



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 4, 2025 – 08:32 AM EST

PDB ID : 5J8A
Title : Structure of the E coli 70S ribosome with the U1052G mutation in 16S rRNA bound to tigecycline
Authors : Cocozaki, A.; Ferguson, A.
Deposited on : 2016-04-07
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-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

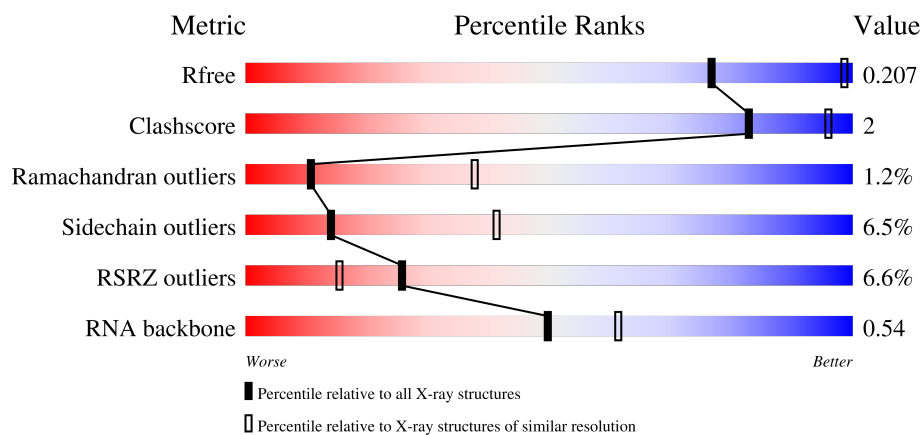
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)
RNA backbone	3690	1021 (3.36-2.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1534	<div> <div>5%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
1	BA	1534	<div> <div>5%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
2	AB	224	<div> <div>3%</div> <div>88%</div> <div>12%</div> <div>.</div> </div>
2	BB	224	<div> <div>6%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	AC	206	<div> <div>3%</div> <div>85%</div> <div>15%</div> </div>
3	BC	206	<div> <div>5%</div> <div>83%</div> <div>17%</div> </div>
4	AD	205	<div> <div>90%</div> <div>10%</div> </div>
4	BD	205	<div> <div>87%</div> <div>13%</div> </div>
5	AE	155	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
5	BE	155	<div> <div>3%</div> <div>71%</div> <div>20%</div> <div>5%</div> <div>..</div> </div>
6	AF	106	<div> <div>84%</div> <div>16%</div> </div>
6	BF	106	<div> <div>3%</div> <div>75%</div> <div>19%</div> <div>6%</div> </div>
7	AG	151	<div> <div>10%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
7	BG	151	<div> <div>19%</div> <div>87%</div> <div>13%</div> </div>
8	AH	129	<div> <div>2%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
8	BH	129	<div> <div>5%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
9	AI	127	<div> <div>9%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
9	BI	127	<div> <div>20%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
10	AJ	99	<div> <div>17%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
10	BJ	99	<div> <div>26%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>
11	AK	117	<div> <div>3%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
11	BK	117	<div> <div>8%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
12	AL	123	<div> <div>%</div> <div>89%</div> <div>11%</div> <div>.</div> </div>
12	BL	123	<div> <div>8%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
13	AM	114	<div> <div>18%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
13	BM	114	<div> <div>10%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>
14	AN	100	<div> <div>23%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
14	BN	100	<div> <div>11%</div> <div>92%</div> <div>8%</div> </div>
15	AO	88	<div> <div>94%</div> <div>6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	BO	88	
16	AP	82	
16	BP	82	
17	AQ	80	
17	BQ	80	
18	AR	55	
18	BR	55	
19	AS	79	
19	BS	79	
20	AT	86	
20	BT	86	
21	AU	56	
21	BU	56	
22	C1	56	
22	D1	56	
23	C2	51	
23	D2	51	
24	C3	46	
24	D3	46	
25	C4	64	
25	D4	64	
26	C5	38	
26	D5	38	
27	C0	58	
27	D0	58	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	CB	120	
28	DB	120	
29	CC	272	
29	DC	272	
30	CD	209	
31	CA	2904	
32	DD	209	
33	CE	201	
33	DE	201	
34	CF	178	
34	DF	178	
35	CG	176	
35	DG	176	
36	CH	149	
36	DH	149	
37	CJ	135	
37	DJ	135	
38	CK	142	
38	DK	142	
39	CL	123	
39	DL	123	
40	CM	144	
40	DM	144	
41	CN	136	
41	DN	136	


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
42	CO	125	<div> <div>24%</div> <div>80%</div> <div>14%</div> <div>• •</div> </div>
42	DO	125	<div> <div>88%</div> <div>12%</div> </div>
43	CP	117	<div> <div>9%</div> <div>87%</div> <div>10%</div> <div>• •</div> </div>
43	DP	117	<div> <div>91%</div> <div>6%</div> <div>•</div> </div>
44	CQ	114	<div> <div>10%</div> <div>89%</div> <div>10%</div> <div>•</div> </div>
44	DQ	114	<div> <div>%</div> <div>88%</div> <div>11%</div> <div>•</div> </div>
45	CR	117	<div> <div>19%</div> <div>85%</div> <div>15%</div> </div>
45	DR	117	<div> <div>86%</div> <div>14%</div> </div>
46	CS	103	<div> <div>14%</div> <div>84%</div> <div>14%</div> <div>• •</div> </div>
46	DS	103	<div> <div>2%</div> <div>94%</div> <div>6%</div> </div>
47	CT	110	<div> <div>21%</div> <div>79%</div> <div>21%</div> </div>
47	DT	110	<div> <div>85%</div> <div>15%</div> </div>
48	CU	93	<div> <div>24%</div> <div>83%</div> <div>15%</div> <div>•</div> </div>
48	DU	93	<div> <div>4%</div> <div>90%</div> <div>10%</div> </div>
49	CV	103	<div> <div>31%</div> <div>81%</div> <div>17%</div> <div>• •</div> </div>
49	DV	103	<div> <div>3%</div> <div>84%</div> <div>14%</div> <div>• •</div> </div>
50	CW	94	<div> <div>5%</div> <div>86%</div> <div>14%</div> </div>
50	DW	94	<div> <div>88%</div> <div>12%</div> </div>
51	CX	83	<div> <div>10%</div> <div>82%</div> <div>8%</div> <div>10%</div> </div>
51	DX	83	<div> <div>%</div> <div>83%</div> <div>7%</div> <div>• 8%</div> </div>
52	CY	77	<div> <div>12%</div> <div>87%</div> <div>13%</div> </div>
52	DY	77	<div> <div>%</div> <div>91%</div> <div>9%</div> </div>
53	CZ	62	<div> <div>10%</div> <div>92%</div> <div>8%</div> </div>
53	DZ	62	<div> <div>3%</div> <div>95%</div> <div>5%</div> </div>
54	DI	135	<div> <div>18%</div> <div>69%</div> <div>27%</div> <div>•</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	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
56	MG	BA	1640	-	-	-	X
56	MG	CA	3021	-	-	-	X
56	MG	CA	3122	-	-	-	X
56	MG	CA	3147	-	-	-	X
56	MG	CA	3148	-	-	-	X
59	PUT	AA	1672	-	-	-	X
67	ACY	DA	3196	-	X	-	-

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 295207 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
			32933	14695	6044	10660	1534			
1	BA	1533	Total	C	N	O	P	0	0	0
			32911	14685	6039	10654	1533			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1052	G	U	engineered mutation	GB 675819282
BA	1052	G	U	engineered mutation	GB 675819282

- 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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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
			2082	1288	423	364	7			
29	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	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			

- 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			

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	DD	209	Total	C	N	O	S	0	1	0
			1576	986	290	296	4			

- Molecule 33 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
33	DE	201	Total	C	N	O	S	0	0	0
			1551	974	283	289	5			

- Molecule 34 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
34	DF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 35 is a protein called 50S ribosomal protein L6.

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

- Molecule 36 is a protein called 50S ribosomal protein L9.

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

- Molecule 37 is a protein called 50S ribosomal protein L11.

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

Continued on next page...

Continued from previous page...

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

- Molecule 38 is a protein called 50S ribosomal protein L13.

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

- Molecule 39 is a protein called 50S ribosomal protein L14.

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

- Molecule 40 is a protein called 50S ribosomal protein L15.

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

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CN	136	Total	C	N	O	S	0	0	0
			1075	686	205	178	6			
41	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	conflict	UNP P0ADY7
DN	81	4D4	ARG	conflict	UNP P0ADY7

- Molecule 42 is a protein called 50S ribosomal protein L17.

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

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L19.

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

- Molecule 45 is a protein called 50S ribosomal protein L20.

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

- Molecule 46 is a protein called 50S ribosomal protein L21.

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

- Molecule 47 is a protein called 50S ribosomal protein L22.

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

Continued on next page...

Continued from previous page...

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

- Molecule 48 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	CU	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
48	DU	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CV	102	Total	C	N	O	S	0	0	0
			779	492	146	141				
49	DV	102	Total	C	N	O	S	0	0	0
			779	492	146	141				

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

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

- Molecule 51 is a protein called 50S ribosomal protein L27.

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

- Molecule 52 is a protein called 50S ribosomal protein L28.

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

- Molecule 53 is a protein called 50S ribosomal protein L29.

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

- Molecule 54 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	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 55 is a RNA chain called 23S rRNA.

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

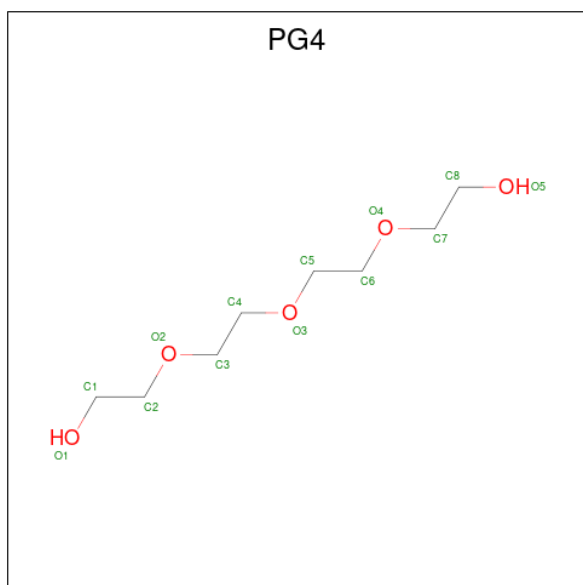
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	72	Total	Mg	0	0
			72	72		
56	BA	45	Total	Mg	0	0
			45	45		
56	CB	3	Total	Mg	0	0
			3	3		
56	CA	156	Total	Mg	0	0
			156	156		
56	DD	1	Total	Mg	0	0
			1	1		
56	DM	1	Total	Mg	0	0
			1	1		
56	DR	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

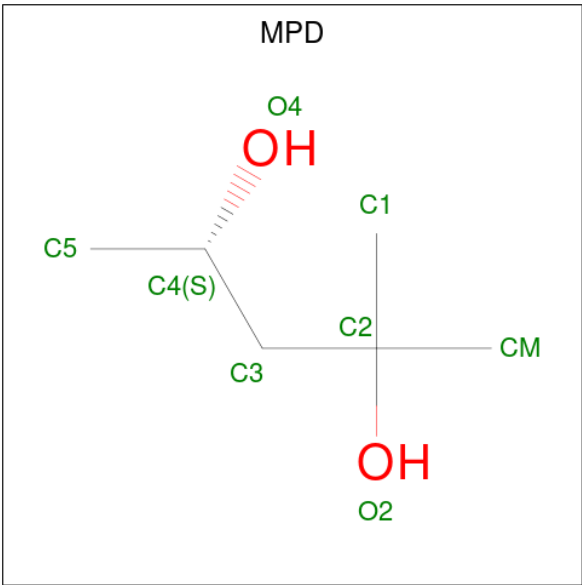
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DB	9	Total	Mg	0	0
			9	9		
56	DA	184	Total	Mg	0	0
			184	184		

- Molecule 57 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



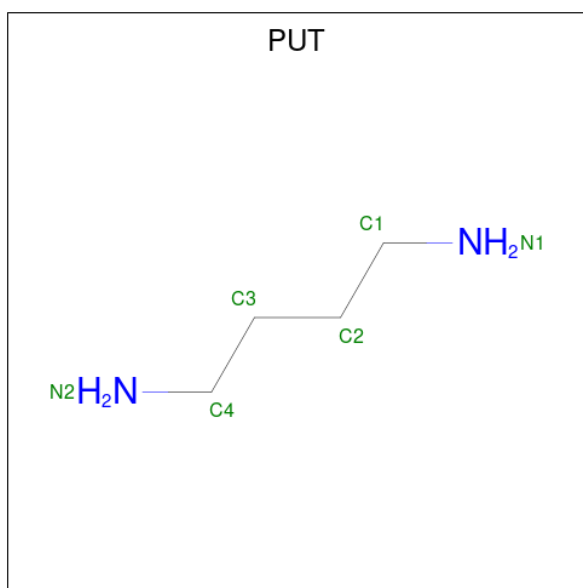
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		

- Molecule 58 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	AA	1	Total	C	O	0	0
			8	6	2		
58	AA	1	Total	C	O	0	0
			8	6	2		
58	DE	1	Total	C	O	0	0
			8	6	2		
58	DE	1	Total	C	O	0	0
			8	6	2		
58	DK	1	Total	C	O	0	0
			8	6	2		
58	DN	1	Total	C	O	0	0
			8	6	2		
58	DS	1	Total	C	O	0	0
			8	6	2		
58	DT	1	Total	C	O	0	0
			8	6	2		
58	DT	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		
58	DA	1	Total	C	O	0	0
			8	6	2		

- Molecule 59 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



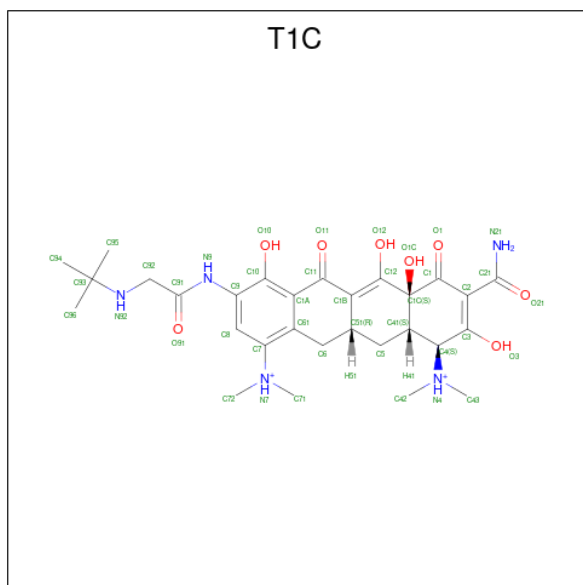
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6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

Continued on next page...

Continued from previous page...

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

- Molecule 60 is TIGECYCLINE (three-letter code: T1C) (formula: $C_{29}H_{41}N_5O_8$).



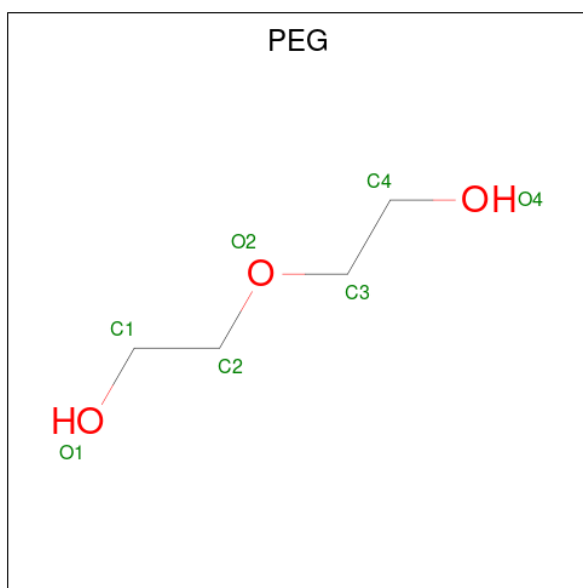
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
60	AA	1	Total	C	N	O	0	0
			42	29	5	8		
60	BA	1	Total	C	N	O	0	0
			42	29	5	8		

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

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

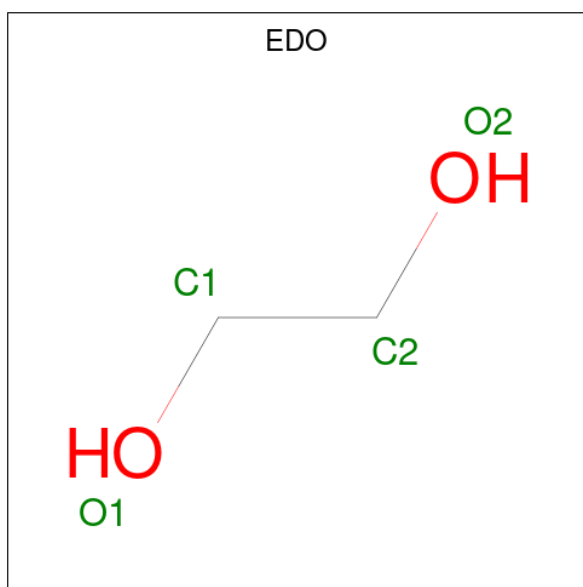
- Molecule 62 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:

C₄H₁₀O₃).



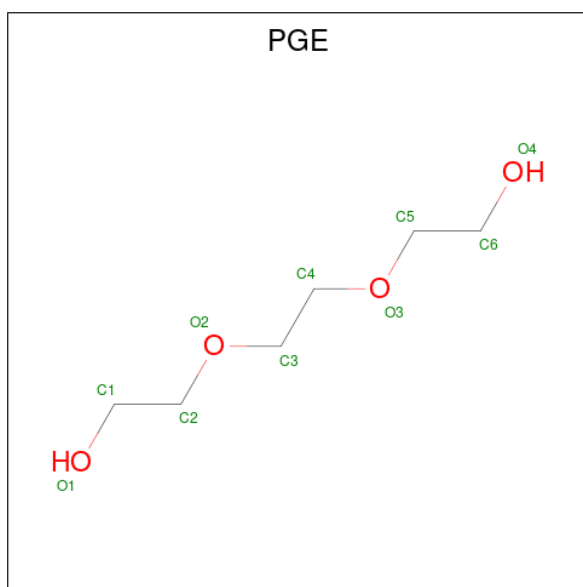
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	AL	1	Total	C	O	0	0
			7	4	3		
62	D1	1	Total	C	O	0	0
			7	4	3		
62	D3	1	Total	C	O	0	0
			7	4	3		
62	DL	1	Total	C	O	0	0
			7	4	3		
62	DP	1	Total	C	O	0	0
			7	4	3		
62	DQ	1	Total	C	O	0	0
			7	4	3		
62	DA	1	Total	C	O	0	0
			7	4	3		
62	DA	1	Total	C	O	0	0
			7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

- Molecule 63 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



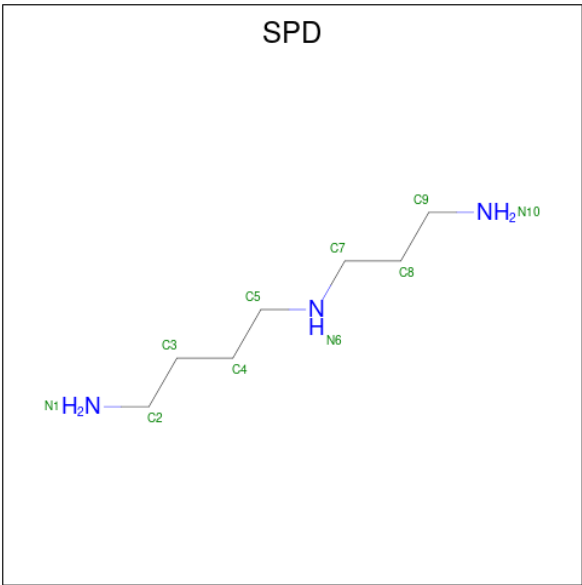
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			4	2	2		
63	DB	1	Total	C	O	0	0
			4	2	2		
63	DB	1	Total	C	O	0	0
			4	2	2		
63	DB	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4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

- Molecule 64 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



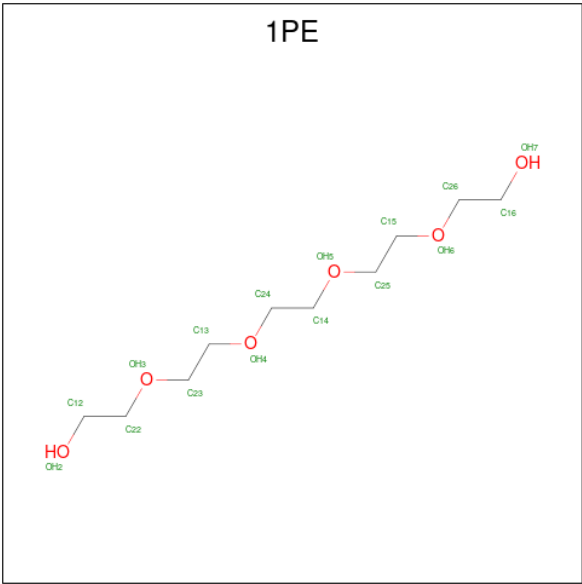
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	D1	1	Total	C	O	0	0
			10	6	4		
64	D3	1	Total	C	O	0	0
			10	6	4		
64	DS	1	Total	C	O	0	0
			10	6	4		
64	DU	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0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

- Molecule 65 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



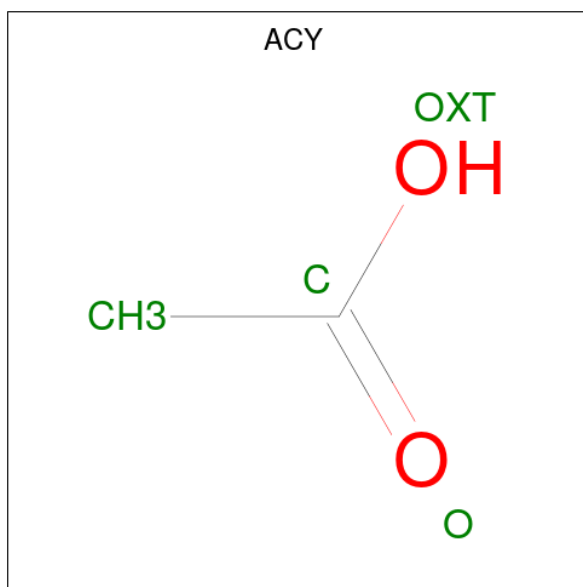
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	N	0	0
			10	7	3		
65	DA	1	Total	C	N	0	0
			10	7	3		
65	DA	1	Total	C	N	0	0
			10	7	3		
65	DA	1	Total	C	N	0	0
			10	7	3		

- Molecule 66 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



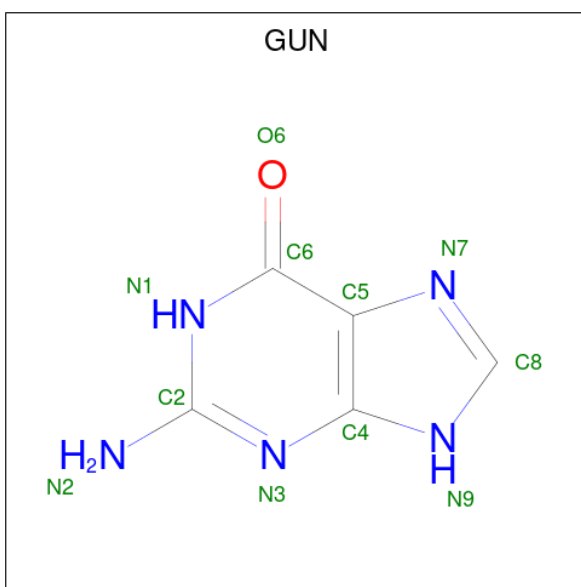
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			16	10	6		
66	DA	1	Total	C	O	0	0
			16	10	6		

- Molecule 67 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



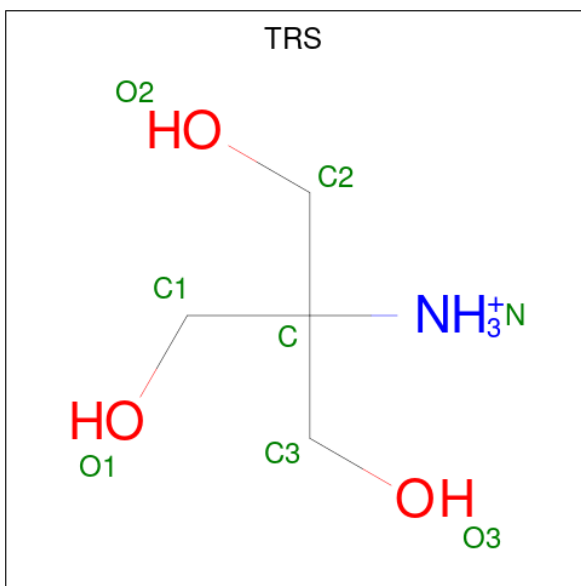
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
67	DA	1	Total	C	O	0	0
			4	2	2		
67	DA	1	Total	C	O	0	0
			4	2	2		
67	DA	1	Total	C	O	0	0
			4	2	2		

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



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

- Molecule 69 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
69	DA	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 70 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
70	AA	500	Total 500	O 500	0	0
70	AC	5	Total 5	O 5	0	0
70	AD	2	Total 2	O 2	0	0
70	AE	4	Total 4	O 4	0	0
70	AF	1	Total 1	O 1	0	0
70	AG	1	Total 1	O 1	0	0
70	AH	1	Total 1	O 1	0	0
70	AJ	2	Total 2	O 2	0	0
70	AK	6	Total 6	O 6	0	0
70	AL	10	Total 10	O 10	0	0
70	AM	4	Total 4	O 4	0	0
70	AN	7	Total 7	O 7	0	0
70	AO	2	Total 2	O 2	0	0
70	AP	2	Total 2	O 2	0	0
70	AR	1	Total 1	O 1	0	0
70	AT	3	Total 3	O 3	0	0
70	AU	2	Total 2	O 2	0	0
70	C3	3	Total 3	O 3	0	0
70	C4	1	Total 1	O 1	0	0
70	BA	288	Total 288	O 288	0	0
70	BD	12	Total 12	O 12	0	0
70	BE	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
70	BF	2	Total	O	0	0
			2	2		
70	BK	2	Total	O	0	0
			2	2		
70	BL	2	Total	O	0	0
			2	2		
70	BN	2	Total	O	0	0
			2	2		
70	BO	1	Total	O	0	0
			1	1		
70	BP	3	Total	O	0	0
			3	3		
70	BT	4	Total	O	0	0
			4	4		
70	BU	1	Total	O	0	0
			1	1		
70	D1	45	Total	O	0	0
			45	45		
70	D2	7	Total	O	0	0
			7	7		
70	D3	23	Total	O	0	0
			23	23		
70	D4	39	Total	O	0	0
			39	39		
70	D5	12	Total	O	0	0
			12	12		
70	D0	21	Total	O	0	0
			21	21		
70	CB	13	Total	O	0	0
			13	13		
70	CC	12	Total	O	0	0
			12	12		
70	CD	6	Total	O	0	0
			6	6		
70	CA	692	Total	O	0	0
			692	692		
70	DC	104	Total	O	0	0
			104	104		
70	DD	92	Total	O	0	0
			92	92		
70	CE	4	Total	O	0	0
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
70	CL	1	Total 1	O 1	0	0
70	CM	4	Total 4	O 4	0	0
70	CO	1	Total 1	O 1	0	0
70	CU	3	Total 3	O 3	0	0
70	CV	1	Total 1	O 1	0	0
70	CW	1	Total 1	O 1	0	0
70	CY	1	Total 1	O 1	0	0
70	DE	60	Total 60	O 60	0	0
70	DF	15	Total 15	O 15	0	0
70	DG	6	Total 6	O 6	0	0
70	DH	2	Total 2	O 2	0	0
70	DK	64	Total 64	O 64	0	0
70	DL	51	Total 51	O 51	0	0
70	DM	64	Total 64	O 64	0	0
70	DN	73	Total 73	O 73	0	0
70	DO	46	Total 46	O 46	0	0
70	DP	40	Total 40	O 40	0	0
70	DQ	32	Total 32	O 32	0	0
70	DR	63	Total 63	O 63	0	0
70	DS	44	Total 44	O 44	0	0
70	DT	69	Total 69	O 69	0	0

Continued on next page...

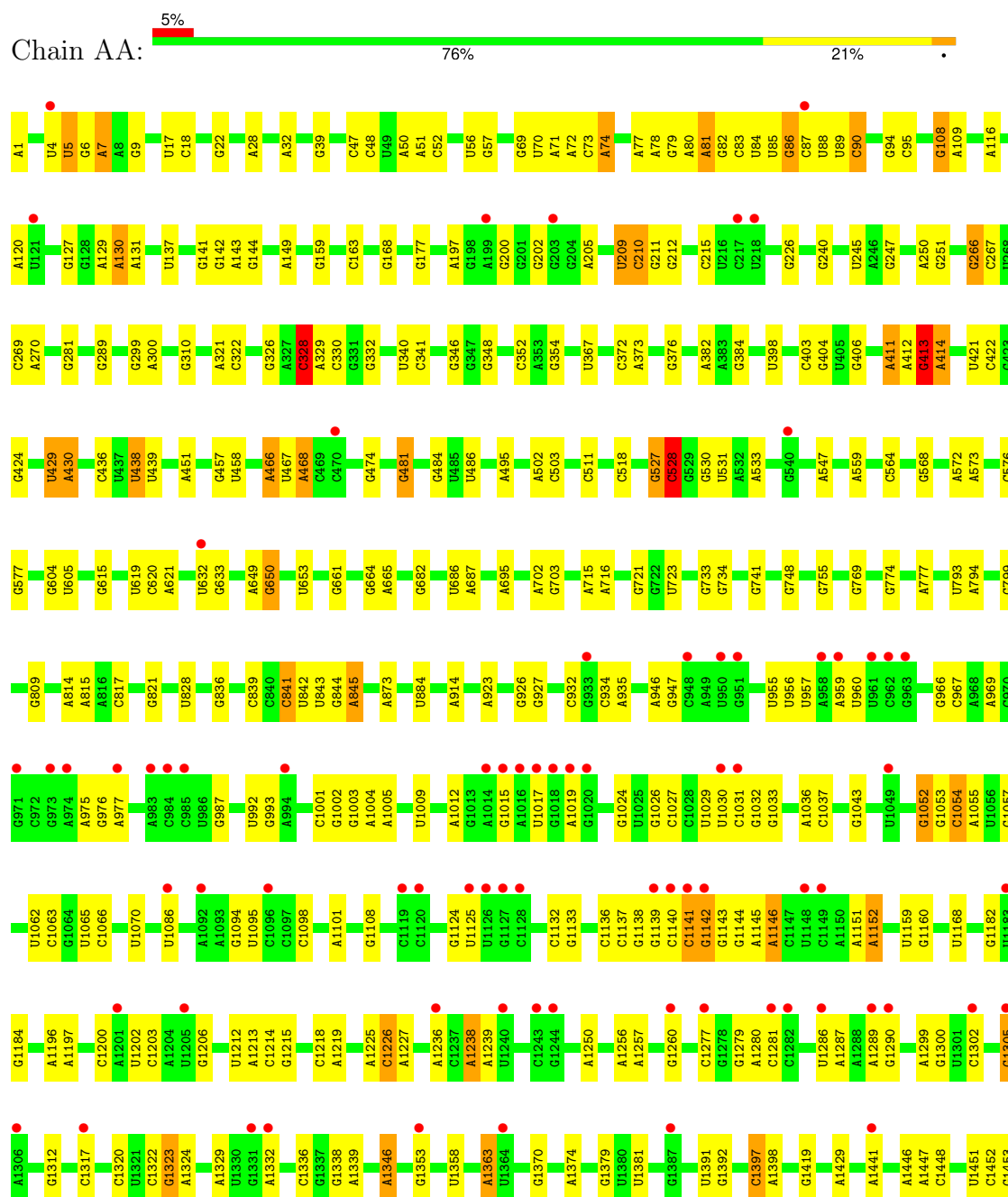
Continued from previous page...

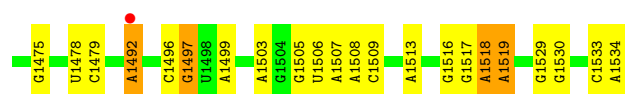
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
70	DU	21	Total 21	O 21	0	0
70	DV	20	Total 20	O 20	0	0
70	DW	31	Total 31	O 31	0	0
70	DX	26	Total 26	O 26	0	0
70	DY	11	Total 11	O 11	0	0
70	DZ	7	Total 7	O 7	0	0
70	DB	213	Total 213	O 213	0	0
70	DA	4829	Total 4829	O 4829	0	0

3 Residue-property plots [i](#)

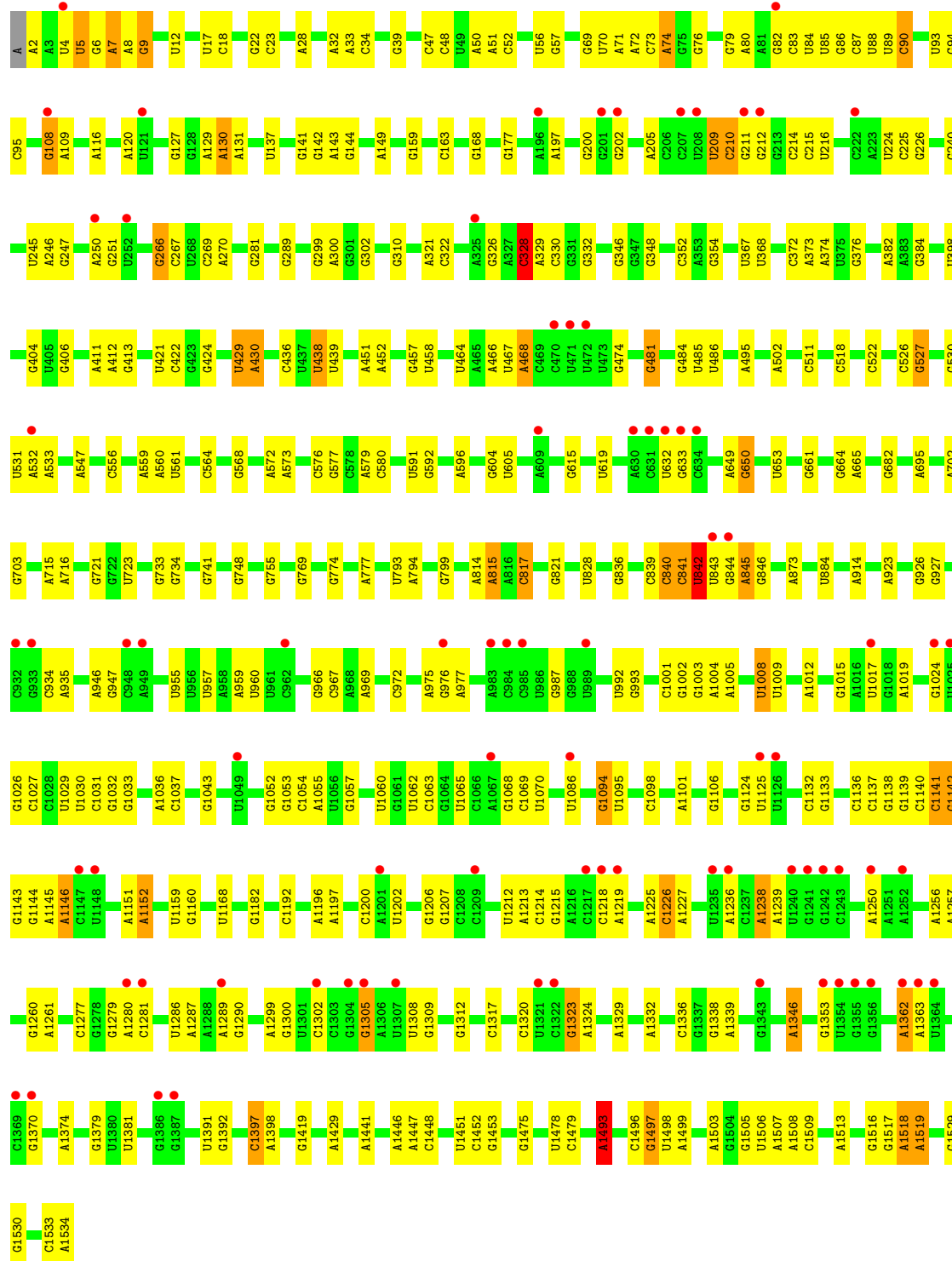
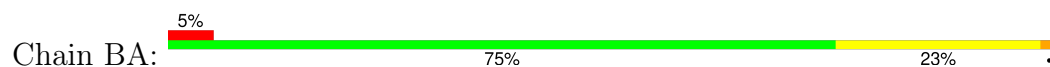
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA

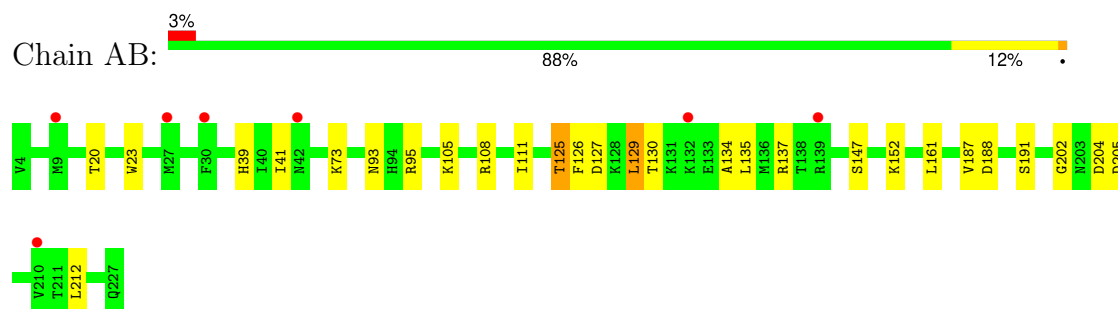




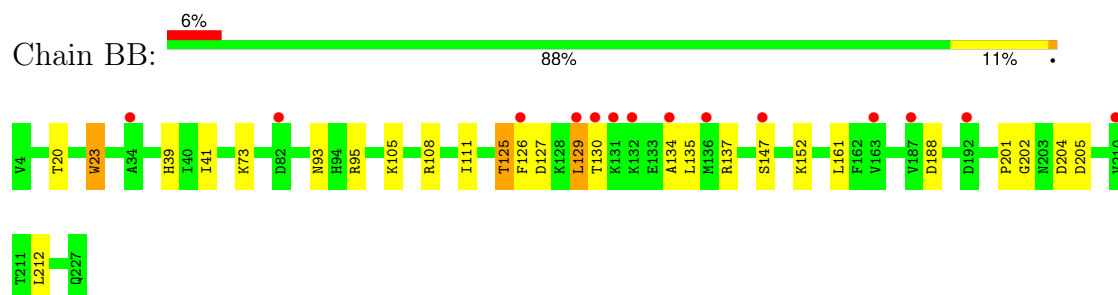
• Molecule 1: 16S rRNA



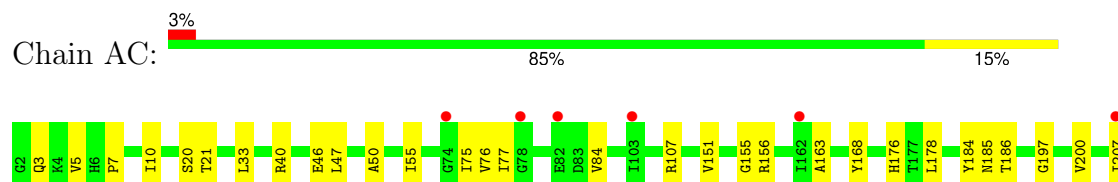
- Molecule 2: 30S ribosomal protein S2



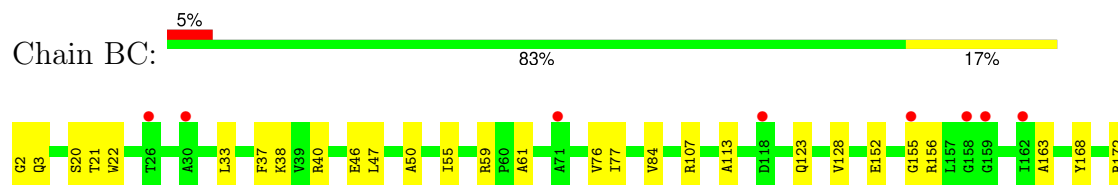
- Molecule 2: 30S ribosomal protein S2



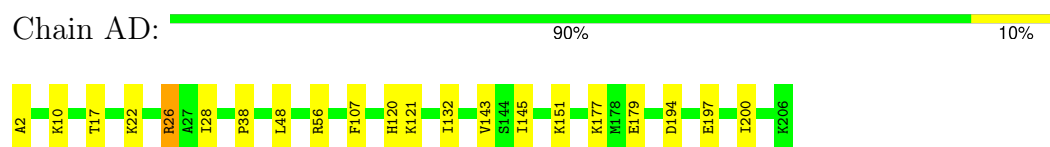
- Molecule 3: 30S ribosomal protein S3



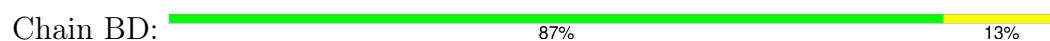
- Molecule 3: 30S ribosomal protein S3



- Molecule 4: 30S ribosomal protein S4

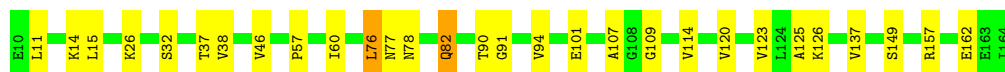
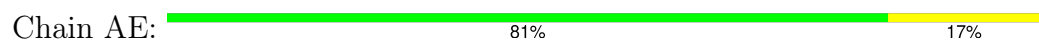


- Molecule 4: 30S ribosomal protein S4

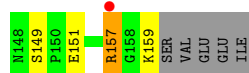
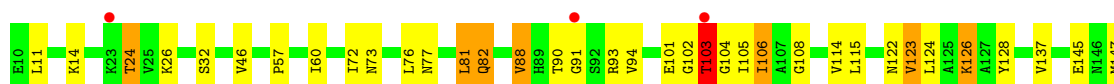
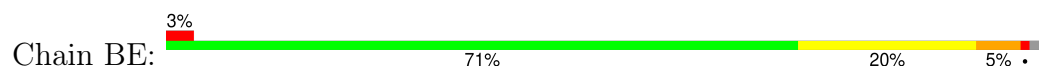




- Molecule 5: 30S ribosomal protein S5



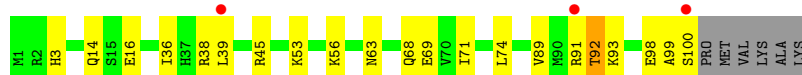
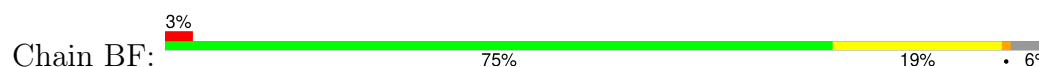
- Molecule 5: 30S ribosomal protein S5



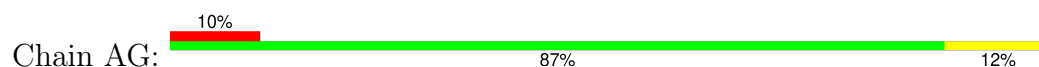
- Molecule 6: 30S ribosomal protein S6



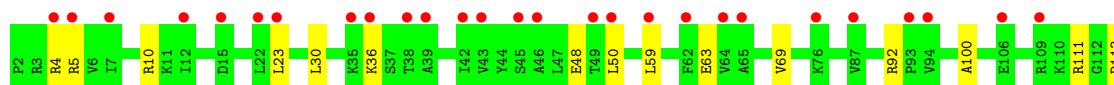
- Molecule 6: 30S ribosomal protein S6

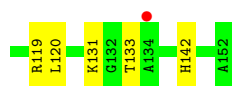


- Molecule 7: 30S ribosomal protein S7

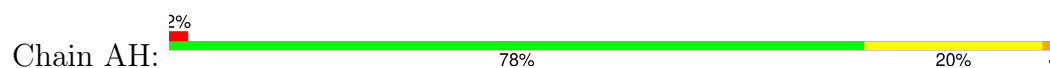


- Molecule 7: 30S ribosomal protein S7





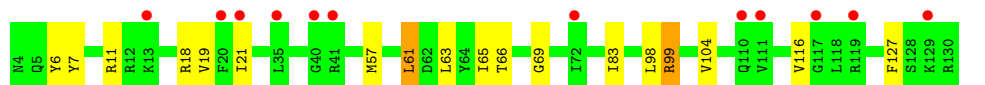
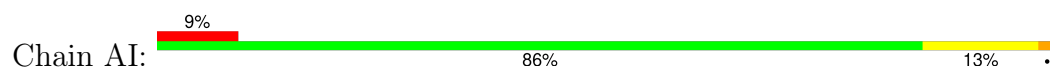
- Molecule 8: 30S ribosomal protein S8



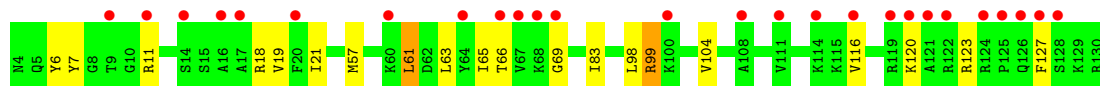
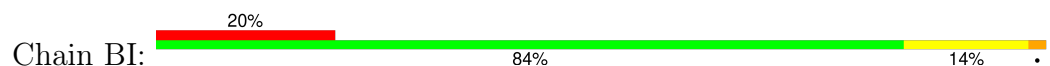
- Molecule 8: 30S ribosomal protein S8



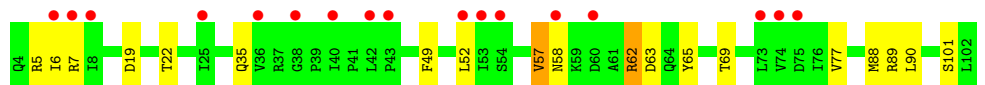
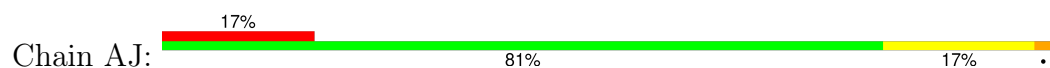
- Molecule 9: 30S ribosomal protein S9



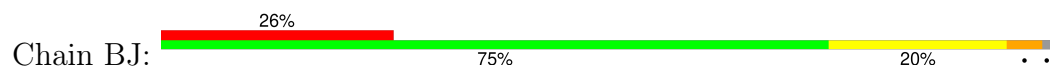
- Molecule 9: 30S ribosomal protein S9

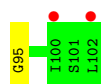


- Molecule 10: 30S ribosomal protein S10

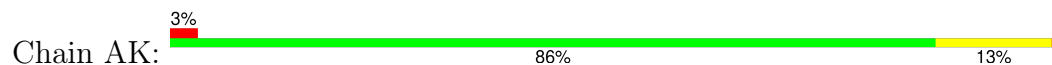


- Molecule 10: 30S ribosomal protein S10

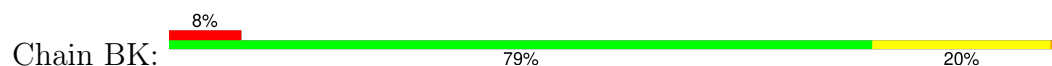




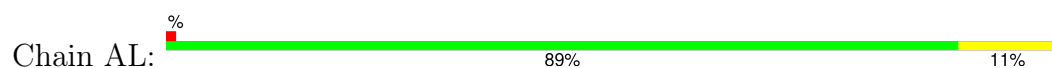
- Molecule 11: 30S ribosomal protein S11



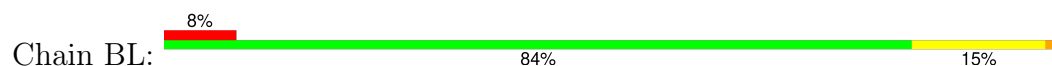
- Molecule 11: 30S ribosomal protein S11



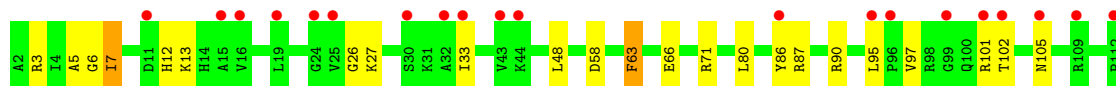
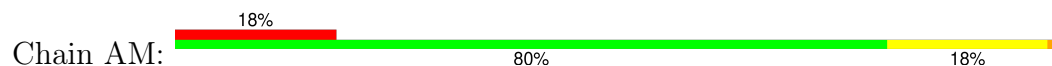
- Molecule 12: 30S ribosomal protein S12



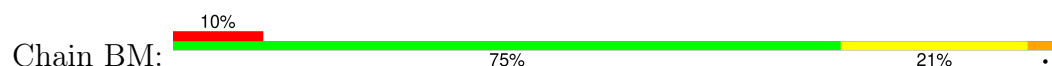
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

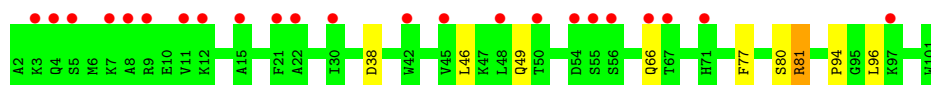


- Molecule 13: 30S ribosomal protein S13





- Molecule 14: 30S ribosomal protein S14



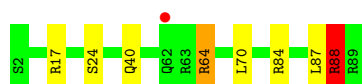
- Molecule 14: 30S ribosomal protein S14



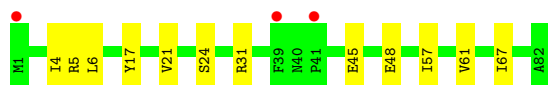
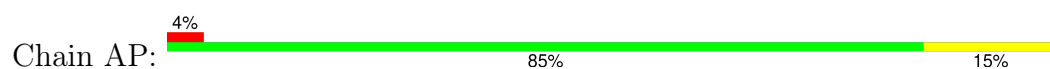
- Molecule 15: 30S ribosomal protein S15



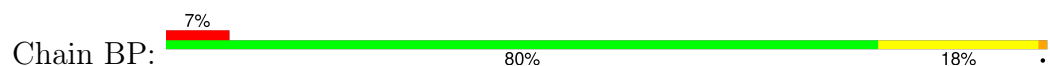
- Molecule 15: 30S ribosomal protein S15




- Molecule 16: 30S ribosomal protein S16

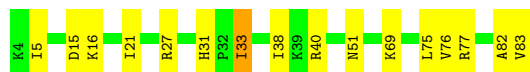


- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

Chain AQ:  80% 19%




- Molecule 17: 30S ribosomal protein S17

Chain BQ:  5% 64% 31%




- Molecule 18: 30S ribosomal protein S18

Chain AR:  2% 87% 13%




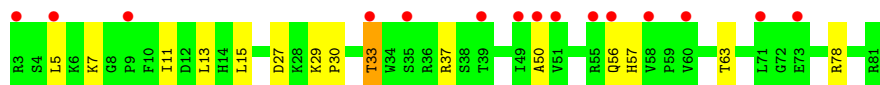
- Molecule 18: 30S ribosomal protein S18

Chain BR:  7% 89% 11%




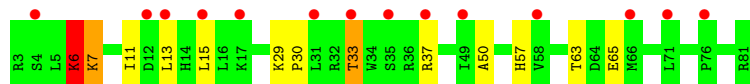
- Molecule 19: 30S ribosomal protein S19

Chain AS:  19% 81% 18%



- Molecule 19: 30S ribosomal protein S19

Chain BS:  18% 84% 13%

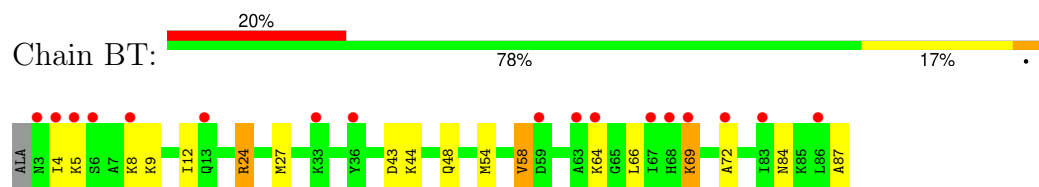


- Molecule 20: 30S ribosomal protein S20

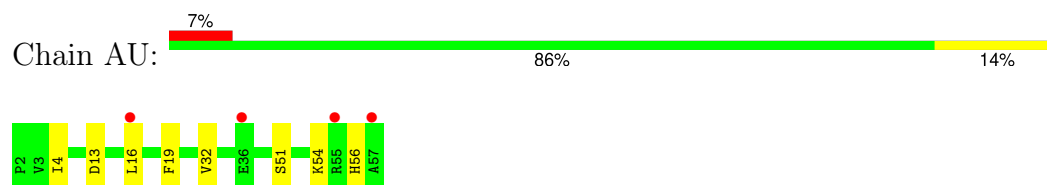
Chain AT:  2% 93% 6%



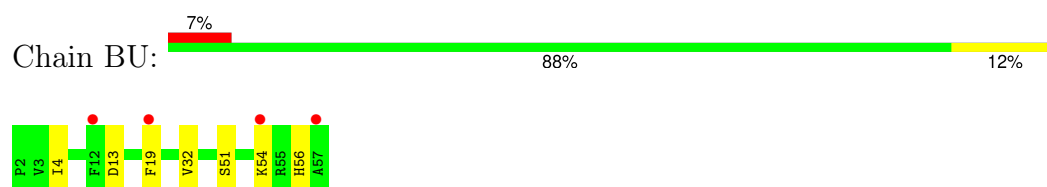
- Molecule 20: 30S ribosomal protein S20



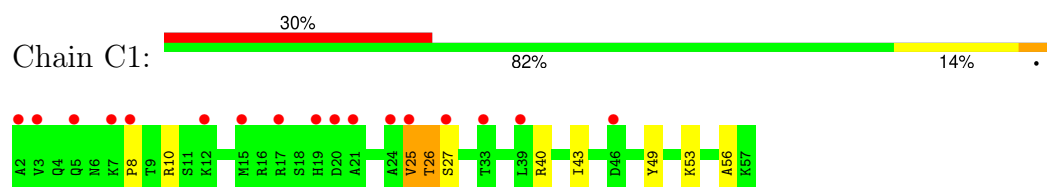
- Molecule 21: 30S ribosomal protein S21



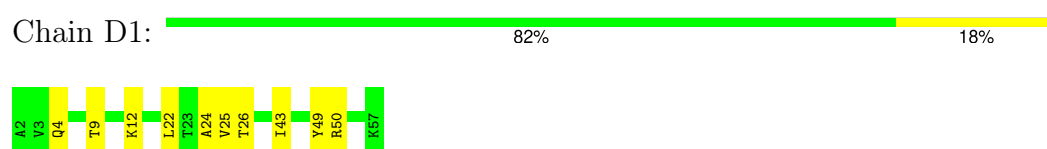
- Molecule 21: 30S ribosomal protein S21



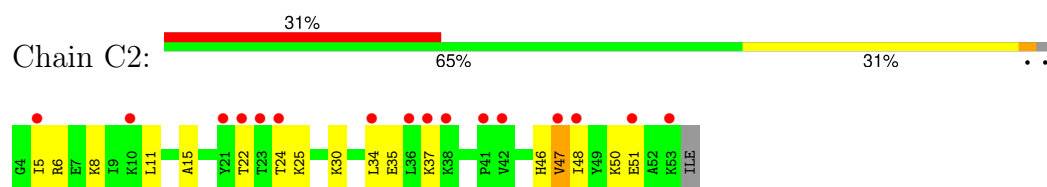
- Molecule 22: 50S ribosomal protein L32



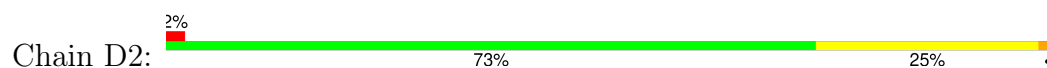
- Molecule 22: 50S ribosomal protein L32



- Molecule 23: 50S ribosomal protein L33

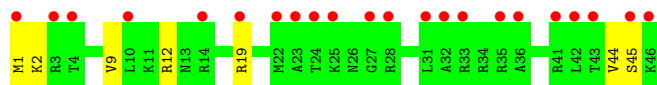
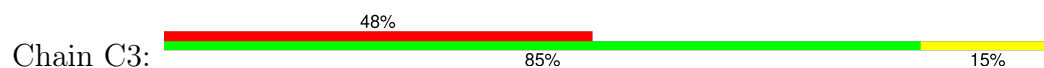


- Molecule 23: 50S ribosomal protein L33

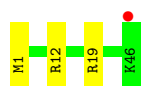




- Molecule 24: 50S ribosomal protein L34



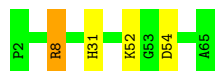
- Molecule 24: 50S ribosomal protein L34



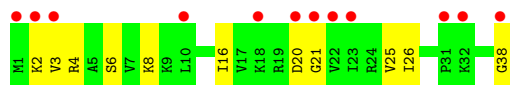
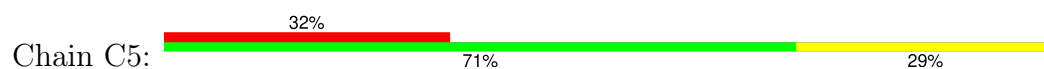
- Molecule 25: 50S ribosomal protein L35



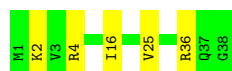
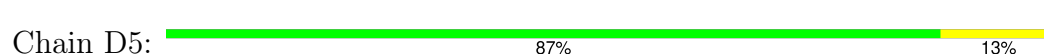
- Molecule 25: 50S ribosomal protein L35



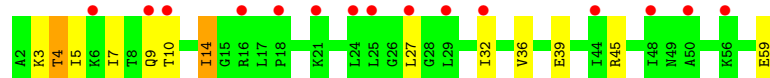
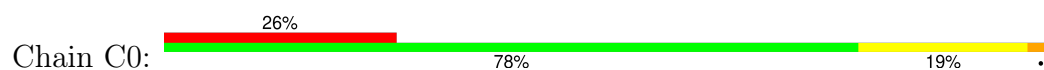
- Molecule 26: 50S ribosomal protein L36



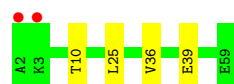
- Molecule 26: 50S ribosomal protein L36



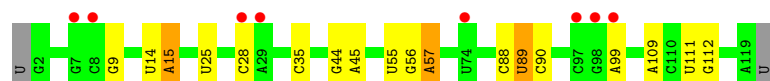
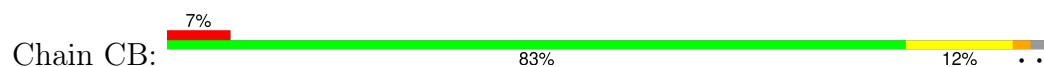
- Molecule 27: 50S ribosomal protein L30



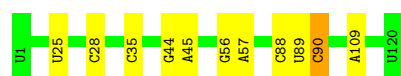
- Molecule 27: 50S ribosomal protein L30



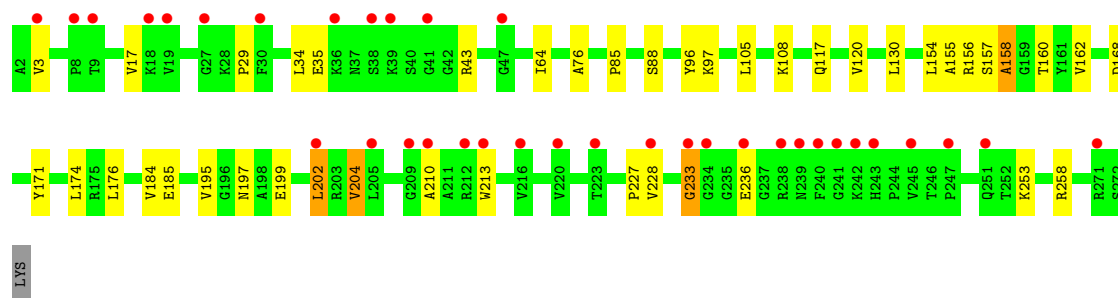
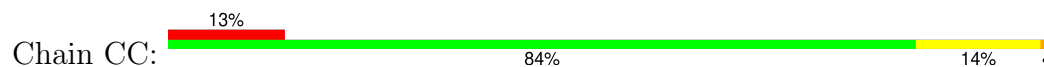
- Molecule 28: 5S rRNA



- Molecule 28: 5S rRNA



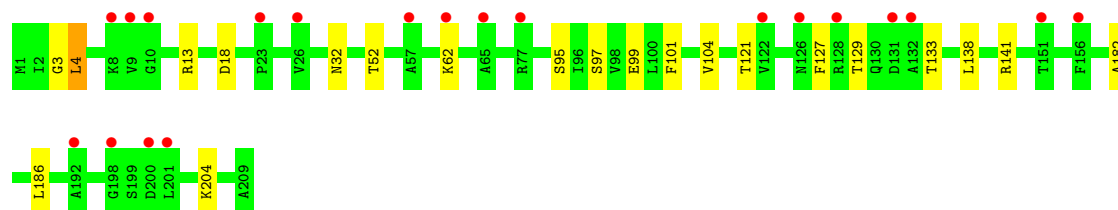
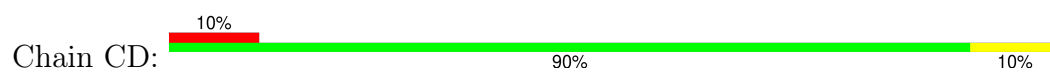
- Molecule 29: 50S ribosomal protein L2



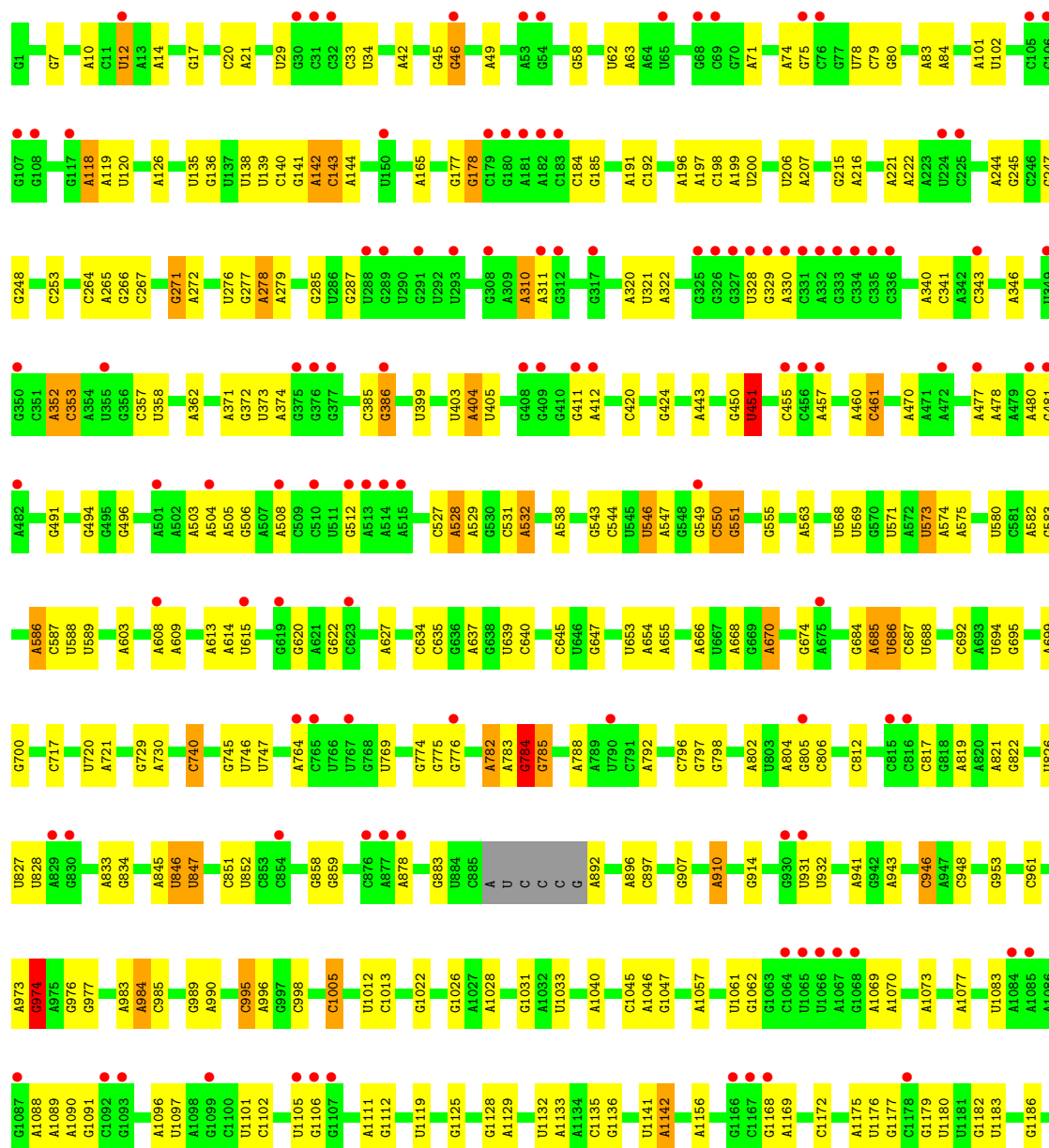
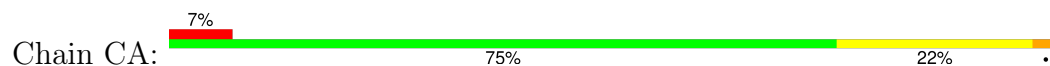
- Molecule 29: 50S ribosomal protein L2

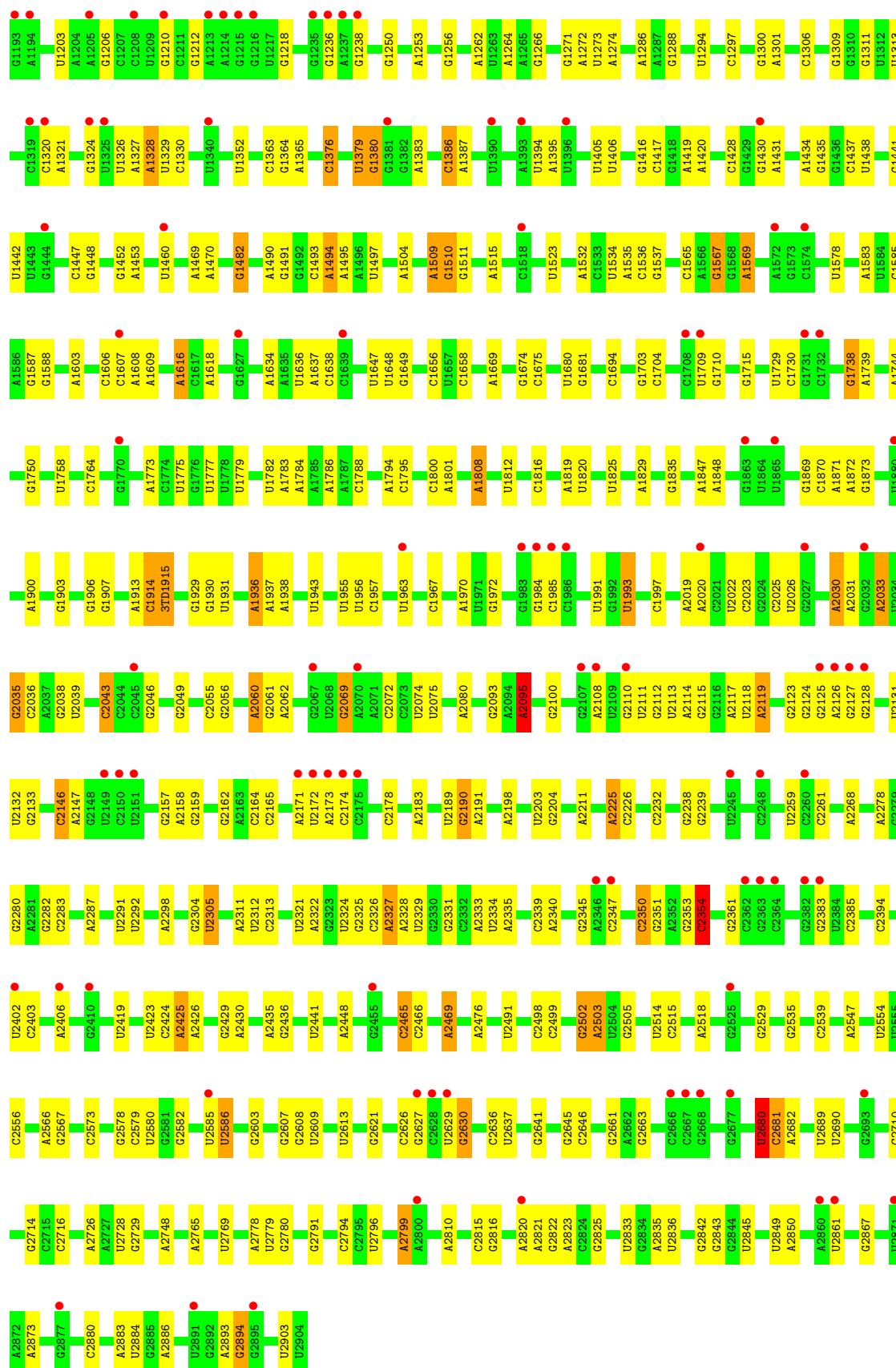


- Molecule 30: 50S ribosomal protein L3



• Molecule 31: 23S rRNA






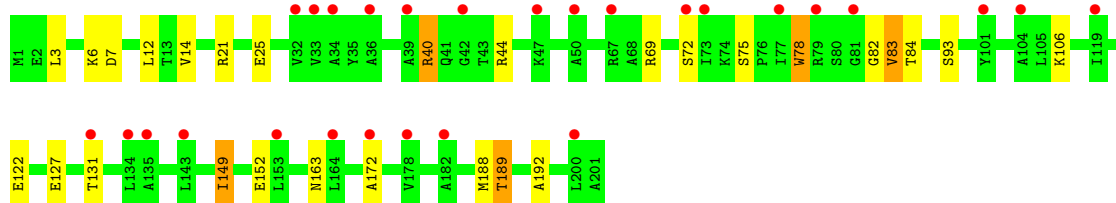
- Molecule 32: 50S ribosomal protein L3

Chain DD:  91% 8%



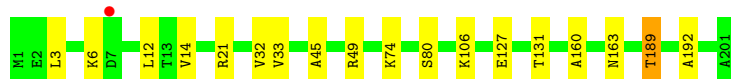
- Molecule 33: 50S ribosomal protein L4

Chain CE:  13% 86% 11%




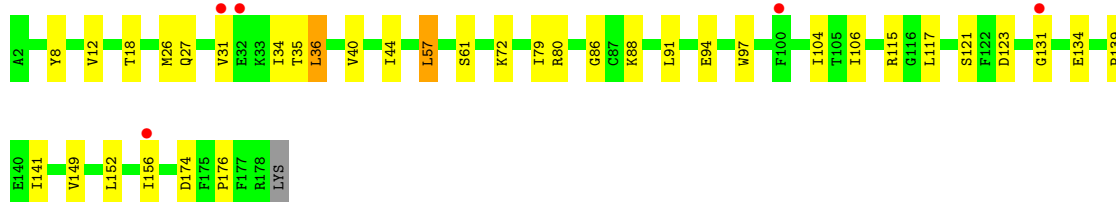
- Molecule 33: 50S ribosomal protein L4

Chain DE:  91% 8%




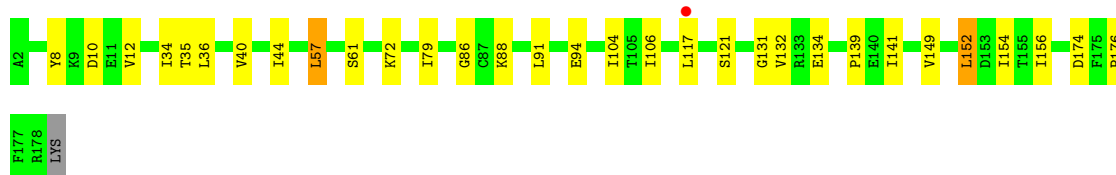
- Molecule 34: 50S ribosomal protein L5

Chain CF:  3% 79% 19%




- Molecule 34: 50S ribosomal protein L5

Chain DF:  2% 82% 16%



- Molecule 35: 50S ribosomal protein L6

Chain CG:  2% 88% 13%

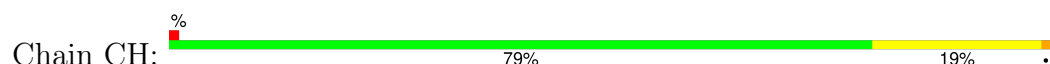




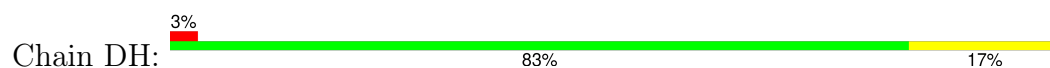
- Molecule 35: 50S ribosomal protein L6



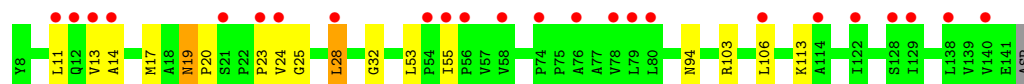
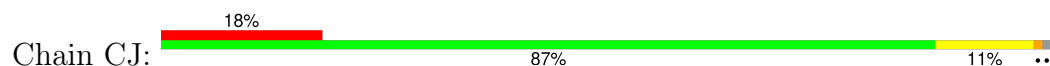
- Molecule 36: 50S ribosomal protein L9



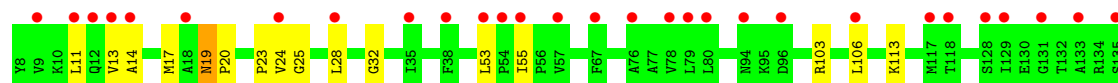
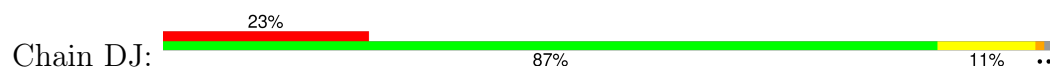
- Molecule 36: 50S ribosomal protein L9



- Molecule 37: 50S ribosomal protein L11



- Molecule 37: 50S ribosomal protein L11



- Molecule 38: 50S ribosomal protein L13

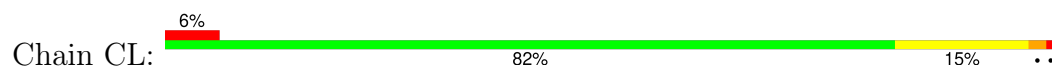




- Molecule 38: 50S ribosomal protein L13



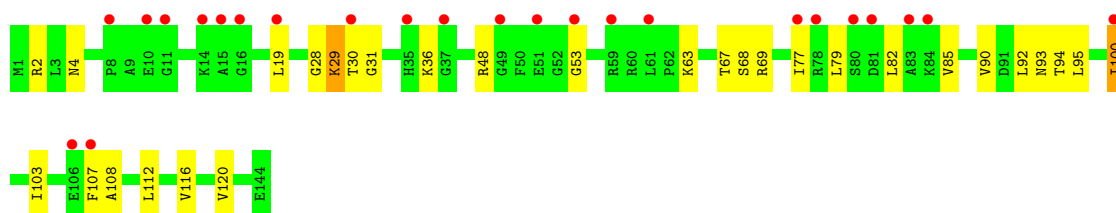
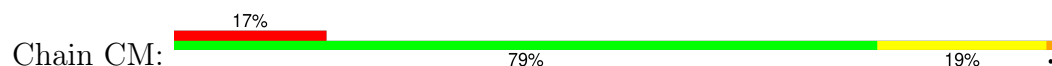
- Molecule 39: 50S ribosomal protein L14



- Molecule 39: 50S ribosomal protein L14



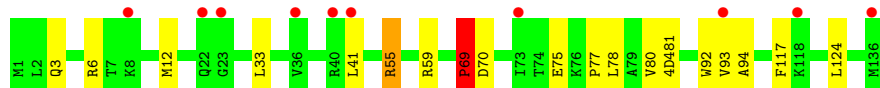
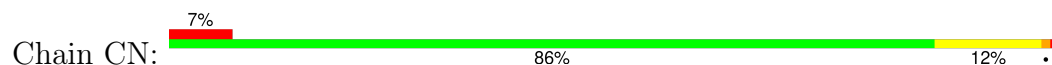
- Molecule 40: 50S ribosomal protein L15



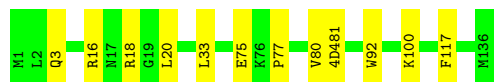
- Molecule 40: 50S ribosomal protein L15




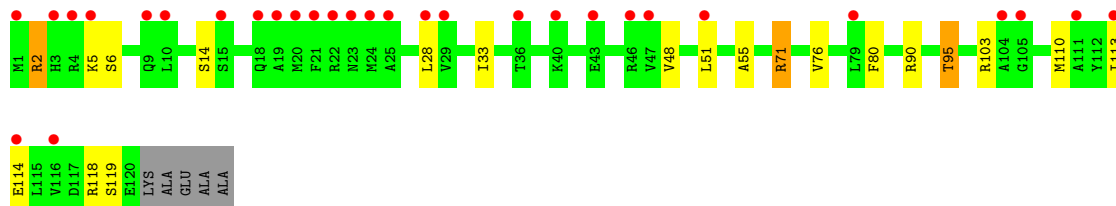
- Molecule 41: 50S ribosomal protein L16



● Molecule 41: 50S ribosomal protein L16

Chain DN:  91% 9%


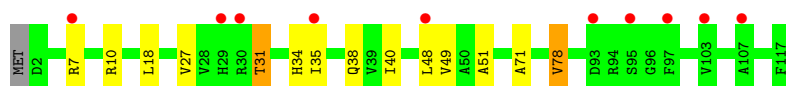
● Molecule 42: 50S ribosomal protein L17

Chain CO:  24% 80% 14% . .

● Molecule 42: 50S ribosomal protein L17

Chain DO:  88% 12%

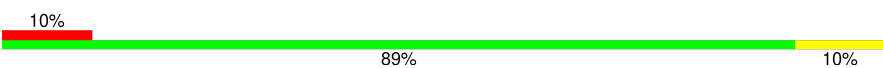
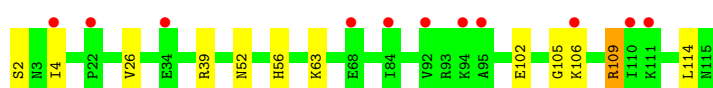
● Molecule 43: 50S ribosomal protein L18

Chain CP:  9% 87% 10% . .

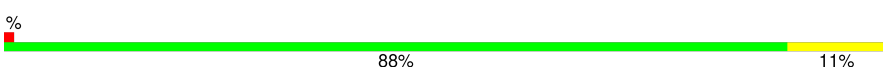
● Molecule 43: 50S ribosomal protein L18

Chain DP:  91% 6% .

● Molecule 44: 50S ribosomal protein L19

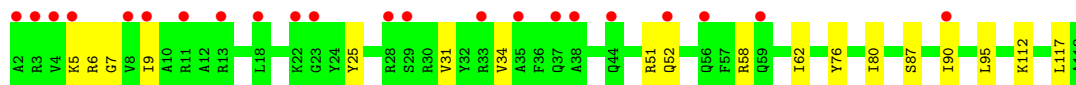
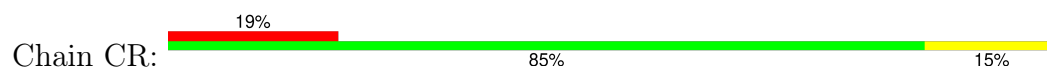
Chain CQ:  10% 89% 10% .

● Molecule 44: 50S ribosomal protein L19

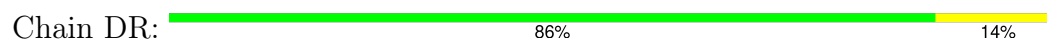
Chain DQ:  % 88% 11% .



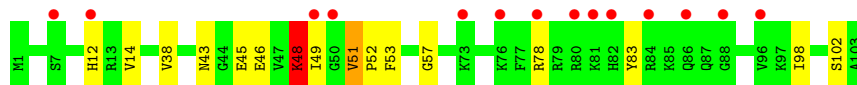
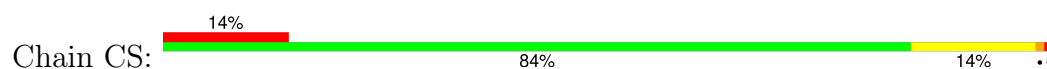
- Molecule 45: 50S ribosomal protein L20



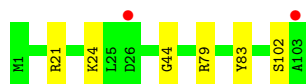
- Molecule 45: 50S ribosomal protein L20



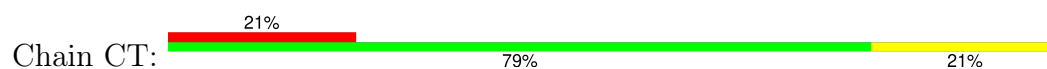
- Molecule 46: 50S ribosomal protein L21



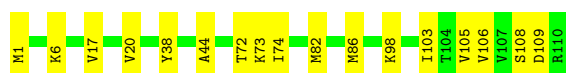
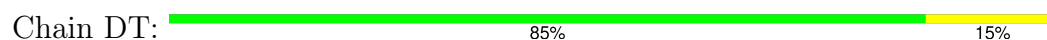
- Molecule 46: 50S ribosomal protein L21



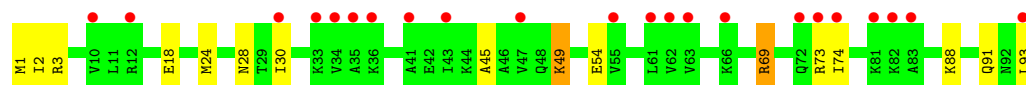
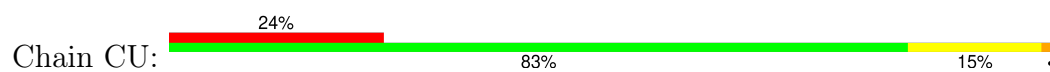
- Molecule 47: 50S ribosomal protein L22



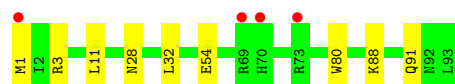
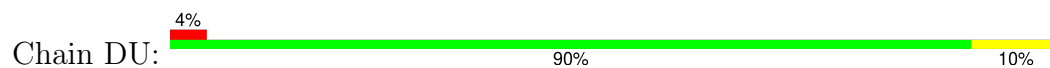
- Molecule 47: 50S ribosomal protein L22



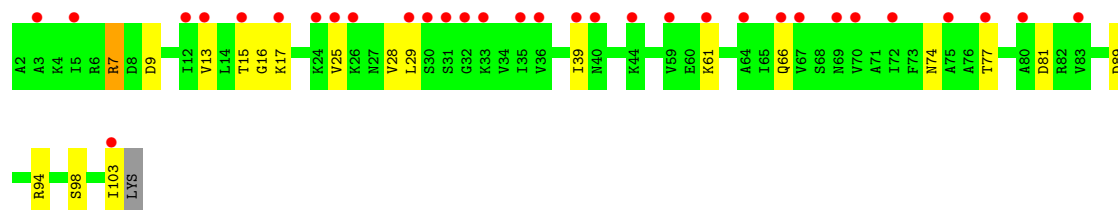
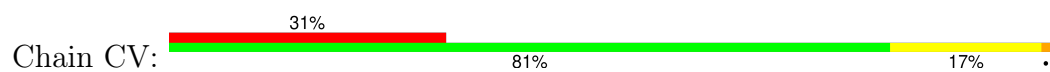
- Molecule 48: 50S ribosomal protein L23



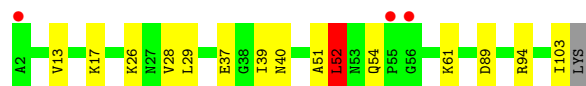
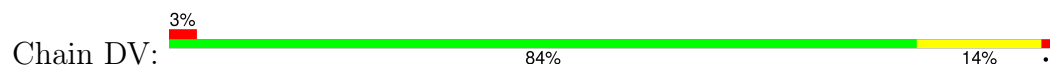
- Molecule 48: 50S ribosomal protein L23



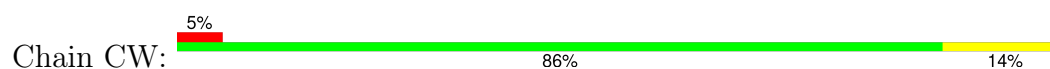
- Molecule 49: 50S ribosomal protein L24



- Molecule 49: 50S ribosomal protein L24



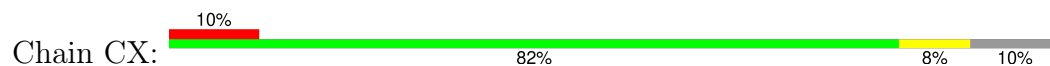
- Molecule 50: 50S ribosomal protein L25



- Molecule 50: 50S ribosomal protein L25

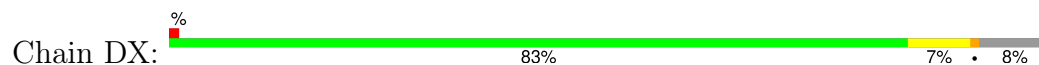


- Molecule 51: 50S ribosomal protein L27

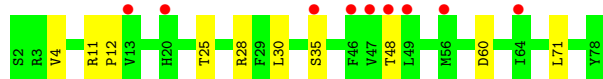
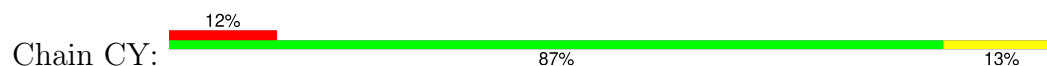




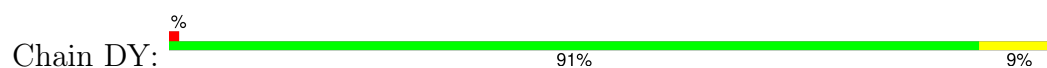
- Molecule 51: 50S ribosomal protein L27



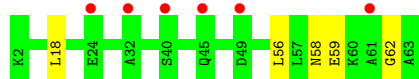
- Molecule 52: 50S ribosomal protein L28



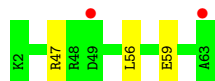
- Molecule 52: 50S ribosomal protein L28



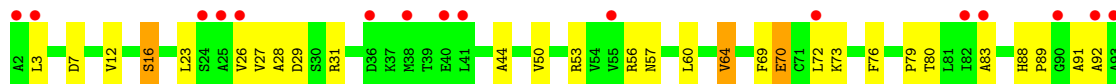
- Molecule 53: 50S ribosomal protein L29



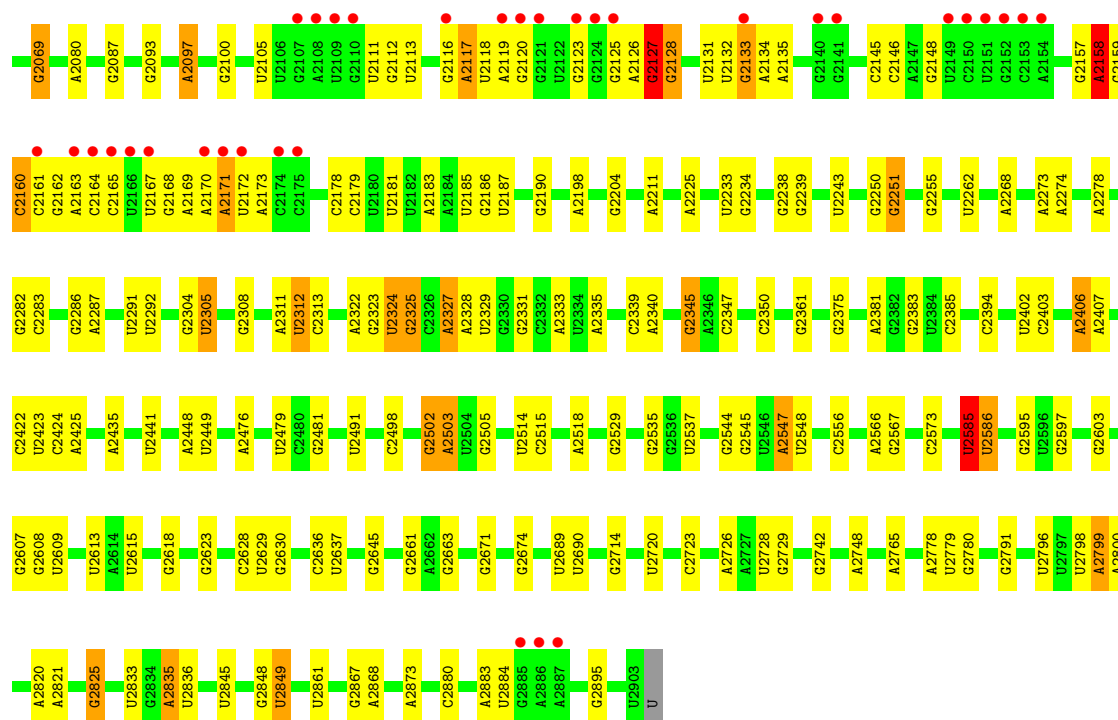
- Molecule 53: 50S ribosomal protein L29



- Molecule 54: 50S ribosomal protein L10







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.72Å 435.19Å 622.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.53 – 3.10 48.53 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.53-3.10) 99.7 (48.53-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 3.12Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, R_{free}	0.171 , 0.192 0.185 , 0.207	Depositor DCC
R_{free} test set	4087 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 106.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	295207	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, ACY, 7MG, OMU, MG, MA6, GUN, 5MC, PEG, OMC, OMG, MEQ, PGE, 5MU, ZN, 4OC, PSU, T1C, 2MG, H2U, TRS, EDO, PG4, 3TD, 1MG, 4D4, UR3, 1PE, D2T, PUT, 2MA, SPD, 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	0.95	7/36597 (0.0%)	0.85	6/57088 (0.0%)
1	BA	0.96	5/36572 (0.0%)	0.85	6/57049 (0.0%)
2	AB	0.43	0/1784	0.62	0/2403
2	BB	0.42	0/1784	0.63	0/2403
3	AC	0.45	0/1652	0.65	0/2225
3	BC	0.44	0/1652	0.65	0/2225
4	AD	0.41	0/1665	0.65	0/2227
4	BD	0.41	0/1665	0.66	0/2227
5	AE	0.44	0/1157	0.74	0/1557
5	BE	0.47	0/1118	0.77	0/1504
6	AF	0.42	0/881	0.66	0/1189
6	BF	0.44	0/835	0.74	0/1128
7	AG	0.44	0/1196	0.61	0/1602
7	BG	0.44	0/1196	0.62	0/1602
8	AH	0.40	0/989	0.66	0/1326
8	BH	0.40	0/989	0.66	0/1326
9	AI	0.42	0/1034	0.64	0/1375
9	BI	0.42	0/1034	0.64	0/1375
10	AJ	0.41	0/806	0.64	0/1089
10	BJ	0.46	0/797	0.69	0/1077
11	AK	0.43	0/893	0.61	0/1205
11	BK	0.41	0/893	0.65	0/1205
12	AL	0.42	0/960	0.69	0/1286
12	BL	0.42	0/960	0.70	0/1286
13	AM	0.47	0/893	0.70	0/1193
13	BM	0.48	0/893	0.70	0/1193
14	AN	0.44	0/817	0.63	0/1088
14	BN	0.42	0/817	0.62	0/1088
15	AO	0.43	0/722	0.59	0/964
15	BO	0.42	0/722	0.59	0/964

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	AP	0.43	0/659	0.68	0/884
16	BP	0.46	0/659	0.74	0/884
17	AQ	0.44	0/658	0.70	0/881
17	BQ	0.48	0/658	0.74	0/881
18	AR	0.46	0/463	0.63	0/621
18	BR	0.46	0/463	0.62	0/621
19	AS	0.46	0/653	0.59	0/877
19	BS	0.46	0/653	0.60	0/877
20	AT	0.45	0/676	0.64	0/895
20	BT	0.49	0/671	0.67	0/888
21	AU	0.40	0/472	0.60	0/627
21	BU	0.37	0/472	0.61	0/627
22	C1	0.48	0/450	0.66	0/599
22	D1	0.51	0/450	0.72	0/599
23	C2	0.44	0/416	0.68	0/554
23	D2	0.45	0/421	0.66	0/561
24	C3	0.40	0/380	0.67	0/498
24	D3	0.50	0/380	0.70	0/498
25	C4	0.41	0/513	0.62	0/676
25	D4	0.47	0/513	0.65	0/676
26	C5	0.41	0/303	0.76	0/397
26	D5	0.46	0/303	0.72	0/397
27	C0	0.47	0/453	0.79	0/605
27	D0	0.53	0/467	0.78	0/623
28	CB	0.92	0/2828	0.87	2/4410 (0.0%)
28	DB	0.94	0/2872	0.86	0/4478
29	CC	0.41	0/2121	0.70	0/2852
29	DC	0.43	0/2121	0.70	0/2852
30	CD	0.40	0/1586	0.65	0/2134
31	CA	0.97	29/69165 (0.0%)	0.86	10/107896 (0.0%)
32	DD	0.44	0/1576	0.65	0/2119
33	CE	0.42	0/1571	0.68	0/2113
33	DE	0.44	0/1570	0.66	0/2113
34	CF	0.40	0/1434	0.65	0/1926
34	DF	0.43	0/1434	0.67	0/1926
35	CG	0.39	0/1343	0.64	0/1816
35	DG	0.41	0/1343	0.62	0/1816
36	CH	0.45	0/1121	0.67	0/1515
36	DH	0.45	0/1121	0.66	0/1515
37	CJ	0.48	0/993	0.62	0/1341
37	DJ	0.48	0/993	0.62	0/1341
38	CK	0.39	0/1152	0.65	0/1551
38	DK	0.47	0/1152	0.66	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	CL	0.43	0/947	0.69	0/1268
39	DL	0.46	0/955	0.68	0/1279
40	CM	0.42	0/1062	0.71	2/1413 (0.1%)
40	DM	0.42	0/1062	0.67	0/1413
41	CN	0.42	0/1081	0.71	1/1443 (0.1%)
41	DN	0.47	0/1092	0.71	0/1457
42	CO	0.41	0/973	0.67	0/1301
42	DO	0.48	0/1006	0.72	0/1345
43	CP	0.41	0/902	0.68	0/1209
43	DP	0.44	0/910	0.68	0/1219
44	CQ	0.38	0/929	0.68	0/1242
44	DQ	0.43	0/929	0.66	0/1242
45	CR	0.43	0/960	0.64	0/1278
45	DR	0.49	0/960	0.65	0/1278
46	CS	0.39	0/829	0.71	0/1107
46	DS	0.43	0/829	0.75	0/1107
47	CT	0.38	0/864	0.70	0/1156
47	DT	0.45	0/864	0.70	0/1156
48	CU	0.41	0/745	0.67	0/994
48	DU	0.43	0/744	0.68	0/994
49	CV	0.42	0/787	0.72	0/1051
49	DV	0.42	0/787	0.71	0/1051
50	CW	0.38	0/766	0.62	0/1025
50	DW	0.44	0/766	0.65	0/1025
51	CX	0.36	0/576	0.59	0/762
51	DX	0.43	0/598	0.63	0/790
52	CY	0.40	0/635	0.70	0/848
52	DY	0.44	0/635	0.69	0/848
53	CZ	0.40	0/502	0.60	0/667
53	DZ	0.42	0/502	0.59	0/667
54	DI	0.49	0/1037	0.73	1/1402 (0.1%)
55	DA	1.02	20/69364 (0.0%)	0.88	10/108207 (0.0%)
All	All	0.86	61/309273 (0.0%)	0.81	38/462224 (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
41	CN	0	1
55	DA	0	25
All	All	0	26

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	CA	2095	A	O5'-C5'	-9.11	1.28	1.42
31	CA	2425	A	C3'-O3'	8.77	1.54	1.42
55	DA	12	U	C1'-N1	8.01	1.60	1.48
31	CA	1936	A	N9-C4	-7.92	1.33	1.37
55	DA	2097	A	O5'-C5'	-7.38	1.31	1.42

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CB	15	A	O4'-C1'-N9	9.58	115.86	108.20
55	DA	1936	A	O4'-C1'-N9	7.65	114.32	108.20
1	AA	1	A	OP1-P-OP2	-7.18	108.83	119.60
54	DI	132	TYR	C-N-CA	7.11	139.46	121.70
1	AA	413	G	C1'-O4'-C4'	-7.07	104.24	109.90

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	CN	69	PRO	Mainchain
55	DA	15	G	Sidechain
55	DA	177	G	Sidechain
55	DA	221	A	Sidechain
55	DA	249	C	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	32933	0	16593	81	0
1	BA	32911	0	16582	95	0
2	AB	1753	0	1780	7	0
2	BB	1753	0	1780	8	0
3	AC	1625	0	1696	12	0
3	BC	1625	0	1696	13	0
4	AD	1643	0	1707	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BD	1643	0	1707	16	0
5	AE	1144	0	1185	10	0
5	BE	1105	0	1148	19	0
6	AF	862	0	864	6	0
6	BF	817	0	808	7	0
7	AG	1182	0	1238	5	0
7	BG	1182	0	1238	3	0
8	AH	979	0	1031	11	0
8	BH	979	0	1031	8	0
9	AI	1022	0	1070	10	0
9	BI	1022	0	1070	11	0
10	AJ	796	0	836	10	0
10	BJ	787	0	828	8	0
11	AK	877	0	887	11	0
11	BK	877	0	887	13	0
12	AL	957	0	1017	6	0
12	BL	957	0	1017	8	0
13	AM	884	0	941	10	0
13	BM	884	0	941	15	0
14	AN	805	0	844	6	0
14	BN	805	0	844	5	0
15	AO	714	0	734	0	0
15	BO	714	0	734	1	0
16	AP	649	0	666	6	0
16	BP	649	0	666	6	0
17	AQ	649	0	691	4	0
17	BQ	649	0	691	11	0
18	AR	456	0	478	2	0
18	BR	456	0	478	3	0
19	AS	638	0	665	4	0
19	BS	638	0	665	6	0
20	AT	670	0	719	1	0
20	BT	665	0	714	6	0
21	AU	465	0	491	3	0
21	BU	465	0	491	3	0
22	C1	444	0	458	4	0
22	D1	444	0	458	10	0
23	C2	409	0	440	7	0
23	D2	414	0	442	5	0
24	C3	377	0	418	4	0
24	D3	377	0	418	2	0
25	C4	504	0	572	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	D4	504	0	572	2	0
26	C5	302	0	340	9	0
26	D5	302	0	340	3	0
27	C0	449	0	488	3	0
27	D0	463	0	504	0	0
28	CB	2529	0	1281	7	0
28	DB	2569	0	1301	2	0
29	CC	2082	0	2154	20	0
29	DC	2082	0	2154	10	0
30	CD	1565	0	1616	12	0
31	CA	62229	0	31319	205	0
32	DD	1576	0	1627	11	0
33	CE	1552	0	1619	13	0
33	DE	1551	0	1619	10	0
34	CF	1410	0	1444	18	0
34	DF	1410	0	1444	13	0
35	CG	1323	0	1371	7	0
35	DG	1323	0	1371	6	0
36	CH	1110	0	1148	10	0
36	DH	1110	0	1148	7	0
37	CJ	979	0	1028	7	0
37	DJ	979	0	1028	5	0
38	CK	1129	0	1162	6	0
38	DK	1129	0	1162	6	0
39	CL	938	0	1012	8	0
39	DL	946	0	1023	7	0
40	CM	1053	0	1129	15	0
40	DM	1053	0	1129	7	0
41	CN	1075	0	1154	8	0
41	DN	1092	0	1177	8	0
42	CO	960	0	1000	7	0
42	DO	993	0	1034	6	0
43	CP	892	0	923	6	0
43	DP	900	0	935	6	0
44	CQ	917	0	962	4	0
44	DQ	917	0	962	7	0
45	CR	947	0	1019	11	0
45	DR	947	0	1019	13	0
46	CS	816	0	839	8	0
46	DS	816	0	839	4	0
47	CT	857	0	922	12	0
47	DT	857	0	922	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	CU	739	0	807	6	0
48	DU	738	0	807	4	0
49	CV	779	0	831	6	0
49	DV	779	0	831	6	0
50	CW	753	0	780	7	0
50	DW	753	0	780	7	0
51	CX	569	0	581	4	0
51	DX	591	0	606	4	0
52	CY	625	0	652	4	0
52	DY	625	0	652	3	0
53	CZ	501	0	531	1	0
53	DZ	501	0	531	2	0
54	DI	1023	0	1052	20	0
55	DA	62423	0	31412	164	0
56	AA	72	0	0	0	0
56	BA	45	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	184	0	0	0	0
56	DB	9	0	0	0	0
56	DD	1	0	0	0	0
56	DM	1	0	0	0	0
56	DR	1	0	0	0	0
57	AA	13	0	18	1	0
57	BA	13	0	18	1	0
57	DA	26	0	36	0	0
57	DQ	13	0	18	0	0
57	DR	13	0	18	4	0
57	DS	13	0	18	1	0
58	AA	16	0	28	0	0
58	DA	40	0	70	2	0
58	DE	16	0	28	0	0
58	DK	8	0	14	0	0
58	DN	8	0	14	1	0
58	DS	8	0	14	0	0
58	DT	16	0	28	0	0
59	AA	24	0	48	0	0
59	DA	72	0	144	3	0
60	AA	42	0	39	2	0
60	BA	42	0	38	0	0
61	AB	1	0	0	0	0
61	C5	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	D5	1	0	0	0	0
62	AL	7	0	10	0	0
62	D1	7	0	10	1	0
62	D3	7	0	10	0	0
62	DA	35	0	50	0	0
62	DL	7	0	10	0	0
62	DP	7	0	10	0	0
62	DQ	7	0	10	0	0
63	D1	4	0	6	0	0
63	DA	28	0	42	1	0
63	DB	16	0	24	0	0
64	D1	10	0	14	2	0
64	D3	10	0	14	0	0
64	DA	50	0	70	5	0
64	DS	10	0	14	1	0
64	DU	10	0	14	1	0
65	DA	40	0	76	2	0
66	DA	32	0	44	3	0
67	DA	12	0	9	0	0
68	DA	11	0	5	0	0
69	DA	8	0	12	1	0
70	AA	500	0	0	0	0
70	AC	5	0	0	0	0
70	AD	2	0	0	0	0
70	AE	4	0	0	0	0
70	AF	1	0	0	0	0
70	AG	1	0	0	0	0
70	AH	1	0	0	0	0
70	AJ	2	0	0	0	0
70	AK	6	0	0	0	0
70	AL	10	0	0	0	0
70	AM	4	0	0	1	0
70	AN	7	0	0	1	0
70	AO	2	0	0	0	0
70	AP	2	0	0	0	0
70	AR	1	0	0	0	0
70	AT	3	0	0	0	0
70	AU	2	0	0	0	0
70	BA	288	0	0	1	0
70	BD	12	0	0	0	0
70	BE	1	0	0	0	0
70	BF	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	BK	2	0	0	0	0
70	BL	2	0	0	0	0
70	BN	2	0	0	0	0
70	BO	1	0	0	0	0
70	BP	3	0	0	0	0
70	BT	4	0	0	0	0
70	BU	1	0	0	0	0
70	C3	3	0	0	0	0
70	C4	1	0	0	0	0
70	CA	692	0	0	2	0
70	CB	13	0	0	0	0
70	CC	12	0	0	0	0
70	CD	6	0	0	0	0
70	CE	4	0	0	0	0
70	CL	1	0	0	0	0
70	CM	4	0	0	0	0
70	CO	1	0	0	0	0
70	CU	3	0	0	0	0
70	CV	1	0	0	0	0
70	CW	1	0	0	0	0
70	CY	1	0	0	0	0
70	D0	21	0	0	0	0
70	D1	45	0	0	0	0
70	D2	7	0	0	0	0
70	D3	23	0	0	0	0
70	D4	39	0	0	0	0
70	D5	12	0	0	0	0
70	DA	4829	0	0	13	0
70	DB	213	0	0	0	0
70	DC	104	0	0	0	0
70	DD	92	0	0	2	0
70	DE	60	0	0	2	0
70	DF	15	0	0	0	0
70	DG	6	0	0	0	0
70	DH	2	0	0	0	0
70	DK	64	0	0	2	0
70	DL	51	0	0	0	0
70	DM	64	0	0	0	0
70	DN	73	0	0	0	0
70	DO	46	0	0	0	0
70	DP	40	0	0	0	0
70	DQ	32	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	DR	63	0	0	1	0
70	DS	44	0	0	0	0
70	DT	69	0	0	1	0
70	DU	21	0	0	0	0
70	DV	20	0	0	0	0
70	DW	31	0	0	0	0
70	DX	26	0	0	0	0
70	DY	11	0	0	0	0
70	DZ	7	0	0	1	0
All	All	295207	0	194493	1128	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 1128 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)
46:CS:14:VAL:HG21	46:CS:98:ILE:HG13	1.26	1.10
31:CA:1936:A:H2	31:CA:1943:U:H3	1.01	0.98
2:BB:20:THR:HA	2:BB:39:HIS:CE1	1.98	0.97
1:BA:1052:G:H22	1:BA:1206:G:H1	0.98	0.94
55:DA:2796:U:H3	55:DA:2799:A:H61	1.20	0.88

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	222/224 (99%)	207 (93%)	11 (5%)	4 (2%)	7	29
2	BB	222/224 (99%)	207 (93%)	11 (5%)	4 (2%)	7	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	204/206 (99%)	194 (95%)	9 (4%)	1 (0%)	25	58
3	BC	204/206 (99%)	195 (96%)	7 (3%)	2 (1%)	13	42
4	AD	203/205 (99%)	197 (97%)	6 (3%)	0	100	100
4	BD	203/205 (99%)	197 (97%)	6 (3%)	0	100	100
5	AE	153/155 (99%)	144 (94%)	7 (5%)	2 (1%)	10	36
5	BE	148/155 (96%)	131 (88%)	14 (10%)	3 (2%)	6	26
6	AF	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
6	BF	98/106 (92%)	91 (93%)	5 (5%)	2 (2%)	6	26
7	AG	149/151 (99%)	135 (91%)	13 (9%)	1 (1%)	19	51
7	BG	149/151 (99%)	137 (92%)	12 (8%)	0	100	100
8	AH	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	48
8	BH	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	8	31
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%)	89 (92%)	7 (7%)	1 (1%)	13	42
10	BJ	96/99 (97%)	77 (80%)	13 (14%)	6 (6%)	1	7
11	AK	115/117 (98%)	105 (91%)	9 (8%)	1 (1%)	14	45
11	BK	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	14	45
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	111 (92%)	8 (7%)	1 (1%)	16	48
13	AM	112/114 (98%)	102 (91%)	7 (6%)	3 (3%)	4	21
13	BM	112/114 (98%)	101 (90%)	6 (5%)	5 (4%)	2	12
14	AN	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	6	26
14	BN	98/100 (98%)	87 (89%)	10 (10%)	1 (1%)	13	42
15	AO	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
15	BO	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	11	38
16	AP	80/82 (98%)	73 (91%)	5 (6%)	2 (2%)	4	22
16	BP	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	4	22
17	AQ	78/80 (98%)	71 (91%)	6 (8%)	1 (1%)	10	36
17	BQ	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	1	10
18	AR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
19	BS	77/79 (98%)	66 (86%)	10 (13%)	1 (1%)	10	36
20	AT	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
20	BT	83/86 (96%)	79 (95%)	3 (4%)	1 (1%)	11	38
21	AU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
21	BU	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
22	C1	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	1	8
22	D1	54/56 (96%)	54 (100%)	0	0	100	100
23	C2	48/51 (94%)	43 (90%)	3 (6%)	2 (4%)	2	13
23	D2	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
24	C3	44/46 (96%)	42 (96%)	1 (2%)	1 (2%)	5	23
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	C4	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
25	D4	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	20
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	51 (91%)	3 (5%)	2 (4%)	3	16
27	D0	57/58 (98%)	53 (93%)	4 (7%)	0	100	100
29	CC	269/272 (99%)	249 (93%)	15 (6%)	5 (2%)	6	27
29	DC	269/272 (99%)	251 (93%)	16 (6%)	2 (1%)	19	51
30	CD	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
32	DD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
33	CE	199/201 (99%)	189 (95%)	7 (4%)	3 (2%)	8	33
33	DE	199/201 (99%)	191 (96%)	7 (4%)	1 (0%)	25	58
34	CF	175/178 (98%)	166 (95%)	9 (5%)	0	100	100
34	DF	175/178 (98%)	166 (95%)	9 (5%)	0	100	100
35	CG	174/176 (99%)	162 (93%)	7 (4%)	5 (3%)	3	20
35	DG	174/176 (99%)	165 (95%)	7 (4%)	2 (1%)	12	39
36	CH	147/149 (99%)	130 (88%)	11 (8%)	6 (4%)	2	13
36	DH	147/149 (99%)	133 (90%)	11 (8%)	3 (2%)	6	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	CJ	132/135 (98%)	125 (95%)	3 (2%)	4 (3%)	3	19
37	DJ	132/135 (98%)	125 (95%)	3 (2%)	4 (3%)	3	19
38	CK	140/142 (99%)	135 (96%)	2 (1%)	3 (2%)	5	25
38	DK	140/142 (99%)	136 (97%)	2 (1%)	2 (1%)	9	34
39	CL	120/123 (98%)	114 (95%)	4 (3%)	2 (2%)	7	30
39	DL	121/123 (98%)	116 (96%)	4 (3%)	1 (1%)	16	48
40	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	5	25
40	DM	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	19	51
41	CN	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	16	48
41	DN	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
42	CO	118/125 (94%)	110 (93%)	6 (5%)	2 (2%)	7	30
42	DO	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
43	CP	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
43	DP	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
44	CQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	14	45
44	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	14	45
45	CR	115/117 (98%)	110 (96%)	4 (4%)	1 (1%)	14	45
45	DR	115/117 (98%)	110 (96%)	4 (4%)	1 (1%)	14	45
46	CS	101/103 (98%)	91 (90%)	7 (7%)	3 (3%)	3	19
46	DS	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	13	42
47	CT	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
47	DT	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
48	CU	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
48	DU	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
49	CV	100/103 (97%)	90 (90%)	6 (6%)	4 (4%)	2	14
49	DV	100/103 (97%)	96 (96%)	2 (2%)	2 (2%)	6	26
50	CW	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
50	DW	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
51	CX	73/83 (88%)	72 (99%)	1 (1%)	0	100	100
51	DX	75/83 (90%)	74 (99%)	1 (1%)	0	100	100
52	CY	75/77 (97%)	72 (96%)	3 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	DY	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
53	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	30
53	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
54	DI	133/135 (98%)	112 (84%)	15 (11%)	6 (4%)	2	12
All	All	11407/11651 (98%)	10682 (94%)	590 (5%)	135 (1%)	11	38

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	126	PHE
3	AC	156	ARG
13	AM	5	ALA
17	AQ	82	ALA
22	C1	25	VAL

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%)	172 (92%)	14 (8%)	11	36
2	BB	186/186 (100%)	171 (92%)	15 (8%)	9	33
3	AC	170/170 (100%)	159 (94%)	11 (6%)	14	41
3	BC	170/170 (100%)	157 (92%)	13 (8%)	11	36
4	AD	172/172 (100%)	165 (96%)	7 (4%)	26	57
4	BD	172/172 (100%)	165 (96%)	7 (4%)	26	57
5	AE	118/118 (100%)	105 (89%)	13 (11%)	5	21
5	BE	113/118 (96%)	92 (81%)	21 (19%)	1	6
6	AF	92/92 (100%)	84 (91%)	8 (9%)	8	31
6	BF	87/92 (95%)	76 (87%)	11 (13%)	3	15
7	AG	124/124 (100%)	112 (90%)	12 (10%)	6	25
7	BG	124/124 (100%)	109 (88%)	15 (12%)	4	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AH	104/104 (100%)	90 (86%)	14 (14%)	3	13
8	BH	104/104 (100%)	91 (88%)	13 (12%)	3	15
9	AI	105/105 (100%)	100 (95%)	5 (5%)	21	51
9	BI	105/105 (100%)	100 (95%)	5 (5%)	21	51
10	AJ	87/87 (100%)	80 (92%)	7 (8%)	10	34
10	BJ	86/87 (99%)	76 (88%)	10 (12%)	4	18
11	AK	90/90 (100%)	90 (100%)	0	100	100
11	BK	90/90 (100%)	84 (93%)	6 (7%)	13	40
12	AL	102/102 (100%)	96 (94%)	6 (6%)	16	44
12	BL	102/102 (100%)	95 (93%)	7 (7%)	13	39
13	AM	92/92 (100%)	83 (90%)	9 (10%)	6	25
13	BM	92/92 (100%)	85 (92%)	7 (8%)	11	36
14	AN	83/83 (100%)	82 (99%)	1 (1%)	67	83
14	BN	83/83 (100%)	81 (98%)	2 (2%)	44	70
15	AO	76/76 (100%)	71 (93%)	5 (7%)	14	41
15	BO	76/76 (100%)	68 (90%)	8 (10%)	5	22
16	AP	65/65 (100%)	64 (98%)	1 (2%)	60	80
16	BP	65/65 (100%)	60 (92%)	5 (8%)	10	35
17	AQ	74/74 (100%)	65 (88%)	9 (12%)	4	16
17	BQ	74/74 (100%)	63 (85%)	11 (15%)	2	10
18	AR	48/48 (100%)	45 (94%)	3 (6%)	15	42
18	BR	48/48 (100%)	47 (98%)	1 (2%)	48	72
19	AS	70/70 (100%)	61 (87%)	9 (13%)	3	15
19	BS	70/70 (100%)	63 (90%)	7 (10%)	6	24
20	AT	65/65 (100%)	59 (91%)	6 (9%)	7	28
20	BT	65/65 (100%)	56 (86%)	9 (14%)	3	13
21	AU	48/48 (100%)	45 (94%)	3 (6%)	15	42
21	BU	48/48 (100%)	46 (96%)	2 (4%)	25	56
22	C1	47/47 (100%)	45 (96%)	2 (4%)	25	55
22	D1	47/47 (100%)	46 (98%)	1 (2%)	48	72
23	C2	45/46 (98%)	42 (93%)	3 (7%)	13	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	D2	45/46 (98%)	40 (89%)	5 (11%)	5	20
24	C3	38/38 (100%)	37 (97%)	1 (3%)	41	68
24	D3	38/38 (100%)	37 (97%)	1 (3%)	41	68
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%)	40 (83%)	8 (17%)	2	7
27	D0	49/48 (102%)	45 (92%)	4 (8%)	9	33
29	CC	216/217 (100%)	203 (94%)	13 (6%)	16	44
29	DC	216/217 (100%)	208 (96%)	8 (4%)	29	59
30	CD	164/164 (100%)	156 (95%)	8 (5%)	21	51
32	DD	163/163 (100%)	157 (96%)	6 (4%)	29	59
33	CE	165/165 (100%)	150 (91%)	15 (9%)	7	28
33	DE	165/165 (100%)	160 (97%)	5 (3%)	36	64
34	CF	148/149 (99%)	133 (90%)	15 (10%)	6	23
34	DF	148/149 (99%)	137 (93%)	11 (7%)	11	36
35	CG	137/137 (100%)	132 (96%)	5 (4%)	30	60
35	DG	137/137 (100%)	133 (97%)	4 (3%)	37	65
36	CH	114/114 (100%)	101 (89%)	13 (11%)	4	19
36	DH	114/114 (100%)	104 (91%)	10 (9%)	8	30
37	CJ	104/105 (99%)	99 (95%)	5 (5%)	21	51
37	DJ	104/105 (99%)	99 (95%)	5 (5%)	21	51
38	CK	116/116 (100%)	112 (97%)	4 (3%)	32	62
38	DK	116/116 (100%)	114 (98%)	2 (2%)	56	78
39	CL	103/104 (99%)	95 (92%)	8 (8%)	10	35
39	DL	104/104 (100%)	97 (93%)	7 (7%)	13	40
40	CM	103/103 (100%)	95 (92%)	8 (8%)	10	35
40	DM	103/103 (100%)	98 (95%)	5 (5%)	21	51
41	CN	108/108 (100%)	103 (95%)	5 (5%)	23	52
41	DN	109/108 (101%)	107 (98%)	2 (2%)	54	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	CO	100/102 (98%)	92 (92%)	8 (8%)	10	34
42	DO	102/102 (100%)	98 (96%)	4 (4%)	27	58
43	CP	86/87 (99%)	80 (93%)	6 (7%)	12	39
43	DP	87/87 (100%)	84 (97%)	3 (3%)	32	62
44	CQ	99/99 (100%)	92 (93%)	7 (7%)	12	39
44	DQ	99/99 (100%)	94 (95%)	5 (5%)	20	49
45	CR	89/89 (100%)	84 (94%)	5 (6%)	17	46
45	DR	89/89 (100%)	86 (97%)	3 (3%)	32	62
46	CS	84/84 (100%)	78 (93%)	6 (7%)	12	39
46	DS	84/84 (100%)	83 (99%)	1 (1%)	67	83
47	CT	93/93 (100%)	90 (97%)	3 (3%)	34	63
47	DT	93/93 (100%)	90 (97%)	3 (3%)	34	63
48	CU	80/80 (100%)	71 (89%)	9 (11%)	4	20
48	DU	80/80 (100%)	78 (98%)	2 (2%)	42	69
49	CV	83/84 (99%)	77 (93%)	6 (7%)	12	38
49	DV	83/84 (99%)	79 (95%)	4 (5%)	21	51
50	CW	78/78 (100%)	74 (95%)	4 (5%)	20	49
50	DW	78/78 (100%)	75 (96%)	3 (4%)	28	59
51	CX	56/62 (90%)	54 (96%)	2 (4%)	30	60
51	DX	58/62 (94%)	54 (93%)	4 (7%)	13	39
52	CY	67/67 (100%)	63 (94%)	4 (6%)	16	44
52	DY	67/67 (100%)	65 (97%)	2 (3%)	36	64
53	CZ	54/54 (100%)	52 (96%)	2 (4%)	29	59
53	DZ	54/54 (100%)	54 (100%)	0	100	100
54	DI	103/103 (100%)	97 (94%)	6 (6%)	17	45
All	All	9461/9494 (100%)	8844 (94%)	617 (6%)	14	41

5 of 617 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	CN	78	LEU
40	DM	107	PHE
43	CP	49	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	CN	75	GLU
52	CY	25	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
8	BH	4	GLN
20	BT	3	ASN
35	DG	116	GLN
17	BQ	51	ASN
35	CG	38	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	263 (17%)	31 (2%)
1	BA	1529/1534 (99%)	264 (17%)	36 (2%)
28	CB	117/120 (97%)	12 (10%)	0
28	DB	119/120 (99%)	10 (8%)	0
31	CA	2892/2904 (99%)	466 (16%)	78 (2%)
55	DA	2880/2904 (99%)	404 (14%)	62 (2%)
All	All	9067/9116 (99%)	1419 (15%)	207 (2%)

5 of 1419 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	6	G
1	AA	9	G
1	AA	22	G

5 of 207 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	CA	1536	C
31	CA	2873	A
55	DA	2406	A
31	CA	1647	U
31	CA	2157	G

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

75 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$
55	PSU	DA	2605	55	18,21,22	0.45	0	21,30,33	0.53	0
1	2MG	BA	1207	1	18,26,27	0.82	1 (5%)	16,38,41	0.58	0
1	MA6	BA	1518	1	19,26,27	0.80	0	18,38,41	1.29	2 (11%)
1	2MG	BA	1516	1	18,26,27	0.82	1 (5%)	16,38,41	0.65	0
55	H2U	DA	2449	55	18,21,22	0.47	0	19,30,33	0.67	1 (5%)
55	PSU	DA	955	55	18,21,22	0.67	0	21,30,33	0.53	0
55	PSU	DA	1917	55	18,21,22	0.35	0	21,30,33	0.41	0
55	1MG	DA	745	55	19,26,27	1.25	3 (15%)	18,39,42	0.58	0
31	2MA	CA	2503	31	17,25,26	0.94	1 (5%)	16,37,40	2.22	1 (6%)
55	5MU	DA	1939	55	19,22,23	0.48	0	27,32,35	0.43	0
55	5MC	DA	1962	55	19,22,23	0.54	0	26,32,35	0.44	0
1	MA6	BA	1519	1	19,26,27	0.95	0	18,38,41	1.11	2 (11%)
1	5MC	AA	1407	1	19,22,23	0.40	0	26,32,35	0.53	0
1	MA6	AA	1519	1	19,26,27	0.95	0	18,38,41	1.11	2 (11%)
1	2MG	AA	1207	1	18,26,27	0.89	0	16,38,41	0.60	0
55	2MG	DA	1835	55	18,26,27	0.95	1 (5%)	16,38,41	0.54	0
31	6MZ	CA	1618	31	17,25,26	0.99	0	15,36,39	0.98	1 (6%)
1	2MG	AA	1516	1	18,26,27	0.83	1 (5%)	16,38,41	0.62	0
55	2MA	DA	2503	55,56	17,25,26	0.96	1 (5%)	16,37,40	2.21	1 (6%)
1	2MG	AA	966	1	18,26,27	0.77	0	16,38,41	0.73	0
31	PSU	CA	2605	31	18,21,22	0.45	0	21,30,33	0.58	0
1	4OC	AA	1402	1	20,23,24	0.34	0	25,32,35	0.44	0
12	D2T	BL	89	12	8,9,10	1.24	1 (12%)	6,11,13	1.33	1 (16%)
1	UR3	BA	1498	1	19,22,23	0.85	0	26,32,35	0.72	1 (3%)
55	PSU	DA	746	55,56	18,21,22	0.94	1 (5%)	21,30,33	0.32	0
12	D2T	AL	89	12	8,9,10	1.37	2 (25%)	6,11,13	1.15	0
31	PSU	CA	2504	31	18,21,22	0.36	0	21,30,33	0.43	0
55	6MZ	DA	1618	55	17,25,26	0.88	1 (5%)	15,36,39	2.04	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PSU	DA	2604	55	18,21,22	0.79	0	21,30,33	0.52	0
31	2MG	CA	2445	31	18,26,27	0.96	0	16,38,41	0.62	0
55	3TD	DA	1915	55	19,22,23	0.51	0	23,32,35	0.90	1 (4%)
31	PSU	CA	1911	31	18,21,22	0.27	0	21,30,33	0.40	0
1	PSU	BA	516	1	18,21,22	0.37	0	21,30,33	0.46	0
1	5MC	BA	1407	1	19,22,23	0.41	0	26,32,35	0.51	0
31	3TD	CA	1915	31	19,22,23	0.51	0	23,32,35	0.85	1 (4%)
55	5MU	DA	747	55	19,22,23	0.41	0	27,32,35	0.32	0
55	OMU	DA	2552	55	19,22,23	0.47	0	25,31,34	0.31	0
55	6MZ	DA	2030	55	17,25,26	1.16	2 (11%)	15,36,39	1.09	2 (13%)
31	5MC	CA	1962	31	19,22,23	0.28	0	26,32,35	0.37	0
1	5MC	BA	967	1	19,22,23	0.30	0	26,32,35	0.40	0
1	UR3	AA	1498	1	19,22,23	0.48	0	26,32,35	0.33	0
31	PSU	CA	746	56,31	18,21,22	0.54	1 (5%)	21,30,33	0.43	0
31	PSU	CA	955	31	18,21,22	0.31	0	21,30,33	0.50	0
55	2MG	DA	2445	55	18,26,27	0.88	0	16,38,41	0.63	0
55	OMC	DA	2498	55,56	19,22,23	0.34	0	25,31,34	0.52	0
1	2MG	BA	966	1	18,26,27	0.79	0	16,38,41	0.60	0
31	1MG	CA	745	31	19,26,27	1.20	2 (10%)	18,39,42	0.72	1 (5%)
1	7MG	BA	527	1	23,26,27	4.15	2 (8%)	27,39,42	2.58	6 (22%)
55	PSU	DA	2504	55	18,21,22	0.46	0	21,30,33	0.41	0
55	7MG	DA	2069	55	23,26,27	4.17	3 (13%)	27,39,42	2.19	6 (22%)
55	PSU	DA	1911	55	18,21,22	0.28	0	21,30,33	0.39	0
1	MA6	AA	1518	1	19,26,27	0.85	0	18,38,41	1.27	2 (11%)
31	5MU	CA	1939	31	19,22,23	0.43	0	27,32,35	0.36	0
31	PSU	CA	2457	31	18,21,22	0.66	0	21,30,33	0.48	0
31	OMG	CA	2251	31	19,26,27	0.78	0	21,38,41	0.67	0
31	PSU	CA	2580	31	18,21,22	0.50	0	21,30,33	0.60	0
55	PSU	DA	2457	55	18,21,22	0.54	0	21,30,33	0.46	0
1	PSU	AA	516	56,1	18,21,22	0.33	0	21,30,33	0.48	0
1	5MC	AA	967	1	19,22,23	0.32	0	26,32,35	0.42	0
55	OMG	DA	2251	55	19,26,27	1.03	1 (5%)	21,38,41	0.51	0
1	4OC	BA	1402	1	20,23,24	0.34	0	25,32,35	0.45	0
31	7MG	CA	2069	31	23,26,27	4.11	3 (13%)	27,39,42	2.35	6 (22%)
1	7MG	AA	527	1	23,26,27	4.19	2 (8%)	27,39,42	2.57	6 (22%)
31	5MU	CA	747	31	19,22,23	0.39	0	27,32,35	0.30	0
31	OMU	CA	2552	31	19,22,23	0.30	0	25,31,34	0.28	0
32	MEQ	DD	150[A]	32	8,9,10	0.39	0	5,10,12	0.53	0
55	PSU	DA	2580	55	18,21,22	0.74	0	21,30,33	0.63	0
41	4D4	DN	81[A]	-	9,11,12	1.77	2 (22%)	7,13,15	2.46	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	4D4	DN	81[B]	-	9,11,12	1.85	2 (22%)	7,13,15	2.69	2 (28%)
31	6MZ	CA	2030	31	17,25,26	0.87	0	15,36,39	0.93	1 (6%)
41	4D4	CN	81	41	9,11,12	2.30	2 (22%)	7,13,15	2.55	2 (28%)
31	2MG	CA	1835	31	18,26,27	0.97	2 (11%)	16,38,41	0.49	0
32	MEQ	DD	150[B]	32	8,9,10	0.98	1 (12%)	5,10,12	0.73	0
31	PSU	CA	1917	31	18,21,22	0.31	0	21,30,33	0.40	0
31	OMC	CA	2498	56,31	19,22,23	0.46	0	25,31,34	0.52	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
55	PSU	DA	2605	55	-	0/7/25/26	0/2/2/2
1	2MG	BA	1207	1	-	0/5/27/28	0/3/3/3
1	MA6	BA	1518	1	-	0/7/29/30	0/3/3/3
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
55	H2U	DA	2449	55	-	0/7/38/39	0/2/2/2
55	PSU	DA	955	55	-	0/7/25/26	0/2/2/2
55	PSU	DA	1917	55	-	0/7/25/26	0/2/2/2
55	1MG	DA	745	55	-	0/3/25/26	0/3/3/3
31	2MA	CA	2503	31	-	1/3/25/26	0/3/3/3
55	5MU	DA	1939	55	-	0/7/25/26	0/2/2/2
55	5MC	DA	1962	55	-	2/7/25/26	0/2/2/2
1	MA6	BA	1519	1	-	3/7/29/30	0/3/3/3
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	3/7/29/30	0/3/3/3
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
55	2MG	DA	1835	55	-	2/5/27/28	0/3/3/3
31	6MZ	CA	1618	31	-	1/5/27/28	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
55	2MA	DA	2503	55,56	-	1/3/25/26	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1	-	1/9/29/30	0/2/2/2
12	D2T	BL	89	12	-	4/7/12/14	-
1	UR3	BA	1498	1	-	0/7/25/26	0/2/2/2
55	PSU	DA	746	55,56	-	2/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	1/7/12/14	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PSU	CA	2504	31	-	1/7/25/26	0/2/2/2
55	6MZ	DA	1618	55	-	0/5/27/28	0/3/3/3
55	PSU	DA	2604	55	-	0/7/25/26	0/2/2/2
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3
55	3TD	DA	1915	55	-	0/7/25/26	0/2/2/2
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
1	5MC	BA	1407	1	-	0/7/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
55	5MU	DA	747	55	-	1/7/25/26	0/2/2/2
55	OMU	DA	2552	55	-	1/9/27/28	0/2/2/2
55	6MZ	DA	2030	55	-	2/5/27/28	0/3/3/3
31	5MC	CA	1962	31	-	0/7/25/26	0/2/2/2
1	5MC	BA	967	1	-	0/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
31	PSU	CA	746	56,31	-	2/7/25/26	0/2/2/2
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
55	2MG	DA	2445	55	-	2/5/27/28	0/3/3/3
55	OMC	DA	2498	55,56	-	0/9/27/28	0/2/2/2
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
1	7MG	BA	527	1	-	2/7/37/38	0/3/3/3
55	PSU	DA	2504	55	-	1/7/25/26	0/2/2/2
55	7MG	DA	2069	55	-	1/7/37/38	0/3/3/3
55	PSU	DA	1911	55	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
31	5MU	CA	1939	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	OMG	CA	2251	31	-	0/5/27/28	0/3/3/3
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
55	PSU	DA	2457	55	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	56,1	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
55	OMG	DA	2251	55	-	1/5/27/28	0/3/3/3
1	4OC	BA	1402	1	-	1/9/29/30	0/2/2/2
31	7MG	CA	2069	31	-	0/7/37/38	0/3/3/3
1	7MG	AA	527	1	-	2/7/37/38	0/3/3/3
31	5MU	CA	747	31	-	0/7/25/26	0/2/2/2
31	OMU	CA	2552	31	-	1/9/27/28	0/2/2/2
32	MEQ	DD	150[A]	32	-	4/8/9/11	-
55	PSU	DA	2580	55	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	4D4	DN	81[A]	-	-	1/11/12/14	-
41	4D4	DN	81[B]	-	-	3/11/12/14	-
31	6MZ	CA	2030	31	-	2/5/27/28	0/3/3/3
41	4D4	CN	81	41	-	1/11/12/14	-
31	2MG	CA	1835	31	-	1/5/27/28	0/3/3/3
32	MEQ	DD	150[B]	32	-	4/8/9/11	-
31	PSU	CA	1917	31	-	0/7/25/26	0/2/2/2
31	OMC	CA	2498	56,31	-	0/9/27/28	0/2/2/2

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	527	7MG	C8-N9	-19.65	1.33	1.45
55	DA	2069	7MG	C8-N9	-19.53	1.33	1.45
1	BA	527	7MG	C8-N9	-19.48	1.33	1.45
31	CA	2069	7MG	C8-N9	-19.17	1.33	1.45
41	CN	81	4D4	CZ-NE	6.24	1.45	1.33

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	CA	2503	2MA	C4-N3-C2	-8.53	116.75	123.30
55	DA	2503	2MA	C4-N3-C2	-8.44	116.82	123.30
55	DA	1618	6MZ	C9-N6-C6	-7.33	116.06	122.85
1	BA	527	7MG	C6-C5-N7	-6.55	121.78	131.93
1	AA	527	7MG	O4'-C1'-N9	6.49	118.14	109.30

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	7MG	O4'-C4'-C5'-O5'
1	BA	527	7MG	O4'-C4'-C5'-O5'
1	BA	527	7MG	C3'-C4'-C5'-O5'
32	DD	150[A]	MEQ	N-CA-CB-CG
32	DD	150[A]	MEQ	C-CA-CB-CG

There are no ring outliers.

18 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	BA	1518	MA6	1	0
55	DA	745	1MG	1	0
31	CA	2503	2MA	1	0
1	BA	1519	MA6	1	0
1	AA	1519	MA6	1	0
55	DA	2503	2MA	1	0
31	CA	1915	3TD	1	0
55	DA	2030	6MZ	1	0
1	BA	967	5MC	1	0
55	DA	2498	OMC	1	0
1	AA	1518	MA6	1	0
31	CA	2580	PSU	1	0
1	AA	967	5MC	1	0
55	DA	2251	OMG	1	0
32	DD	150[A]	MEQ	3	0
31	CA	2030	6MZ	1	0
32	DD	150[B]	MEQ	1	0
31	CA	2498	OMC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 557 ligands modelled in this entry, 475 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	$\# Z > 2$
62	PEG	AL	201	-	6,6,6	0.23	0	5,5,5	0.12	0
64	PGE	DA	3203	-	9,9,9	0.21	0	8,8,8	0.20	0
63	EDO	DA	3194	-	3,3,3	0.72	0	2,2,2	0.15	0
58	MPD	DE	301	-	7,7,7	0.72	0	9,10,10	0.60	0
57	PG4	BA	1642	-	12,12,12	0.15	0	11,11,11	0.19	0
67	ACY	DA	3191	-	3,3,3	0.59	0	3,3,3	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	PUT	DA	3223	-	5,5,5	0.16	0	4,4,4	0.12	0
69	TRS	DA	3220	-	7,7,7	0.31	0	9,9,9	0.34	0
64	PGE	DA	3186	-	9,9,9	0.24	0	8,8,8	0.29	0
63	EDO	DA	3002	-	3,3,3	0.62	0	2,2,2	0.24	0
59	PUT	AA	1672	-	5,5,5	0.19	0	4,4,4	0.21	0
63	EDO	DB	211	-	3,3,3	0.64	0	2,2,2	0.14	0
59	PUT	DA	3188	-	5,5,5	0.20	0	4,4,4	0.13	0
62	PEG	DP	201	-	6,6,6	0.16	0	5,5,5	0.08	0
64	PGE	D1	102	-	9,9,9	0.20	0	8,8,8	0.14	0
63	EDO	DA	3215	-	3,3,3	0.62	0	2,2,2	0.23	0
65	SPD	DA	3187	-	9,9,9	0.21	0	8,8,8	0.19	0
59	PUT	DA	3205	-	5,5,5	0.11	0	4,4,4	0.10	0
58	MPD	DA	3207	-	7,7,7	0.68	0	9,10,10	0.53	0
59	PUT	DA	3184	-	5,5,5	0.15	0	4,4,4	0.11	0
68	GUN	DA	3211	-	7,12,12	0.36	0	8,17,17	0.71	0
59	PUT	AA	1675	-	5,5,5	0.20	0	4,4,4	0.13	0
63	EDO	DA	3197	-	3,3,3	0.60	0	2,2,2	0.24	0
59	PUT	AA	1674	-	5,5,5	0.14	0	4,4,4	0.10	0
63	EDO	DB	213	-	3,3,3	0.66	0	2,2,2	0.08	0
58	MPD	AA	1676	-	7,7,7	0.53	0	9,10,10	0.59	0
64	PGE	DU	101	-	9,9,9	0.23	0	8,8,8	0.12	0
66	1PE	DA	3202	-	15,15,15	0.32	0	14,14,14	0.34	0
57	PG4	DA	3216	-	12,12,12	0.10	0	11,11,11	0.17	0
67	ACY	DA	3201	-	3,3,3	0.76	0	3,3,3	1.05	0
57	PG4	DR	202	-	12,12,12	0.26	0	11,11,11	0.36	0
59	PUT	DA	3189	-	5,5,5	0.29	0	4,4,4	0.20	0
59	PUT	DA	3221	-	5,5,5	0.16	0	4,4,4	0.11	0
63	EDO	DA	3198	-	3,3,3	0.59	0	2,2,2	0.24	0
62	PEG	DA	3227	-	6,6,6	0.22	0	5,5,5	0.14	0
64	PGE	D3	101	-	9,9,9	0.23	0	8,8,8	0.22	0
59	PUT	AA	1673	-	5,5,5	0.10	0	4,4,4	0.07	0
58	MPD	DA	3190	-	7,7,7	0.32	0	9,10,10	0.52	0
58	MPD	DT	201	-	7,7,7	0.46	0	9,10,10	0.35	0
58	MPD	AA	1671	-	7,7,7	0.58	0	9,10,10	0.55	0
64	PGE	DA	3217	-	9,9,9	0.16	0	8,8,8	0.13	0
57	PG4	DA	3193	-	12,12,12	0.29	0	11,11,11	0.25	0
62	PEG	D3	102	-	6,6,6	0.21	0	5,5,5	0.19	0
65	SPD	DA	3183	-	9,9,9	0.10	0	8,8,8	0.10	0
57	PG4	DS	202	-	12,12,12	0.46	0	11,11,11	0.29	0
58	MPD	DA	3204	-	7,7,7	0.69	0	9,10,10	0.69	0
67	ACY	DA	3196	-	3,3,3	2.27	1 (33%)	3,3,3	2.32	2 (66%)
58	MPD	DA	3192	-	7,7,7	0.45	0	9,10,10	0.58	0
59	PUT	DA	3222	-	5,5,5	0.44	0	4,4,4	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
66	1PE	DA	3185	-	15,15,15	0.19	0	14,14,14	0.21	0
58	MPD	DE	302	-	7,7,7	0.79	0	9,10,10	0.61	0
64	PGE	DS	201	-	9,9,9	0.25	0	8,8,8	0.20	0
62	PEG	DA	3218	-	6,6,6	0.17	0	5,5,5	0.08	0
62	PEG	DA	3200	-	6,6,6	0.35	0	5,5,5	0.21	0
62	PEG	DA	3226	-	6,6,6	0.24	0	5,5,5	0.12	0
58	MPD	DT	202	-	7,7,7	0.62	0	9,10,10	0.38	0
63	EDO	D1	101	-	3,3,3	0.56	0	2,2,2	0.15	0
59	PUT	DA	3213	-	5,5,5	0.16	0	4,4,4	0.17	0
62	PEG	DA	3199	-	6,6,6	0.24	0	5,5,5	0.15	0
62	PEG	DQ	201	-	6,6,6	0.13	0	5,5,5	0.09	0
62	PEG	DL	201	-	6,6,6	0.07	0	5,5,5	0.10	0
60	T1C	AA	1680	56	45,45,45	1.06	3 (6%)	56,72,72	1.56	4 (7%)
63	EDO	DB	201	-	3,3,3	0.61	0	2,2,2	0.19	0
57	PG4	AA	1670	-	12,12,12	0.31	0	11,11,11	0.28	0
63	EDO	DA	3209	-	3,3,3	0.54	0	2,2,2	0.32	0
60	T1C	BA	1643	56	45,45,45	1.05	3 (6%)	56,72,72	1.64	7 (12%)
59	PUT	DA	3001	-	5,5,5	0.24	0	4,4,4	0.13	0
58	MPD	DK	201	-	7,7,7	0.58	0	9,10,10	0.28	0
59	PUT	DA	3195	-	5,5,5	0.31	0	4,4,4	0.36	0
65	SPD	DA	3206	-	9,9,9	0.20	0	8,8,8	0.17	0
64	PGE	DA	3214	-	9,9,9	0.19	0	8,8,8	0.27	0
59	PUT	DA	3212	-	5,5,5	0.17	0	4,4,4	0.04	0
62	PEG	D1	103	-	6,6,6	0.31	0	5,5,5	0.15	0
65	SPD	DA	3224	-	9,9,9	0.19	0	8,8,8	0.40	0
59	PUT	DA	3219	-	5,5,5	0.16	0	4,4,4	0.20	0
63	EDO	DB	212	-	3,3,3	0.52	0	2,2,2	0.34	0
58	MPD	DS	203	-	7,7,7	0.31	0	9,10,10	0.52	0
57	PG4	DQ	202	-	12,12,12	0.20	0	11,11,11	0.14	0
63	EDO	DA	3208	-	3,3,3	0.60	0	2,2,2	0.22	0
58	MPD	DA	3210	-	7,7,7	0.56	0	9,10,10	0.30	0
58	MPD	DN	201	-	7,7,7	0.79	0	9,10,10	0.54	0
64	PGE	DA	3225	-	9,9,9	0.12	0	8,8,8	0.17	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
62	PEG	AL	201	-	-	2/4/4/4	-
64	PGE	DA	3203	-	-	5/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	EDO	DA	3194	-	-	0/1/1/1	-
58	MPD	DE	301	-	-	2/5/5/5	-
57	PG4	BA	1642	-	-	0/10/10/10	-
59	PUT	DA	3223	-	-	1/3/3/3	-
69	TRS	DA	3220	-	-	0/9/9/9	-
64	PGE	DA	3186	-	-	3/7/7/7	-
63	EDO	DA	3002	-	-	0/1/1/1	-
59	PUT	AA	1672	-	-	0/3/3/3	-
63	EDO	DB	211	-	-	0/1/1/1	-
59	PUT	DA	3188	-	-	0/3/3/3	-
62	PEG	DP	201	-	-	2/4/4/4	-
64	PGE	D1	102	-	-	3/7/7/7	-
63	EDO	DA	3215	-	-	1/1/1/1	-
65	SPD	DA	3187	-	-	2/7/7/7	-
59	PUT	DA	3205	-	-	0/3/3/3	-
58	MPD	DA	3207	-	-	2/5/5/5	-
59	PUT	DA	3184	-	-	0/3/3/3	-
68	GUN	DA	3211	-	-	-	0/2/2/2
59	PUT	AA	1675	-	-	1/3/3/3	-
63	EDO	DA	3197	-	-	0/1/1/1	-
59	PUT	AA	1674	-	-	0/3/3/3	-
63	EDO	DB	213	-	-	0/1/1/1	-
58	MPD	AA	1676	-	-	4/5/5/5	-
64	PGE	DU	101	-	-	3/7/7/7	-
66	1PE	DA	3202	-	-	4/13/13/13	-
57	PG4	DA	3216	-	-	3/10/10/10	-
57	PG4	DR	202	-	-	5/10/10/10	-
59	PUT	DA	3189	-	-	0/3/3/3	-
59	PUT	DA	3221	-	-	0/3/3/3	-
63	EDO	DA	3198	-	-	1/1/1/1	-
62	PEG	DA	3227	-	-	0/4/4/4	-
64	PGE	D3	101	-	-	2/7/7/7	-
59	PUT	AA	1673	-	-	0/3/3/3	-
58	MPD	DA	3190	-	-	2/5/5/5	-
58	MPD	DT	201	-	-	3/5/5/5	-
58	MPD	AA	1671	-	-	0/5/5/5	-
64	PGE	DA	3217	-	-	4/7/7/7	-
57	PG4	DA	3193	-	-	5/10/10/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PEG	D3	102	-	-	1/4/4/4	-
65	SPD	DA	3183	-	-	1/7/7/7	-
57	PG4	DS	202	-	-	5/10/10/10	-
58	MPD	DA	3204	-	-	4/5/5/5	-
58	MPD	DA	3192	-	-	1/5/5/5	-
59	PUT	DA	3222	-	-	0/3/3/3	-
66	1PE	DA	3185	-	-	5/13/13/13	-
58	MPD	DE	302	-	-	2/5/5/5	-
64	PGE	DS	201	-	-	3/7/7/7	-
62	PEG	DA	3218	-	-	1/4/4/4	-
62	PEG	DA	3200	-	-	2/4/4/4	-
62	PEG	DA	3226	-	-	2/4/4/4	-
58	MPD	DT	202	-	-	2/5/5/5	-
63	EDO	D1	101	-	-	0/1/1/1	-
59	PUT	DA	3213	-	-	0/3/3/3	-
62	PEG	DA	3199	-	-	2/4/4/4	-
62	PEG	DQ	201	-	-	1/4/4/4	-
62	PEG	DL	201	-	-	2/4/4/4	-
60	T1C	AA	1680	56	-	6/22/80/80	0/4/4/4
63	EDO	DB	201	-	-	1/1/1/1	-
57	PG4	AA	1670	-	-	4/10/10/10	-
63	EDO	DA	3209	-	-	0/1/1/1	-
60	T1C	BA	1643	56	-	11/22/80/80	0/4/4/4
59	PUT	DA	3001	-	-	0/3/3/3	-
58	MPD	DK	201	-	-	2/5/5/5	-
59	PUT	DA	3195	-	-	1/3/3/3	-
65	SPD	DA	3206	-	-	3/7/7/7	-
64	PGE	DA	3214	-	-	2/7/7/7	-
59	PUT	DA	3212	-	-	0/3/3/3	-
62	PEG	D1	103	-	-	0/4/4/4	-
65	SPD	DA	3224	-	-	3/7/7/7	-
59	PUT	DA	3219	-	-	0/3/3/3	-
63	EDO	DB	212	-	-	1/1/1/1	-
58	MPD	DS	203	-	-	1/5/5/5	-
57	PG4	DQ	202	-	-	1/10/10/10	-
63	EDO	DA	3208	-	-	0/1/1/1	-
58	MPD	DA	3210	-	-	0/5/5/5	-
58	MPD	DN	201	-	-	2/5/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	PGE	DA	3225	-	-	4/7/7/7	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	DA	3196	ACY	O-C	3.74	1.38	1.22
60	BA	1643	T1C	C4-C3	3.30	1.58	1.51
60	AA	1680	T1C	C4-C3	2.99	1.57	1.51
60	AA	1680	T1C	C7-C61	2.96	1.43	1.40
60	BA	1643	T1C	C7-C61	2.91	1.43	1.40

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	1643	T1C	C92-N92-C93	7.92	125.80	115.77
60	AA	1680	T1C	C92-N92-C93	7.68	125.49	115.77
60	AA	1680	T1C	C8-C9-C10	-5.29	115.41	120.53
60	BA	1643	T1C	C8-C9-C10	-4.69	115.98	120.53
60	BA	1643	T1C	C61-C6-C51	-3.60	108.36	113.12

There are no chirality outliers.

5 of 136 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AA	1676	MPD	C2-C3-C4-C5
58	DA	3192	MPD	C2-C3-C4-O4
60	AA	1680	T1C	C95-C93-N92-C92
60	AA	1680	T1C	C96-C93-N92-C92
60	AA	1680	T1C	C91-C92-N92-C93

There are no ring outliers.

24 monomers are involved in 32 short contacts:

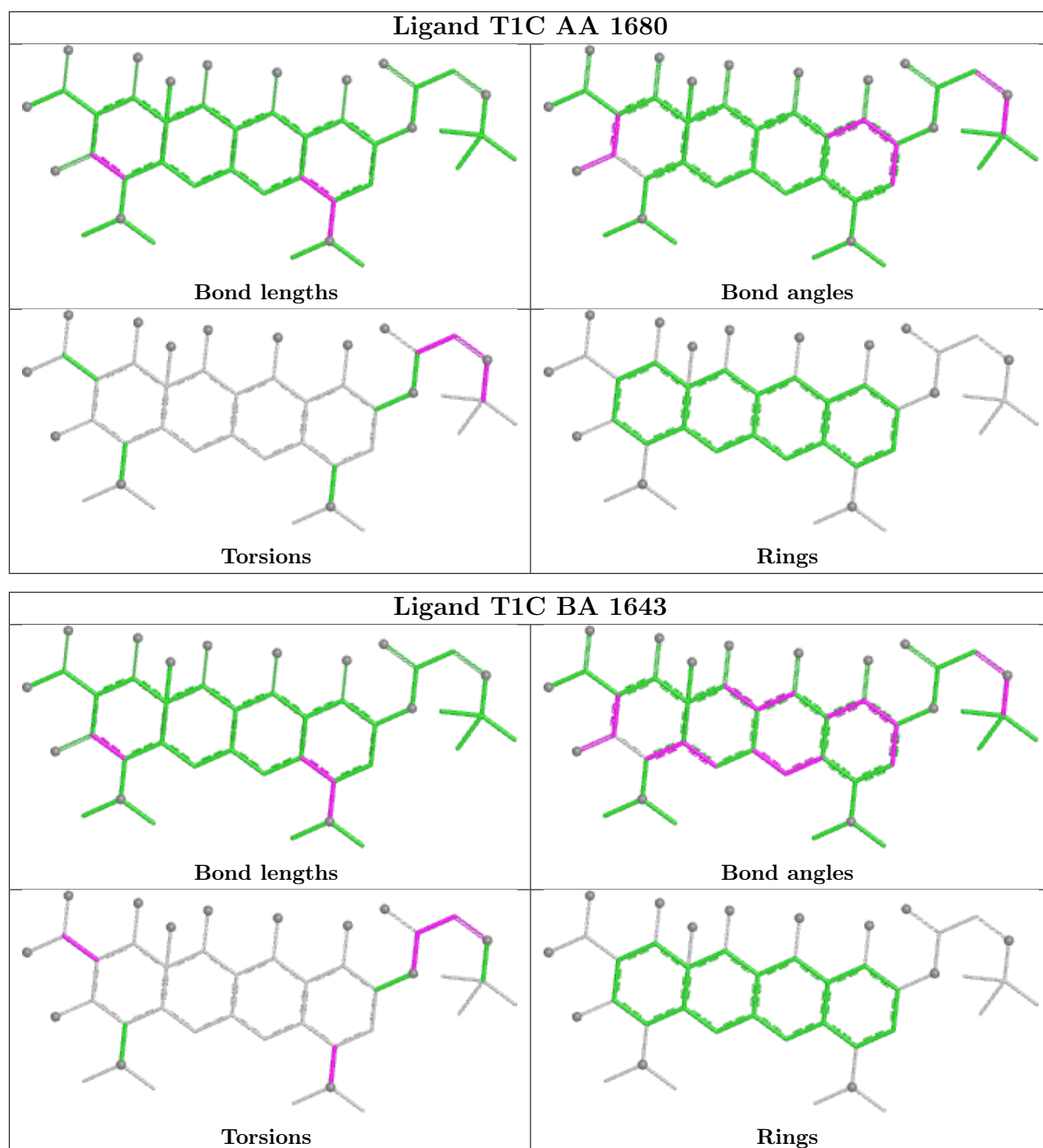
Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	DA	3203	PGE	1	0
57	BA	1642	PG4	1	0
59	DA	3223	PUT	1	0
69	DA	3220	TRS	1	0
64	D1	102	PGE	2	0
64	DU	101	PGE	1	0
66	DA	3202	1PE	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	DR	202	PG4	4	0
64	DA	3217	PGE	1	0
57	DS	202	PG4	1	0
58	DA	3204	MPD	1	0
58	DA	3192	MPD	1	0
66	DA	3185	1PE	1	0
64	DS	201	PGE	1	0
60	AA	1680	T1C	2	0
57	AA	1670	PG4	1	0
63	DA	3209	EDO	1	0
59	DA	3195	PUT	1	0
64	DA	3214	PGE	1	0
62	D1	103	PEG	1	0
65	DA	3224	SPD	2	0
59	DA	3219	PUT	1	0
58	DN	201	MPD	1	0
64	DA	3225	PGE	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1523/1534 (99%)	0.06	77 (5%) 34 20	43, 96, 240, 296	0
1	BA	1522/1534 (99%)	0.30	81 (5%) 33 20	59, 109, 268, 280	0
2	AB	224/224 (100%)	0.36	7 (3%) 51 32	72, 125, 197, 249	0
2	BB	224/224 (100%)	0.56	14 (6%) 27 16	101, 143, 205, 240	0
3	AC	206/206 (100%)	0.14	6 (2%) 54 34	78, 108, 137, 154	0
3	BC	206/206 (100%)	0.46	11 (5%) 33 20	103, 151, 181, 204	0
4	AD	205/205 (100%)	0.00	0 100 100	71, 104, 137, 164	0
4	BD	205/205 (100%)	-0.22	0 100 100	51, 77, 108, 132	0
5	AE	155/155 (100%)	-0.13	0 100 100	59, 84, 116, 155	0
5	BE	150/155 (96%)	0.27	4 (2%) 56 36	68, 94, 135, 207	0
6	AF	106/106 (100%)	0.15	0 100 100	78, 107, 128, 148	0
6	BF	100/106 (94%)	0.19	3 (3%) 52 33	88, 124, 147, 160	0
7	AG	151/151 (100%)	0.82	15 (9%) 14 8	108, 141, 166, 178	0
7	BG	151/151 (100%)	1.20	28 (18%) 4 2	145, 205, 222, 231	0
8	AH	129/129 (100%)	0.05	3 (2%) 61 42	67, 89, 116, 132	0
8	BH	129/129 (100%)	0.19	6 (4%) 37 22	90, 113, 141, 157	0
9	AI	127/127 (100%)	0.90	12 (9%) 15 9	86, 142, 167, 175	0
9	BI	127/127 (100%)	1.33	26 (20%) 3 2	141, 172, 209, 221	0
10	AJ	99/99 (100%)	1.04	17 (17%) 5 3	91, 129, 150, 161	0
10	BJ	98/99 (98%)	1.39	26 (26%) 2 1	144, 175, 196, 202	0
11	AK	117/117 (100%)	0.33	4 (3%) 48 28	59, 117, 141, 150	0
11	BK	117/117 (100%)	0.50	9 (7%) 21 11	69, 115, 149, 175	0
12	AL	122/123 (99%)	-0.16	1 (0%) 82 68	50, 70, 99, 133	0
12	BL	122/123 (99%)	0.40	10 (8%) 19 11	71, 86, 117, 143	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.99	20 (17%) 5 3	116, 139, 175, 182	0
13	BM	114/114 (100%)	1.03	11 (9%) 15 9	202, 239, 248, 254	0
14	AN	100/100 (100%)	1.31	23 (23%) 2 1	84, 124, 192, 203	0
14	BN	100/100 (100%)	1.23	11 (11%) 12 7	134, 185, 229, 236	0
15	AO	88/88 (100%)	0.08	0 100 100	68, 92, 115, 136	0
15	BO	88/88 (100%)	0.18	1 (1%) 77 61	79, 113, 132, 152	0
16	AP	82/82 (100%)	0.28	3 (3%) 45 27	62, 86, 128, 142	0
16	BP	82/82 (100%)	0.81	6 (7%) 22 13	77, 94, 149, 159	0
17	AQ	80/80 (100%)	0.02	0 100 100	64, 88, 118, 134	0
17	BQ	80/80 (100%)	0.58	4 (5%) 35 21	83, 120, 149, 157	0
18	AR	55/55 (100%)	0.31	1 (1%) 67 49	74, 101, 142, 166	0
18	BR	55/55 (100%)	0.41	4 (7%) 22 13	75, 97, 134, 166	0
19	AS	79/79 (100%)	1.28	15 (18%) 4 2	123, 139, 159, 165	0
19	BS	79/79 (100%)	1.02	14 (17%) 4 2	217, 233, 247, 254	0
20	AT	86/86 (100%)	0.30	2 (2%) 61 42	68, 86, 116, 133	0
20	BT	85/86 (98%)	1.10	17 (20%) 3 2	90, 119, 151, 161	0
21	AU	56/56 (100%)	0.49	4 (7%) 23 14	81, 118, 163, 176	0
21	BU	56/56 (100%)	0.50	4 (7%) 23 14	75, 110, 147, 155	0
22	C1	56/56 (100%)	1.59	17 (30%) 1 1	93, 147, 170, 185	0
22	D1	56/56 (100%)	-0.61	0 100 100	21, 47, 72, 112	0
23	C2	50/51 (98%)	1.48	16 (32%) 1 1	145, 160, 172, 198	0
23	D2	51/51 (100%)	-0.04	1 (1%) 64 45	56, 69, 100, 116	0
24	C3	46/46 (100%)	2.24	22 (47%) 0 0	102, 130, 139, 152	0
24	D3	46/46 (100%)	-0.50	1 (2%) 62 42	30, 40, 58, 116	0
25	C4	64/64 (100%)	2.86	42 (65%) 0 0	108, 134, 150, 160	0
25	D4	64/64 (100%)	-0.42	0 100 100	32, 41, 57, 75	0
26	C5	38/38 (100%)	1.73	12 (31%) 1 1	115, 134, 145, 151	0
26	D5	38/38 (100%)	-0.50	0 100 100	43, 55, 72, 99	0
27	C0	58/58 (100%)	1.63	15 (25%) 2 1	109, 132, 151, 162	0
27	D0	58/58 (100%)	-0.47	2 (3%) 48 28	27, 37, 61, 83	2 (3%)
28	CB	118/120 (98%)	0.64	8 (6%) 25 14	110, 181, 234, 243	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DB	120/120 (100%)	-0.62	0 100 100	34, 63, 99, 131	0
29	CC	271/272 (99%)	0.61	35 (12%) 9 5	73, 100, 126, 136	0
29	DC	271/272 (99%)	-0.48	4 (1%) 71 54	26, 57, 84, 99	0
30	CD	209/209 (100%)	0.84	20 (9%) 15 9	79, 116, 143, 158	0
31	CA	2876/2904 (99%)	0.70	210 (7%) 22 13	64, 133, 248, 291	0
32	DD	208/209 (99%)	-0.70	1 (0%) 87 75	20, 41, 71, 100	0
33	CE	201/201 (100%)	1.05	27 (13%) 8 5	90, 160, 190, 200	0
33	DE	201/201 (100%)	-0.51	1 (0%) 87 75	25, 62, 104, 136	0
34	CF	177/178 (99%)	0.56	5 (2%) 55 35	201, 219, 227, 235	0
34	DF	177/178 (99%)	0.01	1 (0%) 85 72	54, 89, 132, 150	0
35	CG	176/176 (100%)	0.49	4 (2%) 61 42	140, 167, 194, 206	0
35	DG	176/176 (100%)	-0.19	4 (2%) 61 42	44, 75, 103, 136	0
36	CH	149/149 (100%)	0.32	2 (1%) 74 58	89, 149, 175, 187	0
36	DH	149/149 (100%)	0.47	4 (2%) 56 36	71, 150, 190, 207	0
37	CJ	134/135 (99%)	1.21	24 (17%) 4 2	241, 258, 269, 276	0
37	DJ	134/135 (99%)	1.28	31 (23%) 2 1	210, 234, 245, 252	0
38	CK	142/142 (100%)	0.70	9 (6%) 27 16	84, 109, 134, 142	0
38	DK	142/142 (100%)	-0.75	0 100 100	23, 37, 67, 88	0
39	CL	122/123 (99%)	0.50	7 (5%) 30 18	76, 99, 141, 159	0
39	DL	123/123 (100%)	-0.71	0 100 100	28, 44, 71, 110	0
40	CM	144/144 (100%)	1.19	24 (16%) 5 3	94, 152, 193, 222	0
40	DM	144/144 (100%)	-0.35	1 (0%) 84 70	18, 56, 88, 121	0
41	CN	135/136 (99%)	0.58	10 (7%) 22 13	76, 111, 139, 174	0
41	DN	135/136 (99%)	-0.64	0 100 100	18, 43, 73, 95	1 (0%)
42	CO	120/125 (96%)	1.20	30 (25%) 2 1	93, 124, 143, 189	0
42	DO	125/125 (100%)	-0.66	0 100 100	27, 40, 76, 125	0
43	CP	116/117 (99%)	0.70	10 (8%) 18 10	142, 164, 181, 187	0
43	DP	117/117 (100%)	-0.36	0 100 100	42, 61, 90, 99	0
44	CQ	114/114 (100%)	0.62	11 (9%) 15 9	96, 113, 138, 154	0
44	DQ	114/114 (100%)	-0.45	1 (0%) 81 66	28, 52, 86, 125	0
45	CR	117/117 (100%)	1.02	22 (18%) 4 2	82, 109, 134, 148	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	DR	117/117 (100%)	-0.80	0 100 100	19, 34, 52, 82	0
46	CS	103/103 (100%)	0.89	14 (13%) 8 5	101, 124, 166, 174	0
46	DS	103/103 (100%)	-0.69	2 (1%) 66 47	22, 45, 74, 101	0
47	CT	110/110 (100%)	1.36	23 (20%) 3 2	99, 126, 157, 172	0
47	DT	110/110 (100%)	-0.49	0 100 100	26, 37, 67, 120	0
48	CU	93/93 (100%)	1.46	22 (23%) 2 1	124, 154, 178, 190	0
48	DU	93/93 (100%)	0.05	4 (4%) 40 24	41, 63, 120, 139	0
49	CV	102/103 (99%)	1.57	32 (31%) 1 1	132, 164, 197, 206	0
49	DV	102/103 (99%)	-0.19	3 (2%) 54 34	49, 67, 116, 143	0
50	CW	94/94 (100%)	0.35	5 (5%) 33 20	122, 144, 158, 167	0
50	DW	94/94 (100%)	-0.48	0 100 100	38, 58, 88, 96	0
51	CX	75/83 (90%)	0.91	8 (10%) 12 7	95, 126, 138, 176	0
51	DX	76/83 (91%)	-0.44	1 (1%) 74 58	20, 43, 72, 108	1 (1%)
52	CY	77/77 (100%)	0.99	9 (11%) 10 7	87, 116, 146, 163	0
52	DY	77/77 (100%)	-0.33	1 (1%) 74 58	34, 58, 96, 112	0
53	CZ	62/62 (100%)	1.06	6 (9%) 15 8	139, 171, 185, 191	0
53	DZ	62/62 (100%)	0.30	2 (3%) 50 31	51, 81, 123, 140	0
54	DI	135/135 (100%)	1.14	24 (17%) 4 2	82, 161, 211, 226	1 (0%)
55	DA	2873/2904 (98%)	-0.70	71 (2%) 58 39	18, 47, 217, 299	11 (0%)
All	All	20634/20767 (99%)	0.25	1361 (6%) 26 15	18, 106, 237, 299	16 (0%)

The worst 5 of 1361 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	CA	2172	U	10.7
7	AG	5	ARG	10.5
1	AA	121	U	9.5
25	C4	36	LYS	9.1
31	CA	331	C	8.4

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

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	2MG	BA	966	24/25	0.62	0.14	161,163,169,169	0
1	2MG	BA	1207	24/25	0.64	0.13	169,172,175,177	0
1	5MC	BA	967	21/22	0.72	0.14	156,162,165,165	0
31	PSU	CA	1917	20/21	0.79	0.12	106,115,121,121	0
1	2MG	AA	1207	24/25	0.82	0.12	124,129,130,132	0
31	3TD	CA	1915	21/22	0.85	0.08	132,137,140,141	0
31	PSU	CA	2457	20/21	0.87	0.14	83,88,93,96	0
31	PSU	CA	2504	20/21	0.87	0.15	87,89,95,96	0
1	PSU	BA	516	20/21	0.88	0.10	93,98,101,102	0
31	2MA	CA	2503	23/24	0.88	0.15	90,95,99,100	0
31	PSU	CA	1911	20/21	0.88	0.07	112,123,126,126	0
1	2MG	AA	966	24/25	0.89	0.13	84,94,103,105	0
31	PSU	CA	955	20/21	0.89	0.12	92,93,95,95	0
31	6MZ	CA	1618	23/24	0.90	0.14	112,116,119,120	0
55	PSU	DA	1917	20/21	0.90	0.09	79,84,93,93	0
1	PSU	AA	516	20/21	0.91	0.09	81,85,86,87	0
31	PSU	CA	2580	20/21	0.91	0.09	86,88,93,94	0
55	3TD	DA	1915	21/22	0.91	0.09	105,109,117,117	0
31	6MZ	CA	2030	23/24	0.91	0.12	82,91,100,102	0
12	D2T	AL	89	10/11	0.92	0.12	61,65,85,86	0
1	5MC	BA	1407	21/22	0.92	0.11	81,92,94,95	0
55	PSU	DA	1911	20/21	0.92	0.08	82,85,87,88	0
12	D2T	BL	89	10/11	0.92	0.13	77,82,93,93	0
31	PSU	CA	746	20/21	0.92	0.08	98,101,104,104	0
31	2MG	CA	2445	24/25	0.93	0.15	74,83,85,89	0
31	1MG	CA	745	24/25	0.93	0.10	92,96,97,98	0
1	5MC	AA	967	21/22	0.93	0.12	90,100,103,105	0
31	7MG	CA	2069	24/25	0.93	0.15	84,89,94,94	0
41	4D4	CN	81	12/13	0.93	0.12	85,88,108,110	0
31	OMC	CA	2498	21/22	0.94	0.13	82,84,89,92	0
1	UR3	BA	1498	21/22	0.94	0.09	81,84,87,88	0
31	5MC	CA	1962	21/22	0.94	0.12	67,69,73,76	0
31	5MU	CA	747	21/22	0.94	0.10	95,101,103,106	0
1	7MG	AA	527	24/25	0.95	0.08	60,65,72,74	0
31	OMU	CA	2552	21/22	0.95	0.14	80,82,86,88	0
31	OMG	CA	2251	24/25	0.95	0.10	69,79,82,84	0
1	2MG	BA	1516	24/25	0.95	0.08	67,75,78,81	0
31	5MU	CA	1939	21/22	0.95	0.09	70,73,82,85	0
31	2MG	CA	1835	24/25	0.95	0.09	61,72,77,78	0
1	7MG	BA	527	24/25	0.95	0.08	76,81,88,89	0
31	PSU	CA	2605	20/21	0.96	0.07	73,75,78,80	0
1	MA6	BA	1518	24/25	0.96	0.08	67,73,76,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	MA6	BA	1519	24/25	0.96	0.09	74,77,81,83	0
1	MA6	AA	1518	24/25	0.96	0.08	51,55,58,61	0
1	UR3	AA	1498	21/22	0.96	0.09	58,63,67,70	0
41	4D4	DN	81[A]	12/13	0.96	0.10	32,40,49,51	9
41	4D4	DN	81[B]	12/13	0.96	0.10	12,25,36,36	9
1	5MC	AA	1407	21/22	0.97	0.07	55,57,60,62	0
55	PSU	DA	2604	20/21	0.97	0.07	41,46,56,56	0
1	4OC	BA	1402	22/23	0.97	0.07	79,83,83,84	0
1	4OC	AA	1402	22/23	0.97	0.07	53,61,66,66	0
1	2MG	AA	1516	24/25	0.97	0.07	58,62,63,63	0
32	MEQ	DD	150[B]	10/11	0.98	0.08	23,32,41,41	10
55	5MU	DA	1939	21/22	0.98	0.07	35,37,41,47	0
55	5MC	DA	1962	21/22	0.98	0.08	36,44,48,49	0
55	7MG	DA	2069	24/25	0.98	0.08	32,37,41,43	0
55	2MG	DA	2445	24/25	0.98	0.07	26,29,35,37	0
55	2MA	DA	2503	23/24	0.98	0.06	21,35,41,42	0
55	PSU	DA	2504	20/21	0.98	0.09	37,40,44,44	0
55	OMU	DA	2552	21/22	0.98	0.07	31,34,39,46	0
55	5MU	DA	747	21/22	0.98	0.06	28,33,36,41	0
55	PSU	DA	2605	20/21	0.98	0.06	31,41,43,43	0
55	2MG	DA	1835	24/25	0.98	0.06	41,47,52,52	0
1	MA6	AA	1519	24/25	0.98	0.07	53,56,61,64	0
32	MEQ	DD	150[A]	10/11	0.98	0.08	7,15,29,31	10
55	OMC	DA	2498	21/22	0.99	0.05	21,26,29,30	0
55	PSU	DA	746	20/21	0.99	0.04	21,28,31,35	0
55	1MG	DA	745	24/25	0.99	0.05	25,29,37,41	0
55	6MZ	DA	2030	23/24	0.99	0.05	22,25,29,34	0
55	PSU	DA	2580	20/21	0.99	0.06	20,25,32,34	0
55	PSU	DA	955	20/21	0.99	0.06	25,27,30,30	0
55	OMG	DA	2251	24/25	0.99	0.05	27,32,37,42	0
55	6MZ	DA	1618	23/24	0.99	0.05	26,33,36,36	0
55	H2U	DA	2449	20/21	0.99	0.06	25,29,31,32	0
55	PSU	DA	2457	20/21	0.99	0.04	27,31,37,37	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
56	MG	DA	3168	1/1	0.26	0.31	141,141,141,141	0
56	MG	CA	3154	1/1	0.32	0.36	147,147,147,147	0
56	MG	BA	1624	1/1	0.34	0.14	262,262,262,262	0
56	MG	AA	1628	1/1	0.38	0.18	159,159,159,159	0
56	MG	BA	1639	1/1	0.40	0.32	94,94,94,94	0
56	MG	AA	1677	1/1	0.41	0.18	194,194,194,194	0
56	MG	CA	3122	1/1	0.43	0.58	126,126,126,126	0
56	MG	CA	3038	1/1	0.46	0.11	263,263,263,263	0
56	MG	BA	1641	1/1	0.48	0.23	120,120,120,120	0
56	MG	CA	3132	1/1	0.49	0.27	105,105,105,105	0
56	MG	BA	1640	1/1	0.50	0.54	124,124,124,124	0
56	MG	CA	3060	1/1	0.52	0.15	234,234,234,234	0
56	MG	CA	3075	1/1	0.53	0.26	230,230,230,230	0
56	MG	CA	3077	1/1	0.54	0.15	249,249,249,249	0
56	MG	BA	1603	1/1	0.57	0.13	263,263,263,263	0
56	MG	CA	3124	1/1	0.58	0.20	118,118,118,118	0
56	MG	BA	1625	1/1	0.65	0.18	256,256,256,256	0
56	MG	CA	3005	1/1	0.66	0.21	237,237,237,237	0
56	MG	CA	3061	1/1	0.67	0.12	247,247,247,247	0
56	MG	CA	3028	1/1	0.67	0.17	278,278,278,278	0
56	MG	CA	3115	1/1	0.68	0.20	84,84,84,84	0
56	MG	CA	3155	1/1	0.69	0.16	156,156,156,156	0
56	MG	CA	3021	1/1	0.69	0.51	264,264,264,264	0
56	MG	CA	3139	1/1	0.70	0.28	87,87,87,87	0
58	MPD	DE	301	8/8	0.70	0.25	139,140,142,142	0
63	EDO	DB	212	4/4	0.71	0.31	115,115,116,116	0
56	MG	CA	3067	1/1	0.72	0.14	277,277,277,277	0
56	MG	AA	1678	1/1	0.72	0.22	78,78,78,78	0
56	MG	CA	3156	1/1	0.72	0.17	232,232,232,232	0
56	MG	DA	3146	1/1	0.73	0.28	122,122,122,122	0
56	MG	CA	3009	1/1	0.73	0.25	243,243,243,243	0
56	MG	BA	1606	1/1	0.74	0.21	227,227,227,227	0
56	MG	CA	3002	1/1	0.75	0.16	265,265,265,265	0
56	MG	DA	3143	1/1	0.75	0.31	114,114,114,114	0
56	MG	AA	1622	1/1	0.75	0.36	100,100,100,100	0
56	MG	DA	3129	1/1	0.76	0.38	102,102,102,102	0
62	PEG	DP	201	7/7	0.76	0.16	126,127,131,132	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3145	1/1	0.76	0.20	73,73,73,73	0
67	ACY	DA	3196	4/4	0.76	0.25	84,85,87,87	0
59	PUT	AA	1672	6/6	0.77	0.41	99,100,102,103	0
56	MG	CA	3034	1/1	0.77	0.25	246,246,246,246	0
56	MG	CA	3129	1/1	0.78	0.24	104,104,104,104	0
56	MG	CA	3147	1/1	0.78	0.52	58,58,58,58	1
56	MG	CA	3148	1/1	0.78	0.53	51,51,51,51	1
56	MG	CA	3112	1/1	0.79	0.10	75,75,75,75	0
56	MG	BA	1623	1/1	0.79	0.26	248,248,248,248	0
56	MG	CA	3146	1/1	0.79	0.19	144,144,144,144	0
56	MG	BA	1612	1/1	0.79	0.36	182,182,182,182	0
56	MG	DA	3180	1/1	0.79	0.28	106,106,106,106	0
56	MG	CA	3130	1/1	0.80	0.31	89,89,89,89	0
56	MG	BA	1646	1/1	0.80	0.15	108,108,108,108	0
56	MG	CA	3135	1/1	0.80	0.36	101,101,101,101	0
56	MG	AA	1660	1/1	0.80	0.17	284,284,284,284	0
56	MG	CA	3014	1/1	0.80	0.14	216,216,216,216	0
56	MG	CA	3003	1/1	0.80	0.33	278,278,278,278	0
56	MG	CA	3104	1/1	0.80	0.16	258,258,258,258	0
56	MG	CA	3142	1/1	0.81	0.10	78,78,78,78	0
56	MG	AA	1614	1/1	0.81	0.21	85,85,85,85	0
56	MG	CA	3068	1/1	0.81	0.17	216,216,216,216	0
56	MG	CA	3123	1/1	0.81	0.11	113,113,113,113	0
56	MG	AA	1654	1/1	0.81	0.34	262,262,262,262	0
56	MG	CA	3126	1/1	0.81	0.24	86,86,86,86	0
56	MG	CA	3032	1/1	0.82	0.12	241,241,241,241	0
56	MG	CA	3106	1/1	0.82	0.12	83,83,83,83	0
56	MG	CA	3108	1/1	0.82	0.19	83,83,83,83	0
56	MG	AA	1661	1/1	0.82	0.16	173,173,173,173	0
56	MG	CA	3152	1/1	0.82	0.10	151,151,151,151	0
56	MG	CA	3007	1/1	0.82	0.10	214,214,214,214	0
58	MPD	DK	201	8/8	0.83	0.17	120,121,123,124	0
56	MG	CA	3125	1/1	0.83	0.19	89,89,89,89	0
59	PUT	AA	1675	6/6	0.83	0.24	106,109,109,109	0
56	MG	DA	3061	1/1	0.83	0.13	233,233,233,233	0
56	MG	AA	1608	1/1	0.83	0.39	96,96,96,96	0
56	MG	CA	3090	1/1	0.83	0.13	185,185,185,185	0
60	T1C	BA	1643	42/42	0.84	0.18	170,174,179,179	0
56	MG	CA	3072	1/1	0.84	0.12	249,249,249,249	0
63	EDO	DB	211	4/4	0.84	0.36	88,90,92,92	0
56	MG	CA	3140	1/1	0.84	0.10	84,84,84,84	0
64	PGE	D1	102	10/10	0.84	0.28	122,127,128,128	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3047	1/1	0.84	0.32	229,229,229,229	0
59	PUT	DA	3222	6/6	0.85	0.20	48,52,57,58	0
56	MG	AA	1603	1/1	0.85	0.12	83,83,83,83	0
62	PEG	D3	102	7/7	0.85	0.28	114,119,124,125	0
56	MG	BA	1629	1/1	0.85	0.18	168,168,168,168	0
56	MG	CA	3107	1/1	0.85	0.26	83,83,83,83	0
56	MG	CA	3026	1/1	0.85	0.20	173,173,173,173	0
56	MG	CA	3080	1/1	0.85	0.18	151,151,151,151	0
56	MG	BA	1636	1/1	0.85	0.23	72,72,72,72	0
56	MG	DA	3178	1/1	0.86	0.38	88,88,88,88	0
56	MG	CA	3056	1/1	0.86	0.39	71,71,71,71	0
56	MG	AA	1609	1/1	0.86	0.31	89,89,89,89	0
58	MPD	DE	302	8/8	0.86	0.26	93,97,102,102	0
56	MG	AA	1611	1/1	0.86	0.22	108,108,108,108	0
58	MPD	DA	3190	8/8	0.86	0.19	95,97,99,102	0
56	MG	CA	3151	1/1	0.86	0.18	71,71,71,71	0
56	MG	AA	1624	1/1	0.86	0.19	95,95,95,95	0
56	MG	CA	3036	1/1	0.86	0.15	193,193,193,193	0
56	MG	CA	3037	1/1	0.86	0.25	189,189,189,189	0
56	MG	CA	3111	1/1	0.86	0.12	83,83,83,83	0
56	MG	CA	3022	1/1	0.86	0.21	195,195,195,195	0
56	MG	CA	3076	1/1	0.86	0.13	182,182,182,182	0
56	MG	CA	3116	1/1	0.86	0.25	95,95,95,95	0
56	MG	CA	3117	1/1	0.86	0.30	67,67,67,67	0
56	MG	BA	1647	1/1	0.86	0.38	91,91,91,91	0
67	ACY	DA	3201	4/4	0.86	0.25	78,79,79,79	0
69	TRS	DA	3220	8/8	0.86	0.17	125,128,134,134	0
56	MG	CA	3099	1/1	0.87	0.13	160,160,160,160	0
59	PUT	AA	1673	6/6	0.87	0.11	100,102,103,104	0
59	PUT	AA	1674	6/6	0.87	0.33	133,134,135,135	0
56	MG	CA	3136	1/1	0.87	0.37	84,84,84,84	0
56	MG	CA	3149	1/1	0.87	0.13	67,67,67,67	0
56	MG	CA	3137	1/1	0.87	0.17	106,106,106,106	0
56	MG	DA	3176	1/1	0.87	0.28	98,98,98,98	0
56	MG	AA	1618	1/1	0.87	0.32	92,92,92,92	0
56	MG	AA	1664	1/1	0.87	0.15	212,212,212,212	0
57	PG4	AA	1670	13/13	0.87	0.12	78,87,97,97	0
63	EDO	DA	3002	4/4	0.87	0.43	93,94,95,95	0
56	MG	AA	1605	1/1	0.87	0.51	89,89,89,89	0
56	MG	CA	3055	1/1	0.87	0.07	169,169,169,169	0
56	MG	BA	1607	1/1	0.87	0.17	207,207,207,207	0
56	MG	DA	3125	1/1	0.87	0.31	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3084	1/1	0.88	0.20	174,174,174,174	0
56	MG	BA	1604	1/1	0.88	0.09	153,153,153,153	0
56	MG	CA	3110	1/1	0.88	0.09	93,93,93,93	0
56	MG	CA	3094	1/1	0.88	0.13	105,105,105,105	0
57	PG4	DA	3193	13/13	0.88	0.24	85,95,100,101	0
56	MG	DA	3126	1/1	0.88	0.31	61,61,61,61	0
62	PEG	DQ	201	7/7	0.88	0.18	124,127,128,129	0
62	PEG	DA	3199	7/7	0.88	0.21	80,89,93,95	0
56	MG	AA	1615	1/1	0.88	0.33	83,83,83,83	0
56	MG	BA	1644	1/1	0.88	0.18	133,133,133,133	0
58	MPD	DN	201	8/8	0.88	0.18	106,111,116,117	0
56	MG	CA	3127	1/1	0.88	0.24	73,73,73,73	0
58	MPD	DA	3204	8/8	0.88	0.25	112,114,117,117	0
56	MG	DA	3152	1/1	0.88	0.54	66,66,66,66	0
56	MG	BA	1614	1/1	0.88	0.15	171,171,171,171	0
56	MG	CA	3039	1/1	0.89	0.13	175,175,175,175	0
56	MG	DA	3132	1/1	0.89	0.12	70,70,70,70	0
60	T1C	AA	1680	42/42	0.89	0.15	96,107,123,124	0
57	PG4	DQ	202	13/13	0.89	0.11	60,63,76,76	0
61	ZN	C5	101	1/1	0.89	0.10	149,149,149,149	0
62	PEG	AL	201	7/7	0.89	0.13	83,85,94,95	0
56	MG	DA	3136	1/1	0.89	0.27	77,77,77,77	0
56	MG	CA	3073	1/1	0.89	0.17	222,222,222,222	0
56	MG	AA	1616	1/1	0.89	0.54	85,85,85,85	0
56	MG	CA	3092	1/1	0.89	0.07	152,152,152,152	0
56	MG	DA	3164	1/1	0.89	0.32	71,71,71,71	0
58	MPD	DT	201	8/8	0.89	0.27	102,108,109,109	0
56	MG	DA	3167	1/1	0.89	0.29	102,102,102,102	0
56	MG	CA	3138	1/1	0.89	0.20	66,66,66,66	0
64	PGE	DS	201	10/10	0.89	0.12	77,89,91,92	0
56	MG	DA	3170	1/1	0.89	0.25	77,77,77,77	0
56	MG	CB	201	1/1	0.89	0.08	168,168,168,168	0
68	GUN	DA	3211	11/11	0.89	0.18	98,100,101,102	0
56	MG	CA	3001	1/1	0.89	0.17	296,296,296,296	0
57	PG4	DA	3216	13/13	0.90	0.16	99,104,109,110	0
56	MG	AA	1627	1/1	0.90	0.34	91,91,91,91	0
56	MG	CA	3141	1/1	0.90	0.38	80,80,80,80	0
56	MG	DA	3163	1/1	0.90	0.36	91,91,91,91	0
56	MG	BA	1638	1/1	0.90	0.40	78,78,78,78	0
56	MG	CA	3131	1/1	0.90	0.26	78,78,78,78	0
56	MG	AA	1612	1/1	0.90	0.32	77,77,77,77	0
56	MG	CA	3006	1/1	0.90	0.10	155,155,155,155	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	1645	1/1	0.90	0.21	102,102,102,102	0
56	MG	CA	3083	1/1	0.90	0.17	204,204,204,204	0
64	PGE	D3	101	10/10	0.90	0.18	97,99,102,103	0
56	MG	CA	3113	1/1	0.90	0.32	71,71,71,71	0
64	PGE	DA	3203	10/10	0.90	0.19	83,85,88,90	0
56	MG	DA	3141	1/1	0.90	0.33	86,86,86,86	0
57	PG4	BA	1642	13/13	0.90	0.11	88,89,99,100	0
56	MG	CA	3105	1/1	0.90	0.21	262,262,262,262	0
56	MG	DA	3145	1/1	0.90	0.18	79,79,79,79	0
56	MG	CA	3029	1/1	0.91	0.15	143,143,143,143	0
59	PUT	DA	3223	6/6	0.91	0.22	61,62,65,67	0
56	MG	CA	3010	1/1	0.91	0.10	234,234,234,234	0
57	PG4	DS	202	13/13	0.91	0.12	43,51,72,73	0
56	MG	CA	3114	1/1	0.91	0.14	66,66,66,66	0
56	MG	DA	3110	1/1	0.91	0.27	295,295,295,295	0
56	MG	DA	3120	1/1	0.91	0.20	70,70,70,70	0
62	PEG	DL	201	7/7	0.91	0.15	82,85,87,87	0
56	MG	DA	3124	1/1	0.91	0.24	65,65,65,65	0
56	MG	AA	1647	1/1	0.91	0.11	179,179,179,179	0
56	MG	AA	1642	1/1	0.91	0.13	158,158,158,158	0
62	PEG	DA	3226	7/7	0.91	0.23	89,91,98,98	0
56	MG	CA	3150	1/1	0.91	0.19	75,75,75,75	0
56	MG	DA	3172	1/1	0.91	0.49	103,103,103,103	0
58	MPD	DA	3192	8/8	0.91	0.27	95,100,104,105	0
63	EDO	DA	3198	4/4	0.91	0.24	78,81,83,83	0
56	MG	CA	3064	1/1	0.91	0.17	249,249,249,249	0
56	MG	DA	3177	1/1	0.91	0.41	77,77,77,77	0
56	MG	CA	3054	1/1	0.91	0.12	156,156,156,156	0
56	MG	DA	3137	1/1	0.91	0.50	37,37,37,37	1
65	SPD	DA	3183	10/10	0.91	0.15	79,83,87,87	0
56	MG	CA	3078	1/1	0.91	0.09	149,149,149,149	0
59	PUT	DA	3189	6/6	0.91	0.16	45,54,56,56	0
59	PUT	DA	3212	6/6	0.91	0.24	81,84,85,85	0
59	PUT	DA	3221	6/6	0.91	0.25	138,140,141,141	0
59	PUT	DA	3213	6/6	0.92	0.27	105,107,110,110	0
59	PUT	DA	3219	6/6	0.92	0.18	70,75,78,79	0
56	MG	CA	3109	1/1	0.92	0.13	62,62,62,62	0
56	MG	AA	1679	1/1	0.92	0.20	77,77,77,77	0
56	MG	DA	3142	1/1	0.92	0.16	62,62,62,62	0
56	MG	AA	1656	1/1	0.92	0.10	196,196,196,196	0
57	PG4	DR	202	13/13	0.92	0.24	109,117,120,121	0
56	MG	AA	1602	1/1	0.92	0.24	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	BA	1627	1/1	0.92	0.14	124,124,124,124	0
62	PEG	D1	103	7/7	0.92	0.26	85,90,91,91	0
56	MG	AA	1623	1/1	0.92	0.14	69,69,69,69	0
56	MG	DA	3158	1/1	0.92	0.18	191,191,191,191	0
56	MG	DA	3160	1/1	0.92	0.36	74,74,74,74	0
56	MG	DA	3162	1/1	0.92	0.11	85,85,85,85	0
56	MG	DA	3122	1/1	0.92	0.32	100,100,100,100	0
62	PEG	DA	3200	7/7	0.92	0.30	83,85,95,96	0
62	PEG	DA	3218	7/7	0.92	0.33	123,129,133,134	0
56	MG	DA	3123	1/1	0.92	0.30	62,62,62,62	0
58	MPD	DT	202	8/8	0.92	0.25	128,128,130,130	0
56	MG	CA	3008	1/1	0.92	0.17	136,136,136,136	0
56	MG	CA	3057	1/1	0.92	0.09	133,133,133,133	0
56	MG	AA	1621	1/1	0.92	0.46	77,77,77,77	0
58	MPD	DA	3207	8/8	0.92	0.21	77,78,80,80	0
56	MG	DA	3171	1/1	0.92	0.10	73,73,73,73	0
56	MG	CA	3118	1/1	0.92	0.26	59,59,59,59	0
56	MG	DA	3131	1/1	0.92	0.21	62,62,62,62	0
56	MG	AA	1625	1/1	0.92	0.17	86,86,86,86	0
56	MG	AA	1626	1/1	0.92	0.11	99,99,99,99	0
59	PUT	DA	3195	6/6	0.92	0.28	87,91,91,92	0
59	PUT	DA	3205	6/6	0.92	0.35	108,109,111,111	0
56	MG	DA	3179	1/1	0.92	0.22	104,104,104,104	0
62	PEG	DA	3227	7/7	0.93	0.20	97,99,103,104	0
56	MG	CA	3119	1/1	0.93	0.25	89,89,89,89	0
56	MG	CA	3012	1/1	0.93	0.08	95,95,95,95	0
56	MG	DB	208	1/1	0.93	0.10	76,76,76,76	0
56	MG	DA	3173	1/1	0.93	0.20	98,98,98,98	0
63	EDO	DA	3209	4/4	0.93	0.26	135,136,137,138	0
56	MG	DA	3147	1/1	0.93	0.34	65,65,65,65	0
56	MG	DB	209	1/1	0.93	0.12	66,66,66,66	0
56	MG	CA	3065	1/1	0.93	0.09	109,109,109,109	0
64	PGE	DU	101	10/10	0.93	0.15	89,97,104,105	0
56	MG	CA	3101	1/1	0.93	0.08	151,151,151,151	0
56	MG	DA	3133	1/1	0.93	0.13	91,91,91,91	0
65	SPD	DA	3224	10/10	0.93	0.15	50,54,66,68	0
66	1PE	DA	3185	16/16	0.93	0.12	50,55,84,87	0
56	MG	DA	3119	1/1	0.93	0.26	57,57,57,57	0
56	MG	BA	1637	1/1	0.93	0.12	85,85,85,85	0
56	MG	AA	1606	1/1	0.93	0.31	91,91,91,91	0
56	MG	CB	203	1/1	0.93	0.06	145,145,145,145	0
56	MG	DA	3155	1/1	0.94	0.15	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3134	1/1	0.94	0.16	108,108,108,108	0
56	MG	DA	3130	1/1	0.94	0.29	54,54,54,54	0
56	MG	AA	1601	1/1	0.94	0.35	67,67,67,67	0
63	EDO	DB	201	4/4	0.94	0.23	94,97,98,99	0
56	MG	AA	1636	1/1	0.94	0.09	97,97,97,97	0
56	MG	CA	3071	1/1	0.94	0.06	166,166,166,166	0
63	EDO	DB	213	4/4	0.94	0.20	82,82,84,84	0
56	MG	DA	3118	1/1	0.94	0.14	68,68,68,68	0
58	MPD	AA	1671	8/8	0.94	0.24	88,88,90,92	0
58	MPD	AA	1676	8/8	0.94	0.22	95,99,100,101	0
56	MG	AA	1659	1/1	0.94	0.08	115,115,115,115	0
56	MG	DA	3169	1/1	0.94	0.20	69,69,69,69	0
56	MG	AA	1619	1/1	0.94	0.22	92,92,92,92	0
56	MG	AA	1617	1/1	0.94	0.33	96,96,96,96	0
56	MG	CA	3153	1/1	0.94	0.10	64,64,64,64	0
64	PGE	DA	3214	10/10	0.94	0.13	72,73,77,78	0
64	PGE	DA	3225	10/10	0.94	0.16	73,83,94,96	0
56	MG	CA	3093	1/1	0.94	0.07	88,88,88,88	0
65	SPD	DA	3206	10/10	0.94	0.25	87,102,109,110	0
56	MG	BA	1633	1/1	0.94	0.15	229,229,229,229	0
56	MG	BA	1616	1/1	0.94	0.10	122,122,122,122	0
66	1PE	DA	3202	16/16	0.94	0.15	61,64,72,73	0
56	MG	DA	3150	1/1	0.94	0.18	51,51,51,51	0
56	MG	DA	3151	1/1	0.94	0.28	82,82,82,82	0
56	MG	DA	3128	1/1	0.94	0.26	72,72,72,72	0
56	MG	DA	3182	1/1	0.94	0.20	61,61,61,61	0
56	MG	CA	3066	1/1	0.95	0.10	89,89,89,89	0
56	MG	CA	3019	1/1	0.95	0.08	58,58,58,58	0
56	MG	CA	3133	1/1	0.95	0.17	72,72,72,72	0
56	MG	BA	1619	1/1	0.95	0.09	96,96,96,96	0
63	EDO	D1	101	4/4	0.95	0.07	59,60,60,60	0
56	MG	CA	3070	1/1	0.95	0.07	91,91,91,91	0
56	MG	DA	3138	1/1	0.95	0.13	59,59,59,59	0
56	MG	DR	201	1/1	0.95	0.11	42,42,42,42	0
59	PUT	DA	3188	6/6	0.95	0.15	50,53,55,56	0
56	MG	DB	206	1/1	0.95	0.32	80,80,80,80	0
56	MG	DB	207	1/1	0.95	0.13	92,92,92,92	0
56	MG	BA	1635	1/1	0.95	0.07	102,102,102,102	0
63	EDO	DA	3215	4/4	0.95	0.12	65,66,68,70	0
56	MG	CA	3051	1/1	0.95	0.07	80,80,80,80	0
56	MG	CA	3023	1/1	0.95	0.09	158,158,158,158	0
56	MG	CA	3120	1/1	0.95	0.14	102,102,102,102	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3121	1/1	0.95	0.10	64,64,64,64	0
56	MG	CA	3074	1/1	0.95	0.07	131,131,131,131	0
56	MG	AA	1655	1/1	0.95	0.07	163,163,163,163	0
56	MG	DA	3157	1/1	0.95	0.23	73,73,73,73	0
56	MG	CA	3143	1/1	0.95	0.08	70,70,70,70	0
56	MG	BA	1609	1/1	0.95	0.07	166,166,166,166	0
56	MG	AA	1665	1/1	0.95	0.13	161,161,161,161	0
56	MG	CB	202	1/1	0.95	0.12	116,116,116,116	0
56	MG	AA	1604	1/1	0.95	0.42	70,70,70,70	0
56	MG	DA	3165	1/1	0.95	0.26	62,62,62,62	0
56	MG	CA	3128	1/1	0.95	0.13	75,75,75,75	0
56	MG	AA	1657	1/1	0.95	0.14	136,136,136,136	0
56	MG	BA	1630	1/1	0.95	0.12	153,153,153,153	0
56	MG	CA	3016	1/1	0.96	0.14	107,107,107,107	0
56	MG	DA	3181	1/1	0.96	0.33	83,83,83,83	0
59	PUT	DA	3184	6/6	0.96	0.16	78,80,81,82	0
56	MG	AA	1644	1/1	0.96	0.17	106,106,106,106	0
56	MG	DA	3156	1/1	0.96	0.27	62,62,62,62	0
56	MG	CA	3062	1/1	0.96	0.06	175,175,175,175	0
56	MG	CA	3063	1/1	0.96	0.15	125,125,125,125	0
63	EDO	DA	3194	4/4	0.96	0.13	76,77,78,78	0
63	EDO	DA	3197	4/4	0.96	0.12	65,67,68,69	0
56	MG	CA	3031	1/1	0.96	0.05	64,64,64,64	0
63	EDO	DA	3208	4/4	0.96	0.18	89,90,90,91	0
56	MG	DA	3161	1/1	0.96	0.17	61,61,61,61	0
56	MG	DA	3011	1/1	0.96	0.07	115,115,115,115	0
56	MG	DA	3036	1/1	0.96	0.10	24,24,24,24	0
56	MG	CA	3048	1/1	0.96	0.06	76,76,76,76	0
56	MG	DA	3097	1/1	0.96	0.12	128,128,128,128	0
56	MG	DA	3166	1/1	0.96	0.22	81,81,81,81	0
64	PGE	DA	3186	10/10	0.96	0.09	39,48,55,57	0
56	MG	BA	1618	1/1	0.96	0.07	129,129,129,129	0
56	MG	DA	3140	1/1	0.96	0.10	54,54,54,54	0
64	PGE	DA	3217	10/10	0.96	0.13	85,88,91,92	0
56	MG	AA	1669	1/1	0.96	0.08	134,134,134,134	0
56	MG	CA	3082	1/1	0.96	0.14	114,114,114,114	0
56	MG	CA	3035	1/1	0.96	0.18	91,91,91,91	0
56	MG	DA	3144	1/1	0.96	0.09	72,72,72,72	0
56	MG	DA	3121	1/1	0.96	0.45	68,68,68,68	0
56	MG	CA	3069	1/1	0.96	0.08	88,88,88,88	0
67	ACY	DA	3191	4/4	0.96	0.10	68,70,70,71	0
56	MG	CA	3088	1/1	0.96	0.09	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
58	MPD	DA	3210	8/8	0.96	0.15	87,89,90,91	0
56	MG	AA	1663	1/1	0.96	0.04	90,90,90,90	0
56	MG	AA	1607	1/1	0.96	0.20	65,65,65,65	0
56	MG	CA	3018	1/1	0.97	0.05	85,85,85,85	0
56	MG	DA	3116	1/1	0.97	0.24	72,72,72,72	0
56	MG	CA	3058	1/1	0.97	0.12	98,98,98,98	0
56	MG	CA	3004	1/1	0.97	0.08	159,159,159,159	0
56	MG	AA	1630	1/1	0.97	0.10	134,134,134,134	0
56	MG	BA	1622	1/1	0.97	0.05	85,85,85,85	0
61	ZN	AB	301	1/1	0.97	0.09	171,171,171,171	0
56	MG	BA	1610	1/1	0.97	0.05	93,93,93,93	0
56	MG	CA	3102	1/1	0.97	0.06	113,113,113,113	0
56	MG	CA	3046	1/1	0.97	0.10	111,111,111,111	0
56	MG	DA	3174	1/1	0.97	0.11	74,74,74,74	0
56	MG	AA	1658	1/1	0.97	0.12	98,98,98,98	0
56	MG	CA	3079	1/1	0.97	0.06	115,115,115,115	0
56	MG	DA	3127	1/1	0.97	0.43	53,53,53,53	0
56	MG	DA	3153	1/1	0.97	0.23	52,52,52,52	0
56	MG	DA	3154	1/1	0.97	0.20	59,59,59,59	0
56	MG	BA	1605	1/1	0.97	0.07	107,107,107,107	0
56	MG	AA	1633	1/1	0.97	0.06	123,123,123,123	0
56	MG	BA	1617	1/1	0.97	0.05	131,131,131,131	0
56	MG	DB	210	1/1	0.97	0.13	97,97,97,97	0
56	MG	AA	1610	1/1	0.97	0.21	90,90,90,90	0
56	MG	CA	3086	1/1	0.97	0.05	68,68,68,68	0
56	MG	DA	3135	1/1	0.97	0.14	72,72,72,72	0
56	MG	BA	1632	1/1	0.97	0.09	75,75,75,75	0
56	MG	CA	3089	1/1	0.97	0.11	68,68,68,68	0
56	MG	BA	1631	1/1	0.98	0.03	55,55,55,55	0
56	MG	DA	3117	1/1	0.98	0.03	56,56,56,56	0
56	MG	BA	1613	1/1	0.98	0.08	73,73,73,73	0
56	MG	AA	1613	1/1	0.98	0.35	65,65,65,65	0
56	MG	CA	3042	1/1	0.98	0.04	88,88,88,88	0
56	MG	BA	1601	1/1	0.98	0.06	106,106,106,106	0
58	MPD	DS	203	8/8	0.98	0.11	48,52,58,59	0
56	MG	BA	1602	1/1	0.98	0.04	68,68,68,68	0
56	MG	CA	3097	1/1	0.98	0.05	90,90,90,90	0
56	MG	CA	3098	1/1	0.98	0.04	77,77,77,77	0
56	MG	AA	1651	1/1	0.98	0.05	76,76,76,76	0
56	MG	CA	3100	1/1	0.98	0.12	92,92,92,92	0
56	MG	AA	1638	1/1	0.98	0.05	114,114,114,114	0
56	MG	CA	3053	1/1	0.98	0.09	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3024	1/1	0.98	0.08	102,102,102,102	0
56	MG	AA	1639	1/1	0.98	0.05	118,118,118,118	0
56	MG	AA	1641	1/1	0.98	0.05	67,67,67,67	0
56	MG	AA	1667	1/1	0.98	0.07	47,47,47,47	0
59	PUT	DA	3001	6/6	0.98	0.09	46,50,58,60	0
56	MG	BA	1608	1/1	0.98	0.06	102,102,102,102	0
56	MG	DA	3134	1/1	0.98	0.04	96,96,96,96	0
56	MG	CA	3059	1/1	0.98	0.04	86,86,86,86	0
56	MG	AA	1629	1/1	0.98	0.07	93,93,93,93	0
56	MG	CA	3081	1/1	0.98	0.04	104,104,104,104	0
56	MG	DA	3005	1/1	0.98	0.05	94,94,94,94	0
56	MG	DA	3139	1/1	0.98	0.11	67,67,67,67	0
56	MG	DA	3007	1/1	0.98	0.05	82,82,82,82	0
56	MG	CA	3033	1/1	0.98	0.14	110,110,110,110	0
56	MG	AA	1634	1/1	0.98	0.07	130,130,130,130	0
65	SPD	DA	3187	10/10	0.98	0.10	34,42,45,48	0
56	MG	DA	3042	1/1	0.98	0.09	40,40,40,40	0
56	MG	DA	3043	1/1	0.98	0.08	80,80,80,80	0
56	MG	DA	3053	1/1	0.98	0.07	89,89,89,89	0
56	MG	AA	1645	1/1	0.98	0.06	66,66,66,66	0
56	MG	DA	3079	1/1	0.98	0.07	119,119,119,119	0
56	MG	DA	3148	1/1	0.98	0.06	61,61,61,61	0
56	MG	DA	3149	1/1	0.98	0.07	62,62,62,62	0
56	MG	CA	3085	1/1	0.98	0.04	74,74,74,74	0
56	MG	CA	3013	1/1	0.98	0.04	86,86,86,86	0
56	MG	AA	1640	1/1	0.99	0.05	73,73,73,73	0
56	MG	CA	3025	1/1	0.99	0.04	82,82,82,82	0
56	MG	DA	3003	1/1	0.99	0.05	85,85,85,85	0
56	MG	DA	3004	1/1	0.99	0.09	77,77,77,77	0
56	MG	AA	1648	1/1	0.99	0.05	70,70,70,70	0
56	MG	DA	3006	1/1	0.99	0.03	87,87,87,87	0
56	MG	CA	3091	1/1	0.99	0.06	68,68,68,68	0
56	MG	BA	1634	1/1	0.99	0.08	99,99,99,99	0
56	MG	DA	3014	1/1	0.99	0.03	45,45,45,45	0
56	MG	DA	3025	1/1	0.99	0.06	108,108,108,108	0
56	MG	DA	3027	1/1	0.99	0.05	94,94,94,94	0
56	MG	DA	3029	1/1	0.99	0.04	46,46,46,46	0
56	MG	AA	1649	1/1	0.99	0.04	68,68,68,68	0
56	MG	CA	3030	1/1	0.99	0.05	78,78,78,78	0
56	MG	CA	3095	1/1	0.99	0.07	63,63,63,63	0
56	MG	DA	3048	1/1	0.99	0.04	57,57,57,57	0
56	MG	DA	3051	1/1	0.99	0.03	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	CA	3096	1/1	0.99	0.02	61,61,61,61	0
56	MG	DA	3159	1/1	0.99	0.07	72,72,72,72	0
56	MG	AA	1662	1/1	0.99	0.05	79,79,79,79	0
56	MG	DA	3063	1/1	0.99	0.12	72,72,72,72	0
56	MG	DA	3064	1/1	0.99	0.03	25,25,25,25	0
56	MG	DA	3069	1/1	0.99	0.08	79,79,79,79	0
56	MG	DA	3071	1/1	0.99	0.07	68,68,68,68	0
56	MG	DA	3073	1/1	0.99	0.04	45,45,45,45	0
56	MG	DA	3077	1/1	0.99	0.04	63,63,63,63	0
56	MG	DA	3078	1/1	0.99	0.04	96,96,96,96	0
56	MG	AA	1650	1/1	0.99	0.04	114,114,114,114	0
56	MG	DA	3080	1/1	0.99	0.03	44,44,44,44	0
56	MG	DA	3081	1/1	0.99	0.04	65,65,65,65	0
56	MG	DA	3084	1/1	0.99	0.07	54,54,54,54	0
56	MG	DA	3092	1/1	0.99	0.09	35,35,35,35	0
56	MG	DA	3093	1/1	0.99	0.05	20,20,20,20	0
56	MG	DA	3094	1/1	0.99	0.09	80,80,80,80	0
56	MG	DA	3175	1/1	0.99	0.06	63,63,63,63	0
56	MG	BA	1620	1/1	0.99	0.03	94,94,94,94	0
56	MG	BA	1621	1/1	0.99	0.12	33,33,33,33	0
56	MG	AA	1635	1/1	0.99	0.04	104,104,104,104	0
56	MG	CA	3011	1/1	0.99	0.03	59,59,59,59	0
56	MG	CA	3103	1/1	0.99	0.06	82,82,82,82	0
56	MG	AA	1632	1/1	0.99	0.04	94,94,94,94	0
56	MG	AA	1666	1/1	0.99	0.04	57,57,57,57	0
56	MG	DA	3230	1/1	0.99	0.05	55,55,55,55	0
56	MG	DA	3231	1/1	0.99	0.12	39,39,39,39	0
56	MG	AA	1643	1/1	0.99	0.03	65,65,65,65	0
56	MG	CA	3040	1/1	0.99	0.05	76,76,76,76	0
56	MG	CA	3144	1/1	0.99	0.03	49,49,49,49	0
56	MG	CA	3041	1/1	0.99	0.05	55,55,55,55	0
56	MG	CA	3015	1/1	0.99	0.13	51,51,51,51	0
56	MG	CA	3043	1/1	0.99	0.05	81,81,81,81	0
56	MG	CA	3044	1/1	0.99	0.06	57,57,57,57	0
56	MG	CA	3045	1/1	0.99	0.06	84,84,84,84	0
56	MG	BA	1626	1/1	0.99	0.03	102,102,102,102	0
56	MG	AA	1668	1/1	0.99	0.09	75,75,75,75	0
56	MG	BA	1628	1/1	0.99	0.05	89,89,89,89	0
56	MG	CA	3049	1/1	0.99	0.03	48,48,48,48	0
56	MG	CA	3050	1/1	0.99	0.04	54,54,54,54	0
56	MG	CA	3020	1/1	0.99	0.06	86,86,86,86	0
56	MG	CA	3052	1/1	0.99	0.06	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	AA	1620	1/1	0.99	0.25	78,78,78,78	0
56	MG	DB	202	1/1	0.99	0.06	62,62,62,62	0
56	MG	AA	1631	1/1	0.99	0.05	53,53,53,53	0
56	MG	AA	1646	1/1	0.99	0.05	66,66,66,66	0
56	MG	CA	3087	1/1	0.99	0.05	77,77,77,77	0
56	MG	DA	3085	1/1	1.00	0.01	31,31,31,31	0
56	MG	DA	3086	1/1	1.00	0.01	34,34,34,34	0
56	MG	DA	3087	1/1	1.00	0.02	54,54,54,54	0
56	MG	DA	3088	1/1	1.00	0.03	24,24,24,24	0
56	MG	DA	3089	1/1	1.00	0.02	26,26,26,26	0
56	MG	DA	3090	1/1	1.00	0.04	24,24,24,24	0
56	MG	DA	3228	1/1	1.00	0.04	41,41,41,41	0
56	MG	DA	3229	1/1	1.00	0.02	54,54,54,54	0
56	MG	DA	3091	1/1	1.00	0.02	30,30,30,30	0
56	MG	DA	3019	1/1	1.00	0.03	65,65,65,65	0
56	MG	DA	3020	1/1	1.00	0.04	31,31,31,31	0
56	MG	DA	3021	1/1	1.00	0.05	34,34,34,34	0
56	MG	DA	3095	1/1	1.00	0.05	36,36,36,36	0
56	MG	DA	3096	1/1	1.00	0.03	33,33,33,33	0
56	MG	DA	3022	1/1	1.00	0.05	36,36,36,36	0
56	MG	DA	3098	1/1	1.00	0.03	23,23,23,23	0
56	MG	DA	3099	1/1	1.00	0.01	31,31,31,31	0
56	MG	DA	3100	1/1	1.00	0.03	61,61,61,61	0
56	MG	DA	3101	1/1	1.00	0.02	42,42,42,42	0
56	MG	DA	3102	1/1	1.00	0.05	34,34,34,34	0
56	MG	DA	3103	1/1	1.00	0.05	30,30,30,30	0
56	MG	DA	3104	1/1	1.00	0.03	29,29,29,29	0
56	MG	DA	3105	1/1	1.00	0.10	37,37,37,37	0
56	MG	DA	3106	1/1	1.00	0.02	36,36,36,36	0
56	MG	DA	3107	1/1	1.00	0.02	39,39,39,39	0
56	MG	DA	3108	1/1	1.00	0.02	30,30,30,30	0
56	MG	DA	3109	1/1	1.00	0.03	26,26,26,26	0
56	MG	DA	3023	1/1	1.00	0.04	29,29,29,29	0
56	MG	DA	3111	1/1	1.00	0.02	25,25,25,25	0
56	MG	DA	3112	1/1	1.00	0.04	83,83,83,83	0
56	MG	DA	3113	1/1	1.00	0.05	37,37,37,37	0
56	MG	DA	3114	1/1	1.00	0.01	31,31,31,31	0
56	MG	DA	3115	1/1	1.00	0.01	32,32,32,32	0
56	MG	DA	3024	1/1	1.00	0.01	39,39,39,39	0
56	MG	AA	1653	1/1	1.00	0.03	50,50,50,50	0
56	MG	DA	3026	1/1	1.00	0.03	51,51,51,51	0
56	MG	CA	3027	1/1	1.00	0.07	73,73,73,73	0

Continued on next page...

Continued from previous page...

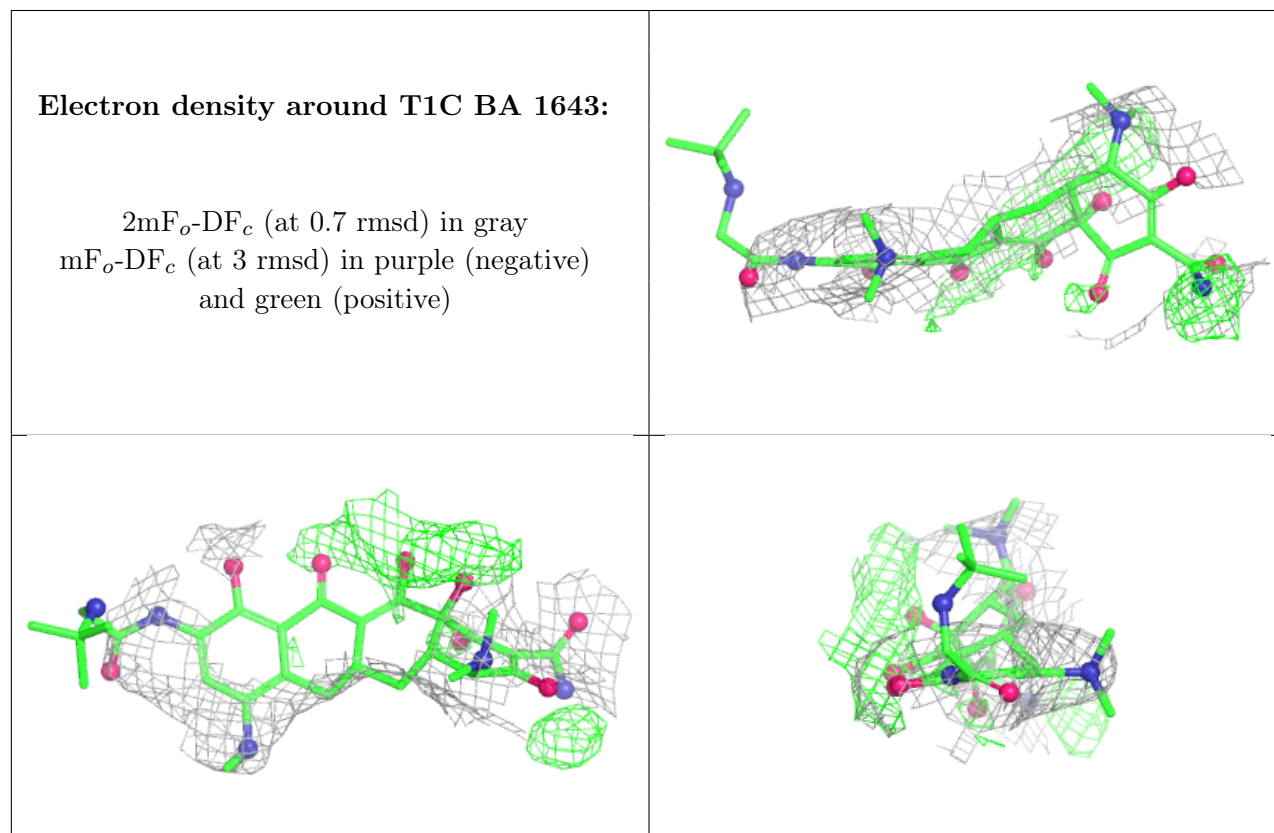
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3028	1/1	1.00	0.08	27,27,27,27	0
56	MG	AA	1637	1/1	1.00	0.03	51,51,51,51	0
56	MG	DA	3030	1/1	1.00	0.02	22,22,22,22	0
56	MG	DA	3031	1/1	1.00	0.07	29,29,29,29	0
56	MG	DA	3032	1/1	1.00	0.02	27,27,27,27	0
56	MG	DA	3033	1/1	1.00	0.01	13,13,13,13	0
56	MG	DA	3034	1/1	1.00	0.06	35,35,35,35	0
56	MG	DA	3035	1/1	1.00	0.04	34,34,34,34	0
56	MG	AA	1652	1/1	1.00	0.14	25,25,25,25	0
56	MG	DA	3037	1/1	1.00	0.03	30,30,30,30	0
56	MG	DA	3038	1/1	1.00	0.07	35,35,35,35	0
56	MG	DA	3039	1/1	1.00	0.07	55,55,55,55	0
56	MG	DA	3040	1/1	1.00	0.14	24,24,24,24	0
56	MG	DA	3041	1/1	1.00	0.03	52,52,52,52	0
61	ZN	D5	101	1/1	1.00	0.02	66,66,66,66	0
56	MG	CA	3017	1/1	1.00	0.08	88,88,88,88	0
56	MG	DD	301	1/1	1.00	0.03	35,35,35,35	0
56	MG	DA	3044	1/1	1.00	0.03	53,53,53,53	0
56	MG	DA	3045	1/1	1.00	0.03	24,24,24,24	0
56	MG	DA	3046	1/1	1.00	0.02	47,47,47,47	0
56	MG	DA	3047	1/1	1.00	0.05	36,36,36,36	0
56	MG	DM	201	1/1	1.00	0.04	56,56,56,56	0
56	MG	DA	3049	1/1	1.00	0.02	20,20,20,20	0
56	MG	DA	3050	1/1	1.00	0.02	24,24,24,24	0
56	MG	BA	1615	1/1	1.00	0.03	72,72,72,72	0
56	MG	DA	3052	1/1	1.00	0.03	41,41,41,41	0
56	MG	BA	1611	1/1	1.00	0.04	53,53,53,53	0
56	MG	DA	3054	1/1	1.00	0.04	30,30,30,30	0
56	MG	DA	3055	1/1	1.00	0.02	34,34,34,34	0
56	MG	DA	3056	1/1	1.00	0.04	23,23,23,23	0
56	MG	DA	3057	1/1	1.00	0.01	27,27,27,27	0
56	MG	DA	3058	1/1	1.00	0.03	27,27,27,27	0
56	MG	DA	3059	1/1	1.00	0.03	33,33,33,33	0
56	MG	DA	3060	1/1	1.00	0.04	41,41,41,41	0
56	MG	DB	203	1/1	1.00	0.04	41,41,41,41	0
56	MG	DA	3062	1/1	1.00	0.04	73,73,73,73	0
56	MG	DA	3008	1/1	1.00	0.03	27,27,27,27	0
56	MG	DA	3009	1/1	1.00	0.04	27,27,27,27	0
56	MG	DA	3065	1/1	1.00	0.06	45,45,45,45	0
56	MG	DA	3066	1/1	1.00	0.03	49,49,49,49	0
56	MG	DA	3067	1/1	1.00	0.06	46,46,46,46	0
56	MG	DA	3068	1/1	1.00	0.09	59,59,59,59	0

Continued on next page...

Continued from previous page...

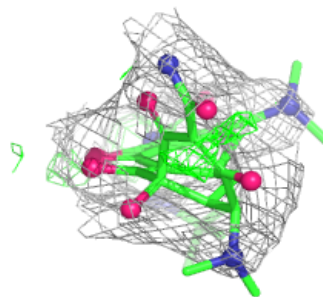
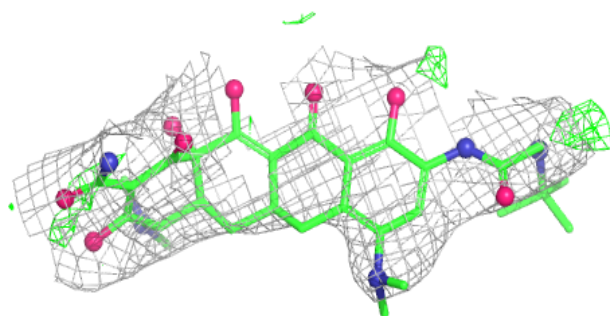
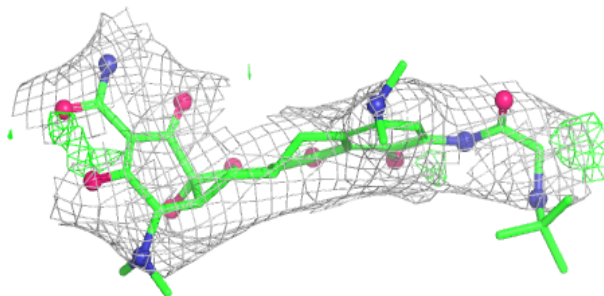
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	DA	3010	1/1	1.00	0.02	26,26,26,26	0
56	MG	DA	3070	1/1	1.00	0.05	55,55,55,55	0
56	MG	DB	204	1/1	1.00	0.06	37,37,37,37	0
56	MG	DA	3072	1/1	1.00	0.01	38,38,38,38	0
56	MG	DA	3012	1/1	1.00	0.03	25,25,25,25	0
56	MG	DA	3074	1/1	1.00	0.02	33,33,33,33	0
56	MG	DA	3075	1/1	1.00	0.03	40,40,40,40	0
56	MG	DA	3076	1/1	1.00	0.03	31,31,31,31	0
56	MG	DA	3013	1/1	1.00	0.02	20,20,20,20	0
56	MG	DB	205	1/1	1.00	0.04	63,63,63,63	0
56	MG	DA	3015	1/1	1.00	0.03	72,72,72,72	0
56	MG	DA	3016	1/1	1.00	0.01	26,26,26,26	0
56	MG	DA	3017	1/1	1.00	0.04	44,44,44,44	0
56	MG	DA	3082	1/1	1.00	0.06	56,56,56,56	0
56	MG	DA	3083	1/1	1.00	0.06	30,30,30,30	0
56	MG	DA	3018	1/1	1.00	0.11	8,8,8,8	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around T1C AA 1680:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.