



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 03:17 pm BST

PDB ID : 5J91  
Title : Structure of the Wild-type 70S E coli ribosome bound to Tigecycline  
Authors : Cocozaki, A.; Ferguson, A.  
Deposited on : 2016-04-08  
Resolution : 2.96 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

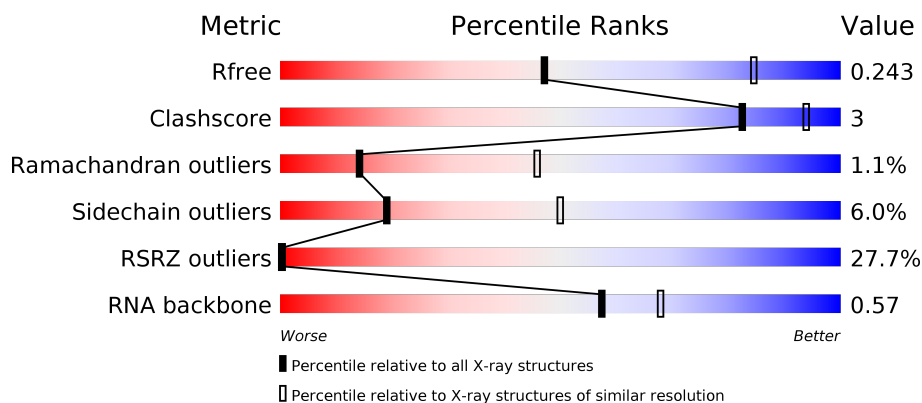
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

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

Mol	Chain	Length	Quality of chain
1	AA	1534	<div> <div>7%</div> <div>78%</div> <div>20%</div> <div>•</div> </div>
1	BA	1534	<div> <div>26%</div> <div>77%</div> <div>20%</div> <div>•</div> </div>
2	AB	224	<div> <div>32%</div> <div>88%</div> <div>11%</div> <div>•</div> </div>
2	BB	224	<div> <div>35%</div> <div>85%</div> <div>13%</div> <div>•</div> </div>

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

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Mol	Chain	Length	Quality of chain
15	BO	88	
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	

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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	134	
37	DJ	134	
38	CK	142	
38	DK	142	
39	CL	123	
39	DL	123	
40	CM	144	
40	DM	144	
41	CN	136	
41	DN	136	

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Mol	Chain	Length	Quality of chain
42	CO	125	
42	DO	125	
43	CP	117	
43	DP	117	
44	CQ	114	
44	DQ	114	
45	CR	117	
45	DR	117	
46	CS	103	
46	DS	103	
47	CT	110	
47	DT	110	
48	CU	93	
48	DU	93	
49	CV	103	
49	DV	103	
50	CW	94	
50	DW	94	
51	CX	76	
51	DX	76	
52	CY	77	
52	DY	77	
53	CZ	62	
53	DZ	62	
54	DI	135	

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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	AA	1602	-	-	-	X
56	MG	AA	1603	-	-	-	X
56	MG	AA	1604	-	-	-	X
56	MG	AA	1605	-	-	-	X
56	MG	AA	1606	-	-	-	X
56	MG	AA	1608	-	-	-	X
56	MG	AA	1612	-	-	-	X
56	MG	AA	1613	-	-	-	X
56	MG	AA	1615	-	-	-	X
56	MG	AA	1616	-	-	-	X
56	MG	AA	1618	-	-	-	X
56	MG	AA	1620	-	-	-	X
56	MG	AA	1621	-	-	-	X
56	MG	AA	1622	-	-	-	X
56	MG	AA	1624	-	-	-	X
56	MG	AA	1626	-	-	-	X
56	MG	AA	1627	-	-	-	X
56	MG	AA	1628	-	-	-	X
56	MG	AA	1642	-	-	-	X
56	MG	BA	1623	-	-	-	X
56	MG	BA	1629	-	-	-	X
56	MG	BA	1637	-	-	-	X
56	MG	BA	1638	-	-	-	X
56	MG	BA	1639	-	-	-	X
56	MG	BA	1641	-	-	-	X
56	MG	CA	3003	-	-	-	X
56	MG	CA	3005	-	-	-	X
56	MG	CA	3007	-	-	-	X
56	MG	CA	3010	-	-	-	X
56	MG	CA	3026	-	-	-	X
56	MG	CA	3028	-	-	-	X
56	MG	CA	3032	-	-	-	X
56	MG	CA	3047	-	-	-	X
56	MG	CA	3056	-	-	-	X
56	MG	CA	3068	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	CA	3075	-	-	-	X
56	MG	CA	3082	-	-	-	X
56	MG	CA	3090	-	-	-	X
56	MG	CA	3105	-	-	-	X
56	MG	CA	3106	-	-	-	X
56	MG	CA	3108	-	-	-	X
56	MG	CA	3109	-	-	-	X
56	MG	CA	3110	-	-	-	X
56	MG	CA	3111	-	-	-	X
56	MG	CA	3113	-	-	-	X
56	MG	CA	3115	-	-	-	X
56	MG	CA	3121	-	-	-	X
56	MG	CA	3122	-	-	-	X
56	MG	CA	3123	-	-	-	X
56	MG	CA	3124	-	-	-	X
56	MG	CA	3128	-	-	-	X
56	MG	CA	3130	-	-	-	X
56	MG	CA	3131	-	-	-	X
56	MG	CA	3132	-	-	-	X
56	MG	CA	3133	-	-	-	X
56	MG	CA	3134	-	-	-	X
56	MG	CA	3135	-	-	-	X
56	MG	CA	3137	-	-	-	X
56	MG	CA	3139	-	-	-	X
56	MG	CA	3140	-	-	-	X
56	MG	CA	3141	-	-	-	X
56	MG	CA	3142	-	-	-	X
56	MG	CA	3148	-	-	-	X
56	MG	CA	3149	-	-	-	X
56	MG	CA	3154	-	-	-	X
56	MG	DA	3125	-	-	-	X
56	MG	DA	3131	-	-	-	X
56	MG	DA	3143	-	-	-	X
56	MG	DA	3145	-	-	-	X
56	MG	DA	3147	-	-	-	X
56	MG	DA	3155	-	-	-	X
56	MG	DA	3157	-	-	-	X
56	MG	DA	3159	-	-	-	X
56	MG	DA	3161	-	-	-	X
56	MG	DA	3167	-	-	-	X
56	MG	DA	3168	-	-	-	X
56	MG	DA	3171	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	DA	3173	-	-	-	X
56	MG	DA	3178	-	-	-	X
56	MG	DA	3179	-	-	-	X
56	MG	DA	3180	-	-	-	X
56	MG	DA	3182	-	-	-	X
56	MG	DB	206	-	-	-	X
56	MG	DB	207	-	-	-	X
57	PG4	DA	3215	-	-	-	X
58	MPD	DA	3203	-	-	-	X
58	MPD	DA	3206	-	-	-	X
58	MPD	DE	302	-	-	-	X
58	MPD	DT	201	-	-	-	X
58	MPD	DT	202	-	-	-	X
59	PUT	AA	1672	-	-	-	X
59	PUT	AA	1673	-	-	-	X
59	PUT	AA	1674	-	-	-	X
59	PUT	AA	1675	-	-	-	X
59	PUT	DA	3218	-	-	-	X
62	PEG	D1	103	-	-	-	X
62	PEG	D3	102	-	-	-	X
62	PEG	DA	3217	-	-	-	X
62	PEG	DP	201	-	-	-	X
62	PEG	DQ	201	-	-	-	X
63	EDO	DA	3004	-	-	-	X
63	EDO	DA	3208	-	-	-	X
63	EDO	DB	210	-	-	-	X
64	PGE	D1	102	-	-	-	X
64	PGE	D3	101	-	-	-	X
69	TRS	DA	3219	-	-	-	X

## 2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 295202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CC	271	Total	C	N	O	S	0	0	0
			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
			1552	974	283	290	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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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
			739	466	139	132	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		0	0	0
			779	492	146	141				
49	DV	102	Total	C	N	O		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).

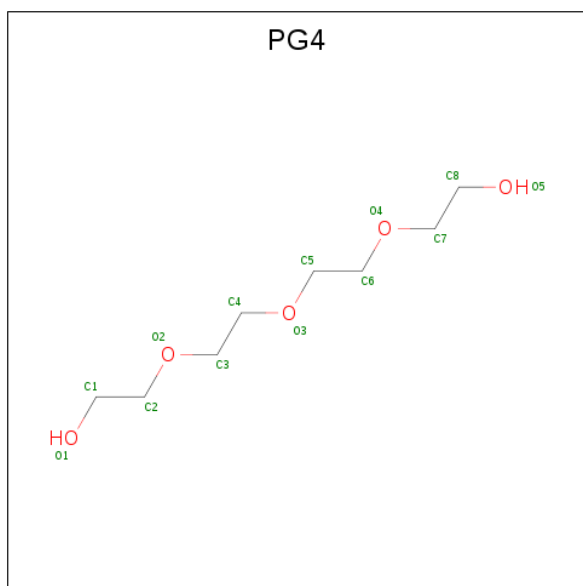
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	BA	43	Total	Mg	0	0
			43	43		
56	CA	156	Total	Mg	0	0
			156	156		
56	CB	3	Total	Mg	0	0
			3	3		
56	DM	1	Total	Mg	0	0
			1	1		
56	DR	2	Total	Mg	0	0
			2	2		
56	AA	71	Total	Mg	0	0
			71	71		
56	DA	182	Total	Mg	0	0
			182	182		
56	DB	9	Total	Mg	0	0
			9	9		

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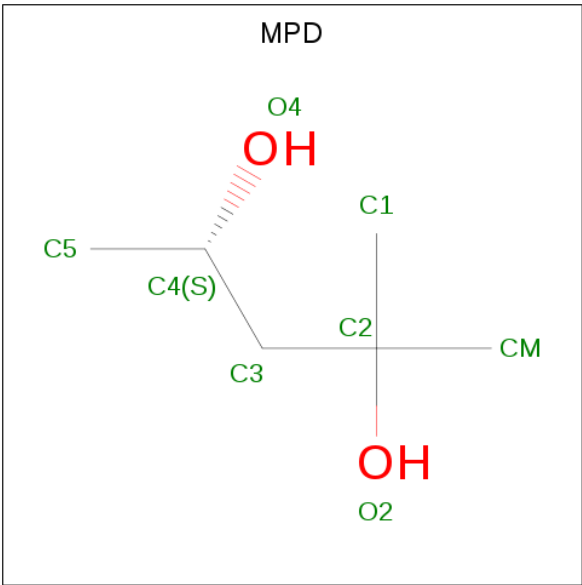
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	DD	2	Total	Mg	0	0
			2	2		

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



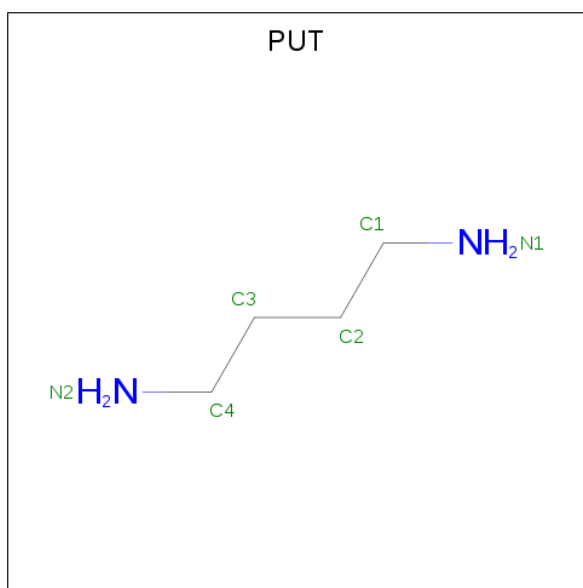
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	AA	1	Total	C	O	0	0
			13	8	5		
57	BA	1	Total	C	O	0	0
			13	8	5		
57	DQ	1	Total	C	O	0	0
			13	8	5		
57	DR	1	Total	C	O	0	0
			13	8	5		
57	DS	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		
57	DA	1	Total	C	O	0	0
			13	8	5		

- 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-DIAMINOBTANE (three-letter code: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>).



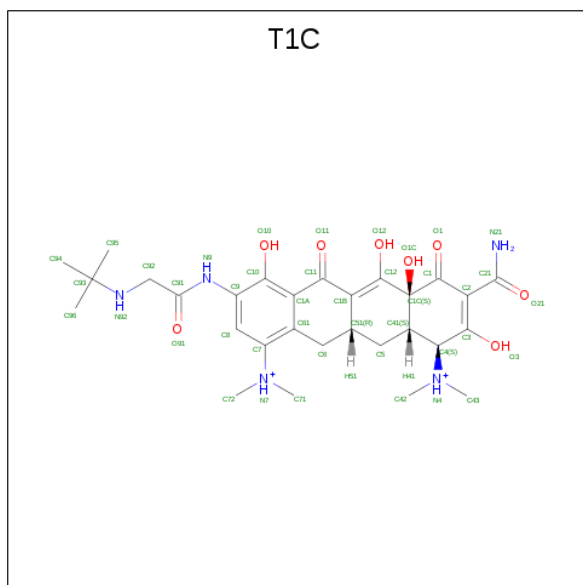
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	AA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6	4	2		
59	DA	1	Total	C	N	0	0
			6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

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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:  $C_{29}H_{41}N_5O_8$ ).



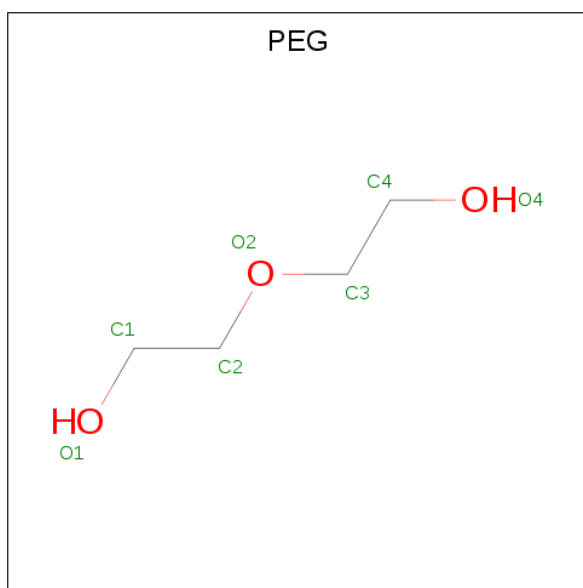
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
60	AA	1	Total	C	N	O	0	0
			42	29	5	8		
60	BA	1	Total	C	N	O	0	0
			42	29	5	8		

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

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

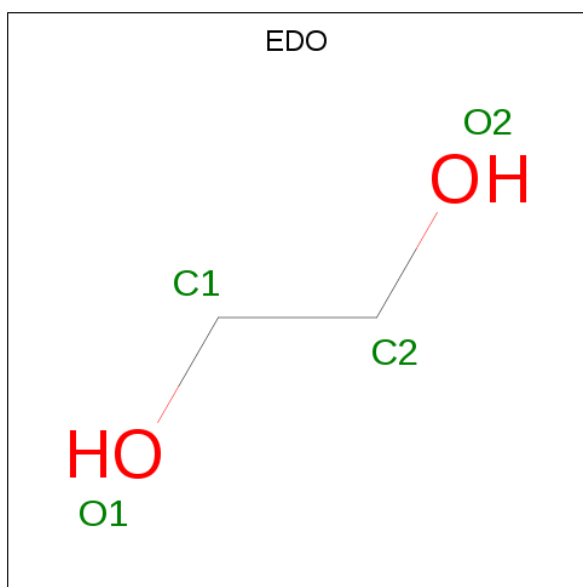
- Molecule 62 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:

C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



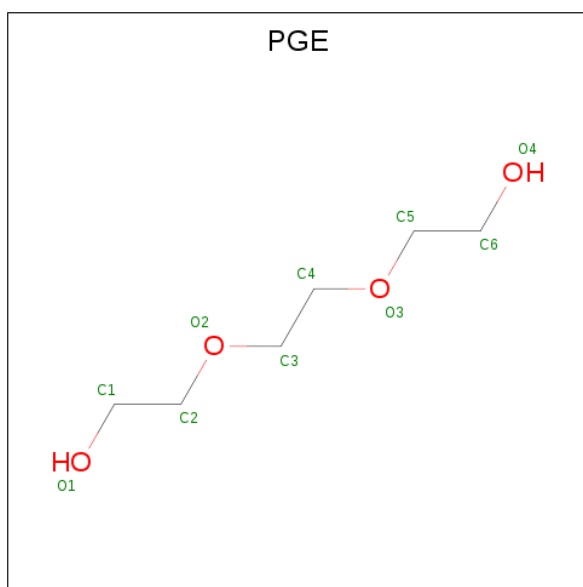
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	AL	1	Total	C	O	0	0
			7	4	3		
62	D1	1	Total	C	O	0	0
			7	4	3		
62	D3	1	Total	C	O	0	0
			7	4	3		
62	DL	1	Total	C	O	0	0
			7	4	3		
62	DP	1	Total	C	O	0	0
			7	4	3		
62	DQ	1	Total	C	O	0	0
			7	4	3		
62	DA	1	Total	C	O	0	0
			7	4	3		
62	DA	1	Total	C	O	0	0
			7	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: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



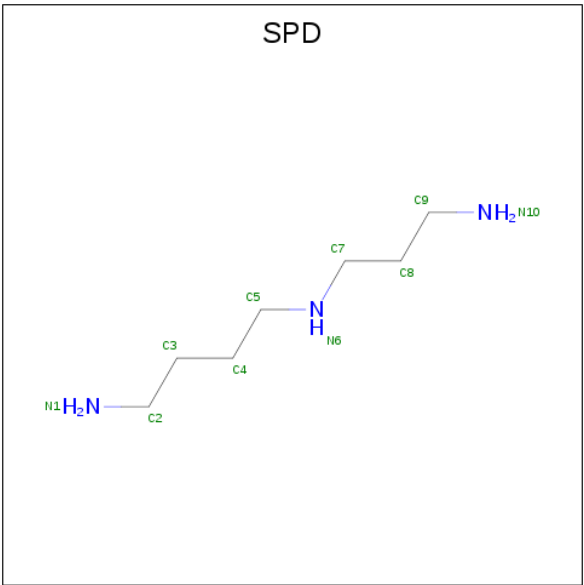
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
63	D1	1	Total	C	O	0	0
			4	2	2		
63	DB	1	Total	C	O	0	0
			4	2	2		
63	DB	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4	2	2		
63	DA	1	Total	C	O	0	0
			4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

- Molecule 64 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



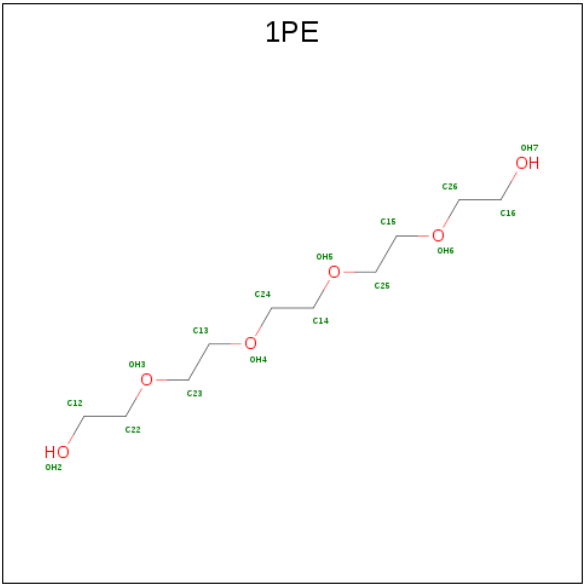
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
64	D1	1	Total	C	O	0	0
			10	6	4		
64	D3	1	Total	C	O	0	0
			10	6	4		
64	DD	1	Total	C	O	0	0
			10	6	4		
64	DS	1	Total	C	O	0	0
			10	6	4		
64	DU	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0	0
			10	6	4		
64	DA	1	Total	C	O	0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

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



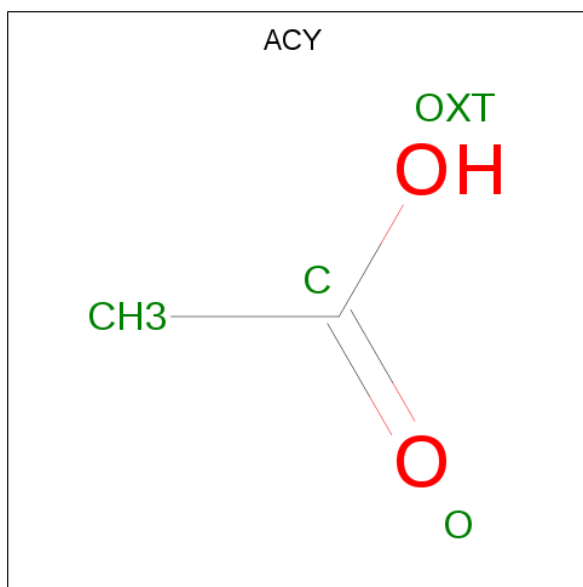
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
65	DA	1	Total	C	N	0	0
			10	7	3		
65	DA	1	Total	C	N	0	0
			10	7	3		
65	DA	1	Total	C	N	0	0
			10	7	3		
65	DA	1	Total	C	N	0	0
			10	7	3		

- Molecule 66 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



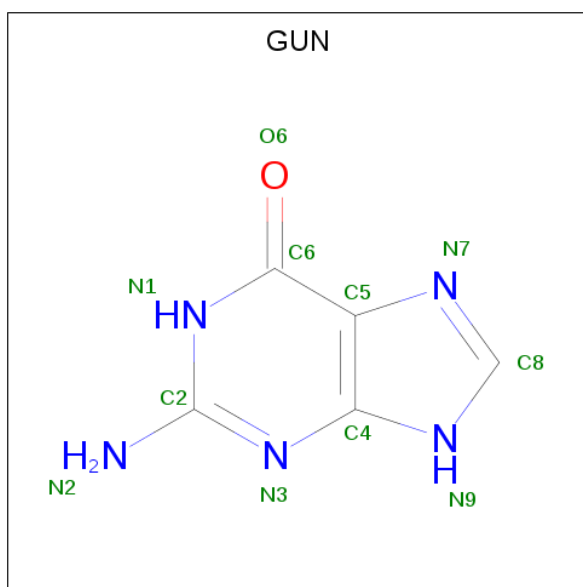
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
66	DA	1	Total	C	O	0	0
			16	10	6		
66	DA	1	Total	C	O	0	0
			16	10	6		

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



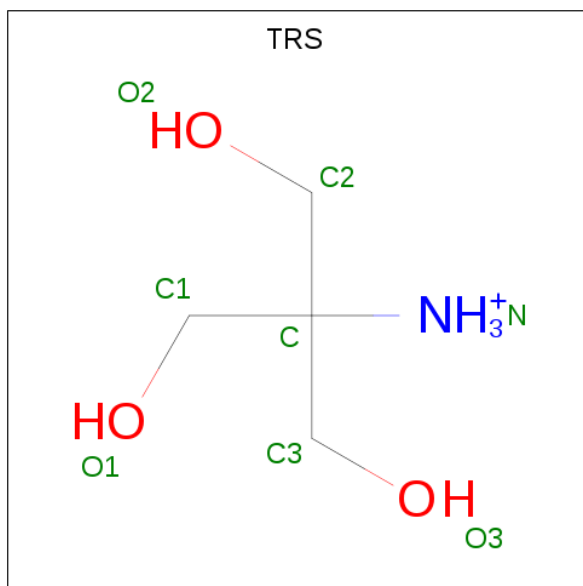
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
67	DA	1	Total	C	O	0	0
			4	2	2		
67	DA	1	Total	C	O	0	0
			4	2	2		
67	DA	1	Total	C	O	0	0
			4	2	2		

- 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	507	Total 507	O 507	0	0
70	AC	4	Total 4	O 4	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	5	Total 5	O 5	0	0
70	AL	8	Total 8	O 8	0	0
70	AM	4	Total 4	O 4	0	0
70	AN	5	Total 5	O 5	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	AS	1	Total 1	O 1	0	0
70	AT	2	Total 2	O 2	0	0
70	AU	3	Total 3	O 3	0	0
70	C3	3	Total 3	O 3	0	0
70	C4	1	Total 1	O 1	0	0
70	BA	287	Total 287	O 287	0	0
70	BD	13	Total 13	O 13	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
70	BE	1	Total 1	O 1	0	0
70	BF	1	Total 1	O 1	0	0
70	BK	1	Total 1	O 1	0	0
70	BL	3	Total 3	O 3	0	0
70	BN	2	Total 2	O 2	0	0
70	BO	1	Total 1	O 1	0	0
70	BP	3	Total 3	O 3	0	0
70	BR	1	Total 1	O 1	0	0
70	BT	4	Total 4	O 4	0	0
70	BU	2	Total 2	O 2	0	0
70	D1	42	Total 42	O 42	0	0
70	D2	7	Total 7	O 7	0	0
70	D3	25	Total 25	O 25	0	0
70	D4	32	Total 32	O 32	0	0
70	D5	13	Total 13	O 13	0	0
70	D0	25	Total 25	O 25	0	0
70	CB	13	Total 13	O 13	0	0
70	CC	10	Total 10	O 10	0	0
70	CD	5	Total 5	O 5	0	0
70	CA	694	Total 694	O 694	0	0
70	DC	102	Total 102	O 102	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
70	DD	105	Total 105	O 105	0	0
70	CE	6	Total 6	O 6	0	0
70	CL	1	Total 1	O 1	0	0
70	CM	3	Total 3	O 3	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	63	Total 63	O 63	0	0
70	DF	14	Total 14	O 14	0	0
70	DG	6	Total 6	O 6	0	0
70	DH	2	Total 2	O 2	0	0
70	DK	58	Total 58	O 58	0	0
70	DL	51	Total 51	O 51	0	0
70	DM	60	Total 60	O 60	0	0
70	DN	71	Total 71	O 71	0	0
70	DO	44	Total 44	O 44	0	0
70	DP	35	Total 35	O 35	0	0
70	DQ	27	Total 27	O 27	0	0
70	DR	64	Total 64	O 64	0	0

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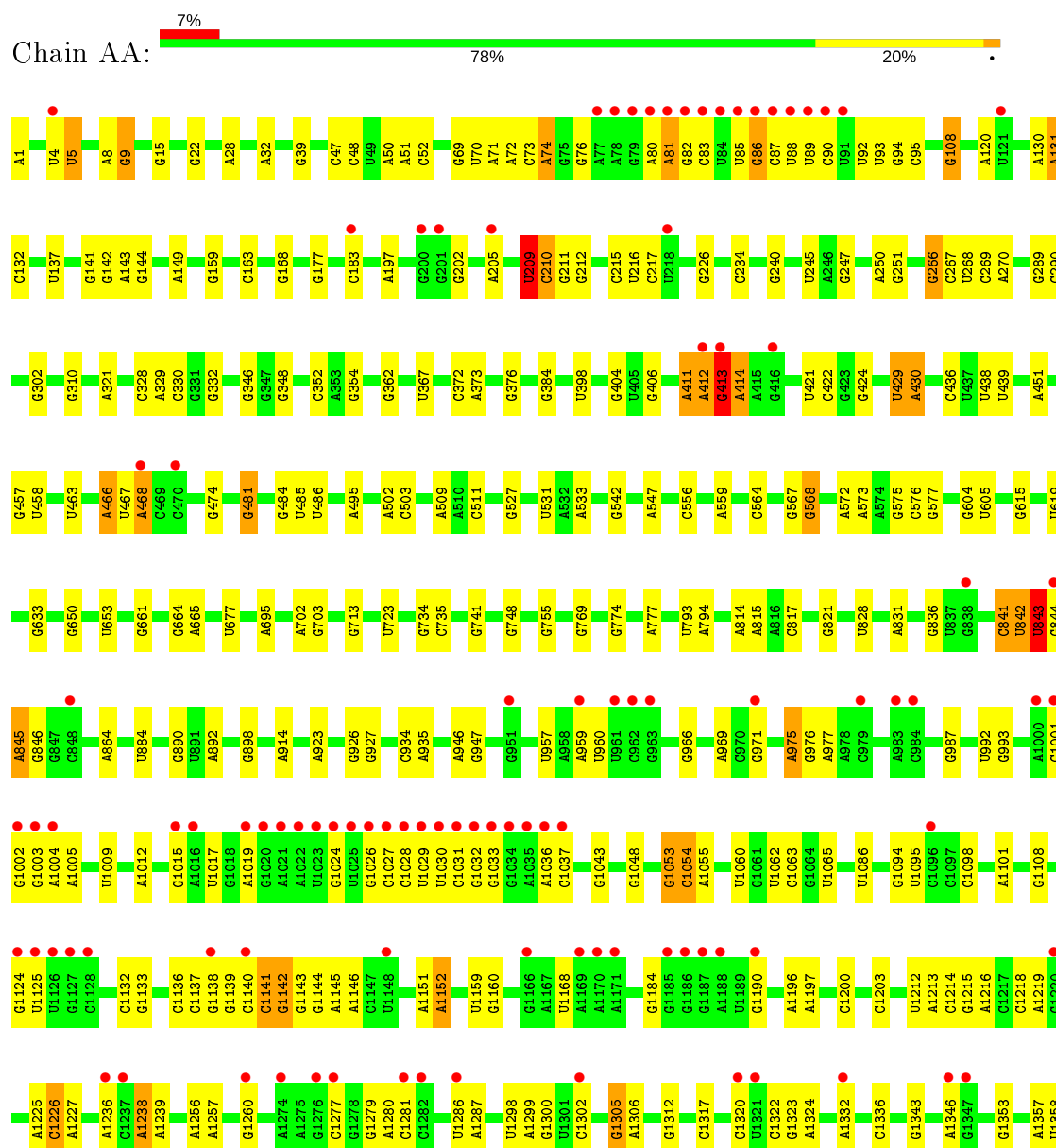
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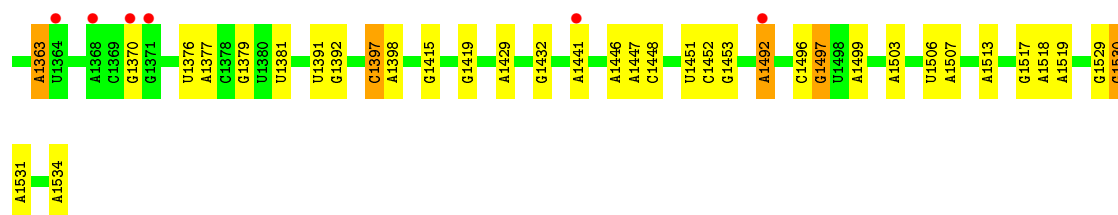
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
70	DS	51	Total 51	O 51	0	0
70	DT	70	Total 70	O 70	0	0
70	DU	17	Total 17	O 17	0	0
70	DV	19	Total 19	O 19	0	0
70	DW	31	Total 31	O 31	0	0
70	DX	30	Total 30	O 30	0	0
70	DY	9	Total 9	O 9	0	0
70	DZ	7	Total 7	O 7	0	0
70	DB	213	Total 213	O 213	0	0
70	DA	4836	Total 4836	O 4836	0	0

### 3 Residue-property plots [i](#)

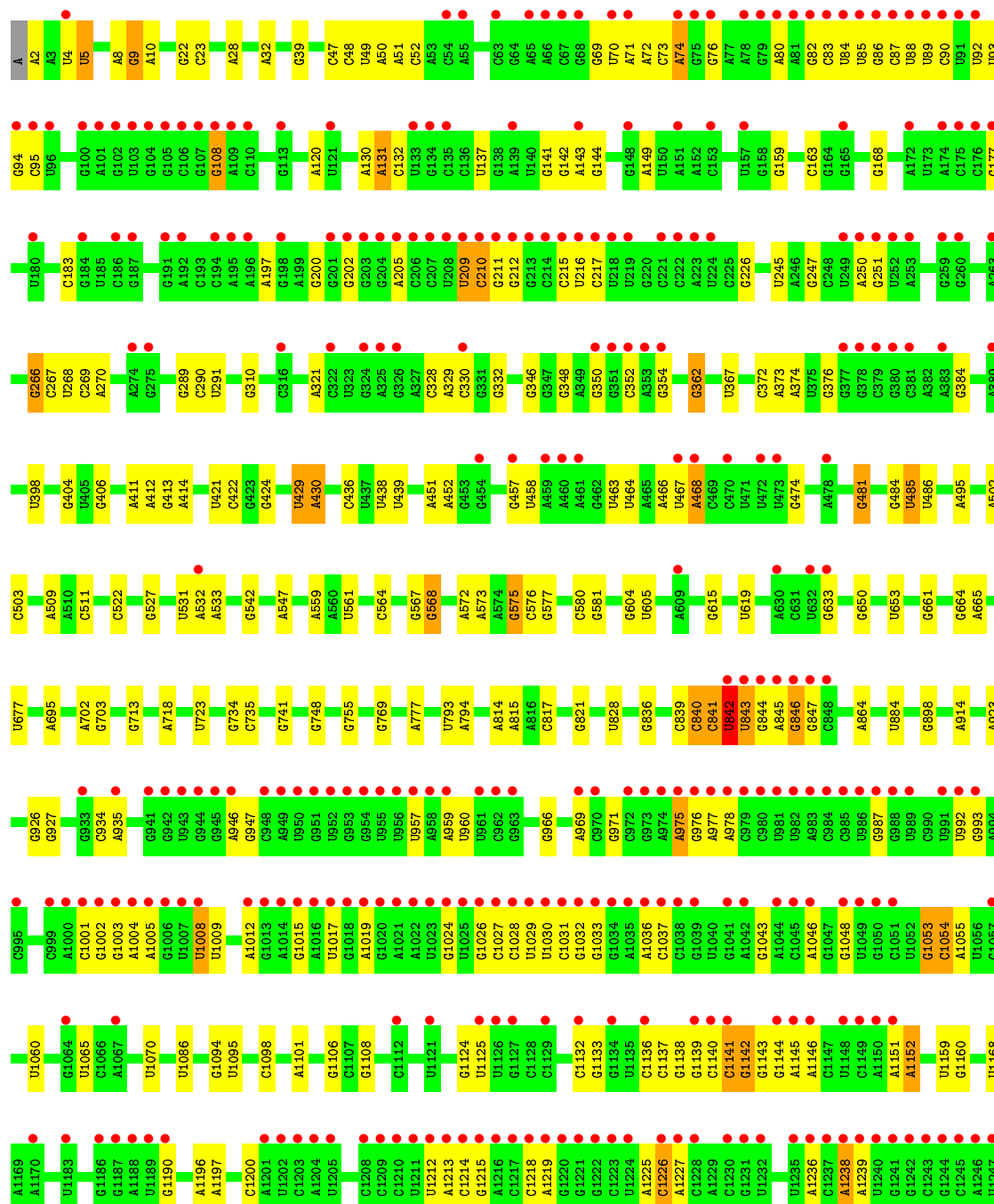
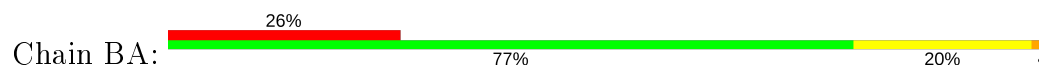
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ( $\text{RSRZ} > 2$ ). 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.

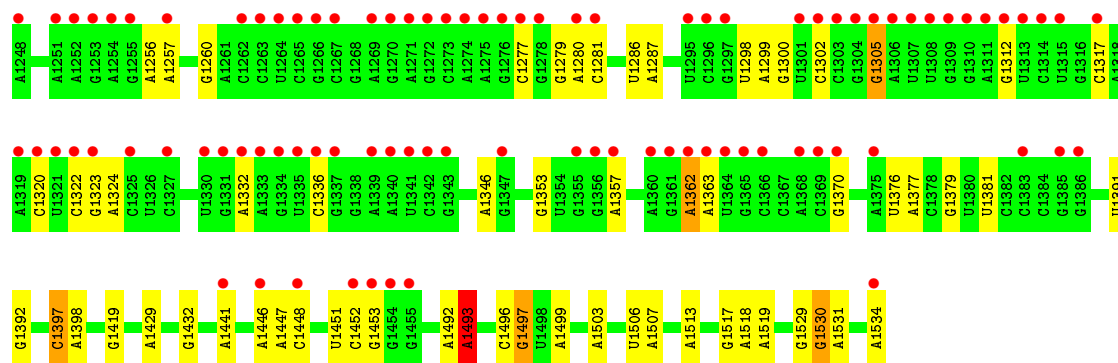
#### • Molecule 1: 16S rRNA



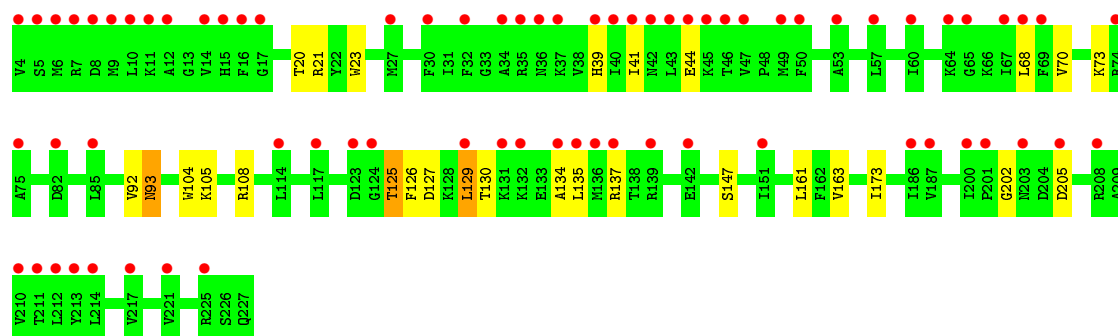
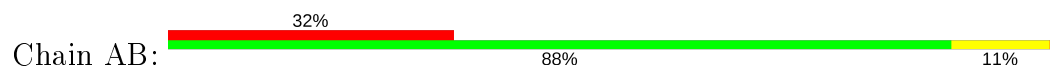


• Molecule 1: 16S rRNA

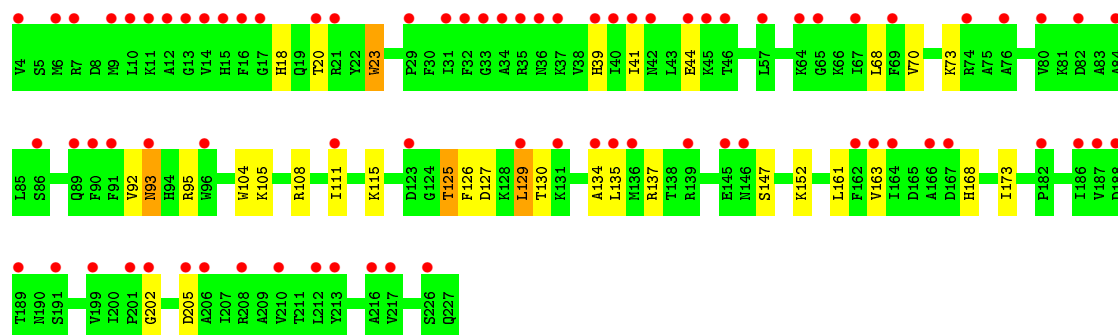
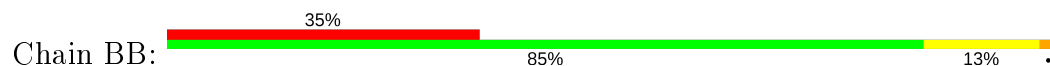




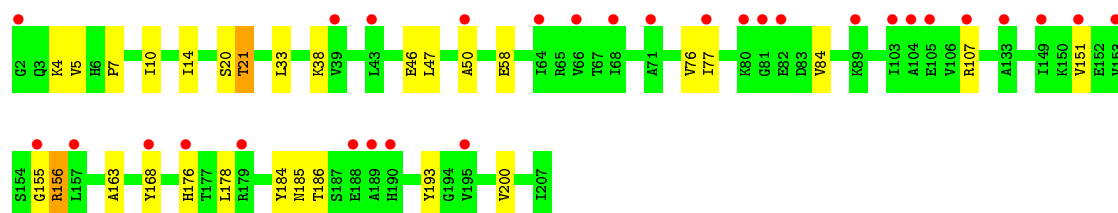
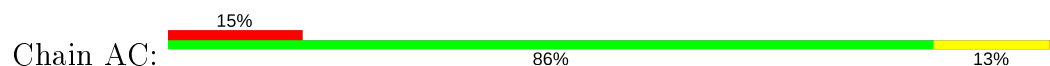
• Molecule 2: 30S ribosomal protein S2



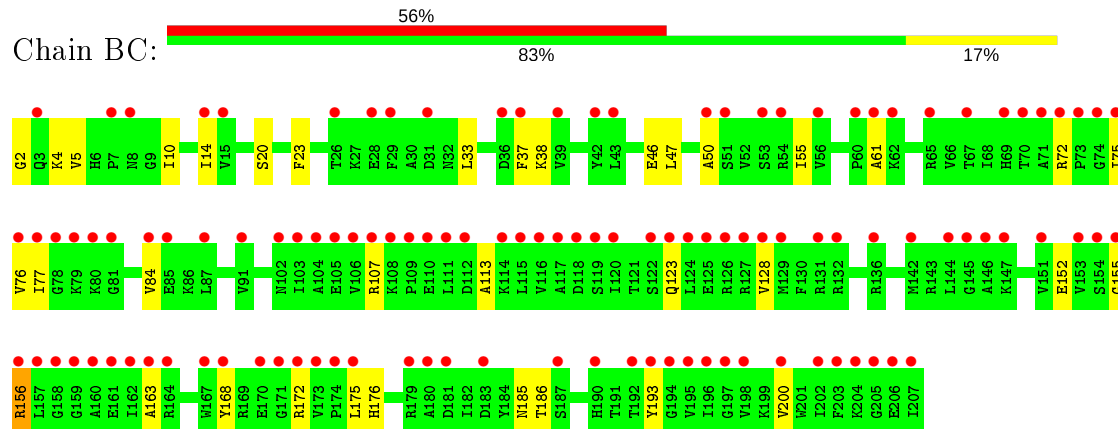
• Molecule 2: 30S ribosomal protein S2



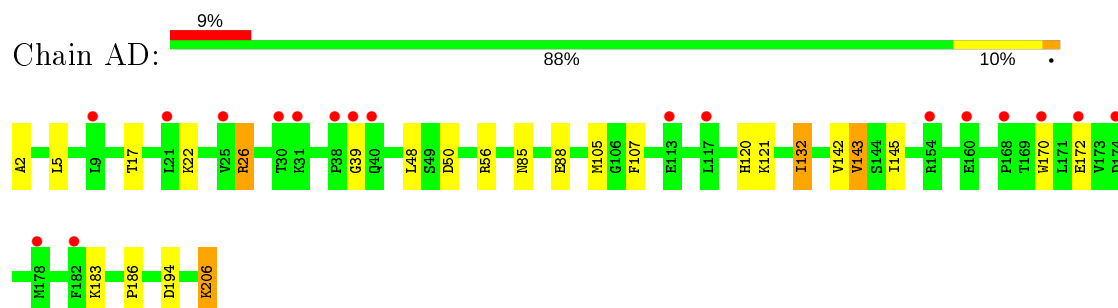
• Molecule 3: 30S ribosomal protein S3



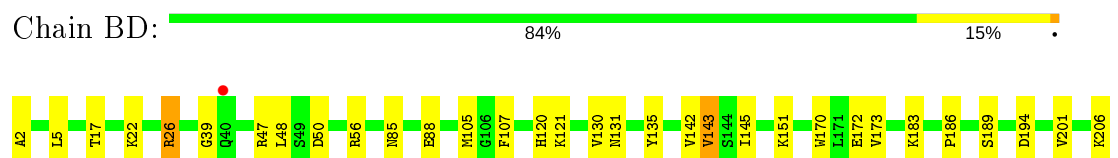
- Molecule 3: 30S ribosomal protein S3



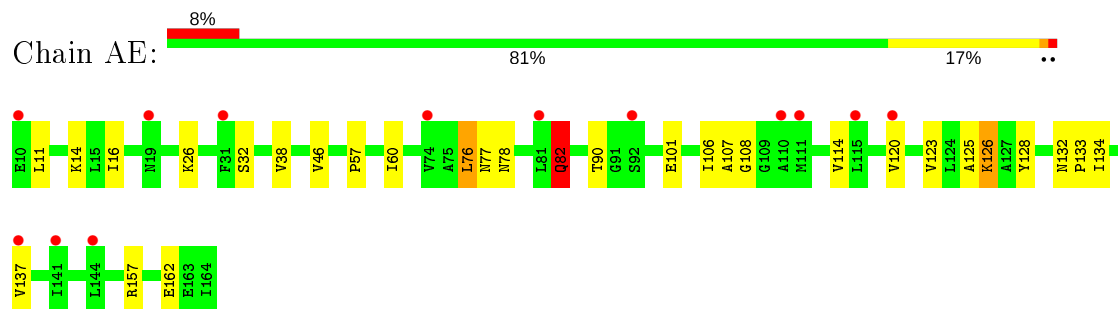
- Molecule 4: 30S ribosomal protein S4



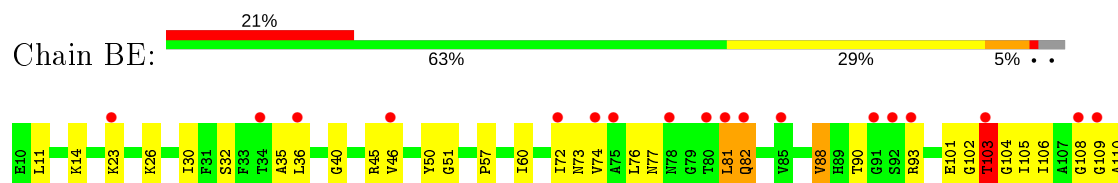
- Molecule 4: 30S ribosomal protein S4

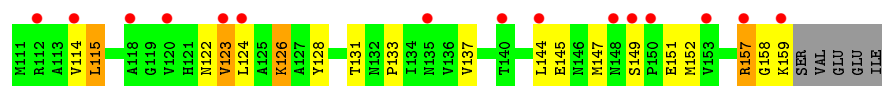


- Molecule 5: 30S ribosomal protein S5

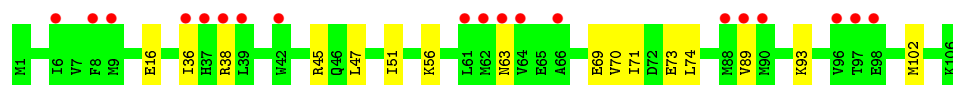
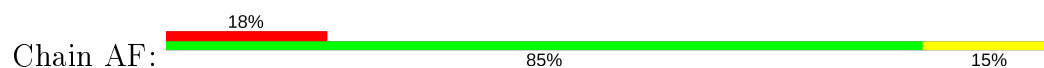


- Molecule 5: 30S ribosomal protein S5

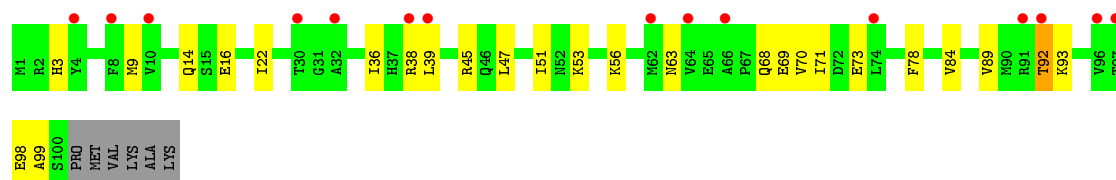




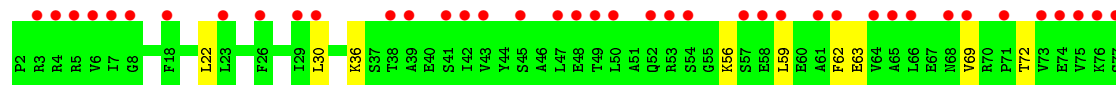
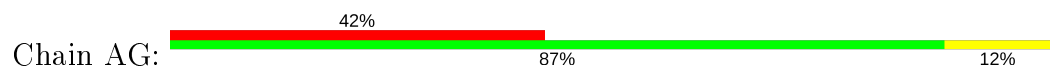
- Molecule 6: 30S ribosomal protein S6



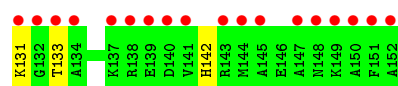
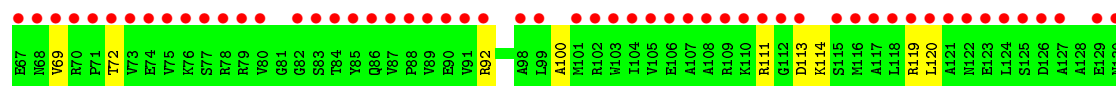
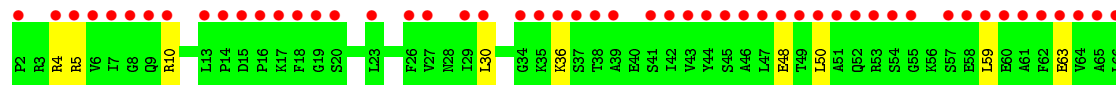
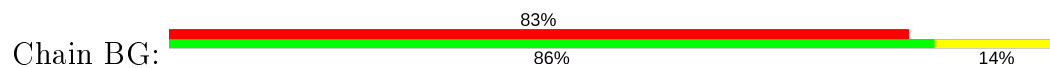
- Molecule 6: 30S ribosomal protein S6



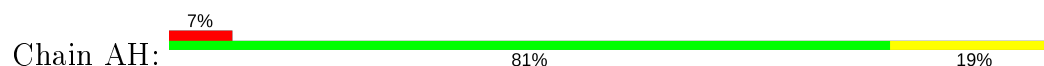
- Molecule 7: 30S ribosomal protein S7



- Molecule 7: 30S ribosomal protein S7

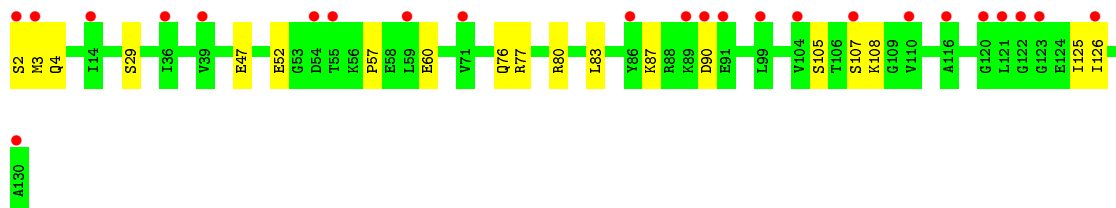
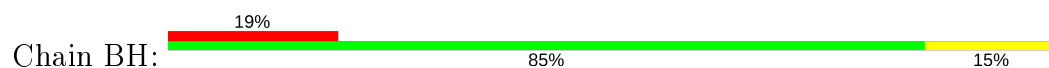


- Molecule 8: 30S ribosomal protein S8

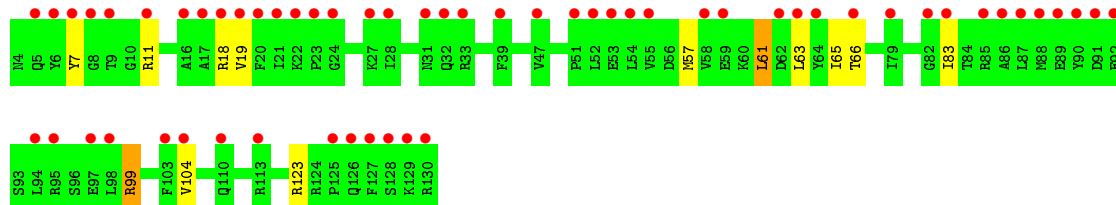
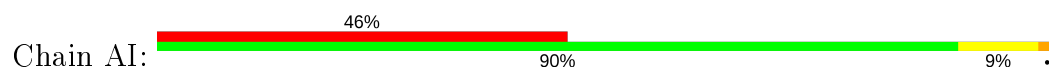




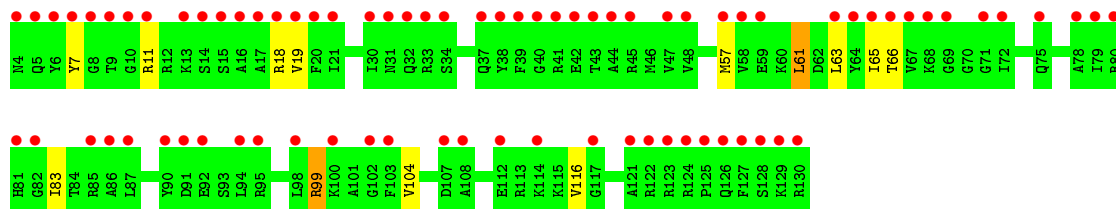
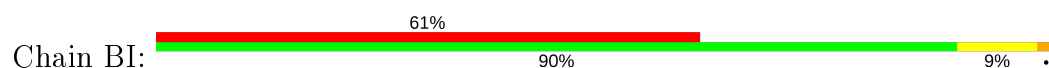
- Molecule 8: 30S ribosomal protein S8



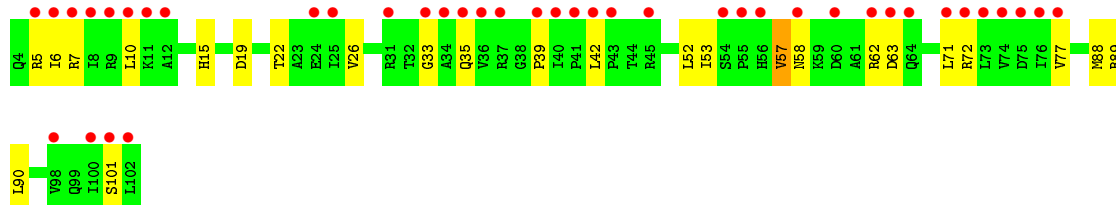
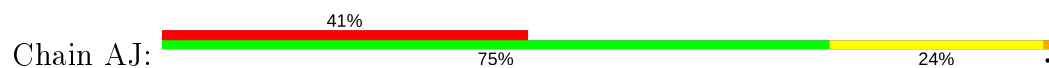
- Molecule 9: 30S ribosomal protein S9



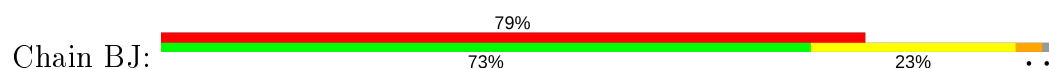
- Molecule 9: 30S ribosomal protein S9

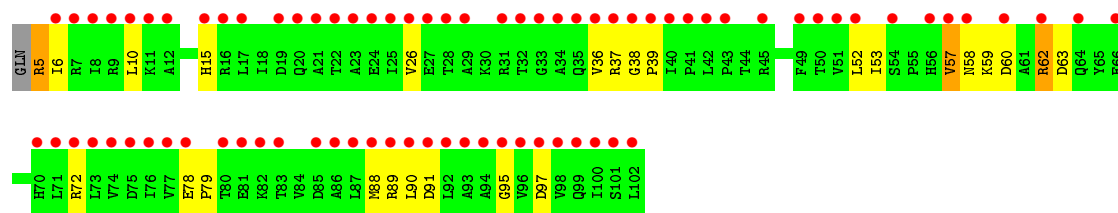


- Molecule 10: 30S ribosomal protein S10

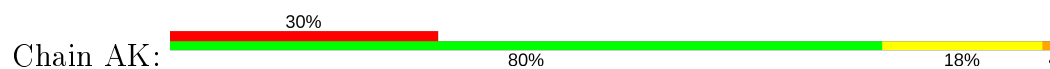


- Molecule 10: 30S ribosomal protein S10

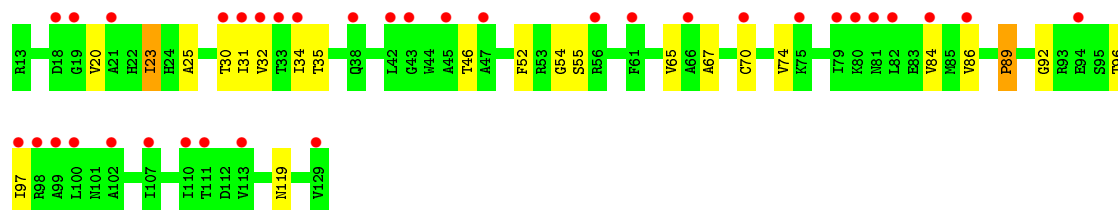




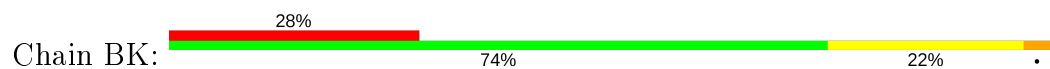
- Molecule 11: 30S ribosomal protein S11



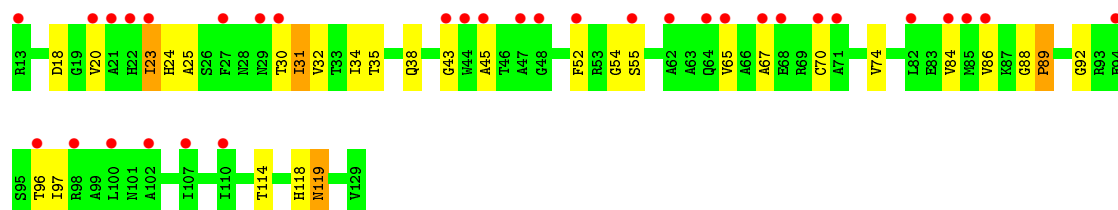
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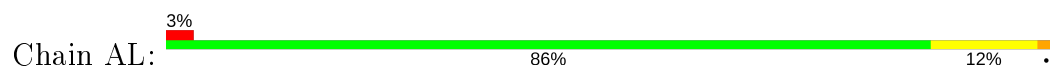
- Molecule 11: 30S ribosomal protein S11



Chain BK:



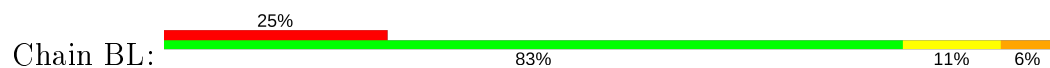
- Molecule 12: 30S ribosomal protein S12



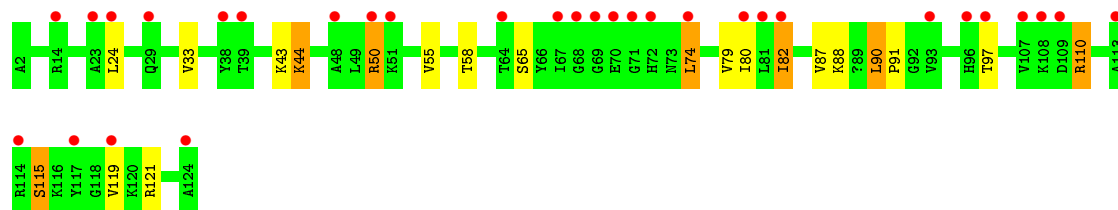
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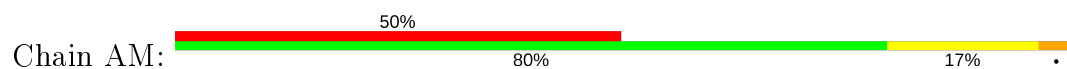
- Molecule 12: 30S ribosomal protein S12



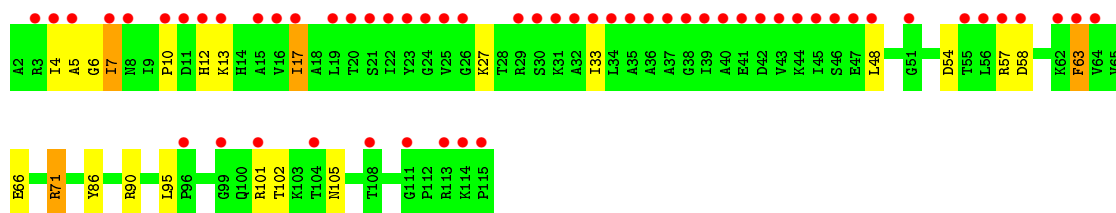
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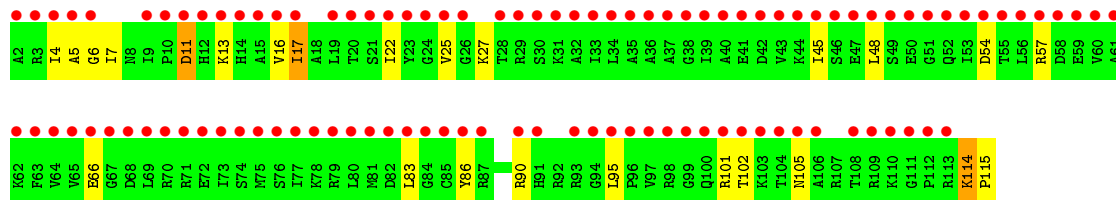
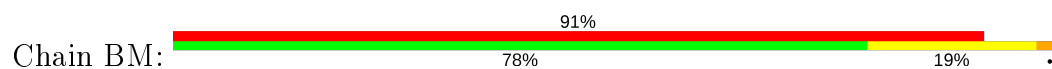
- Molecule 13: 30S ribosomal protein S13



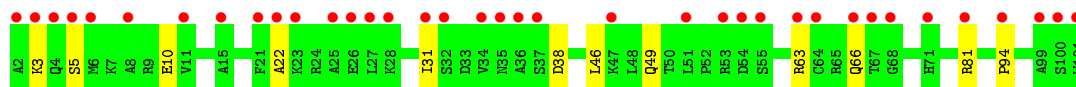
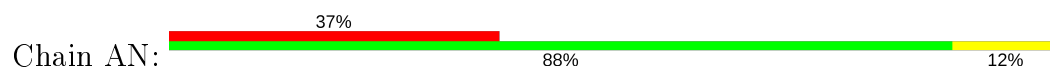
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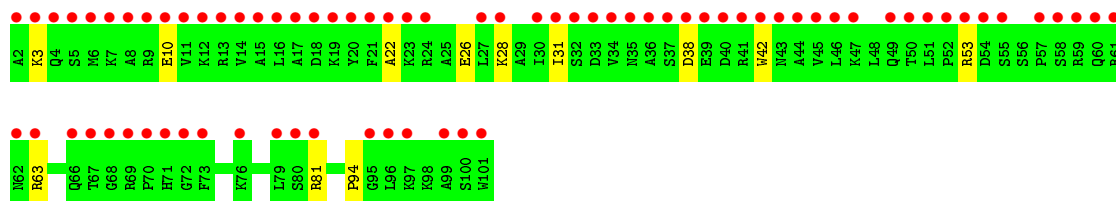
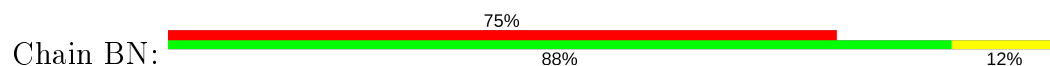
● Molecule 13: 30S ribosomal protein S13



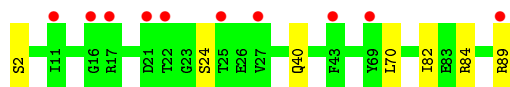
● Molecule 14: 30S ribosomal protein S14



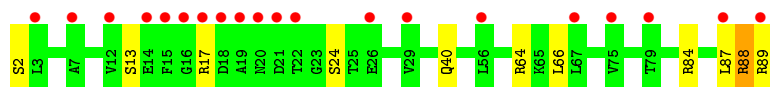
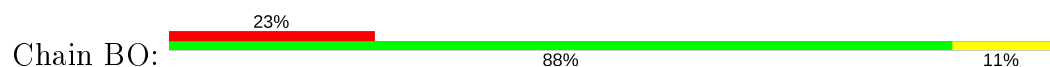
● Molecule 14: 30S ribosomal protein S14



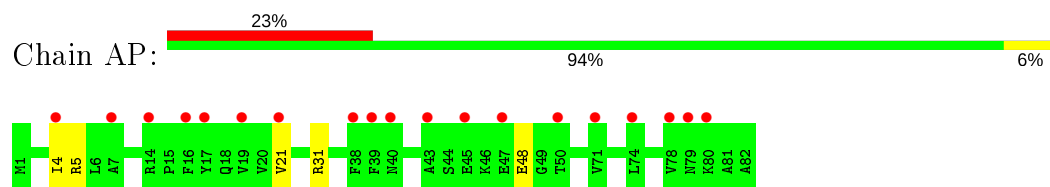
● Molecule 15: 30S ribosomal protein S15



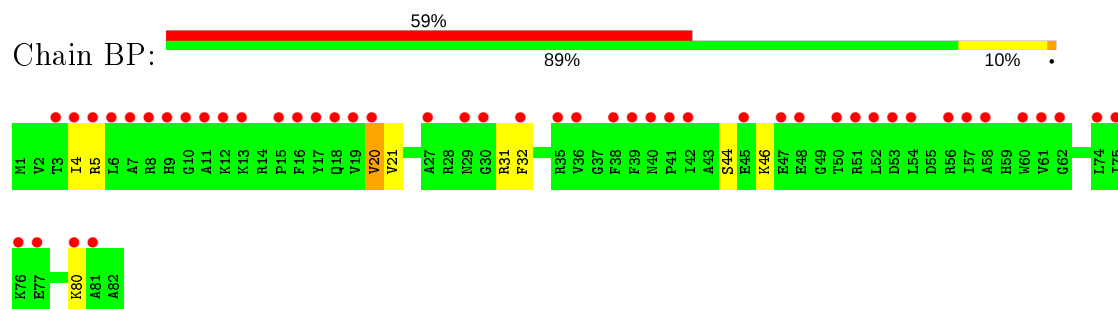
● Molecule 15: 30S ribosomal protein S15



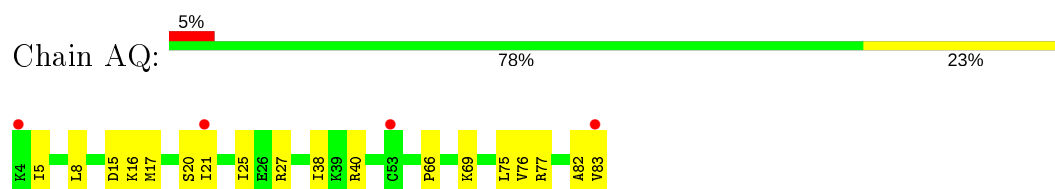
- Molecule 16: 30S ribosomal protein S16



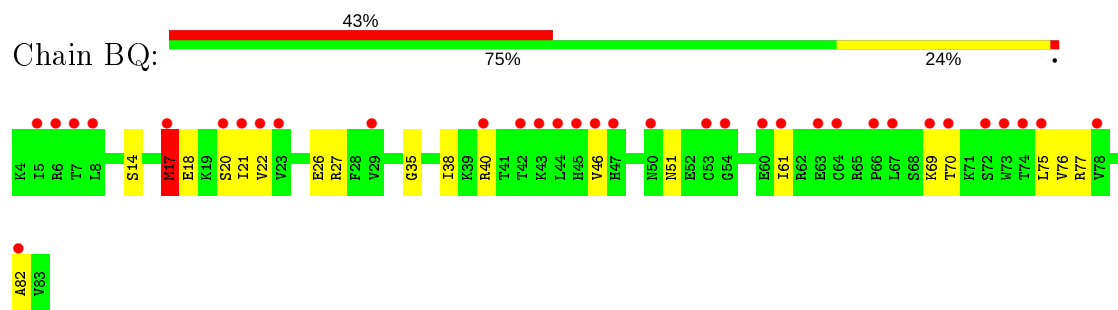
- Molecule 16: 30S ribosomal protein S16



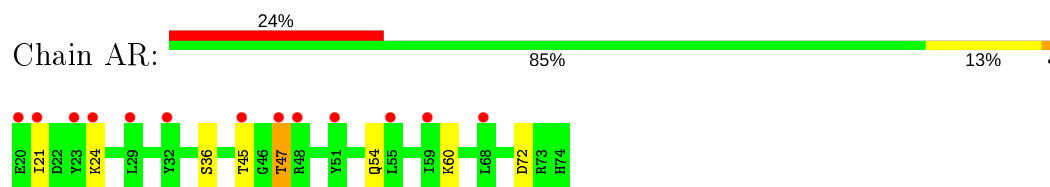
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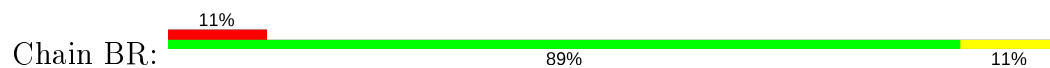
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

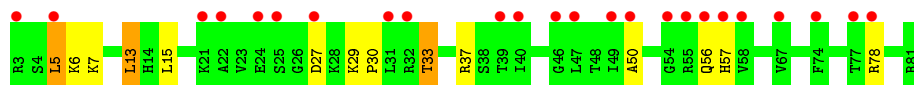
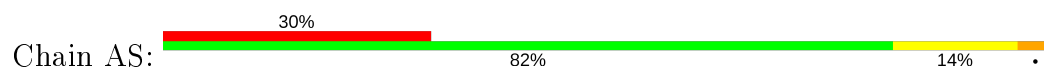


- Molecule 18: 30S ribosomal protein S18

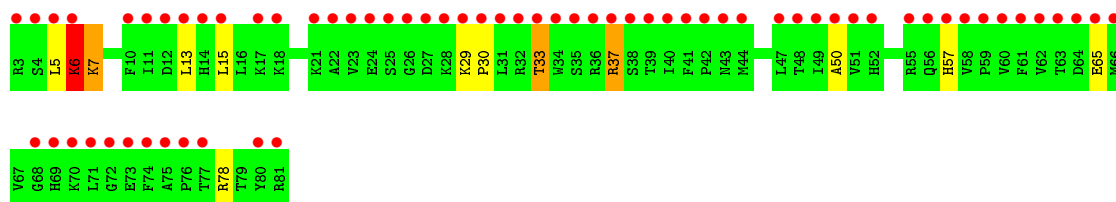
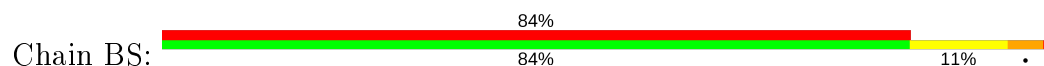




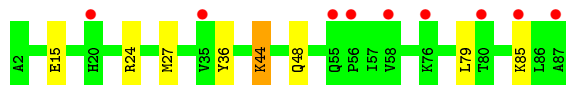
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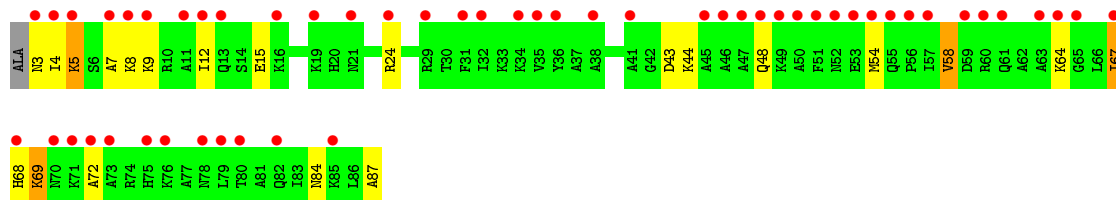
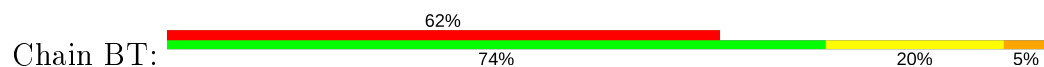
- Molecule 19: 30S ribosomal protein S19



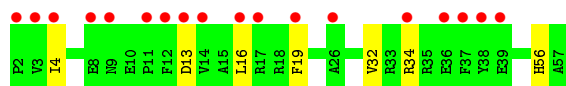
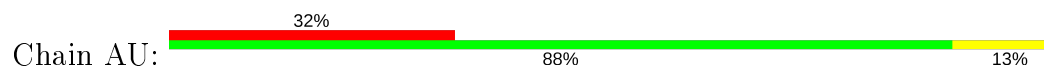
- Molecule 20: 30S ribosomal protein S20



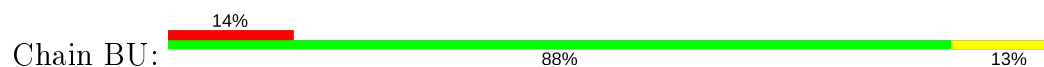
- Molecule 20: 30S ribosomal protein S20

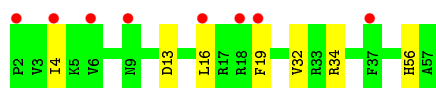


- Molecule 21: 30S ribosomal protein S21

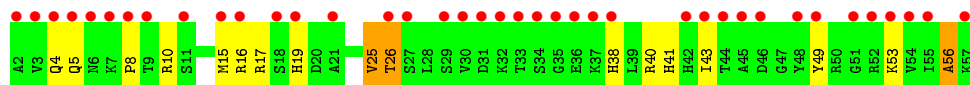
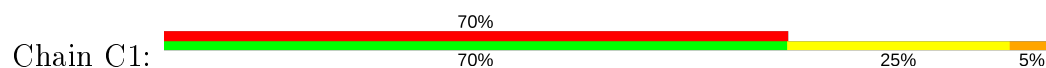


- Molecule 21: 30S ribosomal protein S21

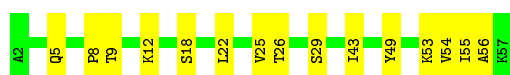




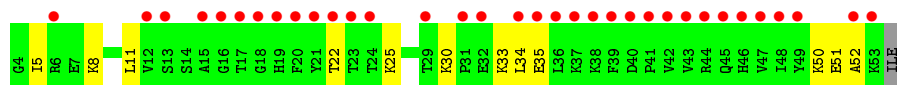
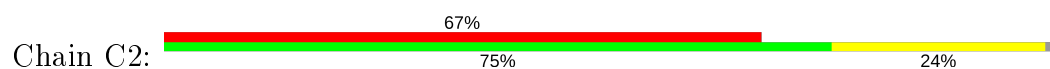
- Molecule 22: 50S ribosomal protein L32



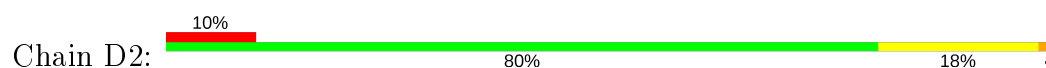
- Molecule 22: 50S ribosomal protein L32



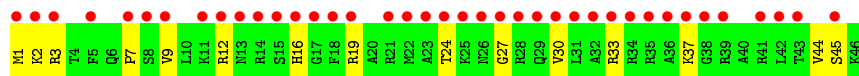
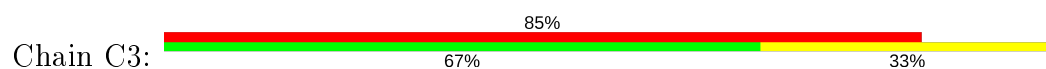
- Molecule 23: 50S ribosomal protein L33



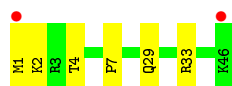
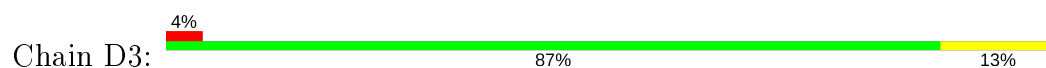
- Molecule 23: 50S ribosomal protein L33



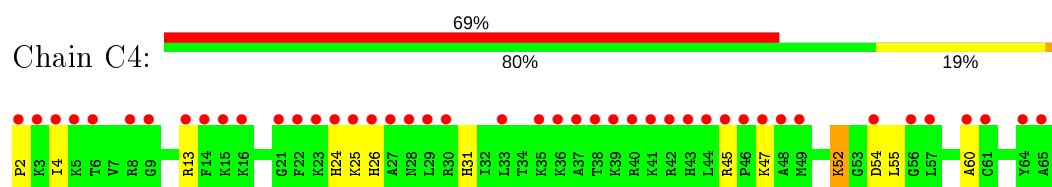
- Molecule 24: 50S ribosomal protein L34



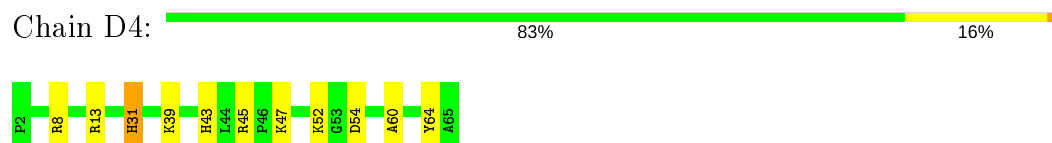
- Molecule 24: 50S ribosomal protein L34



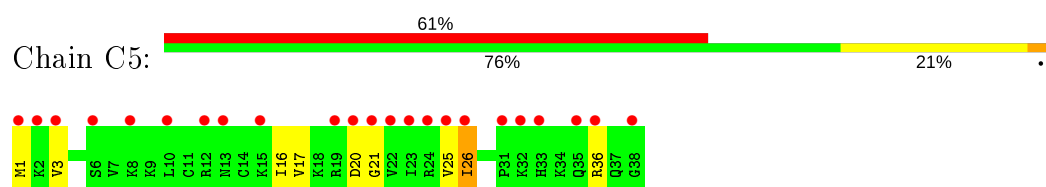
- Molecule 25: 50S ribosomal protein L35



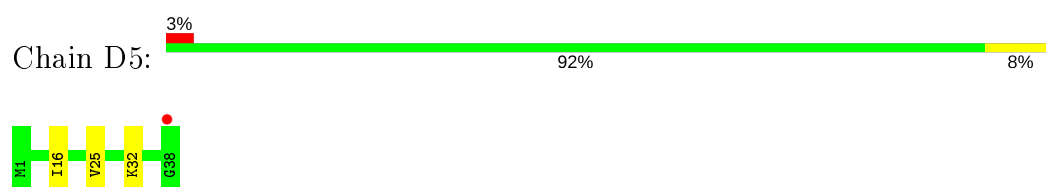
- Molecule 25: 50S ribosomal protein L35



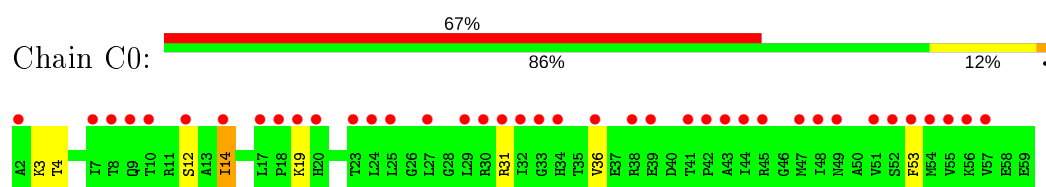
- Molecule 26: 50S ribosomal protein L36



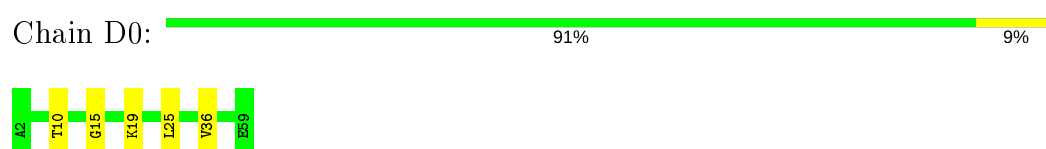
- Molecule 26: 50S ribosomal protein L36



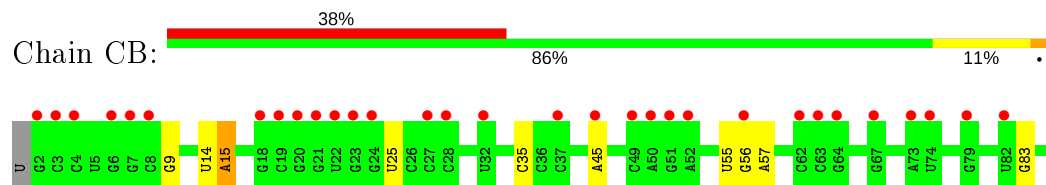
- Molecule 27: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L30



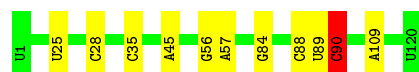
- Molecule 28: 5S rRNA





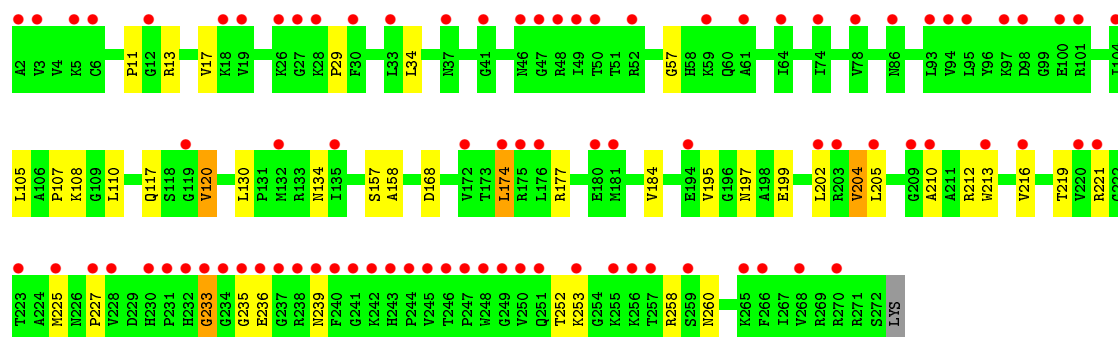
• Molecule 28: 5S rRNA

Chain DB: 91% 8% .



• Molecule 29: 50S ribosomal protein L2

Chain CC: 32% 84% 14% .



• Molecule 29: 50S ribosomal protein L2

Chain DC: 2% 90% 8% .



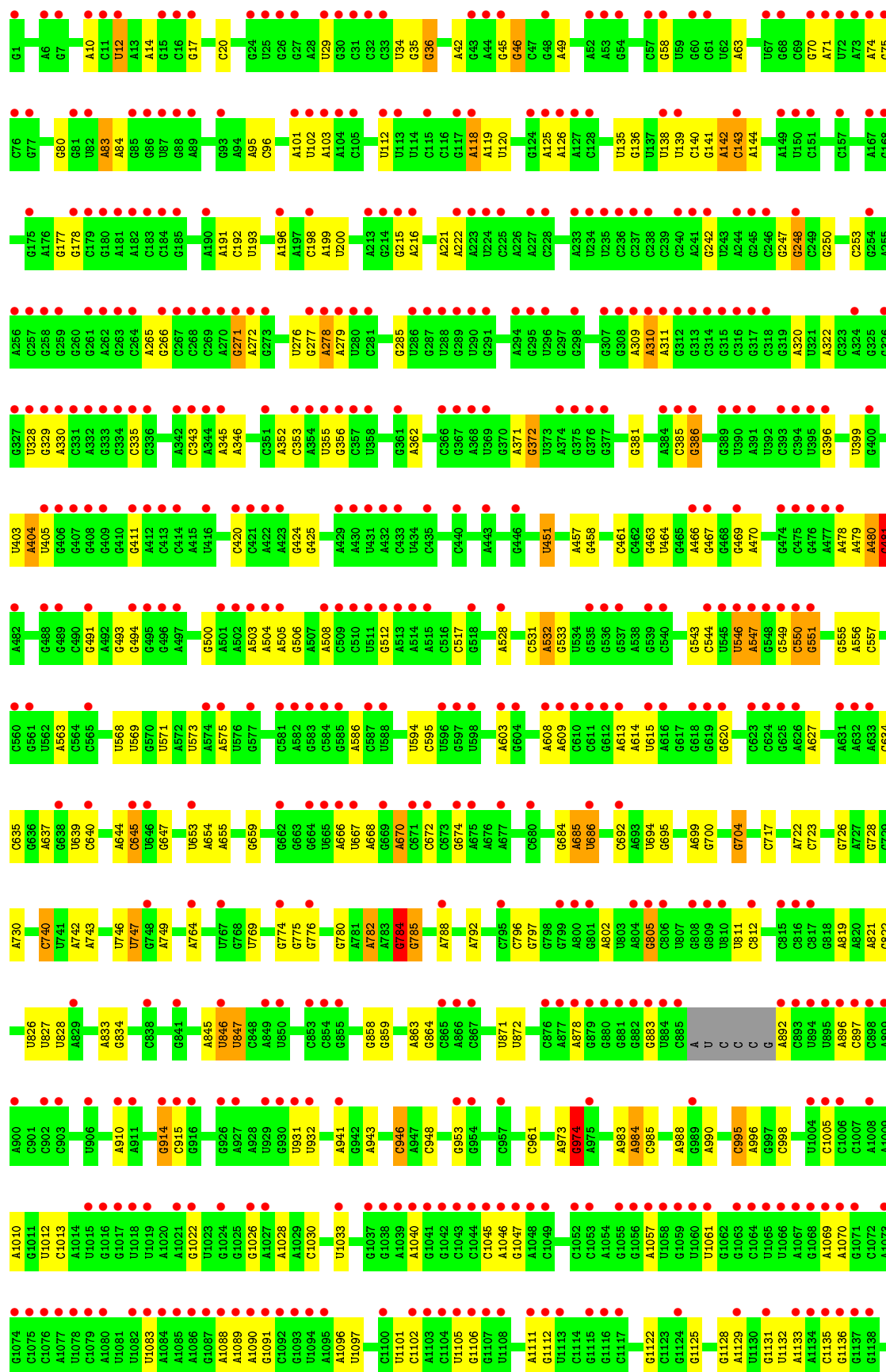
• Molecule 30: 50S ribosomal protein L3

Chain CD: 62% 89% 11% .

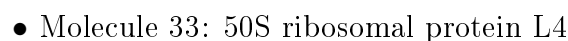


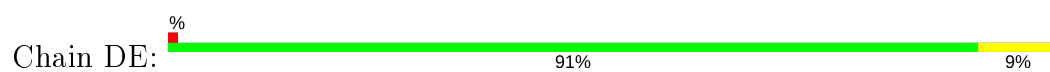
• Molecule 31: 23S rRNA

Chain CA: 35% 75% 22% .

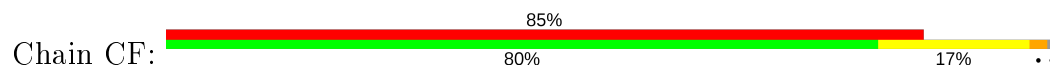


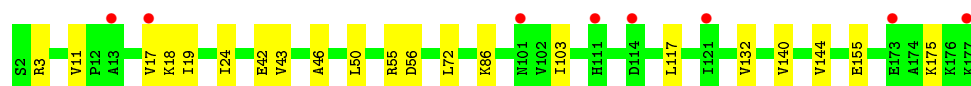
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G2282	C2175	U2109	G2029	G1930	A1789	G1675	A1583	G1492	U1394	A1307	G1228	A1142
C2283	A2176	A2030	A2031	U1931	A1794	U1693	U1584	A1493	A1395	G1309	G1229	A1143
G2286	C2177	U2111	A2032	A1936	C1795	U1694	C1585	A1494	U1396	G1310	G1233	G1149
A2287	C2178	G2112	A2033	A1937	C1796	U1695	G1586	A1495	G1401	G1311	U1234	C1150
G2288	C2179	U2113	U2034	A1938	C1800	G1695	G1587	A1496	G1402	U1312	U1235	G1156
U2291	U2180	A2114	G2035	A1938	A1801	G1696	U1588	U1497	G1403	U1313	G1236	C1157
U2292	U2181	G2115	G2036	U1943	G1807	G1703	G1589	A1508	U1406	C1314	G1237	A1158
G2293	A2182	G2116	A2037	G1954	A1808	C1704	A1596	A1509	G1407	G1319	A1237	G1162
G2294	A2183	U2117	G2038	G1955	A1809	U1708	A1597	G1510	G1408	G1320	G1238	G1163
C2295	U2185	A2119	U2039	U1956	A1810	U1709	U1598	G1511	U1409	A1321	G1239	G1164
U2296	G2186	G2120	G2040	C1957	G1811	G1715	C1600	U1513	G1416	A1322	A1244	A1165
A2297	G2187	G2121	A2042	C1958	U1812	G1716	G1601	A1514	G1417	G1323	G1245	G1166
G2298	U2189	U2122	C2043	U1963	C1816	U1719	A1603	A1515	G1418	G1324	A1246	A1167
A2299	G2190	G2123	C2044	U1964	U1820	U1720	G1606	G1516	A1420	U1325	G1248	G1168
C2300	A2191	G2124	C2045	C1965	U1821	G1721	G1607	G1517	A1421	U1326	U1249	C1169
C2301	G2192	G2125	G2046	C1966	U1822	A1722	C1608	G1518	G1422	A1327	G1250	G1170
U2302	U2193	A2126	C2047	C1967	U1823	U1723	G1609	G1519	G1423	U1328	C1251	G1171
G2303	G2127	G2127	G2048	A1966	C1822	A1724	A1607	G1520	G1424	G1330	G1252	C1172
U2304	G2128	U2129	C2049	C1967	U1823	U1725	A1609	A1521	A1431	G1331	A1254	U1173
C2305	G2129	C2130	C2050	A1970	U1825	U1729	G1612	U1523	C1437	U1255	U1256	U1174
G2306	U2130	U2131	A2051	G1971	U1826	G1730	G1613	G1524	U1438	G1339	A1260	A1175
A2309	U2132	G2132	G2052	G1972	A1829	C1732	A1614	A1525	A1439	U1340	A1261	U1176
C2310	G2133	G2133	A2053	U1973	A1830	G1733	A1615	A1526	G1443	U1341	A1262	G1177
A2311	U2134	A2134	C2055	G1983	A1847	U1734	G1616	A1528	C1444	U1352	A1263	G1178
G2312	G2135	A2135	C2056	G1984	A1848	A1735	A1617	G1529	G1445	A1353	G1266	G1179
C2313	G2136	G2136	C2057	C1985	U1854	U1738	G1619	G1530	U1446	A1354	G1267	U1180
A2317	C2143	C2144	A2059	C1986	U1854	G1738	G1620	C1531	C1447	G1355	C1270	U1181
G2318	G2145	G2145	G2061	U1991	G1861	U1742	G1621	A1532	G1448	A1356	A1271	U1182
C2322	C2146	A2147	A2062	G1992	G1862	G1743	G1622	U1534	G1449	G1357	U1272	U1183
A2323	G2147	G2148	G2069	U1993	U1864	A1744	U1629	A1535	G1452	U1358	A1274	G1184
G2325	U2149	U2149	C2072	C1997	U1865	U1748	G1633	C1536	A1453	A1359	A1275	G1185
C2326	G2150	U2151	C2073	G2000	U1866	G1749	A1634	G1537	C1454	G1360	A1276	G1186
A2328	U2152	G2152	C2074	U2003	G1867	G1750	A1635	G1538	G1455	G1361	G1277	G1189
G2333	C2153	G2153	U2075	A2003	U1868	U1758	U1636	U1539	G1456	C1362	G1278	U1201
U2334	A2154	A2154	G2076	G2004	G1869	U1759	A1637	G1540	U1460	G1363	G1279	G1202
G2335	U2155	U2155	A2077	A2005	A1870	C1764	C1638	C1541	U1467	A1364	A1284	U1203
U2336	G2157	G2157	C2078	C2006	A1872	U1765	G1642	G1543	U1468	A1365	A1285	A1204
A2339	U2158	A2158	A2080	G2010	C1873	C1771	G1643	G1546	A1469	U1372	A1286	A1205
C2340	G2159	G2159	G2088	A2013	G1874	A1772	G1644	C1547	G1470	A1373	A1287	G1206
G2345	C2160	G2160	A2088	A2014	G1875	U1773	G1645	A1548	C1471	U1374	G1288	G1207
A2346	G2161	A2162	G2093	A2015	U1880	G1774	U1646	G1551	G1472	U1375	C1289	C1208
C2347	A2163	G2163	A2094	U2016	A1900	U1775	U1648	G1552	G1475	G1376	U1290	U1209
U2348	C2164	C2164	A2095	A2019	G1906	U1776	G1649	G1555	A1476	U1379	G1291	G1210
G2349	G2165	A2166	G2100	A2020	G1907	U1777	U1650	C1556	A1477	G1380	G1292	G1211
C2350	U2167	U2167	A2101	C1908	G1907	U1779	G1651	C1557	G1478	G1381	G1293	A1212
G2351	G2168	U2168	U2022	C1909	C1908	U1782	A1652	C1565	G1482	G1382	G1294	A1213
A2354	C2169	C2169	C2023	G1910	G1909	U1783	G1653	A1566	U1487	A1383	C1297	A1214
G2355	A2170	G2170	G2024	A1913	G1910	A1784	G1654	A1567	C1488	A1384	G1300	G1215
C2356	U2171	U2171	C2025	A1914	G1913	U1785	G1655	A1569	C1489	A1385	A1302	G1216
A2358	U2172	U2172	U2026	C1914	A1914	A1786	U1656	U1578	G1490	A1387	G1301	U1217
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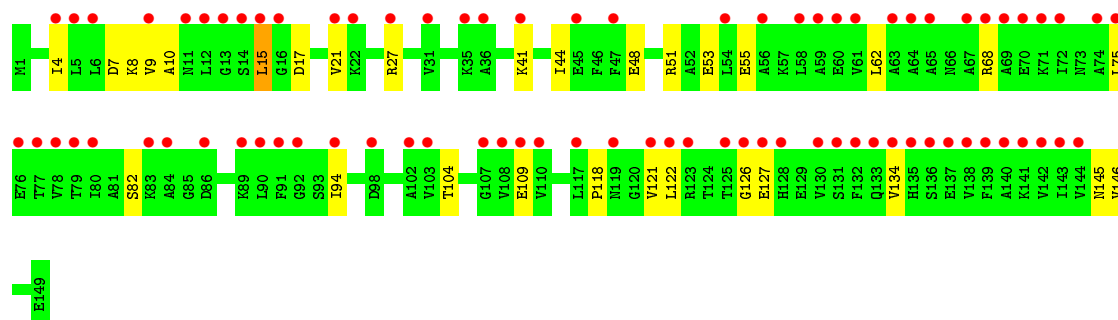
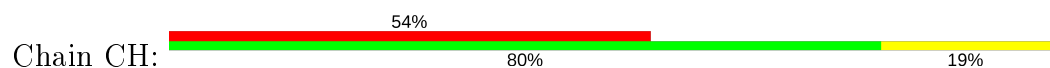


• Molecule 34: 50S ribosomal protein L5

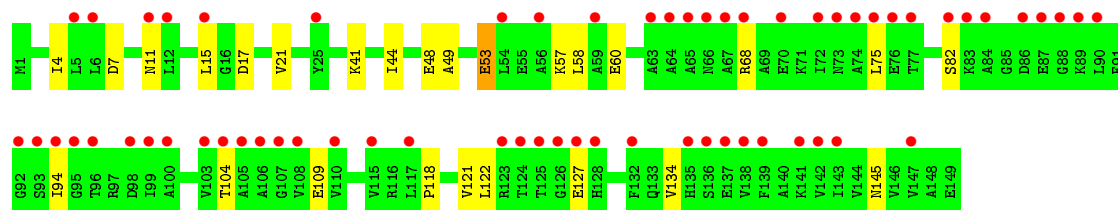
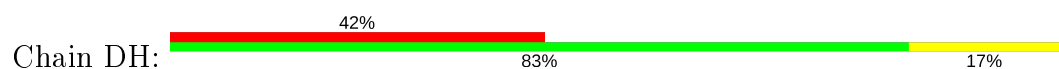




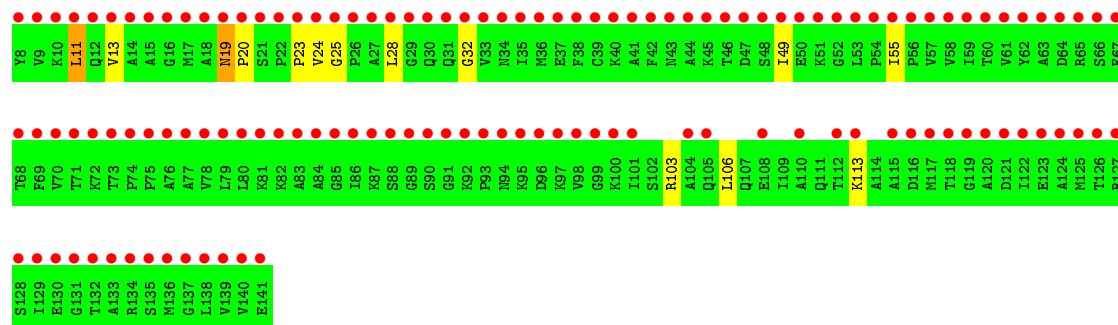
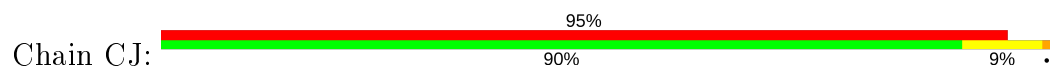
- Molecule 36: 50S ribosomal protein L9



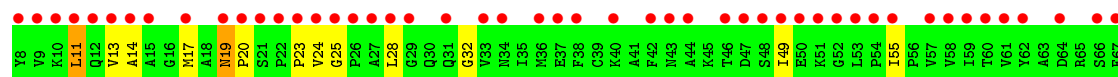
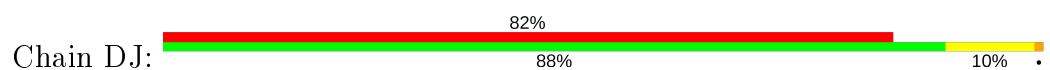
- Molecule 36: 50S ribosomal protein L9

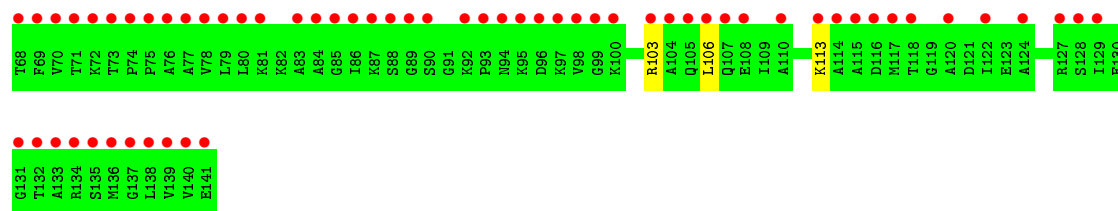


- Molecule 37: 50S ribosomal protein L11

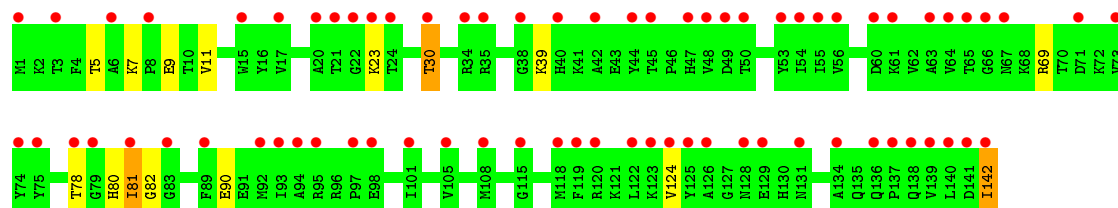
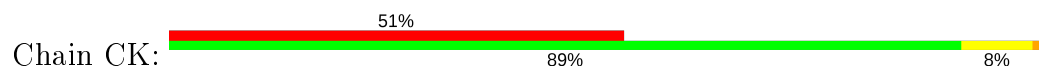


- Molecule 37: 50S ribosomal protein L11

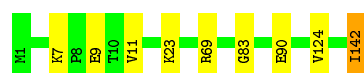




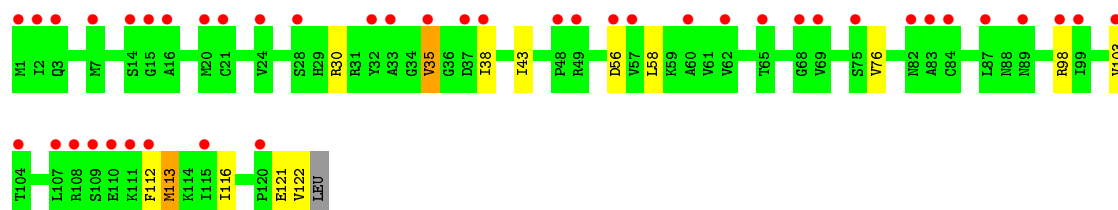
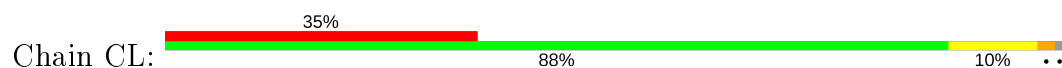
• Molecule 38: 50S ribosomal protein L13



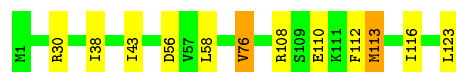
• Molecule 38: 50S ribosomal protein L13



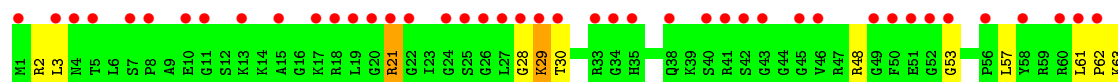
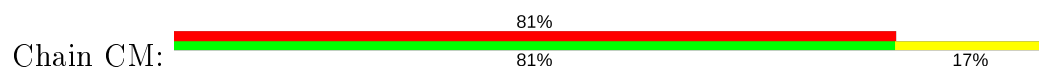
• Molecule 39: 50S ribosomal protein L14

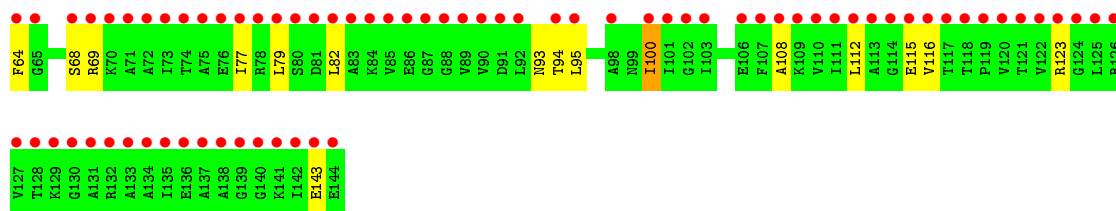


• Molecule 39: 50S ribosomal protein L14

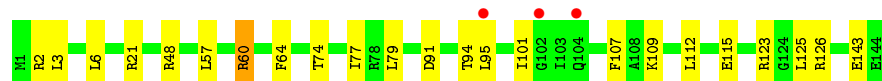
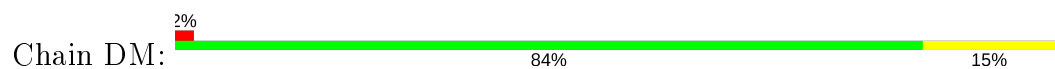


• Molecule 40: 50S ribosomal protein L15

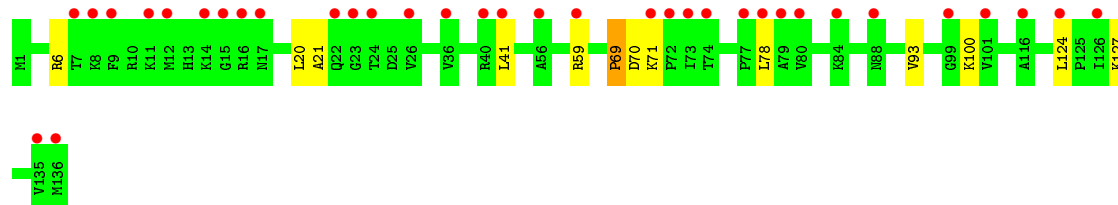
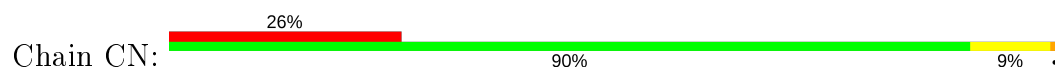




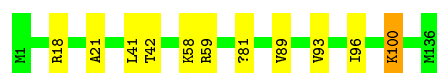
- Molecule 40: 50S ribosomal protein L15



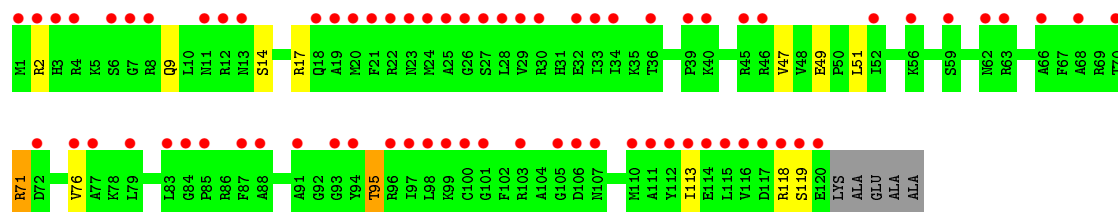
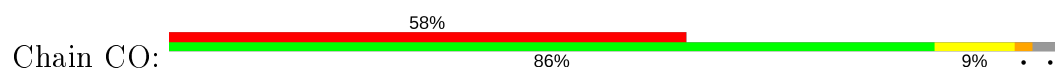
- Molecule 41: 50S ribosomal protein L16



- Molecule 41: 50S ribosomal protein L16



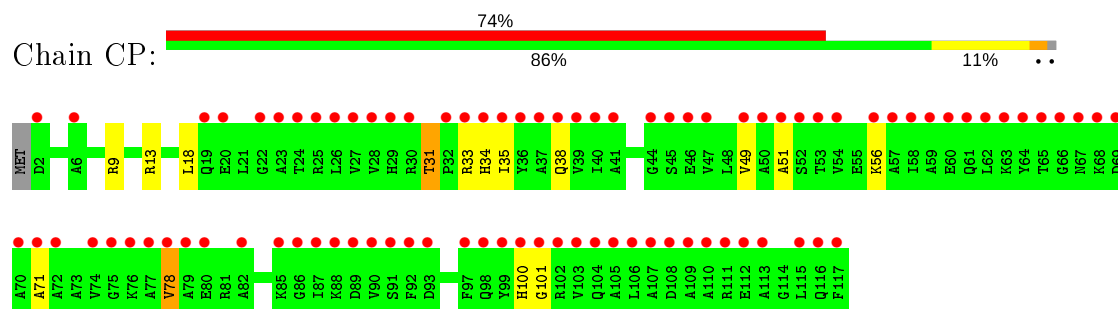
- Molecule 42: 50S ribosomal protein L17



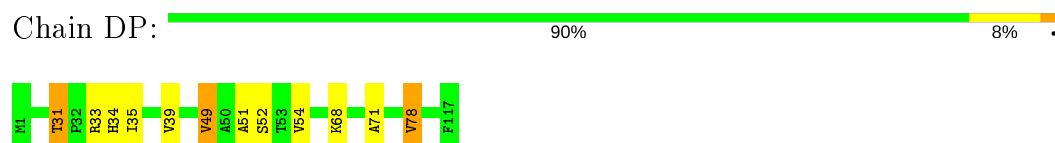
- Molecule 42: 50S ribosomal protein L17



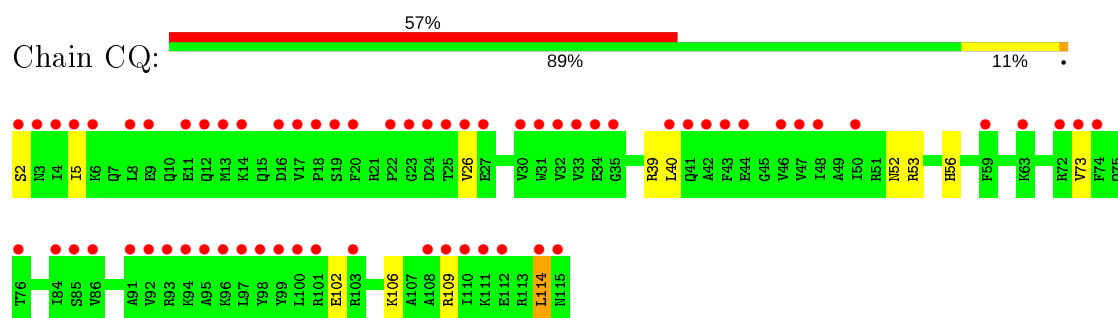
- Molecule 43: 50S ribosomal protein L18



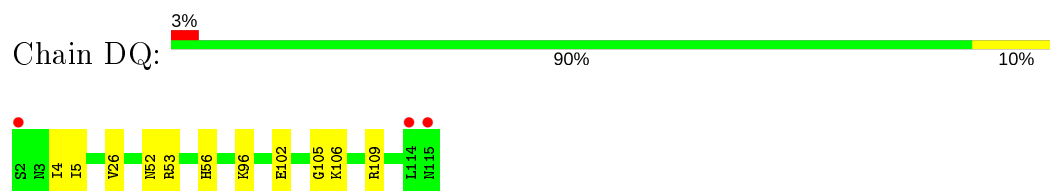
- Molecule 43: 50S ribosomal protein L18



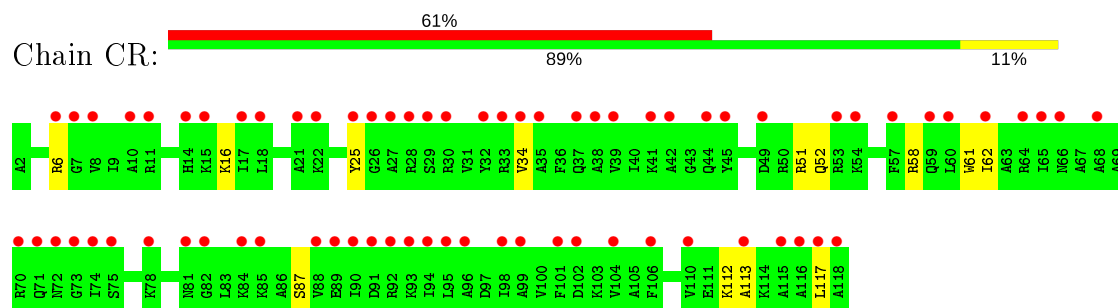
- Molecule 44: 50S ribosomal protein L19



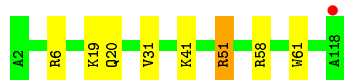
- Molecule 44: 50S ribosomal protein L19



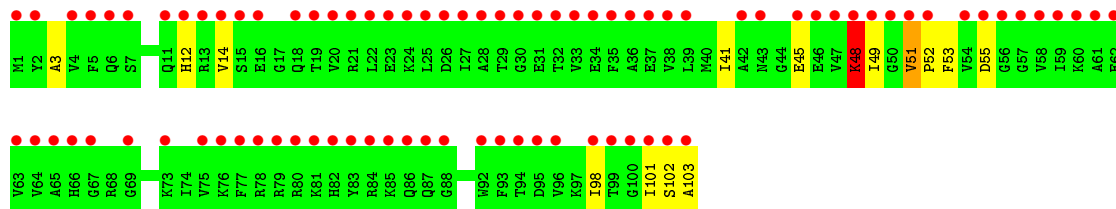
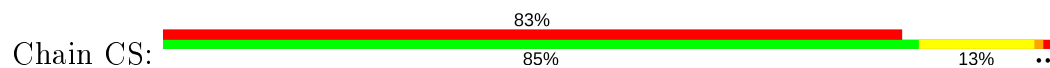
- Molecule 45: 50S ribosomal protein L20



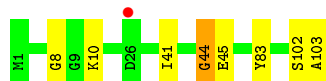
- Molecule 45: 50S ribosomal protein L20



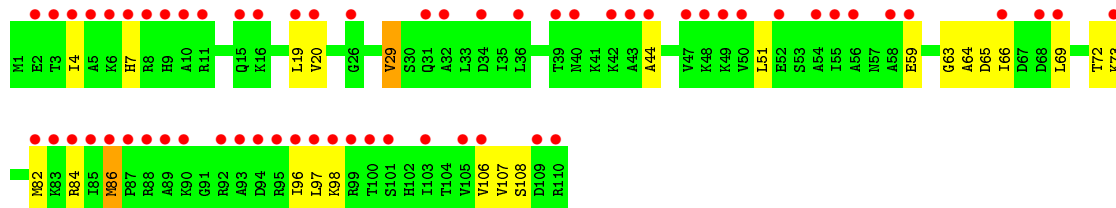
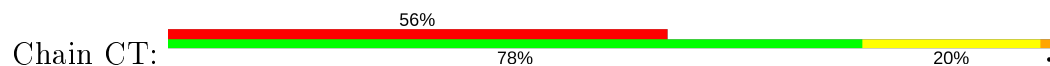
- Molecule 46: 50S ribosomal protein L21



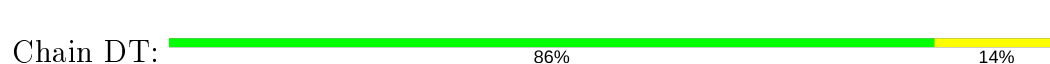
- Molecule 46: 50S ribosomal protein L21



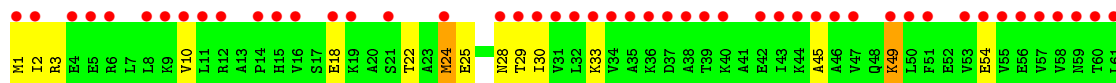
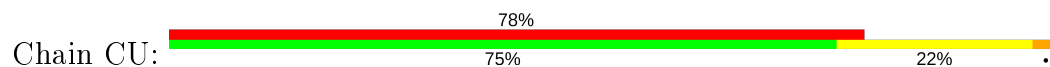
- Molecule 47: 50S ribosomal protein L22

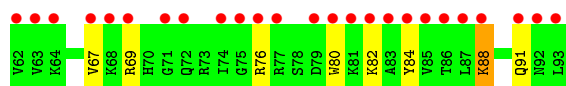


- Molecule 47: 50S ribosomal protein L22

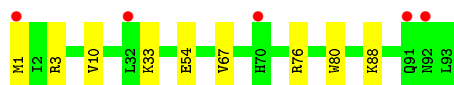
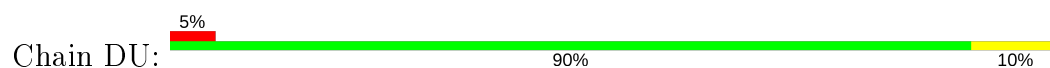


- Molecule 48: 50S ribosomal protein L23

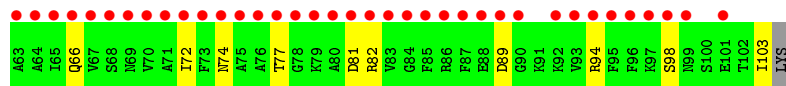
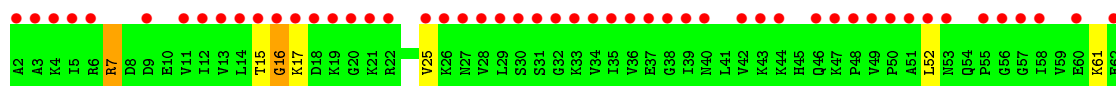
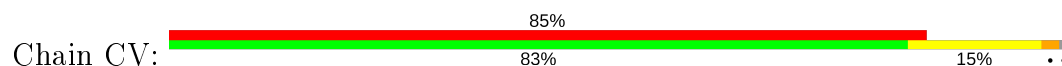




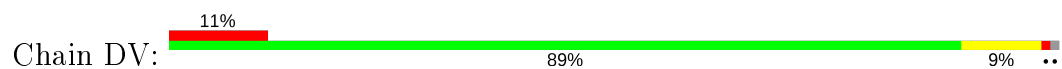
- Molecule 48: 50S ribosomal protein L23



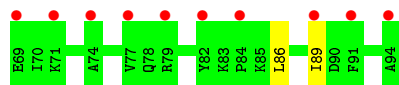
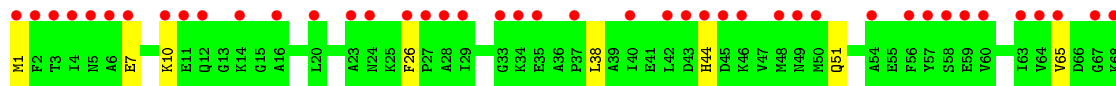
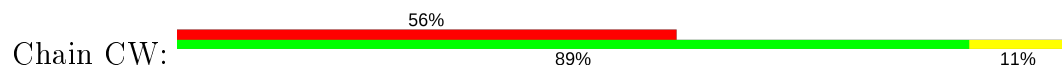
- Molecule 49: 50S ribosomal protein L24



- Molecule 49: 50S ribosomal protein L24



- Molecule 50: 50S ribosomal protein L25

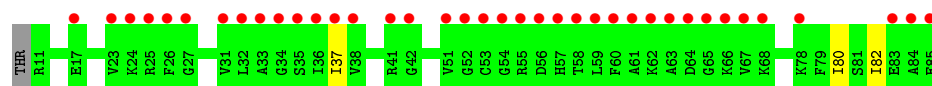


- Molecule 50: 50S ribosomal protein L25

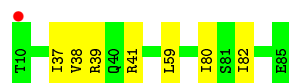


- Molecule 51: 50S ribosomal protein L27

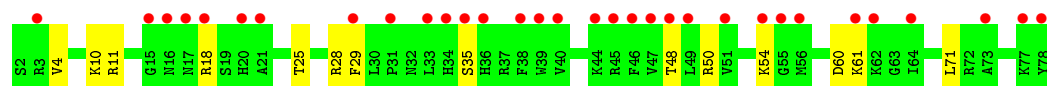
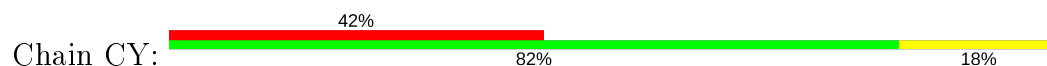




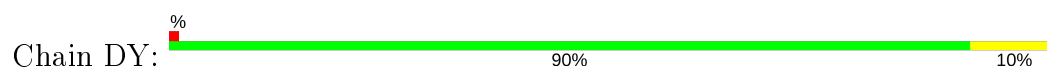
- Molecule 51: 50S ribosomal protein L27



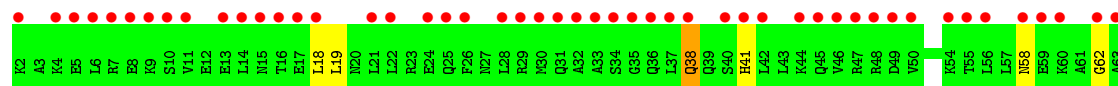
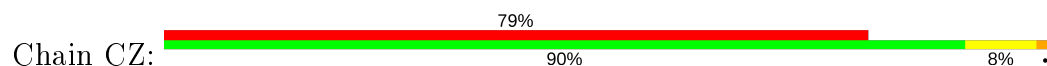
- Molecule 52: 50S ribosomal protein L28



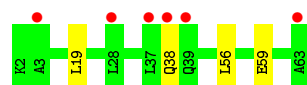
- Molecule 52: 50S ribosomal protein L28



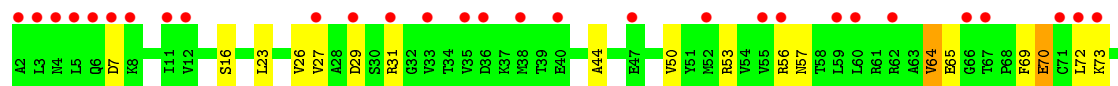
- Molecule 53: 50S ribosomal protein L29

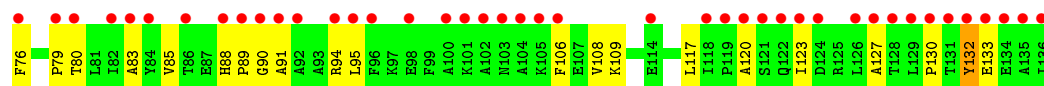


- Molecule 53: 50S ribosomal protein L29

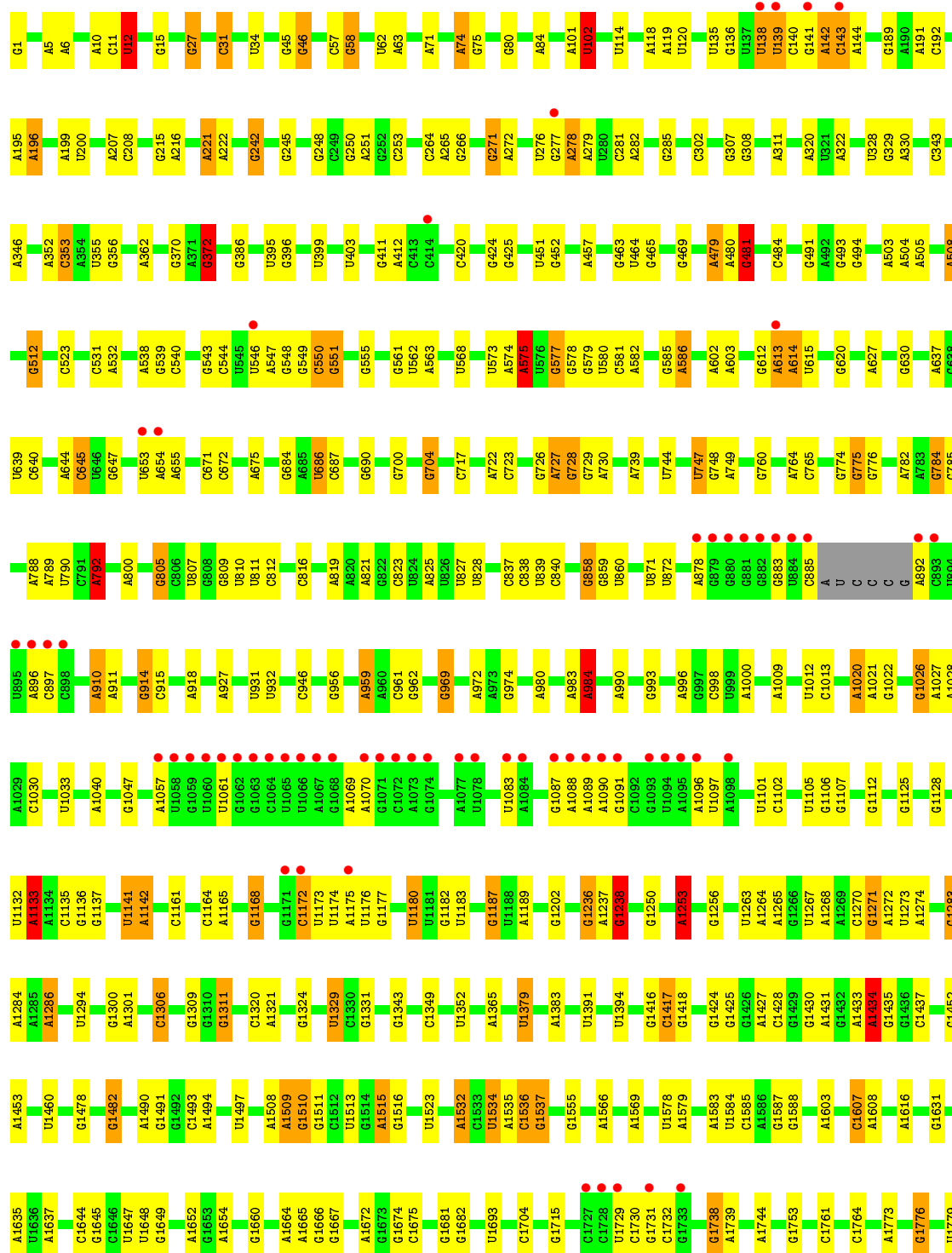
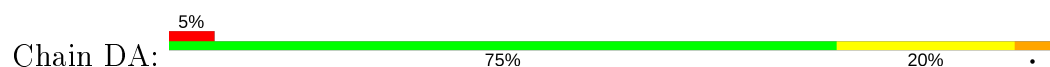


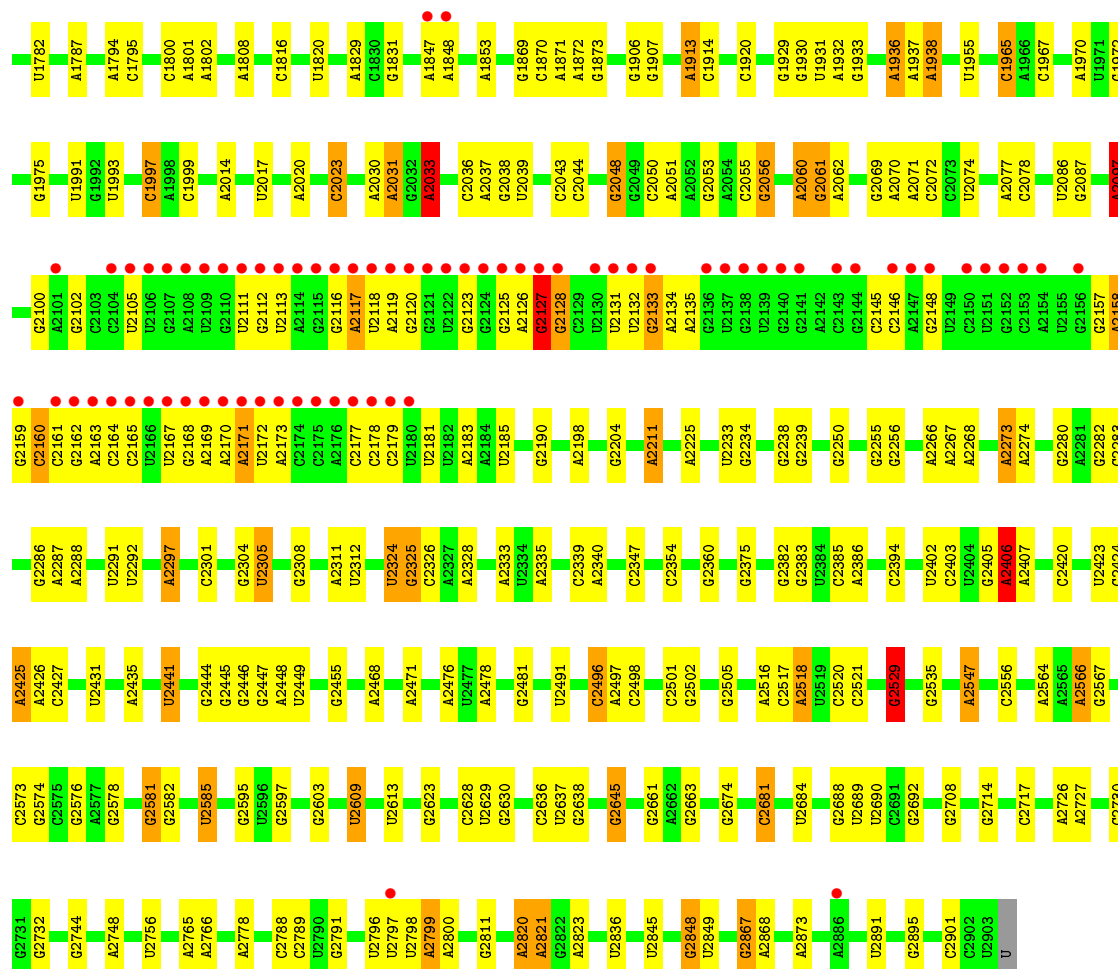
- Molecule 54: 50S ribosomal protein L10





• Molecule 55: 23S rRNA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.18Å 434.82Å 624.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.51 – 2.96 48.28 – 2.96	Depositor EDS
% Data completeness (in resolution range)	88.6 (48.51-2.96) 88.6 (48.28-2.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	21.17 (at 2.96Å)	Xtriage
Refinement program	BUSTER-TNT 2.11.6	Depositor
R, $R_{free}$	0.208 , 0.221 0.227 , 0.243	Depositor DCC
$R_{free}$ test set	4163 reflections (0.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 89.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	295202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, GUN, 1PE, 2MA, 2MG, ACY, PEG, 1MG, 3TD, PGE, G7M, D2T, UR3, SPD, 4D4, 5MU, ZN, 5MC, MPD, PG4, 6MZ, TRS, OMC, MG, OMG, T1C, H2U, EDO, MEQ, OMU, PUT, 4OC, PSU

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	AP	0.48	0/659	0.70	0/884
16	BP	0.50	0/659	0.76	0/884
17	AQ	0.48	0/658	0.73	0/881
17	BQ	0.51	0/658	0.78	0/881
18	AR	0.53	0/463	0.65	0/621
18	BR	0.50	0/463	0.64	0/621
19	AS	0.46	0/653	0.59	0/877
19	BS	0.45	0/653	0.60	0/877
20	AT	0.48	0/676	0.66	0/895
20	BT	0.52	0/671	0.68	0/888
21	AU	0.45	0/472	0.61	0/627
21	BU	0.43	0/472	0.63	0/627
22	C1	0.49	0/450	0.71	0/599
22	D1	0.61	0/450	0.79	0/599
23	C2	0.46	0/416	0.73	0/554
23	D2	0.51	0/421	0.73	0/561
24	C3	0.46	0/380	0.69	0/498
24	D3	0.55	0/380	0.76	0/498
25	C4	0.46	0/513	0.67	0/676
25	D4	0.56	0/513	0.71	0/676
26	C5	0.43	0/303	0.77	0/397
26	D5	0.53	0/303	0.76	0/397
27	C0	0.52	0/453	0.77	0/605
27	D0	0.62	0/467	0.81	0/623
28	CB	0.98	0/2828	0.88	2/4410 (0.0%)
28	DB	1.13	1/2872 (0.0%)	0.90	0/4478
29	CC	0.45	0/2121	0.76	0/2852
29	DC	0.50	0/2121	0.76	1/2852 (0.0%)
30	CD	0.43	0/1586	0.70	0/2134
31	CA	1.07	44/69165 (0.1%)	0.87	17/107896 (0.0%)
32	DD	0.54	0/1576	0.73	0/2119
33	CE	0.45	0/1571	0.72	0/2113
33	DE	0.52	0/1571	0.72	0/2113
34	CF	0.43	0/1434	0.68	0/1926
34	DF	0.46	0/1434	0.70	0/1926
35	CG	0.42	0/1343	0.66	0/1816
35	DG	0.44	0/1343	0.64	0/1816
36	CH	0.48	0/1121	0.68	0/1515
36	DH	0.48	0/1121	0.68	0/1515
37	CJ	0.48	0/993	0.62	0/1341
37	DJ	0.48	0/993	0.61	0/1341
38	CK	0.43	0/1152	0.70	0/1551
38	DK	0.56	0/1152	0.74	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	CL	0.47	0/947	0.74	0/1268
39	DL	0.54	0/955	0.75	0/1279
40	CM	0.46	0/1062	0.74	1/1413 (0.1%)
40	DM	0.50	0/1062	0.75	1/1413 (0.1%)
41	CN	0.45	0/1081	0.75	1/1443 (0.1%)
41	DN	0.59	0/1092	0.81	0/1457
42	CO	0.46	0/973	0.72	0/1301
42	DO	0.58	0/1006	0.80	0/1345
43	CP	0.43	0/902	0.73	0/1209
43	DP	0.47	0/910	0.73	0/1219
44	CQ	0.41	0/929	0.71	0/1242
44	DQ	0.48	0/929	0.72	0/1242
45	CR	0.48	0/960	0.69	0/1278
45	DR	0.62	0/960	0.76	0/1278
46	CS	0.44	0/829	0.74	0/1107
46	DS	0.55	0/829	0.78	0/1107
47	CT	0.43	0/864	0.74	0/1156
47	DT	0.55	0/864	0.75	0/1156
48	CU	0.44	0/745	0.72	0/994
48	DU	0.48	0/745	0.72	0/994
49	CV	0.44	0/787	0.76	0/1051
49	DV	0.49	0/787	0.77	0/1051
50	CW	0.40	0/766	0.65	0/1025
50	DW	0.50	0/766	0.69	0/1025
51	CX	0.39	0/576	0.65	0/762
51	DX	0.53	0/598	0.73	0/790
52	CY	0.43	0/635	0.73	0/848
52	DY	0.46	0/635	0.72	0/848
53	CZ	0.42	0/502	0.61	0/667
53	DZ	0.43	0/502	0.60	0/667
54	DI	0.51	0/1037	0.74	1/1402 (0.1%)
55	DA	1.27	148/69364 (0.2%)	0.97	26/108207 (0.0%)
All	All	0.98	212/309267 (0.1%)	0.85	60/462210 (0.0%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	AE	0	1
10	BJ	0	1
31	CA	0	12
55	DA	0	87
All	All	0	108

The worst 5 of 212 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	1020	A	N3-C4	9.93	1.40	1.34
31	CA	1936	A	N9-C4	-9.29	1.32	1.37
31	CA	2095	A	O5'-C5'	-9.00	1.28	1.42
55	DA	539	G	N7-C5	7.77	1.44	1.39
55	DA	12	U	C1'-N1	7.58	1.60	1.48

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	CB	15	A	O4'-C1'-N9	10.06	116.25	108.20
55	DA	512	G	O4'-C1'-N9	8.55	115.04	108.20
1	AA	413	G	C1'-O4'-C4'	-8.26	103.29	109.90
55	DA	784	G	P-O3'-C3'	7.86	129.13	119.70
41	CN	69	PRO	C-N-CA	7.39	140.18	121.70

There are no chirality outliers.

5 of 108 planarity outliers are listed below:

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

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16591	90	0
1	BA	32908	0	16580	97	0
2	AB	1753	0	1780	10	0
2	BB	1753	0	1780	15	0
3	AC	1625	0	1696	14	0
3	BC	1625	0	1696	18	0
4	AD	1643	0	1707	13	0
4	BD	1643	0	1707	17	0
5	AE	1144	0	1185	15	0
5	BE	1105	0	1148	30	0
6	AF	862	0	864	7	0
6	BF	817	0	808	9	0
7	AG	1182	0	1238	7	0
7	BG	1182	0	1238	4	0
8	AH	979	0	1031	8	0
8	BH	979	0	1031	4	0
9	AI	1022	0	1070	6	0
9	BI	1022	0	1070	6	0
10	AJ	796	0	836	11	0
10	BJ	787	0	828	10	0
11	AK	877	0	887	14	0
11	BK	877	0	887	17	0
12	AL	957	0	1017	7	0
12	BL	957	0	1017	9	0
13	AM	884	0	941	11	0
13	BM	884	0	941	11	0
14	AN	805	0	844	8	0
14	BN	805	0	844	8	0
15	AO	714	0	734	1	0
15	BO	714	0	734	0	0
16	AP	649	0	666	3	0
16	BP	649	0	666	5	0
17	AQ	649	0	691	6	0
17	BQ	649	0	691	5	0
18	AR	456	0	478	5	0
18	BR	456	0	478	3	0
19	AS	638	0	665	7	0
19	BS	638	0	665	8	0
20	AT	670	0	719	2	0
20	BT	665	0	714	8	0
21	AU	465	0	491	2	0
21	BU	465	0	491	2	0
22	C1	444	0	458	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	D1	444	0	458	13	0
23	C2	409	0	440	5	0
23	D2	414	0	442	5	0
24	C3	377	0	418	17	0
24	D3	377	0	418	6	0
25	C4	504	0	572	13	0
25	D4	504	0	572	12	0
26	C5	302	0	340	9	0
26	D5	302	0	340	2	0
27	C0	449	0	488	4	0
27	D0	463	0	504	1	0
28	CB	2529	0	1281	4	0
28	DB	2569	0	1301	5	0
29	CC	2082	0	2154	17	0
29	DC	2082	0	2154	11	0
30	CD	1565	0	1616	16	0
31	CA	62229	0	31318	236	0
32	DD	1576	0	1627	16	0
33	CE	1552	0	1619	14	0
33	DE	1552	0	1619	11	0
34	CF	1410	0	1444	16	0
34	DF	1410	0	1444	12	0
35	CG	1323	0	1371	9	0
35	DG	1323	0	1371	9	0
36	CH	1110	0	1148	8	0
36	DH	1110	0	1148	6	0
37	CJ	979	0	1028	4	0
37	DJ	979	0	1028	5	0
38	CK	1129	0	1162	9	0
38	DK	1129	0	1162	5	0
39	CL	938	0	1012	8	0
39	DL	946	0	1023	6	0
40	CM	1053	0	1129	19	0
40	DM	1053	0	1129	15	0
41	CN	1075	0	1154	5	0
41	DN	1092	0	1177	7	0
42	CO	960	0	1000	5	0
42	DO	993	0	1034	5	0
43	CP	892	0	923	7	0
43	DP	900	0	935	9	0
44	CQ	917	0	962	7	0
44	DQ	917	0	962	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	CR	947	0	1019	13	0
45	DR	947	0	1019	9	0
46	CS	816	0	839	8	0
46	DS	816	0	839	5	0
47	CT	857	0	922	12	0
47	DT	857	0	922	10	0
48	CU	739	0	807	10	0
48	DU	739	0	807	4	0
49	CV	779	0	831	8	0
49	DV	779	0	831	5	0
50	CW	753	0	780	5	0
50	DW	753	0	780	3	0
51	CX	569	0	581	1	0
51	DX	591	0	606	5	0
52	CY	625	0	652	8	0
52	DY	625	0	652	4	0
53	CZ	501	0	531	2	0
53	DZ	501	0	531	1	0
54	DI	1023	0	1052	19	0
55	DA	62423	0	31411	173	0
56	AA	71	0	0	0	0
56	BA	43	0	0	0	0
56	CA	156	0	0	0	0
56	CB	3	0	0	0	0
56	DA	182	0	0	0	0
56	DB	9	0	0	0	0
56	DD	2	0	0	0	0
56	DM	1	0	0	0	0
56	DR	2	0	0	0	0
57	AA	13	0	18	1	0
57	BA	13	0	18	0	0
57	DA	26	0	36	2	0
57	DQ	13	0	18	0	0
57	DR	13	0	18	5	0
57	DS	13	0	18	1	0
58	AA	16	0	28	0	0
58	DA	40	0	70	5	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	AA	24	0	48	0	0
59	DA	72	0	144	10	0
60	AA	42	0	38	0	0
60	BA	42	0	38	0	0
61	AB	1	0	0	0	0
61	C5	1	0	0	0	0
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	2	0
62	DA	35	0	50	1	0
62	DL	7	0	10	0	0
62	DP	7	0	10	1	0
62	DQ	7	0	10	0	0
63	D1	4	0	6	0	0
63	DA	36	0	54	2	0
63	DB	8	0	12	1	0
64	D1	10	0	14	2	0
64	D3	10	0	14	0	0
64	DA	40	0	56	5	0
64	DD	10	0	14	2	0
64	DS	10	0	14	0	0
64	DU	10	0	14	1	0
65	DA	40	0	76	4	0
66	DA	32	0	44	0	0
67	DA	12	0	12	0	0
68	DA	11	0	5	0	0
69	DA	8	0	12	1	0
70	AA	507	0	0	0	0
70	AC	4	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	5	0	0	0	0
70	AL	8	0	0	0	0
70	AM	4	0	0	1	0
70	AN	5	0	0	1	0
70	AO	2	0	0	0	0
70	AP	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	AR	1	0	0	0	0
70	AS	1	0	0	0	0
70	AT	2	0	0	0	0
70	AU	3	0	0	0	0
70	BA	287	0	0	1	0
70	BD	13	0	0	0	0
70	BE	1	0	0	0	0
70	BF	1	0	0	0	0
70	BK	1	0	0	0	0
70	BL	3	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	BR	1	0	0	0	0
70	BT	4	0	0	0	0
70	BU	2	0	0	0	0
70	C3	3	0	0	1	0
70	C4	1	0	0	0	0
70	CA	694	0	0	1	0
70	CB	13	0	0	0	0
70	CC	10	0	0	0	0
70	CD	5	0	0	0	0
70	CE	6	0	0	0	0
70	CL	1	0	0	0	0
70	CM	3	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	25	0	0	0	0
70	D1	42	0	0	0	0
70	D2	7	0	0	0	0
70	D3	25	0	0	0	0
70	D4	32	0	0	1	0
70	D5	13	0	0	0	0
70	DA	4836	0	0	8	0
70	DB	213	0	0	0	0
70	DC	102	0	0	0	0
70	DD	105	0	0	1	0
70	DE	63	0	0	0	0
70	DF	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	DG	6	0	0	0	0
70	DH	2	0	0	0	0
70	DK	58	0	0	0	0
70	DL	51	0	0	0	0
70	DM	60	0	0	0	0
70	DN	71	0	0	0	0
70	DO	44	0	0	0	0
70	DP	35	0	0	0	0
70	DQ	27	0	0	1	0
70	DR	64	0	0	0	0
70	DS	51	0	0	0	0
70	DT	70	0	0	1	0
70	DU	17	0	0	0	0
70	DV	19	0	0	0	0
70	DW	31	0	0	0	0
70	DX	30	0	0	1	0
70	DY	9	0	0	0	0
70	DZ	7	0	0	0	0
All	All	295202	0	194489	1207	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 3.

The worst 5 of 1207 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)
26:C5:3:VAL:HG11	31:CA:2539:C:H5'	1.32	1.05
46:CS:14:VAL:HG21	46:CS:98:ILE:HG13	1.32	1.05
4:BD:85:ASN:HA	5:BE:102:GLY:HA2	1.43	0.99
31:CA:1936:A:H2	31:CA:1943:U:H3	1.01	0.98
48:CU:28:ASN:HD21	48:CU:91:GLN:HB3	1.29	0.96

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%)	210 (95%)	9 (4%)	3 (1%)	11	39
2	BB	222/224 (99%)	211 (95%)	7 (3%)	4 (2%)	8	33
3	AC	204/206 (99%)	192 (94%)	11 (5%)	1 (0%)	29	64
3	BC	204/206 (99%)	194 (95%)	8 (4%)	2 (1%)	15	48
4	AD	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
4	BD	203/205 (99%)	198 (98%)	5 (2%)	0	100	100
5	AE	153/155 (99%)	147 (96%)	5 (3%)	1 (1%)	22	56
5	BE	148/155 (96%)	132 (89%)	12 (8%)	4 (3%)	5	23
6	AF	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
6	BF	98/106 (92%)	91 (93%)	5 (5%)	2 (2%)	7	30
7	AG	149/151 (99%)	137 (92%)	11 (7%)	1 (1%)	22	56
7	BG	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
8	AH	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
8	BH	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
9	AI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
9	BI	125/127 (98%)	110 (88%)	15 (12%)	0	100	100
10	AJ	97/99 (98%)	88 (91%)	7 (7%)	2 (2%)	7	29
10	BJ	96/99 (97%)	77 (80%)	14 (15%)	5 (5%)	2	9
11	AK	115/117 (98%)	107 (93%)	6 (5%)	2 (2%)	9	34
11	BK	115/117 (98%)	104 (90%)	9 (8%)	2 (2%)	9	34
12	AL	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
12	BL	120/123 (98%)	114 (95%)	5 (4%)	1 (1%)	19	53
13	AM	112/114 (98%)	103 (92%)	6 (5%)	3 (3%)	5	23
13	BM	112/114 (98%)	102 (91%)	5 (4%)	5 (4%)	2	12
14	AN	98/100 (98%)	88 (90%)	8 (8%)	2 (2%)	7	30
14	BN	98/100 (98%)	90 (92%)	6 (6%)	2 (2%)	7	30
15	AO	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
15	BO	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	13	43
16	AP	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
16	BP	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	5	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	78/80 (98%)	70 (90%)	7 (9%)	1 (1%)	12	41
17	BQ	78/80 (98%)	68 (87%)	5 (6%)	5 (6%)	1	5
18	AR	53/55 (96%)	53 (100%)	0	0	100	100
18	BR	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
19	AS	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	12	41
19	BS	77/79 (98%)	68 (88%)	7 (9%)	2 (3%)	5	24
20	AT	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
20	BT	83/86 (96%)	79 (95%)	3 (4%)	1 (1%)	13	43
21	AU	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
21	BU	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
22	C1	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	2	8
22	D1	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
23	C2	48/51 (94%)	44 (92%)	2 (4%)	2 (4%)	3	13
23	D2	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
24	C3	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	6	27
24	D3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
25	C4	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
25	D4	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
26	C5	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	5	22
26	D5	36/38 (95%)	36 (100%)	0	0	100	100
27	C0	56/58 (97%)	54 (96%)	0	2 (4%)	3	16
27	D0	57/58 (98%)	56 (98%)	1 (2%)	0	100	100
29	CC	269/272 (99%)	252 (94%)	12 (4%)	5 (2%)	8	32
29	DC	269/272 (99%)	257 (96%)	10 (4%)	2 (1%)	22	56
30	CD	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
32	DD	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
33	CE	199/201 (99%)	191 (96%)	5 (2%)	3 (2%)	10	38
33	DE	199/201 (99%)	194 (98%)	4 (2%)	1 (0%)	29	64
34	CF	175/178 (98%)	168 (96%)	6 (3%)	1 (1%)	25	60
34	DF	175/178 (98%)	169 (97%)	5 (3%)	1 (1%)	25	60
35	CG	174/176 (99%)	162 (93%)	7 (4%)	5 (3%)	4	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	DG	174/176 (99%)	165 (95%)	8 (5%)	1 (1%)	25	60
36	CH	147/149 (99%)	136 (92%)	6 (4%)	5 (3%)	3	17
36	DH	147/149 (99%)	138 (94%)	6 (4%)	3 (2%)	7	30
37	CJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	4	20
37	DJ	132/134 (98%)	125 (95%)	3 (2%)	4 (3%)	4	20
38	CK	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	22	56
38	DK	140/142 (99%)	137 (98%)	2 (1%)	1 (1%)	22	56
39	CL	120/123 (98%)	112 (93%)	7 (6%)	1 (1%)	19	53
39	DL	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	19	53
40	CM	142/144 (99%)	132 (93%)	7 (5%)	3 (2%)	7	29
40	DM	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
41	CN	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	19	53
41	DN	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
42	CO	118/125 (94%)	111 (94%)	5 (4%)	2 (2%)	9	34
42	DO	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
43	CP	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
43	DP	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
44	CQ	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
44	DQ	112/114 (98%)	107 (96%)	4 (4%)	1 (1%)	17	51
45	CR	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
45	DR	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
46	CS	101/103 (98%)	93 (92%)	5 (5%)	3 (3%)	4	20
46	DS	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	15	48
47	CT	108/110 (98%)	101 (94%)	5 (5%)	2 (2%)	8	32
47	DT	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
48	CU	91/93 (98%)	86 (94%)	4 (4%)	1 (1%)	14	46
48	DU	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
49	CV	100/103 (97%)	91 (91%)	4 (4%)	5 (5%)	2	10
49	DV	100/103 (97%)	96 (96%)	2 (2%)	2 (2%)	7	30
50	CW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
50	DW	92/94 (98%)	91 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	CX	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
51	DX	75/76 (99%)	74 (99%)	1 (1%)	0	100	100
52	CY	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
52	DY	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
53	CZ	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	34
53	DZ	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
54	DI	133/135 (98%)	114 (86%)	13 (10%)	6 (4%)	2	12
All	All	11407/11635 (98%)	10791 (95%)	485 (4%)	131 (1%)	14	46

5 of 131 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/186 (100%)	173 (93%)	13 (7%)	15	43
2	BB	186/186 (100%)	173 (93%)	13 (7%)	15	43
3	AC	170/170 (100%)	159 (94%)	11 (6%)	17	46
3	BC	170/170 (100%)	156 (92%)	14 (8%)	11	36
4	AD	172/172 (100%)	162 (94%)	10 (6%)	20	51
4	BD	172/172 (100%)	160 (93%)	12 (7%)	15	43
5	AE	118/118 (100%)	107 (91%)	11 (9%)	9	30
5	BE	113/118 (96%)	95 (84%)	18 (16%)	2	10
6	AF	92/92 (100%)	86 (94%)	6 (6%)	17	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	BF	87/92 (95%)	77 (88%)	10 (12%)	5	21
7	AG	124/124 (100%)	115 (93%)	9 (7%)	14	41
7	BG	124/124 (100%)	109 (88%)	15 (12%)	5	19
8	AH	104/104 (100%)	93 (89%)	11 (11%)	6	24
8	BH	104/104 (100%)	93 (89%)	11 (11%)	6	24
9	AI	105/105 (100%)	100 (95%)	5 (5%)	25	59
9	BI	105/105 (100%)	100 (95%)	5 (5%)	25	59
10	AJ	87/87 (100%)	81 (93%)	6 (7%)	15	44
10	BJ	86/87 (99%)	78 (91%)	8 (9%)	9	30
11	AK	90/90 (100%)	87 (97%)	3 (3%)	38	70
11	BK	90/90 (100%)	83 (92%)	7 (8%)	12	38
12	AL	102/102 (100%)	92 (90%)	10 (10%)	8	27
12	BL	102/102 (100%)	90 (88%)	12 (12%)	5	20
13	AM	92/92 (100%)	83 (90%)	9 (10%)	8	27
13	BM	92/92 (100%)	85 (92%)	7 (8%)	13	39
14	AN	83/83 (100%)	82 (99%)	1 (1%)	71	88
14	BN	83/83 (100%)	82 (99%)	1 (1%)	71	88
15	AO	76/76 (100%)	71 (93%)	5 (7%)	16	46
15	BO	76/76 (100%)	65 (86%)	11 (14%)	3	13
16	AP	65/65 (100%)	64 (98%)	1 (2%)	65	85
16	BP	65/65 (100%)	63 (97%)	2 (3%)	40	71
17	AQ	74/74 (100%)	67 (90%)	7 (10%)	8	29
17	BQ	74/74 (100%)	66 (89%)	8 (11%)	6	23
18	AR	48/48 (100%)	47 (98%)	1 (2%)	53	80
18	BR	48/48 (100%)	47 (98%)	1 (2%)	53	80
19	AS	70/70 (100%)	63 (90%)	7 (10%)	7	26
19	BS	70/70 (100%)	65 (93%)	5 (7%)	14	43
20	AT	65/65 (100%)	59 (91%)	6 (9%)	9	30
20	BT	65/65 (100%)	55 (85%)	10 (15%)	2	11
21	AU	48/48 (100%)	44 (92%)	4 (8%)	11	35
21	BU	48/48 (100%)	44 (92%)	4 (8%)	11	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	C1	47/47 (100%)	45 (96%)	2 (4%)	29	62
22	D1	47/47 (100%)	44 (94%)	3 (6%)	17	47
23	C2	45/46 (98%)	44 (98%)	1 (2%)	52	79
23	D2	45/46 (98%)	43 (96%)	2 (4%)	28	62
24	C3	38/38 (100%)	37 (97%)	1 (3%)	46	75
24	D3	38/38 (100%)	37 (97%)	1 (3%)	46	75
25	C4	51/51 (100%)	48 (94%)	3 (6%)	19	50
25	D4	51/51 (100%)	48 (94%)	3 (6%)	19	50
26	C5	34/34 (100%)	32 (94%)	2 (6%)	19	50
26	D5	34/34 (100%)	34 (100%)	0	100	100
27	C0	48/48 (100%)	45 (94%)	3 (6%)	18	48
27	D0	49/48 (102%)	45 (92%)	4 (8%)	11	36
29	CC	216/217 (100%)	202 (94%)	14 (6%)	17	46
29	DC	216/217 (100%)	210 (97%)	6 (3%)	43	74
30	CD	164/164 (100%)	160 (98%)	4 (2%)	49	77
32	DD	163/163 (100%)	160 (98%)	3 (2%)	59	82
33	CE	165/165 (100%)	152 (92%)	13 (8%)	12	37
33	DE	165/165 (100%)	161 (98%)	4 (2%)	49	77
34	CF	148/149 (99%)	133 (90%)	15 (10%)	7	26
34	DF	148/149 (99%)	137 (93%)	11 (7%)	13	41
35	CG	137/137 (100%)	134 (98%)	3 (2%)	52	79
35	DG	137/137 (100%)	132 (96%)	5 (4%)	35	67
36	CH	114/114 (100%)	101 (89%)	13 (11%)	5	21
36	DH	114/114 (100%)	101 (89%)	13 (11%)	5	21
37	CJ	104/104 (100%)	100 (96%)	4 (4%)	33	66
37	DJ	104/104 (100%)	100 (96%)	4 (4%)	33	66
38	CK	116/116 (100%)	110 (95%)	6 (5%)	23	56
38	DK	116/116 (100%)	114 (98%)	2 (2%)	60	83
39	CL	103/104 (99%)	99 (96%)	4 (4%)	32	65
39	DL	104/104 (100%)	99 (95%)	5 (5%)	25	59
40	CM	103/103 (100%)	97 (94%)	6 (6%)	20	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	DM	103/103 (100%)	99 (96%)	4 (4%)	32	65
41	CN	108/108 (100%)	104 (96%)	4 (4%)	34	66
41	DN	109/108 (101%)	106 (97%)	3 (3%)	43	74
42	CO	100/102 (98%)	95 (95%)	5 (5%)	24	57
42	DO	102/102 (100%)	99 (97%)	3 (3%)	42	73
43	CP	86/87 (99%)	80 (93%)	6 (7%)	15	43
43	DP	87/87 (100%)	84 (97%)	3 (3%)	37	69
44	CQ	99/99 (100%)	93 (94%)	6 (6%)	18	49
44	DQ	99/99 (100%)	97 (98%)	2 (2%)	55	80
45	CR	89/89 (100%)	86 (97%)	3 (3%)	37	69
45	DR	89/89 (100%)	87 (98%)	2 (2%)	52	79
46	CS	84/84 (100%)	79 (94%)	5 (6%)	19	50
46	DS	84/84 (100%)	83 (99%)	1 (1%)	71	88
47	CT	93/93 (100%)	88 (95%)	5 (5%)	22	54
47	DT	93/93 (100%)	92 (99%)	1 (1%)	73	89
48	CU	80/80 (100%)	72 (90%)	8 (10%)	7	26
48	DU	80/80 (100%)	77 (96%)	3 (4%)	33	66
49	CV	83/84 (99%)	79 (95%)	4 (5%)	25	59
49	DV	83/84 (99%)	81 (98%)	2 (2%)	49	77
50	CW	78/78 (100%)	75 (96%)	3 (4%)	33	66
50	DW	78/78 (100%)	76 (97%)	2 (3%)	46	75
51	CX	56/58 (97%)	55 (98%)	1 (2%)	59	82
51	DX	58/58 (100%)	57 (98%)	1 (2%)	60	83
52	CY	67/67 (100%)	63 (94%)	4 (6%)	19	50
52	DY	67/67 (100%)	65 (97%)	2 (3%)	41	72
53	CZ	54/54 (100%)	50 (93%)	4 (7%)	13	41
53	DZ	54/54 (100%)	52 (96%)	2 (4%)	34	66
54	DI	103/103 (100%)	98 (95%)	5 (5%)	25	58
All	All	9461/9484 (100%)	8897 (94%)	564 (6%)	19	50

5 of 564 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	BK	23	ILE
20	BT	67	ILE
38	DK	124	VAL
12	BL	44	LYS
15	BO	64	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
2	BB	168	HIS
7	BG	97	ASN
51	CX	57	HIS
4	BD	131	ASN
5	BE	70	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	239 (15%)	27 (1%)
1	BA	1529/1534 (99%)	246 (16%)	28 (1%)
28	CB	117/120 (97%)	11 (9%)	0
28	DB	119/120 (99%)	9 (7%)	0
31	CA	2892/2904 (99%)	426 (14%)	72 (2%)
55	DA	2880/2904 (99%)	367 (12%)	57 (1%)
All	All	9067/9116 (99%)	1298 (14%)	184 (2%)

5 of 1298 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	9	G
1	AA	22	G
1	AA	32	A

5 of 184 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	CA	1070	A
31	CA	1730	C
55	DA	2158	A

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Mol	Chain	Res	Type
31	CA	1089	A
31	CA	1379	U

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

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$
1	5MC	AA	1407	1	15,22,23	0.86	0	19,32,35	1.20	2 (10%)
55	2MG	DA	2445	55	19,26,27	1.25	3 (15%)	21,38,41	2.55	4 (19%)
31	PSU	CA	1917	31	17,21,22	1.21	2 (11%)	20,30,33	5.35	4 (20%)
1	2MG	BA	1207	1	19,26,27	1.25	2 (10%)	21,38,41	2.39	4 (19%)
1	MA6	BA	1518	1	19,26,27	0.86	0	18,38,41	0.96	1 (5%)
31	PSU	CA	2605	31	17,21,22	1.18	2 (11%)	20,30,33	5.33	5 (25%)
32	MEQ	DD	150[A]	32	8,9,10	0.58	0	5,10,12	0.45	0
31	G7M	CA	2069	31	20,26,27	0.98	1 (5%)	20,39,42	2.89	4 (20%)
1	MA6	BA	1519	1	19,26,27	0.73	0	18,38,41	1.31	1 (5%)
55	1MG	DA	745	55	18,26,27	1.44	3 (16%)	19,39,42	1.29	3 (15%)
1	PSU	AA	516	1,56	17,21,22	1.20	2 (11%)	20,30,33	5.29	4 (20%)
31	2MG	CA	2445	31	19,26,27	1.42	2 (10%)	21,38,41	2.39	4 (19%)
31	2MG	CA	1835	31	19,26,27	1.19	2 (10%)	21,38,41	2.32	4 (19%)
1	2MG	AA	1207	1	19,26,27	1.17	2 (10%)	21,38,41	2.41	4 (19%)
55	6MZ	DA	1618	55	18,25,26	0.90	0	16,36,39	1.80	2 (12%)
55	2MA	DA	2503	55,56	17,25,26	0.81	0	19,37,40	2.00	3 (15%)
55	PSU	DA	746	55,56	17,21,22	1.64	4 (23%)	20,30,33	5.29	4 (20%)
31	6MZ	CA	2030	31	18,25,26	0.84	0	16,36,39	0.96	2 (12%)
55	2MG	DA	1835	55	19,26,27	1.12	2 (10%)	21,38,41	2.37	4 (19%)
12	D2T	AL	89	12	4,9,10	0.51	0	3,11,13	0.86	0
1	2MG	BA	966	1	19,26,27	1.14	2 (10%)	21,38,41	2.36	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
41	4D4	CN	81	41	9,11,12	2.00	2 (22%)	8,13,15	2.39	2 (25%)
1	UR3	AA	1498	1	14,22,23	0.84	0	15,32,35	0.53	0
55	5MU	DA	1939	55	15,22,23	1.23	1 (6%)	16,32,35	3.70	2 (12%)
55	PSU	DA	2604	55	17,21,22	1.32	2 (11%)	20,30,33	5.30	4 (20%)
31	6MZ	CA	1618	31	18,25,26	0.84	0	16,36,39	1.12	2 (12%)
1	2MG	AA	966	1	19,26,27	1.26	2 (10%)	21,38,41	2.33	3 (14%)
31	2MA	CA	2503	31	17,25,26	0.85	0	19,37,40	2.07	2 (10%)
1	2MG	AA	1516	1	19,26,27	1.39	2 (10%)	21,38,41	2.35	4 (19%)
31	5MC	CA	1962	31	15,22,23	0.81	1 (6%)	19,32,35	1.12	1 (5%)
55	5MC	DA	1962	55	15,22,23	0.91	0	19,32,35	1.12	1 (5%)
55	PSU	DA	2580	55	17,21,22	1.49	4 (23%)	20,30,33	5.33	4 (20%)
1	4OC	AA	1402	1	16,23,24	0.82	0	17,32,35	0.92	1 (5%)
55	OMU	DA	2552	55	14,22,23	1.19	2 (14%)	14,31,34	1.11	1 (7%)
55	6MZ	DA	2030	55	18,25,26	0.88	1 (5%)	16,36,39	0.92	1 (6%)
31	1MG	CA	745	31	18,26,27	1.33	1 (5%)	19,39,42	1.21	2 (10%)
31	PSU	CA	2580	31	17,21,22	1.31	2 (11%)	20,30,33	5.33	5 (25%)
55	PSU	DA	1917	55	17,21,22	1.31	3 (17%)	20,30,33	5.32	4 (20%)
1	5MC	BA	967	1	15,22,23	0.81	0	19,32,35	1.15	2 (10%)
55	G7M	DA	2069	55	20,26,27	1.05	1 (5%)	20,39,42	2.86	4 (20%)
55	OMG	DA	2251	55	18,26,27	1.05	1 (5%)	20,38,41	2.47	5 (25%)
31	PSU	CA	955	31	17,21,22	1.21	2 (11%)	20,30,33	5.31	4 (20%)
1	PSU	BA	516	1	17,21,22	1.25	2 (11%)	20,30,33	5.33	4 (20%)
1	G7M	BA	527	1	20,26,27	1.25	2 (10%)	20,39,42	3.16	5 (25%)
1	4OC	BA	1402	1	16,23,24	0.88	1 (6%)	17,32,35	0.89	1 (5%)
1	MA6	AA	1519	1	19,26,27	0.75	0	18,38,41	1.33	1 (5%)
1	2MG	BA	1516	1	19,26,27	1.28	2 (10%)	21,38,41	2.37	4 (19%)
31	PSU	CA	2504	31	17,21,22	1.23	3 (17%)	20,30,33	5.30	4 (20%)
31	OMU	CA	2552	31	14,22,23	1.23	2 (14%)	14,31,34	1.09	1 (7%)
41	4D4	DN	81[A]	-	9,11,12	2.14	2 (22%)	8,13,15	2.19	2 (25%)
31	OMG	CA	2251	31	18,26,27	1.25	2 (11%)	20,38,41	2.52	4 (20%)
41	4D4	DN	81[B]	-	9,11,12	1.42	1 (11%)	8,13,15	2.41	2 (25%)
1	G7M	AA	527	1	20,26,27	1.22	2 (10%)	20,39,42	3.10	6 (30%)
31	PSU	CA	2457	31	17,21,22	1.26	3 (17%)	20,30,33	5.29	4 (20%)
31	PSU	CA	1911	31	17,21,22	1.21	2 (11%)	20,30,33	5.29	4 (20%)
55	PSU	DA	2504	55	17,21,22	1.35	3 (17%)	20,30,33	5.34	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MA6	AA	1518	1	19,26,27	0.86	0	18,38,41	0.93	1 (5%)
32	MEQ	DD	150[B]	32	8,9,10	2.22	1 (12%)	5,10,12	1.71	1 (20%)
1	5MC	AA	967	1	15,22,23	0.82	0	19,32,35	1.14	2 (10%)
31	3TD	CA	1915	31	17,22,23	1.27	3 (17%)	19,32,35	1.49	2 (10%)
1	UR3	BA	1498	1	14,22,23	1.13	2 (14%)	15,32,35	0.48	0
55	PSU	DA	955	55	17,21,22	1.45	4 (23%)	20,30,33	5.31	5 (25%)
31	5MU	CA	1939	31	15,22,23	1.26	1 (6%)	16,32,35	3.70	2 (12%)
55	OMC	DA	2498	55,56	15,22,23	0.87	1 (6%)	17,31,34	1.28	1 (5%)
12	D2T	BL	89	12	4,9,10	0.57	0	3,11,13	0.87	0
31	PSU	CA	746	31,56	17,21,22	1.39	3 (17%)	20,30,33	5.32	4 (20%)
55	H2U	DA	2449	55	18,21,22	0.47	0	21,30,33	0.50	0
1	5MC	BA	1407	1	15,22,23	0.84	0	19,32,35	1.18	2 (10%)
31	OMC	CA	2498	31,56	15,22,23	0.98	1 (6%)	17,31,34	1.18	1 (5%)
55	PSU	DA	1911	55	17,21,22	1.19	3 (17%)	20,30,33	5.28	4 (20%)
55	3TD	DA	1915	55	17,22,23	1.32	3 (17%)	19,32,35	1.53	2 (10%)
55	5MU	DA	747	55	15,22,23	1.23	1 (6%)	16,32,35	3.64	2 (12%)
55	PSU	DA	2605	55	17,21,22	1.18	2 (11%)	20,30,33	5.31	5 (25%)
31	5MU	CA	747	31	15,22,23	1.17	1 (6%)	16,32,35	3.70	2 (12%)
55	PSU	DA	2457	55	17,21,22	1.14	3 (17%)	20,30,33	5.29	4 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	AA	1407	1	-	0/5/25/26	0/2/2/2
55	2MG	DA	2445	55	-	0/5/27/28	0/3/3/3
31	PSU	CA	1917	31	-	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
31	PSU	CA	2605	31	-	0/7/25/26	0/2/2/2
32	MEQ	DD	150[A]	32	-	3/8/9/11	-
31	G7M	CA	2069	31	-	2/3/25/26	0/3/3/3
1	MA6	BA	1519	1	-	1/7/29/30	0/3/3/3
55	1MG	DA	745	55	-	0/3/25/26	0/3/3/3
1	PSU	AA	516	1,56	-	0/7/25/26	0/2/2/2
31	2MG	CA	2445	31	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	2MG	CA	1835	31	-	2/5/27/28	0/3/3/3
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
55	6MZ	DA	1618	55	-	0/5/27/28	0/3/3/3
55	2MA	DA	2503	55,56	-	2/3/25/26	0/3/3/3
55	PSU	DA	746	55,56	-	3/7/25/26	0/2/2/2
31	6MZ	CA	2030	31	-	1/5/27/28	0/3/3/3
55	2MG	DA	1835	55	-	2/5/27/28	0/3/3/3
12	D2T	AL	89	12	-	1/3/12/14	-
1	2MG	BA	966	1	-	0/5/27/28	0/3/3/3
41	4D4	CN	81	41	-	1/11/12/14	-
1	UR3	AA	1498	1	-	0/5/25/26	0/2/2/2
55	5MU	DA	1939	55	-	0/5/25/26	0/2/2/2
55	PSU	DA	2604	55	-	0/7/25/26	0/2/2/2
31	6MZ	CA	1618	31	-	0/5/27/28	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
31	2MA	CA	2503	31	-	2/3/25/26	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
31	5MC	CA	1962	31	-	2/5/25/26	0/2/2/2
55	5MC	DA	1962	55	-	2/5/25/26	0/2/2/2
55	PSU	DA	2580	55	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	1	-	0/9/29/30	0/2/2/2
55	OMU	DA	2552	55	-	1/7/27/28	0/2/2/2
55	6MZ	DA	2030	55	-	2/5/27/28	0/3/3/3
31	1MG	CA	745	31	-	0/3/25/26	0/3/3/3
31	PSU	CA	2580	31	-	0/7/25/26	0/2/2/2
55	PSU	DA	1917	55	-	0/7/25/26	0/2/2/2
1	5MC	BA	967	1	-	0/5/25/26	0/2/2/2
55	G7M	DA	2069	55	-	2/3/25/26	0/3/3/3
55	OMG	DA	2251	55	-	1/5/27/28	0/3/3/3
31	PSU	CA	955	31	-	0/7/25/26	0/2/2/2
1	PSU	BA	516	1	-	0/7/25/26	0/2/2/2
1	G7M	BA	527	1	-	2/3/25/26	0/3/3/3
1	4OC	BA	1402	1	-	0/9/29/30	0/2/2/2
1	MA6	AA	1519	1	-	1/7/29/30	0/3/3/3
1	2MG	BA	1516	1	-	0/5/27/28	0/3/3/3
31	PSU	CA	2504	31	-	1/7/25/26	0/2/2/2
31	OMU	CA	2552	31	-	1/7/27/28	0/2/2/2
41	4D4	DN	81[A]	-	-	0/11/12/14	-
31	OMG	CA	2251	31	-	1/5/27/28	0/3/3/3
41	4D4	DN	81[B]	-	-	2/11/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
31	PSU	CA	2457	31	-	0/7/25/26	0/2/2/2
31	PSU	CA	1911	31	-	0/7/25/26	0/2/2/2
55	PSU	DA	2504	55	-	1/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
32	MEQ	DD	150[B]	32	-	4/8/9/11	-
1	5MC	AA	967	1	-	0/5/25/26	0/2/2/2
31	3TD	CA	1915	31	-	0/7/25/26	0/2/2/2
1	UR3	BA	1498	1	-	0/5/25/26	0/2/2/2
55	PSU	DA	955	55	-	0/7/25/26	0/2/2/2
31	5MU	CA	1939	31	-	0/5/25/26	0/2/2/2
55	OMC	DA	2498	55,56	-	0/7/27/28	0/2/2/2
12	D2T	BL	89	12	-	1/3/12/14	-
31	PSU	CA	746	31,56	-	3/7/25/26	0/2/2/2
55	H2U	DA	2449	55	-	1/7/38/39	0/2/2/2
1	5MC	BA	1407	1	-	0/5/25/26	0/2/2/2
31	OMC	CA	2498	31,56	-	0/7/27/28	0/2/2/2
55	PSU	DA	1911	55	-	0/7/25/26	0/2/2/2
55	3TD	DA	1915	55	-	0/7/25/26	0/2/2/2
55	5MU	DA	747	55	-	0/5/25/26	0/2/2/2
55	PSU	DA	2605	55	-	0/7/25/26	0/2/2/2
31	5MU	CA	747	31	-	0/5/25/26	0/2/2/2
55	PSU	DA	2457	55	-	0/7/25/26	0/2/2/2

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	DD	150[B]	MEQ	CB-CA	6.11	1.61	1.53
41	DN	81[A]	4D4	CZ-NE	5.93	1.45	1.33
41	CN	81	4D4	CZ-NE	5.45	1.44	1.33
31	CA	745	1MG	C6-C5	4.40	1.48	1.41
55	DA	1915	3TD	C4-C5	3.90	1.49	1.41

The worst 5 of 203 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	516	PSU	N1-C2-N3	-17.23	114.73	128.43
55	DA	2504	PSU	N1-C2-N3	-17.22	114.74	128.43
31	CA	1917	PSU	N1-C2-N3	-17.18	114.78	128.43
31	CA	2605	PSU	N1-C2-N3	-17.17	114.78	128.43
31	CA	746	PSU	N1-C2-N3	-17.17	114.78	128.43

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	AL	89	D2T	CG-CB-SB-CB1
55	DA	746	PSU	O4'-C1'-C5-C6
31	CA	1962	5MC	O4'-C1'-N1-C6
31	CA	1962	5MC	C2'-C1'-N1-C6
55	DA	1962	5MC	O4'-C1'-N1-C6

There are no ring outliers.

15 monomers are involved in 13 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 554 ligands modelled in this entry, 472 are monoatomic - leaving 82 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
62	PEG	DQ	201	-	6,6,6	0.21	0	5,5,5	0.15	0
59	PUT	AA	1673	-	5,5,5	0.16	0	4,4,4	0.15	0
64	PGE	DU	101	-	9,9,9	0.25	0	8,8,8	0.38	0
59	PUT	DA	3189	-	5,5,5	0.47	0	4,4,4	0.42	0
66	1PE	DA	3185	-	15,15,15	0.16	0	14,14,14	0.16	0
59	PUT	DA	3184	-	5,5,5	0.24	0	4,4,4	0.16	0
58	MPD	DE	301	-	7,7,7	0.87	0	9,10,10	0.78	0
58	MPD	DA	3209	-	7,7,7	0.72	0	9,10,10	0.39	0
57	PG4	DA	3215	-	12,12,12	0.17	0	11,11,11	0.13	0
58	MPD	DA	3203	-	7,7,7	0.92	0	9,10,10	0.65	0
69	TRS	DA	3219	-	7,7,7	0.29	0	9,9,9	0.29	0
59	PUT	DA	3221	-	5,5,5	0.45	0	4,4,4	0.62	0
63	EDO	DA	3207	-	3,3,3	0.72	0	2,2,2	0.16	0
58	MPD	DS	203	-	7,7,7	0.42	0	9,10,10	0.69	0
60	T1C	BA	1643	56	44,45,45	0.99	3 (6%)	53,72,72	1.41	2 (3%)
59	PUT	DA	3204	-	5,5,5	0.35	0	4,4,4	0.28	0
59	PUT	DA	3220	-	5,5,5	0.19	0	4,4,4	0.13	0
62	PEG	DL	201	-	6,6,6	0.13	0	5,5,5	0.12	0
63	EDO	DA	3198	-	3,3,3	0.68	0	2,2,2	0.38	0
58	MPD	DA	3206	-	7,7,7	1.05	1 (14%)	9,10,10	0.54	0
64	PGE	DA	3213	-	9,9,9	0.16	0	8,8,8	0.18	0
58	MPD	DK	201	-	7,7,7	0.76	0	9,10,10	0.26	0
62	PEG	D3	102	-	6,6,6	0.33	0	5,5,5	0.25	0
64	PGE	D1	102	-	9,9,9	0.30	0	8,8,8	0.30	0
59	PUT	AA	1674	-	5,5,5	0.16	0	4,4,4	0.15	0
63	EDO	DA	3001	-	3,3,3	0.86	0	2,2,2	0.10	0
58	MPD	DN	201	-	7,7,7	1.12	1 (14%)	9,10,10	0.60	0
63	EDO	DA	3194	-	3,3,3	0.66	0	2,2,2	0.07	0
59	PUT	DA	3222	-	5,5,5	0.29	0	4,4,4	0.30	0
59	PUT	DA	3212	-	5,5,5	0.37	0	4,4,4	0.31	0
59	PUT	AA	1672	-	5,5,5	0.22	0	4,4,4	0.18	0
64	PGE	D3	101	-	9,9,9	0.29	0	8,8,8	0.23	0
63	EDO	DB	211	-	3,3,3	0.61	0	2,2,2	0.17	0
58	MPD	DT	201	-	7,7,7	0.63	0	9,10,10	0.20	0
62	PEG	DP	201	-	6,6,6	0.29	0	5,5,5	0.17	0
65	SPD	DA	3187	-	9,9,9	0.17	0	8,8,8	0.42	0
63	EDO	DA	3004	-	3,3,3	0.74	0	2,2,2	0.12	0
64	PGE	DD	301	-	9,9,9	0.29	0	8,8,8	0.33	0
63	EDO	DA	3208	-	3,3,3	0.59	0	2,2,2	0.30	0
64	PGE	DS	201	-	9,9,9	0.48	0	8,8,8	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
62	PEG	DA	3217	-	6,6,6	0.29	0	5,5,5	0.09	0
65	SPD	DA	3223	-	9,9,9	0.18	0	8,8,8	0.67	0
59	PUT	DA	3211	-	5,5,5	0.31	0	4,4,4	0.16	0
59	PUT	DA	3188	-	5,5,5	0.43	0	4,4,4	0.27	0
59	PUT	DA	3002	-	5,5,5	0.19	0	4,4,4	0.09	0
65	SPD	DA	3183	-	9,9,9	0.13	0	8,8,8	0.20	0
58	MPD	DE	302	-	7,7,7	0.93	1 (14%)	9,10,10	0.47	0
64	PGE	DA	3186	-	9,9,9	0.35	0	8,8,8	0.56	0
67	ACY	DA	3191	-	1,3,3	2.16	1 (100%)	0,3,3	0.00	-
62	PEG	DA	3200	-	6,6,6	0.51	0	5,5,5	0.28	0
62	PEG	DA	3199	-	6,6,6	0.30	0	5,5,5	0.21	0
57	PG4	DA	3193	-	12,12,12	0.30	0	11,11,11	0.43	0
63	EDO	DA	3003	-	3,3,3	0.77	0	2,2,2	0.11	0
59	PUT	DA	3218	-	5,5,5	0.14	0	4,4,4	0.12	0
64	PGE	DA	3216	-	9,9,9	0.13	0	8,8,8	0.25	0
59	PUT	AA	1675	-	5,5,5	0.21	0	4,4,4	0.22	0
57	PG4	AA	1670	-	12,12,12	0.27	0	11,11,11	0.41	0
58	MPD	DA	3190	-	7,7,7	0.49	0	9,10,10	0.47	0
57	PG4	BA	1642	-	12,12,12	0.20	0	11,11,11	0.22	0
62	PEG	D1	103	-	6,6,6	0.42	0	5,5,5	0.15	0
64	PGE	DA	3224	-	9,9,9	0.24	0	8,8,8	0.18	0
67	ACY	DA	3201	-	1,3,3	2.01	1 (100%)	0,3,3	0.00	-
58	MPD	AA	1671	-	7,7,7	0.72	0	9,10,10	0.45	0
63	EDO	DA	3197	-	3,3,3	0.65	0	2,2,2	0.22	0
65	SPD	DA	3205	-	9,9,9	0.24	0	8,8,8	0.18	0
62	PEG	DA	3225	-	6,6,6	0.49	0	5,5,5	0.27	0
67	ACY	DA	3196	-	1,3,3	3.04	1 (100%)	0,3,3	0.00	-
63	EDO	DA	3214	-	3,3,3	0.68	0	2,2,2	0.23	0
58	MPD	DA	3192	-	7,7,7	0.71	0	9,10,10	0.81	0
57	PG4	DQ	202	-	12,12,12	0.15	0	11,11,11	0.16	0
63	EDO	DB	210	-	3,3,3	0.61	0	2,2,2	0.22	0
59	PUT	DA	3195	-	5,5,5	0.32	0	4,4,4	0.51	0
58	MPD	DT	202	-	7,7,7	0.84	0	9,10,10	0.43	0
63	EDO	D1	101	-	3,3,3	0.68	0	2,2,2	0.15	0
58	MPD	AA	1676	-	7,7,7	0.62	0	9,10,10	0.42	0
62	PEG	DA	3226	-	6,6,6	0.42	0	5,5,5	0.28	0
60	T1C	AA	1677	56	44,45,45	1.01	4 (9%)	53,72,72	1.43	3 (5%)
62	PEG	AL	201	-	6,6,6	0.25	0	5,5,5	0.13	0
57	PG4	DS	202	-	12,12,12	0.47	0	11,11,11	0.43	0
66	1PE	DA	3202	-	15,15,15	0.35	0	14,14,14	0.40	0
57	PG4	DR	202	-	12,12,12	0.43	0	11,11,11	0.54	0
68	GUN	DA	3210	-	9,12,12	2.26	2 (22%)	8,17,17	3.97	4 (50%)

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	DQ	201	-	-	2/4/4/4	-
59	PUT	AA	1673	-	-	0/3/3/3	-
64	PGE	DU	101	-	-	4/7/7/7	-
59	PUT	DA	3189	-	-	0/3/3/3	-
66	1PE	DA	3185	-	-	5/13/13/13	-
59	PUT	DA	3184	-	-	0/3/3/3	-
58	MPD	DE	301	-	-	5/5/5/5	-
58	MPD	DA	3209	-	-	1/5/5/5	-
57	PG4	DA	3215	-	-	4/10/10/10	-
58	MPD	DA	3203	-	-	1/5/5/5	-
69	TRS	DA	3219	-	-	0/9/9/9	-
59	PUT	DA	3221	-	-	1/3/3/3	-
63	EDO	DA	3207	-	-	0/1/1/1	-
58	MPD	DS	203	-	-	0/5/5/5	-
60	T1C	BA	1643	56	-	11/22/80/80	0/4/4/4
59	PUT	DA	3204	-	-	1/3/3/3	-
59	PUT	DA	3220	-	-	0/3/3/3	-
62	PEG	DL	201	-	-	2/4/4/4	-
63	EDO	DA	3198	-	-	1/1/1/1	-
58	MPD	DA	3206	-	-	1/5/5/5	-
64	PGE	DA	3213	-	-	2/7/7/7	-
58	MPD	DK	201	-	-	2/5/5/5	-
62	PEG	D3	102	-	-	2/4/4/4	-
64	PGE	D1	102	-	-	4/7/7/7	-
59	PUT	AA	1674	-	-	0/3/3/3	-
63	EDO	DA	3001	-	-	1/1/1/1	-
58	MPD	DN	201	-	-	4/5/5/5	-
63	EDO	DA	3194	-	-	1/1/1/1	-
59	PUT	DA	3222	-	-	1/3/3/3	-
59	PUT	DA	3212	-	-	1/3/3/3	-
59	PUT	AA	1672	-	-	0/3/3/3	-
64	PGE	D3	101	-	-	2/7/7/7	-
63	EDO	DB	211	-	-	0/1/1/1	-
58	MPD	DT	201	-	-	2/5/5/5	-
62	PEG	DP	201	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
65	SPD	DA	3187	-	-	0/7/7/7	-
63	EDO	DA	3004	-	-	0/1/1/1	-
64	PGE	DD	301	-	-	4/7/7/7	-
63	EDO	DA	3208	-	-	0/1/1/1	-
64	PGE	DS	201	-	-	3/7/7/7	-
65	SPD	DA	3223	-	-	4/7/7/7	-
59	PUT	DA	3211	-	-	0/3/3/3	-
59	PUT	DA	3188	-	-	0/3/3/3	-
59	PUT	DA	3002	-	-	0/3/3/3	-
65	SPD	DA	3183	-	-	1/7/7/7	-
64	PGE	DA	3186	-	-	4/7/7/7	-
58	MPD	DE	302	-	-	2/5/5/5	-
62	PEG	DA	3200	-	-	3/4/4/4	-
62	PEG	DA	3199	-	-	3/4/4/4	-
57	PG4	DA	3193	-	-	8/10/10/10	-
63	EDO	DA	3003	-	-	0/1/1/1	-
59	PUT	DA	3218	-	-	0/3/3/3	-
64	PGE	DA	3216	-	-	4/7/7/7	-
59	PUT	AA	1675	-	-	1/3/3/3	-
57	PG4	AA	1670	-	-	4/10/10/10	-
58	MPD	DA	3190	-	-	2/5/5/5	-
57	PG4	BA	1642	-	-	0/10/10/10	-
62	PEG	D1	103	-	-	1/4/4/4	-
64	PGE	DA	3224	-	-	4/7/7/7	-
62	PEG	DA	3217	-	-	3/4/4/4	-
58	MPD	AA	1671	-	-	1/5/5/5	-
63	EDO	DA	3197	-	-	0/1/1/1	-
65	SPD	DA	3205	-	-	5/7/7/7	-
62	PEG	DA	3225	-	-	2/4/4/4	-
63	EDO	DA	3214	-	-	0/1/1/1	-
58	MPD	DA	3192	-	-	2/5/5/5	-
57	PG4	DQ	202	-	-	1/10/10/10	-
63	EDO	DB	210	-	-	0/1/1/1	-
59	PUT	DA	3195	-	-	1/3/3/3	-
58	MPD	DT	202	-	-	2/5/5/5	-
63	EDO	D1	101	-	-	0/1/1/1	-
58	MPD	AA	1676	-	-	2/5/5/5	-
62	PEG	DA	3226	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	T1C	AA	1677	56	-	8/22/80/80	0/4/4/4
62	PEG	AL	201	-	-	2/4/4/4	-
57	PG4	DS	202	-	-	2/10/10/10	-
66	1PE	DA	3202	-	-	8/13/13/13	-
57	PG4	DR	202	-	-	6/10/10/10	-
68	GUN	DA	3210	-	-	-	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	DA	3210	GUN	C6-C5	5.28	1.50	1.41
68	DA	3210	GUN	C6-N1	3.43	1.39	1.33
60	BA	1643	T1C	C4-C3	3.26	1.58	1.51
67	DA	3196	ACY	CH3-C	3.04	1.52	1.48
60	AA	1677	T1C	C4-C3	2.87	1.57	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	DA	3210	GUN	C5-C6-N1	-8.35	112.02	123.43
60	BA	1643	T1C	C92-N92-C93	6.96	124.57	115.84
60	AA	1677	T1C	C92-N92-C93	6.83	124.40	115.84
68	DA	3210	GUN	C6-N1-C2	5.79	125.12	115.93
60	BA	1643	T1C	C8-C9-C10	-4.64	115.88	120.49

There are no chirality outliers.

5 of 156 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	DN	201	MPD	CM-C2-C3-C4
58	DT	202	MPD	C2-C3-C4-C5
58	DA	3190	MPD	C2-C3-C4-O4
58	DA	3190	MPD	C2-C3-C4-C5
58	DE	301	MPD	C1-C2-C3-C4

There are no ring outliers.

30 monomers are involved in 48 short contacts:

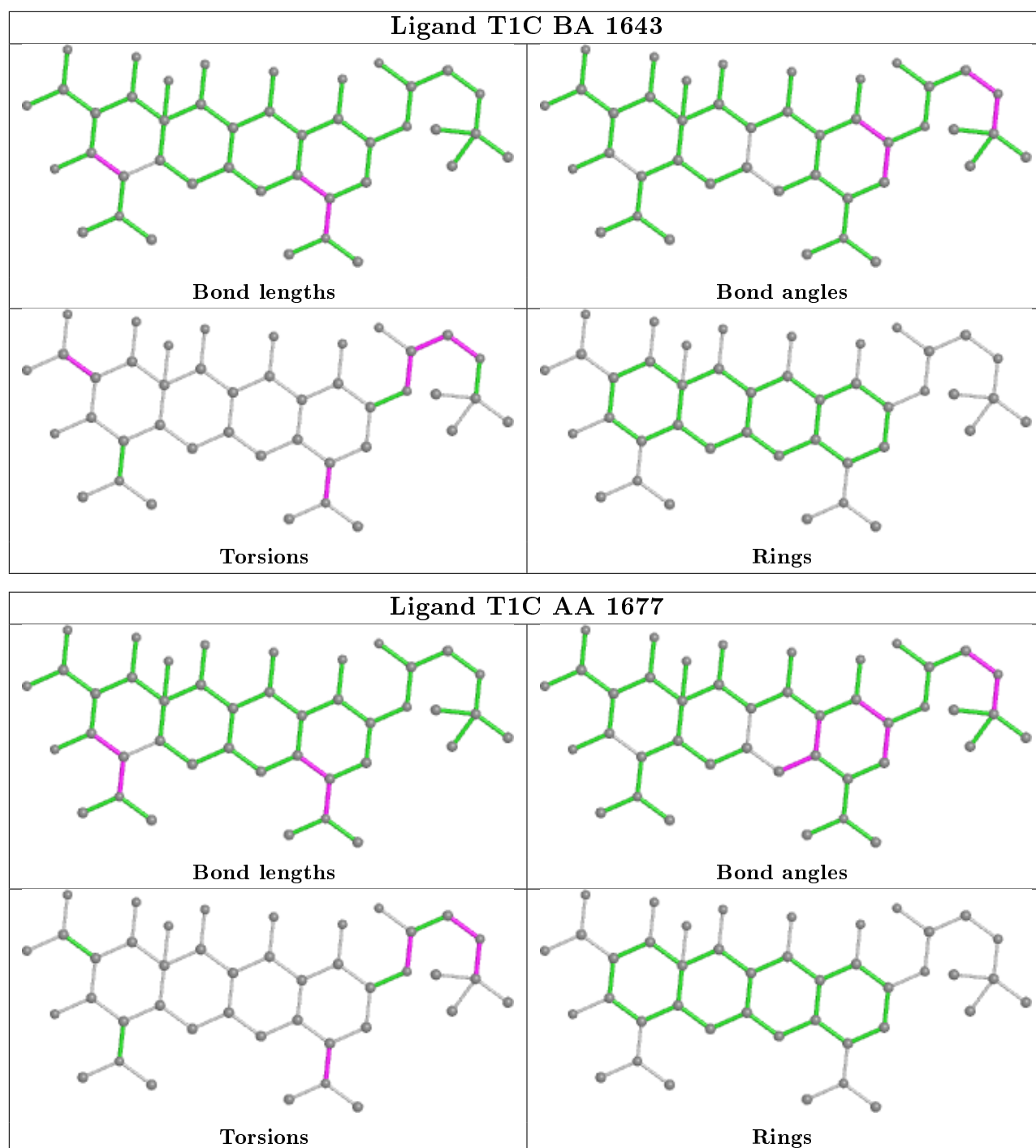
Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	DU	101	PGE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	DA	3189	PUT	1	0
57	DA	3215	PG4	1	0
58	DA	3203	MPD	2	0
69	DA	3219	TRS	1	0
59	DA	3221	PUT	3	0
64	DA	3213	PGE	1	0
62	D3	102	PEG	2	0
64	D1	102	PGE	2	0
58	DN	201	MPD	1	0
63	DA	3194	EDO	1	0
59	DA	3222	PUT	1	0
59	DA	3212	PUT	1	0
63	DB	211	EDO	1	0
62	DP	201	PEG	1	0
64	DD	301	PGE	2	0
65	DA	3223	SPD	4	0
62	DA	3200	PEG	1	0
57	DA	3193	PG4	1	0
59	DA	3218	PUT	1	0
64	DA	3216	PGE	1	0
57	AA	1670	PG4	1	0
58	DA	3190	MPD	1	0
62	D1	103	PEG	1	0
64	DA	3224	PGE	3	0
63	DA	3197	EDO	1	0
58	DA	3192	MPD	2	0
59	DA	3195	PUT	3	0
57	DS	202	PG4	1	0
57	DR	202	PG4	5	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1523/1534 (99%)	0.70	105 (6%) 16 10	46, 105, 241, 293	0
1	BA	1522/1534 (99%)	1.53	397 (26%) 0 0	61, 140, 279, 284	0
2	AB	224/224 (100%)	1.62	72 (32%) 0 0	83, 127, 202, 270	0
2	BB	224/224 (100%)	1.76	78 (34%) 0 0	99, 144, 211, 261	0
3	AC	206/206 (100%)	0.82	30 (14%) 2 1	80, 108, 141, 163	0
3	BC	206/206 (100%)	2.64	116 (56%) 0 0	115, 151, 190, 231	0
4	AD	205/205 (100%)	0.62	18 (8%) 10 5	64, 103, 131, 154	0
4	BD	205/205 (100%)	0.20	1 (0%) 91 81	61, 81, 107, 131	0
5	AE	155/155 (100%)	0.77	13 (8%) 11 6	67, 91, 133, 169	0
5	BE	150/155 (96%)	1.17	33 (22%) 0 0	77, 97, 144, 227	0
6	AF	106/106 (100%)	0.83	19 (17%) 1 1	82, 105, 128, 142	0
6	BF	100/106 (94%)	0.97	15 (15%) 2 1	86, 121, 146, 154	0
7	AG	151/151 (100%)	2.15	64 (42%) 0 0	107, 137, 166, 179	0
7	BG	151/151 (100%)	5.30	125 (82%) 0 0	147, 203, 218, 228	0
8	AH	129/129 (100%)	0.64	9 (6%) 16 9	71, 91, 118, 136	0
8	BH	129/129 (100%)	1.02	24 (18%) 1 0	91, 116, 150, 168	0
9	AI	127/127 (100%)	2.31	58 (45%) 0 0	96, 132, 169, 200	0
9	BI	127/127 (100%)	3.78	78 (61%) 0 0	138, 176, 209, 229	0
10	AJ	99/99 (100%)	2.03	41 (41%) 0 0	94, 121, 153, 168	0
10	BJ	98/99 (98%)	4.86	78 (79%) 0 0	141, 171, 197, 207	0
11	AK	117/117 (100%)	1.61	35 (29%) 0 0	68, 112, 147, 163	0
11	BK	117/117 (100%)	1.47	33 (28%) 0 0	83, 116, 148, 168	0
12	AL	122/123 (99%)	0.60	4 (3%) 46 30	55, 72, 104, 132	0
12	BL	122/123 (99%)	1.39	31 (25%) 0 0	79, 97, 118, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)		Q<0.9	
13	AM	114/114 (100%)	2.48	57 (50%)	0	0	106, 131, 182, 202	0
13	BM	114/114 (100%)	5.54	104 (91%)	0	0	203, 237, 245, 249	0
14	AN	100/100 (100%)	1.81	37 (37%)	0	0	90, 117, 206, 215	0
14	BN	100/100 (100%)	3.85	75 (75%)	0	0	132, 181, 239, 250	0
15	AO	88/88 (100%)	0.69	10 (11%)	5	3	72, 94, 112, 132	0
15	BO	88/88 (100%)	1.25	20 (22%)	0	0	79, 112, 132, 150	0
16	AP	82/82 (100%)	1.27	19 (23%)	0	0	67, 86, 121, 139	0
16	BP	82/82 (100%)	2.79	48 (58%)	0	0	94, 111, 157, 166	0
17	AQ	80/80 (100%)	0.65	4 (5%)	28	18	70, 86, 119, 143	0
17	BQ	80/80 (100%)	2.17	34 (42%)	0	0	100, 128, 151, 156	0
18	AR	55/55 (100%)	1.21	13 (23%)	0	0	79, 99, 135, 164	0
18	BR	55/55 (100%)	1.07	6 (10%)	5	3	80, 96, 129, 157	0
19	AS	79/79 (100%)	1.56	24 (30%)	0	0	103, 119, 156, 164	0
19	BS	79/79 (100%)	5.06	66 (83%)	0	0	215, 232, 243, 251	0
20	AT	86/86 (100%)	1.04	9 (10%)	6	4	70, 85, 120, 133	0
20	BT	85/86 (98%)	3.27	53 (62%)	0	0	108, 128, 165, 179	0
21	AU	56/56 (100%)	1.59	18 (32%)	0	0	83, 123, 159, 172	0
21	BU	56/56 (100%)	1.01	8 (14%)	2	1	80, 106, 149, 160	0
22	C1	56/56 (100%)	3.35	39 (69%)	0	0	110, 150, 178, 195	0
22	D1	56/56 (100%)	0.59	0	100	100	26, 46, 71, 102	0
23	C2	50/51 (98%)	3.69	34 (68%)	0	0	133, 148, 161, 183	0
23	D2	51/51 (100%)	0.72	5 (9%)	7	4	55, 69, 95, 110	0
24	C3	46/46 (100%)	4.62	39 (84%)	0	0	108, 117, 127, 138	0
24	D3	46/46 (100%)	0.61	2 (4%)	35	22	38, 46, 61, 104	0
25	C4	64/64 (100%)	3.11	44 (68%)	0	0	112, 130, 142, 148	0
25	D4	64/64 (100%)	0.57	0	100	100	36, 44, 53, 68	0
26	C5	38/38 (100%)	2.71	23 (60%)	0	0	108, 122, 133, 143	0
26	D5	38/38 (100%)	0.64	1 (2%)	56	39	43, 54, 68, 91	0
27	C0	58/58 (100%)	3.36	39 (67%)	0	0	104, 121, 140, 143	0
27	D0	58/58 (100%)	0.52	0	100	100	33, 40, 60, 72	0
28	CB	118/120 (98%)	1.71	45 (38%)	0	0	140, 195, 250, 254	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DB	120/120 (100%)	0.30	0 100 100	33, 60, 99, 143	0
29	CC	271/272 (99%)	1.49	88 (32%) 0 0	88, 119, 152, 165	0
29	DC	271/272 (99%)	0.30	6 (2%) 62 45	31, 57, 83, 96	0
30	CD	209/209 (100%)	3.00	130 (62%) 0 0	103, 134, 170, 190	0
31	CA	2876/2904 (99%)	1.90	1023 (35%) 0 0	73, 178, 274, 295	0
32	DD	208/209 (99%)	0.16	0 100 100	22, 41, 69, 91	0
33	CE	201/201 (100%)	3.31	140 (69%) 0 0	119, 167, 201, 218	0
33	DE	201/201 (100%)	0.38	3 (1%) 73 57	31, 59, 101, 141	0
34	CF	177/178 (99%)	4.96	152 (85%) 0 0	204, 217, 226, 233	0
34	DF	177/178 (99%)	0.68	16 (9%) 9 5	58, 84, 125, 138	0
35	CG	176/176 (100%)	4.32	144 (81%) 0 0	140, 181, 219, 228	0
35	DG	176/176 (100%)	0.34	8 (4%) 33 21	49, 73, 99, 128	0
36	CH	149/149 (100%)	2.34	80 (53%) 0 0	86, 156, 175, 183	0
36	DH	149/149 (100%)	2.10	63 (42%) 0 0	79, 157, 193, 208	0
37	CJ	134/134 (100%)	7.53	127 (94%) 0 0	236, 253, 264, 272	0
37	DJ	134/134 (100%)	5.79	110 (82%) 0 0	204, 229, 238, 246	0
38	CK	142/142 (100%)	2.31	72 (50%) 0 0	105, 129, 168, 221	0
38	DK	142/142 (100%)	0.11	0 100 100	25, 37, 61, 75	0
39	CL	122/123 (99%)	1.70	43 (35%) 0 0	95, 116, 149, 167	0
39	DL	123/123 (100%)	0.09	0 100 100	30, 46, 71, 109	0
40	CM	144/144 (100%)	4.11	116 (80%) 0 0	113, 163, 214, 236	0
40	DM	144/144 (100%)	0.32	3 (2%) 63 46	21, 58, 88, 117	0
41	CN	135/136 (99%)	1.38	35 (25%) 0 0	98, 119, 150, 189	0
41	DN	135/136 (99%)	-0.02	0 100 100	29, 43, 69, 88	0
42	CO	120/125 (96%)	2.71	72 (60%) 0 0	110, 132, 155, 186	0
42	DO	125/125 (100%)	0.22	1 (0%) 86 73	29, 39, 68, 111	0
43	CP	116/117 (99%)	3.84	87 (75%) 0 0	147, 171, 185, 189	0
43	DP	117/117 (100%)	0.28	0 100 100	47, 60, 87, 97	0
44	CQ	114/114 (100%)	2.53	65 (57%) 0 0	108, 126, 156, 172	0
44	DQ	114/114 (100%)	0.14	3 (2%) 56 39	34, 52, 82, 114	0
45	CR	117/117 (100%)	2.82	71 (60%) 0 0	98, 138, 174, 199	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	DR	117/117 (100%)	0.29	1 (0%) 84 71	23, 33, 48, 70	0
46	CS	103/103 (100%)	4.11	85 (82%) 0 0	114, 143, 185, 201	0
46	DS	103/103 (100%)	0.13	1 (0%) 82 68	26, 45, 71, 93	0
47	CT	110/110 (100%)	2.50	62 (56%) 0 0	109, 137, 180, 193	0
47	DT	110/110 (100%)	0.10	0 100 100	21, 36, 60, 118	0
48	CU	93/93 (100%)	3.96	73 (78%) 0 0	131, 156, 184, 194	0
48	DU	93/93 (100%)	0.63	5 (5%) 25 16	37, 60, 114, 130	0
49	CV	102/103 (99%)	5.48	88 (86%) 0 0	119, 167, 203, 213	0
49	DV	102/103 (99%)	0.55	11 (10%) 5 3	47, 64, 112, 144	0
50	CW	94/94 (100%)	2.59	53 (56%) 0 0	125, 145, 165, 170	0
50	DW	94/94 (100%)	0.06	0 100 100	38, 56, 80, 92	0
51	CX	75/76 (98%)	2.94	38 (50%) 0 0	111, 134, 148, 178	0
51	DX	76/76 (100%)	0.09	1 (1%) 77 61	31, 45, 69, 107	0
52	CY	77/77 (100%)	1.91	32 (41%) 0 0	103, 122, 147, 168	0
52	DY	77/77 (100%)	0.30	1 (1%) 77 61	37, 59, 92, 108	0
53	CZ	62/62 (100%)	4.42	49 (79%) 0 0	134, 171, 184, 195	0
53	DZ	62/62 (100%)	0.77	6 (9%) 7 4	52, 75, 111, 132	0
54	DI	135/135 (100%)	2.40	71 (52%) 0 0	82, 158, 202, 211	1 (0%)
55	DA	2873/2904 (98%)	0.64	135 (4%) 31 20	22, 48, 215, 300	0
All	All	20634/20751 (99%)	1.61	5723 (27%) 0 0	21, 116, 247, 300	1 (0%)

The worst 5 of 5723 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	DJ	54	PRO	42.4
9	BI	128	SER	22.8
37	CJ	13	VAL	22.8
37	DJ	76	ALA	22.6
37	DJ	55	ILE	21.9

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

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	5MC	BA	967	21/22	0.67	0.39	153,164,167,167	0
1	2MG	BA	966	24/25	0.75	0.36	153,160,171,171	0
1	2MG	BA	1207	24/25	0.80	0.29	158,161,165,168	0
31	PSU	CA	1917	20/21	0.81	0.21	119,125,134,135	0
31	2MA	CA	2503	23/24	0.83	0.26	110,115,118,118	0
31	6MZ	CA	2030	23/24	0.85	0.24	108,114,116,117	0
1	PSU	BA	516	20/21	0.85	0.16	88,99,102,104	0
31	OMU	CA	2552	21/22	0.85	0.45	91,96,100,101	0
31	3TD	CA	1915	21/22	0.86	0.28	150,155,157,157	0
31	PSU	CA	2504	20/21	0.86	0.25	98,108,110,111	0
31	PSU	CA	955	20/21	0.86	0.26	107,112,115,115	0
31	PSU	CA	1911	20/21	0.86	0.24	123,137,138,139	0
31	G7M	CA	2069	24/25	0.87	0.26	109,112,115,116	0
31	2MG	CA	2445	24/25	0.87	0.31	105,110,112,113	0
31	PSU	CA	2580	20/21	0.87	0.22	102,105,109,109	0
31	PSU	CA	746	20/21	0.87	0.25	120,123,126,127	0
1	5MC	AA	967	21/22	0.88	0.20	90,106,107,108	0
31	5MU	CA	747	21/22	0.88	0.28	126,128,130,131	0
31	OMG	CA	2251	24/25	0.89	0.26	90,95,100,101	0
31	PSU	CA	2457	20/21	0.89	0.25	106,107,108,109	0
1	5MC	BA	1407	21/22	0.89	0.21	100,109,114,117	0
1	2MG	BA	1516	24/25	0.89	0.21	82,90,99,100	0
41	4D4	CN	81	12/13	0.90	0.34	112,122,143,143	0
31	1MG	CA	745	24/25	0.90	0.25	106,113,118,121	0
1	2MG	AA	1207	24/25	0.91	0.16	114,118,121,124	0
12	D2T	BL	89	10/11	0.91	0.28	86,88,94,95	0
31	6MZ	CA	1618	23/24	0.91	0.30	136,143,148,149	0
1	2MG	AA	966	24/25	0.91	0.19	95,98,107,108	0
55	PSU	DA	1911	20/21	0.91	0.18	78,88,91,91	0
55	3TD	DA	1915	21/22	0.91	0.22	103,106,112,113	0
12	D2T	AL	89	10/11	0.91	0.27	66,71,78,78	0
31	PSU	CA	2605	20/21	0.92	0.22	82,84,86,87	0
31	OMC	CA	2498	21/22	0.92	0.28	97,102,104,106	0
1	UR3	BA	1498	21/22	0.92	0.18	89,93,97,98	0
1	MA6	BA	1518	24/25	0.92	0.25	84,88,95,96	0
31	2MG	CA	1835	24/25	0.92	0.18	74,76,78,78	0
31	5MU	CA	1939	21/22	0.93	0.19	75,79,81,82	0
1	4OC	BA	1402	22/23	0.93	0.17	78,81,84,85	0
1	MA6	BA	1519	24/25	0.93	0.26	84,87,91,92	0
31	5MC	CA	1962	21/22	0.93	0.16	72,78,79,82	0
1	PSU	AA	516	20/21	0.94	0.16	88,92,97,97	0
55	PSU	DA	1917	20/21	0.94	0.17	74,82,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	UR3	AA	1498	21/22	0.95	0.19	64,68,72,73	0
32	MEQ	DD	150[A]	10/11	0.96	0.24	14,23,32,32	10
1	4OC	AA	1402	22/23	0.96	0.18	61,68,72,73	0
1	2MG	AA	1516	24/25	0.96	0.17	58,61,62,63	0
55	2MG	DA	1835	24/25	0.96	0.23	49,55,56,56	0
41	4D4	DN	81[A]	12/13	0.96	0.24	33,38,53,55	9
1	G7M	BA	527	24/25	0.96	0.15	75,80,83,84	0
41	4D4	DN	81[B]	12/13	0.96	0.24	27,32,34,35	9
1	G7M	AA	527	24/25	0.96	0.17	63,67,73,74	0
55	5MC	DA	1962	21/22	0.96	0.23	43,46,50,52	0
1	MA6	AA	1519	24/25	0.96	0.19	61,62,70,71	0
32	MEQ	DD	150[B]	10/11	0.96	0.24	27,32,45,50	10
1	MA6	AA	1518	24/25	0.97	0.16	60,61,62,64	0
55	PSU	DA	2604	20/21	0.97	0.19	37,42,54,55	0
1	5MC	AA	1407	21/22	0.97	0.15	60,61,63,64	0
55	OMG	DA	2251	24/25	0.98	0.21	29,33,35,39	0
55	5MU	DA	1939	21/22	0.98	0.22	35,38,40,43	0
55	OMU	DA	2552	21/22	0.98	0.22	33,37,39,43	0
55	PSU	DA	2605	20/21	0.98	0.19	35,41,43,44	0
55	PSU	DA	2504	20/21	0.98	0.21	33,41,49,52	0
55	2MA	DA	2503	23/24	0.99	0.20	33,36,39,43	0
55	OMC	DA	2498	21/22	0.99	0.21	20,27,31,37	0
55	PSU	DA	746	20/21	0.99	0.19	28,32,36,38	0
55	PSU	DA	2580	20/21	0.99	0.21	25,30,33,35	0
55	H2U	DA	2449	20/21	0.99	0.22	27,30,36,39	0
55	G7M	DA	2069	24/25	0.99	0.20	26,35,36,37	0
55	2MG	DA	2445	24/25	0.99	0.21	25,29,33,34	0
55	1MG	DA	745	24/25	0.99	0.21	28,31,33,38	0
55	6MZ	DA	2030	23/24	0.99	0.22	24,28,32,39	0
55	5MU	DA	747	21/22	0.99	0.20	28,31,37,38	0
55	6MZ	DA	1618	23/24	0.99	0.20	25,30,32,35	0
55	PSU	DA	955	20/21	0.99	0.21	27,28,32,35	0
55	PSU	DA	2457	20/21	0.99	0.19	25,29,31,35	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
56	MG	CA	3140	1/1	-0.34	0.60	147,147,147,147	0
56	MG	AA	1622	1/1	-0.17	1.84	130,130,130,130	0
56	MG	CA	3033	1/1	-0.13	0.30	200,200,200,200	0
56	MG	CA	3038	1/1	-0.04	0.22	268,268,268,268	0
56	MG	CA	3123	1/1	-0.03	0.99	188,188,188,188	0
56	MG	CA	3077	1/1	0.00	0.48	252,252,252,252	0
56	MG	CA	3142	1/1	0.03	0.56	133,133,133,133	0
56	MG	AA	1626	1/1	0.05	1.41	111,111,111,111	0
56	MG	CA	3156	1/1	0.09	0.18	246,246,246,246	0
56	MG	CA	3149	1/1	0.10	1.20	92,92,92,92	0
56	MG	CA	3104	1/1	0.13	0.32	263,263,263,263	0
56	MG	CA	3028	1/1	0.14	0.73	283,283,283,283	0
56	MG	DA	3180	1/1	0.14	1.27	97,97,97,97	0
56	MG	CA	3130	1/1	0.17	1.11	141,141,141,141	0
56	MG	CA	3139	1/1	0.19	1.21	139,139,139,139	0
56	MG	CA	3061	1/1	0.20	0.21	274,274,274,274	0
56	MG	CA	3141	1/1	0.20	0.60	109,109,109,109	0
56	MG	AA	1603	1/1	0.21	1.09	119,119,119,119	0
56	MG	CA	3146	1/1	0.25	0.38	247,247,247,247	0
56	MG	AA	1604	1/1	0.26	0.85	82,82,82,82	0
56	MG	DA	3168	1/1	0.27	0.48	108,108,108,108	0
56	MG	AA	1642	1/1	0.27	0.51	165,165,165,165	0
56	MG	BA	1630	1/1	0.29	0.14	221,221,221,221	0
56	MG	AA	1628	1/1	0.29	0.95	142,142,142,142	0
56	MG	CA	3113	1/1	0.30	0.78	94,94,94,94	0
56	MG	DA	3131	1/1	0.32	0.76	87,87,87,87	0
56	MG	DA	3138	1/1	0.33	0.39	89,89,89,89	0
56	MG	CA	3110	1/1	0.34	0.83	188,188,188,188	0
56	MG	AA	1614	1/1	0.35	0.20	131,131,131,131	0
56	MG	CA	3124	1/1	0.35	0.53	202,202,202,202	0
56	MG	DA	3179	1/1	0.35	0.48	102,102,102,102	0
56	MG	CA	3056	1/1	0.35	0.72	100,100,100,100	0
56	MG	CA	3003	1/1	0.35	2.62	284,284,284,284	0
56	MG	CA	3002	1/1	0.37	0.31	259,259,259,259	0
56	MG	DA	3145	1/1	0.40	0.76	101,101,101,101	0
56	MG	CA	3005	1/1	0.44	1.15	253,253,253,253	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3133	1/1	0.45	0.63	140,140,140,140	0
56	MG	AA	1606	1/1	0.46	0.49	120,120,120,120	0
62	PEG	DQ	201	7/7	0.47	1.03	107,109,110,110	0
56	MG	DB	207	1/1	0.48	0.77	105,105,105,105	0
56	MG	CA	3092	1/1	0.50	0.23	202,202,202,202	0
56	MG	DA	3163	1/1	0.50	0.36	84,84,84,84	0
56	MG	AA	1616	1/1	0.51	0.93	88,88,88,88	0
56	MG	BA	1629	1/1	0.52	0.58	157,157,157,157	0
56	MG	CA	3039	1/1	0.52	0.36	153,153,153,153	0
56	MG	CA	3068	1/1	0.53	0.43	253,253,253,253	0
56	MG	DA	3130	1/1	0.53	0.36	87,87,87,87	0
56	MG	CA	3097	1/1	0.54	0.16	125,125,125,125	0
56	MG	CA	3134	1/1	0.54	0.52	204,204,204,204	0
56	MG	DA	3178	1/1	0.55	0.67	101,101,101,101	0
56	MG	DB	206	1/1	0.56	0.47	102,102,102,102	0
56	MG	CA	3075	1/1	0.57	1.37	253,253,253,253	0
56	MG	CA	3154	1/1	0.58	0.45	155,155,155,155	0
56	MG	AA	1605	1/1	0.58	0.71	99,99,99,99	0
56	MG	DA	3182	1/1	0.58	0.54	73,73,73,73	0
56	MG	CA	3047	1/1	0.58	1.53	240,240,240,240	0
56	MG	CA	3090	1/1	0.59	0.57	215,215,215,215	0
56	MG	BA	1641	1/1	0.59	0.97	140,140,140,140	0
56	MG	CA	3131	1/1	0.59	0.57	111,111,111,111	0
56	MG	BA	1638	1/1	0.59	0.93	110,110,110,110	0
56	MG	CA	3054	1/1	0.59	0.21	140,140,140,140	0
56	MG	CA	3122	1/1	0.61	0.77	136,136,136,136	0
56	MG	CA	3126	1/1	0.61	0.38	136,136,136,136	0
56	MG	DA	3147	1/1	0.61	0.42	89,89,89,89	0
56	MG	BA	1639	1/1	0.62	0.63	106,106,106,106	0
56	MG	CA	3071	1/1	0.62	0.20	207,207,207,207	0
56	MG	AA	1627	1/1	0.62	0.56	99,99,99,99	0
56	MG	CA	3034	1/1	0.62	0.17	256,256,256,256	0
56	MG	CA	3132	1/1	0.62	0.75	152,152,152,152	0
56	MG	DA	3134	1/1	0.62	0.37	78,78,78,78	0
56	MG	CA	3115	1/1	0.63	0.46	108,108,108,108	0
56	MG	AA	1661	1/1	0.63	0.33	190,190,190,190	0
56	MG	AA	1624	1/1	0.63	0.80	93,93,93,93	0
56	MG	CA	3027	1/1	0.63	0.31	137,137,137,137	0
56	MG	AA	1632	1/1	0.64	0.08	124,124,124,124	0
56	MG	AA	1602	1/1	0.64	0.55	88,88,88,88	0
59	PUT	AA	1675	6/6	0.64	0.62	90,92,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1612	1/1	0.65	0.73	81,81,81,81	0
56	MG	CA	3079	1/1	0.65	0.16	143,143,143,143	0
56	MG	CA	3135	1/1	0.65	0.54	104,104,104,104	0
56	MG	BA	1637	1/1	0.65	0.59	93,93,93,93	0
56	MG	CA	3018	1/1	0.65	0.16	133,133,133,133	0
56	MG	AA	1608	1/1	0.66	0.50	119,119,119,119	0
56	MG	CA	3007	1/1	0.66	0.46	257,257,257,257	0
56	MG	AA	1621	1/1	0.66	0.45	83,83,83,83	0
56	MG	AA	1615	1/1	0.67	0.55	90,90,90,90	0
56	MG	BA	1623	1/1	0.67	1.44	235,235,235,235	0
56	MG	CA	3078	1/1	0.67	0.19	195,195,195,195	0
56	MG	CA	3031	1/1	0.67	0.23	127,127,127,127	0
56	MG	BA	1624	1/1	0.68	0.26	275,275,275,275	0
56	MG	AA	1617	1/1	0.68	0.36	98,98,98,98	0
56	MG	CA	3108	1/1	0.68	0.52	109,109,109,109	0
56	MG	CA	3076	1/1	0.69	0.21	213,213,213,213	0
56	MG	CA	3129	1/1	0.69	0.23	141,141,141,141	0
56	MG	CA	3105	1/1	0.69	0.41	254,254,254,254	0
56	MG	DA	3157	1/1	0.69	0.53	73,73,73,73	0
56	MG	CA	3013	1/1	0.70	0.18	135,135,135,135	0
56	MG	BA	1604	1/1	0.70	0.19	182,182,182,182	0
56	MG	CB	203	1/1	0.70	0.10	155,155,155,155	0
64	PGE	D1	102	10/10	0.70	0.59	95,96,100,100	0
65	SPD	DA	3205	10/10	0.70	0.38	75,81,84,85	0
56	MG	AA	1613	1/1	0.71	1.50	85,85,85,85	0
56	MG	DA	3125	1/1	0.71	0.42	83,83,83,83	0
62	PEG	DA	3217	7/7	0.71	0.55	89,93,98,99	0
56	MG	BA	1626	1/1	0.71	0.32	111,111,111,111	0
56	MG	BA	1606	1/1	0.72	0.21	251,251,251,251	0
59	PUT	AA	1672	6/6	0.72	0.66	110,112,114,114	0
56	MG	AA	1611	1/1	0.72	0.25	113,113,113,113	0
56	MG	CA	3014	1/1	0.72	0.18	262,262,262,262	0
59	PUT	AA	1674	6/6	0.72	0.72	98,99,100,100	0
56	MG	CA	3137	1/1	0.72	0.59	168,168,168,168	0
58	MPD	DT	201	8/8	0.72	0.41	73,82,84,86	0
56	MG	CA	3099	1/1	0.72	0.28	235,235,235,235	0
58	MPD	DT	202	8/8	0.73	0.41	87,88,89,91	0
56	MG	BA	1608	1/1	0.73	0.13	122,122,122,122	0
56	MG	CA	3032	1/1	0.73	0.53	269,269,269,269	0
56	MG	CA	3121	1/1	0.73	0.50	101,101,101,101	0
56	MG	DA	3161	1/1	0.73	0.43	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3167	1/1	0.73	0.40	75,75,75,75	0
56	MG	CA	3106	1/1	0.73	0.60	103,103,103,103	0
56	MG	DA	3155	1/1	0.73	0.57	74,74,74,74	0
56	MG	CA	3055	1/1	0.73	0.10	195,195,195,195	0
56	MG	CA	3016	1/1	0.74	0.34	148,148,148,148	0
56	MG	AA	1618	1/1	0.74	0.83	91,91,91,91	0
56	MG	CA	3049	1/1	0.74	0.24	100,100,100,100	0
56	MG	AA	1679	1/1	0.75	0.25	189,189,189,189	0
62	PEG	D3	102	7/7	0.75	1.24	72,74,83,84	0
56	MG	BA	1614	1/1	0.75	0.17	147,147,147,147	0
63	EDO	DA	3208	4/4	0.75	0.48	98,99,100,101	0
56	MG	DA	3159	1/1	0.75	0.44	80,80,80,80	0
56	MG	CA	3060	1/1	0.75	0.38	242,242,242,242	0
56	MG	CA	3111	1/1	0.75	1.00	159,159,159,159	0
56	MG	BA	1625	1/1	0.76	0.39	274,274,274,274	0
56	MG	DA	3170	1/1	0.76	0.39	73,73,73,73	0
57	PG4	DA	3215	13/13	0.76	0.43	95,103,104,104	0
58	MPD	DE	302	8/8	0.76	0.57	96,97,98,98	0
58	MPD	DA	3203	8/8	0.76	0.75	96,99,102,104	0
56	MG	DA	3136	1/1	0.76	0.12	92,92,92,92	0
56	MG	CA	3151	1/1	0.76	0.36	84,84,84,84	0
56	MG	AA	1620	1/1	0.76	0.46	83,83,83,83	0
64	PGE	D3	101	10/10	0.76	0.66	87,88,88,88	0
62	PEG	DA	3225	7/7	0.76	0.39	62,65,70,70	0
63	EDO	DA	3004	4/4	0.76	0.45	107,107,108,109	0
56	MG	CA	3109	1/1	0.76	0.58	93,93,93,93	0
69	TRS	DA	3219	8/8	0.76	0.56	98,99,102,104	0
56	MG	AA	1663	1/1	0.77	0.19	110,110,110,110	0
56	MG	CA	3010	1/1	0.77	0.52	231,231,231,231	0
56	MG	CA	3001	1/1	0.77	0.38	299,299,299,299	0
59	PUT	DA	3218	6/6	0.77	0.42	75,77,80,81	0
68	GUN	DA	3210	11/11	0.77	0.38	71,73,74,74	0
62	PEG	D1	103	7/7	0.77	0.47	56,60,61,62	0
67	ACY	DA	3196	4/4	0.77	0.32	75,79,79,80	0
56	MG	CA	3148	1/1	0.77	0.79	86,86,86,86	1
56	MG	CB	201	1/1	0.77	0.10	166,166,166,166	0
59	PUT	AA	1673	6/6	0.78	0.49	125,126,127,128	0
56	MG	DA	3126	1/1	0.78	0.37	76,76,76,76	0
56	MG	CA	3006	1/1	0.78	0.19	227,227,227,227	0
64	PGE	DA	3224	10/10	0.78	0.34	74,81,83,83	0
60	T1C	BA	1643	42/42	0.78	0.23	169,175,185,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
57	PG4	AA	1670	13/13	0.78	0.30	80,92,101,102	0
63	EDO	DB	210	4/4	0.78	0.43	85,85,85,86	0
56	MG	CA	3120	1/1	0.78	0.25	195,195,195,195	0
58	MPD	DA	3206	8/8	0.79	0.51	89,93,94,94	0
62	PEG	DP	201	7/7	0.79	0.53	94,94,99,100	0
56	MG	DA	3173	1/1	0.79	0.56	81,81,81,81	0
56	MG	CA	3093	1/1	0.79	0.23	123,123,123,123	0
56	MG	CA	3128	1/1	0.79	0.42	87,87,87,87	0
59	PUT	DA	3211	6/6	0.79	0.34	65,66,72,74	0
56	MG	CA	3063	1/1	0.79	0.24	207,207,207,207	0
56	MG	CA	3026	1/1	0.79	1.03	197,197,197,197	0
56	MG	DA	3171	1/1	0.79	0.57	82,82,82,82	0
56	MG	CA	3082	1/1	0.79	0.45	160,160,160,160	0
56	MG	CA	3145	1/1	0.79	0.38	75,75,75,75	0
56	MG	BA	1631	1/1	0.80	0.07	71,71,71,71	0
58	MPD	DE	301	8/8	0.80	0.61	102,104,107,109	0
56	MG	CA	3065	1/1	0.80	0.25	122,122,122,122	0
56	MG	CA	3107	1/1	0.80	0.72	106,106,106,106	0
56	MG	CA	3069	1/1	0.80	0.21	115,115,115,115	0
56	MG	DA	3143	1/1	0.80	0.46	95,95,95,95	0
62	PEG	DA	3200	7/7	0.80	0.51	55,58,65,65	0
56	MG	AA	1625	1/1	0.81	0.30	78,78,78,78	0
56	MG	CA	3009	1/1	0.81	0.16	248,248,248,248	0
56	MG	CA	3057	1/1	0.81	0.16	132,132,132,132	0
56	MG	CA	3044	1/1	0.81	0.18	84,84,84,84	0
56	MG	CA	3147	1/1	0.81	0.40	91,91,91,91	1
56	MG	BA	1603	1/1	0.81	0.70	261,261,261,261	0
59	PUT	DA	3189	6/6	0.81	0.38	47,48,49,49	0
56	MG	CA	3083	1/1	0.81	0.34	241,241,241,241	0
57	PG4	BA	1642	13/13	0.81	0.42	96,102,107,107	0
56	MG	AA	1655	1/1	0.81	0.16	115,115,115,115	0
56	MG	AA	1644	1/1	0.82	0.14	94,94,94,94	0
56	MG	CA	3008	1/1	0.82	0.10	179,179,179,179	0
59	PUT	DA	3204	6/6	0.82	0.43	66,66,70,71	0
56	MG	CA	3112	1/1	0.82	0.33	110,110,110,110	0
61	ZN	C5	101	1/1	0.82	0.06	148,148,148,148	0
56	MG	BA	1618	1/1	0.82	0.19	106,106,106,106	0
56	MG	CA	3119	1/1	0.82	0.72	134,134,134,134	0
58	MPD	DK	201	8/8	0.82	0.27	93,94,95,95	0
59	PUT	DA	3195	6/6	0.82	0.54	51,53,62,65	0
56	MG	CA	3023	1/1	0.82	0.14	150,150,150,150	0
56	MG	CA	3067	1/1	0.82	0.44	289,289,289,289	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	BA	1622	1/1	0.82	0.12	95,95,95,95	0
56	MG	DA	3153	1/1	0.82	0.33	100,100,100,100	0
56	MG	DA	3181	1/1	0.83	0.70	91,91,91,91	0
56	MG	CA	3048	1/1	0.83	0.17	107,107,107,107	0
56	MG	CA	3072	1/1	0.83	0.88	272,272,272,272	0
57	PG4	DQ	202	13/13	0.83	0.30	64,66,71,72	0
56	MG	AA	1659	1/1	0.83	0.09	97,97,97,97	0
56	MG	CA	3022	1/1	0.83	0.70	188,188,188,188	0
58	MPD	DN	201	8/8	0.83	0.41	87,89,92,93	0
56	MG	CA	3066	1/1	0.83	0.14	125,125,125,125	0
56	MG	DA	3176	1/1	0.83	0.32	93,93,93,93	0
56	MG	DA	3123	1/1	0.83	0.51	77,77,77,77	0
56	MG	AA	1654	1/1	0.83	0.49	252,252,252,252	0
59	PUT	DA	3212	6/6	0.83	0.45	55,57,64,66	0
56	MG	BA	1627	1/1	0.83	0.78	129,129,129,129	0
56	MG	CA	3155	1/1	0.83	0.31	204,204,204,204	0
56	MG	DA	3133	1/1	0.83	0.41	78,78,78,78	0
56	MG	DA	3151	1/1	0.84	0.10	58,58,58,58	0
67	ACY	DA	3201	4/4	0.84	0.33	60,64,64,66	0
56	MG	DA	3124	1/1	0.84	0.38	114,114,114,114	0
56	MG	AA	1640	1/1	0.84	0.13	62,62,62,62	0
56	MG	DA	3172	1/1	0.84	0.37	89,89,89,89	0
56	MG	BA	1610	1/1	0.84	0.08	109,109,109,109	0
56	MG	BA	1612	1/1	0.84	0.26	137,137,137,137	0
63	EDO	D1	101	4/4	0.84	0.34	67,67,68,68	0
57	PG4	DR	202	13/13	0.84	0.46	61,63,75,75	0
66	1PE	DA	3202	16/16	0.84	0.37	60,63,65,65	0
64	PGE	DS	201	10/10	0.84	0.37	56,66,68,69	0
56	MG	CA	3059	1/1	0.84	0.36	147,147,147,147	0
56	MG	DA	3112	1/1	0.84	0.44	293,293,293,293	0
63	EDO	DA	3194	4/4	0.84	0.30	51,56,59,60	0
56	MG	AA	1665	1/1	0.85	0.43	168,168,168,168	0
64	PGE	DA	3213	10/10	0.85	0.48	84,86,90,90	0
56	MG	AA	1639	1/1	0.85	0.09	132,132,132,132	0
56	MG	BA	1601	1/1	0.85	0.17	95,95,95,95	0
56	MG	CA	3040	1/1	0.85	0.09	126,126,126,126	0
63	EDO	DA	3214	4/4	0.85	0.31	77,78,79,79	0
56	MG	AA	1657	1/1	0.85	0.47	162,162,162,162	0
58	MPD	DA	3190	8/8	0.85	0.34	91,92,93,94	0
56	MG	CA	3050	1/1	0.85	0.13	91,91,91,91	0
56	MG	CA	3051	1/1	0.85	0.12	109,109,109,109	0
56	MG	DA	3065	1/1	0.85	0.16	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
62	PEG	AL	201	7/7	0.85	0.39	74,78,85,85	0
56	MG	DA	3007	1/1	0.85	0.12	112,112,112,112	0
56	MG	DD	303	1/1	0.85	0.36	66,66,66,66	0
56	MG	CA	3098	1/1	0.85	0.13	110,110,110,110	0
59	PUT	DA	3184	6/6	0.85	0.37	42,48,50,51	0
56	MG	DA	3128	1/1	0.85	0.48	78,78,78,78	0
57	PG4	DA	3193	13/13	0.85	0.87	63,65,76,77	0
56	MG	DA	3169	1/1	0.85	0.33	73,73,73,73	0
56	MG	CB	202	1/1	0.85	0.12	139,139,139,139	0
56	MG	CA	3125	1/1	0.85	0.27	141,141,141,141	0
56	MG	DA	3063	1/1	0.85	0.13	222,222,222,222	0
56	MG	CA	3080	1/1	0.85	0.35	186,186,186,186	0
65	SPD	DA	3183	10/10	0.85	0.44	57,63,66,66	0
56	MG	CA	3058	1/1	0.85	0.41	135,135,135,135	0
59	PUT	DA	3220	6/6	0.85	0.36	92,92,94,95	0
56	MG	CA	3012	1/1	0.86	0.27	130,130,130,130	0
56	MG	CA	3096	1/1	0.86	0.13	116,116,116,116	0
56	MG	DA	3174	1/1	0.86	0.30	78,78,78,78	0
62	PEG	DA	3226	7/7	0.86	0.33	58,59,65,67	0
56	MG	CA	3094	1/1	0.86	0.26	159,159,159,159	0
56	MG	BA	1607	1/1	0.86	0.38	162,162,162,162	0
56	MG	AA	1609	1/1	0.86	0.38	107,107,107,107	0
56	MG	CA	3086	1/1	0.86	0.16	97,97,97,97	0
56	MG	DA	3165	1/1	0.86	0.45	69,69,69,69	0
56	MG	DA	3148	1/1	0.86	0.24	115,115,115,115	0
56	MG	CA	3064	1/1	0.86	0.57	267,267,267,267	0
64	PGE	DU	101	10/10	0.87	0.50	64,72,83,83	0
56	MG	CA	3088	1/1	0.87	0.10	88,88,88,88	0
56	MG	AA	1664	1/1	0.87	0.35	186,186,186,186	0
56	MG	CA	3062	1/1	0.87	0.19	237,237,237,237	0
62	PEG	DA	3199	7/7	0.87	0.44	60,64,69,70	0
56	MG	CA	3017	1/1	0.87	0.10	106,106,106,106	0
56	MG	CA	3021	1/1	0.87	1.07	278,278,278,278	0
56	MG	DA	3154	1/1	0.87	0.46	59,59,59,59	0
56	MG	CA	3143	1/1	0.87	0.50	107,107,107,107	0
64	PGE	DD	301	10/10	0.87	0.36	63,67,72,73	0
57	PG4	DS	202	13/13	0.87	0.34	43,51,59,61	0
56	MG	AA	1601	1/1	0.87	1.43	104,104,104,104	0
64	PGE	DA	3216	10/10	0.87	0.39	62,64,65,65	0
56	MG	CA	3030	1/1	0.87	0.15	124,124,124,124	0
63	EDO	DA	3001	4/4	0.87	0.37	72,73,75,77	0
56	MG	CA	3020	1/1	0.87	0.11	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	CA	3053	1/1	0.87	0.22	108,108,108,108	0
56	MG	CA	3004	1/1	0.87	0.23	223,223,223,223	0
56	MG	DA	3175	1/1	0.87	0.50	75,75,75,75	0
63	EDO	DA	3207	4/4	0.87	0.26	58,60,62,63	0
56	MG	CA	3036	1/1	0.88	0.33	203,203,203,203	0
58	MPD	DA	3209	8/8	0.88	0.31	68,70,70,71	0
56	MG	CA	3153	1/1	0.88	0.22	90,90,90,90	0
56	MG	BA	1602	1/1	0.88	0.07	100,100,100,100	0
56	MG	AA	1660	1/1	0.88	0.30	286,286,286,286	0
56	MG	CA	3052	1/1	0.88	0.13	97,97,97,97	0
63	EDO	DA	3003	4/4	0.88	0.52	64,64,66,67	0
62	PEG	DL	201	7/7	0.88	0.28	65,69,76,78	0
56	MG	AA	1649	1/1	0.88	0.12	77,77,77,77	0
56	MG	BA	1636	1/1	0.88	0.64	172,172,172,172	0
56	MG	CA	3152	1/1	0.88	0.46	215,215,215,215	0
56	MG	AA	1623	1/1	0.88	0.36	85,85,85,85	0
56	MG	DA	3095	1/1	0.88	0.17	33,33,33,33	0
56	MG	DA	3129	1/1	0.88	1.13	60,60,60,60	0
58	MPD	DA	3192	8/8	0.89	0.59	79,79,82,83	0
56	MG	AA	1610	1/1	0.89	0.40	99,99,99,99	0
56	MG	BA	1633	1/1	0.89	0.28	235,235,235,235	0
59	PUT	DA	3221	6/6	0.89	0.33	44,48,50,50	0
66	1PE	DA	3185	16/16	0.89	0.31	44,53,71,72	0
56	MG	CA	3019	1/1	0.89	0.10	79,79,79,79	0
56	MG	DA	3162	1/1	0.89	0.25	64,64,64,64	0
56	MG	DA	3156	1/1	0.89	0.34	74,74,74,74	0
56	MG	DA	3045	1/1	0.89	0.09	85,85,85,85	0
56	MG	CA	3035	1/1	0.89	0.26	158,158,158,158	0
56	MG	CA	3144	1/1	0.90	0.13	83,83,83,83	0
56	MG	CA	3116	1/1	0.90	0.80	89,89,89,89	0
56	MG	CA	3117	1/1	0.90	0.77	109,109,109,109	0
56	MG	AA	1635	1/1	0.90	0.10	100,100,100,100	0
56	MG	CA	3150	1/1	0.90	0.50	82,82,82,82	0
63	EDO	DB	211	4/4	0.90	0.24	73,73,74,75	0
56	MG	BA	1617	1/1	0.90	0.14	126,126,126,126	0
56	MG	DA	3149	1/1	0.90	0.28	77,77,77,77	0
58	MPD	AA	1676	8/8	0.90	0.57	97,100,100,102	0
56	MG	CA	3045	1/1	0.90	0.07	93,93,93,93	0
56	MG	AA	1656	1/1	0.90	0.16	149,149,149,149	0
56	MG	AA	1647	1/1	0.90	0.13	202,202,202,202	0
65	SPD	DA	3223	10/10	0.90	0.27	40,44,54,55	0
56	MG	CA	3101	1/1	0.90	0.11	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1619	1/1	0.90	0.27	92,92,92,92	0
56	MG	AA	1607	1/1	0.90	0.61	92,92,92,92	0
56	MG	DA	3142	1/1	0.90	0.28	79,79,79,79	0
56	MG	BA	1634	1/1	0.90	0.07	116,116,116,116	0
56	MG	DA	3120	1/1	0.90	0.36	55,55,55,55	0
56	MG	CA	3029	1/1	0.90	0.36	177,177,177,177	0
56	MG	CA	3127	1/1	0.90	0.11	85,85,85,85	0
56	MG	DA	3166	1/1	0.90	0.86	90,90,90,90	0
56	MG	BA	1640	1/1	0.91	0.82	156,156,156,156	0
56	MG	BA	1632	1/1	0.91	0.12	72,72,72,72	0
56	MG	BA	1644	1/1	0.91	0.12	97,97,97,97	0
56	MG	CA	3136	1/1	0.91	0.34	105,105,105,105	0
56	MG	AA	1636	1/1	0.91	0.28	97,97,97,97	0
56	MG	CA	3095	1/1	0.91	0.18	81,81,81,81	0
63	EDO	DA	3197	4/4	0.91	0.26	68,68,69,69	0
56	MG	CA	3084	1/1	0.91	0.34	208,208,208,208	0
56	MG	CA	3100	1/1	0.91	0.31	110,110,110,110	0
56	MG	CA	3089	1/1	0.91	0.22	95,95,95,95	0
56	MG	BA	1609	1/1	0.91	0.16	194,194,194,194	0
56	MG	AA	1634	1/1	0.91	0.19	108,108,108,108	0
56	MG	DA	3103	1/1	0.91	0.12	44,44,44,44	0
56	MG	AA	1630	1/1	0.91	0.15	134,134,134,134	0
56	MG	CA	3103	1/1	0.91	0.15	120,120,120,120	0
56	MG	CA	3011	1/1	0.92	0.28	117,117,117,117	0
64	PGE	DA	3186	10/10	0.92	0.22	39,46,49,50	0
56	MG	BA	1645	1/1	0.92	0.05	98,98,98,98	0
60	T1C	AA	1677	42/42	0.92	0.25	89,96,109,110	0
58	MPD	AA	1671	8/8	0.92	0.53	101,103,104,106	0
56	MG	BA	1635	1/1	0.92	0.10	111,111,111,111	0
56	MG	DR	203	1/1	0.92	0.42	111,111,111,111	0
63	EDO	DA	3198	4/4	0.92	0.35	56,57,58,59	0
59	PUT	DA	3002	6/6	0.92	0.23	45,52,54,55	0
56	MG	DA	3122	1/1	0.92	0.32	80,80,80,80	0
61	ZN	AB	301	1/1	0.92	0.30	209,209,209,209	0
56	MG	BA	1628	1/1	0.92	0.18	111,111,111,111	0
56	MG	CA	3118	1/1	0.92	0.45	90,90,90,90	0
56	MG	DA	3016	1/1	0.92	0.11	44,44,44,44	0
56	MG	DR	201	1/1	0.92	0.60	44,44,44,44	0
56	MG	CA	3043	1/1	0.92	0.14	101,101,101,101	0
56	MG	DA	3053	1/1	0.93	0.12	78,78,78,78	0
56	MG	CA	3081	1/1	0.93	0.17	134,134,134,134	0
56	MG	AA	1651	1/1	0.93	0.13	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3038	1/1	0.93	0.22	29,29,29,29	0
56	MG	DA	3094	1/1	0.93	0.21	35,35,35,35	0
56	MG	DA	3160	1/1	0.93	0.12	72,72,72,72	0
56	MG	AA	1658	1/1	0.93	0.10	100,100,100,100	0
56	MG	AA	1669	1/1	0.93	0.41	118,118,118,118	0
56	MG	DA	3118	1/1	0.93	0.34	76,76,76,76	0
56	MG	CA	3042	1/1	0.93	0.12	91,91,91,91	0
56	MG	CA	3074	1/1	0.93	0.27	206,206,206,206	0
56	MG	DA	3044	1/1	0.93	0.15	36,36,36,36	0
56	MG	CA	3015	1/1	0.93	0.25	83,83,83,83	0
56	MG	CA	3087	1/1	0.93	0.07	97,97,97,97	0
56	MG	CA	3102	1/1	0.93	0.27	114,114,114,114	0
56	MG	DA	3152	1/1	0.94	0.23	47,47,47,47	0
56	MG	DA	3121	1/1	0.94	0.37	91,91,91,91	0
56	MG	CA	3091	1/1	0.94	0.10	96,96,96,96	0
56	MG	AA	1633	1/1	0.94	0.29	101,101,101,101	0
56	MG	DA	3164	1/1	0.94	0.32	72,72,72,72	0
56	MG	DA	3005	1/1	0.94	0.10	81,81,81,81	0
56	MG	DA	3080	1/1	0.94	0.10	109,109,109,109	0
56	MG	DA	3132	1/1	0.94	0.52	77,77,77,77	0
56	MG	BA	1615	1/1	0.94	0.08	76,76,76,76	0
59	PUT	DA	3222	6/6	0.94	0.24	50,54,55,55	0
56	MG	CA	3138	1/1	0.94	0.16	103,103,103,103	0
56	MG	DA	3084	1/1	0.94	0.08	57,57,57,57	0
56	MG	CA	3041	1/1	0.94	0.19	71,71,71,71	0
56	MG	DA	3119	1/1	0.94	0.11	63,63,63,63	0
65	SPD	DA	3187	10/10	0.94	0.24	38,40,48,50	0
56	MG	DA	3021	1/1	0.94	0.07	48,48,48,48	0
56	MG	CA	3070	1/1	0.94	0.08	112,112,112,112	0
59	PUT	DA	3188	6/6	0.94	0.22	32,35,40,41	0
56	MG	AA	1643	1/1	0.94	0.14	78,78,78,78	0
56	MG	DA	3229	1/1	0.94	0.13	55,55,55,55	0
56	MG	DA	3108	1/1	0.95	0.18	36,36,36,36	0
56	MG	DB	201	1/1	0.95	0.14	64,64,64,64	0
56	MG	DB	205	1/1	0.95	0.17	49,49,49,49	0
56	MG	CA	3114	1/1	0.95	0.47	62,62,62,62	0
56	MG	AA	1678	1/1	0.95	0.16	74,74,74,74	0
56	MG	CA	3085	1/1	0.95	0.12	89,89,89,89	0
56	MG	DA	3139	1/1	0.95	0.40	64,64,64,64	1
56	MG	BA	1621	1/1	0.95	0.19	42,42,42,42	0
56	MG	DA	3069	1/1	0.95	0.17	44,44,44,44	0
61	ZN	D5	101	1/1	0.95	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3127	1/1	0.95	0.43	62,62,62,62	0
56	MG	DA	3009	1/1	0.95	0.12	102,102,102,102	0
56	MG	DA	3146	1/1	0.95	0.15	72,72,72,72	0
56	MG	DA	3097	1/1	0.95	0.14	45,45,45,45	0
56	MG	AA	1653	1/1	0.95	0.04	75,75,75,75	0
56	MG	BA	1619	1/1	0.95	0.19	107,107,107,107	0
56	MG	DA	3140	1/1	0.95	0.19	57,57,57,57	0
56	MG	DA	3081	1/1	0.95	0.17	94,94,94,94	0
67	ACY	DA	3191	4/4	0.95	0.27	56,57,58,59	0
56	MG	DA	3082	1/1	0.95	0.08	55,55,55,55	0
56	MG	DB	208	1/1	0.95	0.26	64,64,64,64	0
56	MG	DA	3135	1/1	0.95	0.27	72,72,72,72	0
56	MG	DA	3144	1/1	0.95	0.37	65,65,65,65	0
56	MG	DA	3076	1/1	0.95	0.20	38,38,38,38	0
56	MG	DA	3150	1/1	0.95	0.18	59,59,59,59	0
56	MG	DA	3070	1/1	0.95	0.15	61,61,61,61	0
56	MG	AA	1650	1/1	0.95	0.09	87,87,87,87	0
56	MG	BA	1613	1/1	0.95	0.18	78,78,78,78	0
56	MG	DA	3177	1/1	0.95	0.18	68,68,68,68	0
56	MG	DA	3006	1/1	0.96	0.11	68,68,68,68	0
56	MG	DA	3043	1/1	0.96	0.08	31,31,31,31	0
56	MG	DA	3227	1/1	0.96	0.14	45,45,45,45	0
56	MG	DA	3117	1/1	0.96	0.11	41,41,41,41	0
56	MG	DA	3091	1/1	0.96	0.23	55,55,55,55	0
56	MG	CA	3073	1/1	0.96	0.28	260,260,260,260	0
56	MG	CA	3037	1/1	0.96	0.43	235,235,235,235	0
56	MG	DA	3049	1/1	0.96	0.17	33,33,33,33	0
56	MG	DA	3099	1/1	0.96	0.13	78,78,78,78	0
56	MG	DA	3029	1/1	0.96	0.14	61,61,61,61	0
56	MG	AA	1641	1/1	0.96	0.08	92,92,92,92	0
56	MG	DA	3022	1/1	0.96	0.15	43,43,43,43	0
56	MG	AA	1629	1/1	0.96	0.14	83,83,83,83	0
56	MG	DA	3013	1/1	0.96	0.13	71,71,71,71	0
56	MG	AA	1666	1/1	0.96	0.05	67,67,67,67	0
56	MG	DA	3098	1/1	0.96	0.09	29,29,29,29	0
56	MG	DA	3020	1/1	0.96	0.32	33,33,33,33	0
56	MG	DA	3050	1/1	0.96	0.12	43,43,43,43	0
56	MG	DA	3137	1/1	0.96	0.26	47,47,47,47	0
56	MG	DB	209	1/1	0.96	0.49	80,80,80,80	0
56	MG	DA	3115	1/1	0.96	0.15	49,49,49,49	0
56	MG	DA	3008	1/1	0.96	0.05	82,82,82,82	0
56	MG	DA	3158	1/1	0.96	0.17	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	DA	3090	1/1	0.96	0.18	26,26,26,26	0
56	MG	DM	201	1/1	0.96	0.06	62,62,62,62	0
56	MG	DA	3088	1/1	0.96	0.17	45,45,45,45	0
56	MG	DA	3105	1/1	0.96	0.19	39,39,39,39	0
56	MG	DA	3114	1/1	0.97	0.11	62,62,62,62	0
56	MG	DA	3079	1/1	0.97	0.07	63,63,63,63	0
56	MG	AA	1638	1/1	0.97	0.09	103,103,103,103	0
56	MG	BA	1616	1/1	0.97	0.18	149,149,149,149	0
56	MG	DA	3100	1/1	0.97	0.14	30,30,30,30	0
56	MG	DA	3028	1/1	0.97	0.14	38,38,38,38	0
56	MG	AA	1637	1/1	0.97	0.08	57,57,57,57	0
56	MG	BA	1620	1/1	0.97	0.17	97,97,97,97	0
56	MG	DB	203	1/1	0.97	0.05	39,39,39,39	0
56	MG	DA	3077	1/1	0.97	0.18	42,42,42,42	0
56	MG	DA	3075	1/1	0.97	0.07	49,49,49,49	0
56	MG	AA	1667	1/1	0.97	0.12	49,49,49,49	0
56	MG	DA	3018	1/1	0.97	0.25	29,29,29,29	0
56	MG	DA	3083	1/1	0.97	0.09	69,69,69,69	0
56	MG	CA	3046	1/1	0.97	0.14	143,143,143,143	0
56	MG	BA	1605	1/1	0.97	0.09	125,125,125,125	0
56	MG	AA	1652	1/1	0.97	0.29	57,57,57,57	0
56	MG	DA	3102	1/1	0.97	0.14	56,56,56,56	0
56	MG	CA	3024	1/1	0.97	0.17	141,141,141,141	0
56	MG	DA	3109	1/1	0.97	0.10	29,29,29,29	0
56	MG	DA	3073	1/1	0.97	0.15	47,47,47,47	0
56	MG	DA	3017	1/1	0.97	0.13	56,56,56,56	0
56	MG	DB	202	1/1	0.97	0.13	29,29,29,29	0
56	MG	DA	3230	1/1	0.97	0.35	45,45,45,45	0
56	MG	DA	3078	1/1	0.97	0.10	38,38,38,38	0
56	MG	DD	302	1/1	0.97	0.13	48,48,48,48	0
56	MG	DA	3031	1/1	0.97	0.21	46,46,46,46	0
56	MG	DA	3046	1/1	0.97	0.09	47,47,47,47	0
56	MG	DA	3026	1/1	0.98	0.10	40,40,40,40	0
56	MG	DA	3032	1/1	0.98	0.23	42,42,42,42	0
56	MG	DA	3062	1/1	0.98	0.15	37,37,37,37	0
56	MG	DA	3085	1/1	0.98	0.14	41,41,41,41	0
56	MG	DA	3116	1/1	0.98	0.14	28,28,28,28	0
56	MG	DA	3054	1/1	0.98	0.09	57,57,57,57	0
56	MG	DA	3027	1/1	0.98	0.15	71,71,71,71	0
56	MG	DA	3093	1/1	0.98	0.14	36,36,36,36	0
56	MG	DA	3089	1/1	0.98	0.08	36,36,36,36	0
56	MG	DA	3036	1/1	0.98	0.16	34,34,34,34	0

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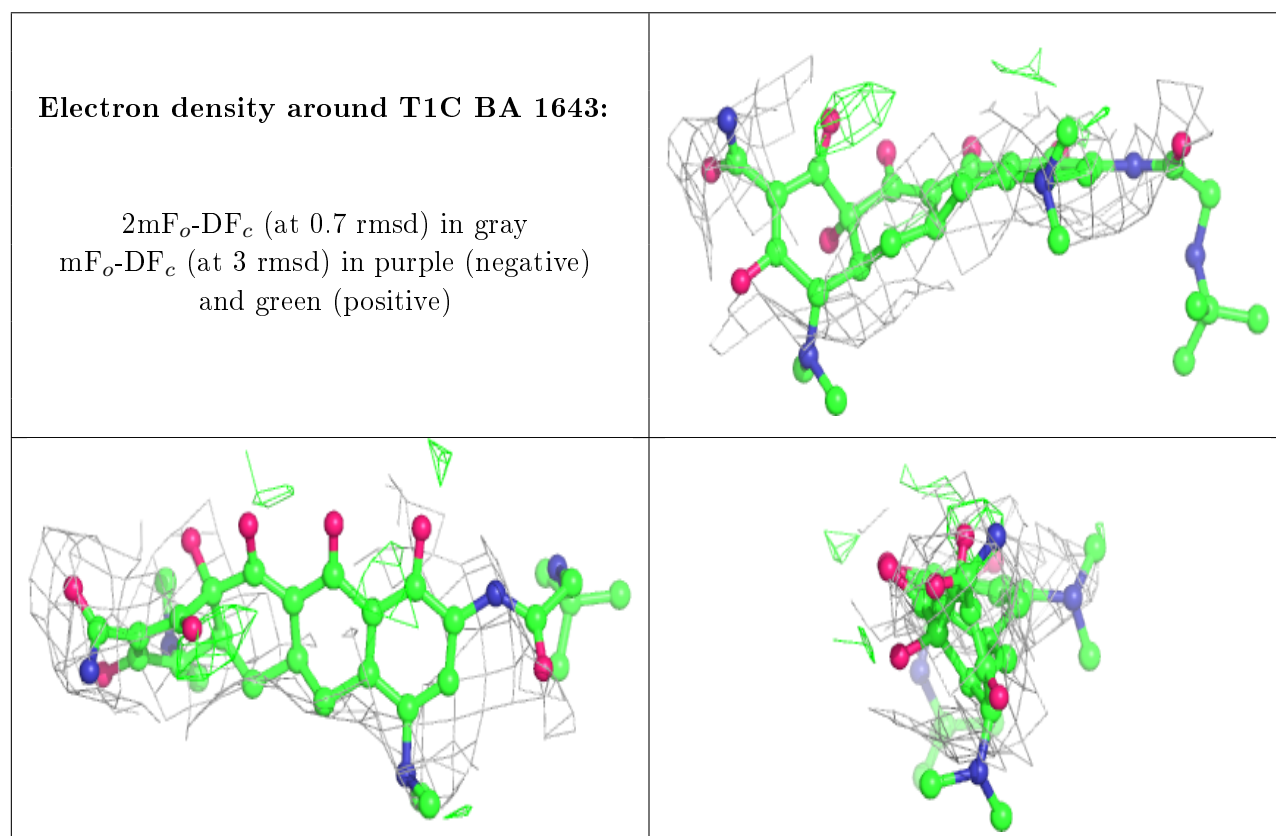
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1662	1/1	0.98	0.22	110,110,110,110	0
56	MG	DA	3141	1/1	0.98	0.22	66,66,66,66	0
56	MG	DA	3055	1/1	0.98	0.08	49,49,49,49	0
56	MG	DA	3039	1/1	0.98	0.12	20,20,20,20	0
56	MG	BA	1611	1/1	0.98	0.11	66,66,66,66	0
56	MG	DA	3111	1/1	0.98	0.15	32,32,32,32	0
56	MG	DA	3040	1/1	0.98	0.14	26,26,26,26	0
56	MG	DA	3107	1/1	0.98	0.17	47,47,47,47	0
56	MG	DA	3015	1/1	0.98	0.18	18,18,18,18	0
56	MG	DA	3066	1/1	0.98	0.19	29,29,29,29	0
56	MG	AA	1631	1/1	0.98	0.06	56,56,56,56	0
56	MG	DA	3101	1/1	0.98	0.22	30,30,30,30	0
56	MG	DA	3071	1/1	0.98	0.06	91,91,91,91	0
56	MG	AA	1646	1/1	0.98	0.08	65,65,65,65	0
56	MG	DA	3041	1/1	0.98	0.09	58,58,58,58	0
58	MPD	DS	203	8/8	0.98	0.21	37,40,44,47	0
56	MG	DA	3010	1/1	0.98	0.14	34,34,34,34	0
56	MG	CA	3025	1/1	0.98	0.28	105,105,105,105	0
56	MG	DA	3057	1/1	0.98	0.23	57,57,57,57	0
56	MG	DA	3034	1/1	0.98	0.17	28,28,28,28	0
56	MG	DA	3068	1/1	0.98	0.11	62,62,62,62	0
56	MG	DA	3086	1/1	0.98	0.12	39,39,39,39	0
56	MG	DA	3023	1/1	0.98	0.21	34,34,34,34	0
56	MG	DA	3228	1/1	0.98	0.09	53,53,53,53	0
56	MG	DA	3037	1/1	0.98	0.23	31,31,31,31	0
56	MG	DA	3067	1/1	0.98	0.19	55,55,55,55	0
56	MG	DA	3106	1/1	0.98	0.20	31,31,31,31	0
56	MG	DA	3074	1/1	0.98	0.15	33,33,33,33	0
56	MG	AA	1645	1/1	0.98	0.12	61,61,61,61	0
56	MG	DA	3019	1/1	0.99	0.10	43,43,43,43	0
56	MG	DA	3047	1/1	0.99	0.19	27,27,27,27	0
56	MG	DA	3052	1/1	0.99	0.15	36,36,36,36	0
56	MG	DA	3033	1/1	0.99	0.19	26,26,26,26	0
56	MG	DA	3024	1/1	0.99	0.20	32,32,32,32	0
56	MG	DA	3056	1/1	0.99	0.17	22,22,22,22	0
56	MG	DA	3096	1/1	0.99	0.11	61,61,61,61	0
56	MG	DA	3104	1/1	0.99	0.09	42,42,42,42	0
56	MG	DA	3064	1/1	0.99	0.08	59,59,59,59	0
56	MG	DA	3061	1/1	0.99	0.15	19,19,19,19	0
56	MG	DA	3014	1/1	0.99	0.25	19,19,19,19	0
56	MG	DA	3058	1/1	0.99	0.08	31,31,31,31	0
56	MG	DA	3030	1/1	0.99	0.14	25,25,25,25	0

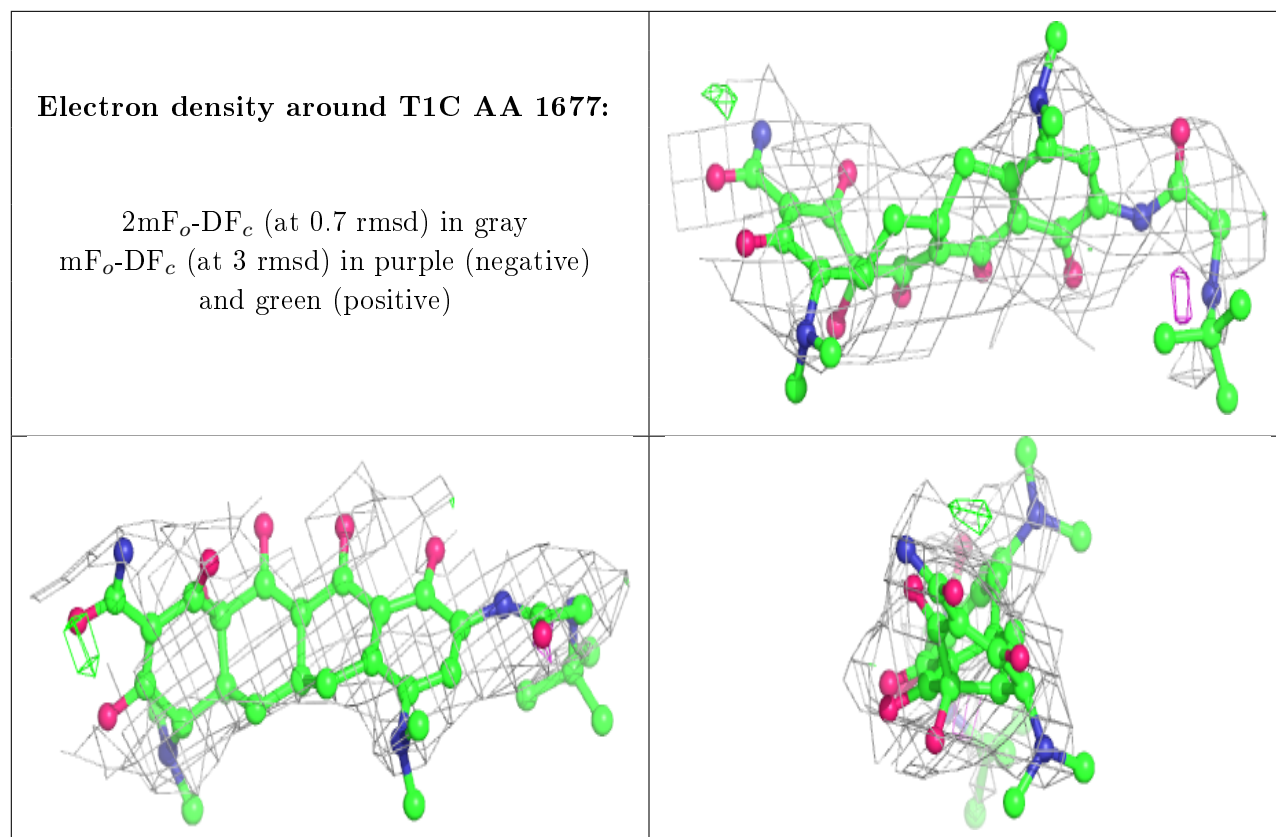
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	AA	1648	1/1	0.99	0.09	76,76,76,76	0
56	MG	DA	3072	1/1	0.99	0.09	47,47,47,47	0
56	MG	DA	3048	1/1	0.99	0.13	42,42,42,42	0
56	MG	DA	3042	1/1	0.99	0.16	20,20,20,20	0
56	MG	AA	1668	1/1	0.99	0.11	54,54,54,54	0
56	MG	DA	3110	1/1	0.99	0.19	19,19,19,19	0
56	MG	DA	3087	1/1	0.99	0.16	48,48,48,48	0
56	MG	DA	3060	1/1	0.99	0.11	16,16,16,16	0
56	MG	DA	3092	1/1	0.99	0.17	31,31,31,31	0
56	MG	DA	3025	1/1	0.99	0.23	25,25,25,25	0
56	MG	DB	204	1/1	0.99	0.15	56,56,56,56	0
56	MG	DA	3035	1/1	1.00	0.18	24,24,24,24	0
56	MG	DA	3012	1/1	1.00	0.09	29,29,29,29	0
56	MG	DA	3113	1/1	1.00	0.22	18,18,18,18	0
56	MG	DA	3051	1/1	1.00	0.14	17,17,17,17	0
56	MG	DA	3011	1/1	1.00	0.17	28,28,28,28	0
56	MG	DA	3059	1/1	1.00	0.15	37,37,37,37	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.