			13	8	5		

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

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



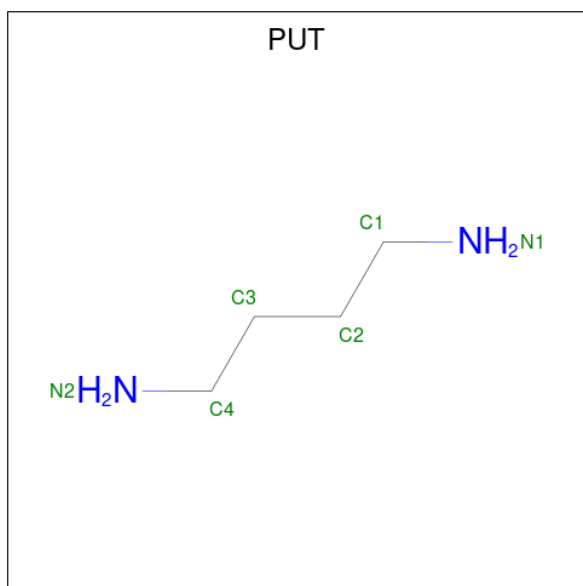
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			8	6	2		
57	AA	1	Total	C	O	0	0
			8	6	2		
57	DE	1	Total	C	O	0	0
			8	6	2		
57	DE	1	Total	C	O	0	0
			8	6	2		
57	DK	1	Total	C	O	0	0
			8	6	2		
57	DN	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	DS	1	Total C O 8 6 2	0	0
57	DT	1	Total C O 8 6 2	0	0
57	DT	1	Total C O 8 6 2	0	0
57	DA	1	Total C O 8 6 2	0	0
57	DA	1	Total C O 8 6 2	0	0
57	DA	1	Total C O 8 6 2	0	0
57	DA	1	Total C O 8 6 2	0	0
57	DA	1	Total C O 8 6 2	0	0

- Molecule 58 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



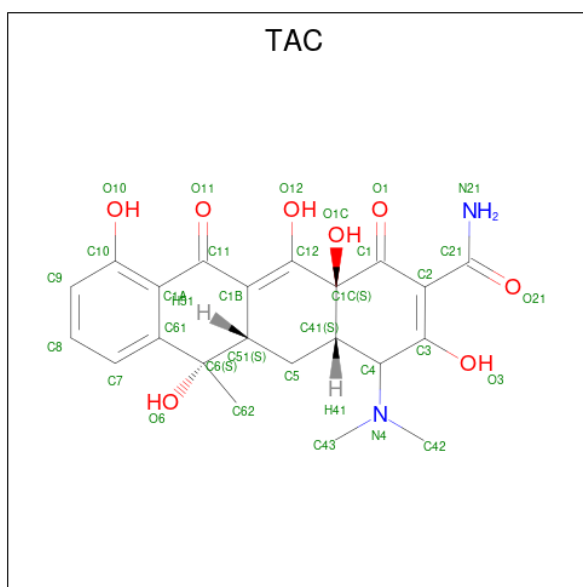
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AA	1	Total C N 6 4 2	0	0
58	AA	1	Total C N 6 4 2	0	0
58	AA	1	Total C N 6 4 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		
58	DA	1	Total	C	N	0	0
			6	4	2		

- Molecule 59 is TETRACYCLINE (three-letter code: TAC) (formula:  $C_{22}H_{24}N_2O_8$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	AA	1	Total 32	C 22	N 2	O 8	0	0
59	BA	1	Total 32	C 22	N 2	O 8	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	AB	1	Total Zn 1 1	0	0
60	C5	1	Total Zn 1 1	0	0
60	D5	1	Total Zn 1 1	0	0

- Molecule 61 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $\text{C}_4\text{H}_{10}\text{O}_3$ ).



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

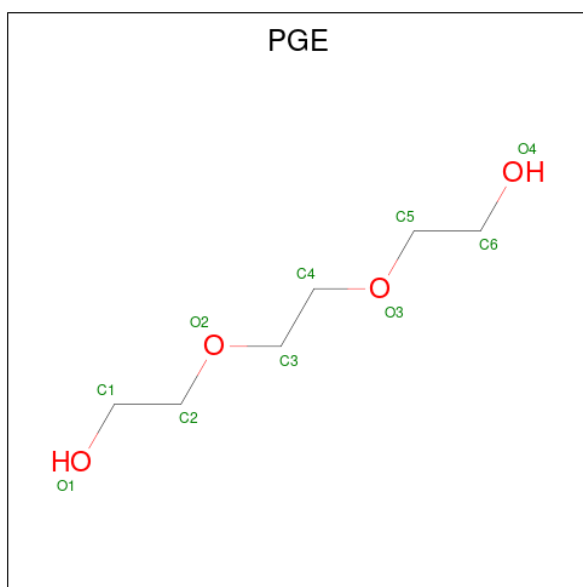
- Molecule 62 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).





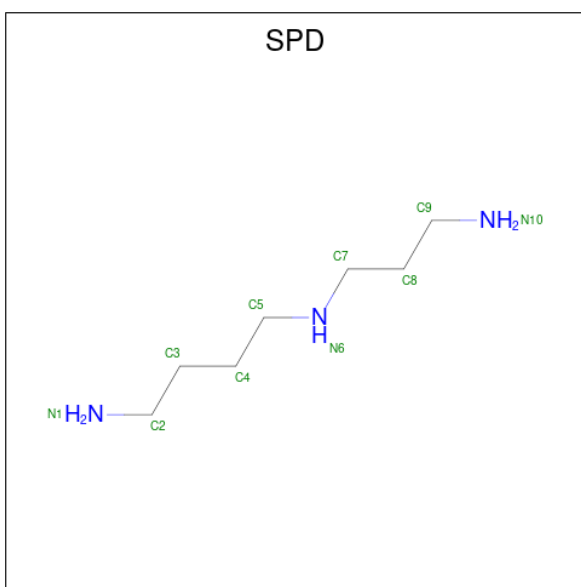
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	D1	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DB	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4	2	2		
62	DA	1	Total	C	O	0	0
			4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

- Molecule 63 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



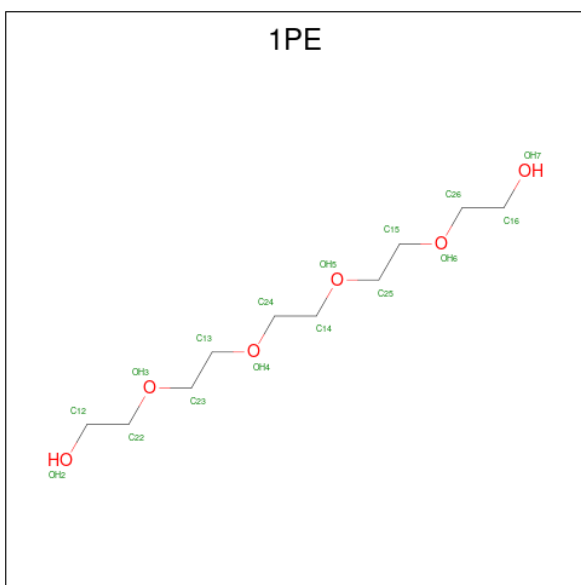
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			10	6	4		
63	D3	1	Total	C	O	0	0
			10	6	4		
63	DD	1	Total	C	O	0	0
			10	6	4		
63	DS	1	Total	C	O	0	0
			10	6	4		
63	DU	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		
63	DA	1	Total	C	O	0	0
			10	6	4		

- Molecule 64 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).



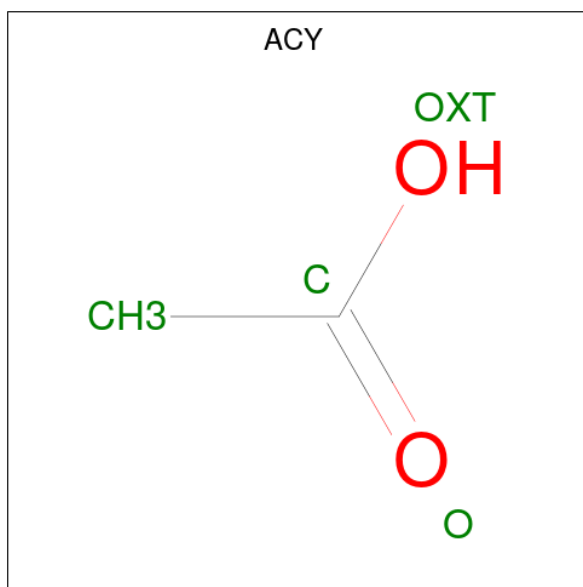
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		
64	DA	1	Total	C	N	0	0
			10	7	3		

- Molecule 65 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



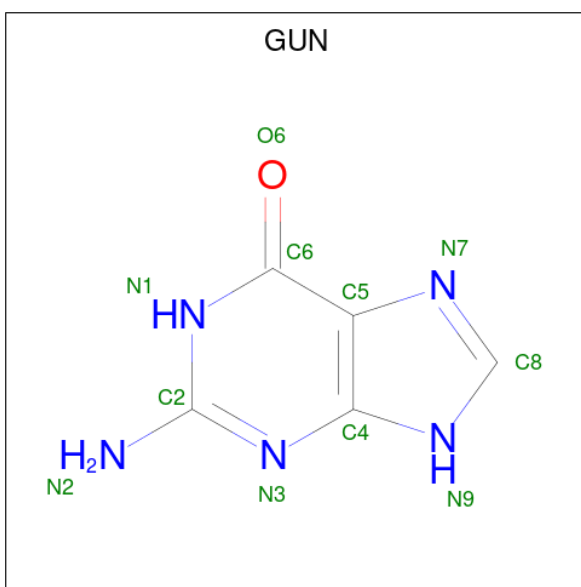
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	O	0	0
			16	10	6		
65	DA	1	Total	C	O	0	0
			16	10	6		

- Molecule 66 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



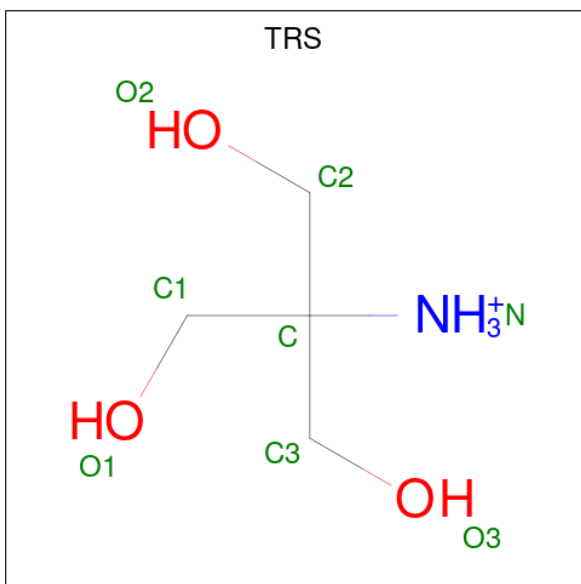
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		
66	DA	1	Total	C	O	0	0
			4	2	2		

- Molecule 67 is GUANINE (three-letter code: GUN) (formula:  $C_5H_5N_5O$ ).



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

- Molecule 68 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
68	DA	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 69 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	AA	507	Total 507	O 507	0	0
69	AC	4	Total 4	O 4	0	0
69	AD	2	Total 2	O 2	0	0
69	AE	4	Total 4	O 4	0	0
69	AF	1	Total 1	O 1	0	0
69	AG	1	Total 1	O 1	0	0
69	AH	1	Total 1	O 1	0	0
69	AJ	2	Total 2	O 2	0	0
69	AK	5	Total 5	O 5	0	0
69	AL	8	Total 8	O 8	0	0
69	AM	4	Total 4	O 4	0	0
69	AN	5	Total 5	O 5	0	0
69	AO	2	Total 2	O 2	0	0
69	AP	2	Total 2	O 2	0	0
69	AR	1	Total 1	O 1	0	0
69	AS	1	Total 1	O 1	0	0
69	AT	2	Total 2	O 2	0	0
69	AU	3	Total 3	O 3	0	0
69	C3	3	Total 3	O 3	0	0
69	C4	2	Total 2	O 2	0	0
69	BA	287	Total 287	O 287	0	0
69	BD	13	Total 13	O 13	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	BE	1	Total 1	O 1	0	0
69	BF	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	BN	2	Total 2	O 2	0	0
69	BO	1	Total 1	O 1	0	0
69	BP	3	Total 3	O 3	0	0
69	BR	1	Total 1	O 1	0	0
69	BT	4	Total 4	O 4	0	0
69	BU	2	Total 2	O 2	0	0
69	D1	42	Total 42	O 42	0	0
69	D2	7	Total 7	O 7	0	0
69	D3	24	Total 24	O 24	0	0
69	D4	33	Total 33	O 33	0	0
69	D5	13	Total 13	O 13	0	0
69	D0	27	Total 27	O 27	0	0
69	CB	13	Total 13	O 13	0	0
69	CC	10	Total 10	O 10	0	0
69	CD	5	Total 5	O 5	0	0
69	CA	692	Total 692	O 692	0	0
69	DC	102	Total 102	O 102	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DD	105	Total 105	O 105	0	0
69	CE	7	Total 7	O 7	0	0
69	CL	1	Total 1	O 1	0	0
69	CM	3	Total 3	O 3	0	0
69	CO	1	Total 1	O 1	0	0
69	CU	3	Total 3	O 3	0	0
69	CV	1	Total 1	O 1	0	0
69	CW	1	Total 1	O 1	0	0
69	CY	1	Total 1	O 1	0	0
69	DE	63	Total 63	O 63	0	0
69	DF	14	Total 14	O 14	0	0
69	DG	6	Total 6	O 6	0	0
69	DH	2	Total 2	O 2	0	0
69	DK	58	Total 58	O 58	0	0
69	DL	51	Total 51	O 51	0	0
69	DM	62	Total 62	O 62	0	0
69	DN	71	Total 71	O 71	0	0
69	DO	44	Total 44	O 44	0	0
69	DP	35	Total 35	O 35	0	0
69	DQ	27	Total 27	O 27	0	0
69	DR	64	Total 64	O 64	0	0

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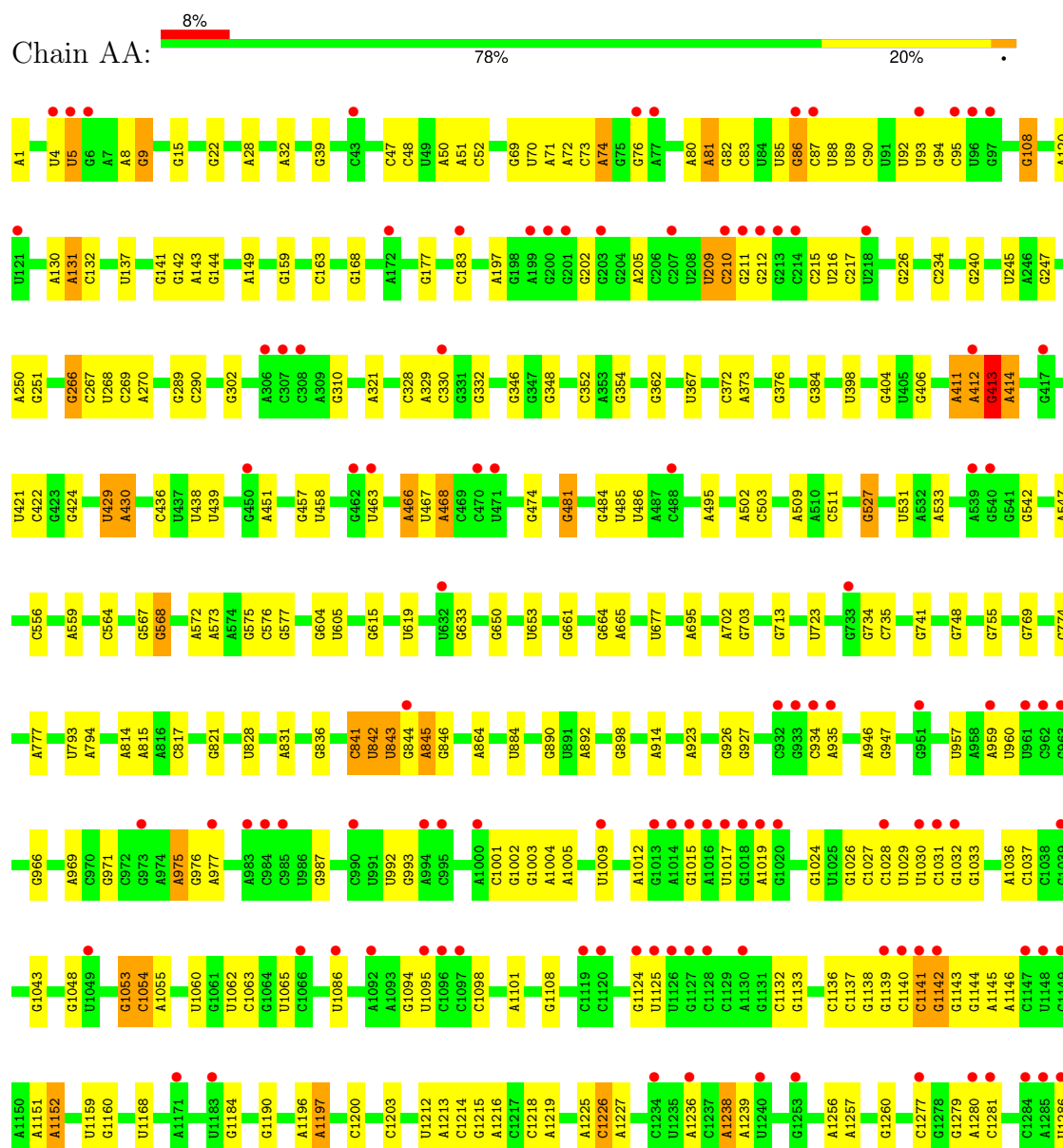
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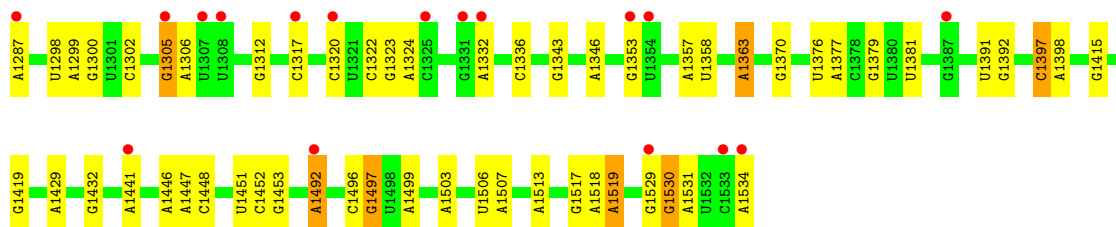
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
69	DS	51	Total 51	O 51	0	0
69	DT	69	Total 69	O 69	0	0
69	DU	17	Total 17	O 17	0	0
69	DV	19	Total 19	O 19	0	0
69	DW	31	Total 31	O 31	0	0
69	DX	30	Total 30	O 30	0	0
69	DY	9	Total 9	O 9	0	0
69	DZ	7	Total 7	O 7	0	0
69	DB	212	Total 212	O 212	0	0
69	DA	4834	Total 4834	O 4834	0	0

### 3 Residue-property plots

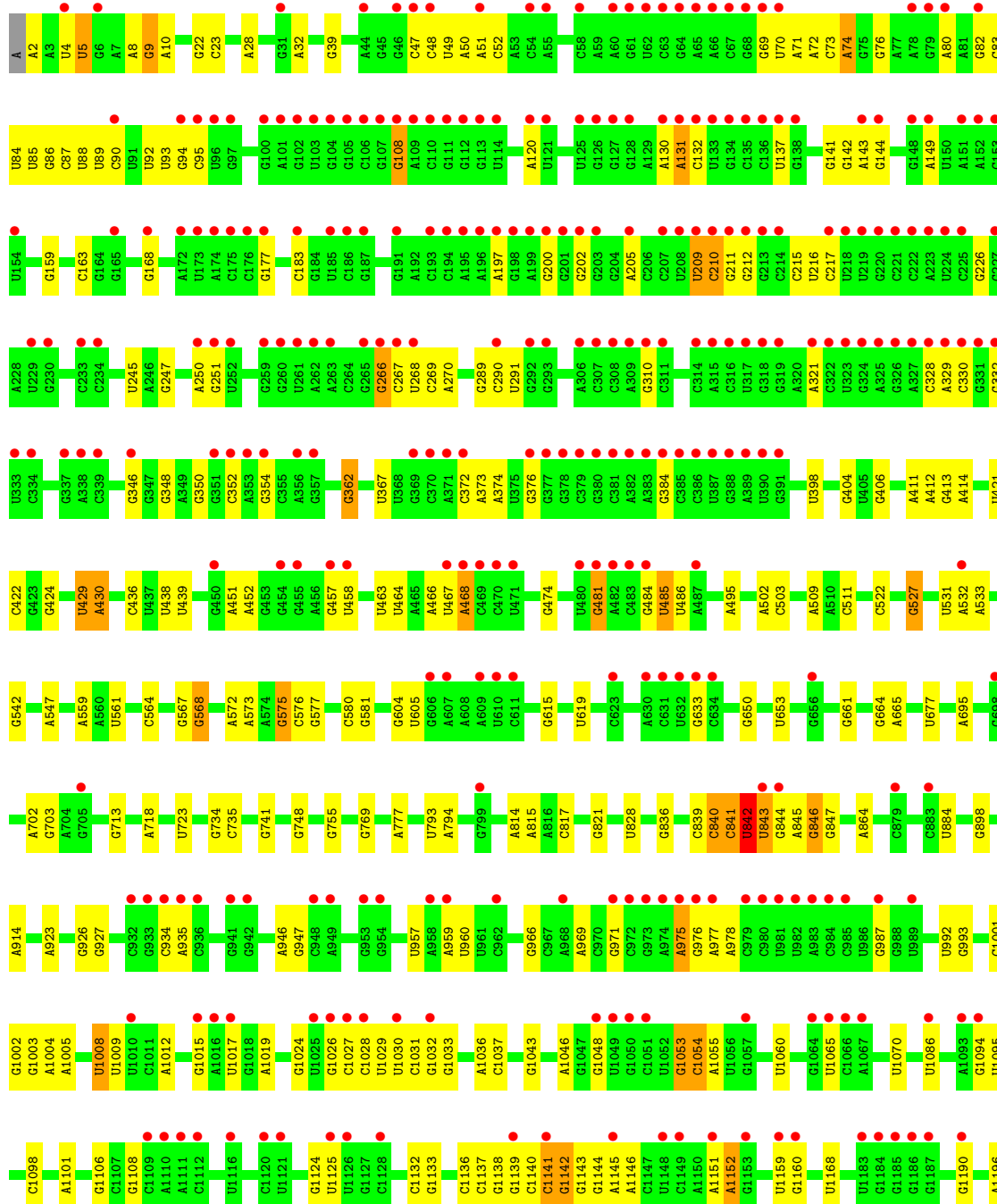
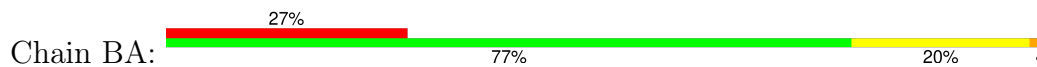
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

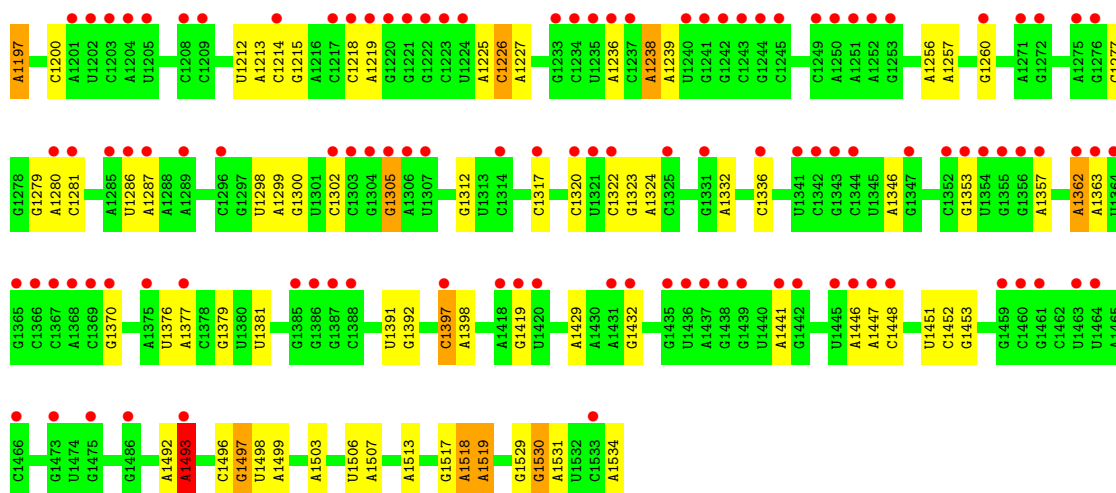
#### • Molecule 1: 16S rRNA



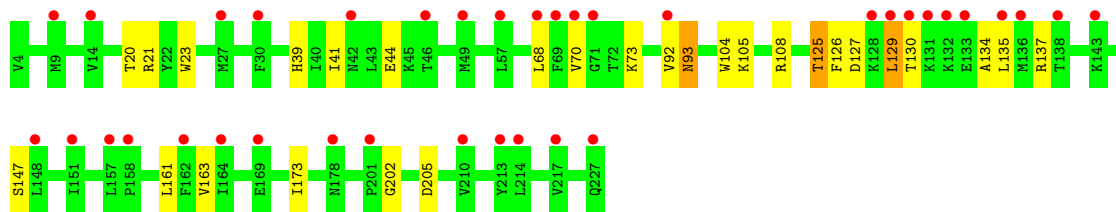
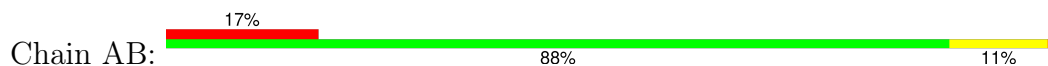


• Molecule 1: 16S rRNA

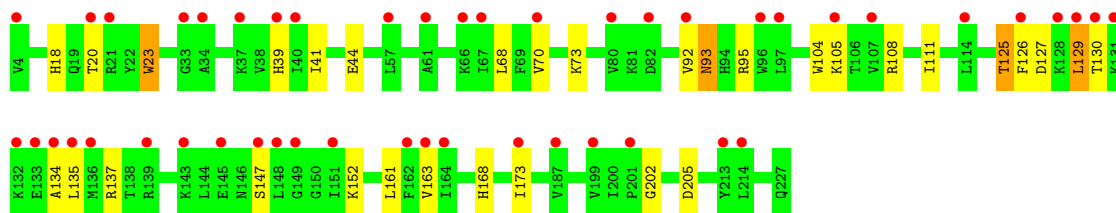
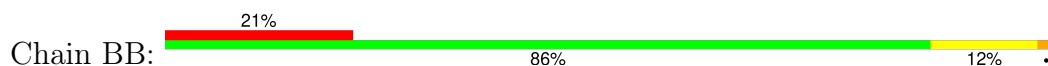




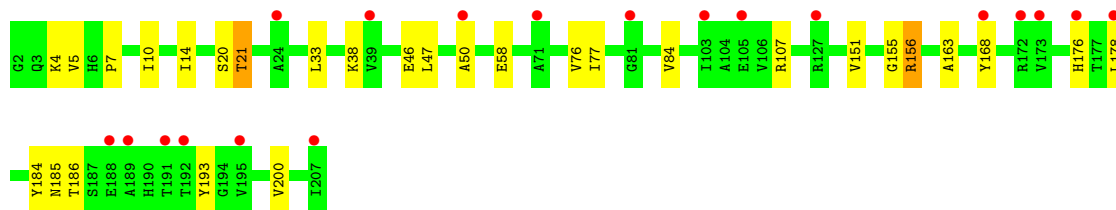
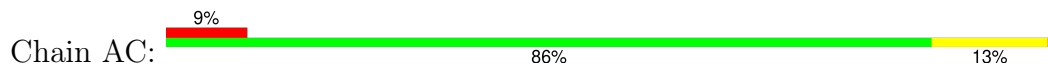
• Molecule 2: 30S ribosomal protein S2



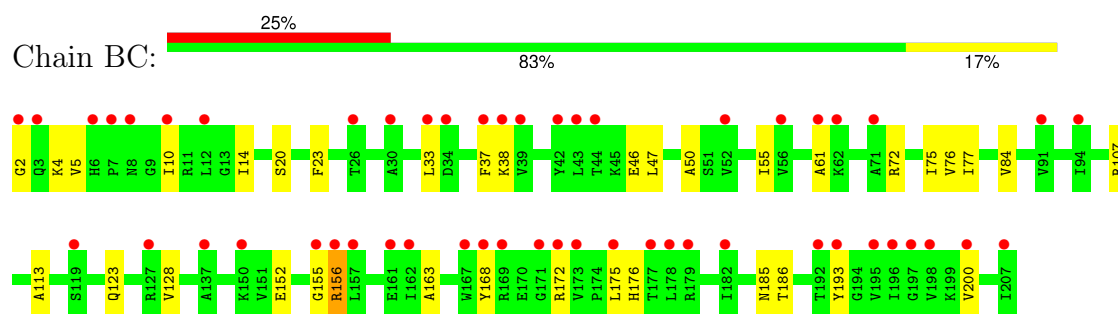
• Molecule 2: 30S ribosomal protein S2



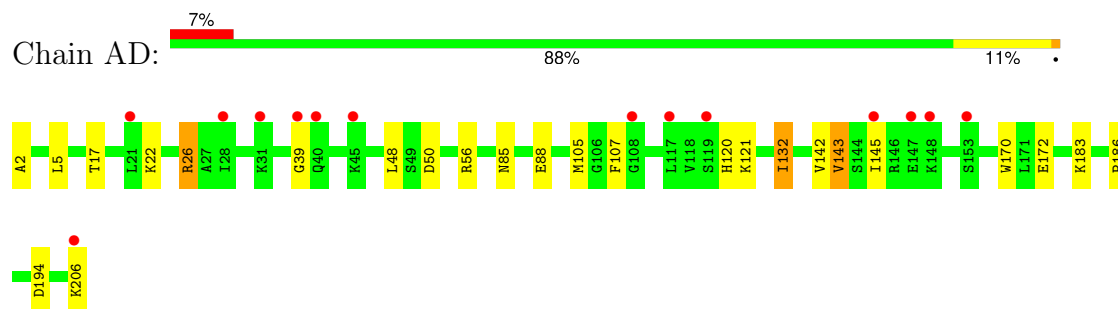
• Molecule 3: 30S ribosomal protein S3



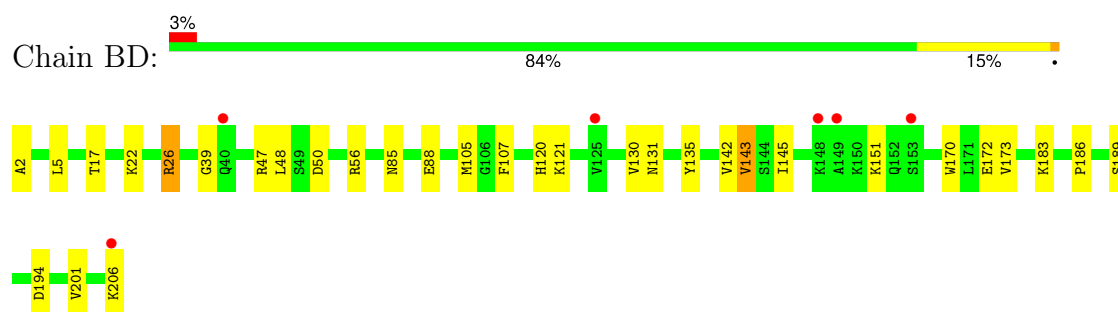
• Molecule 3: 30S ribosomal protein S3



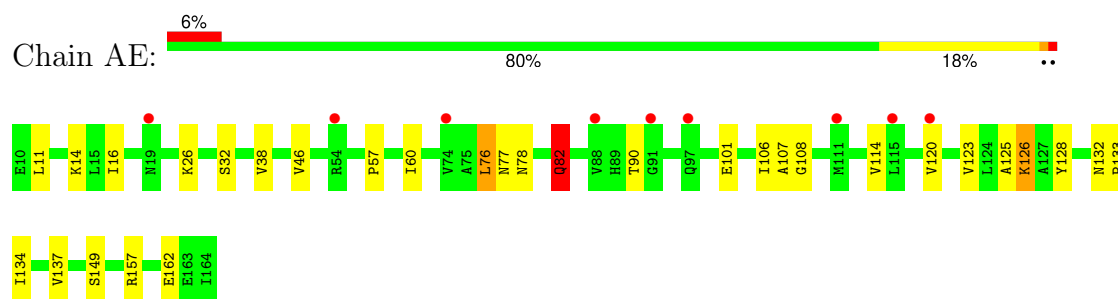
- Molecule 4: 30S ribosomal protein S4



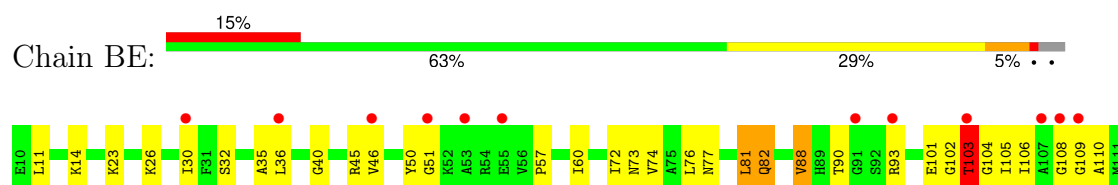
- Molecule 4: 30S ribosomal protein S4



- Molecule 5: 30S ribosomal protein S5

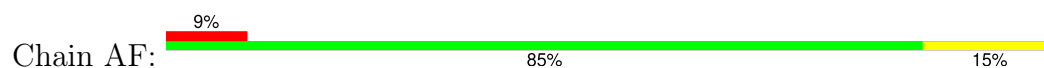


- Molecule 5: 30S ribosomal protein S5





- Molecule 6: 30S ribosomal protein S6



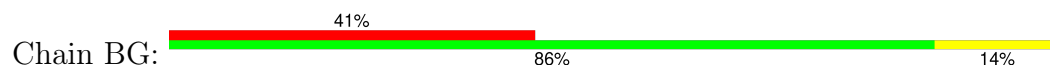
- Molecule 6: 30S ribosomal protein S6



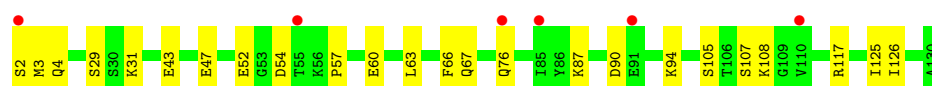
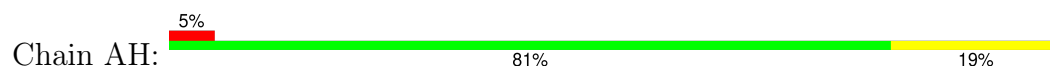
- Molecule 7: 30S ribosomal protein S7



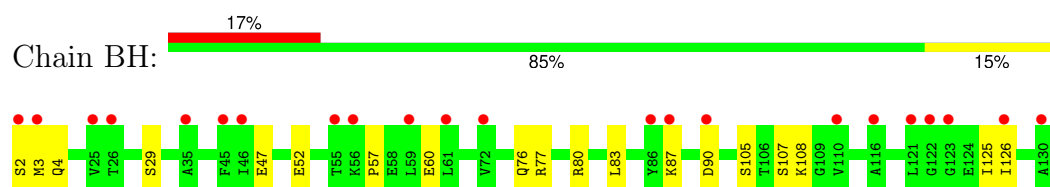
- Molecule 7: 30S ribosomal protein S7



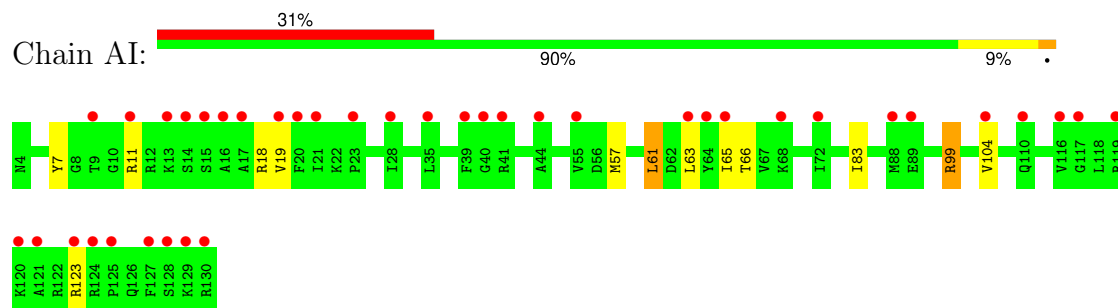
- Molecule 8: 30S ribosomal protein S8



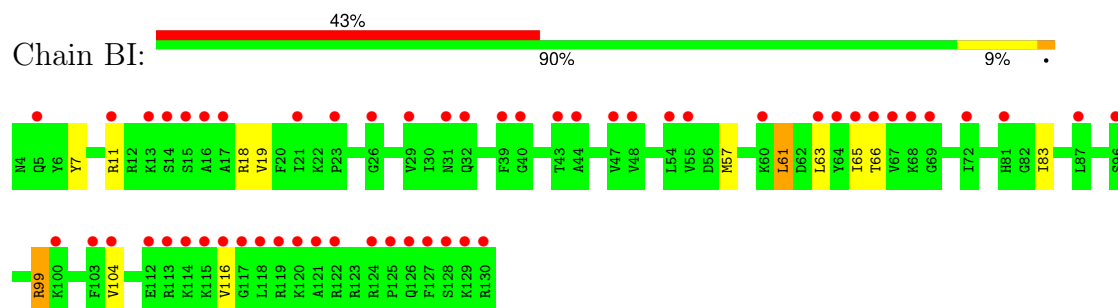
- Molecule 8: 30S ribosomal protein S8



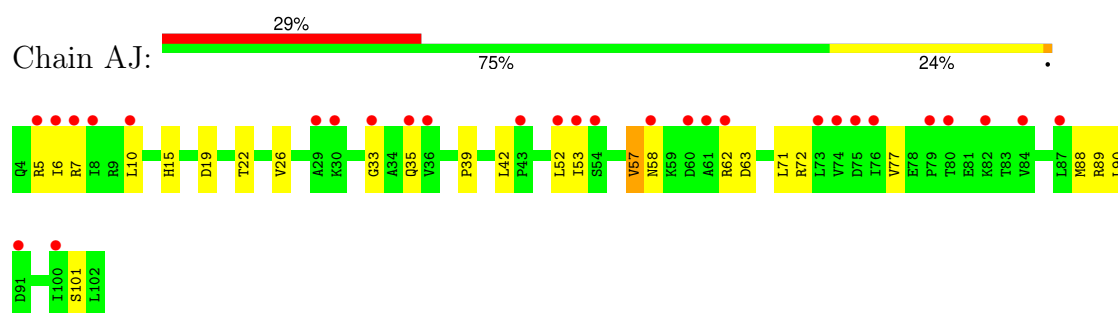
• Molecule 9: 30S ribosomal protein S9



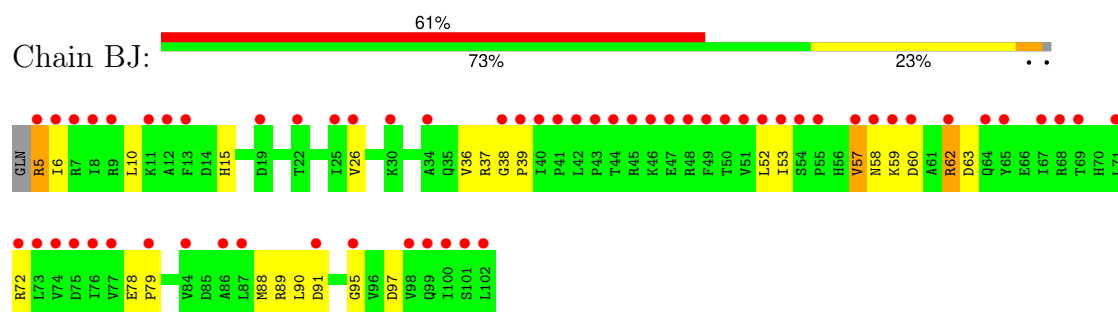
• Molecule 9: 30S ribosomal protein S9



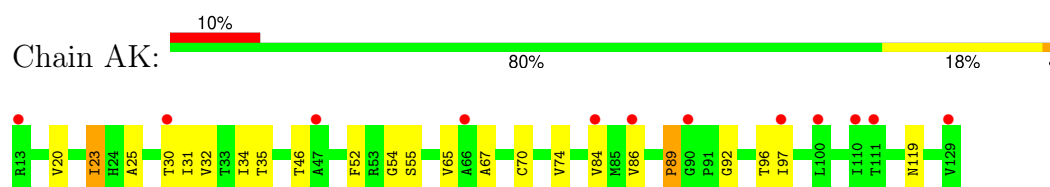
• Molecule 10: 30S ribosomal protein S10



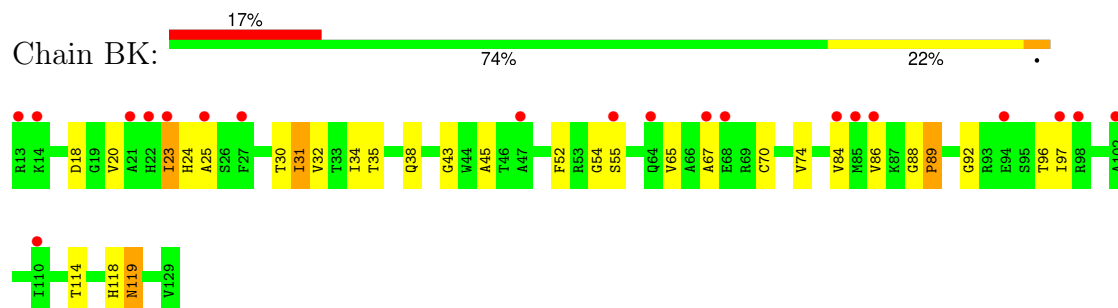
• Molecule 10: 30S ribosomal protein S10



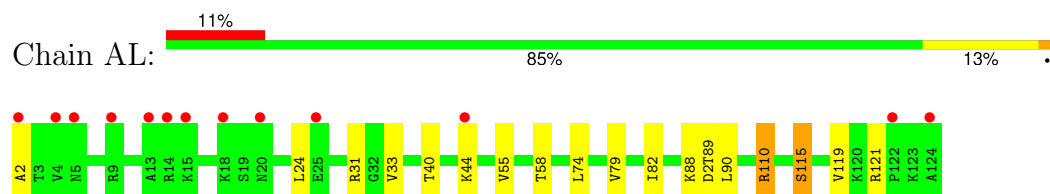
• Molecule 11: 30S ribosomal protein S11



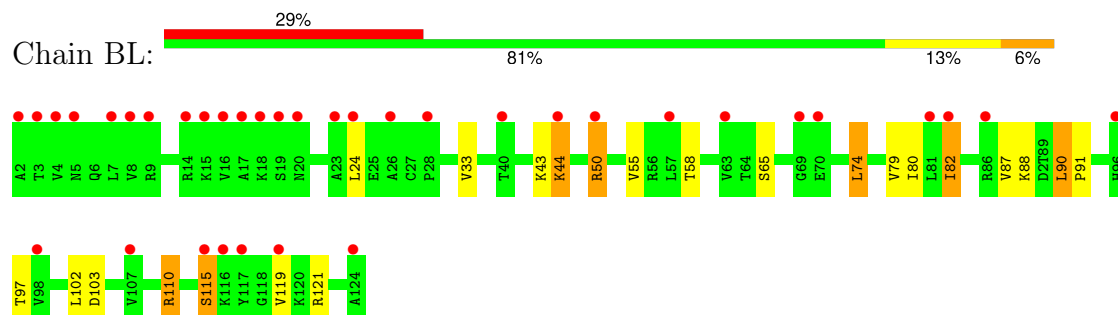
- Molecule 11: 30S ribosomal protein S11



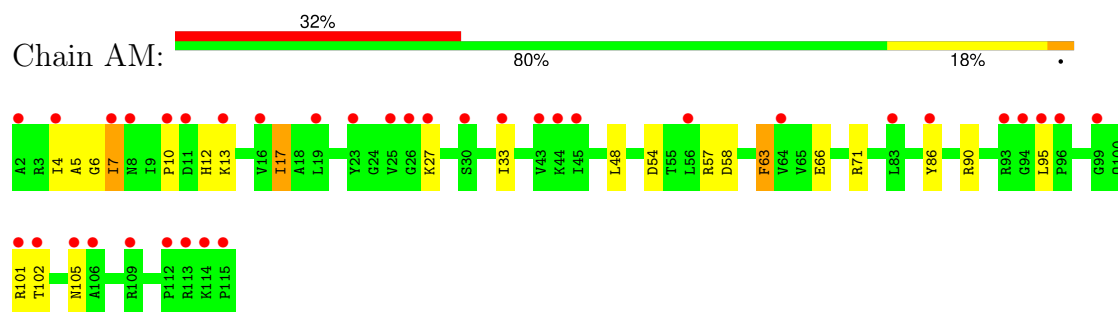
- Molecule 12: 30S ribosomal protein S12



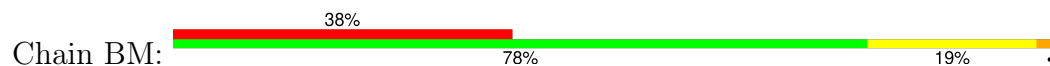
- Molecule 12: 30S ribosomal protein S12



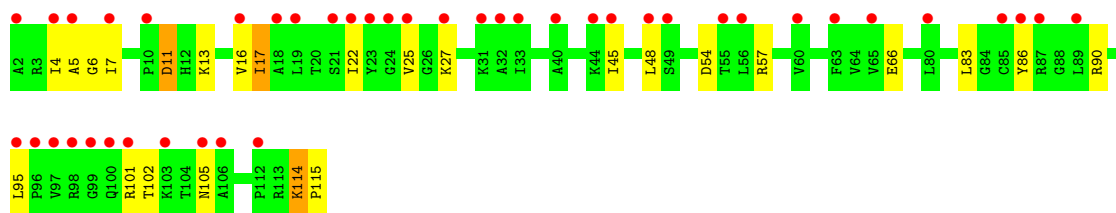
- Molecule 13: 30S ribosomal protein S13



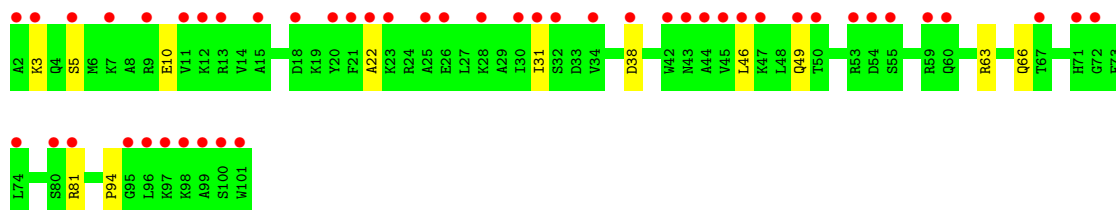
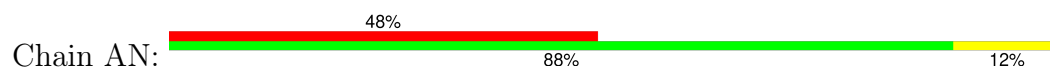
- Molecule 13: 30S ribosomal protein S13



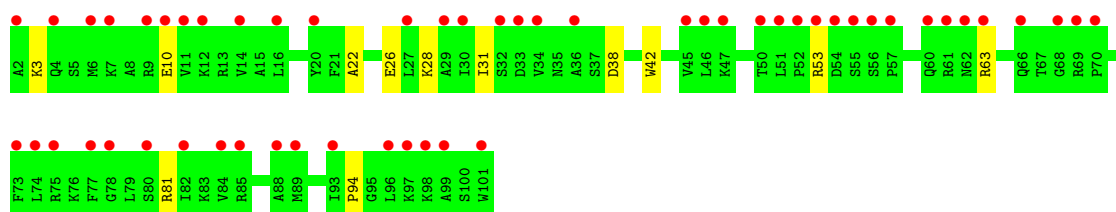




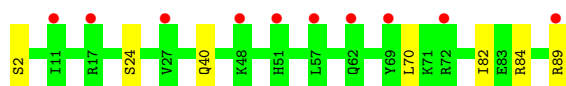
● Molecule 14: 30S ribosomal protein S14



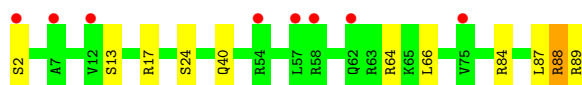
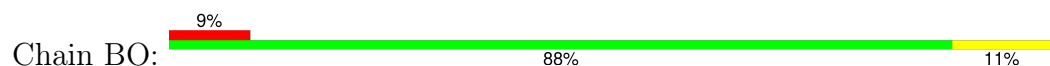
● Molecule 14: 30S ribosomal protein S14



● Molecule 15: 30S ribosomal protein S15



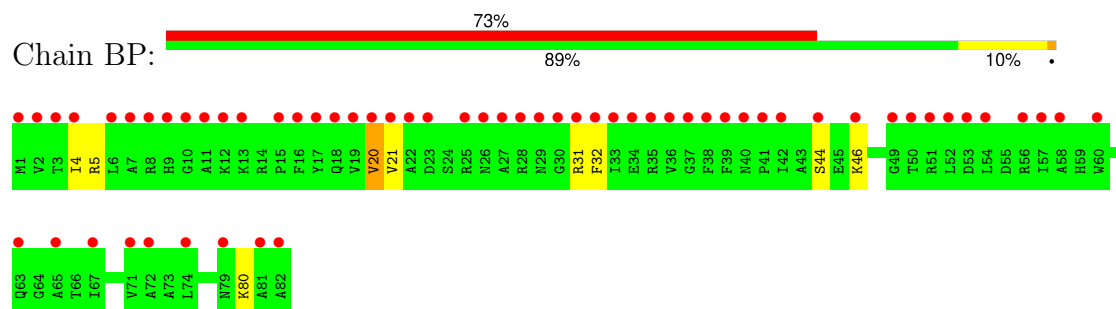
● Molecule 15: 30S ribosomal protein S15



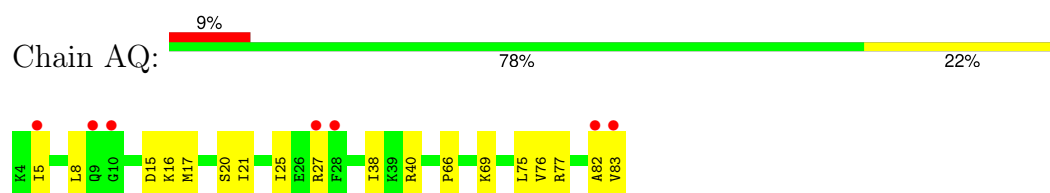
● Molecule 16: 30S ribosomal protein S16



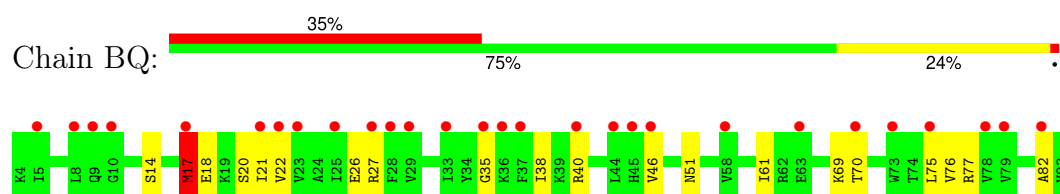
- Molecule 16: 30S ribosomal protein S16



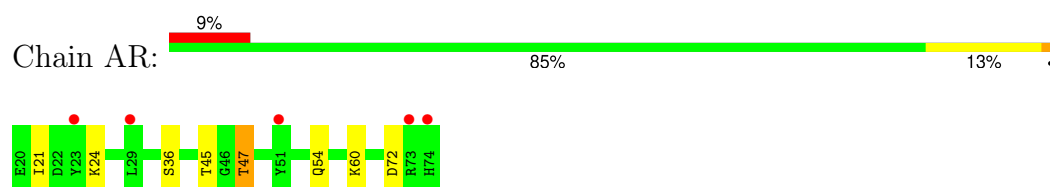
- Molecule 17: 30S ribosomal protein S17



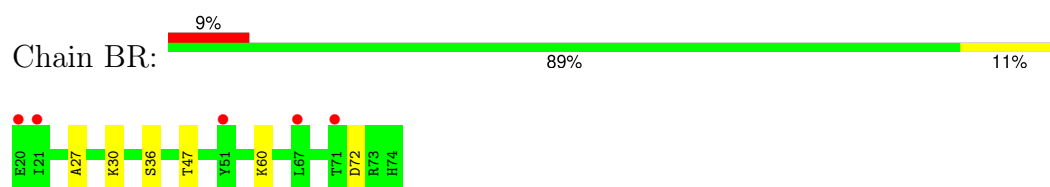
- Molecule 17: 30S ribosomal protein S17



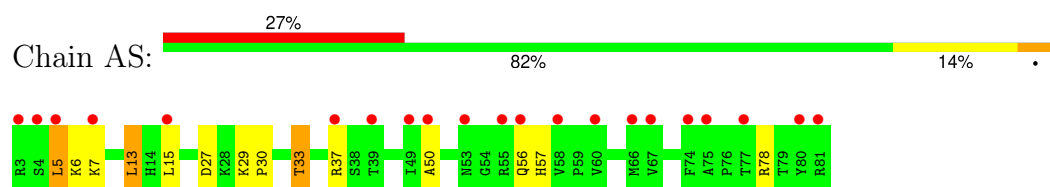
- Molecule 18: 30S ribosomal protein S18



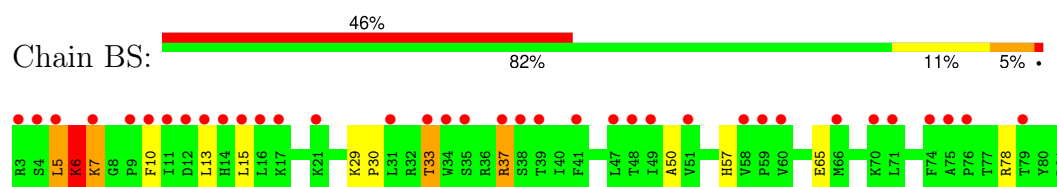
- Molecule 18: 30S ribosomal protein S18



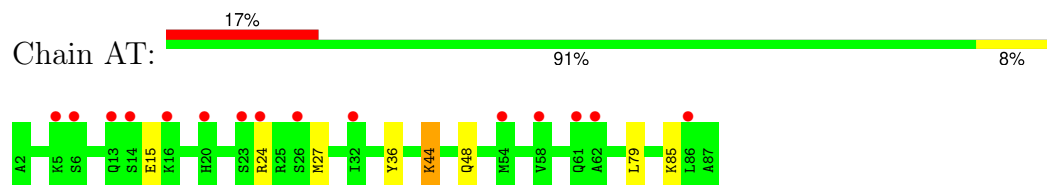
- Molecule 19: 30S ribosomal protein S19



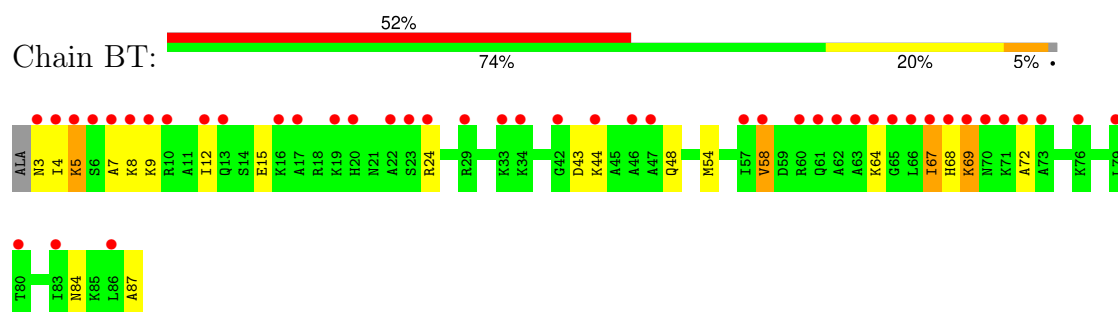
- Molecule 19: 30S ribosomal protein S19



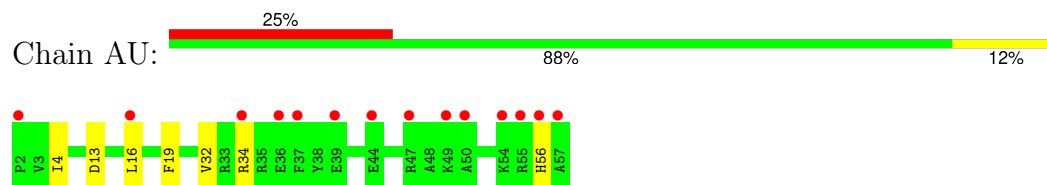
- Molecule 20: 30S ribosomal protein S20



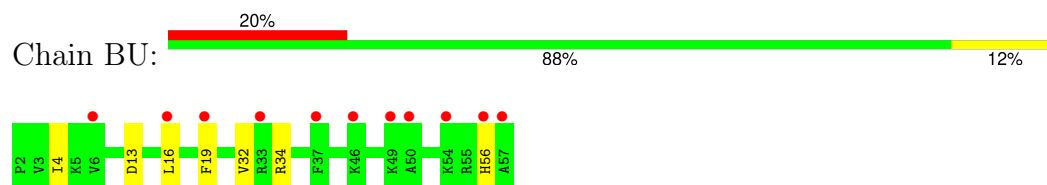
- Molecule 20: 30S ribosomal protein S20



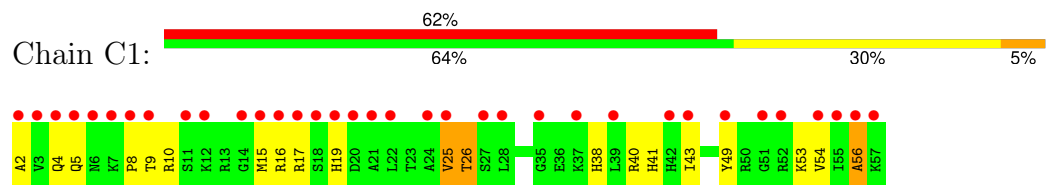
- Molecule 21: 30S ribosomal protein S21



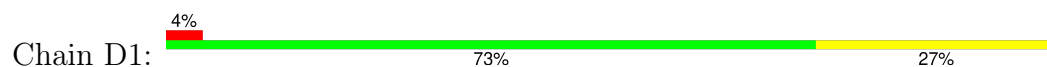
- Molecule 21: 30S ribosomal protein S21

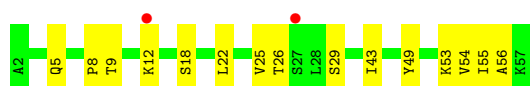


- Molecule 22: 50S ribosomal protein L32

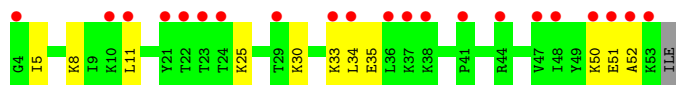
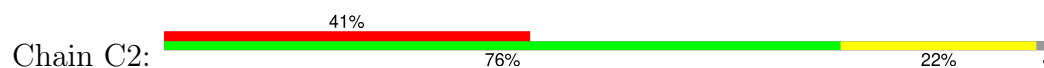


- Molecule 22: 50S ribosomal protein L32

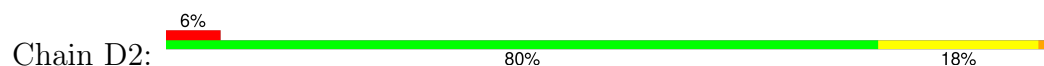




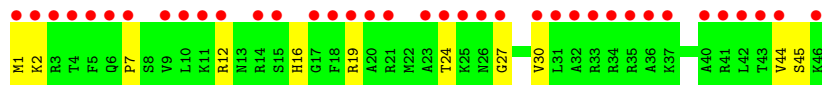
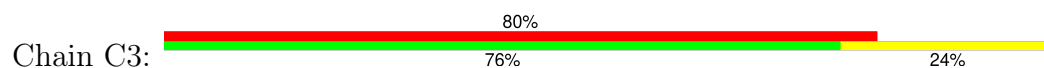
- Molecule 23: 50S ribosomal protein L33



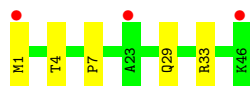
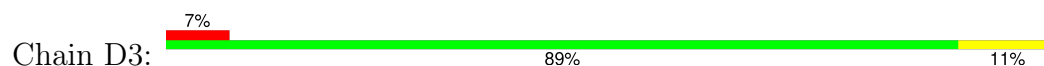
- Molecule 23: 50S ribosomal protein L33



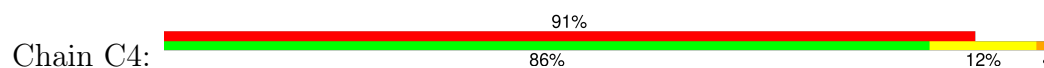
- Molecule 24: 50S ribosomal protein L34



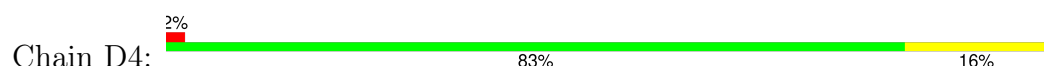
- Molecule 24: 50S ribosomal protein L34

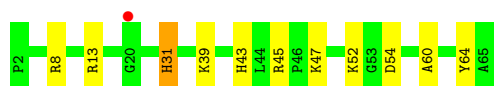


- Molecule 25: 50S ribosomal protein L35

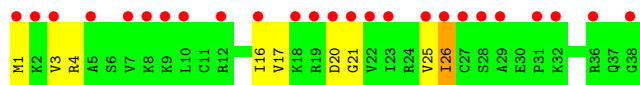
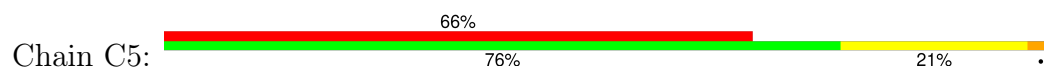


- Molecule 25: 50S ribosomal protein L35





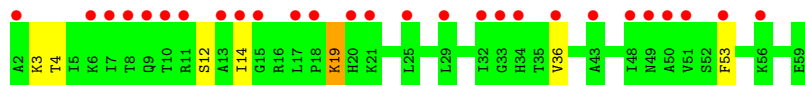
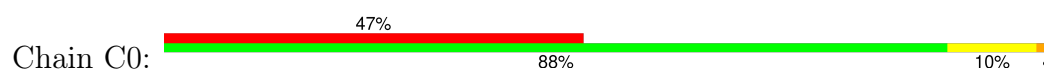
- Molecule 26: 50S ribosomal protein L36



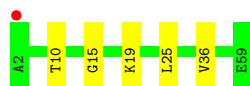
- Molecule 26: 50S ribosomal protein L36



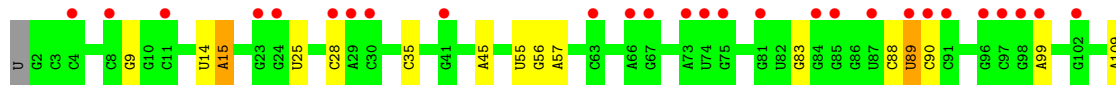
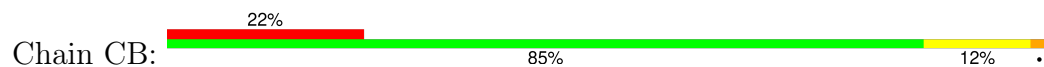
- Molecule 27: 50S ribosomal protein L30



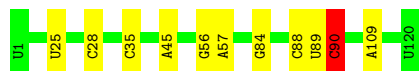
- Molecule 27: 50S ribosomal protein L30



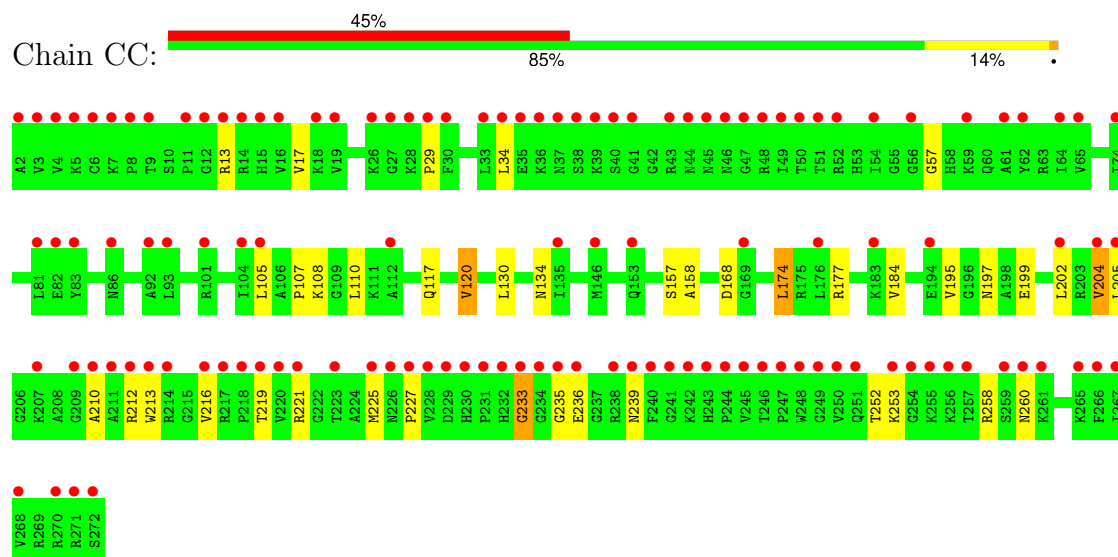
- Molecule 28: 5S rRNA



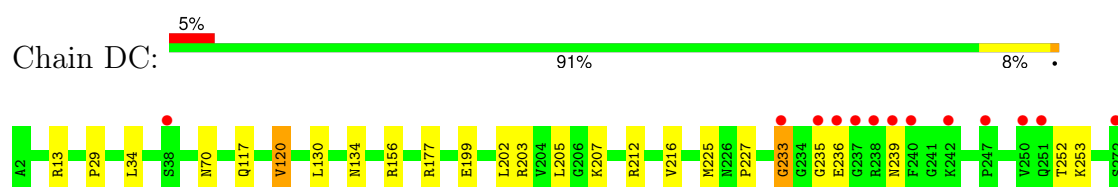
- Molecule 28: 5S rRNA



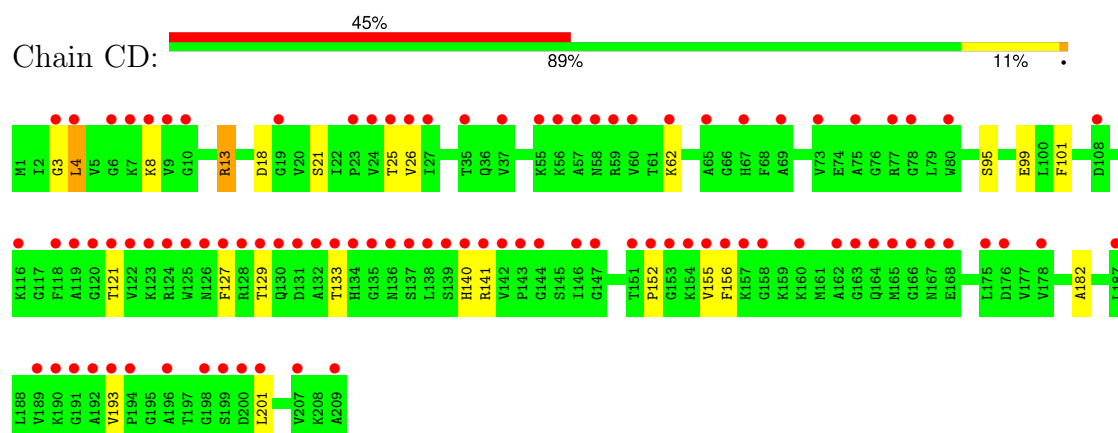
- Molecule 29: 50S ribosomal protein L2



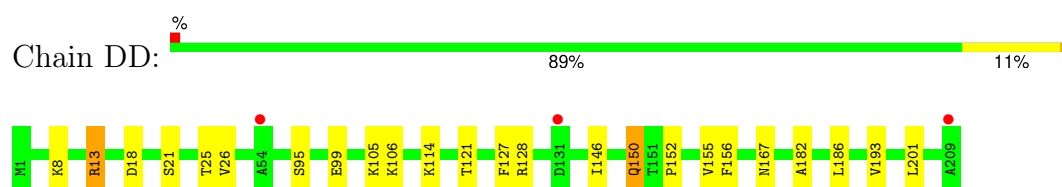
- Molecule 29: 50S ribosomal protein L2



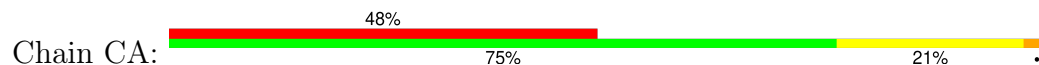
- Molecule 30: 50S ribosomal protein L3



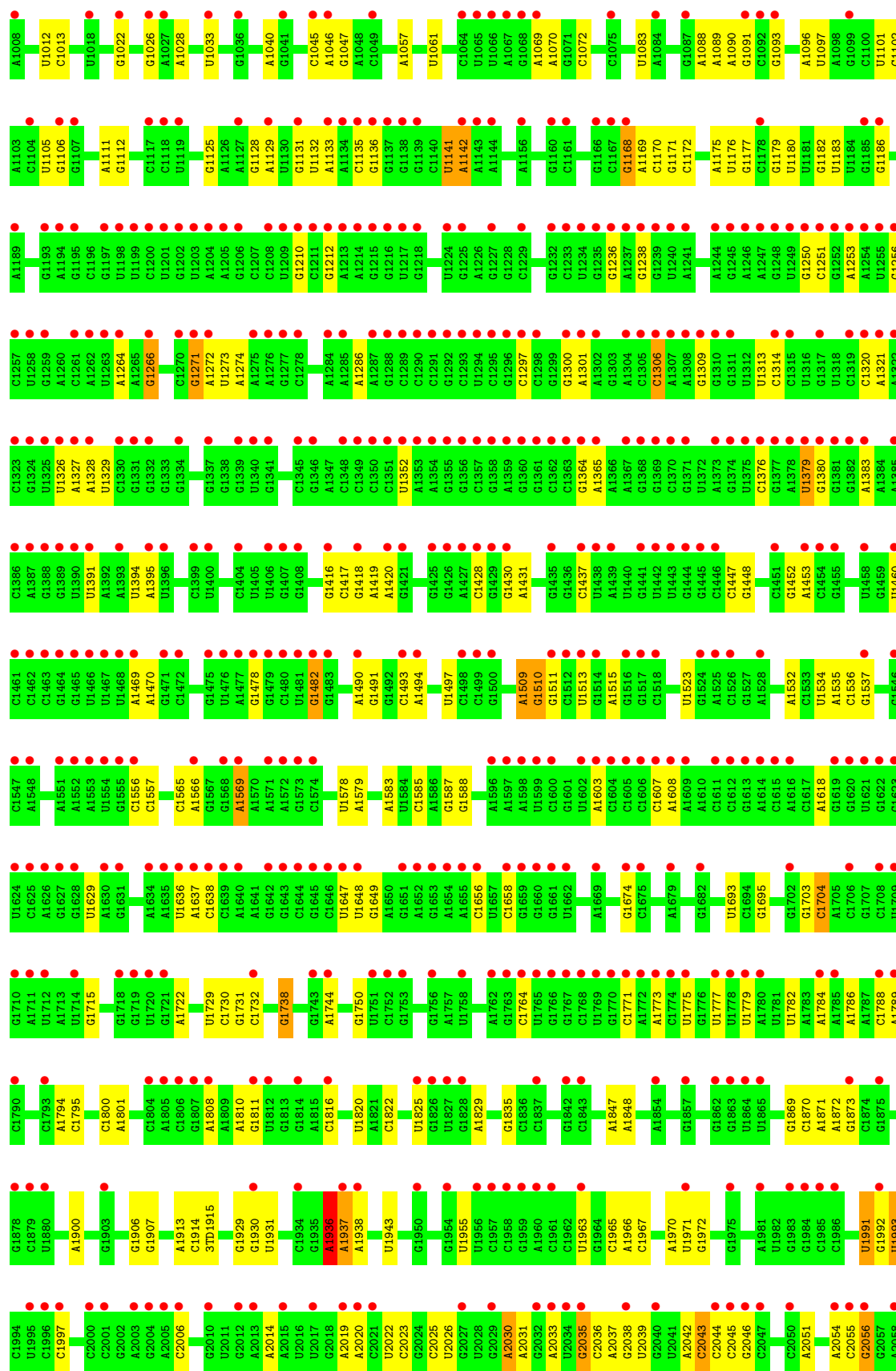
- Molecule 30: 50S ribosomal protein L3



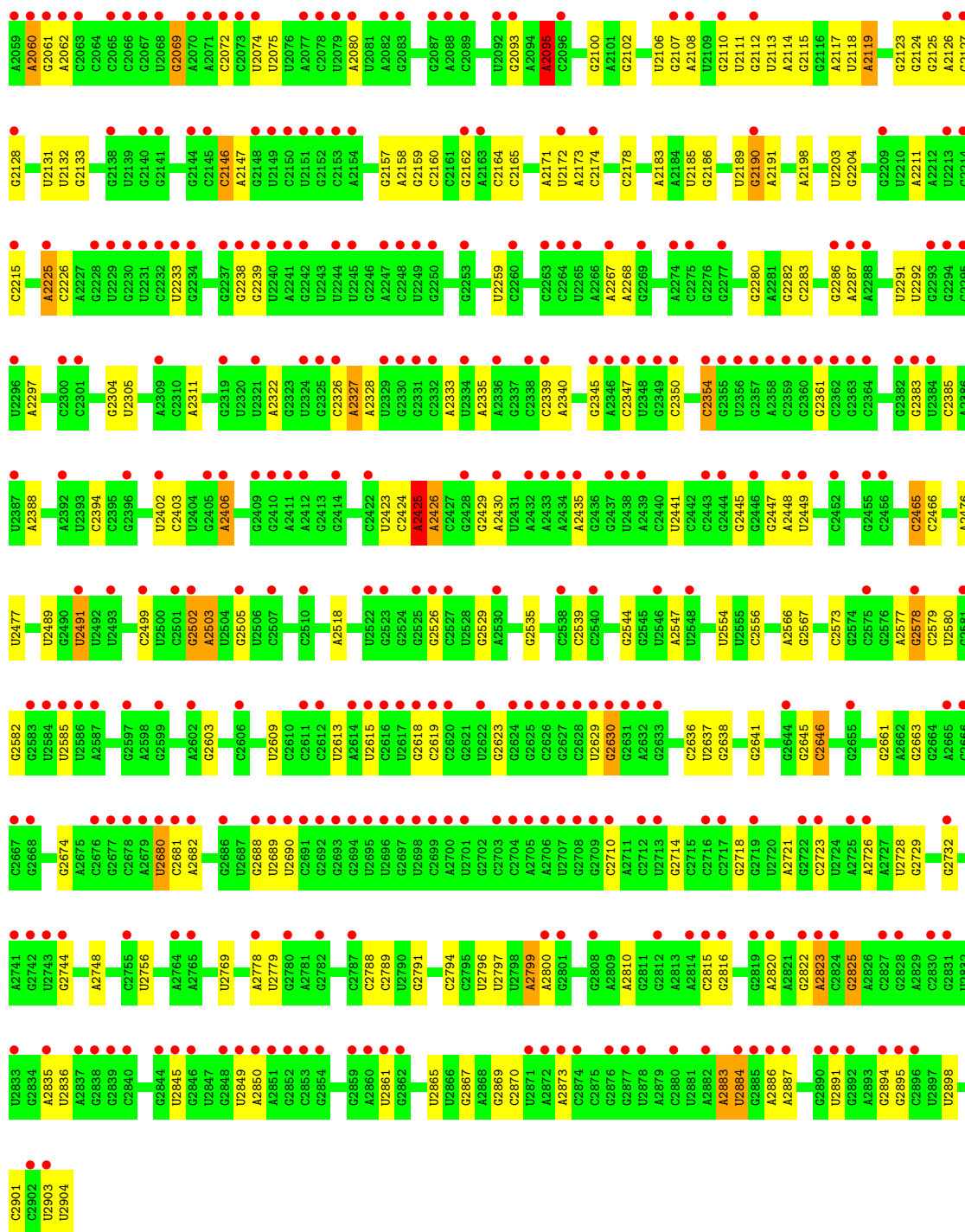
- Molecule 31: 23S rRNA





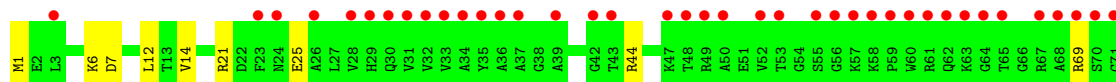


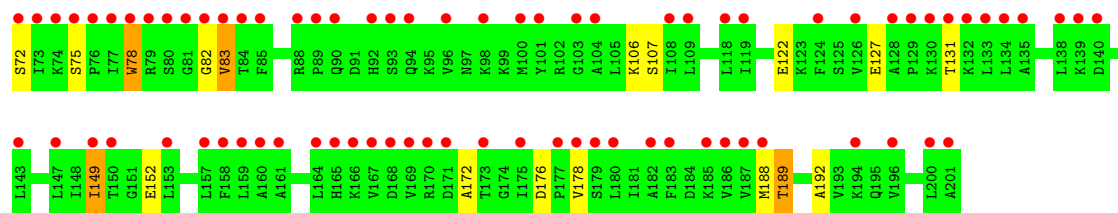




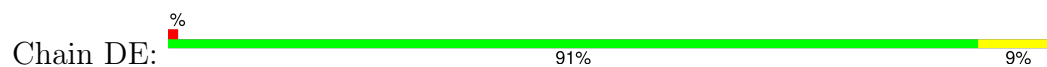
● Molecule 32: 50S ribosomal protein L4

Chain CE:

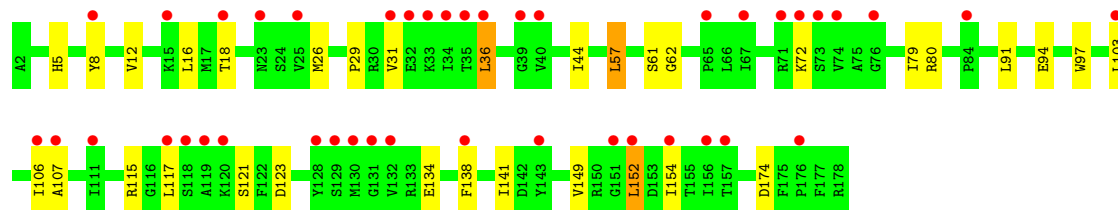
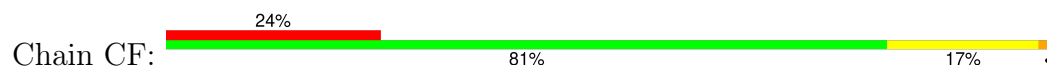




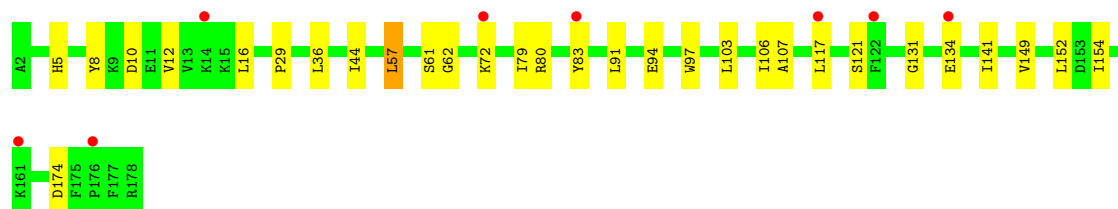
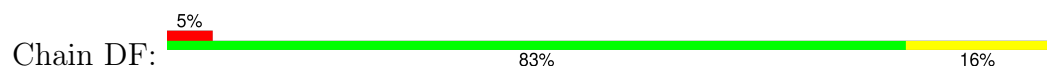
• Molecule 32: 50S ribosomal protein L4



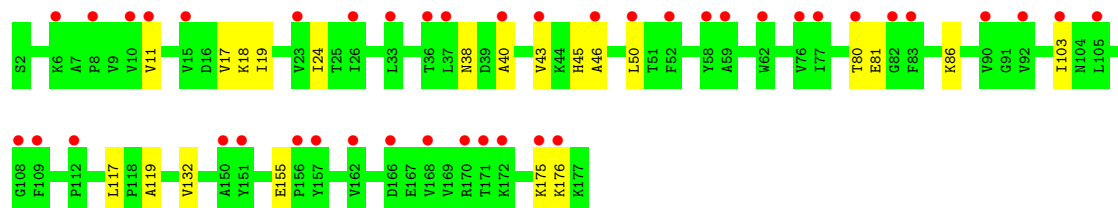
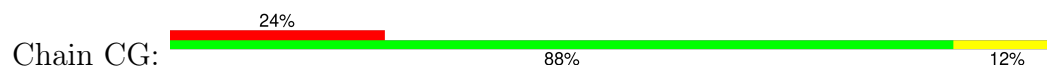
• Molecule 33: 50S ribosomal protein L5



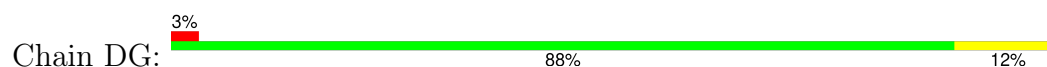
• Molecule 33: 50S ribosomal protein L5



• Molecule 34: 50S ribosomal protein L6

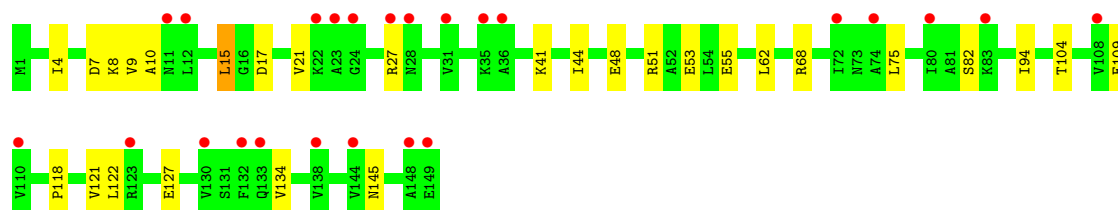
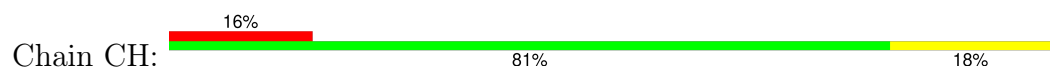


• Molecule 34: 50S ribosomal protein L6

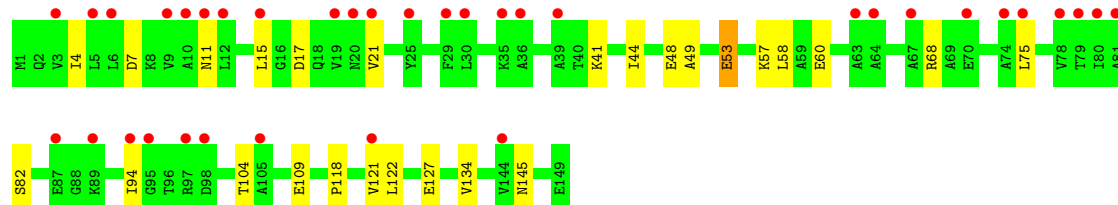
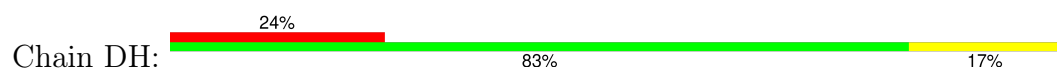




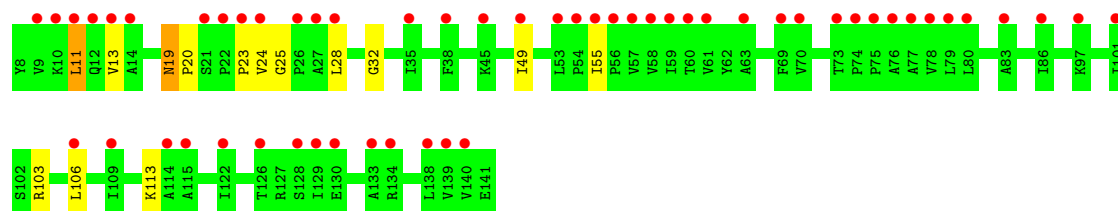
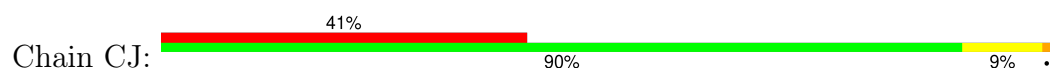
- Molecule 35: 50S ribosomal protein L9



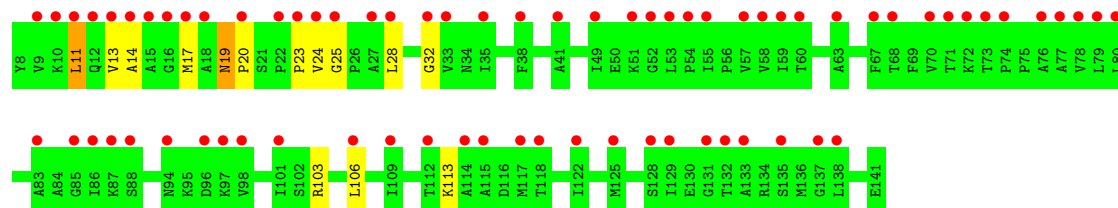
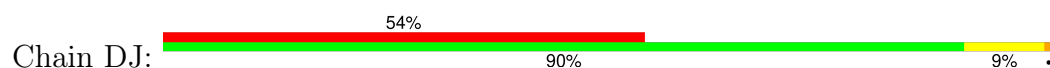
- Molecule 35: 50S ribosomal protein L9



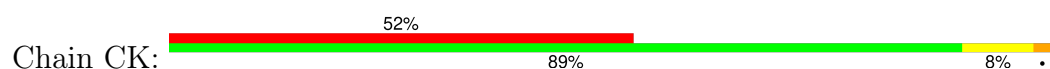
- Molecule 36: 50S ribosomal protein L11

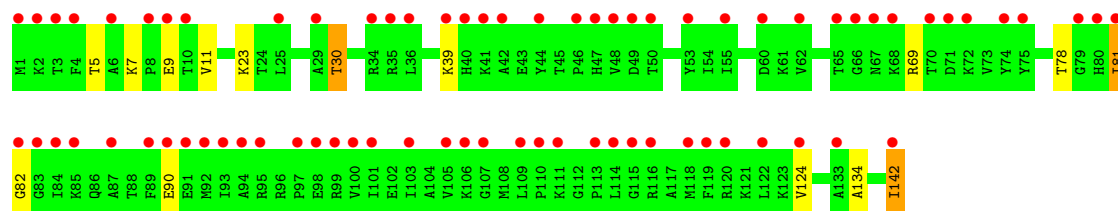


- Molecule 36: 50S ribosomal protein L11



- Molecule 37: 50S ribosomal protein L13





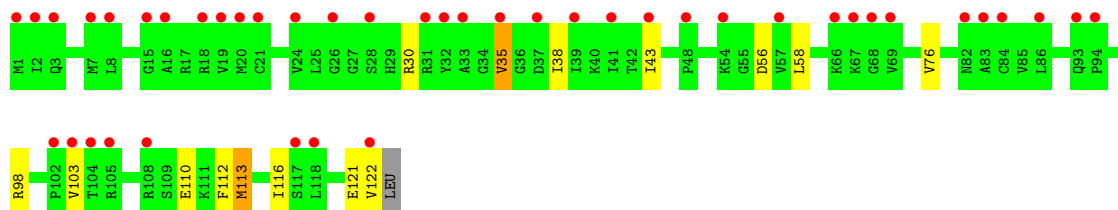
• Molecule 37: 50S ribosomal protein L13

Chain DK: 94% 5% .



• Molecule 38: 50S ribosomal protein L14

Chain CL: 35% 87% 11% ..



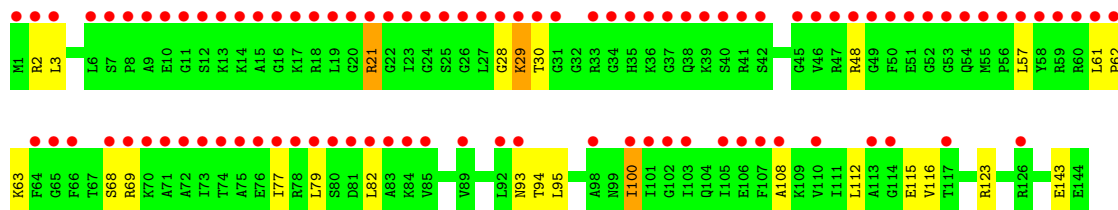
• Molecule 38: 50S ribosomal protein L14

Chain DL: 90% 8% .



• Molecule 39: 50S ribosomal protein L15

Chain CM: 66% 82% 16% .



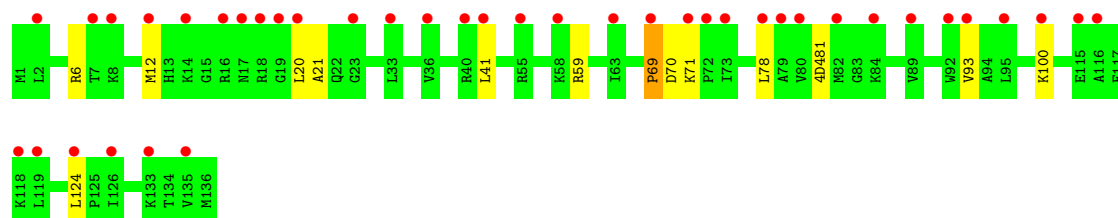
• Molecule 39: 50S ribosomal protein L15

Chain DM: 6% 84% 15% .



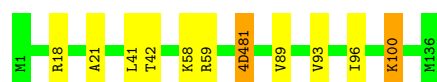
- Molecule 40: 50S ribosomal protein L16

Chain CN: 29% 90% 10%



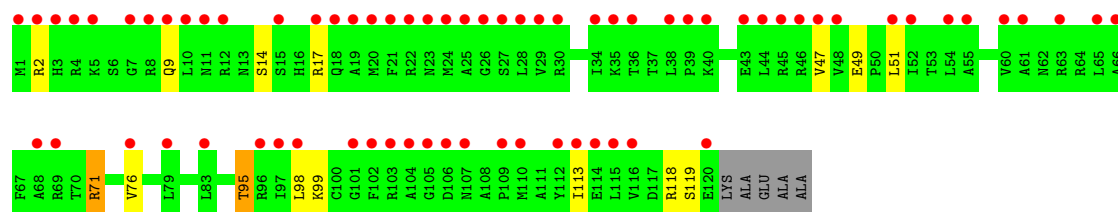
- Molecule 40: 50S ribosomal protein L16

Chain DN: 92% 7%



- Molecule 41: 50S ribosomal protein L17

Chain CO: 56% 84% 10%



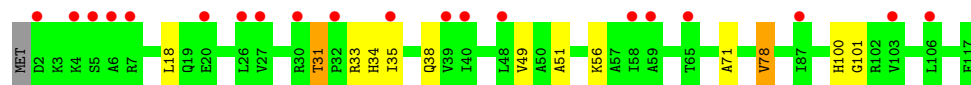
- Molecule 41: 50S ribosomal protein L17

Chain DO: 93% 7%



- Molecule 42: 50S ribosomal protein L18

Chain CP: 17% 88% 9%

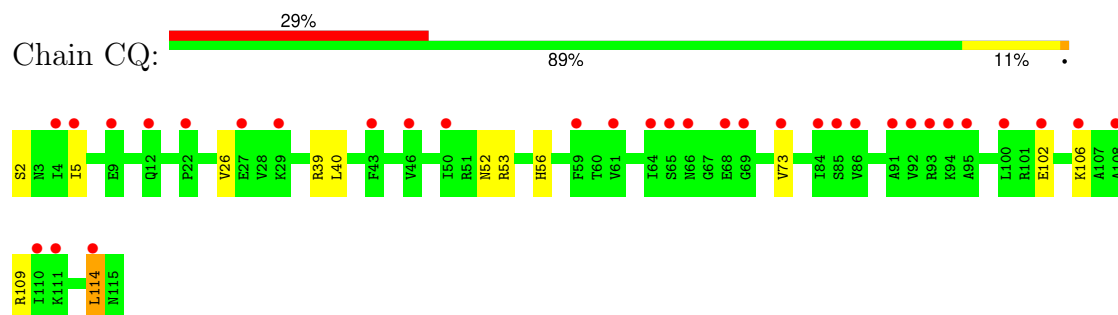


- Molecule 42: 50S ribosomal protein L18

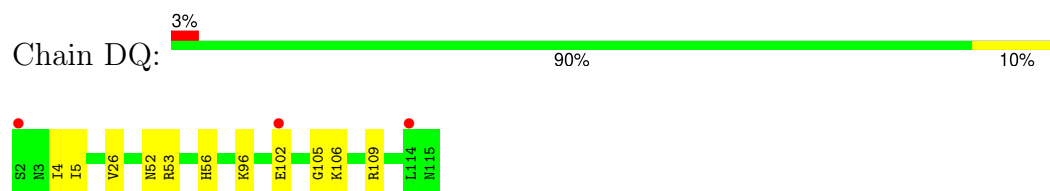
Chain DP: 2% 90% 8%



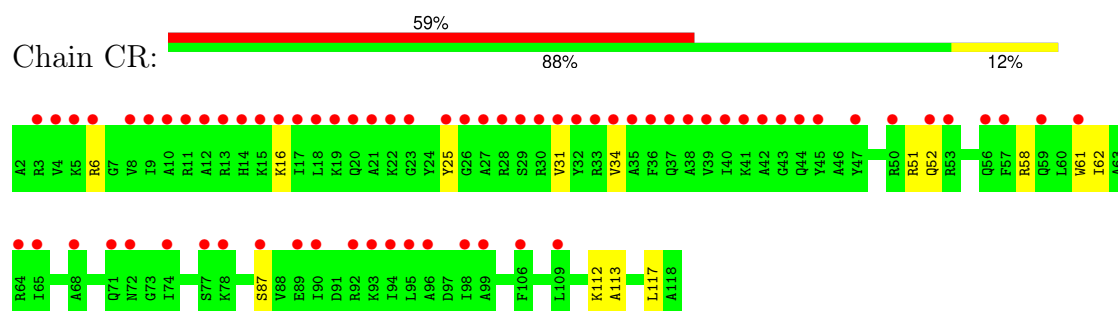
- Molecule 43: 50S ribosomal protein L19



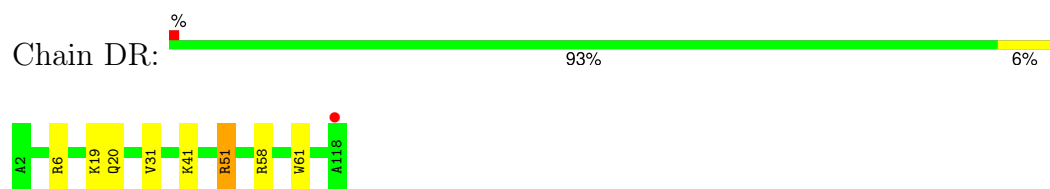
- Molecule 43: 50S ribosomal protein L19



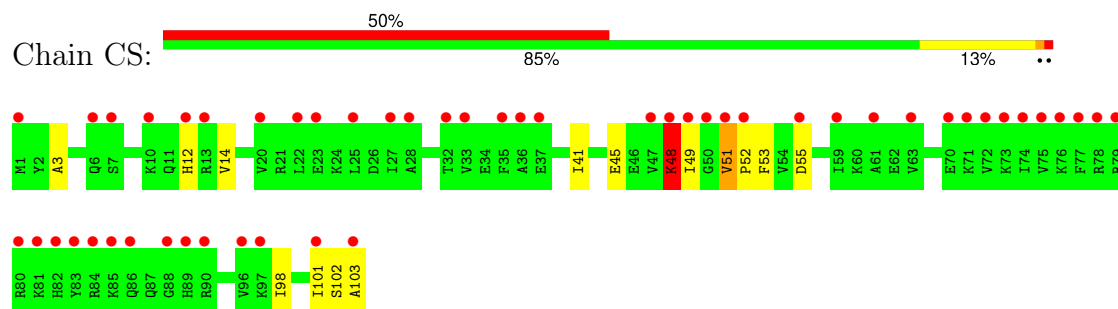
- Molecule 44: 50S ribosomal protein L20



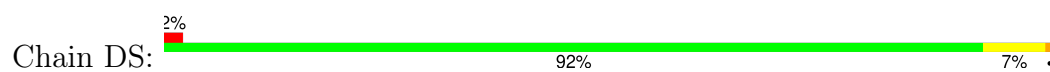
- Molecule 44: 50S ribosomal protein L20



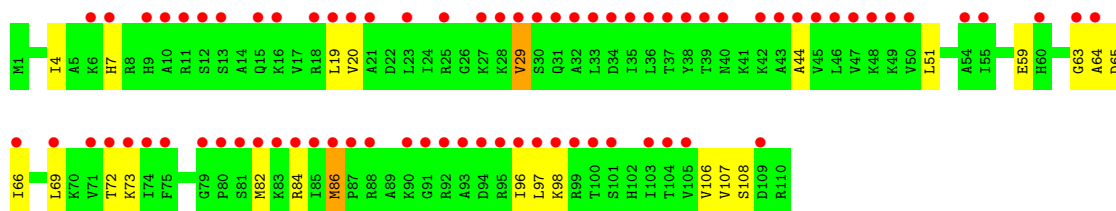
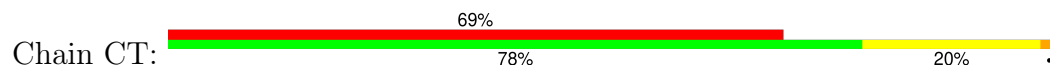
- Molecule 45: 50S ribosomal protein L21



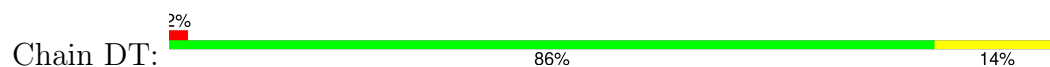
- Molecule 45: 50S ribosomal protein L21



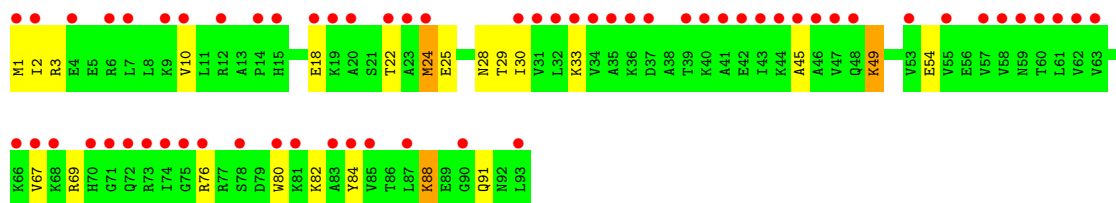
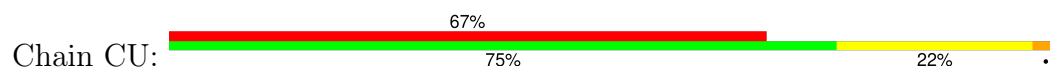
- Molecule 46: 50S ribosomal protein L22



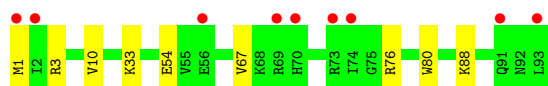
- Molecule 46: 50S ribosomal protein L22



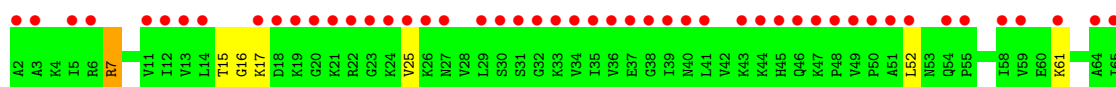
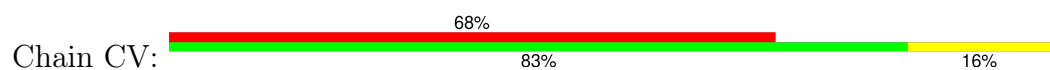
- Molecule 47: 50S ribosomal protein L23

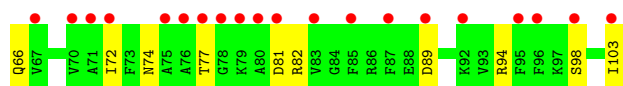


- Molecule 47: 50S ribosomal protein L23

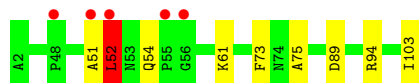


- Molecule 48: 50S ribosomal protein L24

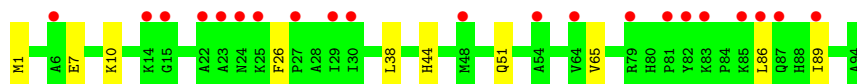




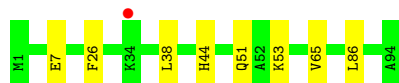
- Molecule 48: 50S ribosomal protein L24



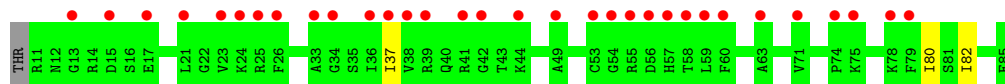
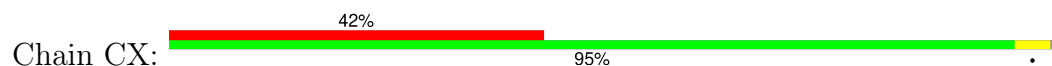
- Molecule 49: 50S ribosomal protein L25



- Molecule 49: 50S ribosomal protein L25



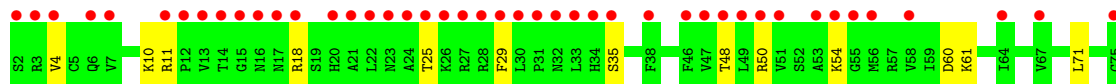
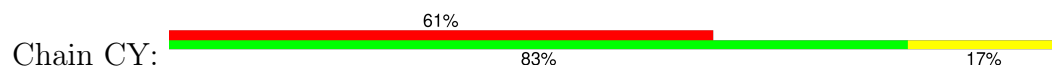
- Molecule 50: 50S ribosomal protein L27



- Molecule 50: 50S ribosomal protein L27



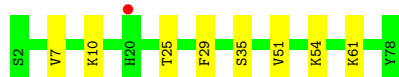
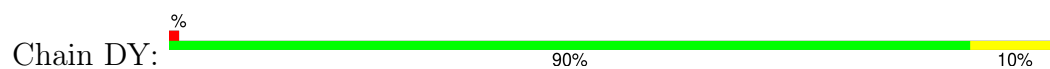
- Molecule 51: 50S ribosomal protein L28



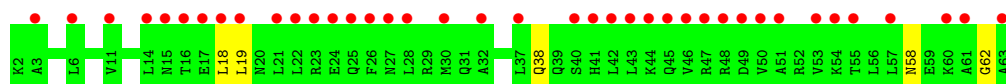




- Molecule 51: 50S ribosomal protein L28



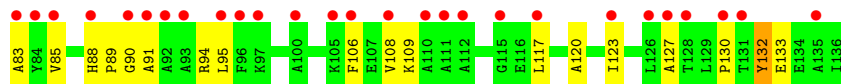
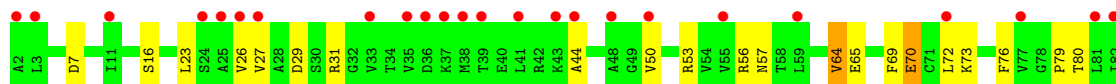
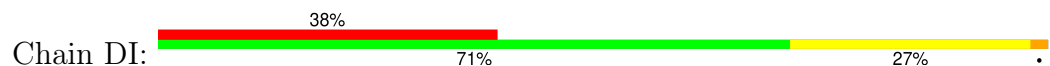
- Molecule 52: 50S ribosomal protein L29



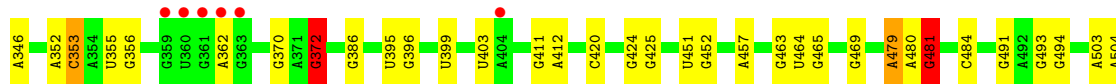
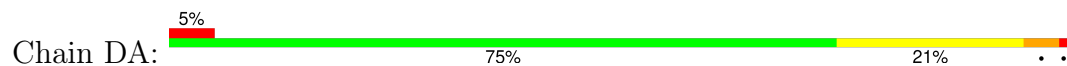
- Molecule 52: 50S ribosomal protein L29

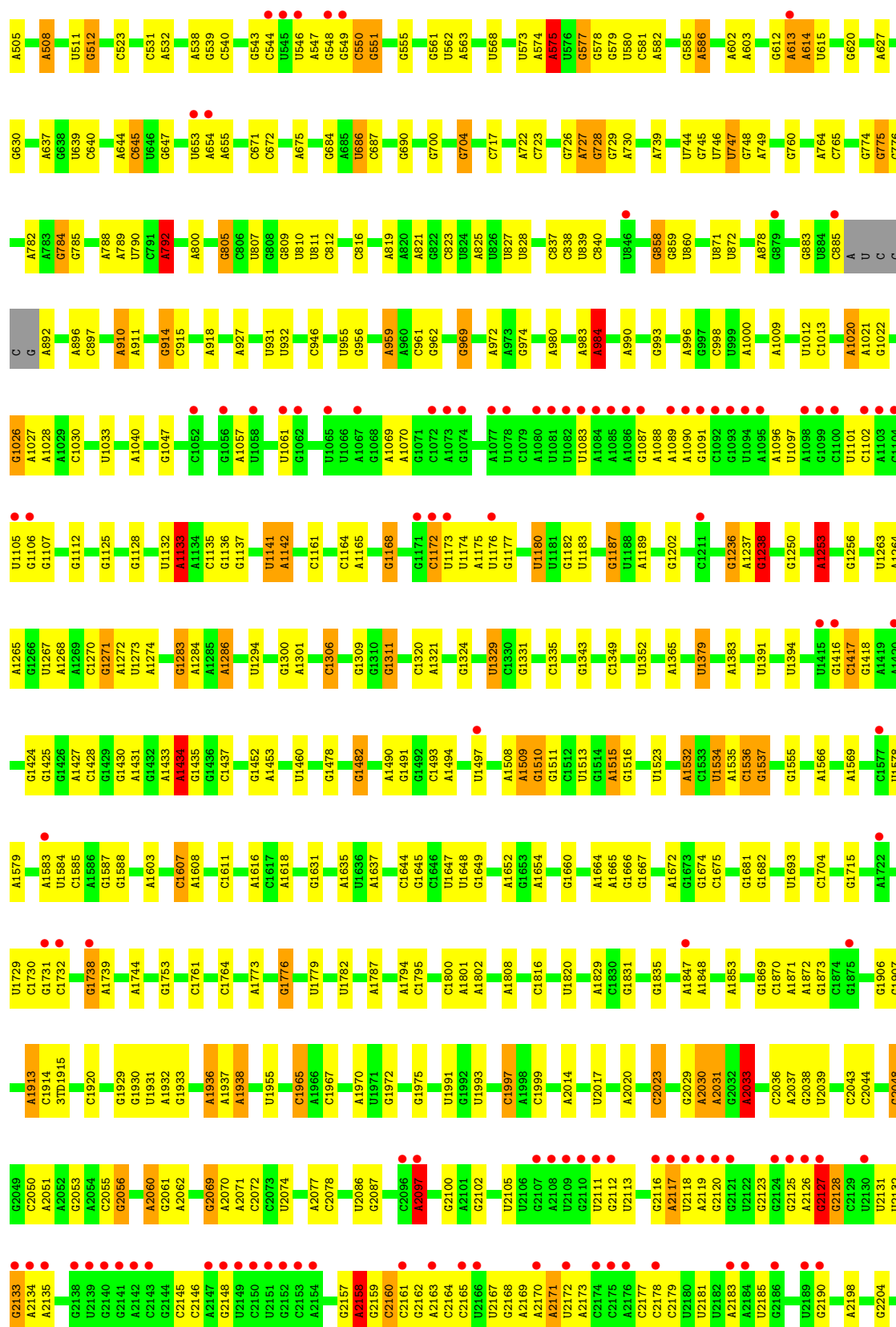


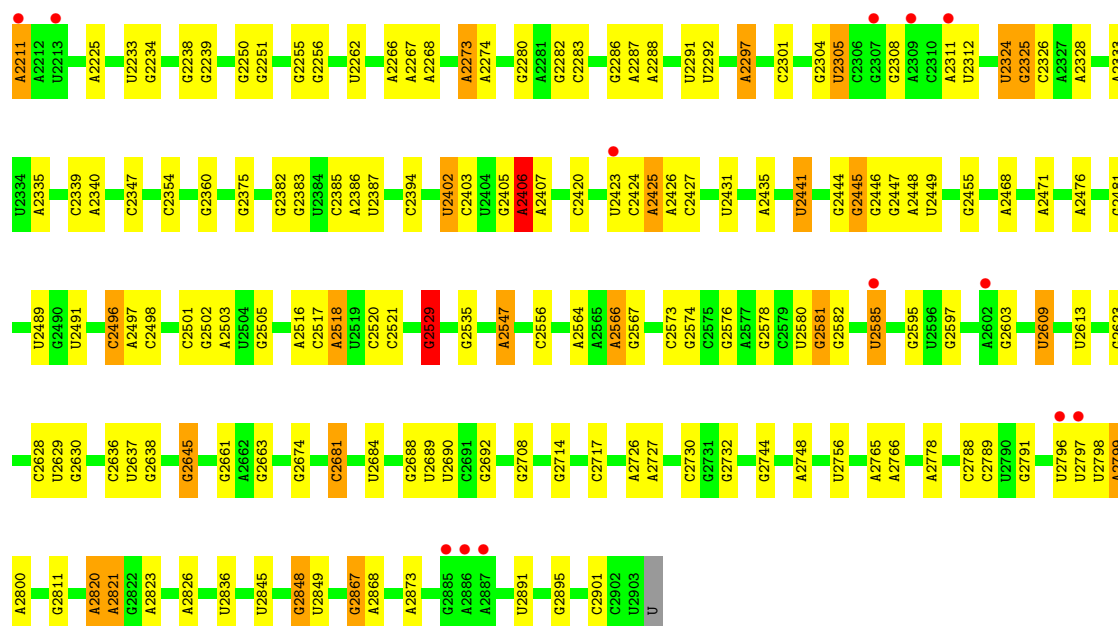
- Molecule 53: 50S ribosomal protein L10



- Molecule 54: 23S rRNA







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.31Å 434.58Å 624.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.16 – 2.80 48.16 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.7 (48.16-2.80) 85.7 (48.16-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	19.79 (at 2.81Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, $R_{free}$	0.209 , 0.219 0.232 , 0.241	Depositor DCC
$R_{free}$ test set	4734 reflections (0.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 93.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	295188	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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: ZN, MA6, OMU, 5MC, 2MA, PSU, TAC, TRS, 5MU, SPD, PEG, MG, 4D4, PGE, 1MG, MPD, ACY, H2U, PUT, OMC, UR3, OMG, EDO, 3TD, D2T, G7M, GUN, 1PE, MEQ, 2MG, PG4, 4OC, 6MZ

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	1.04	7/36593 (0.0%)	0.86	5/57081 (0.0%)
1	BA	1.05	10/36568 (0.0%)	0.86	5/57042 (0.0%)
2	AB	0.48	0/1784	0.65	0/2403
2	BB	0.48	0/1784	0.65	0/2403
3	AC	0.48	0/1652	0.67	0/2225
3	BC	0.47	0/1652	0.67	0/2225
4	AD	0.44	0/1665	0.69	0/2227
4	BD	0.43	0/1665	0.70	0/2227
5	AE	0.48	0/1157	0.77	0/1557
5	BE	0.51	0/1118	0.81	0/1504
6	AF	0.46	0/881	0.69	0/1189
6	BF	0.47	0/835	0.77	0/1128
7	AG	0.45	0/1196	0.61	0/1602
7	BG	0.46	0/1196	0.62	0/1602
8	AH	0.46	0/989	0.71	0/1326
8	BH	0.46	0/989	0.69	0/1326
9	AI	0.44	0/1034	0.66	0/1375
9	BI	0.44	0/1034	0.65	0/1375
10	AJ	0.44	0/806	0.67	0/1089
10	BJ	0.48	0/797	0.71	0/1077
11	AK	0.46	0/893	0.65	0/1205
11	BK	0.45	0/893	0.68	0/1205
12	AL	0.44	0/960	0.74	0/1286
12	BL	0.47	0/960	0.74	0/1286
13	AM	0.51	0/893	0.72	0/1193
13	BM	0.49	0/893	0.71	0/1193
14	AN	0.46	0/817	0.63	0/1088
14	BN	0.44	0/817	0.63	0/1088
15	AO	0.48	0/722	0.60	0/964
15	BO	0.47	0/722	0.63	0/964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	AP	0.48	0/659	0.70	0/884
16	BP	0.50	0/659	0.76	0/884
17	AQ	0.48	0/658	0.73	0/881
17	BQ	0.51	0/658	0.78	0/881
18	AR	0.53	0/463	0.65	0/621
18	BR	0.50	0/463	0.64	0/621
19	AS	0.47	0/653	0.59	0/877
19	BS	0.45	0/653	0.60	0/877
20	AT	0.48	0/676	0.66	0/895
20	BT	0.52	0/671	0.68	0/888
21	AU	0.45	0/472	0.61	0/627
21	BU	0.43	0/472	0.63	0/627
22	C1	0.49	0/450	0.71	0/599
22	D1	0.61	0/450	0.79	0/599
23	C2	0.46	0/416	0.73	0/554
23	D2	0.51	0/421	0.73	0/561
24	C3	0.46	0/380	0.69	0/498
24	D3	0.55	0/380	0.76	0/498
25	C4	0.46	0/513	0.67	0/676
25	D4	0.56	0/513	0.71	0/676
26	C5	0.43	0/303	0.77	0/397
26	D5	0.53	0/303	0.76	0/397
27	C0	0.52	0/453	0.77	0/605
27	D0	0.62	0/467	0.81	0/623
28	CB	0.98	0/2828	0.88	2/4410 (0.0%)
28	DB	1.12	1/2872 (0.0%)	0.90	0/4478
29	CC	0.45	0/2122	0.76	0/2852
29	DC	0.50	0/2122	0.76	1/2852 (0.0%)
30	CD	0.43	0/1576	0.70	0/2119
30	DD	0.54	0/1576	0.73	0/2119
31	CA	1.07	44/69165 (0.1%)	0.87	17/107896 (0.0%)
32	CE	0.45	0/1571	0.72	0/2113
32	DE	0.52	0/1571	0.72	0/2113
33	CF	0.43	0/1435	0.68	0/1926
33	DF	0.46	0/1435	0.70	0/1926
34	CG	0.42	0/1343	0.66	0/1816
34	DG	0.44	0/1343	0.64	0/1816
35	CH	0.48	0/1121	0.68	0/1515
35	DH	0.48	0/1121	0.68	0/1515
36	CJ	0.48	0/993	0.62	0/1341
36	DJ	0.48	0/993	0.62	0/1341
37	CK	0.43	0/1152	0.70	0/1551
37	DK	0.56	0/1152	0.74	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	CL	0.47	0/947	0.74	0/1268
38	DL	0.54	0/955	0.75	0/1279
39	CM	0.46	0/1062	0.74	1/1413 (0.1%)
39	DM	0.50	0/1062	0.75	1/1413 (0.1%)
40	CN	0.45	0/1081	0.75	1/1443 (0.1%)
40	DN	0.59	0/1092	0.81	0/1457
41	CO	0.46	0/973	0.72	0/1301
41	DO	0.58	0/1006	0.81	0/1345
42	CP	0.43	0/902	0.73	0/1209
42	DP	0.47	0/910	0.73	0/1219
43	CQ	0.41	0/929	0.71	0/1242
43	DQ	0.48	0/929	0.72	0/1242
44	CR	0.48	0/960	0.69	0/1278
44	DR	0.62	0/960	0.76	0/1278
45	CS	0.44	0/829	0.73	0/1107
45	DS	0.55	0/829	0.78	0/1107
46	CT	0.43	0/864	0.74	0/1156
46	DT	0.55	0/864	0.75	0/1156
47	CU	0.44	0/745	0.72	0/994
47	DU	0.48	0/745	0.72	0/994
48	CV	0.45	0/788	0.77	0/1051
48	DV	0.49	0/788	0.77	0/1051
49	CW	0.40	0/766	0.65	0/1025
49	DW	0.50	0/766	0.69	0/1025
50	CX	0.39	0/576	0.65	0/762
50	DX	0.53	0/598	0.73	0/790
51	CY	0.43	0/635	0.73	0/848
51	DY	0.46	0/635	0.72	0/848
52	CZ	0.42	0/502	0.60	0/667
52	DZ	0.43	0/502	0.60	0/667
53	DI	0.51	0/1037	0.74	1/1402 (0.1%)
54	DA	1.27	154/69364 (0.2%)	0.97	25/108207 (0.0%)
All	All	0.98	216/309263 (0.1%)	0.85	59/462195 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	3
1	BA	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	AE	0	1
10	BJ	0	1
31	CA	0	12
54	DA	0	89
All	All	0	110

The worst 5 of 216 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	DA	1020	A	N3-C4	9.99	1.40	1.34
31	CA	1936	A	N9-C4	-9.12	1.32	1.37
31	CA	2095	A	O5'-C5'	-9.03	1.28	1.42
54	DA	539	G	N7-C5	7.80	1.44	1.39
54	DA	195	A	N9-C4	7.60	1.42	1.37

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CB	15	A	O4'-C1'-N9	10.09	116.27	108.20
54	DA	512	G	O4'-C1'-N9	8.48	114.99	108.20
1	AA	413	G	C1'-O4'-C4'	-8.21	103.34	109.90
54	DA	784	G	P-O3'-C3'	7.87	129.15	119.70
40	CN	69	PRO	C-N-CA	7.39	140.17	121.70

There are no chirality outliers.

5 of 110 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1432	G	Sidechain
1	AA	362	G	Sidechain
1	AA	898	G	Sidechain
5	AE	82	GLN	Sidechain
1	BA	362	G	Sidechain

## 5.2 Too-close contacts

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16591	90	0
1	BA	32908	0	16580	98	0
2	AB	1753	0	1780	10	0
2	BB	1753	0	1780	14	0
3	AC	1625	0	1696	14	0
3	BC	1625	0	1696	18	0
4	AD	1643	0	1707	13	0
4	BD	1643	0	1707	17	0
5	AE	1144	0	1185	15	0
5	BE	1105	0	1148	30	0
6	AF	862	0	864	7	0
6	BF	817	0	808	8	0
7	AG	1182	0	1238	7	0
7	BG	1182	0	1238	4	0
8	AH	979	0	1031	8	0
8	BH	979	0	1031	4	0
9	AI	1022	0	1070	6	0
9	BI	1022	0	1070	6	0
10	AJ	796	0	836	11	0
10	BJ	787	0	828	10	0
11	AK	877	0	887	14	0
11	BK	877	0	887	17	0
12	AL	957	0	1017	7	0
12	BL	957	0	1017	10	0
13	AM	884	0	941	10	0
13	BM	884	0	941	11	0
14	AN	805	0	844	8	0
14	BN	805	0	844	8	0
15	AO	714	0	734	1	0
15	BO	714	0	734	0	0
16	AP	649	0	666	3	0
16	BP	649	0	666	5	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	5	0
18	AR	456	0	478	5	0
18	BR	456	0	478	3	0
19	AS	638	0	665	7	0
19	BS	638	0	665	9	0
20	AT	670	0	719	2	0
20	BT	665	0	714	8	0
21	AU	465	0	491	2	0
21	BU	465	0	491	2	0
22	C1	444	0	458	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	D1	444	0	458	13	0
23	C2	409	0	440	4	0
23	D2	414	0	442	5	0
24	C3	377	0	418	9	0
24	D3	377	0	418	5	0
25	C4	504	0	572	7	0
25	D4	504	0	572	11	0
26	C5	302	0	340	7	0
26	D5	302	0	340	1	0
27	C0	449	0	488	3	0
27	D0	463	0	504	1	0
28	CB	2529	0	1281	5	0
28	DB	2569	0	1301	5	0
29	CC	2083	0	2154	17	0
29	DC	2083	0	2154	11	0
30	CD	1565	0	1614	16	0
30	DD	1576	0	1627	16	0
31	CA	62229	0	31318	213	0
32	CE	1552	0	1619	13	0
32	DE	1552	0	1619	11	0
33	CF	1411	0	1444	15	0
33	DF	1411	0	1444	11	0
34	CG	1323	0	1371	9	0
34	DG	1323	0	1371	9	0
35	CH	1110	0	1148	7	0
35	DH	1110	0	1148	6	0
36	CJ	979	0	1028	5	0
36	DJ	979	0	1028	4	0
37	CK	1129	0	1162	10	0
37	DK	1129	0	1162	4	0
38	CL	938	0	1012	8	0
38	DL	946	0	1023	6	0
39	CM	1053	0	1129	16	0
39	DM	1053	0	1129	15	0
40	CN	1075	0	1154	5	0
40	DN	1092	0	1177	7	0
41	CO	960	0	1000	7	0
41	DO	993	0	1034	5	0
42	CP	892	0	923	6	0
42	DP	900	0	935	9	0
43	CQ	917	0	962	7	0
43	DQ	917	0	962	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	CR	947	0	1019	13	0
44	DR	947	0	1019	9	0
45	CS	816	0	839	8	0
45	DS	816	0	839	5	0
46	CT	857	0	922	12	0
46	DT	857	0	922	10	0
47	CU	739	0	807	10	0
47	DU	739	0	807	4	0
48	CV	780	0	831	6	0
48	DV	780	0	831	4	0
49	CW	753	0	780	5	0
49	DW	753	0	780	3	0
50	CX	569	0	581	1	0
50	DX	591	0	606	7	0
51	CY	625	0	652	7	0
51	DY	625	0	652	4	0
52	CZ	501	0	531	0	0
52	DZ	501	0	531	1	0
53	DI	1023	0	1052	19	0
54	DA	62423	0	31411	171	0
55	AA	71	0	0	0	0
55	BA	43	0	0	0	0
55	C3	1	0	0	0	0
55	CA	155	0	0	0	0
55	CB	3	0	0	0	0
55	DA	182	0	0	0	0
55	DB	9	0	0	0	0
55	DD	2	0	0	0	0
55	DM	1	0	0	0	0
55	DR	2	0	0	0	0
56	AA	13	0	18	1	0
56	BA	13	0	18	0	0
56	DA	26	0	36	2	0
56	DQ	13	0	18	0	0
56	DR	13	0	18	5	0
56	DS	13	0	18	1	0
57	AA	16	0	28	0	0
57	DA	40	0	70	5	0
57	DE	16	0	28	0	0
57	DK	8	0	14	0	0
57	DN	8	0	14	1	0
57	DS	8	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	DT	16	0	28	0	0
58	AA	24	0	48	0	0
58	DA	72	0	144	10	0
59	AA	32	0	21	1	0
59	BA	32	0	21	1	0
60	AB	1	0	0	0	0
60	C5	1	0	0	0	0
60	D5	1	0	0	0	0
61	AL	7	0	10	0	0
61	D1	7	0	10	1	0
61	D3	7	0	10	2	0
61	DA	35	0	50	1	0
61	DL	7	0	10	0	0
61	DP	7	0	10	1	0
61	DQ	7	0	10	0	0
62	D1	4	0	6	0	0
62	DA	36	0	54	2	0
62	DB	8	0	12	1	0
63	D1	10	0	14	2	0
63	D3	10	0	14	0	0
63	DA	40	0	56	5	0
63	DD	10	0	14	2	0
63	DS	10	0	14	0	0
63	DU	10	0	14	1	0
64	DA	40	0	76	4	0
65	DA	32	0	44	0	0
66	DA	12	0	11	0	0
67	DA	11	0	5	0	0
68	DA	8	0	12	1	0
69	AA	507	0	0	0	0
69	AC	4	0	0	0	0
69	AD	2	0	0	0	0
69	AE	4	0	0	0	0
69	AF	1	0	0	0	0
69	AG	1	0	0	0	0
69	AH	1	0	0	0	0
69	AJ	2	0	0	0	0
69	AK	5	0	0	0	0
69	AL	8	0	0	0	0
69	AM	4	0	0	1	0
69	AN	5	0	0	1	0
69	AO	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	AP	2	0	0	0	0
69	AR	1	0	0	0	0
69	AS	1	0	0	0	0
69	AT	2	0	0	0	0
69	AU	3	0	0	0	0
69	BA	287	0	0	1	0
69	BD	13	0	0	0	0
69	BE	1	0	0	0	0
69	BF	1	0	0	0	0
69	BK	1	0	0	0	0
69	BL	3	0	0	0	0
69	BN	2	0	0	0	0
69	BO	1	0	0	0	0
69	BP	3	0	0	0	0
69	BR	1	0	0	0	0
69	BT	4	0	0	0	0
69	BU	2	0	0	0	0
69	C3	3	0	0	1	0
69	C4	2	0	0	0	0
69	CA	692	0	0	1	0
69	CB	13	0	0	0	0
69	CC	10	0	0	0	0
69	CD	5	0	0	0	0
69	CE	7	0	0	0	0
69	CL	1	0	0	0	0
69	CM	3	0	0	0	0
69	CO	1	0	0	0	0
69	CU	3	0	0	0	0
69	CV	1	0	0	0	0
69	CW	1	0	0	0	0
69	CY	1	0	0	0	0
69	D0	27	0	0	0	0
69	D1	42	0	0	0	0
69	D2	7	0	0	0	0
69	D3	24	0	0	0	0
69	D4	33	0	0	1	0
69	D5	13	0	0	0	0
69	DA	4834	0	0	7	0
69	DB	212	0	0	0	0
69	DC	102	0	0	0	0
69	DD	105	0	0	1	0
69	DE	63	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	DF	14	0	0	0	0
69	DG	6	0	0	0	0
69	DH	2	0	0	0	0
69	DK	58	0	0	0	0
69	DL	51	0	0	0	0
69	DM	62	0	0	0	0
69	DN	71	0	0	0	0
69	DO	44	0	0	0	0
69	DP	35	0	0	0	0
69	DQ	27	0	0	1	0
69	DR	64	0	0	0	0
69	DS	51	0	0	0	0
69	DT	69	0	0	1	0
69	DU	17	0	0	0	0
69	DV	19	0	0	0	0
69	DW	31	0	0	0	0
69	DX	30	0	0	1	0
69	DY	9	0	0	0	0
69	DZ	7	0	0	0	0
All	All	295188	0	194452	1182	0

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 2.

The worst 5 of 1182 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)
45:CS:14:VAL:HG21	45:CS:98:ILE:HG13	1.32	1.05
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.43	0.98
31:CA:1936:A:H2	31:CA:1943:U:H3	1.01	0.98
47:CU:28:ASN:HD21	47:CU:91:GLN:HB3	1.29	0.96
14:AN:66:GLN:HB2	69:AN:205:HOH:O	1.67	0.95

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	210 (95%)	9 (4%)	3 (1%)	9	30
2	BB	222/224 (99%)	211 (95%)	7 (3%)	4 (2%)	7	24
3	AC	204/206 (99%)	192 (94%)	11 (5%)	1 (0%)	25	56
3	BC	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	13	39
4	AD	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
4	BD	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
5	AE	153/155 (99%)	147 (96%)	5 (3%)	1 (1%)	19	48
5	BE	148/155 (96%)	132 (89%)	12 (8%)	4 (3%)	4	15
6	AF	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
6	BF	98/106 (92%)	91 (93%)	5 (5%)	2 (2%)	6	21
7	AG	149/151 (99%)	137 (92%)	11 (7%)	1 (1%)	19	48
7	BG	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
8	AH	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
8	BH	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
9	AI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
9	BI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
10	AJ	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	5	20
10	BJ	96/99 (97%)	77 (80%)	14 (15%)	5 (5%)	1	5
11	AK	115/117 (98%)	107 (93%)	6 (5%)	2 (2%)	7	26
11	BK	115/117 (98%)	104 (90%)	9 (8%)	2 (2%)	7	26
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	114 (95%)	5 (4%)	1 (1%)	16	44
13	AM	112/114 (98%)	103 (92%)	6 (5%)	3 (3%)	4	15
13	BM	112/114 (98%)	102 (91%)	5 (4%)	5 (4%)	2	7
14	AN	98/100 (98%)	88 (90%)	8 (8%)	2 (2%)	6	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	BN	98/100 (98%)	90 (92%)	6 (6%)	2 (2%)	6	21
15	AO	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
15	BO	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	11	34
16	AP	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
16	BP	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	4	17
17	AQ	78/80 (98%)	70 (90%)	7 (9%)	1 (1%)	10	32
17	BQ	78/80 (98%)	68 (87%)	5 (6%)	5 (6%)	1	3
18	AR	53/55 (96%)	53 (100%)	0	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	10	32
19	BS	77/79 (98%)	68 (88%)	7 (9%)	2 (3%)	4	16
20	AT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
20	BT	83/86 (96%)	79 (95%)	3 (4%)	1 (1%)	11	34
21	AU	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
21	BU	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
22	C1	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	1	4
22	D1	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	2	8
23	D2	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
24	C3	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	5	19
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	C4	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
25	D4	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	14
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	54 (96%)	0	2 (4%)	3	10
27	D0	57/58 (98%)	56 (98%)	1 (2%)	0	100	100
29	CC	269/271 (99%)	252 (94%)	12 (4%)	5 (2%)	6	23
29	DC	269/271 (99%)	257 (96%)	10 (4%)	2 (1%)	19	48
30	CD	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
30	DD	206/209 (99%)	202 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	CE	199/201 (99%)	191 (96%)	5 (2%)	3 (2%)	8	29
32	DE	199/201 (99%)	194 (98%)	4 (2%)	1 (0%)	25	56
33	CF	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	22	51
33	DF	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	22	51
34	CG	174/176 (99%)	162 (93%)	7 (4%)	5 (3%)	3	13
34	DG	174/176 (99%)	165 (95%)	8 (5%)	1 (1%)	22	51
35	CH	147/149 (99%)	136 (92%)	6 (4%)	5 (3%)	3	11
35	DH	147/149 (99%)	138 (94%)	6 (4%)	3 (2%)	6	21
36	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3	13
36	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	3	13
37	CK	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	19	48
37	DK	140/142 (99%)	137 (98%)	2 (1%)	1 (1%)	19	48
38	CL	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	7	26
38	DL	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	16	44
39	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	5	20
39	DM	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
40	CN	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	16	44
40	DN	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
41	CO	118/125 (94%)	111 (94%)	5 (4%)	2 (2%)	7	26
41	DO	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
42	CP	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
42	DP	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
43	CQ	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
43	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	14	42
44	CR	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
44	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
45	CS	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	3	13
45	DS	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	13	39
46	CT	108/110 (98%)	101 (94%)	5 (5%)	2 (2%)	6	23
46	DT	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
47	CU	91/93 (98%)	86 (94%)	4 (4%)	1 (1%)	12	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	DU	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
48	CV	100/102 (98%)	91 (91%)	4 (4%)	5 (5%)	1	5
48	DV	100/102 (98%)	96 (96%)	2 (2%)	2 (2%)	6	21
49	CW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
49	DW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
50	CX	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
50	DX	75/76 (99%)	74 (99%)	1 (1%)	0	100	100
51	CY	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
51	DY	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
52	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	26
52	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
53	DI	133/135 (98%)	114 (86%)	13 (10%)	6 (4%)	2	7
All	All	11406/11629 (98%)	10790 (95%)	484 (4%)	132 (1%)	11	34

5 of 132 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE
3	AC	156	ARG
13	AM	5	ALA
22	C1	25	VAL
2	BB	126	PHE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	173 (93%)	13 (7%)	12	36
2	BB	186/186 (100%)	173 (93%)	13 (7%)	12	36
3	AC	170/170 (100%)	159 (94%)	11 (6%)	14	40
3	BC	170/170 (100%)	156 (92%)	14 (8%)	9	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AD	172/172 (100%)	163 (95%)	9 (5%)	19	50
4	BD	172/172 (100%)	160 (93%)	12 (7%)	12	36
5	AE	118/118 (100%)	106 (90%)	12 (10%)	6	19
5	BE	113/118 (96%)	95 (84%)	18 (16%)	2	7
6	AF	92/92 (100%)	86 (94%)	6 (6%)	14	40
6	BF	87/92 (95%)	77 (88%)	10 (12%)	4	15
7	AG	124/124 (100%)	115 (93%)	9 (7%)	11	34
7	BG	124/124 (100%)	109 (88%)	15 (12%)	4	13
8	AH	104/104 (100%)	93 (89%)	11 (11%)	5	18
8	BH	104/104 (100%)	93 (89%)	11 (11%)	5	18
9	AI	105/105 (100%)	100 (95%)	5 (5%)	21	53
9	BI	105/105 (100%)	100 (95%)	5 (5%)	21	53
10	AJ	87/87 (100%)	81 (93%)	6 (7%)	13	37
10	BJ	86/87 (99%)	78 (91%)	8 (9%)	7	23
11	AK	90/90 (100%)	87 (97%)	3 (3%)	33	67
11	BK	90/90 (100%)	83 (92%)	7 (8%)	10	31
12	AL	102/102 (100%)	92 (90%)	10 (10%)	6	21
12	BL	102/102 (100%)	90 (88%)	12 (12%)	4	14
13	AM	92/92 (100%)	83 (90%)	9 (10%)	6	21
13	BM	92/92 (100%)	85 (92%)	7 (8%)	11	32
14	AN	83/83 (100%)	82 (99%)	1 (1%)	67	89
14	BN	83/83 (100%)	82 (99%)	1 (1%)	67	89
15	AO	76/76 (100%)	71 (93%)	5 (7%)	14	39
15	BO	76/76 (100%)	65 (86%)	11 (14%)	2	8
16	AP	65/65 (100%)	64 (98%)	1 (2%)	60	86
16	BP	65/65 (100%)	63 (97%)	2 (3%)	35	69
17	AQ	74/74 (100%)	67 (90%)	7 (10%)	7	22
17	BQ	74/74 (100%)	66 (89%)	8 (11%)	5	17
18	AR	48/48 (100%)	47 (98%)	1 (2%)	48	80
18	BR	48/48 (100%)	47 (98%)	1 (2%)	48	80
19	AS	70/70 (100%)	63 (90%)	7 (10%)	6	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	BS	70/70 (100%)	65 (93%)	5 (7%)	12	35
20	AT	65/65 (100%)	59 (91%)	6 (9%)	7	24
20	BT	65/65 (100%)	55 (85%)	10 (15%)	2	7
21	AU	48/48 (100%)	44 (92%)	4 (8%)	9	28
21	BU	48/48 (100%)	44 (92%)	4 (8%)	9	28
22	C1	47/47 (100%)	45 (96%)	2 (4%)	25	57
22	D1	47/47 (100%)	44 (94%)	3 (6%)	14	41
23	C2	45/46 (98%)	44 (98%)	1 (2%)	47	79
23	D2	45/46 (98%)	43 (96%)	2 (4%)	24	56
24	C3	38/38 (100%)	37 (97%)	1 (3%)	41	75
24	D3	38/38 (100%)	37 (97%)	1 (3%)	41	75
25	C4	51/51 (100%)	48 (94%)	3 (6%)	16	44
25	D4	51/51 (100%)	48 (94%)	3 (6%)	16	44
26	C5	34/34 (100%)	32 (94%)	2 (6%)	16	44
26	D5	34/34 (100%)	34 (100%)	0	100	100
27	C0	48/48 (100%)	45 (94%)	3 (6%)	15	42
27	D0	49/48 (102%)	45 (92%)	4 (8%)	9	29
29	CC	216/216 (100%)	203 (94%)	13 (6%)	16	44
29	DC	216/216 (100%)	210 (97%)	6 (3%)	38	72
30	CD	163/163 (100%)	159 (98%)	4 (2%)	42	75
30	DD	163/163 (100%)	160 (98%)	3 (2%)	54	83
32	CE	165/165 (100%)	152 (92%)	13 (8%)	10	30
32	DE	165/165 (100%)	161 (98%)	4 (2%)	44	77
33	CF	148/148 (100%)	133 (90%)	15 (10%)	6	20
33	DF	148/148 (100%)	137 (93%)	11 (7%)	11	33
34	CG	137/137 (100%)	134 (98%)	3 (2%)	47	79
34	DG	137/137 (100%)	132 (96%)	5 (4%)	30	64
35	CH	114/114 (100%)	101 (89%)	13 (11%)	4	15
35	DH	114/114 (100%)	101 (89%)	13 (11%)	4	15
36	CJ	104/104 (100%)	100 (96%)	4 (4%)	28	62
36	DJ	104/104 (100%)	100 (96%)	4 (4%)	28	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	CK	116/116 (100%)	110 (95%)	6 (5%)	19	50
37	DK	116/116 (100%)	114 (98%)	2 (2%)	56	84
38	CL	103/104 (99%)	99 (96%)	4 (4%)	27	61
38	DL	104/104 (100%)	99 (95%)	5 (5%)	21	53
39	CM	103/103 (100%)	97 (94%)	6 (6%)	17	45
39	DM	103/103 (100%)	99 (96%)	4 (4%)	27	61
40	CN	108/108 (100%)	104 (96%)	4 (4%)	29	63
40	DN	109/108 (101%)	106 (97%)	3 (3%)	38	72
41	CO	100/102 (98%)	95 (95%)	5 (5%)	20	51
41	DO	102/102 (100%)	99 (97%)	3 (3%)	37	71
42	CP	86/87 (99%)	80 (93%)	6 (7%)	12	36
42	DP	87/87 (100%)	84 (97%)	3 (3%)	32	66
43	CQ	99/99 (100%)	93 (94%)	6 (6%)	15	43
43	DQ	99/99 (100%)	97 (98%)	2 (2%)	50	81
44	CR	89/89 (100%)	86 (97%)	3 (3%)	32	66
44	DR	89/89 (100%)	87 (98%)	2 (2%)	47	79
45	CS	84/84 (100%)	79 (94%)	5 (6%)	16	44
45	DS	84/84 (100%)	83 (99%)	1 (1%)	67	89
46	CT	93/93 (100%)	88 (95%)	5 (5%)	18	48
46	DT	93/93 (100%)	92 (99%)	1 (1%)	70	90
47	CU	80/80 (100%)	72 (90%)	8 (10%)	6	20
47	DU	80/80 (100%)	77 (96%)	3 (4%)	28	62
48	CV	83/83 (100%)	79 (95%)	4 (5%)	21	53
48	DV	83/83 (100%)	81 (98%)	2 (2%)	44	77
49	CW	78/78 (100%)	75 (96%)	3 (4%)	28	62
49	DW	78/78 (100%)	76 (97%)	2 (3%)	41	75
50	CX	56/58 (97%)	55 (98%)	1 (2%)	54	83
50	DX	58/58 (100%)	57 (98%)	1 (2%)	56	84
51	CY	67/67 (100%)	63 (94%)	4 (6%)	16	44
51	DY	67/67 (100%)	65 (97%)	2 (3%)	36	70
52	CZ	54/54 (100%)	50 (93%)	4 (7%)	11	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	DZ	54/54 (100%)	52 (96%)	2 (4%)	29	63
53	DI	103/103 (100%)	98 (95%)	5 (5%)	21	52
All	All	9460/9477 (100%)	8897 (94%)	563 (6%)	16	44

5 of 563 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	CU	24	MET
51	CY	35	SER
47	CU	10	VAL
37	DK	124	VAL
5	BE	88	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
20	BT	3	ASN
34	CG	38	ASN
24	D3	26	ASN
29	DC	142	HIS
42	CP	29	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	239 (15%)	27 (1%)
1	BA	1529/1534 (99%)	246 (16%)	28 (1%)
28	CB	117/120 (97%)	11 (9%)	0
28	DB	119/120 (99%)	9 (7%)	0
31	CA	2892/2904 (99%)	425 (14%)	72 (2%)
54	DA	2880/2904 (99%)	367 (12%)	57 (1%)
All	All	9067/9116 (99%)	1297 (14%)	184 (2%)

5 of 1297 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G

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Mol	Chain	Res	Type
1	AA	22	G
1	AA	32	A

5 of 184 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	CA	2286	G
54	DA	1070	A
31	CA	2430	A
54	DA	271	G
54	DA	1175	A

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

76 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$
54	OMG	DA	2251	54	19,26,27	0.95	1 (5%)	21,38,41	0.63	0
31	OMC	CA	2498	55,31	19,22,23	0.46	0	25,31,34	0.47	0
54	PSU	DA	746	55,54	18,21,22	0.99	2 (11%)	21,30,33	0.50	0
40	4D4	DN	81[A]	-	9,11,12	2.24	2 (22%)	7,13,15	2.34	2 (28%)
54	2MA	DA	2503	55,54	17,25,26	0.91	1 (5%)	16,37,40	2.23	1 (6%)
31	6MZ	CA	1618	31	17,25,26	1.01	1 (5%)	15,36,39	1.10	2 (13%)
40	4D4	CN	81	40	9,11,12	2.10	2 (22%)	7,13,15	2.62	2 (28%)
31	5MC	CA	1962	31	19,22,23	0.24	0	26,32,35	0.37	0
31	PSU	CA	2605	31	18,21,22	0.33	0	21,30,33	0.56	0
54	6MZ	DA	1618	54	17,25,26	0.99	0	15,36,39	1.80	2 (13%)
54	3TD	DA	1915	54	19,22,23	0.54	0	23,32,35	0.85	1 (4%)
30	MEQ	DD	150[A]	30	8,9,10	0.55	0	5,10,12	0.45	0
1	G7M	BA	527	1	20,26,27	0.94	1 (5%)	16,39,42	2.11	1 (6%)
31	2MG	CA	1835	31	18,26,27	0.95	1 (5%)	16,38,41	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	PSU	CA	2457	31	18,21,22	0.44	0	21,30,33	0.46	0
31	G7M	CA	2069	31	20,26,27	0.82	1 (5%)	16,39,42	0.98	1 (6%)
1	2MG	AA	1516	1	18,26,27	0.89	0	16,38,41	0.73	0
54	OMC	DA	2498	55,54	19,22,23	0.40	0	25,31,34	0.56	0
54	6MZ	DA	2030	54	17,25,26	0.94	1 (5%)	15,36,39	0.92	1 (6%)
31	2MG	CA	2445	31	18,26,27	0.92	0	16,38,41	0.65	0
54	PSU	DA	2504	54	18,21,22	0.63	0	21,30,33	0.45	0
1	G7M	AA	527	1	20,26,27	0.78	0	16,39,42	1.81	1 (6%)
54	PSU	DA	1917	54	18,21,22	0.40	0	21,30,33	0.50	0
54	1MG	DA	745	54	19,26,27	1.51	2 (10%)	18,39,42	0.74	1 (5%)
31	PSU	CA	746	55,31	18,21,22	0.63	1 (5%)	21,30,33	0.44	0
1	MA6	BA	1519	1	19,26,27	0.81	0	18,38,41	1.32	2 (11%)
31	PSU	CA	955	31	18,21,22	0.29	0	21,30,33	0.53	0
12	D2T	AL	89	12	8,9,10	1.32	1 (12%)	6,11,13	0.68	0
1	4OC	BA	1402	1	20,23,24	0.41	0	25,32,35	0.52	0
31	6MZ	CA	2030	31	17,25,26	0.91	0	15,36,39	1.07	2 (13%)
1	2MG	BA	1516	1	18,26,27	0.83	0	16,38,41	0.71	0
31	1MG	CA	745	31	19,26,27	1.34	3 (15%)	18,39,42	0.64	0
31	OMG	CA	2251	31	19,26,27	0.79	0	21,38,41	0.64	0
1	2MG	BA	966	55,1	18,26,27	0.80	0	16,38,41	0.54	0
31	OMU	CA	2552	31	19,22,23	0.31	0	25,31,34	0.31	0
1	5MC	AA	1407	1	19,22,23	0.34	0	26,32,35	0.46	0
1	MA6	AA	1518	1	19,26,27	0.93	0	18,38,41	1.00	0
31	PSU	CA	1917	31	18,21,22	0.34	0	21,30,33	0.44	0
54	PSU	DA	955	54	18,21,22	0.63	1 (5%)	21,30,33	0.63	0
40	4D4	DN	81[B]	-	9,11,12	1.49	1 (11%)	7,13,15	2.64	2 (28%)
54	PSU	DA	2604	54	18,21,22	0.55	0	21,30,33	0.65	0
1	2MG	AA	966	1	18,26,27	0.76	0	16,38,41	0.67	0
54	OMU	DA	2552	54	19,22,23	0.34	0	25,31,34	0.36	0
54	PSU	DA	2605	54	18,21,22	0.40	0	21,30,33	0.58	0
31	3TD	CA	1915	31	19,22,23	0.50	0	23,32,35	0.80	1 (4%)
30	MEQ	DD	150[B]	30	8,9,10	1.96	1 (12%)	5,10,12	1.71	1 (20%)
54	5MU	DA	747	54	19,22,23	0.46	0	27,32,35	0.44	0
1	PSU	BA	516	1	18,21,22	0.39	0	21,30,33	0.45	0
31	5MU	CA	1939	31	19,22,23	0.48	0	27,32,35	0.41	0
31	2MA	CA	2503	31	17,25,26	0.91	1 (5%)	16,37,40	2.25	1 (6%)
54	G7M	DA	2069	54	20,26,27	0.71	1 (5%)	16,39,42	0.91	1 (6%)
54	PSU	DA	2457	54	18,21,22	0.41	0	21,30,33	0.43	0
54	5MC	DA	1962	54	19,22,23	0.45	0	26,32,35	0.49	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MG	BA	1207	1	18,26,27	0.81	0	16,38,41	0.61	0
1	4OC	AA	1402	1	20,23,24	0.30	0	25,32,35	0.52	0
31	PSU	CA	2504	31	18,21,22	0.40	0	21,30,33	0.47	0
1	5MC	AA	967	1	19,22,23	0.29	0	26,32,35	0.37	0
54	5MU	DA	1939	54	19,22,23	0.34	0	27,32,35	0.41	0
54	H2U	DA	2449	54	18,21,22	0.47	0	19,30,33	0.50	0
1	PSU	AA	516	55,1	18,21,22	0.28	0	21,30,33	0.45	0
54	2MG	DA	1835	54	18,26,27	0.86	1 (5%)	16,38,41	0.63	0
1	5MC	BA	967	1	19,22,23	0.27	0	26,32,35	0.36	0
30	MEQ	CD	150	30	7,8,10	0.39	0	4,9,12	0.38	0
54	2MG	DA	2445	54	18,26,27	0.91	0	16,38,41	0.85	1 (6%)
54	PSU	DA	2580	54	18,21,22	0.78	1 (5%)	21,30,33	0.69	0
31	5MU	CA	747	31	19,22,23	0.34	0	27,32,35	0.38	0
1	2MG	AA	1207	1	18,26,27	0.82	0	16,38,41	0.63	0
1	UR3	BA	1498	1	19,22,23	0.51	0	26,32,35	0.84	1 (3%)
31	PSU	CA	1911	31	18,21,22	0.27	0	21,30,33	0.40	0
1	5MC	BA	1407	1	19,22,23	0.31	0	26,32,35	0.45	0
31	PSU	CA	2580	31	18,21,22	0.40	0	21,30,33	0.68	1 (4%)
1	MA6	AA	1519	1	19,26,27	0.82	0	18,38,41	1.36	2 (11%)
1	MA6	BA	1518	1	19,26,27	0.91	0	18,38,41	1.03	1 (5%)
54	PSU	DA	1911	54	18,21,22	0.30	0	21,30,33	0.39	0
1	UR3	AA	1498	1	19,22,23	0.29	0	26,32,35	0.35	0
12	D2T	BL	89	12	8,9,10	0.77	0	6,11,13	0.66	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
54	OMG	DA	2251	54	-	1/5/27/28	0/3/3/3
31	OMC	CA	2498	55,31	-	0/9/27/28	0/2/2/2
54	PSU	DA	746	55,54	-	2/7/25/26	0/2/2/2
40	4D4	DN	81[A]	-	-	0/11/12/14	-
54	2MA	DA	2503	55,54	-	1/3/25/26	0/3/3/3
31	6MZ	CA	1618	31	-	0/5/27/28	0/3/3/3
40	4D4	CN	81	40	-	1/11/12/14	-
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
54	6MZ	DA	1618	54	-	0/5/27/28	0/3/3/3
54	3TD	DA	1915	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	MEQ	DD	150[A]	30	-	3/8/9/11	-
1	G7M	BA	527	1	-	2/3/25/26	0/3/3/3
31	2MG	CA	1835	31	-	2/5/27/28	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	G7M	CA	2069	31	-	1/3/25/26	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
54	OMC	DA	2498	55,54	-	0/9/27/28	0/2/2/2
54	6MZ	DA	2030	54	-	2/5/27/28	0/3/3/3
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
54	PSU	DA	2504	54	-	1/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
54	PSU	DA	1917	54	-	0/7/25/26	0/2/2/2
54	1MG	DA	745	54	-	0/3/25/26	0/3/3/3
31	PSU	CA	746	55,31	-	2/7/25/26	0/2/2/2
1	MA6	BA	1519	1	-	1/7/29/30	0/3/3/3
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	2/7/12/14	-
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2
31	6MZ	CA	2030	31	-	1/5/27/28	0/3/3/3
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
31	OMG	CA	2251	31	-	1/5/27/28	0/3/3/3
1	2MG	BA	966	55,1	-	0/5/27/28	0/3/3/3
31	OMU	CA	2552	31	-	1/9/27/28	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
54	PSU	DA	955	54	-	0/7/25/26	0/2/2/2
40	4D4	DN	81[B]	-	-	2/11/12/14	-
54	PSU	DA	2604	54	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
54	OMU	DA	2552	54	-	1/9/27/28	0/2/2/2
54	PSU	DA	2605	54	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
30	MEQ	DD	150[B]	30	-	4/8/9/11	-
54	5MU	DA	747	54	-	0/7/25/26	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	0/7/25/26	0/2/2/2
31	2MA	CA	2503	31	-	1/3/25/26	0/3/3/3
54	G7M	DA	2069	54	-	1/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	DA	2457	54	-	0/7/25/26	0/2/2/2
54	5MC	DA	1962	54	-	2/7/25/26	0/2/2/2
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
31	PSU	CA	2504	31	-	1/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
54	5MU	DA	1939	54	-	0/7/25/26	0/2/2/2
54	H2U	DA	2449	54	-	1/7/38/39	0/2/2/2
1	PSU	AA	516	55,1	-	0/7/25/26	0/2/2/2
54	2MG	DA	1835	54	-	2/5/27/28	0/3/3/3
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
30	MEQ	CD	150	30	-	2/6/7/11	-
54	2MG	DA	2445	54	-	0/5/27/28	0/3/3/3
54	PSU	DA	2580	54	-	0/7/25/26	0/2/2/2
31	5MU	CA	747	31	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	1/7/29/30	0/3/3/3
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
54	PSU	DA	1911	54	-	0/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
12	D2T	BL	89	12	-	4/7/12/14	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	DN	81[A]	4D4	CZ-NE	6.08	1.45	1.33
40	CN	81	4D4	CZ-NE	5.62	1.44	1.33
30	DD	150[B]	MEQ	CB-CA	5.34	1.61	1.53
31	CA	745	1MG	C2-N1	4.51	1.45	1.37
54	DA	745	1MG	C2-N1	4.43	1.45	1.37

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2503	2MA	C4-N3-C2	-8.68	116.64	123.30
54	DA	2503	2MA	C4-N3-C2	-8.43	116.83	123.30
1	BA	527	G7M	O4'-C1'-N9	7.94	119.28	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	527	G7M	O4'-C1'-N9	6.83	117.80	108.75
54	DA	1618	6MZ	C9-N6-C6	6.07	128.48	122.85

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
12	AL	89	D2T	SB-CB-CG-OD2
1	BA	527	G7M	O4'-C4'-C5'-O5'
12	BL	89	D2T	CG-CB-SB-CB1
12	BL	89	D2T	CA-CB-CG-OD1

There are no ring outliers.

15 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	DA	2498	OMC	1	0
54	DA	2030	6MZ	1	0
31	CA	2445	2MG	1	0
1	BA	1519	MA6	1	0
31	CA	2030	6MZ	2	0
1	AA	1518	MA6	1	0
40	DN	81[B]	4D4	1	0
30	DD	150[B]	MEQ	1	0
54	DA	747	5MU	1	0
31	CA	2503	2MA	1	0
54	DA	2449	H2U	1	0
54	DA	2445	2MG	1	0
31	CA	747	5MU	1	0
1	AA	1519	MA6	1	0
1	BA	1518	MA6	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 554 ligands modelled in this entry, 472 are monoatomic - leaving 82 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	$\# Z  > 2$
56	PG4	DQ	202	-	12,12,12	0.15	0	11,11,11	0.16	0
67	GUN	DA	3210	-	7,12,12	0.72	0	8,17,17	0.82	0
57	MPD	AA	1676	-	7,7,7	0.54	0	9,10,10	0.45	0
57	MPD	DN	201	-	7,7,7	1.01	1 (14%)	9,10,10	0.63	0
57	MPD	DT	202	-	7,7,7	0.75	0	9,10,10	0.43	0
61	PEG	DA	3225	-	6,6,6	0.50	0	5,5,5	0.27	0
56	PG4	DS	202	-	12,12,12	0.48	0	11,11,11	0.43	0
58	PUT	AA	1674	-	5,5,5	0.15	0	4,4,4	0.14	0
62	EDO	DA	3194	-	3,3,3	0.60	0	2,2,2	0.12	0
58	PUT	AA	1673	-	5,5,5	0.15	0	4,4,4	0.15	0
58	PUT	DA	3211	-	5,5,5	0.31	0	4,4,4	0.20	0
58	PUT	DA	3212	-	5,5,5	0.37	0	4,4,4	0.33	0
61	PEG	DA	3199	-	6,6,6	0.30	0	5,5,5	0.20	0
57	MPD	DA	3190	-	7,7,7	0.44	0	9,10,10	0.51	0
63	PGE	DU	101	-	9,9,9	0.25	0	8,8,8	0.37	0
63	PGE	D3	101	-	9,9,9	0.29	0	8,8,8	0.23	0
61	PEG	DP	201	-	6,6,6	0.30	0	5,5,5	0.15	0
63	PGE	DA	3213	-	9,9,9	0.17	0	8,8,8	0.18	0
58	PUT	DA	3002	-	5,5,5	0.20	0	4,4,4	0.07	0
66	ACY	DA	3191	-	3,3,3	1.01	0	3,3,3	0.90	0
58	PUT	DA	3204	-	5,5,5	0.35	0	4,4,4	0.30	0
56	PG4	DR	202	-	12,12,12	0.43	0	11,11,11	0.54	0
57	MPD	DT	201	-	7,7,7	0.57	0	9,10,10	0.19	0
65	1PE	DA	3185	-	15,15,15	0.16	0	14,14,14	0.16	0
64	SPD	DA	3223	-	9,9,9	0.17	0	8,8,8	0.69	0
62	EDO	DA	3004	-	3,3,3	0.67	0	2,2,2	0.18	0
63	PGE	DA	3186	-	9,9,9	0.35	0	8,8,8	0.56	0
61	PEG	DA	3217	-	6,6,6	0.30	0	5,5,5	0.08	0
57	MPD	DE	301	-	7,7,7	0.79	0	9,10,10	0.81	0
62	EDO	D1	101	-	3,3,3	0.61	0	2,2,2	0.19	0
63	PGE	DA	3224	-	9,9,9	0.25	0	8,8,8	0.17	0
64	SPD	DA	3205	-	9,9,9	0.24	0	8,8,8	0.19	0
62	EDO	DB	211	-	3,3,3	0.54	0	2,2,2	0.22	0
58	PUT	DA	3221	-	5,5,5	0.46	0	4,4,4	0.65	0
62	EDO	DA	3001	-	3,3,3	0.77	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	PUT	DA	3218	-	5,5,5	0.12	0	4,4,4	0.10	0
62	EDO	DA	3198	-	3,3,3	0.62	0	2,2,2	0.39	0
64	SPD	DA	3187	-	9,9,9	0.15	0	8,8,8	0.43	0
58	PUT	AA	1675	-	5,5,5	0.20	0	4,4,4	0.23	0
57	MPD	DA	3209	-	7,7,7	0.64	0	9,10,10	0.42	0
58	PUT	DA	3184	-	5,5,5	0.23	0	4,4,4	0.17	0
66	ACY	DA	3196	-	3,3,3	2.60	1 (33%)	3,3,3	2.25	2 (66%)
63	PGE	D1	102	-	9,9,9	0.29	0	8,8,8	0.30	0
57	MPD	DA	3192	-	7,7,7	0.64	0	9,10,10	0.83	0
56	PG4	BA	1601	-	12,12,12	0.21	0	11,11,11	0.22	0
61	PEG	DA	3200	-	6,6,6	0.51	0	5,5,5	0.28	0
58	PUT	AA	1672	-	5,5,5	0.22	0	4,4,4	0.19	0
61	PEG	DQ	201	-	6,6,6	0.21	0	5,5,5	0.15	0
64	SPD	DA	3183	-	9,9,9	0.12	0	8,8,8	0.20	0
61	PEG	D3	102	-	6,6,6	0.33	0	5,5,5	0.24	0
61	PEG	DA	3226	-	6,6,6	0.43	0	5,5,5	0.27	0
66	ACY	DA	3201	-	3,3,3	0.98	0	3,3,3	0.93	0
58	PUT	DA	3195	-	5,5,5	0.31	0	4,4,4	0.55	0
61	PEG	DL	201	-	6,6,6	0.13	0	5,5,5	0.12	0
63	PGE	DS	201	-	9,9,9	0.49	0	8,8,8	0.48	0
58	PUT	DA	3220	-	5,5,5	0.18	0	4,4,4	0.14	0
62	EDO	DA	3003	-	3,3,3	0.70	0	2,2,2	0.17	0
63	PGE	DA	3216	-	9,9,9	0.15	0	8,8,8	0.25	0
62	EDO	DA	3197	-	3,3,3	0.58	0	2,2,2	0.27	0
56	PG4	DA	3193	-	12,12,12	0.30	0	11,11,11	0.43	0
65	1PE	DA	3202	-	15,15,15	0.35	0	14,14,14	0.39	0
68	TRS	DA	3219	-	7,7,7	0.36	0	9,9,9	0.36	0
58	PUT	DA	3189	-	5,5,5	0.47	0	4,4,4	0.45	0
59	TAC	BA	1602	55	34,35,35	0.42	0	43,58,58	1.10	2 (4%)
57	MPD	DK	201	-	7,7,7	0.68	0	9,10,10	0.25	0
58	PUT	DA	3188	-	5,5,5	0.44	0	4,4,4	0.28	0
56	PG4	DA	3215	-	12,12,12	0.16	0	11,11,11	0.13	0
62	EDO	DA	3207	-	3,3,3	0.65	0	2,2,2	0.21	0
57	MPD	DS	203	-	7,7,7	0.42	0	9,10,10	0.73	0
62	EDO	DB	210	-	3,3,3	0.54	0	2,2,2	0.26	0
63	PGE	DD	301	-	9,9,9	0.29	0	8,8,8	0.32	0
57	MPD	DA	3206	-	7,7,7	0.95	1 (14%)	9,10,10	0.55	0
57	MPD	DE	302	-	7,7,7	0.82	0	9,10,10	0.53	0
62	EDO	DA	3208	-	3,3,3	0.54	0	2,2,2	0.34	0
58	PUT	DA	3222	-	5,5,5	0.30	0	4,4,4	0.29	0
59	TAC	AA	1678	55	34,35,35	0.50	0	43,58,58	1.03	2 (4%)
57	MPD	AA	1671	-	7,7,7	0.64	0	9,10,10	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
62	EDO	DA	3214	-	3,3,3	0.60	0	2,2,2	0.27	0
61	PEG	D1	103	-	6,6,6	0.42	0	5,5,5	0.15	0
56	PG4	AA	1670	-	12,12,12	0.26	0	11,11,11	0.41	0
57	MPD	DA	3203	-	7,7,7	0.84	0	9,10,10	0.66	0
61	PEG	AL	201	-	6,6,6	0.26	0	5,5,5	0.12	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
56	PG4	DQ	202	-	-	1/10/10/10	-
67	GUN	DA	3210	-	-	-	0/2/2/2
57	MPD	AA	1676	-	-	1/5/5/5	-
57	MPD	DN	201	-	-	3/5/5/5	-
57	MPD	DT	202	-	-	3/5/5/5	-
61	PEG	DA	3225	-	-	2/4/4/4	-
56	PG4	DS	202	-	-	2/10/10/10	-
58	PUT	AA	1674	-	-	0/3/3/3	-
62	EDO	DA	3194	-	-	1/1/1/1	-
58	PUT	AA	1673	-	-	0/3/3/3	-
58	PUT	DA	3211	-	-	0/3/3/3	-
58	PUT	DA	3212	-	-	1/3/3/3	-
61	PEG	DA	3199	-	-	3/4/4/4	-
57	MPD	DA	3190	-	-	2/5/5/5	-
63	PGE	DU	101	-	-	4/7/7/7	-
63	PGE	D3	101	-	-	2/7/7/7	-
61	PEG	DP	201	-	-	2/4/4/4	-
63	PGE	DA	3213	-	-	3/7/7/7	-
58	PUT	DA	3002	-	-	0/3/3/3	-
58	PUT	DA	3204	-	-	1/3/3/3	-
56	PG4	DR	202	-	-	6/10/10/10	-
57	MPD	DT	201	-	-	2/5/5/5	-
65	1PE	DA	3185	-	-	5/13/13/13	-
64	SPD	DA	3223	-	-	4/7/7/7	-
62	EDO	DA	3004	-	-	0/1/1/1	-
63	PGE	DA	3186	-	-	4/7/7/7	-
61	PEG	DA	3217	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	DE	301	-	-	5/5/5/5	-
62	EDO	D1	101	-	-	0/1/1/1	-
63	PGE	DA	3224	-	-	4/7/7/7	-
64	SPD	DA	3205	-	-	5/7/7/7	-
62	EDO	DB	211	-	-	0/1/1/1	-
58	PUT	DA	3221	-	-	1/3/3/3	-
62	EDO	DA	3001	-	-	1/1/1/1	-
58	PUT	DA	3218	-	-	0/3/3/3	-
62	EDO	DA	3198	-	-	1/1/1/1	-
64	SPD	DA	3187	-	-	0/7/7/7	-
58	PUT	AA	1675	-	-	1/3/3/3	-
57	MPD	DA	3209	-	-	1/5/5/5	-
58	PUT	DA	3184	-	-	0/3/3/3	-
63	PGE	D1	102	-	-	4/7/7/7	-
57	MPD	DA	3192	-	-	2/5/5/5	-
56	PG4	BA	1601	-	-	0/10/10/10	-
61	PEG	DA	3200	-	-	3/4/4/4	-
58	PUT	AA	1672	-	-	0/3/3/3	-
61	PEG	DQ	201	-	-	2/4/4/4	-
64	SPD	DA	3183	-	-	1/7/7/7	-
61	PEG	D3	102	-	-	2/4/4/4	-
61	PEG	DA	3226	-	-	0/4/4/4	-
58	PUT	DA	3195	-	-	1/3/3/3	-
61	PEG	DL	201	-	-	2/4/4/4	-
63	PGE	DS	201	-	-	3/7/7/7	-
58	PUT	DA	3220	-	-	0/3/3/3	-
62	EDO	DA	3003	-	-	0/1/1/1	-
63	PGE	DA	3216	-	-	4/7/7/7	-
62	EDO	DA	3197	-	-	0/1/1/1	-
56	PG4	DA	3193	-	-	8/10/10/10	-
65	1PE	DA	3202	-	-	8/13/13/13	-
68	TRS	DA	3219	-	-	0/9/9/9	-
58	PUT	DA	3189	-	-	0/3/3/3	-
59	TAC	BA	1602	55	-	6/8/74/74	0/4/4/4
57	MPD	DK	201	-	-	2/5/5/5	-
58	PUT	DA	3188	-	-	0/3/3/3	-
56	PG4	DA	3215	-	-	4/10/10/10	-
62	EDO	DA	3207	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	DS	203	-	-	0/5/5/5	-
62	EDO	DB	210	-	-	0/1/1/1	-
63	PGE	DD	301	-	-	4/7/7/7	-
57	MPD	DA	3206	-	-	2/5/5/5	-
57	MPD	DE	302	-	-	1/5/5/5	-
62	EDO	DA	3208	-	-	0/1/1/1	-
58	PUT	DA	3222	-	-	1/3/3/3	-
59	TAC	AA	1678	55	-	4/8/74/74	0/4/4/4
57	MPD	AA	1671	-	-	1/5/5/5	-
62	EDO	DA	3214	-	-	0/1/1/1	-
61	PEG	D1	103	-	-	1/4/4/4	-
56	PG4	AA	1670	-	-	4/10/10/10	-
57	MPD	DA	3203	-	-	1/5/5/5	-
61	PEG	AL	201	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	DA	3196	ACY	O-C	4.29	1.40	1.22
57	DN	201	MPD	C3-C2	2.23	1.60	1.54
57	DA	3206	MPD	C3-C2	2.09	1.60	1.54

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BA	1602	TAC	C5-C41-C4	-5.40	105.94	113.73
59	AA	1678	TAC	C5-C41-C4	-5.03	106.46	113.73
66	DA	3196	ACY	OXT-C-CH3	2.95	127.42	115.05
59	BA	1602	TAC	O3-C3-C2	-2.61	118.57	122.93
66	DA	3196	ACY	O-C-CH3	-2.50	112.27	122.53

There are no chirality outliers.

5 of 147 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	AA	1676	MPD	C2-C3-C4-O4
57	DE	301	MPD	C1-C2-C3-C4
57	DE	301	MPD	O2-C2-C3-C4
57	DE	301	MPD	C2-C3-C4-O4
57	DE	301	MPD	C2-C3-C4-C5

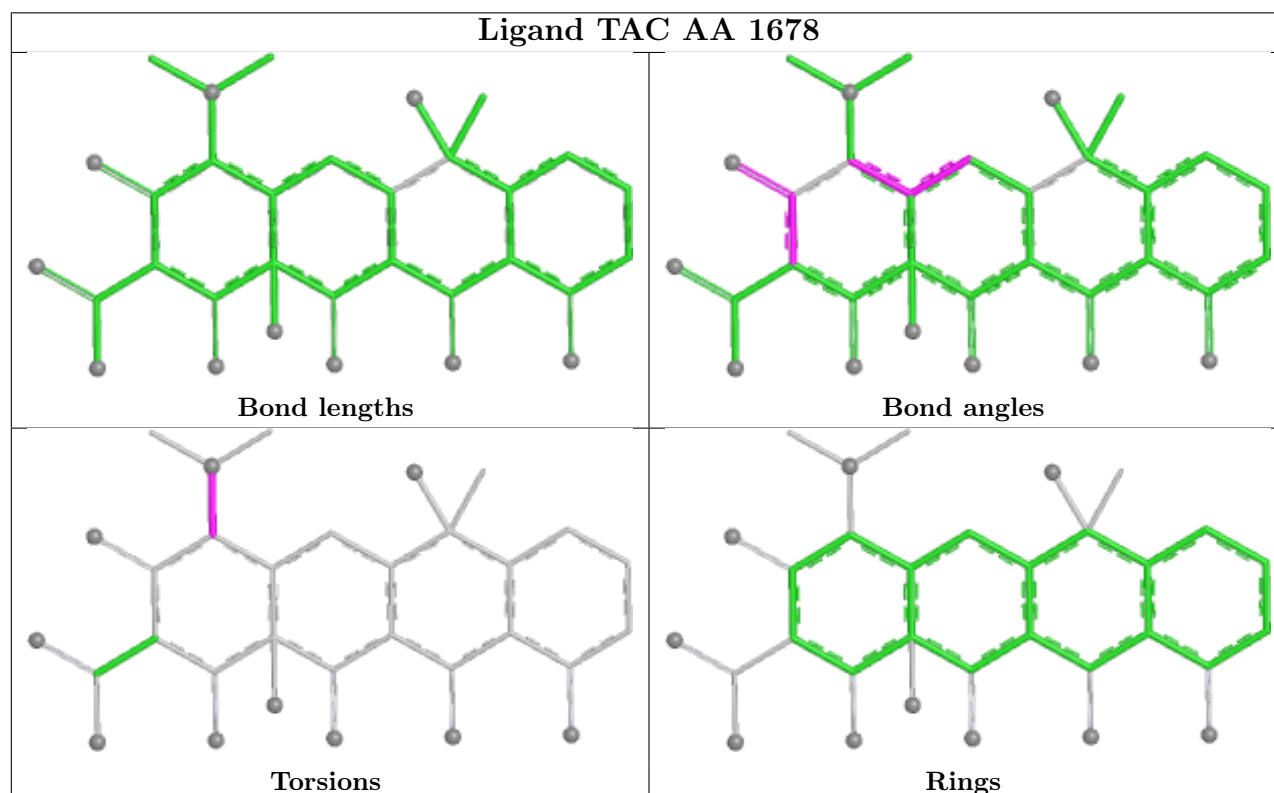
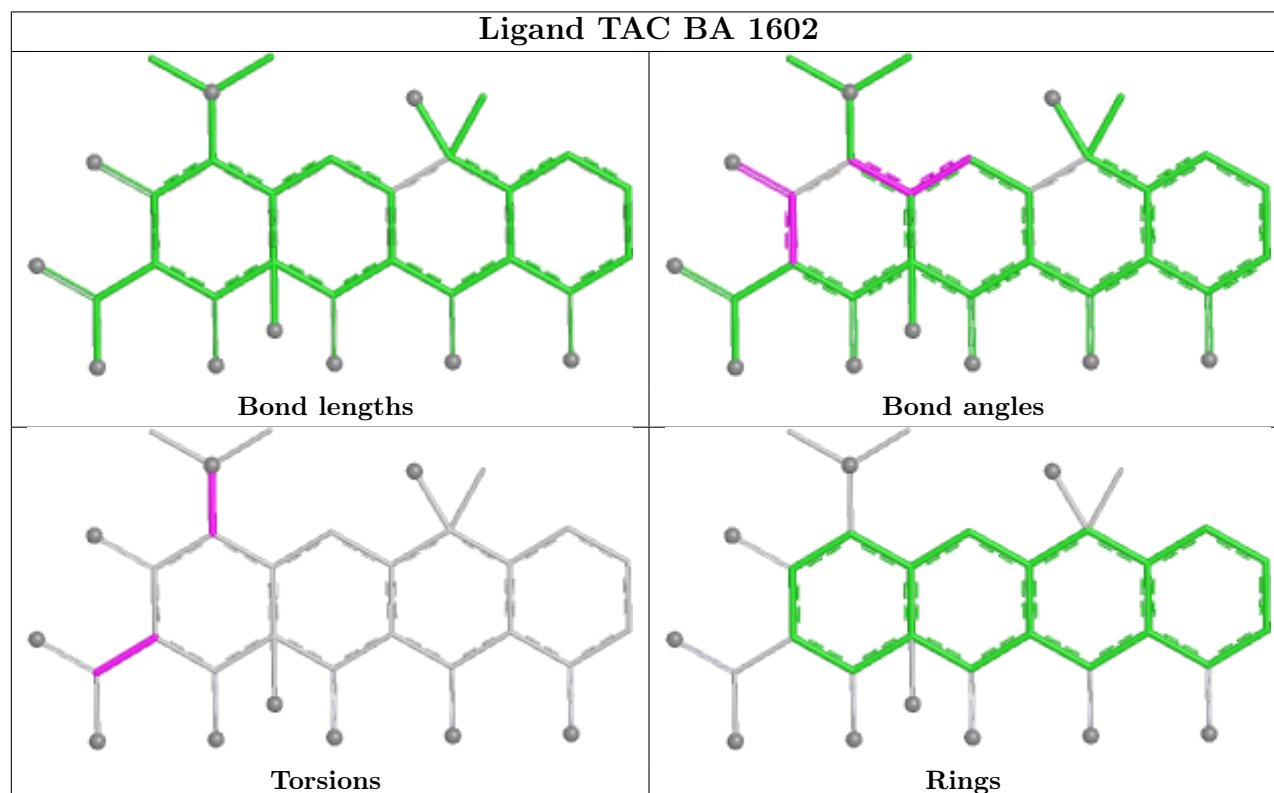
There are no ring outliers.

32 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	DN	201	MPD	1	0
56	DS	202	PG4	1	0
62	DA	3194	EDO	1	0
58	DA	3212	PUT	1	0
57	DA	3190	MPD	1	0
63	DU	101	PGE	1	0
61	DP	201	PEG	1	0
63	DA	3213	PGE	1	0
56	DR	202	PG4	5	0
64	DA	3223	SPD	4	0
63	DA	3224	PGE	3	0
62	DB	211	EDO	1	0
58	DA	3221	PUT	3	0
58	DA	3218	PUT	1	0
63	D1	102	PGE	2	0
57	DA	3192	MPD	2	0
61	DA	3200	PEG	1	0
61	D3	102	PEG	2	0
58	DA	3195	PUT	3	0
63	DA	3216	PGE	1	0
62	DA	3197	EDO	1	0
56	DA	3193	PG4	1	0
68	DA	3219	TRS	1	0
58	DA	3189	PUT	1	0
59	BA	1602	TAC	1	0
56	DA	3215	PG4	1	0
63	DD	301	PGE	2	0
58	DA	3222	PUT	1	0
59	AA	1678	TAC	1	0
61	D1	103	PEG	1	0
56	AA	1670	PG4	1	0
57	DA	3203	MPD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	1523/1534 (99%)	0.73	126 (8%) 19 14	43, 97, 239, 285	0
1	BA	1522/1534 (99%)	1.48	413 (27%) 2 2	52, 139, 267, 278	0
2	AB	224/224 (100%)	1.18	37 (16%) 5 5	78, 123, 207, 275	0
2	BB	224/224 (100%)	1.41	47 (20%) 3 3	93, 139, 208, 261	0
3	AC	206/206 (100%)	0.87	19 (9%) 16 12	73, 101, 135, 157	0
3	BC	206/206 (100%)	1.45	52 (25%) 2 2	103, 141, 180, 219	0
4	AD	205/205 (100%)	0.82	14 (6%) 25 19	53, 96, 127, 158	0
4	BD	205/205 (100%)	0.65	6 (2%) 54 45	53, 77, 106, 135	0
5	AE	155/155 (100%)	0.71	9 (5%) 30 23	60, 87, 139, 174	0
5	BE	150/155 (96%)	1.27	24 (16%) 6 5	71, 91, 142, 229	0
6	AF	106/106 (100%)	0.81	10 (9%) 15 12	72, 97, 120, 134	0
6	BF	100/106 (94%)	1.04	14 (14%) 7 7	79, 112, 139, 147	0
7	AG	151/151 (100%)	1.46	34 (22%) 3 3	99, 128, 157, 169	0
7	BG	151/151 (100%)	1.89	62 (41%) 1 1	139, 193, 209, 220	0
8	AH	129/129 (100%)	0.75	6 (4%) 37 30	66, 85, 113, 128	0
8	BH	129/129 (100%)	1.29	22 (17%) 5 4	86, 110, 145, 164	0
9	AI	127/127 (100%)	1.58	39 (30%) 1 1	85, 123, 161, 188	0
9	BI	127/127 (100%)	2.17	54 (42%) 1 1	130, 168, 201, 223	0
10	AJ	99/99 (100%)	1.63	29 (29%) 1 2	85, 111, 142, 157	0
10	BJ	98/99 (98%)	2.44	60 (61%) 0 0	132, 163, 188, 200	0
11	AK	117/117 (100%)	0.91	12 (10%) 13 10	52, 102, 138, 153	0
11	BK	117/117 (100%)	1.25	20 (17%) 5 4	73, 109, 139, 160	0
12	AL	122/123 (99%)	0.71	13 (10%) 12 10	48, 66, 99, 126	0
12	BL	122/123 (99%)	1.52	36 (29%) 1 2	75, 91, 112, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	AM	114/114 (100%)	1.59	36 (31%)	1	1	90, 118, 167, 184	0
13	BM	114/114 (100%)	1.86	43 (37%)	1	1	195, 228, 237, 241	0
14	AN	100/100 (100%)	2.05	48 (48%)	0	1	82, 108, 198, 210	0
14	BN	100/100 (100%)	2.19	54 (54%)	0	0	125, 173, 232, 242	0
15	AO	88/88 (100%)	0.74	10 (11%)	11	9	63, 87, 108, 128	0
15	BO	88/88 (100%)	1.04	8 (9%)	16	12	75, 105, 125, 144	0
16	AP	82/82 (100%)	1.02	10 (12%)	10	8	60, 79, 114, 133	0
16	BP	82/82 (100%)	2.85	60 (73%)	0	0	89, 105, 151, 161	0
17	AQ	80/80 (100%)	0.82	7 (8%)	17	13	63, 79, 114, 136	0
17	BQ	80/80 (100%)	1.77	28 (35%)	1	1	94, 119, 143, 147	0
18	AR	55/55 (100%)	0.99	5 (9%)	16	12	68, 91, 126, 154	0
18	BR	55/55 (100%)	1.03	5 (9%)	16	12	71, 89, 123, 150	0
19	AS	79/79 (100%)	1.61	21 (26%)	2	2	94, 109, 146, 153	0
19	BS	79/79 (100%)	2.15	36 (45%)	1	1	206, 223, 234, 242	0
20	AT	86/86 (100%)	1.28	15 (17%)	5	4	67, 79, 116, 132	0
20	BT	85/86 (98%)	2.37	45 (52%)	0	0	101, 121, 164, 175	0
21	AU	56/56 (100%)	1.26	14 (25%)	2	2	80, 118, 156, 170	0
21	BU	56/56 (100%)	1.12	11 (19%)	4	4	75, 100, 143, 156	0
22	C1	56/56 (100%)	2.79	35 (62%)	0	0	94, 138, 164, 182	0
22	D1	56/56 (100%)	0.30	2 (3%)	46	38	20, 41, 64, 95	0
23	C2	50/51 (98%)	2.10	21 (42%)	1	1	126, 141, 153, 175	0
23	D2	51/51 (100%)	0.47	3 (5%)	29	22	49, 63, 89, 104	0
24	C3	46/46 (100%)	3.08	37 (80%)	0	0	99, 109, 119, 131	0
24	D3	46/46 (100%)	0.46	3 (6%)	26	20	30, 42, 56, 99	0
25	C4	64/64 (100%)	3.76	58 (90%)	0	0	105, 121, 134, 140	0
25	D4	64/64 (100%)	0.27	1 (1%)	70	63	34, 41, 52, 63	0
26	C5	38/38 (100%)	2.69	25 (65%)	0	0	100, 114, 124, 134	0
26	D5	38/38 (100%)	0.41	1 (2%)	57	49	31, 46, 62, 82	0
27	C0	58/58 (100%)	2.08	27 (46%)	0	1	98, 113, 132, 135	0
27	D0	58/58 (100%)	0.39	1 (1%)	69	61	25, 35, 50, 72	2 (3%)
28	CB	118/120 (98%)	1.51	27 (22%)	2	3	132, 189, 251, 254	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DB	120/120 (100%)	-0.09	0 100 100	29, 56, 101, 148	0
29	CC	271/271 (100%)	2.18	123 (45%) 1 1	80, 112, 146, 165	0
29	DC	271/271 (100%)	0.06	13 (4%) 36 29	28, 56, 84, 100	0
30	CD	208/209 (99%)	2.00	94 (45%) 1 1	86, 121, 156, 181	0
30	DD	208/209 (99%)	-0.19	3 (1%) 73 66	18, 39, 67, 88	0
31	CA	2876/2904 (99%)	2.08	1380 (47%) 0 1	71, 170, 260, 285	0
32	CE	201/201 (100%)	2.45	116 (57%) 0 0	112, 159, 194, 210	0
32	DE	201/201 (100%)	0.08	3 (1%) 71 64	24, 55, 100, 139	0
33	CF	177/177 (100%)	1.48	42 (23%) 2 3	198, 211, 219, 226	0
33	DF	177/177 (100%)	0.76	8 (4%) 39 31	50, 79, 125, 137	0
34	CG	176/176 (100%)	1.44	42 (23%) 2 3	130, 170, 205, 215	0
34	DG	176/176 (100%)	0.35	6 (3%) 48 40	42, 70, 97, 139	0
35	CH	149/149 (100%)	1.26	24 (16%) 5 5	84, 151, 170, 180	0
35	DH	149/149 (100%)	1.46	36 (24%) 2 2	74, 150, 187, 199	0
36	CJ	134/134 (100%)	2.07	55 (41%) 1 1	227, 245, 255, 263	0
36	DJ	134/134 (100%)	2.33	72 (53%) 0 0	196, 220, 229, 237	0
37	CK	142/142 (100%)	2.19	74 (52%) 0 0	95, 117, 152, 194	0
37	DK	142/142 (100%)	-0.37	0 100 100	19, 34, 58, 72	0
38	CL	122/123 (99%)	1.74	43 (35%) 1 1	90, 109, 141, 158	0
38	DL	123/123 (100%)	-0.23	0 100 100	28, 43, 70, 106	0
39	CM	144/144 (100%)	2.90	95 (65%) 0 0	104, 151, 201, 235	0
39	DM	144/144 (100%)	0.34	8 (5%) 31 24	18, 55, 84, 116	0
40	CN	135/136 (99%)	1.64	40 (29%) 1 2	92, 112, 142, 180	0
40	DN	135/136 (99%)	-0.28	0 100 100	16, 39, 67, 86	1 (0%)
41	CO	120/125 (96%)	2.45	70 (58%) 0 0	101, 123, 143, 177	0
41	DO	125/125 (100%)	-0.29	0 100 100	24, 36, 65, 108	0
42	CP	116/117 (99%)	1.44	20 (17%) 5 4	139, 162, 177, 181	0
42	DP	117/117 (100%)	0.23	2 (1%) 69 61	36, 56, 84, 93	0
43	CQ	114/114 (100%)	1.69	33 (28%) 1 2	100, 117, 149, 164	0
43	DQ	114/114 (100%)	0.03	3 (2%) 57 49	30, 49, 77, 109	0
44	CR	117/117 (100%)	2.57	69 (58%) 0 0	89, 122, 157, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	DR	117/117 (100%)	-0.43	1 (0%) 81 75	18, 29, 48, 72	0
45	CS	103/103 (100%)	2.45	51 (49%) 0 1	107, 133, 172, 185	0
45	DS	103/103 (100%)	-0.21	2 (1%) 66 58	19, 41, 69, 91	0
46	CT	110/110 (100%)	2.63	76 (69%) 0 0	99, 127, 167, 182	0
46	DT	110/110 (100%)	-0.18	2 (1%) 67 60	19, 33, 60, 116	0
47	CU	93/93 (100%)	2.62	62 (66%) 0 0	123, 147, 176, 185	0
47	DU	93/93 (100%)	0.53	9 (9%) 15 11	31, 53, 109, 124	0
48	CV	102/102 (100%)	2.75	69 (67%) 0 0	113, 161, 198, 209	0
48	DV	102/102 (100%)	0.38	5 (4%) 36 28	42, 60, 121, 157	0
49	CW	94/94 (100%)	1.32	21 (22%) 3 3	116, 137, 156, 161	0
49	DW	94/94 (100%)	-0.08	1 (1%) 77 71	31, 51, 76, 86	0
50	CX	75/76 (98%)	1.96	32 (42%) 1 1	103, 126, 140, 170	0
50	DX	76/76 (100%)	-0.04	1 (1%) 74 67	18, 39, 64, 104	1 (1%)
51	CY	77/77 (100%)	2.53	47 (61%) 0 0	97, 117, 142, 161	0
51	DY	77/77 (100%)	0.07	1 (1%) 74 67	38, 54, 88, 103	0
52	CZ	62/62 (100%)	2.38	39 (62%) 0 0	127, 163, 175, 186	0
52	DZ	62/62 (100%)	0.52	3 (4%) 36 29	48, 70, 103, 126	0
53	DI	135/135 (100%)	1.85	51 (37%) 1 1	78, 150, 197, 207	1 (0%)
54	DA	2873/2904 (98%)	-0.10	142 (4%) 36 28	17, 44, 217, 299	11 (0%)
All	All	20633/20745 (99%)	1.15	4944 (23%) 2 3	16, 108, 239, 299	16 (0%)

The worst 5 of 4944 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	AG	5	ARG	12.5
41	CO	46	ARG	9.6
10	BJ	74	VAL	9.0
9	BI	124	ARG	8.9
9	BI	16	ALA	8.8

## 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(Å <sup>2</sup> )	Q<0.9
1	2MG	BA	966	24/25	0.63	0.15	149,156,167,168	0
31	PSU	CA	1911	20/21	0.70	0.11	127,137,139,140	0
31	PSU	CA	1917	20/21	0.70	0.13	120,125,134,134	0
31	2MA	CA	2503	23/24	0.71	0.24	107,109,110,110	0
1	2MG	BA	1207	24/25	0.72	0.13	150,152,156,160	0
1	5MC	BA	967	21/22	0.73	0.16	149,158,161,161	0
31	PSU	CA	746	20/21	0.76	0.16	116,118,119,120	0
31	3TD	CA	1915	21/22	0.76	0.11	149,155,157,158	0
31	PSU	CA	2504	20/21	0.77	0.18	93,103,106,106	0
31	PSU	CA	2580	20/21	0.78	0.15	93,99,101,101	0
31	PSU	CA	955	20/21	0.81	0.16	100,105,108,108	0
31	PSU	CA	2457	20/21	0.83	0.13	96,97,99,99	0
31	6MZ	CA	1618	23/24	0.83	0.17	134,138,143,145	0
31	6MZ	CA	2030	23/24	0.84	0.16	101,104,106,107	0
1	PSU	BA	516	20/21	0.85	0.11	80,89,91,94	0
54	3TD	DA	1915	21/22	0.85	0.12	105,110,116,117	0
30	MEQ	CD	150	9/11	0.86	0.20	92,98,133,136	0
31	5MU	CA	1939	21/22	0.86	0.16	70,77,78,80	0
54	PSU	DA	1917	20/21	0.86	0.10	80,84,91,91	0
40	4D4	CN	81	12/13	0.86	0.17	108,112,131,132	0
31	OMU	CA	2552	21/22	0.87	0.23	88,92,94,95	0
12	D2T	AL	89	10/11	0.87	0.14	60,63,71,72	0
1	5MC	BA	1407	21/22	0.87	0.14	98,109,111,115	0
1	2MG	BA	1516	24/25	0.87	0.13	79,86,93,95	0
12	D2T	BL	89	10/11	0.87	0.16	83,85,93,94	0
31	OMG	CA	2251	24/25	0.88	0.16	85,90,93,93	0
31	5MC	CA	1962	21/22	0.88	0.13	70,77,80,82	0
31	OMC	CA	2498	21/22	0.88	0.18	91,94,95,95	0
1	2MG	AA	1207	24/25	0.88	0.11	99,103,105,108	0
31	G7M	CA	2069	24/25	0.88	0.20	102,104,108,109	0
31	2MG	CA	1835	24/25	0.89	0.14	71,73,76,77	0
31	1MG	CA	745	24/25	0.89	0.15	103,107,111,114	0
1	4OC	BA	1402	22/23	0.89	0.12	74,77,79,80	0
31	PSU	CA	2605	20/21	0.89	0.12	79,81,83,84	0
31	5MU	CA	747	21/22	0.89	0.13	116,120,122,123	0
1	G7M	BA	527	24/25	0.89	0.12	70,73,78,79	0
1	UR3	BA	1498	21/22	0.89	0.12	84,87,94,94	0
31	2MG	CA	2445	24/25	0.90	0.21	97,100,102,102	0
1	MA6	BA	1518	24/25	0.90	0.13	84,86,92,93	0
54	PSU	DA	1911	20/21	0.90	0.09	83,90,91,92	0
1	2MG	AA	966	24/25	0.91	0.12	79,84,91,91	0
30	MEQ	DD	150[B]	10/11	0.92	0.13	25,29,41,41	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	G7M	AA	527	24/25	0.92	0.10	55,58,62,63	0
1	PSU	AA	516	20/21	0.92	0.10	76,78,82,82	0
1	MA6	BA	1519	24/25	0.92	0.12	80,82,87,88	0
30	MEQ	DD	150[A]	10/11	0.92	0.13	17,22,27,29	10
1	5MC	AA	967	21/22	0.93	0.12	74,88,90,91	0
54	PSU	DA	2604	20/21	0.94	0.10	36,42,53,53	0
40	4D4	DN	81[A]	12/13	0.94	0.15	30,36,49,50	9
40	4D4	DN	81[B]	12/13	0.94	0.15	26,28,31,32	9
1	5MC	AA	1407	21/22	0.95	0.08	51,52,54,55	0
1	UR3	AA	1498	21/22	0.95	0.09	54,56,61,63	0
1	MA6	AA	1518	24/25	0.95	0.10	50,54,56,57	0
54	5MU	DA	1939	21/22	0.96	0.09	31,36,38,39	0
54	5MC	DA	1962	21/22	0.96	0.09	44,46,49,50	0
54	OMU	DA	2552	21/22	0.96	0.10	35,37,44,47	0
54	2MG	DA	1835	24/25	0.96	0.09	53,55,56,58	0
54	PSU	DA	2605	20/21	0.96	0.09	33,42,46,46	0
1	MA6	AA	1519	24/25	0.96	0.10	53,56,61,65	0
1	2MG	AA	1516	24/25	0.96	0.10	52,54,56,57	0
1	4OC	AA	1402	22/23	0.96	0.08	52,59,61,62	0
54	PSU	DA	2580	20/21	0.97	0.09	24,30,36,37	0
54	5MU	DA	747	21/22	0.97	0.06	26,28,32,37	0
54	2MG	DA	2445	24/25	0.97	0.09	14,25,28,29	0
54	2MA	DA	2503	23/24	0.97	0.08	26,42,46,47	0
54	PSU	DA	2504	20/21	0.97	0.14	45,53,56,57	0
54	PSU	DA	746	20/21	0.97	0.07	28,30,33,36	0
54	PSU	DA	955	20/21	0.98	0.07	25,26,29,30	0
54	6MZ	DA	1618	23/24	0.98	0.07	25,28,31,33	0
54	6MZ	DA	2030	23/24	0.98	0.06	13,23,28,28	0
54	G7M	DA	2069	24/25	0.98	0.08	24,30,37,38	0
54	OMG	DA	2251	24/25	0.98	0.07	23,27,30,30	0
54	1MG	DA	745	24/25	0.98	0.05	19,26,31,33	0
54	H2U	DA	2449	20/21	0.98	0.08	24,27,28,32	0
54	PSU	DA	2457	20/21	0.98	0.06	20,28,30,31	0
54	OMC	DA	2498	21/22	0.98	0.06	21,22,27,29	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
55	MG	CA	3129	1/1	-0.09	0.38	118,118,118,118	0
55	MG	CA	3145	1/1	-0.07	0.34	234,234,234,234	0
55	MG	CA	3109	1/1	-0.06	0.37	175,175,175,175	0
55	MG	CA	3138	1/1	-0.05	0.44	125,125,125,125	0
55	MG	AA	1622	1/1	0.07	0.40	119,119,119,119	0
55	MG	DA	3168	1/1	0.12	0.34	109,109,109,109	0
55	MG	CA	3004	1/1	0.13	0.27	243,243,243,243	0
55	MG	BA	1642	1/1	0.16	0.45	164,164,164,164	0
55	MG	CA	3123	1/1	0.17	0.21	199,199,199,199	0
55	MG	CA	3131	1/1	0.18	0.30	145,145,145,145	0
55	MG	CA	3060	1/1	0.23	0.20	256,256,256,256	0
55	MG	CA	3140	1/1	0.27	0.48	91,91,91,91	0
55	MG	BA	1638	1/1	0.30	0.43	175,175,175,175	0
55	MG	CA	3121	1/1	0.31	0.44	125,125,125,125	0
55	MG	CA	3153	1/1	0.31	0.34	138,138,138,138	0
55	MG	CA	3037	1/1	0.31	0.18	256,256,256,256	0
55	MG	CA	3025	1/1	0.33	0.30	180,180,180,180	0
55	MG	CA	3139	1/1	0.34	0.30	128,128,128,128	0
55	MG	CA	3001	1/1	0.35	0.23	258,258,258,258	0
55	MG	CA	3076	1/1	0.40	0.22	246,246,246,246	0
55	MG	CA	3146	1/1	0.40	1.20	76,76,76,76	1
55	MG	CA	3110	1/1	0.41	0.40	141,141,141,141	0
55	MG	CA	3033	1/1	0.41	0.24	246,246,246,246	0
55	MG	CA	3132	1/1	0.42	0.33	129,129,129,129	0
55	MG	CA	3074	1/1	0.42	0.26	243,243,243,243	0
55	MG	CA	3059	1/1	0.43	0.17	240,240,240,240	0
55	MG	CA	3103	1/1	0.44	0.21	260,260,260,260	0
55	MG	BA	1629	1/1	0.45	0.36	124,124,124,124	0
55	MG	CA	3066	1/1	0.46	0.13	284,284,284,284	0
55	MG	BA	1643	1/1	0.46	0.20	134,134,134,134	0
55	MG	CA	3122	1/1	0.47	0.33	182,182,182,182	0
55	MG	CA	3151	1/1	0.47	0.26	209,209,209,209	0
55	MG	CA	3118	1/1	0.47	0.45	123,123,123,123	0
55	MG	CA	3155	1/1	0.47	0.22	240,240,240,240	0
55	MG	BA	1605	1/1	0.47	0.16	250,250,250,250	0
55	MG	CA	3128	1/1	0.49	0.35	135,135,135,135	0
55	MG	CA	3119	1/1	0.50	0.20	188,188,188,188	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3130	1/1	0.51	0.24	101,101,101,101	0
55	MG	CA	3141	1/1	0.51	0.32	115,115,115,115	0
55	MG	AA	1608	1/1	0.54	0.40	97,97,97,97	0
55	MG	AA	1603	1/1	0.54	0.48	110,110,110,110	0
55	MG	CA	3007	1/1	0.55	0.19	175,175,175,175	0
55	MG	CA	3125	1/1	0.56	0.35	120,120,120,120	0
55	MG	CA	3116	1/1	0.56	0.43	101,101,101,101	0
55	MG	CA	3124	1/1	0.56	0.40	127,127,127,127	0
55	MG	CA	3147	1/1	0.56	0.68	80,80,80,80	1
55	MG	CA	3020	1/1	0.57	0.35	269,269,269,269	0
55	MG	AA	1606	1/1	0.58	0.44	108,108,108,108	0
55	MG	DA	3139	1/1	0.59	0.85	58,58,58,58	1
55	MG	CA	3006	1/1	0.59	0.11	242,242,242,242	0
55	MG	CA	3002	1/1	0.60	0.32	278,278,278,278	0
55	MG	BA	1608	1/1	0.61	0.22	243,243,243,243	0
55	MG	BA	1641	1/1	0.61	0.27	98,98,98,98	0
55	MG	CA	3134	1/1	0.61	0.31	99,99,99,99	0
55	MG	CA	3072	1/1	0.62	0.28	255,255,255,255	0
55	MG	CA	3105	1/1	0.62	0.31	92,92,92,92	0
55	MG	AA	1628	1/1	0.63	0.19	142,142,142,142	0
55	MG	BA	1626	1/1	0.63	0.16	264,264,264,264	0
55	MG	DA	3180	1/1	0.63	0.22	99,99,99,99	0
55	MG	CA	3031	1/1	0.64	0.16	257,257,257,257	0
55	MG	CA	3154	1/1	0.64	0.27	200,200,200,200	0
55	MG	CA	3127	1/1	0.64	0.18	85,85,85,85	0
55	MG	DA	3145	1/1	0.65	0.23	111,111,111,111	0
55	MG	CA	3133	1/1	0.65	0.26	194,194,194,194	0
55	MG	AA	1609	1/1	0.65	0.31	96,96,96,96	0
55	MG	CA	3013	1/1	0.66	0.20	251,251,251,251	0
55	MG	AA	1605	1/1	0.66	0.46	97,97,97,97	0
55	MG	BA	1606	1/1	0.66	0.14	190,190,190,190	0
55	MG	CA	3046	1/1	0.66	0.30	228,228,228,228	0
55	MG	DA	3172	1/1	0.66	0.41	86,86,86,86	0
55	MG	CA	3030	1/1	0.66	0.14	128,128,128,128	0
55	MG	CA	3149	1/1	0.67	0.33	73,73,73,73	0
55	MG	CA	3009	1/1	0.67	0.18	217,217,217,217	0
55	MG	DB	207	1/1	0.67	0.26	99,99,99,99	0
55	MG	BA	1627	1/1	0.67	0.20	264,264,264,264	0
55	MG	CA	3114	1/1	0.68	0.30	102,102,102,102	0
55	MG	CA	3104	1/1	0.68	0.23	252,252,252,252	0
55	MG	AA	1661	1/1	0.68	0.20	182,182,182,182	0
55	MG	CA	3067	1/1	0.68	0.14	239,239,239,239	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3061	1/1	0.68	0.16	227,227,227,227	0
55	MG	CA	3055	1/1	0.69	0.55	94,94,94,94	0
55	MG	AA	1626	1/1	0.69	0.39	104,104,104,104	0
55	MG	CA	3036	1/1	0.69	0.21	235,235,235,235	0
55	MG	DA	3176	1/1	0.69	0.33	91,91,91,91	0
55	MG	CA	3098	1/1	0.69	0.21	231,231,231,231	0
62	EDO	DA	3004	4/4	0.69	0.33	112,113,114,114	0
55	MG	AA	1654	1/1	0.70	0.30	241,241,241,241	0
55	MG	CA	3032	1/1	0.70	0.24	194,194,194,194	0
55	MG	DA	3159	1/1	0.70	0.27	74,74,74,74	0
55	MG	AA	1616	1/1	0.70	0.45	94,94,94,94	0
63	PGE	D1	102	10/10	0.70	0.34	89,92,93,93	0
55	MG	CA	3054	1/1	0.71	0.18	201,201,201,201	0
57	MPD	DE	301	8/8	0.71	0.25	98,102,104,105	0
55	MG	BA	1631	1/1	0.71	0.26	151,151,151,151	0
55	MG	CA	3091	1/1	0.71	0.19	202,202,202,202	0
55	MG	DR	203	1/1	0.72	0.24	108,108,108,108	0
55	MG	CA	3021	1/1	0.72	0.35	182,182,182,182	0
55	MG	DA	3179	1/1	0.72	0.22	100,100,100,100	0
55	MG	AA	1601	1/1	0.72	0.59	100,100,100,100	0
55	MG	CA	3136	1/1	0.72	0.31	156,156,156,156	0
55	MG	CA	3117	1/1	0.72	0.28	85,85,85,85	0
55	MG	CA	3027	1/1	0.72	0.17	277,277,277,277	0
68	TRS	DA	3219	8/8	0.72	0.26	95,98,100,101	0
55	MG	AA	1614	1/1	0.73	0.31	126,126,126,126	0
55	MG	AA	1611	1/1	0.73	0.24	88,88,88,88	0
55	MG	CA	3062	1/1	0.73	0.22	196,196,196,196	0
55	MG	CA	3079	1/1	0.73	0.26	177,177,177,177	0
57	MPD	AA	1676	8/8	0.73	0.43	97,99,100,103	0
55	MG	DA	3147	1/1	0.73	0.36	98,98,98,98	0
55	MG	DA	3148	1/1	0.73	0.24	123,123,123,123	0
55	MG	AA	1617	1/1	0.73	0.38	93,93,93,93	0
67	GUN	DA	3210	11/11	0.73	0.19	66,68,71,71	0
55	MG	CA	3038	1/1	0.73	0.15	154,154,154,154	0
61	PEG	DQ	201	7/7	0.74	0.24	104,105,105,106	0
55	MG	DA	3167	1/1	0.74	0.33	80,80,80,80	0
55	MG	DB	209	1/1	0.74	0.35	87,87,87,87	0
66	ACY	DA	3196	4/4	0.74	0.27	79,80,80,80	0
55	MG	AA	1619	1/1	0.74	0.22	94,94,94,94	0
55	MG	AA	1679	1/1	0.74	0.19	163,163,163,163	0
58	PUT	AA	1672	6/6	0.75	0.42	98,98,100,101	0
55	MG	DA	3173	1/1	0.75	0.33	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3106	1/1	0.75	0.35	83,83,83,83	0
55	MG	DA	3124	1/1	0.75	0.44	102,102,102,102	0
55	MG	CA	3137	1/1	0.75	0.23	95,95,95,95	0
55	MG	CA	3008	1/1	0.75	0.22	244,244,244,244	0
55	MG	C3	101	1/1	0.75	0.37	299,299,299,299	0
55	MG	DA	3153	1/1	0.76	0.41	100,100,100,100	0
55	MG	DA	3182	1/1	0.76	0.25	65,65,65,65	0
55	MG	BA	1640	1/1	0.76	0.48	101,101,101,101	0
55	MG	BA	1625	1/1	0.76	0.28	231,231,231,231	0
55	MG	AA	1624	1/1	0.76	0.28	92,92,92,92	0
58	PUT	AA	1674	6/6	0.76	0.33	88,90,91,91	0
55	MG	DA	3063	1/1	0.77	0.14	219,219,219,219	0
55	MG	CA	3144	1/1	0.77	0.19	62,62,62,62	0
55	MG	CA	3053	1/1	0.77	0.10	134,134,134,134	0
55	MG	CA	3120	1/1	0.77	0.25	75,75,75,75	0
55	MG	CA	3070	1/1	0.77	0.10	188,188,188,188	0
61	PEG	DP	201	7/7	0.77	0.18	90,92,94,94	0
55	MG	BA	1639	1/1	0.78	0.26	88,88,88,88	0
55	MG	DA	3122	1/1	0.78	0.39	86,86,86,86	0
55	MG	BA	1644	1/1	0.78	0.14	87,87,87,87	0
62	EDO	DB	210	4/4	0.78	0.31	76,77,77,78	0
55	MG	DA	3163	1/1	0.78	0.28	76,76,76,76	0
55	MG	CB	203	1/1	0.78	0.12	146,146,146,146	0
55	MG	CA	3071	1/1	0.78	0.14	257,257,257,257	0
55	MG	DA	3171	1/1	0.78	0.17	83,83,83,83	0
55	MG	CA	3089	1/1	0.78	0.17	209,209,209,209	0
55	MG	CA	3077	1/1	0.79	0.19	189,189,189,189	0
55	MG	CA	3075	1/1	0.79	0.16	215,215,215,215	0
55	MG	CA	3081	1/1	0.79	0.24	153,153,153,153	0
55	MG	BA	1632	1/1	0.79	0.17	219,219,219,219	0
55	MG	DA	3134	1/1	0.80	0.14	65,65,65,65	0
57	MPD	DT	201	8/8	0.80	0.30	85,87,92,92	0
55	MG	AA	1615	1/1	0.80	0.31	81,81,81,81	0
55	MG	DA	3130	1/1	0.80	0.29	81,81,81,81	0
55	MG	CA	3112	1/1	0.81	0.41	77,77,77,77	0
55	MG	CA	3082	1/1	0.81	0.19	229,229,229,229	0
55	MG	CA	3115	1/1	0.81	0.39	76,76,76,76	0
61	PEG	DA	3217	7/7	0.81	0.35	92,95,99,99	0
55	MG	CA	3012	1/1	0.81	0.14	134,134,134,134	0
55	MG	AA	1647	1/1	0.81	0.14	201,201,201,201	0
55	MG	CA	3107	1/1	0.81	0.28	90,90,90,90	0
63	PGE	D3	101	10/10	0.81	0.24	82,83,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1630	1/1	0.81	0.13	124,124,124,124	0
55	MG	BA	1609	1/1	0.81	0.24	172,172,172,172	0
58	PUT	AA	1673	6/6	0.81	0.21	122,122,123,123	0
57	MPD	DA	3203	8/8	0.82	0.26	89,92,98,99	0
55	MG	DA	3143	1/1	0.82	0.37	93,93,93,93	0
55	MG	CA	3093	1/1	0.82	0.21	151,151,151,151	0
55	MG	DA	3146	1/1	0.82	0.16	73,73,73,73	0
58	PUT	AA	1675	6/6	0.82	0.22	82,83,84,84	0
59	TAC	BA	1602	32/32	0.82	0.16	170,172,172,172	0
55	MG	CA	3108	1/1	0.82	0.16	72,72,72,72	0
55	MG	AA	1610	1/1	0.82	0.37	97,97,97,97	0
55	MG	BA	1635	1/1	0.82	0.17	226,226,226,226	0
61	PEG	DA	3225	7/7	0.82	0.28	60,63,70,71	0
55	MG	DA	3126	1/1	0.82	0.23	70,70,70,70	0
56	PG4	DR	202	13/13	0.82	0.25	55,64,74,75	0
55	MG	CA	3083	1/1	0.82	0.14	209,209,209,209	0
55	MG	AA	1642	1/1	0.82	0.26	153,153,153,153	0
57	MPD	DE	302	8/8	0.82	0.30	92,94,95,96	0
55	MG	CA	3003	1/1	0.82	0.22	218,218,218,218	0
57	MPD	DT	202	8/8	0.82	0.32	88,89,90,92	0
60	ZN	AB	301	1/1	0.83	0.10	198,198,198,198	0
57	MPD	DK	201	8/8	0.83	0.19	91,92,94,95	0
57	MPD	DN	201	8/8	0.83	0.19	83,88,90,91	0
63	PGE	DU	101	10/10	0.83	0.19	62,68,78,78	0
55	MG	AA	1602	1/1	0.83	0.25	82,82,82,82	0
55	MG	CA	3056	1/1	0.83	0.14	119,119,119,119	0
55	MG	CA	3058	1/1	0.83	0.17	137,137,137,137	0
55	MG	CA	3148	1/1	0.84	0.42	80,80,80,80	0
55	MG	DA	3131	1/1	0.84	0.29	85,85,85,85	0
55	MG	AA	1636	1/1	0.84	0.15	103,103,103,103	0
55	MG	DA	3136	1/1	0.84	0.10	100,100,100,100	0
55	MG	CA	3142	1/1	0.84	0.20	85,85,85,85	0
55	MG	DA	3178	1/1	0.84	0.33	100,100,100,100	0
55	MG	DA	3161	1/1	0.84	0.23	69,69,69,69	0
62	EDO	DA	3003	4/4	0.84	0.34	47,49,50,50	0
55	MG	DA	3162	1/1	0.84	0.15	70,70,70,70	0
62	EDO	DA	3208	4/4	0.84	0.37	88,90,91,91	0
57	MPD	DA	3209	8/8	0.84	0.26	65,68,71,72	0
55	MG	DB	206	1/1	0.84	0.22	106,106,106,106	0
56	PG4	BA	1601	13/13	0.84	0.16	90,95,98,99	0
56	PG4	DQ	202	13/13	0.84	0.15	62,65,71,71	0
66	ACY	DA	3201	4/4	0.84	0.23	53,56,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3101	1/1	0.84	0.13	115,115,115,115	0
58	PUT	DA	3221	6/6	0.84	0.20	45,46,49,51	0
55	MG	CA	3011	1/1	0.85	0.16	120,120,120,120	0
57	MPD	DA	3206	8/8	0.85	0.24	93,94,95,95	0
61	PEG	AL	201	7/7	0.85	0.15	78,79,82,82	0
55	MG	AA	1623	1/1	0.85	0.18	74,74,74,74	0
55	MG	CA	3005	1/1	0.85	0.12	224,224,224,224	0
55	MG	AA	1621	1/1	0.85	0.38	88,88,88,88	0
55	MG	CA	3063	1/1	0.85	0.23	257,257,257,257	0
55	MG	DB	205	1/1	0.85	0.16	64,64,64,64	0
57	MPD	DA	3192	8/8	0.85	0.30	68,72,74,74	0
55	MG	DA	3135	1/1	0.86	0.29	73,73,73,73	0
55	MG	AA	1604	1/1	0.86	0.31	64,64,64,64	0
55	MG	DA	3128	1/1	0.86	0.30	73,73,73,73	0
63	PGE	DD	301	10/10	0.86	0.18	63,66,69,69	0
55	MG	CA	3017	1/1	0.86	0.15	124,124,124,124	0
55	MG	DA	3123	1/1	0.86	0.32	83,83,83,83	0
56	PG4	DA	3193	13/13	0.86	0.19	59,61,70,71	0
55	MG	DA	3133	1/1	0.86	0.23	70,70,70,70	0
55	MG	AA	1677	1/1	0.86	0.21	78,78,78,78	0
55	MG	CA	3057	1/1	0.87	0.11	128,128,128,128	0
55	MG	DA	3127	1/1	0.87	0.35	71,71,71,71	0
61	PEG	DA	3226	7/7	0.87	0.19	55,59,63,64	0
55	MG	DA	3175	1/1	0.87	0.25	85,85,85,85	0
55	MG	CA	3039	1/1	0.87	0.10	124,124,124,124	0
55	MG	DA	3129	1/1	0.87	0.50	69,69,69,69	0
62	EDO	DA	3207	4/4	0.87	0.29	57,58,59,59	0
55	MG	CA	3126	1/1	0.87	0.23	78,78,78,78	0
55	MG	DA	3166	1/1	0.87	0.23	92,92,92,92	0
59	TAC	AA	1678	32/32	0.87	0.13	64,73,81,82	0
55	MG	BA	1610	1/1	0.87	0.14	119,119,119,119	0
56	PG4	AA	1670	13/13	0.87	0.13	80,86,94,94	0
63	PGE	DA	3213	10/10	0.87	0.16	83,85,89,89	0
63	PGE	DA	3216	10/10	0.87	0.17	57,60,68,70	0
57	MPD	DA	3190	8/8	0.87	0.20	87,88,89,93	0
61	PEG	D3	102	7/7	0.87	0.52	73,79,82,82	0
55	MG	CA	3150	1/1	0.87	0.23	80,80,80,80	0
55	MG	AA	1660	1/1	0.87	0.20	275,275,275,275	0
58	PUT	DA	3195	6/6	0.88	0.26	49,55,59,60	0
55	MG	CA	3090	1/1	0.88	0.09	106,106,106,106	0
55	MG	DA	3181	1/1	0.88	0.15	58,58,58,58	0
55	MG	CA	3015	1/1	0.88	0.17	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3125	1/1	0.88	0.32	84,84,84,84	0
65	1PE	DA	3202	16/16	0.88	0.18	52,59,65,67	0
55	MG	BA	1618	1/1	0.88	0.16	144,144,144,144	0
55	MG	DA	3151	1/1	0.88	0.09	54,54,54,54	0
55	MG	CA	3022	1/1	0.88	0.12	142,142,142,142	0
55	MG	DA	3154	1/1	0.88	0.45	58,58,58,58	0
57	MPD	AA	1671	8/8	0.89	0.22	96,98,99,101	0
55	MG	DA	3170	1/1	0.89	0.15	80,80,80,80	0
62	EDO	DA	3214	4/4	0.89	0.19	74,74,74,75	0
55	MG	AA	1665	1/1	0.89	0.12	158,158,158,158	0
55	MG	CA	3065	1/1	0.89	0.12	119,119,119,119	0
55	MG	BA	1611	1/1	0.89	0.11	191,191,191,191	0
63	PGE	DS	201	10/10	0.89	0.11	61,66,67,68	0
55	MG	CA	3024	1/1	0.89	0.16	104,104,104,104	0
55	MG	DA	3138	1/1	0.89	0.31	80,80,80,80	0
55	MG	AA	1657	1/1	0.89	0.17	144,144,144,144	0
64	SPD	DA	3205	10/10	0.89	0.24	76,83,85,85	0
58	PUT	DA	3204	6/6	0.89	0.20	63,65,68,69	0
58	PUT	DA	3218	6/6	0.89	0.20	73,74,75,75	0
62	EDO	DA	3001	4/4	0.89	0.25	74,76,76,77	0
55	MG	DA	3132	1/1	0.89	0.31	66,66,66,66	0
56	PG4	DA	3215	13/13	0.89	0.18	91,98,100,100	0
56	PG4	DS	202	13/13	0.90	0.12	49,51,61,62	0
55	MG	CA	3152	1/1	0.90	0.19	87,87,87,87	0
55	MG	CA	3099	1/1	0.90	0.13	101,101,101,101	0
55	MG	CA	3100	1/1	0.90	0.07	135,135,135,135	0
62	EDO	DA	3194	4/4	0.90	0.20	60,61,62,63	0
62	EDO	DA	3197	4/4	0.90	0.16	66,66,67,67	0
62	EDO	DA	3198	4/4	0.90	0.20	53,55,55,55	0
55	MG	CA	3111	1/1	0.90	0.22	91,91,91,91	0
58	PUT	DA	3211	6/6	0.90	0.19	57,65,66,66	0
55	MG	DR	201	1/1	0.90	0.23	55,55,55,55	0
58	PUT	DA	3220	6/6	0.90	0.24	93,96,99,100	0
55	MG	AA	1618	1/1	0.90	0.47	81,81,81,81	0
55	MG	CA	3068	1/1	0.90	0.09	107,107,107,107	0
55	MG	AA	1627	1/1	0.90	0.28	88,88,88,88	0
55	MG	BA	1620	1/1	0.90	0.11	97,97,97,97	0
55	MG	CA	3092	1/1	0.90	0.09	113,113,113,113	0
55	MG	DA	3013	1/1	0.90	0.12	67,67,67,67	0
63	PGE	DA	3224	10/10	0.90	0.21	79,85,88,88	0
64	SPD	DA	3183	10/10	0.90	0.18	48,57,60,60	0
55	MG	DA	3027	1/1	0.90	0.22	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
65	1PE	DA	3185	16/16	0.90	0.14	42,50,62,64	0
55	MG	DA	3045	1/1	0.90	0.09	90,90,90,90	0
61	PEG	DA	3200	7/7	0.90	0.31	56,57,59,61	0
55	MG	DA	3164	1/1	0.90	0.25	75,75,75,75	0
55	MG	AA	1607	1/1	0.90	0.35	91,91,91,91	0
55	MG	AA	1612	1/1	0.90	0.18	65,65,65,65	0
61	PEG	DA	3199	7/7	0.91	0.23	62,66,69,69	0
58	PUT	DA	3189	6/6	0.91	0.15	38,44,47,47	0
55	MG	BA	1619	1/1	0.91	0.09	122,122,122,122	0
55	MG	DB	208	1/1	0.91	0.22	66,66,66,66	0
55	MG	DD	303	1/1	0.91	0.11	53,53,53,53	0
62	EDO	D1	101	4/4	0.91	0.12	63,64,67,70	0
55	MG	BA	1614	1/1	0.91	0.19	123,123,123,123	0
55	MG	CA	3047	1/1	0.91	0.08	94,94,94,94	0
55	MG	CA	3143	1/1	0.91	0.08	85,85,85,85	0
55	MG	DA	3177	1/1	0.91	0.35	84,84,84,84	0
64	SPD	DA	3223	10/10	0.91	0.18	39,42,46,46	0
55	MG	DA	3165	1/1	0.91	0.20	74,74,74,74	0
55	MG	CA	3135	1/1	0.91	0.22	90,90,90,90	0
55	MG	DA	3152	1/1	0.91	0.17	43,43,43,43	0
55	MG	DA	3112	1/1	0.91	0.31	291,291,291,291	0
55	MG	DA	3169	1/1	0.91	0.26	72,72,72,72	0
58	PUT	DA	3184	6/6	0.91	0.23	45,45,47,48	0
55	MG	DA	3160	1/1	0.92	0.10	56,56,56,56	0
55	MG	CA	3088	1/1	0.92	0.17	90,90,90,90	0
55	MG	DA	3142	1/1	0.92	0.21	73,73,73,73	0
62	EDO	DB	211	4/4	0.92	0.16	74,74,75,75	0
55	MG	CA	3029	1/1	0.92	0.10	113,113,113,113	0
55	MG	AA	1656	1/1	0.92	0.08	124,124,124,124	0
55	MG	CA	3019	1/1	0.92	0.08	102,102,102,102	0
55	MG	CA	3044	1/1	0.92	0.10	93,93,93,93	0
61	PEG	DL	201	7/7	0.92	0.13	69,70,71,71	0
55	MG	DA	3121	1/1	0.92	0.30	90,90,90,90	0
55	MG	AA	1620	1/1	0.92	0.14	67,67,67,67	0
55	MG	CA	3026	1/1	0.92	0.15	123,123,123,123	0
55	MG	CA	3034	1/1	0.92	0.26	144,144,144,144	0
55	MG	AA	1664	1/1	0.92	0.09	161,161,161,161	0
55	MG	CA	3087	1/1	0.92	0.08	91,91,91,91	0
55	MG	AA	1655	1/1	0.93	0.07	100,100,100,100	0
55	MG	BA	1616	1/1	0.93	0.13	136,136,136,136	0
55	MG	CA	3040	1/1	0.93	0.10	71,71,71,71	0
55	MG	CA	3073	1/1	0.93	0.12	197,197,197,197	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	CA	3023	1/1	0.93	0.08	134,134,134,134	0
55	MG	AA	1625	1/1	0.93	0.14	63,63,63,63	0
55	MG	AA	1633	1/1	0.93	0.07	110,110,110,110	0
55	MG	DA	3150	1/1	0.93	0.07	51,51,51,51	0
55	MG	DA	3005	1/1	0.93	0.09	69,69,69,69	0
55	MG	CA	3096	1/1	0.93	0.10	117,117,117,117	0
55	MG	CA	3048	1/1	0.93	0.07	92,92,92,92	0
55	MG	BA	1603	1/1	0.93	0.14	95,95,95,95	0
55	MG	DA	3158	1/1	0.93	0.10	55,55,55,55	0
55	MG	CA	3035	1/1	0.93	0.21	201,201,201,201	0
55	MG	DA	3065	1/1	0.93	0.30	59,59,59,59	0
55	MG	AA	1658	1/1	0.93	0.09	83,83,83,83	0
55	MG	DA	3118	1/1	0.93	0.12	65,65,65,65	0
55	MG	CA	3028	1/1	0.93	0.21	172,172,172,172	0
61	PEG	D1	103	7/7	0.93	0.22	57,60,61,63	0
55	MG	AA	1649	1/1	0.94	0.06	58,58,58,58	0
58	PUT	DA	3222	6/6	0.94	0.16	46,49,51,52	0
55	MG	AA	1613	1/1	0.94	0.38	68,68,68,68	0
55	MG	CA	3016	1/1	0.94	0.06	106,106,106,106	0
55	MG	CA	3049	1/1	0.94	0.09	81,81,81,81	0
55	MG	CB	202	1/1	0.94	0.11	128,128,128,128	0
55	MG	DA	3141	1/1	0.94	0.14	82,82,82,82	0
64	SPD	DA	3187	10/10	0.94	0.15	32,35,43,46	0
58	PUT	DA	3188	6/6	0.94	0.10	30,31,33,39	0
55	MG	CA	3097	1/1	0.94	0.10	110,110,110,110	0
55	MG	DA	3099	1/1	0.94	0.07	81,81,81,81	0
55	MG	CA	3018	1/1	0.94	0.08	78,78,78,78	0
66	ACY	DA	3191	4/4	0.94	0.11	55,55,56,57	0
55	MG	BA	1636	1/1	0.94	0.10	112,112,112,112	0
58	PUT	DA	3212	6/6	0.94	0.32	47,53,59,60	0
55	MG	CA	3064	1/1	0.94	0.10	107,107,107,107	0
55	MG	AA	1632	1/1	0.94	0.12	110,110,110,110	0
55	MG	BA	1637	1/1	0.95	0.08	99,99,99,99	0
55	MG	CB	201	1/1	0.95	0.08	157,157,157,157	0
55	MG	CA	3042	1/1	0.95	0.09	92,92,92,92	0
55	MG	DA	3144	1/1	0.95	0.09	65,65,65,65	0
55	MG	CA	3095	1/1	0.95	0.07	112,112,112,112	0
55	MG	BA	1628	1/1	0.95	0.12	97,97,97,97	0
55	MG	CA	3080	1/1	0.95	0.07	120,120,120,120	0
55	MG	CA	3045	1/1	0.95	0.08	142,142,142,142	0
55	MG	DA	3149	1/1	0.95	0.32	66,66,66,66	0
55	MG	CA	3069	1/1	0.95	0.05	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3038	1/1	0.95	0.12	27,27,27,27	0
55	MG	DA	3043	1/1	0.95	0.07	34,34,34,34	0
55	MG	AA	1635	1/1	0.95	0.07	96,96,96,96	0
55	MG	DA	3053	1/1	0.95	0.09	78,78,78,78	0
55	MG	DA	3156	1/1	0.95	0.30	74,74,74,74	0
55	MG	DA	3157	1/1	0.95	0.17	69,69,69,69	0
55	MG	BA	1623	1/1	0.95	0.19	37,37,37,37	0
55	MG	AA	1634	1/1	0.95	0.08	106,106,106,106	0
55	MG	DA	3081	1/1	0.95	0.09	94,94,94,94	0
55	MG	DA	3097	1/1	0.95	0.08	45,45,45,45	0
55	MG	AA	1639	1/1	0.95	0.08	120,120,120,120	0
55	MG	DA	3137	1/1	0.95	0.19	55,55,55,55	0
55	MG	DA	3100	1/1	0.95	0.07	34,34,34,34	0
55	MG	BA	1607	1/1	0.95	0.07	118,118,118,118	0
55	MG	DA	3230	1/1	0.96	0.09	37,37,37,37	0
55	MG	CA	3085	1/1	0.96	0.14	82,82,82,82	0
55	MG	AA	1651	1/1	0.96	0.07	68,68,68,68	0
55	MG	BA	1633	1/1	0.96	0.05	57,57,57,57	0
55	MG	BA	1613	1/1	0.96	0.06	54,54,54,54	0
55	MG	DA	3140	1/1	0.96	0.07	43,43,43,43	0
55	MG	DA	3114	1/1	0.96	0.14	59,59,59,59	0
55	MG	DA	3006	1/1	0.96	0.05	60,60,60,60	0
55	MG	CA	3113	1/1	0.96	0.19	57,57,57,57	0
55	MG	DA	3016	1/1	0.96	0.07	62,62,62,62	0
55	MG	AA	1669	1/1	0.96	0.07	109,109,109,109	0
55	MG	DA	3029	1/1	0.96	0.07	49,49,49,49	0
55	MG	DA	3036	1/1	0.96	0.08	41,41,41,41	0
60	ZN	C5	101	1/1	0.96	0.06	139,139,139,139	0
63	PGE	DA	3186	10/10	0.96	0.10	29,33,36,37	0
55	MG	CA	3102	1/1	0.96	0.07	115,115,115,115	0
57	MPD	DS	203	8/8	0.96	0.14	36,40,42,44	0
55	MG	CA	3050	1/1	0.96	0.07	102,102,102,102	0
55	MG	CA	3051	1/1	0.96	0.05	82,82,82,82	0
55	MG	DA	3174	1/1	0.96	0.13	79,79,79,79	0
55	MG	BA	1621	1/1	0.96	0.09	103,103,103,103	0
55	MG	CA	3094	1/1	0.96	0.09	73,73,73,73	0
55	MG	BA	1604	1/1	0.96	0.05	99,99,99,99	0
55	MG	DA	3080	1/1	0.96	0.08	105,105,105,105	0
55	MG	DA	3155	1/1	0.96	0.32	71,71,71,71	0
55	MG	BA	1624	1/1	0.96	0.06	97,97,97,97	0
55	MG	DA	3084	1/1	0.96	0.08	44,44,44,44	0
55	MG	DA	3091	1/1	0.96	0.06	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3227	1/1	0.96	0.08	52,52,52,52	0
55	MG	CA	3084	1/1	0.97	0.05	75,75,75,75	0
55	MG	BA	1615	1/1	0.97	0.09	70,70,70,70	0
55	MG	CA	3086	1/1	0.97	0.05	93,93,93,93	0
55	MG	AA	1640	1/1	0.97	0.05	61,61,61,61	0
55	MG	AA	1641	1/1	0.97	0.07	81,81,81,81	0
55	MG	DA	3007	1/1	0.97	0.08	111,111,111,111	0
55	MG	DA	3009	1/1	0.97	0.10	89,89,89,89	0
55	MG	CA	3078	1/1	0.97	0.08	134,134,134,134	0
55	MG	DA	3096	1/1	0.97	0.12	51,51,51,51	0
58	PUT	DA	3002	6/6	0.97	0.11	39,41,44,47	0
55	MG	DD	302	1/1	0.97	0.05	53,53,53,53	0
55	MG	AA	1663	1/1	0.97	0.06	76,76,76,76	0
55	MG	BA	1612	1/1	0.97	0.07	101,101,101,101	0
55	MG	AA	1638	1/1	0.97	0.06	94,94,94,94	0
55	MG	CA	3014	1/1	0.97	0.18	71,71,71,71	0
55	MG	AA	1644	1/1	0.97	0.10	83,83,83,83	0
55	MG	DA	3120	1/1	0.97	0.14	48,48,48,48	0
55	MG	AA	1643	1/1	0.98	0.04	64,64,64,64	0
55	MG	DA	3068	1/1	0.98	0.07	67,67,67,67	0
55	MG	DA	3073	1/1	0.98	0.05	45,45,45,45	0
55	MG	DA	3074	1/1	0.98	0.05	32,32,32,32	0
55	MG	DA	3076	1/1	0.98	0.04	25,25,25,25	0
55	MG	AA	1637	1/1	0.98	0.04	49,49,49,49	0
55	MG	AA	1645	1/1	0.98	0.04	48,48,48,48	0
55	MG	DA	3083	1/1	0.98	0.04	60,60,60,60	0
55	MG	AA	1667	1/1	0.98	0.07	51,51,51,51	0
55	MG	DA	3086	1/1	0.98	0.03	41,41,41,41	0
55	MG	DA	3090	1/1	0.98	0.06	21,21,21,21	0
55	MG	CA	3052	1/1	0.98	0.14	96,96,96,96	0
55	MG	DA	3095	1/1	0.98	0.10	38,38,38,38	0
55	MG	CA	3010	1/1	0.98	0.09	99,99,99,99	0
55	MG	DA	3017	1/1	0.98	0.09	56,56,56,56	0
55	MG	DA	3022	1/1	0.98	0.06	50,50,50,50	0
55	MG	CA	3041	1/1	0.98	0.07	90,90,90,90	0
55	MG	DA	3102	1/1	0.98	0.04	52,52,52,52	0
55	MG	DA	3108	1/1	0.98	0.04	39,39,39,39	0
55	MG	AA	1652	1/1	0.98	0.17	40,40,40,40	0
55	MG	DA	3032	1/1	0.98	0.05	34,34,34,34	0
55	MG	DA	3033	1/1	0.98	0.05	19,19,19,19	0
55	MG	DB	204	1/1	0.98	0.04	65,65,65,65	0
55	MG	CA	3043	1/1	0.98	0.08	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3041	1/1	0.98	0.04	50,50,50,50	0
55	MG	DA	3042	1/1	0.98	0.11	28,28,28,28	0
60	ZN	D5	101	1/1	0.98	0.03	55,55,55,55	0
55	MG	BA	1622	1/1	0.98	0.06	82,82,82,82	0
55	MG	AA	1653	1/1	0.98	0.04	81,81,81,81	0
55	MG	DA	3049	1/1	0.98	0.05	31,31,31,31	0
55	MG	DA	3050	1/1	0.98	0.04	35,35,35,35	0
55	MG	DA	3052	1/1	0.98	0.05	33,33,33,33	0
55	MG	AA	1646	1/1	0.98	0.04	53,53,53,53	0
55	MG	BA	1634	1/1	0.98	0.06	66,66,66,66	0
55	MG	DA	3064	1/1	0.98	0.10	63,63,63,63	0
55	MG	DA	3044	1/1	0.99	0.06	36,36,36,36	0
55	MG	DA	3098	1/1	0.99	0.03	39,39,39,39	0
55	MG	DA	3011	1/1	0.99	0.07	24,24,24,24	0
55	MG	DA	3046	1/1	0.99	0.07	47,47,47,47	0
55	MG	DA	3101	1/1	0.99	0.02	30,30,30,30	0
55	MG	DA	3012	1/1	0.99	0.04	39,39,39,39	0
55	MG	DA	3103	1/1	0.99	0.04	46,46,46,46	0
55	MG	DA	3104	1/1	0.99	0.02	59,59,59,59	0
55	MG	DA	3105	1/1	0.99	0.06	31,31,31,31	0
55	MG	DA	3106	1/1	0.99	0.06	32,32,32,32	0
55	MG	DB	201	1/1	0.99	0.10	63,63,63,63	0
55	MG	DA	3109	1/1	0.99	0.04	29,29,29,29	0
55	MG	DA	3111	1/1	0.99	0.06	38,38,38,38	0
55	MG	DA	3015	1/1	0.99	0.02	17,17,17,17	0
55	MG	DB	203	1/1	0.99	0.03	37,37,37,37	0
55	MG	DA	3115	1/1	0.99	0.06	35,35,35,35	0
55	MG	DA	3116	1/1	0.99	0.07	45,45,45,45	0
55	MG	DA	3054	1/1	0.99	0.03	47,47,47,47	0
55	MG	DA	3119	1/1	0.99	0.05	53,53,53,53	0
55	MG	DA	3055	1/1	0.99	0.09	55,55,55,55	0
55	MG	DA	3056	1/1	0.99	0.06	39,39,39,39	0
55	MG	DA	3057	1/1	0.99	0.04	49,49,49,49	0
55	MG	DA	3061	1/1	0.99	0.03	19,19,19,19	0
55	MG	DA	3062	1/1	0.99	0.02	33,33,33,33	0
55	MG	AA	1662	1/1	0.99	0.07	84,84,84,84	0
55	MG	DA	3021	1/1	0.99	0.04	55,55,55,55	0
55	MG	BA	1630	1/1	0.99	0.05	101,101,101,101	0
55	MG	DA	3229	1/1	0.99	0.03	38,38,38,38	0
55	MG	DA	3066	1/1	0.99	0.03	22,22,22,22	0
55	MG	DA	3023	1/1	0.99	0.08	27,27,27,27	0
55	MG	DA	3069	1/1	0.99	0.04	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	DA	3070	1/1	0.99	0.12	54,54,54,54	0
55	MG	DA	3071	1/1	0.99	0.05	90,90,90,90	0
55	MG	AA	1629	1/1	0.99	0.05	82,82,82,82	0
55	MG	DA	3028	1/1	0.99	0.03	41,41,41,41	0
55	MG	DA	3075	1/1	0.99	0.06	39,39,39,39	0
55	MG	AA	1650	1/1	0.99	0.04	75,75,75,75	0
55	MG	DA	3077	1/1	0.99	0.02	22,22,22,22	0
55	MG	DA	3078	1/1	0.99	0.04	32,32,32,32	0
55	MG	DA	3079	1/1	0.99	0.07	76,76,76,76	0
55	MG	AA	1659	1/1	0.99	0.03	73,73,73,73	0
55	MG	AA	1666	1/1	0.99	0.03	54,54,54,54	0
55	MG	DA	3082	1/1	0.99	0.03	57,57,57,57	0
55	MG	AA	1631	1/1	0.99	0.04	60,60,60,60	0
55	MG	DA	3037	1/1	0.99	0.06	26,26,26,26	0
55	MG	DA	3085	1/1	0.99	0.07	45,45,45,45	0
55	MG	DM	201	1/1	0.99	0.05	55,55,55,55	0
55	MG	DA	3087	1/1	0.99	0.04	45,45,45,45	0
55	MG	DA	3088	1/1	0.99	0.04	56,56,56,56	0
55	MG	DA	3089	1/1	0.99	0.03	46,46,46,46	0
55	MG	DA	3040	1/1	0.99	0.05	30,30,30,30	0
55	MG	AA	1648	1/1	0.99	0.04	63,63,63,63	0
55	MG	DA	3092	1/1	0.99	0.03	18,18,18,18	0
55	MG	DA	3093	1/1	0.99	0.04	31,31,31,31	0
55	MG	DA	3094	1/1	0.99	0.04	25,25,25,25	0
55	MG	DA	3008	1/1	0.99	0.04	73,73,73,73	0
55	MG	BA	1645	1/1	0.99	0.06	87,87,87,87	0
55	MG	DA	3020	1/1	1.00	0.17	11,11,11,11	0
55	MG	DA	3034	1/1	1.00	0.02	29,29,29,29	0
55	MG	DA	3035	1/1	1.00	0.04	20,20,20,20	0
55	MG	DB	202	1/1	1.00	0.06	33,33,33,33	0
55	MG	DA	3014	1/1	1.00	0.08	24,24,24,24	0
55	MG	DA	3010	1/1	1.00	0.04	24,24,24,24	0
55	MG	DA	3058	1/1	1.00	0.08	37,37,37,37	0
55	MG	DA	3107	1/1	1.00	0.07	39,39,39,39	0
55	MG	DA	3059	1/1	1.00	0.05	32,32,32,32	0
55	MG	DA	3060	1/1	1.00	0.02	29,29,29,29	0
55	MG	DA	3110	1/1	1.00	0.02	20,20,20,20	0
55	MG	DA	3039	1/1	1.00	0.04	27,27,27,27	0
55	MG	DA	3024	1/1	1.00	0.08	42,42,42,42	0
55	MG	DA	3113	1/1	1.00	0.04	25,25,25,25	0
55	MG	DA	3025	1/1	1.00	0.06	26,26,26,26	0
55	MG	DA	3026	1/1	1.00	0.03	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	MG	AA	1668	1/1	1.00	0.06	40,40,40,40	0
55	MG	DA	3117	1/1	1.00	0.08	32,32,32,32	0
55	MG	BA	1617	1/1	1.00	0.04	65,65,65,65	0
55	MG	DA	3067	1/1	1.00	0.02	51,51,51,51	0
55	MG	DA	3018	1/1	1.00	0.03	29,29,29,29	0
55	MG	DA	3030	1/1	1.00	0.02	14,14,14,14	0
55	MG	DA	3047	1/1	1.00	0.04	34,34,34,34	0
55	MG	DA	3048	1/1	1.00	0.02	47,47,47,47	0
55	MG	DA	3072	1/1	1.00	0.08	49,49,49,49	0
55	MG	DA	3031	1/1	1.00	0.02	35,35,35,35	0
55	MG	DA	3019	1/1	1.00	0.04	47,47,47,47	0
55	MG	DA	3051	1/1	1.00	0.03	24,24,24,24	0
55	MG	DA	3228	1/1	1.00	0.02	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.