



## Full wwPDB EM Validation Report ⓘ

Dec 17, 2024 – 01:46 AM EST

PDB ID : 7N2V  
EMDB ID : EMD-24134  
Title : Elongating 70S ribosome complex in a spectinomycin-stalled intermediate state of translocation bound to EF-G in an active, GTP conformation (INT1)  
Authors : Rundlet, E.J.; Holm, M.; Schacherl, M.; Natchiar, K.S.; Altman, R.B.; Spahn, C.M.T.; Myasnikov, A.G.; Blanchard, S.C.  
Deposited on : 2021-05-29  
Resolution : 2.54 Å(reported)

This is a Full wwPDB EM Validation 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

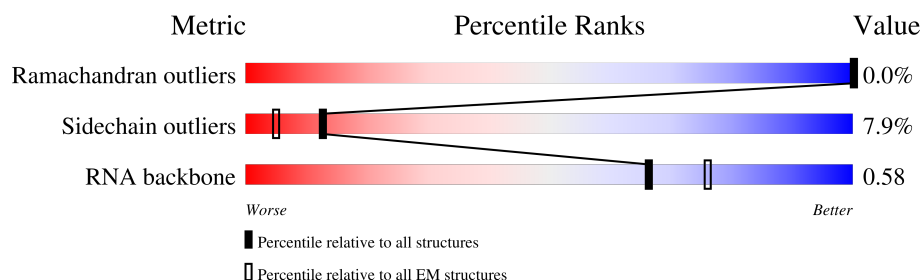
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.54 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.








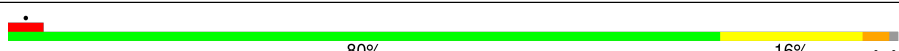
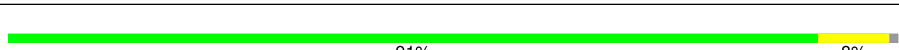
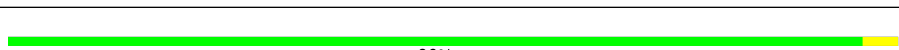
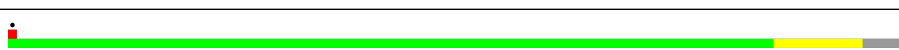

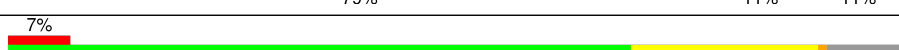
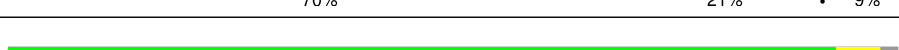
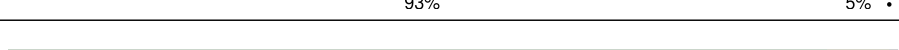
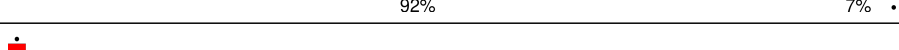
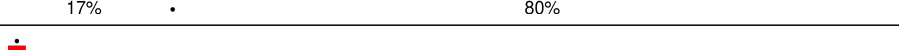
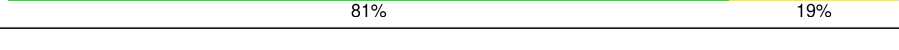

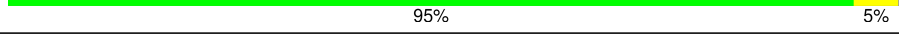
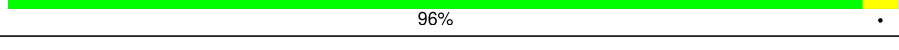
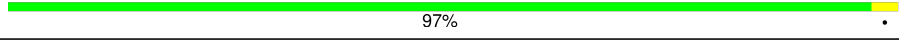
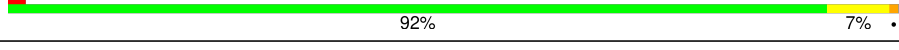
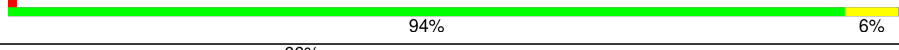
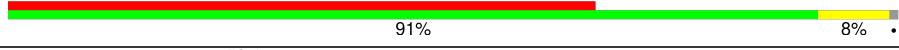


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	16	1534	
2	SB	241	
3	SC	233	
4	SD	206	
5	SE	167	
6	SF	135	
7	SG	179	
8	SH	130	

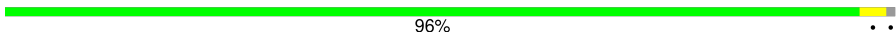
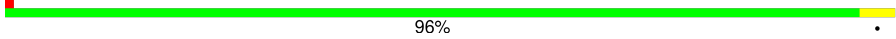
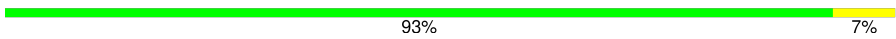

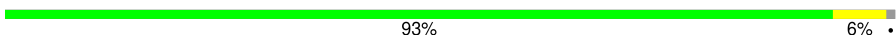
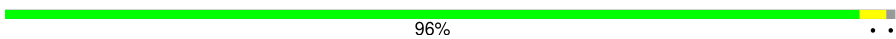
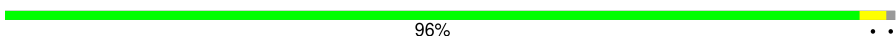
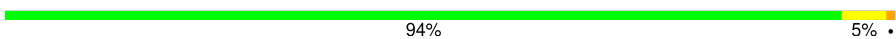
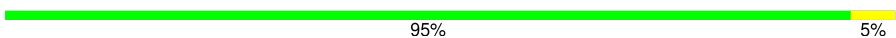

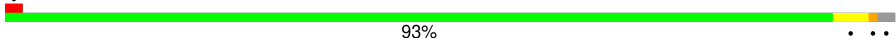


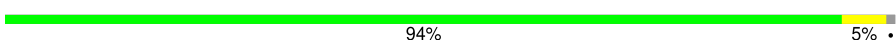
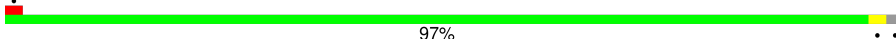


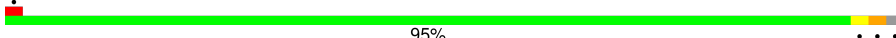


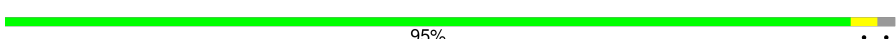

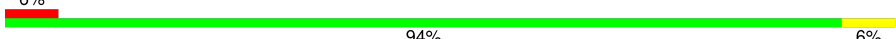


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Mol	Chain	Length	Quality of chain
9	SI	130	
10	SJ	103	
11	SK	129	
12	SL	124	
13	SM	118	
14	SN	101	
15	SO	89	
16	SP	82	
17	SQ	84	
18	SR	75	
19	SS	92	
20	ST	87	
21	SU	71	
22	mR	60	
23	23	2904	
24	5	120	
25	LB	273	
26	LC	209	
27	LD	201	
28	LE	179	
29	LF	177	
30	LI	149	
31	LJ	165	
32	LK	142	
33	LM	142	


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Mol	Chain	Length	Quality of chain
34	LN	123	 96% . .
35	LO	144	 96% .
36	LP	136	 93% 7%
37	LQ	127	 89% 5% • 6%
38	LR	117	 93% 6% .
39	LS	115	 96% . .
40	LT	118	 96% . .
41	LU	103	 94% 5% .
42	LV	110	 95% 5%
43	LW	100	 83% 10% 7%
44	LX	104	 93% . . .
45	LY	94	 93% 7%
46	La	85	 86% . 11%
47	Lb	78	 94% 5% .
48	Lc	63	 97% . .
49	Ld	59	 92% 7% .
50	Le	70	 7% 80% 17% .
51	Lf	57	 95% . . .
52	Lg	55	 85% 9% 5%
53	Lh	46	 96% .
54	Li	65	 95% . .
55	Lj	38	 97% .
56	EF	704	 6% 94% 6%
57	Pp	3	 33% 67%
58	Pt	106	 8% 56% 14% . 28%

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Mol	Chain	Length	Quality of chain
59	Dt	106	

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
64	ATP	23	3003	X	-	-	-

## 2 Entry composition [i](#)

There are 67 unique types of molecules in this entry. The entry contains 154120 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
1	16	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SC	211	Total	C	N	O	S	0	0
			1653	1046	310	293	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SE	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SF	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SG	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SJ	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SK	119	Total	C	N	O	S	0	0
			895	551	179	162	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SM	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SR	67	Total	C	N	O	S	0	0
			555	351	106	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SS	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	ST	85	Total	C	N	O	S	0	0
			664	411	137	113	3		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
21	SU	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	mR	12	Total	C	N	O	P	0	0
			254	114	44	84	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	23	2904	Total	C	N	O	P	0	0
			62355	27824	11469	20158	2904		

- Molecule 24 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	5	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LB	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LC	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LD	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LE	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LF	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LI	148	Total	C	N	O	S	0	0
			1101	694	196	210	1		

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LJ	131	Total	C	N	O	S	0	0
			992	629	175	184	4		

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LK	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LM	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LN	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LO	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LP	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LQ	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LR	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LS	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LT	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LU	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LV	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LW	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LX	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LY	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	La	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lb	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Lc	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Ld	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 50 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Le	68	Total	C	N	O	S	0	0
			533	330	101	96	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lf	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Lg	52	Total	C	N	O	S	0	0
			427	275	78	74			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Lh	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Li	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Lj	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 56 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	EF	704	Total	C	N	O	S	0	0
			5388	3395	938	1033	22		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EF	1	SER	-	expression tag	UNP A0A0H3PU63

- Molecule 57 is a protein called Nascent peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Pp	3	Total	C	N	O	S	0	0
			28	20	4	3	1		

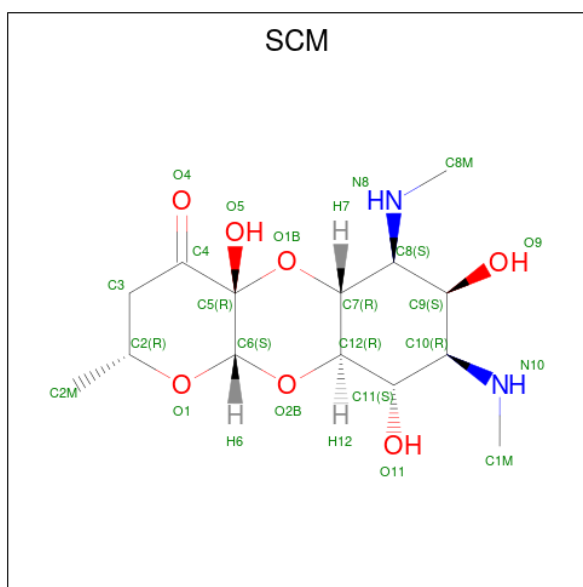
- Molecule 58 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
58	Pt	76	Total	C	N	O	P	S	0	0
			1636	733	284	542	76	1		

- Molecule 59 is a RNA chain called tRNA.

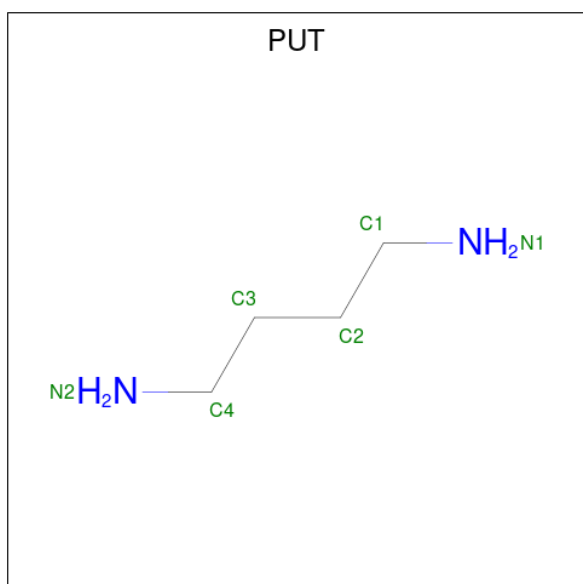
Mol	Chain	Residues	Atoms					AltConf	Trace	
59	Dt	76	Total	C	N	O	P	S	0	0
			1641	735	294	534	76	2		

- Molecule 60 is SPECTINOMYCIN (three-letter code: SCM) (formula: C<sub>14</sub>H<sub>24</sub>N<sub>2</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
60	16	1	Total	C	N	O	0
			23	14	2	7	
60	16	1	Total	C	N	O	0
			23	14	2	7	
60	23	1	Total	C	N	O	0
			23	14	2	7	

- Molecule 61 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula:  $C_4H_{12}N_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
61	16	1	Total	C	N	0
			6	4	2	
61	16	1	Total	C	N	0
			6	4	2	
61	16	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	LC	1	Total	C	N	0
			6	4	2	

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Lig- and of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
62	16	63	Total	Mg	0
			63	63	
62	SK	1	Total	Mg	0
			1	1	

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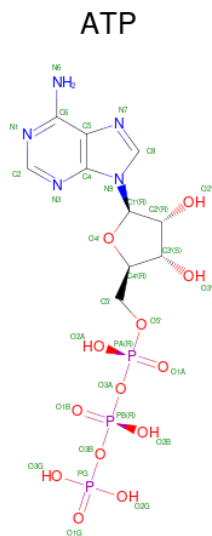
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
62	SN	1	Total 1	Mg 1	0
62	SR	1	Total 1	Mg 1	0
62	23	264	Total 264	Mg 264	0
62	5	6	Total 6	Mg 6	0
62	LB	1	Total 1	Mg 1	0
62	LC	1	Total 1	Mg 1	0
62	LD	1	Total 1	Mg 1	0
62	LO	1	Total 1	Mg 1	0
62	LQ	1	Total 1	Mg 1	0
62	Lf	1	Total 1	Mg 1	0
62	EF	1	Total 1	Mg 1	0
62	Pt	1	Total 1	Mg 1	0

- Molecule 63 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

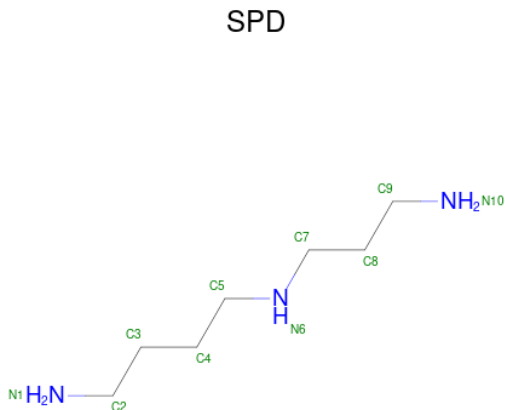
Mol	Chain	Residues	Atoms		AltConf
63	SB	1	Total 1	Zn 1	0
63	Le	1	Total 1	Zn 1	0
63	Lj	1	Total 1	Zn 1	0

- Molecule 64 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
64	23	1	Total 31	C 10	N 5	O 13	P 3	0
64	23	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 65 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ) (labeled as "Ligand of Interest" by depositor).



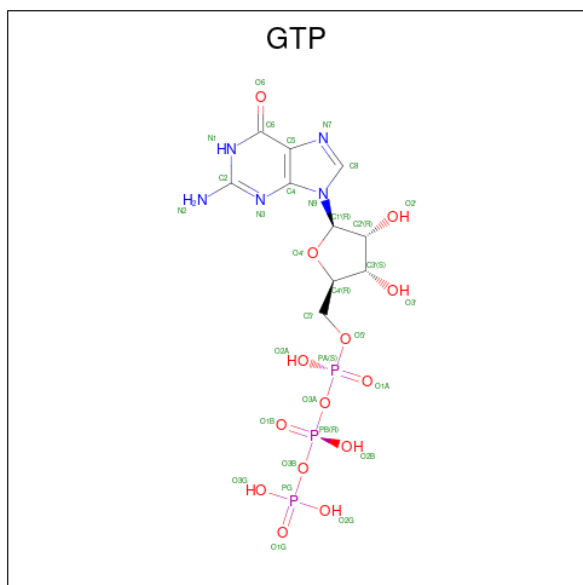
Mol	Chain	Residues	Atoms			AltConf
65	23	1	Total	C	N	0
			10	7	3	

*Continued on next page...*

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Mol	Chain	Residues	Atoms			AltConf
65	23	1	Total	C	N	0
			10	7	3	

- Molecule 66 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
66	EF	1	Total	C	N	O	P	0
			32	10	5	14	3	

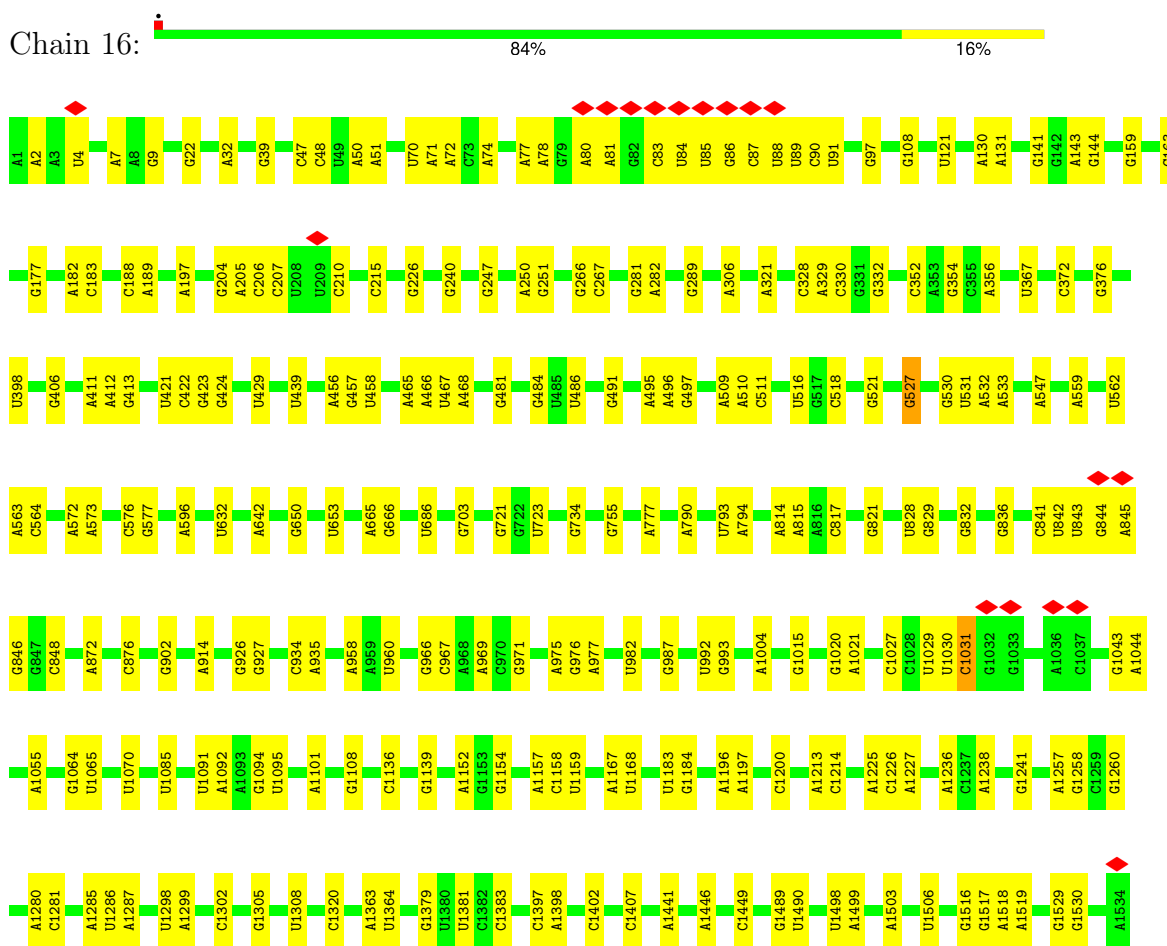
- Molecule 67 is water.

Mol	Chain	Residues	Atoms		AltConf
67	16	1	Total	O	0
			1	1	
67	SB	1	Total	O	0
			1	1	
67	23	22	Total	O	0
			22	22	
67	LB	1	Total	O	0
			1	1	
67	EF	1	Total	O	0
			1	1	

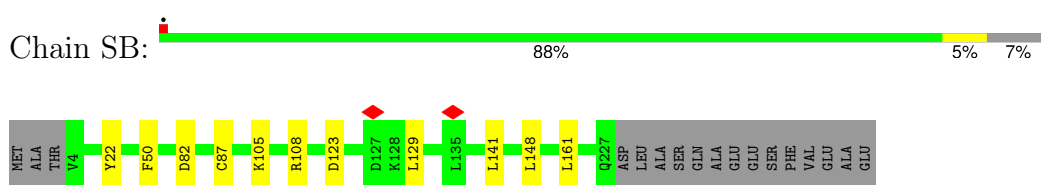
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 2: 30S ribosomal protein S2



- Molecule 3: 30S ribosomal protein S3

Chain SC:  84% 7% 9%



- Molecule 4: 30S ribosomal protein S4

Chain SD:  93% 6%



- Molecule 5: 30S ribosomal protein S5

Chain SE:  90% 7%



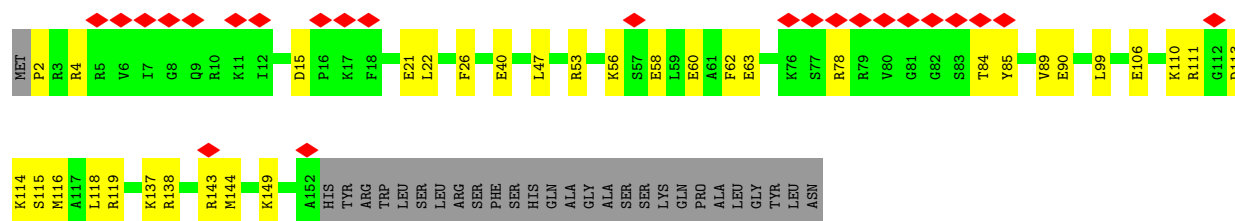
- Molecule 6: 30S ribosomal protein S6

Chain SF:  70% 8% 21%



- Molecule 7: 30S ribosomal protein S7

Chain SG:  13% 65% 19% 16%




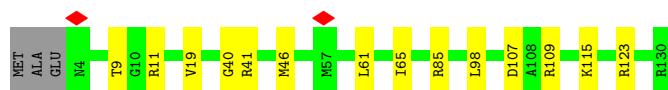
- Molecule 8: 30S ribosomal protein S8

Chain SH:  95% 5%

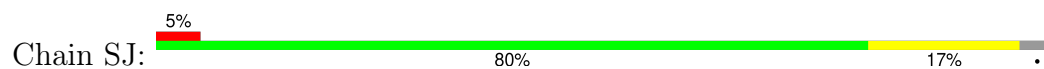


- Molecule 9: 30S ribosomal protein S9

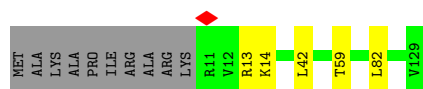
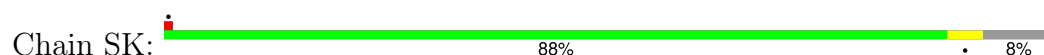
Chain SI:  87% 11% 2%



- Molecule 10: 30S ribosomal protein S10



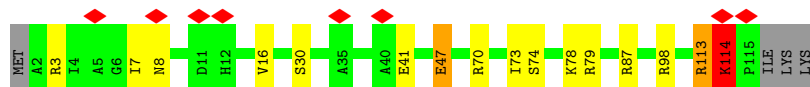
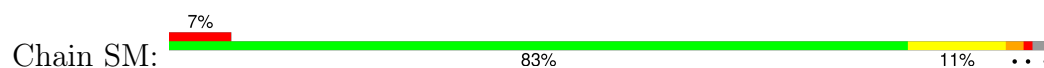
- Molecule 11: 30S ribosomal protein S11



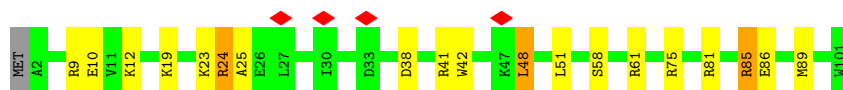
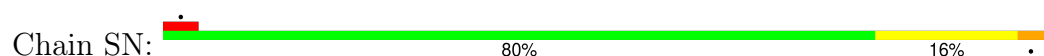
- Molecule 12: 30S ribosomal protein S12



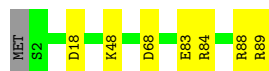
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15




- Molecule 16: 30S ribosomal protein S16

Chain SP:  96%




- Molecule 17: 30S ribosomal protein S17

Chain SQ:  86% 10% 5%



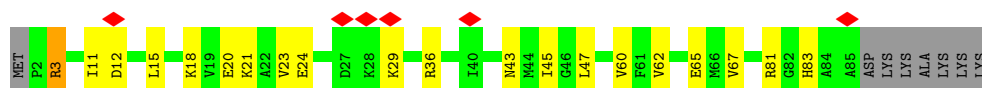
- Molecule 18: 30S ribosomal protein S18

Chain SR:  79% 11% 11%



- Molecule 19: 30S ribosomal protein S19

Chain SS:  7% 70% 21% 9%



- Molecule 20: 30S ribosomal protein S20

Chain ST:  93% 5% 2%



- Molecule 21: 30S ribosomal protein S21

Chain SU:  92% 7% 1%




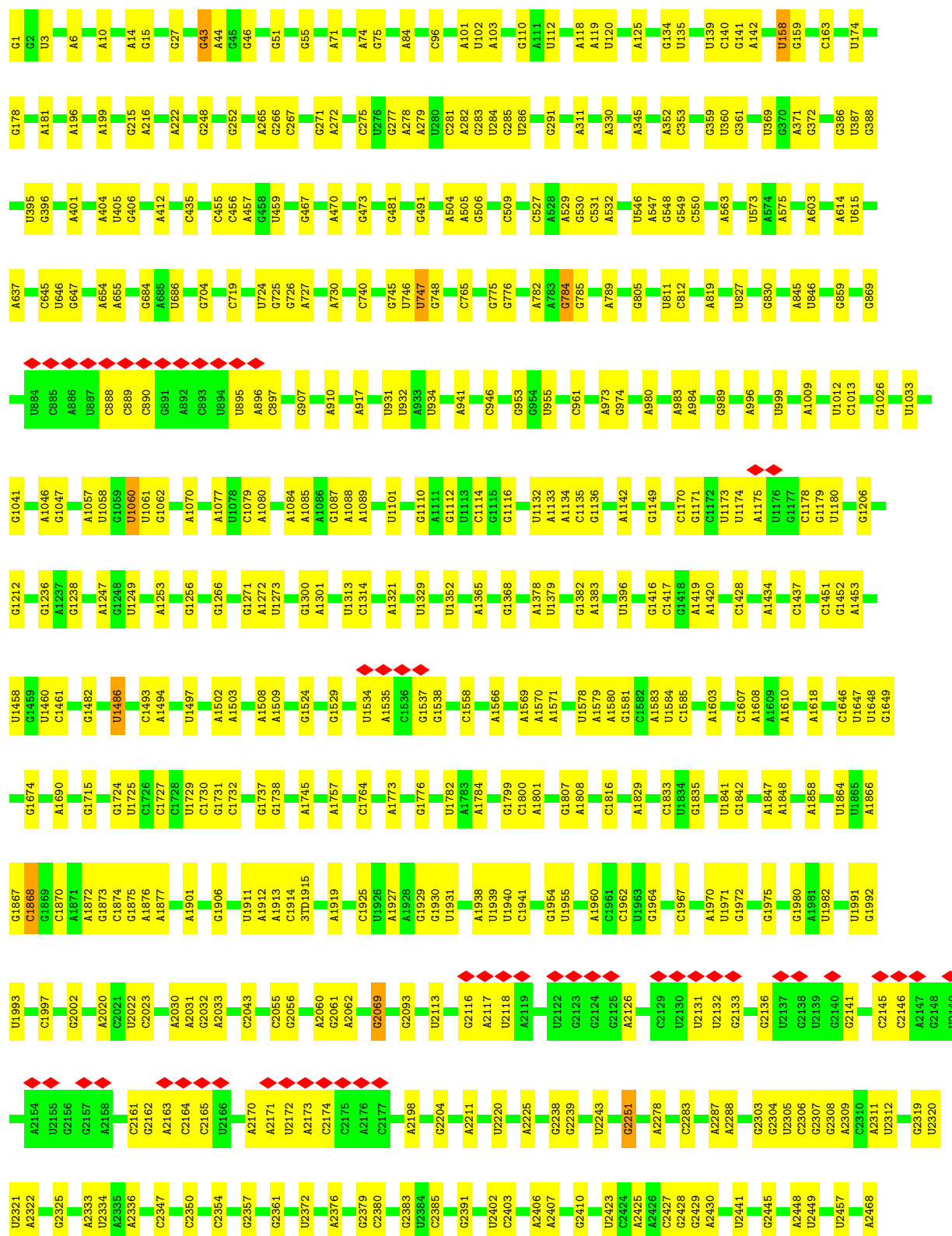
- Molecule 22: mRNA

Chain mR:  17% 80% 3%

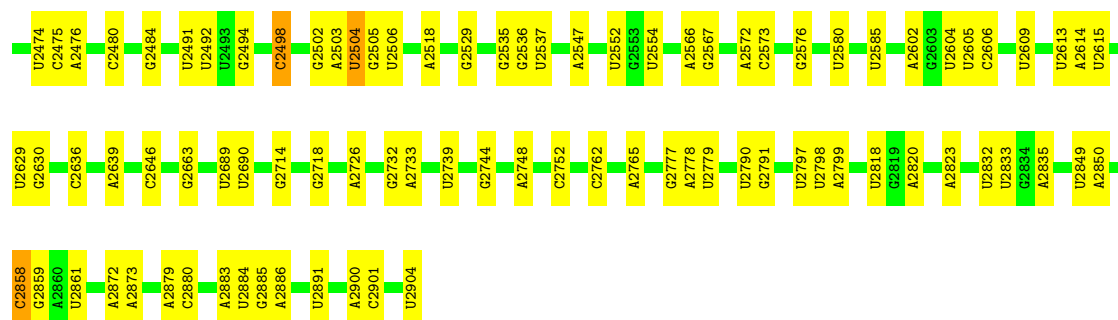


- Molecule 23: 23S rRNA

Chain 23:  81% 19%

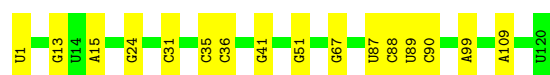






• Molecule 24: 5S rRNA

Chain 5: 87% 13%



• Molecule 25: 50S ribosomal protein L2

Chain LB: 95% 5%



• Molecule 26: 50S ribosomal protein L3

Chain LC: 96%



• Molecule 27: 50S ribosomal protein L4

Chain LD: 97%



• Molecule 28: 50S ribosomal protein L5

Chain LE: 92% 7%

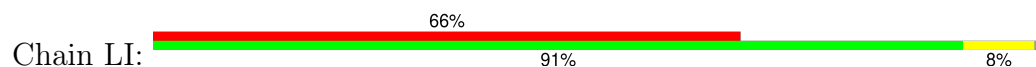


• Molecule 29: 50S ribosomal protein L6

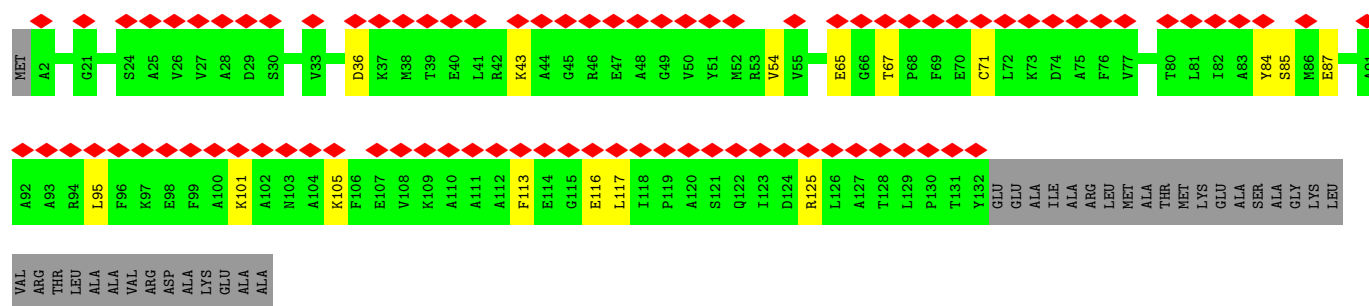
Chain LF: 94% 6%



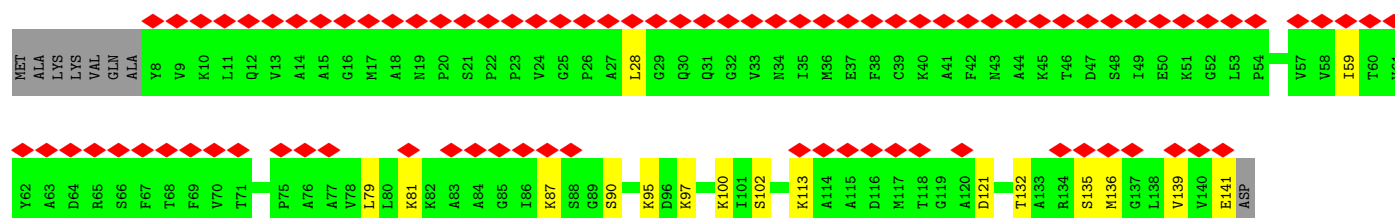
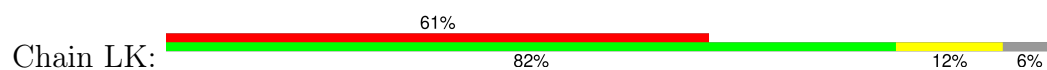
- Molecule 30: 50S ribosomal protein L9



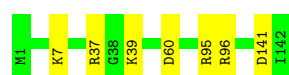
- Molecule 31: 50S ribosomal protein L10



- Molecule 32: 50S ribosomal protein L11



- Molecule 33: 50S ribosomal protein L13



- Molecule 34: 50S ribosomal protein L14





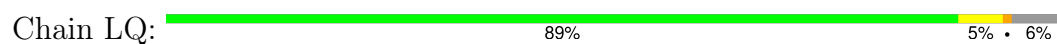
- Molecule 35: 50S ribosomal protein L15



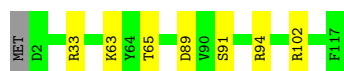
- Molecule 36: 50S ribosomal protein L16



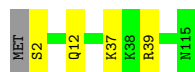
- Molecule 37: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L18



- Molecule 39: 50S ribosomal protein L19

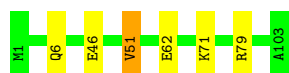


- Molecule 40: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L21





- Molecule 42: 50S ribosomal protein L22

Chain LV: 95% 5%



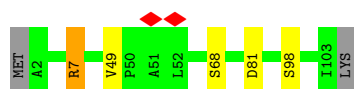
- Molecule 43: 50S ribosomal protein L23

Chain LW: 83% 10% 7%



- Molecule 44: 50S ribosomal protein L24

Chain LX: 93% 7% ..



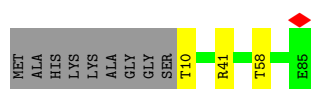
- Molecule 45: 50S ribosomal protein L25

Chain LY: 93% 7%



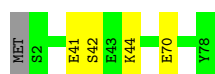
- Molecule 46: 50S ribosomal protein L27

Chain La: 86% 11%



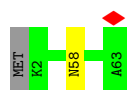
- Molecule 47: 50S ribosomal protein L28

Chain Lb: 94% 5%



- Molecule 48: 50S ribosomal protein L29

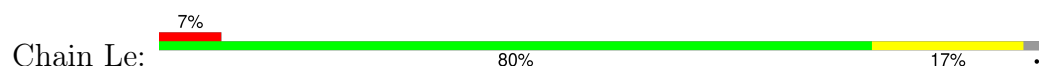
Chain Lc: 97% ..



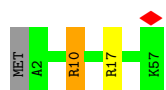
- Molecule 49: 50S ribosomal protein L30



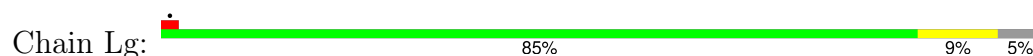
- Molecule 50: 50S ribosomal protein L31



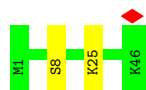
- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33



- Molecule 53: 50S ribosomal protein L34



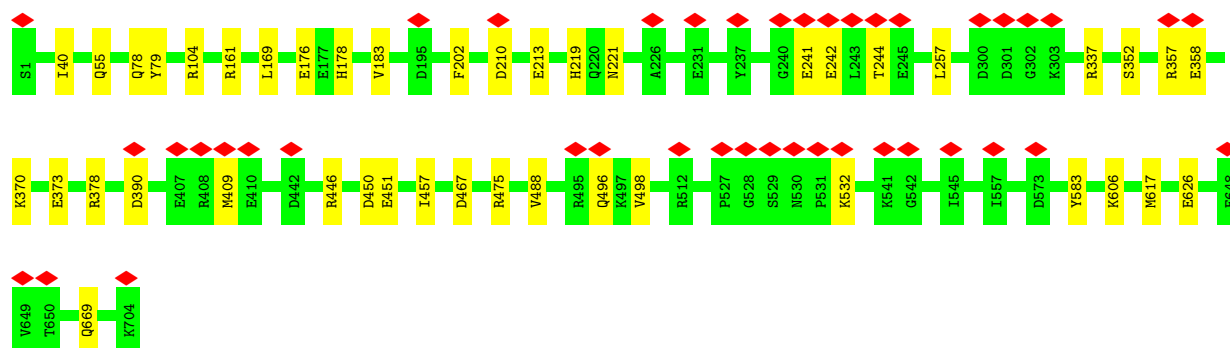
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36

A diagram showing a 4-bit bus with four vertical bars labeled M1, D20, R24, and G38 from left to right. The D20 bar is highlighted in red, and a red diamond is placed above it.

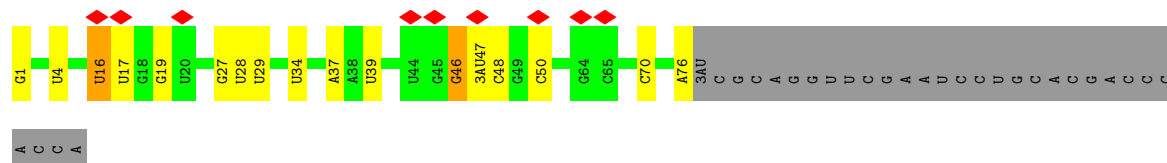
- Chain EF: 



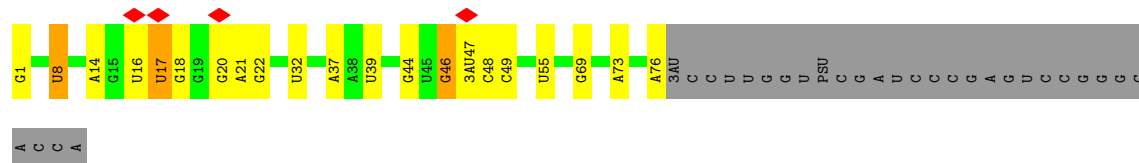
- Chain Pp:  33% 67%



- Chain Pt: 



- Chain Dt: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33688	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	87	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.103	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size ( $\text{\AA}$ )	610.55994, 610.55994, 610.55994	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, 1MG, ZN, T6A, 6MZ, 2MG, 4OC, PUT, 5MC, OMU, PSU, 2MA, ATP, MA6, U8U, 3AU, UR3, 3TD, 4D4, GTP, OMC, SCM, D2T, MIA, OMG, 7MG, MG, H2U, SPD, 5MU

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	16	0.65	1/36619 (0.0%)	0.78	8/57122 (0.0%)
2	SB	0.40	0/1784	0.63	1/2403 (0.0%)
3	SC	0.39	0/1680	0.65	0/2263
4	SD	0.36	0/1665	0.60	0/2227
5	SE	0.42	0/1157	0.63	0/1557
6	SF	0.40	0/881	0.67	1/1189 (0.1%)
7	SG	0.46	0/1195	0.83	5/1602 (0.3%)
8	SH	0.39	0/989	0.57	0/1326
9	SI	0.53	1/1034 (0.1%)	0.71	0/1375
10	SJ	0.40	0/805	0.78	0/1089
11	SK	0.42	0/911	0.70	0/1229
12	SL	0.38	0/960	0.64	0/1286
13	SM	0.46	0/892	0.89	3/1193 (0.3%)
14	SN	0.44	0/817	0.91	3/1088 (0.3%)
15	SO	0.37	0/722	0.59	0/964
16	SP	0.39	0/659	0.61	0/884
17	SQ	0.40	0/657	0.64	0/881
18	SR	0.38	0/564	0.60	0/756
19	SS	0.47	0/685	0.77	1/922 (0.1%)
20	ST	0.32	0/670	0.55	0/888
21	SU	0.50	0/597	0.67	0/792
22	mR	0.55	0/283	0.73	0/438
23	23	0.79	1/69284 (0.0%)	0.78	15/108082 (0.0%)
24	5	0.72	1/2873 (0.0%)	0.76	0/4478
25	LB	0.43	0/2121	0.62	0/2852
26	LC	0.42	0/1586	0.59	0/2134
27	LD	0.39	0/1571	0.58	0/2113
28	LE	0.48	1/1434 (0.1%)	0.72	1/1926 (0.1%)
29	LF	0.37	0/1343	0.62	0/1816
30	LI	0.37	0/1112	0.81	5/1503 (0.3%)
31	LJ	0.42	0/1006	0.67	1/1358 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	LK	0.51	0/993	0.66	0/1341
33	LM	0.43	0/1152	0.57	0/1551
34	LN	0.41	0/947	0.66	0/1268
35	LO	0.41	0/1062	0.63	0/1413
36	LP	0.42	0/1081	0.65	0/1443
37	LQ	0.39	0/973	0.60	0/1301
38	LR	0.41	0/902	0.63	0/1209
39	LS	0.41	0/929	0.61	0/1242
40	LT	0.43	0/960	0.56	0/1278
41	LU	0.43	0/829	0.62	0/1107
42	LV	0.39	0/864	0.59	0/1156
43	LW	0.38	0/744	0.58	0/994
44	LX	0.41	0/787	0.60	0/1051
45	LY	0.40	0/766	0.56	0/1025
46	La	0.41	0/589	0.60	0/779
47	Lb	0.44	0/635	0.69	1/848 (0.1%)
48	Lc	0.43	0/502	0.65	0/667
49	Ld	0.41	0/453	0.65	0/605
50	Le	0.45	0/543	0.72	0/726
51	Lf	0.42	0/450	0.62	0/599
52	Lg	0.42	0/434	0.65	0/576
53	Lh	0.40	0/380	0.67	0/498
54	Li	0.38	0/513	0.64	1/676 (0.1%)
55	Lj	0.39	0/303	0.62	0/397
56	EF	0.40	0/5490	0.61	1/7437 (0.0%)
57	Pp	0.45	0/28	1.11	0/34
58	Pt	0.53	2/1684 (0.1%)	0.78	0/2615
59	Dt	0.60	1/1654 (0.1%)	0.80	1/2572 (0.0%)
All	All	0.65	8/165203 (0.0%)	0.75	48/246144 (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
3	SC	0	2
4	SD	0	3
5	SE	0	1
9	SI	0	3
10	SJ	0	2
12	SL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	SM	0	4
14	SN	0	2
17	SQ	0	3
19	SS	0	1
21	SU	0	1
25	LB	0	3
27	LD	0	1
28	LE	0	3
30	LI	0	2
34	LN	0	2
36	LP	0	2
37	LQ	0	2
38	LR	0	1
41	LU	0	1
44	LX	0	1
45	LY	0	1
46	La	0	1
49	Ld	0	1
51	Lf	0	2
55	Lj	0	1
56	EF	0	3
All	All	0	50

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	Dt	1	G	OP3-P	-10.87	1.48	1.61
23	23	1	G	OP3-P	-10.70	1.48	1.61
24	5	1	U	OP3-P	-10.20	1.49	1.61
58	Pt	1	G	OP3-P	-10.15	1.49	1.61
28	LE	93	GLY	C-N	-8.57	1.14	1.34
58	Pt	16	U	C1'-N1	6.47	1.58	1.48
1	16	1308	U	O3'-P	5.17	1.67	1.61
9	SI	41	ARG	C-O	5.06	1.32	1.23

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16	1490	U	O5'-P-OP1	-29.78	74.96	110.70
1	16	1490	U	OP1-P-OP2	-26.97	79.15	119.60
1	16	1490	U	O5'-P-OP2	17.20	131.33	110.70
14	SN	25	ALA	N-CA-CB	-15.22	88.78	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16	1489	G	OP1-P-O3'	13.97	135.93	105.20
1	16	1489	G	OP2-P-O3'	-13.31	75.92	105.20
13	SM	114	LYS	CB-CA-C	-10.91	88.58	110.40
19	SS	47	LEU	CA-CB-CG	8.48	134.80	115.30
14	SN	24	ARG	N-CA-C	7.70	131.78	111.00
23	23	43	G	C2'-C3'-O3'	7.64	126.31	109.50
23	23	158	U	P-O3'-C3'	7.55	128.76	119.70
30	LI	75	LEU	N-CA-C	7.53	131.34	111.00
30	LI	75	LEU	CB-CA-C	-7.20	96.53	110.20
30	LI	62	LEU	CA-CB-CG	6.98	131.35	115.30
23	23	1060	U	C2'-C3'-O3'	6.92	124.77	113.70
23	23	2858	C	C2'-C3'-O3'	6.72	124.45	113.70
23	23	748	G	O4'-C1'-N9	6.66	113.53	108.20
13	SM	47	GLU	CA-CB-CG	6.61	127.94	113.40
7	SG	47	LEU	CA-CB-CG	6.56	130.39	115.30
23	23	1313	U	C2-N1-C1'	6.52	125.52	117.70
30	LI	122	LEU	CA-CB-CG	6.39	130.00	115.30
23	23	784	G	P-O3'-C3'	6.36	127.33	119.70
13	SM	78	LYS	CD-CE-NZ	-6.20	97.44	111.70
28	LE	93	GLY	C-N-CA	6.19	137.18	121.70
6	SF	54	LEU	CA-CB-CG	6.15	129.45	115.30
23	23	1486	U	C2'-C3'-O3'	6.05	123.38	113.70
7	SG	2	PRO	CA-N-CD	-5.93	103.20	111.50
7	SG	118	LEU	CA-CB-CG	5.90	128.87	115.30
54	Li	32	ILE	CG1-CB-CG2	-5.87	98.48	111.40
56	EF	257	LEU	CA-CB-CG	5.78	128.59	115.30
1	16	1031	C	C2-N1-C1'	5.75	125.13	118.80
23	23	1929	G	O4'-C1'-N9	5.74	112.79	108.20
59	Dt	17	U	C3'-C2'-C1'	-5.68	96.96	101.50
1	16	563	A	O4'-C1'-N9	5.60	112.68	108.20
23	23	984	A	O4'-C1'-N9	5.51	112.61	108.20
14	SN	48	LEU	CA-CB-CG	5.50	127.94	115.30
23	23	435	C	C2-N1-C1'	5.38	124.72	118.80
2	SB	148	LEU	CA-CB-CG	5.38	127.67	115.30
23	23	1060	U	P-O3'-C3'	5.33	126.09	119.70
7	SG	118	LEU	CB-CG-CD2	5.26	119.95	111.00
23	23	1607	C	C5'-C4'-O4'	5.20	115.34	109.10
30	LI	12	LEU	CB-CG-CD2	5.20	119.84	111.00
7	SG	99	LEU	CA-CB-CG	5.19	127.23	115.30
31	LJ	84	TYR	CB-CA-C	-5.18	100.05	110.40
23	23	1868	C	C5'-C4'-O4'	5.17	115.30	109.10
23	23	1101	U	C2-N1-C1'	5.16	123.89	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	Lb	44	LYS	CA-CB-CG	5.15	124.72	113.40
1	16	872	A	O4'-C1'-N9	5.11	112.29	108.20

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
56	EF	104	ARG	Sidechain
56	EF	378	ARG	Sidechain
56	EF	475	ARG	Sidechain
25	LB	221	ARG	Sidechain
25	LB	258	ARG	Sidechain
25	LB	269	ARG	Sidechain
27	LD	69	ARG	Sidechain
28	LE	167	ARG	Sidechain
28	LE	30	ARG	Sidechain
28	LE	71	ARG	Sidechain
30	LI	104	THR	Peptide
30	LI	108	VAL	Peptide
34	LN	31	ARG	Sidechain
34	LN	70	ARG	Sidechain
36	LP	18	ARG	Sidechain
36	LP	59	ARG	Sidechain
37	LQ	118	ARG	Sidechain
37	LQ	2	ARG	Sidechain
38	LR	102	ARG	Sidechain
41	LU	51	VAL	Peptide
44	LX	7	ARG	Sidechain
45	LY	21	ARG	Sidechain
46	La	41	ARG	Sidechain
49	Ld	16	ARG	Sidechain
51	Lf	10	ARG	Sidechain
51	Lf	17	ARG	Sidechain
55	Lj	24	ARG	Sidechain
3	SC	40	ARG	Sidechain
3	SC	88	ARG	Sidechain
4	SD	26	ARG	Sidechain
4	SD	44	ARG	Sidechain
4	SD	56	ARG	Sidechain
5	SE	112	ARG	Sidechain
9	SI	11	ARG	Sidechain
9	SI	123	ARG	Sidechain

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Mol	Chain	Res	Type	Group
9	SI	40	GLY	Mainchain
10	SJ	16	ARG	Sidechain
10	SJ	48	ARG	Sidechain
12	SL	86	ARG	Sidechain
13	SM	113	ARG	Sidechain
13	SM	114	LYS	Peptide
13	SM	70	ARG	Sidechain
13	SM	87	ARG	Sidechain
14	SN	75	ARG	Sidechain
14	SN	85	ARG	Sidechain
17	SQ	40	ARG	Sidechain
17	SQ	6	ARG	Sidechain
17	SQ	65	ARG	Sidechain
19	SS	3	ARG	Sidechain
21	SU	7	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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 PDB entries followed by that with respect to all EM entries.

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	SB	222/241 (92%)	210 (95%)	12 (5%)	0	100	100
3	SC	209/233 (90%)	200 (96%)	9 (4%)	0	100	100
4	SD	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
5	SE	153/167 (92%)	150 (98%)	3 (2%)	0	100	100
6	SF	104/135 (77%)	101 (97%)	3 (3%)	0	100	100
7	SG	149/179 (83%)	141 (95%)	8 (5%)	0	100	100
8	SH	127/130 (98%)	126 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	SI	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
10	SJ	97/103 (94%)	91 (94%)	6 (6%)	0	100	100
11	SK	117/129 (91%)	111 (95%)	6 (5%)	0	100	100
12	SL	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
13	SM	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
14	SN	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
15	SO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	SP	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
17	SQ	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
18	SR	65/75 (87%)	60 (92%)	5 (8%)	0	100	100
19	SS	82/92 (89%)	75 (92%)	7 (8%)	0	100	100
20	ST	83/87 (95%)	83 (100%)	0	0	100	100
21	SU	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
25	LB	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
26	LC	207/209 (99%)	198 (96%)	8 (4%)	1 (0%)	25	34
27	LD	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
28	LE	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
29	LF	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
30	LI	146/149 (98%)	129 (88%)	17 (12%)	0	100	100
31	LJ	129/165 (78%)	121 (94%)	8 (6%)	0	100	100
32	LK	132/142 (93%)	121 (92%)	11 (8%)	0	100	100
33	LM	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
34	LN	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
35	LO	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
36	LP	133/136 (98%)	133 (100%)	0	0	100	100
37	LQ	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
38	LR	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
39	LS	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
40	LT	115/118 (98%)	115 (100%)	0	0	100	100
41	LU	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
42	LV	108/110 (98%)	101 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	LW	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
44	LX	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
45	LY	92/94 (98%)	92 (100%)	0	0	100	100
46	La	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
47	Lb	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
48	Lc	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
49	Ld	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	Le	66/70 (94%)	58 (88%)	8 (12%)	0	100	100
51	Lf	54/57 (95%)	54 (100%)	0	0	100	100
52	Lg	50/55 (91%)	49 (98%)	1 (2%)	0	100	100
53	Lh	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	Li	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
55	Lj	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
56	EF	702/704 (100%)	664 (95%)	38 (5%)	0	100	100
57	Pp	1/3 (33%)	1 (100%)	0	0	100	100
All	All	6575/6927 (95%)	6304 (96%)	270 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	LC	149	ASN

### 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 PDB entries followed by that with respect to all EM entries.

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	SB	186/199 (94%)	176 (95%)	10 (5%)	18	25
3	SC	172/190 (90%)	158 (92%)	14 (8%)	9	12
4	SD	172/173 (99%)	162 (94%)	10 (6%)	17	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	SE	118/126 (94%)	115 (98%)	3 (2%)	42	60
6	SF	92/116 (79%)	82 (89%)	10 (11%)	5	5
7	SG	124/147 (84%)	94 (76%)	30 (24%)	0	0
8	SH	104/105 (99%)	98 (94%)	6 (6%)	17	22
9	SI	105/107 (98%)	95 (90%)	10 (10%)	7	8
10	SJ	87/90 (97%)	72 (83%)	15 (17%)	1	1
11	SK	92/99 (93%)	87 (95%)	5 (5%)	18	25
12	SL	102/103 (99%)	95 (93%)	7 (7%)	13	16
13	SM	92/96 (96%)	79 (86%)	13 (14%)	3	2
14	SN	83/84 (99%)	66 (80%)	17 (20%)	1	1
15	SO	76/77 (99%)	69 (91%)	7 (9%)	7	9
16	SP	65/65 (100%)	62 (95%)	3 (5%)	23	33
17	SQ	74/78 (95%)	69 (93%)	5 (7%)	13	17
18	SR	58/65 (89%)	50 (86%)	8 (14%)	3	2
19	SS	72/79 (91%)	53 (74%)	19 (26%)	0	0
20	ST	65/66 (98%)	61 (94%)	4 (6%)	15	20
21	SU	60/61 (98%)	56 (93%)	4 (7%)	13	17
25	LB	216/218 (99%)	206 (95%)	10 (5%)	23	33
26	LC	164/164 (100%)	156 (95%)	8 (5%)	21	30
27	LD	165/165 (100%)	158 (96%)	7 (4%)	25	37
28	LE	148/150 (99%)	138 (93%)	10 (7%)	13	17
29	LF	137/138 (99%)	127 (93%)	10 (7%)	11	15
30	LI	113/114 (99%)	107 (95%)	6 (5%)	19	26
31	LJ	100/123 (81%)	85 (85%)	15 (15%)	2	2
32	LK	104/110 (94%)	87 (84%)	17 (16%)	2	1
33	LM	116/116 (100%)	109 (94%)	7 (6%)	16	21
34	LN	103/104 (99%)	101 (98%)	2 (2%)	52	70
35	LO	103/103 (100%)	97 (94%)	6 (6%)	17	22
36	LP	108/108 (100%)	102 (94%)	6 (6%)	17	24
37	LQ	100/103 (97%)	94 (94%)	6 (6%)	16	21
38	LR	86/87 (99%)	80 (93%)	6 (7%)	12	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	LS	99/100 (99%)	95 (96%)	4 (4%)	27	40
40	LT	89/90 (99%)	85 (96%)	4 (4%)	23	34
41	LU	84/84 (100%)	78 (93%)	6 (7%)	12	16
42	LV	93/93 (100%)	87 (94%)	6 (6%)	14	18
43	LW	80/84 (95%)	70 (88%)	10 (12%)	3	3
44	LX	83/85 (98%)	78 (94%)	5 (6%)	16	21
45	LY	78/78 (100%)	72 (92%)	6 (8%)	10	13
46	La	58/63 (92%)	56 (97%)	2 (3%)	32	47
47	Lb	67/68 (98%)	64 (96%)	3 (4%)	23	34
48	Lc	54/55 (98%)	53 (98%)	1 (2%)	52	70
49	Ld	48/49 (98%)	45 (94%)	3 (6%)	15	19
50	Le	60/62 (97%)	48 (80%)	12 (20%)	1	1
51	Lf	47/48 (98%)	46 (98%)	1 (2%)	48	66
52	Lg	47/49 (96%)	42 (89%)	5 (11%)	5	6
53	Lh	38/38 (100%)	36 (95%)	2 (5%)	19	26
54	Li	51/52 (98%)	50 (98%)	1 (2%)	50	69
55	Lj	34/34 (100%)	34 (100%)	0	100	100
56	EF	561/578 (97%)	522 (93%)	39 (7%)	12	16
57	Pp	3/3 (100%)	1 (33%)	2 (67%)	0	0
All	All	5436/5642 (96%)	5008 (92%)	428 (8%)	13	13

All (428) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	22	TYR
2	SB	50	PHE
2	SB	82	ASP
2	SB	87	CYS
2	SB	105	LYS
2	SB	108	ARG
2	SB	123	ASP
2	SB	129	LEU
2	SB	141	LEU
2	SB	161	LEU
3	SC	20	SER

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Mol	Chain	Res	Type
3	SC	45	LYS
3	SC	58	GLU
3	SC	63	SER
3	SC	82	GLU
3	SC	89	LYS
3	SC	110	GLU
3	SC	115	LEU
3	SC	118	ASP
3	SC	127	ARG
3	SC	135	LYS
3	SC	185	ASN
3	SC	192	THR
3	SC	211	MET
4	SD	45	LYS
4	SD	73	ARG
4	SD	78	GLU
4	SD	124	MET
4	SD	138	SER
4	SD	151	LYS
4	SD	152	GLN
4	SD	167	LYS
4	SD	191	LEU
4	SD	192	SER
5	SE	130	SER
5	SE	159	LYS
5	SE	164	ILE
6	SF	1	MET
6	SF	2	ARG
6	SF	16	GLU
6	SF	23	GLU
6	SF	41	ASP
6	SF	53	LYS
6	SF	62	MET
6	SF	68	GLN
6	SF	72	ASP
6	SF	102	MET
7	SG	4	ARG
7	SG	15	ASP
7	SG	21	GLU
7	SG	22	LEU
7	SG	26	PHE
7	SG	40	GLU

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Mol	Chain	Res	Type
7	SG	53	ARG
7	SG	56	LYS
7	SG	58	GLU
7	SG	60	GLU
7	SG	62	PHE
7	SG	63	GLU
7	SG	78	ARG
7	SG	84	THR
7	SG	85	TYR
7	SG	89	VAL
7	SG	90	GLU
7	SG	106	GLU
7	SG	110	LYS
7	SG	111	ARG
7	SG	113	ASP
7	SG	114	LYS
7	SG	115	SER
7	SG	116	MET
7	SG	119	ARG
7	SG	137	LYS
7	SG	138	ARG
7	SG	143	ARG
7	SG	144	MET
7	SG	149	LYS
8	SH	41	LYS
8	SH	54	ASP
8	SH	67	GLN
8	SH	105	SER
8	SH	107	SER
8	SH	114	ARG
9	SI	9	THR
9	SI	19	VAL
9	SI	46	MET
9	SI	61	LEU
9	SI	65	ILE
9	SI	85	ARG
9	SI	98	LEU
9	SI	107	ASP
9	SI	109	ARG
9	SI	115	LYS
10	SJ	7	ARG
10	SJ	15	HIS

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Mol	Chain	Res	Type
10	SJ	22	THR
10	SJ	30	LYS
10	SJ	31	ARG
10	SJ	45	ARG
10	SJ	51	VAL
10	SJ	52	LEU
10	SJ	62	ARG
10	SJ	63	ASP
10	SJ	78	GLU
10	SJ	80	THR
10	SJ	81	GLU
10	SJ	88	MET
10	SJ	90	LEU
11	SK	13	ARG
11	SK	14	LYS
11	SK	42	LEU
11	SK	59	THR
11	SK	82	LEU
12	SL	19	SER
12	SL	21	VAL
12	SL	54	ARG
12	SL	56	ARG
12	SL	76	GLU
12	SL	110	ARG
12	SL	123	LYS
13	SM	3	ARG
13	SM	7	ILE
13	SM	8	ASN
13	SM	16	VAL
13	SM	30	SER
13	SM	41	GLU
13	SM	47	GLU
13	SM	73	ILE
13	SM	74	SER
13	SM	79	ARG
13	SM	98	ARG
13	SM	113	ARG
13	SM	114	LYS
14	SN	9	ARG
14	SN	10	GLU
14	SN	12	LYS
14	SN	19	LYS

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Mol	Chain	Res	Type
14	SN	23	LYS
14	SN	24	ARG
14	SN	38	ASP
14	SN	41	ARG
14	SN	42	TRP
14	SN	48	LEU
14	SN	51	LEU
14	SN	58	SER
14	SN	61	ARG
14	SN	81	ARG
14	SN	85	ARG
14	SN	86	GLU
14	SN	89	MET
15	SO	18	ASP
15	SO	48	LYS
15	SO	68	ASP
15	SO	83	GLU
15	SO	84	ARG
15	SO	88	ARG
15	SO	89	ARG
16	SP	8	ARG
16	SP	50	THR
16	SP	76	LYS
17	SQ	7	THR
17	SQ	28	PHE
17	SQ	75	LEU
17	SQ	77	ARG
17	SQ	83	VAL
18	SR	10	PHE
18	SR	11	CYS
18	SR	14	THR
18	SR	19	GLN
18	SR	43	ARG
18	SR	48	ARG
18	SR	73	ARG
18	SR	74	HIS
19	SS	3	ARG
19	SS	11	ILE
19	SS	12	ASP
19	SS	15	LEU
19	SS	18	LYS
19	SS	20	GLU

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Mol	Chain	Res	Type
19	SS	21	LYS
19	SS	23	VAL
19	SS	24	GLU
19	SS	29	LYS
19	SS	36	ARG
19	SS	43	ASN
19	SS	45	ILE
19	SS	60	VAL
19	SS	62	VAL
19	SS	65	GLU
19	SS	67	VAL
19	SS	81	ARG
19	SS	83	HIS
20	ST	4	ILE
20	ST	10	ARG
20	ST	23	SER
20	ST	43	ASP
21	SU	13	ASP
21	SU	20	LYS
21	SU	21	ARG
21	SU	62	ARG
25	LB	37	ASN
25	LB	71	LYS
25	LB	98	ASP
25	LB	118	SER
25	LB	133	ARG
25	LB	167	ARG
25	LB	252	THR
25	LB	259	SER
25	LB	264	ASP
25	LB	265	LYS
26	LC	17	GLU
26	LC	21	SER
26	LC	32	ASN
26	LC	33	ARG
26	LC	165	MET
26	LC	175	LEU
26	LC	184	ARG
26	LC	197	THR
27	LD	6	LYS
27	LD	16	GLU
27	LD	49	ARG

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Mol	Chain	Res	Type
27	LD	69	ARG
27	LD	154	ASP
27	LD	166	LYS
27	LD	191	ASP
28	LE	17	MET
28	LE	23	ASN
28	LE	115	ARG
28	LE	117	LEU
28	LE	120	LYS
28	LE	123	ASP
28	LE	134	GLU
28	LE	153	ASP
28	LE	167	ARG
28	LE	175	PHE
29	LF	16	ASP
29	LF	32	GLU
29	LF	35	ARG
29	LF	50	LEU
29	LF	56	ASP
29	LF	60	ASP
29	LF	95	ARG
29	LF	99	LYS
29	LF	124	GLU
29	LF	134	LYS
30	LI	15	LEU
30	LI	40	THR
30	LI	45	GLU
30	LI	50	ARG
30	LI	82	SER
30	LI	147	VAL
31	LJ	36	ASP
31	LJ	43	LYS
31	LJ	54	VAL
31	LJ	65	GLU
31	LJ	67	THR
31	LJ	71	CYS
31	LJ	85	SER
31	LJ	87	GLU
31	LJ	95	LEU
31	LJ	101	LYS
31	LJ	105	LYS
31	LJ	113	PHE

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Mol	Chain	Res	Type
31	LJ	116	GLU
31	LJ	117	LEU
31	LJ	125	ARG
32	LK	28	LEU
32	LK	59	ILE
32	LK	79	LEU
32	LK	81	LYS
32	LK	87	LYS
32	LK	90	SER
32	LK	95	LYS
32	LK	97	LYS
32	LK	100	LYS
32	LK	102	SER
32	LK	113	LYS
32	LK	121	ASP
32	LK	132	THR
32	LK	135	SER
32	LK	136	MET
32	LK	139	VAL
32	LK	141	GLU
33	LM	7	LYS
33	LM	37	ARG
33	LM	39	LYS
33	LM	60	ASP
33	LM	95	ARG
33	LM	96	ARG
33	LM	141	ASP
34	LN	110	GLU
34	LN	114	LYS
35	LO	42	SER
35	LO	67	THR
35	LO	70	LYS
35	LO	73	ILE
35	LO	89	VAL
35	LO	121	THR
36	LP	1	MET
36	LP	3	GLN
36	LP	6	ARG
36	LP	58	LYS
36	LP	102	LEU
36	LP	123	LYS
37	LQ	2	ARG

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Mol	Chain	Res	Type
37	LQ	14	SER
37	LQ	15	SER
37	LQ	27	SER
37	LQ	57	THR
37	LQ	89	SER
38	LR	33	ARG
38	LR	63	LYS
38	LR	65	THR
38	LR	89	ASP
38	LR	91	SER
38	LR	94	ARG
39	LS	2	SER
39	LS	12	GLN
39	LS	37	LYS
39	LS	39	ARG
40	LT	13	ARG
40	LT	51	ARG
40	LT	75	SER
40	LT	112	LYS
41	LU	6	GLN
41	LU	46	GLU
41	LU	51	VAL
41	LU	62	GLU
41	LU	71	LYS
41	LU	79	ARG
42	LV	59	GLU
42	LV	65	ASP
42	LV	70	LYS
42	LV	95	ARG
42	LV	101	SER
42	LV	108	SER
43	LW	3	ARG
43	LW	6	ARG
43	LW	17	SER
43	LW	37	ASP
43	LW	48	GLN
43	LW	49	LYS
43	LW	72	GLN
43	LW	73	ARG
43	LW	88	LYS
43	LW	89	GLU
44	LX	7	ARG

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Mol	Chain	Res	Type
44	LX	49	VAL
44	LX	68	SER
44	LX	81	ASP
44	LX	98	SER
45	LY	24	ASN
45	LY	25	LYS
45	LY	43	ASP
45	LY	68	LYS
45	LY	71	LYS
45	LY	87	GLN
46	La	10	THR
46	La	58	THR
47	Lb	41	GLU
47	Lb	42	SER
47	Lb	70	GLU
48	Lc	58	ASN
49	Ld	5	ILE
49	Ld	11	ARG
49	Ld	45	ARG
50	Le	4	ASP
50	Le	5	ILE
50	Le	25	ARG
50	Le	32	LEU
50	Le	35	ASP
50	Le	49	ARG
50	Le	50	ASP
50	Le	51	VAL
50	Le	57	VAL
50	Le	58	ASP
50	Le	59	ARG
50	Le	64	PHE
51	Lf	10	ARG
52	Lg	7	GLU
52	Lg	25	LYS
52	Lg	30	LYS
52	Lg	44	ARG
52	Lg	50	LYS
53	Lh	8	SER
53	Lh	25	LYS
54	Li	31	HIS
56	EF	40	ILE
56	EF	55	GLN

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Mol	Chain	Res	Type
56	EF	78	GLN
56	EF	79	TYR
56	EF	161	ARG
56	EF	169	LEU
56	EF	176	GLU
56	EF	178	HIS
56	EF	183	VAL
56	EF	202	PHE
56	EF	210	ASP
56	EF	213	GLU
56	EF	219	HIS
56	EF	221	ASN
56	EF	241	GLU
56	EF	242	GLU
56	EF	244	THR
56	EF	337	ARG
56	EF	352	SER
56	EF	357	ARG
56	EF	358	GLU
56	EF	370	LYS
56	EF	373	GLU
56	EF	390	ASP
56	EF	409	MET
56	EF	446	ARG
56	EF	450	ASP
56	EF	451	GLU
56	EF	457	ILE
56	EF	467	ASP
56	EF	488	VAL
56	EF	496	GLN
56	EF	498	VAL
56	EF	532	LYS
56	EF	583	TYR
56	EF	606	LYS
56	EF	617	MET
56	EF	626	GLU
56	EF	669	GLN
57	Pp	1	MET
57	Pp	3	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
6	SF	68	GLN
7	SG	9	GLN
7	SG	122	ASN
9	SI	50	GLN
9	SI	126	GLN
10	SJ	58	ASN
12	SL	77	HIS
14	SN	35	ASN
19	SS	43	ASN
25	LB	53	HIS
25	LB	90	ASN
29	LF	48	ASN
29	LF	143	GLN
31	LJ	103	ASN
32	LK	31	GLN
32	LK	94	ASN
33	LM	135	GLN
37	LQ	62	ASN
39	LS	66	ASN
42	LV	15	GLN
45	LY	24	ASN
45	LY	51	GLN
48	Lc	36	GLN
50	Le	6	HIS
56	EF	55	GLN
56	EF	78	GLN
56	EF	530	ASN
56	EF	558	GLN
56	EF	560	GLN
56	EF	645	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1530/1534 (99%)	234 (15%)	10 (0%)
22	mR	11/60 (18%)	2 (18%)	0
23	23	2899/2904 (99%)	517 (17%)	28 (0%)
24	5	119/120 (99%)	15 (12%)	1 (0%)
58	Pt	73/106 (68%)	12 (16%)	0
59	Dt	73/106 (68%)	15 (20%)	0
All	All	4705/4830 (97%)	795 (16%)	39 (0%)

All (795) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	2	A
1	16	4	U
1	16	7	A
1	16	9	G
1	16	22	G
1	16	32	A
1	16	39	G
1	16	47	C
1	16	48	C
1	16	50	A
1	16	51	A
1	16	70	U
1	16	71	A
1	16	72	A
1	16	74	A
1	16	77	A
1	16	78	A
1	16	80	A
1	16	81	A
1	16	83	C
1	16	84	U
1	16	85	U
1	16	86	G
1	16	87	C
1	16	88	U
1	16	89	U
1	16	90	C
1	16	91	U
1	16	97	G
1	16	108	G
1	16	121	U
1	16	130	A
1	16	131	A
1	16	141	G
1	16	143	A
1	16	144	G
1	16	159	G
1	16	163	C
1	16	177	G
1	16	182	A
1	16	183	C
1	16	188	C
1	16	189	A

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Mol	Chain	Res	Type
1	16	197	A
1	16	204	G
1	16	205	A
1	16	206	C
1	16	207	C
1	16	210	C
1	16	215	C
1	16	226	G
1	16	240	G
1	16	247	G
1	16	251	G
1	16	266	G
1	16	267	C
1	16	281	G
1	16	282	A
1	16	289	G
1	16	306	A
1	16	321	A
1	16	328	C
1	16	329	A
1	16	330	C
1	16	332	G
1	16	352	C
1	16	354	G
1	16	356	A
1	16	367	U
1	16	372	C
1	16	376	G
1	16	398	U
1	16	406	G
1	16	411	A
1	16	412	A
1	16	413	G
1	16	421	U
1	16	422	C
1	16	423	G
1	16	424	G
1	16	429	U
1	16	439	U
1	16	456	A
1	16	457	G
1	16	458	U

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Mol	Chain	Res	Type
1	16	465	A
1	16	466	A
1	16	467	U
1	16	468	A
1	16	481	G
1	16	484	G
1	16	486	U
1	16	491	G
1	16	495	A
1	16	496	A
1	16	497	G
1	16	509	A
1	16	510	A
1	16	511	C
1	16	518	C
1	16	521	G
1	16	527	7MG
1	16	530	G
1	16	531	U
1	16	533	A
1	16	547	A
1	16	559	A
1	16	562	U
1	16	564	C
1	16	572	A
1	16	573	A
1	16	576	C
1	16	577	G
1	16	596	A
1	16	632	U
1	16	642	A
1	16	650	G
1	16	653	U
1	16	665	A
1	16	666	G
1	16	686	U
1	16	703	G
1	16	721	G
1	16	723	U
1	16	734	G
1	16	755	G
1	16	777	A

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Mol	Chain	Res	Type
1	16	790	A
1	16	793	U
1	16	794	A
1	16	814	A
1	16	815	A
1	16	817	C
1	16	821	G
1	16	828	U
1	16	829	G
1	16	832	G
1	16	836	G
1	16	841	C
1	16	842	U
1	16	843	U
1	16	844	G
1	16	845	A
1	16	846	G
1	16	848	C
1	16	876	C
1	16	902	G
1	16	914	A
1	16	926	G
1	16	927	G
1	16	934	C
1	16	935	A
1	16	958	A
1	16	960	U
1	16	969	A
1	16	971	G
1	16	975	A
1	16	976	G
1	16	977	A
1	16	982	U
1	16	987	G
1	16	992	U
1	16	993	G
1	16	1004	A
1	16	1015	G
1	16	1020	G
1	16	1021	A
1	16	1027	C
1	16	1029	U

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Mol	Chain	Res	Type
1	16	1030	U
1	16	1031	C
1	16	1043	G
1	16	1044	A
1	16	1055	A
1	16	1064	G
1	16	1065	U
1	16	1070	U
1	16	1085	U
1	16	1091	U
1	16	1092	A
1	16	1094	G
1	16	1095	U
1	16	1101	A
1	16	1108	G
1	16	1136	C
1	16	1139	G
1	16	1152	A
1	16	1154	G
1	16	1157	A
1	16	1158	C
1	16	1159	U
1	16	1167	A
1	16	1168	U
1	16	1184	G
1	16	1196	A
1	16	1197	A
1	16	1200	C
1	16	1213	A
1	16	1214	C
1	16	1225	A
1	16	1226	C
1	16	1227	A
1	16	1236	A
1	16	1238	A
1	16	1241	G
1	16	1257	A
1	16	1258	G
1	16	1260	G
1	16	1280	A
1	16	1281	C
1	16	1285	A

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Mol	Chain	Res	Type
1	16	1286	U
1	16	1287	A
1	16	1298	U
1	16	1299	A
1	16	1302	C
1	16	1305	G
1	16	1320	C
1	16	1363	A
1	16	1364	U
1	16	1379	G
1	16	1381	U
1	16	1383	C
1	16	1397	C
1	16	1398	A
1	16	1441	A
1	16	1446	A
1	16	1449	C
1	16	1499	A
1	16	1503	A
1	16	1506	U
1	16	1517	G
1	16	1529	G
1	16	1530	G
22	mR	39	G
22	mR	48	C
23	23	3	U
23	23	6	A
23	23	10	A
23	23	14	A
23	23	15	G
23	23	27	G
23	23	44	A
23	23	46	G
23	23	51	G
23	23	55	G
23	23	71	A
23	23	74	A
23	23	75	G
23	23	84	A
23	23	96	C
23	23	101	A
23	23	102	U

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Mol	Chain	Res	Type
23	23	103	A
23	23	110	G
23	23	112	U
23	23	118	A
23	23	119	A
23	23	120	U
23	23	125	A
23	23	135	U
23	23	139	U
23	23	140	C
23	23	141	G
23	23	142	A
23	23	159	G
23	23	163	C
23	23	174	U
23	23	178	G
23	23	181	A
23	23	196	A
23	23	199	A
23	23	215	G
23	23	216	A
23	23	222	A
23	23	248	G
23	23	252	G
23	23	265	A
23	23	266	G
23	23	267	C
23	23	271	G
23	23	272	A
23	23	275	C
23	23	277	G
23	23	278	A
23	23	279	A
23	23	281	C
23	23	282	A
23	23	283	G
23	23	284	U
23	23	285	G
23	23	286	U
23	23	291	G
23	23	311	A
23	23	330	A

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Mol	Chain	Res	Type
23	23	345	A
23	23	353	C
23	23	359	G
23	23	360	U
23	23	361	G
23	23	369	U
23	23	371	A
23	23	372	G
23	23	386	G
23	23	387	U
23	23	388	G
23	23	395	U
23	23	396	G
23	23	401	A
23	23	404	A
23	23	405	U
23	23	406	G
23	23	412	A
23	23	455	C
23	23	456	C
23	23	457	A
23	23	459	U
23	23	467	G
23	23	470	A
23	23	473	G
23	23	481	G
23	23	491	G
23	23	504	A
23	23	505	A
23	23	506	G
23	23	509	C
23	23	527	C
23	23	529	A
23	23	530	G
23	23	531	C
23	23	532	A
23	23	546	U
23	23	547	A
23	23	548	G
23	23	549	G
23	23	550	C
23	23	563	A

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Mol	Chain	Res	Type
23	23	573	U
23	23	575	A
23	23	603	A
23	23	614	A
23	23	615	U
23	23	637	A
23	23	645	C
23	23	646	U
23	23	647	G
23	23	654	A
23	23	655	A
23	23	684	G
23	23	686	U
23	23	704	G
23	23	719	C
23	23	724	U
23	23	725	G
23	23	726	G
23	23	727	A
23	23	730	A
23	23	740	C
23	23	747	5MU
23	23	765	C
23	23	775	G
23	23	776	G
23	23	782	A
23	23	784	G
23	23	785	G
23	23	789	A
23	23	805	G
23	23	811	U
23	23	812	C
23	23	819	A
23	23	827	U
23	23	830	G
23	23	845	A
23	23	846	U
23	23	859	G
23	23	869	G
23	23	888	C
23	23	889	C
23	23	890	C

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Mol	Chain	Res	Type
23	23	895	U
23	23	896	A
23	23	897	C
23	23	907	G
23	23	910	A
23	23	917	A
23	23	931	U
23	23	932	U
23	23	934	U
23	23	941	A
23	23	946	C
23	23	953	G
23	23	961	C
23	23	973	A
23	23	974	G
23	23	980	A
23	23	983	A
23	23	989	G
23	23	996	A
23	23	999	U
23	23	1009	A
23	23	1012	U
23	23	1013	C
23	23	1026	G
23	23	1033	U
23	23	1041	G
23	23	1046	A
23	23	1047	G
23	23	1057	A
23	23	1058	U
23	23	1060	U
23	23	1061	U
23	23	1062	G
23	23	1070	A
23	23	1077	A
23	23	1079	C
23	23	1080	A
23	23	1084	A
23	23	1085	A
23	23	1087	G
23	23	1088	A
23	23	1089	A

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Mol	Chain	Res	Type
23	23	1110	G
23	23	1112	G
23	23	1114	C
23	23	1116	G
23	23	1132	U
23	23	1133	A
23	23	1134	A
23	23	1135	C
23	23	1136	G
23	23	1142	A
23	23	1149	G
23	23	1170	C
23	23	1171	G
23	23	1173	U
23	23	1174	U
23	23	1175	A
23	23	1178	C
23	23	1179	G
23	23	1180	U
23	23	1206	G
23	23	1212	G
23	23	1236	G
23	23	1238	G
23	23	1247	A
23	23	1249	U
23	23	1253	A
23	23	1256	G
23	23	1266	G
23	23	1271	G
23	23	1272	A
23	23	1273	U
23	23	1300	G
23	23	1301	A
23	23	1314	C
23	23	1321	A
23	23	1329	U
23	23	1352	U
23	23	1365	A
23	23	1368	G
23	23	1378	A
23	23	1379	U
23	23	1382	G

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Mol	Chain	Res	Type
23	23	1383	A
23	23	1396	U
23	23	1416	G
23	23	1417	C
23	23	1419	A
23	23	1420	A
23	23	1428	C
23	23	1434	A
23	23	1437	C
23	23	1451	C
23	23	1452	G
23	23	1453	A
23	23	1458	U
23	23	1460	U
23	23	1461	C
23	23	1482	G
23	23	1486	U
23	23	1493	C
23	23	1494	A
23	23	1497	U
23	23	1502	A
23	23	1503	A
23	23	1509	A
23	23	1524	G
23	23	1529	G
23	23	1534	U
23	23	1535	A
23	23	1537	G
23	23	1538	G
23	23	1558	C
23	23	1566	A
23	23	1569	A
23	23	1570	A
23	23	1571	A
23	23	1578	U
23	23	1579	A
23	23	1580	A
23	23	1581	G
23	23	1583	A
23	23	1584	U
23	23	1585	C
23	23	1603	A

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Mol	Chain	Res	Type
23	23	1608	A
23	23	1610	A
23	23	1646	C
23	23	1647	U
23	23	1648	U
23	23	1649	G
23	23	1674	G
23	23	1690	A
23	23	1715	G
23	23	1724	G
23	23	1725	U
23	23	1727	C
23	23	1729	U
23	23	1730	C
23	23	1731	G
23	23	1732	C
23	23	1737	G
23	23	1738	G
23	23	1745	A
23	23	1757	A
23	23	1764	C
23	23	1773	A
23	23	1776	G
23	23	1782	U
23	23	1784	A
23	23	1799	G
23	23	1800	C
23	23	1801	A
23	23	1807	G
23	23	1808	A
23	23	1816	C
23	23	1829	A
23	23	1833	C
23	23	1841	U
23	23	1842	G
23	23	1847	A
23	23	1848	A
23	23	1858	A
23	23	1864	U
23	23	1866	A
23	23	1867	G
23	23	1868	C

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Mol	Chain	Res	Type
23	23	1870	C
23	23	1872	A
23	23	1873	G
23	23	1874	C
23	23	1875	G
23	23	1876	A
23	23	1877	A
23	23	1901	A
23	23	1906	G
23	23	1912	A
23	23	1913	A
23	23	1914	C
23	23	1919	A
23	23	1925	C
23	23	1927	A
23	23	1930	G
23	23	1931	U
23	23	1938	A
23	23	1940	U
23	23	1941	C
23	23	1954	G
23	23	1955	U
23	23	1960	A
23	23	1964	G
23	23	1967	C
23	23	1970	A
23	23	1971	U
23	23	1972	G
23	23	1975	G
23	23	1982	U
23	23	1991	U
23	23	1992	G
23	23	1993	U
23	23	1997	C
23	23	2002	G
23	23	2020	A
23	23	2022	U
23	23	2023	C
23	23	2031	A
23	23	2032	G
23	23	2033	A
23	23	2043	C

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Mol	Chain	Res	Type
23	23	2055	C
23	23	2056	G
23	23	2060	A
23	23	2061	G
23	23	2062	A
23	23	2069	7MG
23	23	2093	G
23	23	2113	U
23	23	2116	G
23	23	2117	A
23	23	2118	U
23	23	2126	A
23	23	2131	U
23	23	2132	U
23	23	2133	G
23	23	2136	G
23	23	2141	G
23	23	2145	C
23	23	2146	C
23	23	2161	C
23	23	2162	G
23	23	2163	A
23	23	2164	C
23	23	2165	C
23	23	2170	A
23	23	2171	A
23	23	2172	U
23	23	2173	A
23	23	2174	C
23	23	2198	A
23	23	2204	G
23	23	2211	A
23	23	2220	U
23	23	2225	A
23	23	2238	G
23	23	2239	G
23	23	2243	U
23	23	2251	OMG
23	23	2278	A
23	23	2283	C
23	23	2287	A
23	23	2288	A

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Mol	Chain	Res	Type
23	23	2303	G
23	23	2304	G
23	23	2305	U
23	23	2306	C
23	23	2307	G
23	23	2308	G
23	23	2309	A
23	23	2311	A
23	23	2312	U
23	23	2319	G
23	23	2320	U
23	23	2321	U
23	23	2322	A
23	23	2325	G
23	23	2333	A
23	23	2334	U
23	23	2336	A
23	23	2347	C
23	23	2350	C
23	23	2354	C
23	23	2357	G
23	23	2361	G
23	23	2372	U
23	23	2376	A
23	23	2379	G
23	23	2380	C
23	23	2383	G
23	23	2385	C
23	23	2391	G
23	23	2402	U
23	23	2403	C
23	23	2406	A
23	23	2407	A
23	23	2410	G
23	23	2423	U
23	23	2425	A
23	23	2427	C
23	23	2428	G
23	23	2429	G
23	23	2430	A
23	23	2441	U
23	23	2448	A

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Mol	Chain	Res	Type
23	23	2474	U
23	23	2475	C
23	23	2476	A
23	23	2480	C
23	23	2484	G
23	23	2491	U
23	23	2492	U
23	23	2494	G
23	23	2498	OMC
23	23	2502	G
23	23	2504	PSU
23	23	2505	G
23	23	2506	U
23	23	2518	A
23	23	2529	G
23	23	2535	G
23	23	2537	U
23	23	2547	A
23	23	2554	U
23	23	2566	A
23	23	2567	G
23	23	2572	A
23	23	2573	C
23	23	2576	G
23	23	2602	A
23	23	2606	C
23	23	2609	U
23	23	2613	U
23	23	2614	A
23	23	2615	U
23	23	2629	U
23	23	2630	G
23	23	2636	C
23	23	2639	A
23	23	2646	C
23	23	2663	G
23	23	2689	U
23	23	2690	U
23	23	2714	G
23	23	2718	G
23	23	2726	A
23	23	2732	G

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Mol	Chain	Res	Type
23	23	2733	A
23	23	2739	U
23	23	2744	G
23	23	2748	A
23	23	2752	C
23	23	2762	C
23	23	2765	A
23	23	2777	G
23	23	2778	A
23	23	2779	U
23	23	2790	U
23	23	2791	G
23	23	2797	U
23	23	2798	U
23	23	2799	A
23	23	2818	U
23	23	2820	A
23	23	2823	A
23	23	2832	U
23	23	2833	U
23	23	2835	A
23	23	2849	U
23	23	2850	A
23	23	2858	C
23	23	2859	G
23	23	2861	U
23	23	2872	A
23	23	2873	A
23	23	2879	A
23	23	2880	C
23	23	2883	A
23	23	2884	U
23	23	2885	G
23	23	2886	A
23	23	2891	U
23	23	2900	A
23	23	2901	C
23	23	2904	U
24	5	13	G
24	5	15	A
24	5	24	G
24	5	31	C

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Mol	Chain	Res	Type
24	5	35	C
24	5	36	C
24	5	41	G
24	5	51	G
24	5	67	G
24	5	87	U
24	5	88	C
24	5	89	U
24	5	90	C
24	5	99	A
24	5	109	A
58	Pt	4	U
58	Pt	16	U
58	Pt	17	U
58	Pt	19	G
58	Pt	27	G
58	Pt	28	U
58	Pt	29	U
58	Pt	46	7MG
58	Pt	48	C
58	Pt	50	C
58	Pt	70	C
58	Pt	76	A
59	Dt	8	4SU
59	Dt	14	A
59	Dt	16	U
59	Dt	17	U
59	Dt	18	G
59	Dt	20	G
59	Dt	21	A
59	Dt	22	G
59	Dt	44	G
59	Dt	46	7MG
59	Dt	48	C
59	Dt	49	C
59	Dt	69	G
59	Dt	73	A
59	Dt	76	A

All (39) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	16	250	A
1	16	251	G
1	16	281	G
1	16	496	A
1	16	532	A
1	16	653	U
1	16	845	A
1	16	1157	A
1	16	1183	U
1	16	1397	C
23	23	43	G
23	23	134	G
23	23	158	U
23	23	277	G
23	23	352	A
23	23	369	U
23	23	395	U
23	23	404	A
23	23	405	U
23	23	784	G
23	23	1057	A
23	23	1060	U
23	23	1088	A
23	23	1089	A
23	23	1266	G
23	23	1416	G
23	23	1452	G
23	23	1486	U
23	23	1508	A
23	23	1570	A
23	23	1876	A
23	23	1980	G
23	23	2145	C
23	23	2311	A
23	23	2468	A
23	23	2536	G
23	23	2585	U
23	23	2858	C
24	5	15	A



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

47 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	2MG	16	966	1	18,26,27	2.43	7 (38%)	16,38,41	1.74	5 (31%)
23	H2U	23	2449	23	18,21,22	2.93	5 (27%)	19,30,33	1.53	4 (21%)
23	PSU	23	2604	23	18,21,22	4.13	7 (38%)	21,30,33	2.10	5 (23%)
1	5MC	16	1407	1	19,22,23	3.66	8 (42%)	26,32,35	1.03	2 (7%)
59	PSU	Dt	32	59	18,21,22	4.29	7 (38%)	21,30,33	2.07	5 (23%)
58	3AU	Pt	47	58	24,28,29	1.02	1 (4%)	30,40,43	1.51	4 (13%)
1	7MG	16	527	1	23,26,27	1.37	3 (13%)	27,39,42	2.65	7 (25%)
1	MA6	16	1518	1	19,26,27	1.66	3 (15%)	18,38,41	3.36	3 (16%)
23	7MG	23	2069	23	23,26,27	1.38	3 (13%)	27,39,42	2.67	6 (22%)
23	OMU	23	2552	23	19,22,23	2.88	8 (42%)	25,31,34	2.02	5 (20%)
59	7MG	Dt	46	59	23,26,27	3.43	10 (43%)	27,39,42	2.14	9 (33%)
23	1MG	23	745	23	19,26,27	3.12	6 (31%)	18,39,42	1.59	4 (22%)
1	4OC	16	1402	62,1	20,23,24	3.01	8 (40%)	25,32,35	0.93	1 (4%)
1	PSU	16	516	1	18,21,22	4.23	7 (38%)	21,30,33	1.92	5 (23%)
23	PSU	23	2504	23	18,21,22	4.17	7 (38%)	21,30,33	2.00	5 (23%)
59	PSU	Dt	39	59	18,21,22	4.27	7 (38%)	21,30,33	2.06	5 (23%)
59	3AU	Dt	47	59	24,28,29	1.06	1 (4%)	30,40,43	1.58	3 (10%)
12	D2T	SL	89	12	8,9,10	2.40	1 (12%)	6,11,13	2.29	2 (33%)
23	2MA	23	2503	62,23	17,25,26	2.35	5 (29%)	16,37,40	1.96	5 (31%)
1	MA6	16	1519	1	19,26,27	1.28	2 (10%)	18,38,41	2.65	8 (44%)
23	PSU	23	955	23	18,21,22	4.16	7 (38%)	21,30,33	2.19	5 (23%)
1	2MG	16	1516	1	18,26,27	2.47	7 (38%)	16,38,41	1.79	5 (31%)
58	T6A	Pt	37	58	26,34,35	1.90	7 (26%)	28,49,52	2.36	7 (25%)
1	5MC	16	967	1	19,22,23	3.66	8 (42%)	26,32,35	1.01	1 (3%)
23	OMC	23	2498	62,23	19,22,23	2.84	8 (42%)	25,31,34	0.79	0
23	PSU	23	1911	23	18,21,22	4.21	8 (44%)	21,30,33	1.89	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	5MU	23	1939	23	19,22,23	4.78	7 (36%)	27,32,35	3.81	9 (33%)
23	PSU	23	2605	23	18,21,22	4.20	8 (44%)	21,30,33	2.05	5 (23%)
23	PSU	23	2580	23	18,21,22	4.19	8 (44%)	21,30,33	2.11	6 (28%)
23	6MZ	23	1618	23	17,25,26	1.62	2 (11%)	15,36,39	3.26	5 (33%)
23	2MG	23	1835	23	18,26,27	2.36	7 (38%)	16,38,41	1.87	5 (31%)
23	6MZ	23	2030	23	17,25,26	1.72	3 (17%)	15,36,39	3.56	4 (26%)
23	OMG	23	2251	58,23	19,26,27	2.31	8 (42%)	21,38,41	1.49	4 (19%)
23	2MG	23	2445	23	18,26,27	2.36	7 (38%)	16,38,41	1.96	5 (31%)
59	PSU	Dt	55	59	18,21,22	4.43	7 (38%)	21,30,33	2.09	5 (23%)
58	PSU	Pt	39	58	18,21,22	4.32	7 (38%)	21,30,33	2.09	5 (23%)
36	4D4	LP	81	36	9,11,12	2.57	3 (33%)	7,13,15	0.93	0
59	4SU	Dt	8	59	18,21,22	4.29	8 (44%)	25,30,33	2.40	5 (20%)
23	PSU	23	2457	23	18,21,22	4.17	8 (44%)	21,30,33	2.33	5 (23%)
23	PSU	23	746	62,23	18,21,22	4.21	7 (38%)	21,30,33	1.84	5 (23%)
23	5MC	23	1962	23	19,22,23	3.64	8 (42%)	26,32,35	0.97	1 (3%)
59	MIA	Dt	37	59	24,31,32	2.28	3 (12%)	22,44,47	2.58	7 (31%)
1	UR3	16	1498	1	19,22,23	2.75	7 (36%)	26,32,35	1.61	3 (11%)
23	3TD	23	1915	23	19,22,23	4.34	6 (31%)	23,32,35	1.87	3 (13%)
58	U8U	Pt	34	22,58	20,24,25	1.63	4 (20%)	22,34,37	1.12	4 (18%)
23	5MU	23	747	23	19,22,23	4.78	7 (36%)	27,32,35	3.72	10 (37%)
58	7MG	Pt	46	58	23,26,27	3.53	10 (43%)	27,39,42	2.25	9 (33%)

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	2MG	16	966	1	-	0/5/27/28	0/3/3/3
23	H2U	23	2449	23	-	1/7/38/39	0/2/2/2
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
59	PSU	Dt	32	59	-	0/7/25/26	0/2/2/2
58	3AU	Pt	47	58	-	10/16/34/35	0/2/2/2
1	7MG	16	527	1	-	3/7/37/38	0/3/3/3
1	MA6	16	1518	1	-	0/7/29/30	0/3/3/3
23	7MG	23	2069	23	-	0/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	OMU	23	2552	23	-	0/9/27/28	0/2/2/2
59	7MG	Dt	46	59	-	2/7/37/38	0/3/3/3
23	1MG	23	745	23	-	0/3/25/26	0/3/3/3
1	4OC	16	1402	62,1	-	1/9/29/30	0/2/2/2
1	PSU	16	516	1	-	0/7/25/26	0/2/2/2
23	PSU	23	2504	23	-	0/7/25/26	0/2/2/2
59	PSU	Dt	39	59	-	0/7/25/26	0/2/2/2
59	3AU	Dt	47	59	-	9/16/34/35	0/2/2/2
12	D2T	SL	89	12	-	1/7/12/14	-
23	2MA	23	2503	62,23	-	2/3/25/26	0/3/3/3
1	MA6	16	1519	1	-	5/7/29/30	0/3/3/3
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
1	2MG	16	1516	1	-	0/5/27/28	0/3/3/3
58	T6A	Pt	37	58	-	10/19/41/42	0/3/3/3
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
23	OMC	23	2498	62,23	-	2/9/27/28	0/2/2/2
23	PSU	23	1911	23	-	2/7/25/26	0/2/2/2
23	5MU	23	1939	23	-	0/7/25/26	0/2/2/2
23	PSU	23	2605	23	-	0/7/25/26	0/2/2/2
23	PSU	23	2580	23	-	1/7/25/26	0/2/2/2
23	6MZ	23	1618	23	-	4/5/27/28	0/3/3/3
23	2MG	23	1835	23	-	2/5/27/28	0/3/3/3
23	6MZ	23	2030	23	-	2/5/27/28	0/3/3/3
23	OMG	23	2251	58,23	-	3/5/27/28	0/3/3/3
23	2MG	23	2445	23	-	0/5/27/28	0/3/3/3
59	PSU	Dt	55	59	-	0/7/25/26	0/2/2/2
58	PSU	Pt	39	58	-	0/7/25/26	0/2/2/2
36	4D4	LP	81	36	-	1/11/12/14	-
59	4SU	Dt	8	59	-	0/7/25/26	0/2/2/2
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
23	PSU	23	746	62,23	-	2/7/25/26	0/2/2/2
23	5MC	23	1962	23	-	2/7/25/26	0/2/2/2
59	MIA	Dt	37	59	-	6/11/33/34	0/3/3/3
1	UR3	16	1498	1	-	2/7/25/26	0/2/2/2
23	3TD	23	1915	23	-	2/7/25/26	0/2/2/2
58	U8U	Pt	34	22,58	-	2/10/28/29	0/2/2/2
23	5MU	23	747	23	-	1/7/25/26	0/2/2/2
58	7MG	Pt	46	58	-	4/7/37/38	0/3/3/3

All (286) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	1915	3TD	C6-C5	13.19	1.49	1.35
59	Dt	55	PSU	C6-C5	11.60	1.48	1.35
58	Pt	39	PSU	C6-C5	11.39	1.47	1.35
59	Dt	39	PSU	C6-C5	11.24	1.47	1.35
59	Dt	32	PSU	C6-C5	11.24	1.47	1.35
23	23	2504	PSU	C6-C5	11.14	1.47	1.35
23	23	1911	PSU	C6-C5	11.12	1.47	1.35
23	23	2605	PSU	C6-C5	11.07	1.47	1.35
1	16	516	PSU	C6-C5	11.06	1.47	1.35
23	23	2457	PSU	C6-C5	11.04	1.47	1.35
23	23	2580	PSU	C6-C5	11.04	1.47	1.35
23	23	746	PSU	C6-C5	10.87	1.47	1.35
23	23	955	PSU	C6-C5	10.84	1.47	1.35
23	23	2604	PSU	C6-C5	10.74	1.47	1.35
23	23	747	5MU	C2-N1	10.72	1.55	1.38
23	23	1939	5MU	C2-N1	10.67	1.55	1.38
23	23	747	5MU	C6-N1	10.45	1.55	1.38
23	23	1939	5MU	C6-N1	10.38	1.55	1.38
23	23	1915	3TD	C2-N1	10.34	1.49	1.37
59	Dt	55	PSU	C2-N1	10.07	1.49	1.36
59	Dt	32	PSU	C2-N1	9.74	1.49	1.36
23	23	747	5MU	C4-C5	9.70	1.60	1.44
58	Pt	39	PSU	C2-N1	9.68	1.49	1.36
23	23	1939	5MU	C4-C5	9.63	1.60	1.44
23	23	746	PSU	C2-N1	9.54	1.49	1.36
59	Dt	39	PSU	C2-N1	9.52	1.49	1.36
23	23	955	PSU	C2-N1	9.50	1.49	1.36
23	23	2605	PSU	C2-N1	9.37	1.48	1.36
23	23	1911	PSU	C2-N1	9.36	1.48	1.36
1	16	516	PSU	C2-N1	9.36	1.48	1.36
23	23	2604	PSU	C2-N1	9.31	1.48	1.36
23	23	2457	PSU	C2-N1	9.28	1.48	1.36
23	23	2580	PSU	C2-N1	9.23	1.48	1.36
23	23	2504	PSU	C2-N1	9.08	1.48	1.36
59	Dt	8	4SU	C2-N1	9.04	1.52	1.38
1	16	1407	5MC	C6-C5	8.86	1.49	1.34
1	16	967	5MC	C6-C5	8.85	1.49	1.34
23	23	2449	H2U	C2-N1	8.79	1.47	1.35
23	23	1962	5MC	C6-C5	8.77	1.48	1.34
23	23	745	1MG	C2-N2	8.64	1.49	1.34
58	Pt	46	7MG	C8-N9	8.48	1.51	1.45
59	Dt	8	4SU	C4-N3	8.39	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	Dt	46	7MG	C8-N9	7.86	1.51	1.45
23	23	1939	5MU	C4-N3	-7.73	1.24	1.38
59	Dt	55	PSU	C2-N3	7.66	1.50	1.37
23	23	747	5MU	C4-N3	-7.63	1.24	1.38
1	16	516	PSU	C2-N3	7.51	1.49	1.37
59	Dt	37	MIA	C2-S10	-7.47	1.69	1.75
59	Dt	39	PSU	C2-N3	7.43	1.49	1.37
58	Pt	39	PSU	C2-N3	7.42	1.49	1.37
59	Dt	8	4SU	C5-C4	7.26	1.51	1.42
23	23	746	PSU	C2-N3	7.25	1.49	1.37
59	Dt	32	PSU	C2-N3	7.24	1.49	1.37
23	23	2504	PSU	C2-N3	7.17	1.49	1.37
23	23	2580	PSU	C2-N3	7.12	1.49	1.37
23	23	2604	PSU	C2-N3	7.10	1.49	1.37
23	23	2605	PSU	C2-N3	7.07	1.49	1.37
23	23	2457	PSU	C2-N3	7.03	1.49	1.37
23	23	955	PSU	C2-N3	7.02	1.49	1.37
23	23	1911	PSU	C2-N3	6.95	1.48	1.37
59	Dt	46	7MG	C5-N7	6.85	1.44	1.35
59	Dt	37	MIA	C13-C14	6.76	1.52	1.32
59	Dt	8	4SU	C2-N3	6.68	1.49	1.38
58	Pt	46	7MG	C5-N7	6.67	1.44	1.35
1	16	1402	4OC	C4-N3	6.63	1.43	1.32
1	16	1498	UR3	C2-N1	6.55	1.47	1.38
1	16	967	5MC	C4-N3	6.52	1.44	1.34
1	16	1498	UR3	C6-C5	6.51	1.50	1.35
23	23	2552	OMU	C2-N1	6.48	1.48	1.38
1	16	1407	5MC	C4-N3	6.48	1.44	1.34
23	23	1962	5MC	C4-N3	6.47	1.44	1.34
23	23	2552	OMU	C2-N3	6.36	1.49	1.38
59	Dt	8	4SU	C6-C5	6.32	1.49	1.35
23	23	2503	2MA	C2-N3	6.24	1.45	1.31
23	23	1939	5MU	C6-C5	6.18	1.44	1.34
23	23	745	1MG	C2-N3	6.16	1.43	1.33
12	SL	89	D2T	CB-CA	-6.16	1.52	1.54
23	23	747	5MU	C6-C5	6.15	1.44	1.34
23	23	1962	5MC	C5-C4	6.14	1.48	1.44
1	16	1402	4OC	C6-C5	6.08	1.49	1.35
1	16	967	5MC	C5-C4	6.07	1.48	1.44
23	23	2498	OMC	C2-N3	6.01	1.48	1.36
1	16	1407	5MC	C2-N3	5.98	1.48	1.36
1	16	967	5MC	C2-N3	5.95	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	2449	H2U	C2-N3	5.95	1.48	1.38
58	Pt	46	7MG	C2-N3	5.94	1.47	1.33
1	16	1407	5MC	C5-C4	5.91	1.48	1.44
36	LP	81	4D4	CZ-NE	5.86	1.44	1.33
23	23	1962	5MC	C2-N3	5.83	1.47	1.36
1	16	1402	4OC	C2-N3	5.80	1.47	1.36
59	Dt	46	7MG	C2-N3	5.74	1.47	1.33
58	Pt	46	7MG	C4-N3	5.73	1.47	1.34
23	23	2498	OMC	C6-C5	5.65	1.48	1.35
23	23	1915	3TD	C6-N1	5.58	1.45	1.36
59	Dt	46	7MG	C4-N3	5.56	1.47	1.34
1	16	1516	2MG	C2-N2	5.54	1.45	1.33
23	23	2030	6MZ	C6-C5	-5.53	1.36	1.44
1	16	966	2MG	C2-N2	5.46	1.44	1.33
23	23	2552	OMU	C6-C5	5.39	1.47	1.35
59	Dt	55	PSU	C6-N1	5.22	1.44	1.36
23	23	1835	2MG	C2-N2	5.22	1.44	1.33
1	16	1498	UR3	C2-N3	5.21	1.49	1.39
23	23	2445	2MG	C2-N2	5.19	1.44	1.33
59	Dt	8	4SU	C4-S4	-5.14	1.59	1.68
58	Pt	34	U8U	C2-S2	-5.12	1.59	1.67
58	Pt	46	7MG	C4-N9	5.08	1.44	1.37
23	23	2251	OMG	C2-N3	5.06	1.45	1.33
23	23	1618	6MZ	C6-C5	-5.05	1.37	1.44
58	Pt	39	PSU	C6-N1	5.04	1.44	1.36
59	Dt	32	PSU	C6-N1	5.03	1.44	1.36
23	23	746	PSU	C6-N1	4.98	1.44	1.36
58	Pt	46	7MG	C2-N2	4.96	1.45	1.34
58	Pt	37	T6A	C10-N6	4.93	1.48	1.37
1	16	516	PSU	C6-N1	4.92	1.44	1.36
59	Dt	46	7MG	C2-N2	4.91	1.45	1.34
59	Dt	39	PSU	C6-N1	4.90	1.44	1.36
23	23	2503	2MA	C4-N3	4.88	1.49	1.37
23	23	1911	PSU	C6-N1	4.88	1.44	1.36
23	23	955	PSU	C6-N1	4.82	1.44	1.36
23	23	2580	PSU	C6-N1	4.82	1.44	1.36
23	23	2498	OMC	C4-N3	4.80	1.44	1.34
23	23	2504	PSU	C6-N1	4.77	1.44	1.36
23	23	2604	PSU	C6-N1	4.77	1.44	1.36
23	23	2457	PSU	C6-N1	4.75	1.44	1.36
58	Pt	37	T6A	C10-N11	4.75	1.48	1.35
1	16	1516	2MG	C4-N3	4.74	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	966	2MG	C4-N3	4.74	1.48	1.37
1	16	1518	MA6	C6-C5	-4.73	1.37	1.44
23	23	2605	PSU	C6-N1	4.70	1.44	1.36
23	23	745	1MG	C2-N1	4.66	1.45	1.37
23	23	1835	2MG	C4-N3	4.64	1.48	1.37
23	23	1915	3TD	C2-N3	4.63	1.48	1.38
59	Dt	46	7MG	C4-N9	4.58	1.43	1.37
23	23	2449	H2U	C4-N3	4.55	1.45	1.37
1	16	1402	4OC	C4-N4	4.54	1.45	1.36
23	23	2445	2MG	C4-N3	4.52	1.48	1.37
1	16	1516	2MG	C2-N1	4.51	1.43	1.36
23	23	2498	OMC	C4-N4	4.50	1.44	1.33
1	16	966	2MG	C2-N1	4.49	1.43	1.36
23	23	2251	OMG	C4-N3	4.48	1.48	1.37
23	23	745	1MG	C4-N3	4.46	1.48	1.37
1	16	967	5MC	C4-N4	4.31	1.45	1.34
23	23	2445	2MG	C2-N1	4.27	1.43	1.36
23	23	1835	2MG	C2-N1	4.26	1.43	1.36
1	16	1407	5MC	C4-N4	4.24	1.44	1.34
23	23	1962	5MC	C4-N4	4.23	1.44	1.34
1	16	1407	5MC	C6-N1	4.23	1.45	1.38
1	16	967	5MC	C6-N1	4.22	1.45	1.38
23	23	1962	5MC	C6-N1	4.20	1.45	1.38
23	23	2498	OMC	C2-N1	4.15	1.48	1.40
1	16	1518	MA6	C6-N6	4.13	1.47	1.37
58	Pt	37	T6A	C6-C5	-4.07	1.38	1.44
1	16	1407	5MC	C2-N1	4.05	1.48	1.40
23	23	745	1MG	O6-C6	-3.90	1.14	1.22
23	23	2552	OMU	C4-N3	3.90	1.45	1.38
59	Dt	46	7MG	C2-N1	3.86	1.47	1.37
58	Pt	46	7MG	C2-N1	3.81	1.46	1.37
1	16	1402	4OC	C2-N1	3.80	1.48	1.40
59	Dt	55	PSU	C4-N3	3.80	1.46	1.38
23	23	2251	OMG	C2-N2	3.79	1.43	1.34
1	16	967	5MC	C2-N1	3.73	1.47	1.40
23	23	1962	5MC	C2-N1	3.68	1.47	1.40
1	16	516	PSU	C4-N3	3.67	1.45	1.38
36	LP	81	4D4	CZ-NH2	3.63	1.45	1.32
58	Pt	39	PSU	C4-N3	3.62	1.45	1.38
59	Dt	39	PSU	C4-N3	3.55	1.45	1.38
58	Pt	46	7MG	C5-C6	3.54	1.52	1.43
59	Dt	46	7MG	C5-C6	3.51	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	Dt	32	PSU	C4-N3	3.51	1.45	1.38
23	23	746	PSU	C4-N3	3.49	1.45	1.38
1	16	1402	4OC	C5-C4	3.42	1.48	1.41
23	23	2504	PSU	C4-N3	3.40	1.45	1.38
23	23	1911	PSU	C4-N3	3.38	1.45	1.38
23	23	2069	7MG	C4-N9	-3.37	1.33	1.37
1	16	1516	2MG	C6-N1	3.37	1.43	1.37
23	23	2251	OMG	C6-N1	3.37	1.42	1.37
1	16	1519	MA6	C6-C5	3.32	1.49	1.44
23	23	2604	PSU	C4-N3	3.31	1.45	1.38
23	23	1939	5MU	O4-C4	-3.24	1.17	1.23
1	16	966	2MG	C6-N1	3.23	1.42	1.37
1	16	527	7MG	C5-C4	3.22	1.47	1.37
23	23	2605	PSU	C4-N3	3.21	1.44	1.38
23	23	2580	PSU	C4-N3	3.17	1.44	1.38
58	Pt	46	7MG	C6-N1	3.14	1.44	1.38
23	23	2251	OMG	C5-C4	-3.14	1.35	1.43
23	23	1835	2MG	C6-N1	3.13	1.42	1.37
23	23	955	PSU	C4-N3	3.13	1.44	1.38
23	23	1962	5MC	O2-C2	-3.12	1.17	1.23
23	23	2552	OMU	O4-C4	-3.12	1.18	1.24
23	23	2069	7MG	C5-C4	3.11	1.47	1.37
23	23	2449	H2U	O2-C2	-3.11	1.17	1.23
23	23	2503	2MA	C5-C4	-3.10	1.35	1.43
23	23	2445	2MG	C6-N1	3.09	1.42	1.37
59	Dt	46	7MG	C6-N1	3.09	1.44	1.38
23	23	2457	PSU	C4-N3	3.09	1.44	1.38
1	16	527	7MG	C4-N9	-3.08	1.34	1.37
23	23	2445	2MG	C5-C4	-3.06	1.35	1.43
23	23	1939	5MU	O2-C2	-3.06	1.17	1.23
1	16	967	5MC	O2-C2	-3.06	1.18	1.23
1	16	1402	4OC	O2-C2	-3.06	1.18	1.23
1	16	1498	UR3	C6-N1	3.05	1.45	1.38
1	16	1407	5MC	O2-C2	-3.02	1.18	1.23
23	23	1835	2MG	C5-C4	-3.01	1.35	1.43
1	16	1516	2MG	C5-C4	-2.98	1.35	1.43
23	23	747	5MU	O4-C4	-2.98	1.17	1.23
23	23	955	PSU	O4-C4	-2.97	1.17	1.23
1	16	1516	2MG	C5-C6	2.96	1.53	1.47
1	16	1402	4OC	C6-N1	2.93	1.45	1.38
23	23	2605	PSU	O4-C4	-2.93	1.18	1.23
23	23	2457	PSU	O4-C4	-2.92	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	2498	OMC	O2-C2	-2.91	1.18	1.23
23	23	2552	OMU	O2-C2	-2.91	1.17	1.23
23	23	747	5MU	O2-C2	-2.88	1.18	1.23
23	23	2504	PSU	O4-C4	-2.88	1.18	1.23
23	23	1911	PSU	O4-C4	-2.88	1.18	1.23
23	23	2580	PSU	O4-C4	-2.88	1.18	1.23
23	23	2503	2MA	C6-N1	2.87	1.43	1.37
23	23	2498	OMC	C6-N1	2.87	1.44	1.38
23	23	1915	3TD	C4-N3	2.87	1.46	1.40
1	16	966	2MG	C5-C4	-2.87	1.36	1.43
23	23	2604	PSU	O4-C4	-2.86	1.18	1.23
1	16	966	2MG	C5-C6	2.82	1.53	1.47
59	Dt	8	4SU	O2-C2	-2.79	1.18	1.23
58	Pt	34	U8U	C4-N3	-2.78	1.33	1.38
23	23	746	PSU	O4-C4	-2.77	1.18	1.23
23	23	745	1MG	C5-C4	-2.74	1.36	1.43
59	Dt	32	PSU	O4-C4	-2.73	1.18	1.23
59	Dt	39	PSU	O4-C4	-2.67	1.18	1.23
1	16	516	PSU	O4-C4	-2.66	1.18	1.23
58	Pt	39	PSU	O4-C4	-2.65	1.18	1.23
59	Dt	46	7MG	O6-C6	-2.62	1.18	1.23
23	23	1835	2MG	C5-C6	2.62	1.52	1.47
23	23	2445	2MG	C5-C6	2.62	1.52	1.47
23	23	2251	OMG	C5-C6	2.55	1.52	1.47
23	23	2457	PSU	O2-C2	-2.54	1.18	1.23
23	23	955	PSU	O2-C2	-2.53	1.18	1.23
58	Pt	46	7MG	O6-C6	-2.51	1.18	1.23
23	23	1915	3TD	O2-C2	-2.50	1.18	1.23
23	23	2503	2MA	C2-N1	2.50	1.43	1.36
23	23	2580	PSU	O2-C2	-2.50	1.18	1.23
23	23	2069	7MG	C6-N1	-2.49	1.34	1.38
36	LP	81	4D4	CZ-NH1	-2.49	1.25	1.34
59	Dt	55	PSU	O4-C4	-2.47	1.18	1.23
1	16	527	7MG	C6-N1	-2.47	1.34	1.38
59	Dt	8	4SU	C6-N1	2.46	1.43	1.38
23	23	2605	PSU	O2-C2	-2.43	1.18	1.23
23	23	2251	OMG	O6-C6	-2.43	1.17	1.23
23	23	2604	PSU	O2-C2	-2.43	1.18	1.23
58	Pt	37	T6A	C2-N3	2.42	1.35	1.32
58	Pt	34	U8U	C6-N1	-2.42	1.33	1.38
23	23	2580	PSU	O4'-C1'	-2.41	1.40	1.43
23	23	2552	OMU	C6-N1	2.40	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	Dt	32	PSU	O2-C2	-2.40	1.18	1.23
59	Dt	39	PSU	O2-C2	-2.38	1.18	1.23
23	23	2504	PSU	O2-C2	-2.38	1.18	1.23
58	Pt	37	T6A	ODA-C13	2.37	1.29	1.22
1	16	1519	MA6	O4'-C1'	2.34	1.44	1.40
23	23	1911	PSU	O2-C2	-2.32	1.18	1.23
58	Pt	39	PSU	O2-C2	-2.31	1.18	1.23
23	23	2445	2MG	O6-C6	-2.30	1.18	1.23
1	16	1518	MA6	C2-N3	2.29	1.35	1.32
23	23	1835	2MG	O6-C6	-2.25	1.18	1.23
23	23	2251	OMG	C2-N1	2.24	1.43	1.37
23	23	2449	H2U	O4-C4	-2.20	1.18	1.23
59	Dt	37	MIA	O4'-C1'	2.20	1.43	1.40
1	16	516	PSU	O2-C2	-2.19	1.18	1.23
23	23	2498	OMC	C5-C4	2.18	1.48	1.42
23	23	2552	OMU	C5-C4	2.17	1.48	1.43
59	Dt	47	3AU	C2-N1	2.17	1.41	1.38
23	23	746	PSU	O2-C2	-2.17	1.18	1.23
23	23	1911	PSU	O4'-C1'	-2.17	1.40	1.43
1	16	1498	UR3	O2-C2	-2.16	1.18	1.22
23	23	2457	PSU	O4'-C1'	-2.15	1.40	1.43
1	16	1498	UR3	C4-N3	2.15	1.44	1.40
23	23	2030	6MZ	C5-N7	-2.14	1.32	1.39
23	23	2030	6MZ	C2-N3	2.13	1.35	1.32
58	Pt	47	3AU	C2-N1	2.13	1.41	1.38
59	Dt	55	PSU	O2-C2	-2.13	1.18	1.23
1	16	1516	2MG	O6-C6	-2.10	1.18	1.23
58	Pt	37	T6A	O10-C10	-2.10	1.18	1.23
1	16	966	2MG	O6-C6	-2.10	1.18	1.23
23	23	1618	6MZ	C2-N3	2.09	1.35	1.32
23	23	2605	PSU	O4'-C1'	-2.08	1.41	1.43
58	Pt	34	U8U	C-N	-2.07	1.43	1.46
1	16	1498	UR3	C5-C4	2.05	1.49	1.43
58	Pt	37	T6A	C2-N1	2.03	1.37	1.33

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	1939	5MU	C5-C4-N3	12.60	126.27	115.32
1	16	1518	MA6	N1-C6-N6	-12.10	102.86	116.83
23	23	747	5MU	C5-C4-N3	12.05	125.80	115.32
23	23	2030	6MZ	C1'-N9-C4	-11.73	106.03	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	1939	5MU	C5-C6-N1	-10.26	112.17	123.31
23	23	747	5MU	C5-C6-N1	-10.12	112.31	123.31
23	23	1618	6MZ	C1'-N9-C4	-9.49	109.96	126.64
1	16	527	7MG	N9-C4-N3	8.86	138.44	125.46
59	Dt	37	MIA	C12-C13-C14	-8.82	111.18	127.01
23	23	2069	7MG	N9-C4-N3	8.50	137.92	125.46
59	Dt	8	4SU	C4-N3-C2	-8.32	119.34	127.31
58	Pt	37	T6A	N6-C10-N11	6.47	122.67	113.77
1	16	1518	MA6	N3-C2-N1	-6.45	119.91	128.67
23	23	2552	OMU	C4-N3-C2	-6.42	118.64	126.61
58	Pt	37	T6A	N3-C2-N1	-6.42	119.96	128.67
23	23	1618	6MZ	N3-C2-N1	-6.24	120.21	128.67
1	16	1519	MA6	C2-N1-C6	6.13	122.85	116.84
59	Dt	8	4SU	C5-C4-N3	5.93	120.27	114.75
23	23	1915	3TD	N1-C2-N3	5.73	120.30	116.13
1	16	527	7MG	C5-C4-N3	-5.45	117.89	128.13
1	16	1498	UR3	C4-N3-C2	-5.44	120.20	124.58
23	23	2457	PSU	C4-N3-C2	-5.44	118.88	126.37
23	23	2457	PSU	N1-C2-N3	5.40	120.86	115.17
23	23	1939	5MU	C4-N3-C2	-5.37	120.29	127.34
23	23	2069	7MG	N9-C8-N7	-5.34	95.82	103.37
23	23	2069	7MG	C5-C4-N3	-5.29	118.21	128.13
23	23	955	PSU	C4-N3-C2	-5.28	119.09	126.37
23	23	2030	6MZ	N3-C2-N1	-5.27	121.52	128.67
1	16	527	7MG	N9-C8-N7	-5.27	95.92	103.37
59	Dt	32	PSU	C4-N3-C2	-5.20	119.21	126.37
23	23	2604	PSU	C4-N3-C2	-5.16	119.27	126.37
58	Pt	46	7MG	C5-C6-N1	5.15	120.00	110.94
23	23	1939	5MU	O4-C4-C5	-5.14	119.04	124.92
58	Pt	39	PSU	C4-N3-C2	-5.09	119.37	126.37
23	23	747	5MU	O4-C4-C5	-5.08	119.10	124.92
23	23	2605	PSU	C4-N3-C2	-5.05	119.41	126.37
23	23	955	PSU	N1-C2-N3	5.02	120.46	115.17
23	23	747	5MU	C4-N3-C2	-4.98	120.81	127.34
59	Dt	55	PSU	C4-N3-C2	-4.97	119.53	126.37
59	Dt	46	7MG	C5-C6-N1	4.95	119.66	110.94
23	23	1911	PSU	C4-N3-C2	-4.94	119.57	126.37
23	23	2580	PSU	C4-N3-C2	-4.92	119.59	126.37
23	23	746	PSU	C4-N3-C2	-4.91	119.60	126.37
59	Dt	47	3AU	C4-N3-C2	-4.89	118.92	124.66
23	23	2504	PSU	C4-N3-C2	-4.80	119.75	126.37
59	Dt	39	PSU	C4-N3-C2	-4.80	119.75	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	2580	PSU	N1-C2-N3	4.79	120.22	115.17
58	Pt	47	3AU	C4-N3-C2	-4.78	119.05	124.66
23	23	2605	PSU	N1-C2-N3	4.73	120.16	115.17
23	23	2604	PSU	N1-C2-N3	4.72	120.14	115.17
58	Pt	39	PSU	N1-C2-N3	4.69	120.12	115.17
23	23	2503	2MA	C4-N3-C2	-4.69	119.70	123.30
59	Dt	39	PSU	N1-C2-N3	4.67	120.09	115.17
58	Pt	46	7MG	C2-N3-C4	4.67	120.34	112.30
1	16	516	PSU	C4-N3-C2	-4.65	119.97	126.37
23	23	1939	5MU	N3-C2-N1	4.65	120.94	114.89
23	23	2069	7MG	C2-N3-C4	4.62	120.26	112.30
23	23	2504	PSU	N1-C2-N3	4.62	120.04	115.17
59	Dt	32	PSU	N1-C2-N3	4.59	120.01	115.17
59	Dt	55	PSU	N1-C2-N3	4.56	119.98	115.17
1	16	527	7MG	C2-N3-C4	4.48	120.01	112.30
23	23	1911	PSU	N1-C2-N3	4.45	119.87	115.17
23	23	747	5MU	N3-C2-N1	4.42	120.64	114.89
58	Pt	46	7MG	C5-C4-N3	-4.41	119.85	128.13
59	Dt	46	7MG	C2-N3-C4	4.39	119.85	112.30
23	23	2445	2MG	N1-C2-N2	4.33	120.98	116.56
58	Pt	37	T6A	C2-N1-C6	4.30	119.94	116.60
23	23	2552	OMU	N3-C2-N1	4.28	120.47	114.89
23	23	745	1MG	C5-C6-N1	4.26	120.13	113.96
1	16	516	PSU	N1-C2-N3	4.24	119.64	115.17
23	23	2457	PSU	C6-C5-C4	4.23	121.03	118.17
1	16	1516	2MG	N1-C2-N2	4.15	120.80	116.56
1	16	1519	MA6	C4-C5-N7	-4.14	104.96	109.34
23	23	1835	2MG	N1-C2-N2	4.10	120.75	116.56
23	23	746	PSU	N1-C2-N3	4.06	119.45	115.17
59	Dt	37	MIA	C15-C14-C13	-4.05	110.50	122.66
1	16	1519	MA6	C4'-O4'-C1'	4.04	113.63	109.92
23	23	1915	3TD	C1'-C5-C4	4.04	123.73	117.61
59	Dt	46	7MG	C5-C4-N3	-4.02	120.59	128.13
58	Pt	46	7MG	C4-C5-N7	3.98	110.08	105.38
23	23	747	5MU	C5M-C5-C6	-3.98	117.47	122.85
59	Dt	55	PSU	C6-C5-C4	3.95	120.84	118.17
1	16	1498	UR3	C5-C4-N3	3.92	120.21	115.04
1	16	1519	MA6	C10-N6-C6	-3.91	108.63	119.40
23	23	2552	OMU	C5-C4-N3	3.91	120.27	114.80
23	23	1915	3TD	C4-N3-C2	-3.89	120.50	124.61
12	SL	89	D2T	CB1-SB-CB	3.89	109.35	102.36
59	Dt	8	4SU	N3-C2-N1	3.82	119.86	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	747	5MU	C5M-C5-C4	3.77	122.80	118.78
59	Dt	8	4SU	C5-C4-S4	-3.74	120.03	124.31
59	Dt	46	7MG	C4-C5-N7	3.72	109.77	105.38
23	23	2503	2MA	C8-N7-C5	3.72	108.88	102.55
58	Pt	37	T6A	N6-C6-N1	3.72	122.89	118.71
59	Dt	37	MIA	C11-S10-C2	-3.69	99.48	102.25
59	Dt	37	MIA	C16-C14-C13	-3.67	111.63	122.66
23	23	2504	PSU	C6-N1-C2	-3.65	119.30	122.69
23	23	1939	5MU	C5M-C5-C6	-3.65	117.90	122.85
1	16	967	5MC	C5-C6-N1	-3.64	119.36	123.31
1	16	966	2MG	N1-C2-N2	3.61	120.24	116.56
23	23	2580	PSU	C6-N1-C2	-3.57	119.38	122.69
1	16	516	PSU	C6-N1-C2	-3.57	119.38	122.69
23	23	955	PSU	C6-C5-C4	3.57	120.58	118.17
1	16	1519	MA6	N3-C2-N1	-3.53	123.88	128.67
58	Pt	39	PSU	C6-C5-C4	3.52	120.55	118.17
23	23	1939	5MU	C5M-C5-C4	3.48	122.50	118.78
23	23	2030	6MZ	C6-C5-C4	3.47	121.36	117.68
23	23	955	PSU	C6-N1-C2	-3.44	119.50	122.69
59	Dt	39	PSU	C6-C5-C4	3.41	120.48	118.17
59	Dt	39	PSU	C6-N1-C2	-3.39	119.54	122.69
23	23	1962	5MC	C5-C6-N1	-3.39	119.63	123.31
23	23	2605	PSU	C6-N1-C2	-3.39	119.55	122.69
23	23	2449	H2U	C5-C4-N3	3.39	120.29	116.69
23	23	2457	PSU	C6-N1-C2	-3.39	119.55	122.69
23	23	2251	OMG	C8-N7-C5	3.38	108.30	102.55
23	23	2503	2MA	C5-C6-N1	3.36	120.38	114.12
23	23	2604	PSU	C6-C5-C4	3.36	120.44	118.17
23	23	745	1MG	C8-N7-C5	3.35	108.26	102.55
1	16	1518	MA6	C2-N1-C6	3.35	120.12	116.84
59	Dt	32	PSU	C6-C5-C4	3.33	120.42	118.17
23	23	2449	H2U	N3-C2-N1	3.32	119.99	116.65
23	23	2251	OMG	C5-C6-N1	3.28	120.34	114.07
23	23	2445	2MG	C5-C6-N1	3.26	120.30	114.07
1	16	1516	2MG	C8-N7-C5	3.26	108.10	102.55
23	23	2580	PSU	C6-C5-C4	3.25	120.37	118.17
23	23	2251	OMG	C2-N1-C6	-3.24	119.18	125.11
23	23	1835	2MG	C5-C6-N1	3.24	120.25	114.07
23	23	2604	PSU	C6-N1-C2	-3.22	119.70	122.69
23	23	1835	2MG	C8-N7-C5	3.21	108.01	102.55
1	16	966	2MG	C5-C6-N1	3.19	120.16	114.07
59	Dt	46	7MG	C5-C4-N9	3.16	110.38	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	2445	2MG	CM2-N2-C2	-3.15	116.87	123.65
23	23	2445	2MG	C8-N7-C5	3.14	107.90	102.55
1	16	1516	2MG	C5-C6-N1	3.14	120.06	114.07
1	16	966	2MG	C8-N7-C5	3.07	107.78	102.55
23	23	1618	6MZ	C6-C5-C4	3.07	120.93	117.68
23	23	1835	2MG	CM2-N2-C2	-3.06	117.08	123.65
58	Pt	46	7MG	N9-C4-N3	3.05	129.93	125.46
59	Dt	39	PSU	O2-C2-N1	-3.04	119.65	122.79
58	Pt	46	7MG	C2-N1-C6	-3.04	119.60	125.11
58	Pt	46	7MG	C5-C4-N9	3.03	110.22	106.33
58	Pt	39	PSU	C6-N1-C2	-3.03	119.88	122.69
59	Dt	55	PSU	C6-N1-C2	-3.00	119.91	122.69
23	23	1911	PSU	C6-N1-C2	-2.97	119.93	122.69
23	23	1939	5MU	O2-C2-N1	-2.96	118.94	122.80
1	16	1407	5MC	C5-C6-N1	-2.94	120.12	123.31
1	16	516	PSU	O2-C2-N1	-2.93	119.77	122.79
12	SL	89	D2T	OD2-CG-CB	2.90	119.42	113.15
23	23	1939	5MU	O4-C4-N3	-2.88	114.69	120.11
58	Pt	46	7MG	O6-C6-C5	-2.88	120.56	127.62
59	Dt	46	7MG	C2-N1-C6	-2.87	119.90	125.11
23	23	2552	OMU	O4-C4-C5	-2.87	120.21	125.16
23	23	2457	PSU	O2-C2-N1	-2.87	119.83	122.79
58	Pt	39	PSU	O2-C2-N1	-2.85	119.85	122.79
23	23	2069	7MG	C5-C6-N1	2.85	115.96	110.94
23	23	2605	PSU	C6-C5-C4	2.85	120.10	118.17
59	Dt	32	PSU	C6-N1-C2	-2.85	120.05	122.69
23	23	1618	6MZ	C9-N6-C6	-2.84	120.22	122.85
23	23	2449	H2U	C5-C6-N1	2.81	120.02	111.52
59	Dt	46	7MG	O6-C6-C5	-2.79	120.77	127.62
23	23	747	5MU	O2-C2-N1	-2.78	119.18	122.80
23	23	746	PSU	C6-N1-C2	-2.78	120.11	122.69
58	Pt	37	T6A	O10-C10-N6	-2.77	118.72	123.64
59	Dt	55	PSU	O2-C2-N1	-2.77	119.94	122.79
1	16	527	7MG	C5-C6-N1	2.74	115.76	110.94
59	Dt	47	3AU	C5-C4-N3	2.74	119.42	115.64
23	23	2605	PSU	O2-C2-N1	-2.74	119.97	122.79
23	23	955	PSU	O2-C2-N1	-2.74	119.97	122.79
23	23	2504	PSU	O2-C2-N1	-2.73	119.97	122.79
58	Pt	37	T6A	C12-N11-C10	-2.71	117.47	121.99
1	16	1519	MA6	C10-N6-C9	-2.69	107.54	116.18
58	Pt	47	3AU	C5-C4-N3	2.68	119.35	115.64
23	23	2552	OMU	O2-C2-N1	-2.67	119.32	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	747	5MU	O4-C4-N3	-2.67	115.10	120.11
23	23	745	1MG	O6-C6-C5	-2.61	119.88	124.18
23	23	2449	H2U	O2-C2-N1	-2.56	120.03	123.10
58	Pt	34	U8U	O4-C4-C5	-2.55	120.42	124.71
23	23	746	PSU	O2-C2-N1	-2.54	120.17	122.79
59	Dt	32	PSU	O2-C2-N1	-2.52	120.19	122.79
23	23	2604	PSU	O2-C2-N1	-2.52	120.19	122.79
23	23	1618	6MZ	C2-N1-C6	2.51	118.55	116.60
58	Pt	37	T6A	C6-C5-C4	2.51	120.34	117.68
23	23	746	PSU	C6-C5-C4	2.50	119.86	118.17
23	23	2580	PSU	O2-C2-N1	-2.48	120.23	122.79
23	23	2069	7MG	O4'-C1'-N9	2.45	112.64	109.30
59	Dt	46	7MG	N9-C4-N3	2.43	129.02	125.46
58	Pt	47	3AU	C3'-C2'-C1'	2.41	106.02	101.46
58	Pt	46	7MG	N9-C8-N7	2.41	106.78	103.37
1	16	1519	MA6	O3'-C3'-C4'	2.40	117.97	111.08
23	23	1911	PSU	O2-C2-N1	-2.39	120.32	122.79
1	16	966	2MG	CM2-N2-C2	-2.39	118.52	123.65
1	16	1402	4OC	C6-C5-C4	2.38	119.87	117.00
23	23	2030	6MZ	C2-N1-C6	2.37	118.44	116.60
1	16	966	2MG	O6-C6-C5	-2.35	119.65	124.32
23	23	2504	PSU	C6-C5-C4	2.33	119.75	118.17
1	16	1516	2MG	CM2-N2-C2	-2.31	118.69	123.65
23	23	2445	2MG	O6-C6-C5	-2.30	119.75	124.32
23	23	2251	OMG	O6-C6-C5	-2.27	119.83	124.32
58	Pt	34	U8U	C5-C4-N3	2.25	118.65	115.21
59	Dt	37	MIA	N3-C2-N1	-2.24	122.93	127.03
59	Dt	37	MIA	C4-C5-N7	-2.24	106.97	109.34
59	Dt	46	7MG	N9-C8-N7	2.22	106.52	103.37
1	16	527	7MG	O4'-C1'-N9	2.22	112.32	109.30
23	23	2503	2MA	CM2-C2-N1	2.21	120.86	116.27
1	16	1519	MA6	C2'-C3'-C4'	2.20	106.86	102.61
23	23	2580	PSU	O4'-C1'-C2'	2.19	108.18	105.15
23	23	1835	2MG	O6-C6-C5	-2.19	119.98	124.32
59	Dt	37	MIA	C2-N1-C6	2.18	121.30	117.42
59	Dt	47	3AU	C1'-N1-C2	2.13	120.53	117.04
59	Dt	8	4SU	O2-C2-N1	-2.12	120.04	122.80
58	Pt	34	U8U	C5-C6-N1	-2.11	120.11	122.94
1	16	1516	2MG	O6-C6-C5	-2.09	120.19	124.32
23	23	2503	2MA	N1-C2-N3	-2.08	119.86	123.15
1	16	527	7MG	C5-C4-N9	-2.08	103.67	106.33
23	23	745	1MG	CM1-N1-C6	2.07	120.35	117.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Pt	34	U8U	C3'-C2'-C1'	2.07	105.38	101.46
23	23	747	5MU	C6-C5-C4	2.07	119.72	118.02
1	16	1498	UR3	C6-N1-C2	-2.06	120.11	121.80
1	16	1407	5MC	CM5-C5-C6	-2.06	120.06	122.85
1	16	516	PSU	C6-C5-C4	2.02	119.54	118.17
58	Pt	47	3AU	C10-N3-C2	2.01	120.61	117.64

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	1519	MA6	O4'-C4'-C5'-O5'
1	16	1519	MA6	C3'-C4'-C5'-O5'
23	23	1618	6MZ	C5-C6-N6-C9
23	23	1618	6MZ	N1-C6-N6-C9
23	23	1911	PSU	O4'-C1'-C5-C4
23	23	1911	PSU	O4'-C1'-C5-C6
23	23	1915	3TD	O4'-C1'-C5-C4
23	23	1915	3TD	O4'-C1'-C5-C6
23	23	2251	OMG	O4'-C4'-C5'-O5'
23	23	2251	OMG	C1'-C2'-O2'-CM2
58	Pt	37	T6A	N11-C12-C14-O14
58	Pt	37	T6A	N11-C12-C14-C15
58	Pt	37	T6A	C13-C12-C14-O14
58	Pt	37	T6A	C13-C12-C14-C15
58	Pt	47	3AU	N3-C10-C11-C12
59	Dt	37	MIA	O4'-C4'-C5'-O5'
59	Dt	37	MIA	C3'-C4'-C5'-O5'
59	Dt	37	MIA	C12-C13-C14-C15
59	Dt	37	MIA	C12-C13-C14-C16
59	Dt	47	3AU	N3-C10-C11-C12
59	Dt	47	3AU	C10-C11-C12-N40
59	Dt	47	3AU	N40-C12-C13-O30
59	Dt	47	3AU	O4'-C4'-C5'-O5'
1	16	527	7MG	C3'-C4'-C5'-O5'
23	23	2251	OMG	C3'-C4'-C5'-O5'
23	23	2498	OMC	C3'-C4'-C5'-O5'
23	23	2503	2MA	O4'-C4'-C5'-O5'
58	Pt	37	T6A	O4'-C4'-C5'-O5'
58	Pt	37	T6A	C3'-C4'-C5'-O5'
59	Dt	47	3AU	C3'-C4'-C5'-O5'
58	Pt	47	3AU	N40-C12-C13-O31

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Mol	Chain	Res	Type	Atoms
23	23	2498	OMC	O4'-C4'-C5'-O5'
23	23	2503	2MA	C3'-C4'-C5'-O5'
1	16	1519	MA6	N1-C6-N6-C10
59	Dt	47	3AU	N40-C12-C13-O31
1	16	527	7MG	O4'-C4'-C5'-O5'
58	Pt	37	T6A	C14-C12-C13-ODA
58	Pt	37	T6A	C14-C12-C13-ODB
23	23	1618	6MZ	C3'-C4'-C5'-O5'
23	23	2030	6MZ	O4'-C4'-C5'-O5'
23	23	2030	6MZ	C3'-C4'-C5'-O5'
58	Pt	47	3AU	C3'-C4'-C5'-O5'
58	Pt	47	3AU	C11-C10-N3-C4
58	Pt	37	T6A	N11-C12-C13-ODA
23	23	1835	2MG	O4'-C4'-C5'-O5'
58	Pt	34	U8U	O4'-C4'-C5'-O5'
58	Pt	46	7MG	O4'-C4'-C5'-O5'
58	Pt	47	3AU	O4'-C4'-C5'-O5'
58	Pt	47	3AU	C11-C10-N3-C2
23	23	1618	6MZ	O4'-C4'-C5'-O5'
23	23	1835	2MG	C3'-C4'-C5'-O5'
58	Pt	34	U8U	C3'-C4'-C5'-O5'
58	Pt	46	7MG	C3'-C4'-C5'-O5'
58	Pt	47	3AU	C4'-C5'-O5'-P
59	Dt	47	3AU	C4'-C5'-O5'-P
59	Dt	37	MIA	N1-C6-N6-C12
58	Pt	47	3AU	N40-C12-C13-O30
58	Pt	37	T6A	N11-C12-C13-ODB
58	Pt	46	7MG	C2'-C1'-N9-C8
59	Dt	46	7MG	C2'-C1'-N9-C8
12	SL	89	D2T	CG-CB-SB-CB1
59	Dt	47	3AU	C11-C12-C13-O31
23	23	747	5MU	C3'-C4'-C5'-O5'
1	16	1402	4OC	O4'-C4'-C5'-O5'
1	16	1498	UR3	O4'-C4'-C5'-O5'
1	16	1519	MA6	C5-C6-N6-C10
1	16	1519	MA6	C4'-C5'-O5'-P
59	Dt	47	3AU	C11-C12-C13-O30
23	23	2449	H2U	C4'-C5'-O5'-P
1	16	527	7MG	C4'-C5'-O5'-P
58	Pt	46	7MG	O4'-C1'-N9-C8
23	23	746	PSU	O4'-C1'-C5-C6
23	23	1962	5MC	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
23	23	1962	5MC	O4'-C1'-N1-C6
23	23	2580	PSU	O4'-C4'-C5'-O5'
59	Dt	46	7MG	O4'-C1'-N9-C8
23	23	746	PSU	C2'-C1'-C5-C6
58	Pt	47	3AU	C11-C12-C13-O30
58	Pt	47	3AU	C11-C12-C13-O31
36	LP	81	4D4	O-C-CA-CB
59	Dt	37	MIA	C5-C6-N6-C12
1	16	1498	UR3	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 372 ligands modelled in this entry, 347 are monoatomic - leaving 25 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$
61	PUT	23	3013	-	5,5,5	0.15	0	4,4,4	0.60	0
60	SCM	16	1602	-	23,25,25	1.37	3 (13%)	27,39,39	1.43	3 (11%)
66	GTP	EF	901	62	29,34,34	4.25	16 (55%)	35,54,54	1.73	9 (25%)
61	PUT	23	3015	-	5,5,5	0.23	0	4,4,4	0.41	0
61	PUT	23	3014	-	5,5,5	0.20	0	4,4,4	0.41	0
61	PUT	23	3009	-	5,5,5	0.22	0	4,4,4	0.48	0
61	PUT	16	1604	-	5,5,5	0.16	0	4,4,4	0.22	0
64	ATP	23	3003	-	28,33,33	0.74	0	34,52,52	0.75	1 (2%)
60	SCM	16	1601	-	23,25,25	1.35	3 (13%)	27,39,39	1.50	3 (11%)
61	PUT	LC	301	-	5,5,5	0.22	0	4,4,4	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
61	PUT	23	3004	-	5,5,5	0.18	0	4,4,4	0.54	0
61	PUT	23	3007	-	5,5,5	0.14	0	4,4,4	0.22	0
65	SPD	23	3018	-	9,9,9	0.31	0	8,8,8	0.95	0
65	SPD	23	3017	-	9,9,9	0.31	0	8,8,8	0.91	0
60	SCM	23	3001	-	23,25,25	1.38	4 (17%)	27,39,39	1.65	5 (18%)
61	PUT	23	3011	-	5,5,5	0.23	0	4,4,4	0.44	0
61	PUT	16	1605	-	5,5,5	0.15	0	4,4,4	0.23	0
61	PUT	16	1603	-	5,5,5	0.23	0	4,4,4	0.47	0
64	ATP	23	3002	-	28,33,33	0.77	0	34,52,52	0.75	1 (2%)
61	PUT	23	3005	-	5,5,5	0.23	0	4,4,4	0.42	0
61	PUT	23	3008	-	5,5,5	0.22	0	4,4,4	0.49	0
61	PUT	23	3010	-	5,5,5	0.20	0	4,4,4	0.54	0
61	PUT	23	3016	-	5,5,5	0.22	0	4,4,4	0.47	0
61	PUT	23	3006	-	5,5,5	0.21	0	4,4,4	0.48	0
61	PUT	23	3012	-	5,5,5	0.22	0	4,4,4	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PUT	23	3013	-	-	2/3/3/3	-
60	SCM	16	1602	-	-	0/4/57/57	0/3/3/3
66	GTP	EF	901	62	-	2/18/38/38	0/3/3/3
61	PUT	23	3015	-	-	2/3/3/3	-
61	PUT	23	3014	-	-	1/3/3/3	-
61	PUT	23	3009	-	-	1/3/3/3	-
61	PUT	16	1604	-	-	0/3/3/3	-
64	ATP	23	3003	-	1/1/7/7	6/18/38/38	0/3/3/3
60	SCM	16	1601	-	-	2/4/57/57	0/3/3/3
61	PUT	LC	301	-	-	1/3/3/3	-
61	PUT	23	3004	-	-	2/3/3/3	-
61	PUT	23	3007	-	-	2/3/3/3	-
65	SPD	23	3018	-	-	0/7/7/7	-
65	SPD	23	3017	-	-	4/7/7/7	-
60	SCM	23	3001	-	-	0/4/57/57	0/3/3/3
61	PUT	23	3011	-	-	1/3/3/3	-
61	PUT	16	1605	-	-	3/3/3/3	-
61	PUT	16	1603	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	ATP	23	3002	-	-	3/18/38/38	0/3/3/3
61	PUT	23	3005	-	-	0/3/3/3	-
61	PUT	23	3008	-	-	0/3/3/3	-
61	PUT	23	3010	-	-	1/3/3/3	-
61	PUT	23	3016	-	-	1/3/3/3	-
61	PUT	23	3006	-	-	1/3/3/3	-
61	PUT	23	3012	-	-	2/3/3/3	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	EF	901	GTP	O4'-C1'	15.48	1.61	1.40
66	EF	901	GTP	PB-O3B	7.21	1.67	1.59
66	EF	901	GTP	O4'-C4'	-6.51	1.30	1.45
66	EF	901	GTP	C2-N3	6.15	1.48	1.33
66	EF	901	GTP	PA-O3A	5.26	1.65	1.59
66	EF	901	GTP	C4-N3	4.78	1.48	1.37
66	EF	901	GTP	C2-N2	4.47	1.44	1.34
66	EF	901	GTP	C6-N1	3.79	1.43	1.37
66	EF	901	GTP	C5-C6	3.17	1.53	1.47
66	EF	901	GTP	O3'-C3'	-2.92	1.35	1.43
66	EF	901	GTP	PB-O3A	2.77	1.62	1.59
60	16	1601	SCM	C10-N10	-2.58	1.43	1.47
66	EF	901	GTP	C2-N1	2.56	1.43	1.37
66	EF	901	GTP	O5'-C5'	-2.49	1.35	1.44
60	23	3001	SCM	C10-N10	-2.38	1.43	1.47
60	16	1602	SCM	C10-N10	-2.33	1.43	1.47
66	EF	901	GTP	O6-C6	-2.32	1.17	1.23
66	EF	901	GTP	C5-C4	-2.29	1.37	1.43
66	EF	901	GTP	O2'-C2'	2.28	1.48	1.43
60	23	3001	SCM	C11-C10	2.26	1.57	1.53
60	23	3001	SCM	C3-C4	-2.18	1.47	1.50
60	23	3001	SCM	C9-C8	2.06	1.56	1.53
60	16	1601	SCM	C3-C4	-2.04	1.47	1.50
60	16	1602	SCM	C3-C4	-2.03	1.47	1.50
60	16	1602	SCM	C12-C7	2.02	1.56	1.52
60	16	1601	SCM	C8-N8	-2.01	1.44	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	16	1601	SCM	C8M-N8-C8	-4.74	108.11	114.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	EF	901	GTP	C4'-O4'-C1'	-4.36	105.93	109.92
60	23	3001	SCM	C1M-N10-C10	-3.79	109.34	114.23
60	16	1601	SCM	C1M-N10-C10	-3.70	109.46	114.23
60	16	1602	SCM	C8M-N8-C8	-3.57	109.61	114.23
66	EF	901	GTP	C5-C6-N1	3.54	120.83	114.07
60	16	1602	SCM	C1M-N10-C10	-3.54	109.67	114.23
66	EF	901	GTP	C2-N1-C6	-3.45	118.79	125.11
60	23	3001	SCM	C8M-N8-C8	-3.38	109.86	114.23
66	EF	901	GTP	C8-N7-C5	3.31	108.19	102.55
60	23	3001	SCM	O1B-C7-C12	3.29	114.71	108.94
66	EF	901	GTP	C5'-C4'-C3'	-2.95	104.60	115.21
66	EF	901	GTP	O4'-C1'-N9	2.89	112.58	108.75
60	23	3001	SCM	C2M-C2-C3	-2.61	108.57	113.27
60	16	1602	SCM	C2M-C2-C3	-2.59	108.62	113.27
64	23	3002	ATP	C5-C6-N6	2.39	123.96	120.31
60	16	1601	SCM	C2M-C2-C3	-2.37	109.01	113.27
60	23	3001	SCM	O2B-C12-C7	2.37	113.19	108.23
64	23	3003	ATP	C5-C6-N6	2.34	123.88	120.31
66	EF	901	GTP	O3A-PB-O1B	-2.25	103.93	110.70
66	EF	901	GTP	O6-C6-C5	-2.12	120.12	124.32
66	EF	901	GTP	C2'-C3'-C4'	-2.06	98.63	102.61

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
64	23	3003	ATP	C4'

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
64	23	3002	ATP	PB-O3B-PG-O3G
64	23	3002	ATP	O4'-C4'-C5'-O5'
64	23	3003	ATP	C5'-O5'-PA-O1A
64	23	3003	ATP	C5'-O5'-PA-O3A
66	EF	901	GTP	C5'-O5'-PA-O3A
61	23	3015	PUT	C1-C2-C3-C4
64	23	3003	ATP	O4'-C4'-C5'-O5'
65	23	3017	SPD	C3-C4-C5-N6
64	23	3003	ATP	C3'-C4'-C5'-O5'
64	23	3002	ATP	C3'-C4'-C5'-O5'
61	23	3016	PUT	C1-C2-C3-C4
61	23	3013	PUT	C1-C2-C3-C4

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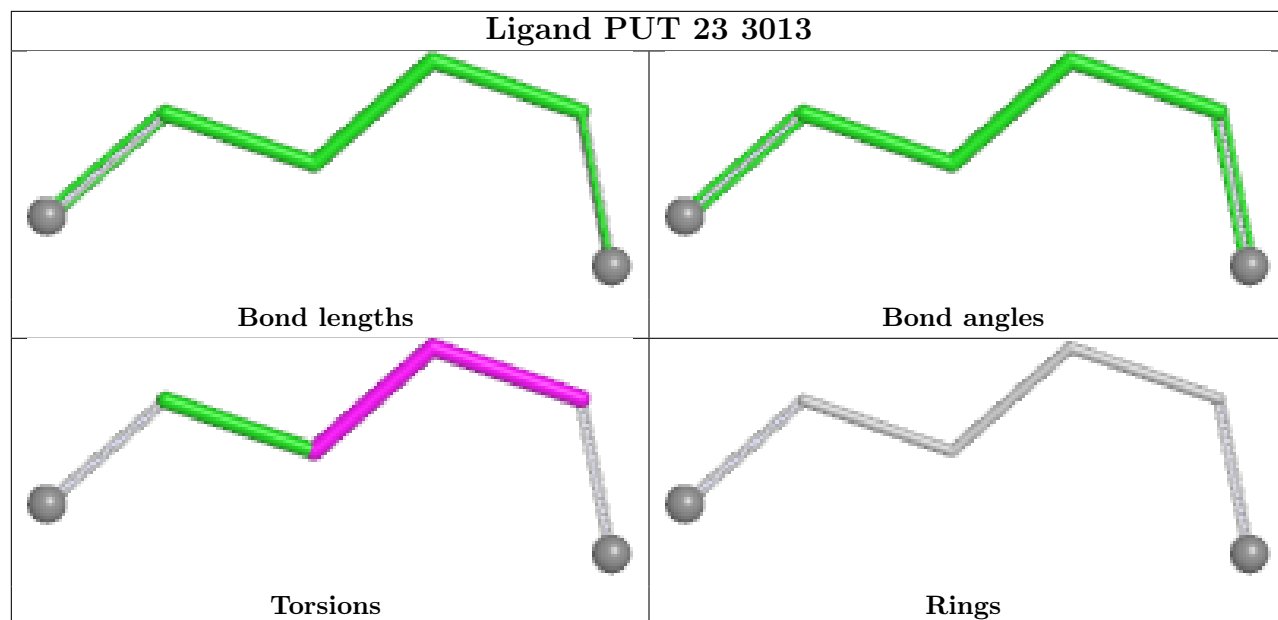
Mol	Chain	Res	Type	Atoms
60	16	1601	SCM	C9-C10-N10-C1M
60	16	1601	SCM	C11-C10-N10-C1M
61	16	1605	PUT	N1-C1-C2-C3
65	23	3017	SPD	C8-C7-N6-C5
61	23	3007	PUT	C1-C2-C3-C4
61	LC	301	PUT	C1-C2-C3-C4
61	23	3006	PUT	C1-C2-C3-C4
61	23	3011	PUT	C1-C2-C3-C4
61	16	1605	PUT	C1-C2-C3-C4
61	23	3007	PUT	N1-C1-C2-C3
61	23	3014	PUT	N1-C1-C2-C3
65	23	3017	SPD	C7-C8-C9-N10
61	23	3004	PUT	C1-C2-C3-C4
61	23	3012	PUT	C1-C2-C3-C4
66	EF	901	GTP	C5'-O5'-PA-O1A
65	23	3017	SPD	N1-C2-C3-C4
64	23	3003	ATP	C4'-C5'-O5'-PA
61	23	3013	PUT	C2-C3-C4-N2
61	23	3010	PUT	C2-C3-C4-N2
61	23	3015	PUT	C2-C3-C4-N2
64	23	3003	ATP	PB-O3B-PG-O3G
61	23	3012	PUT	N1-C1-C2-C3
61	23	3009	PUT	C1-C2-C3-C4
61	16	1605	PUT	C2-C3-C4-N2
61	23	3004	PUT	N1-C1-C2-C3

There are no ring outliers.

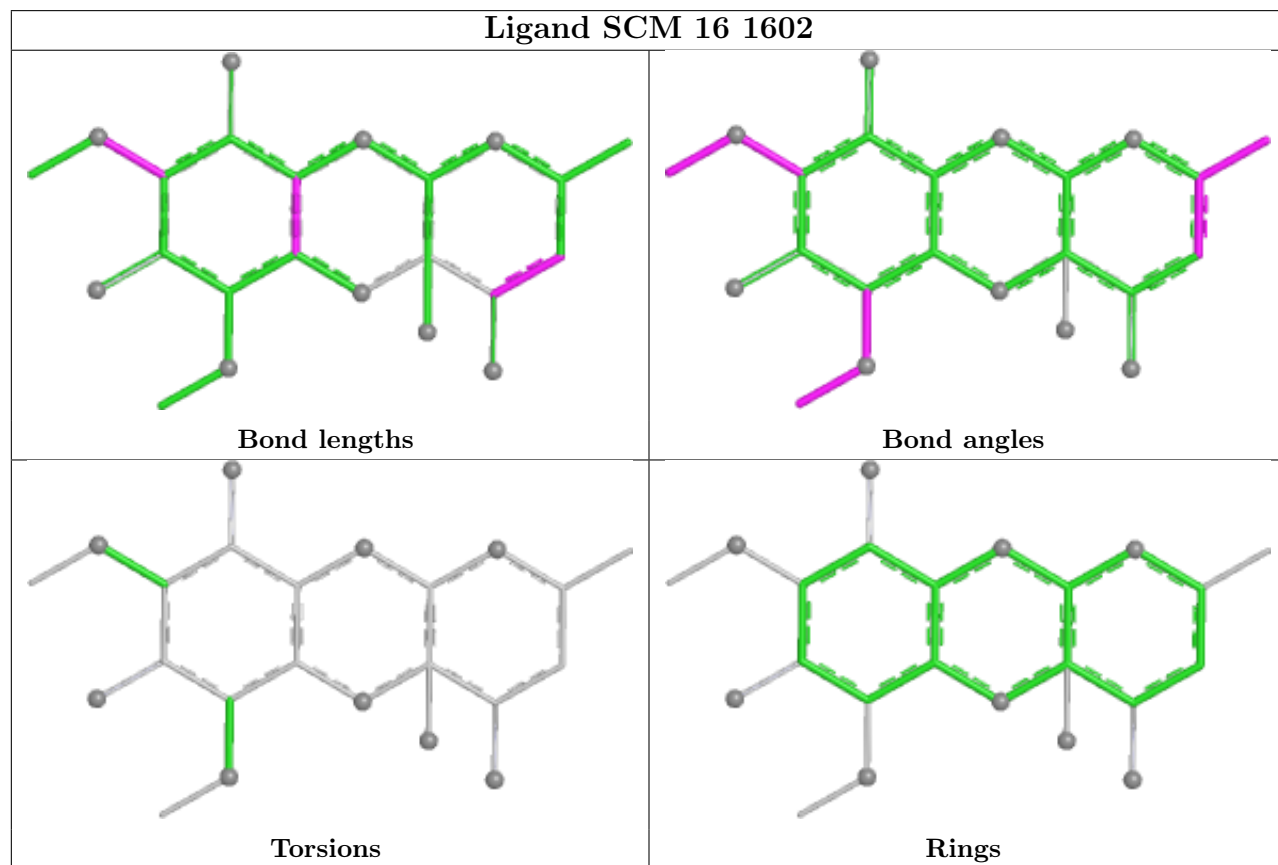
No monomer is involved in short contacts.

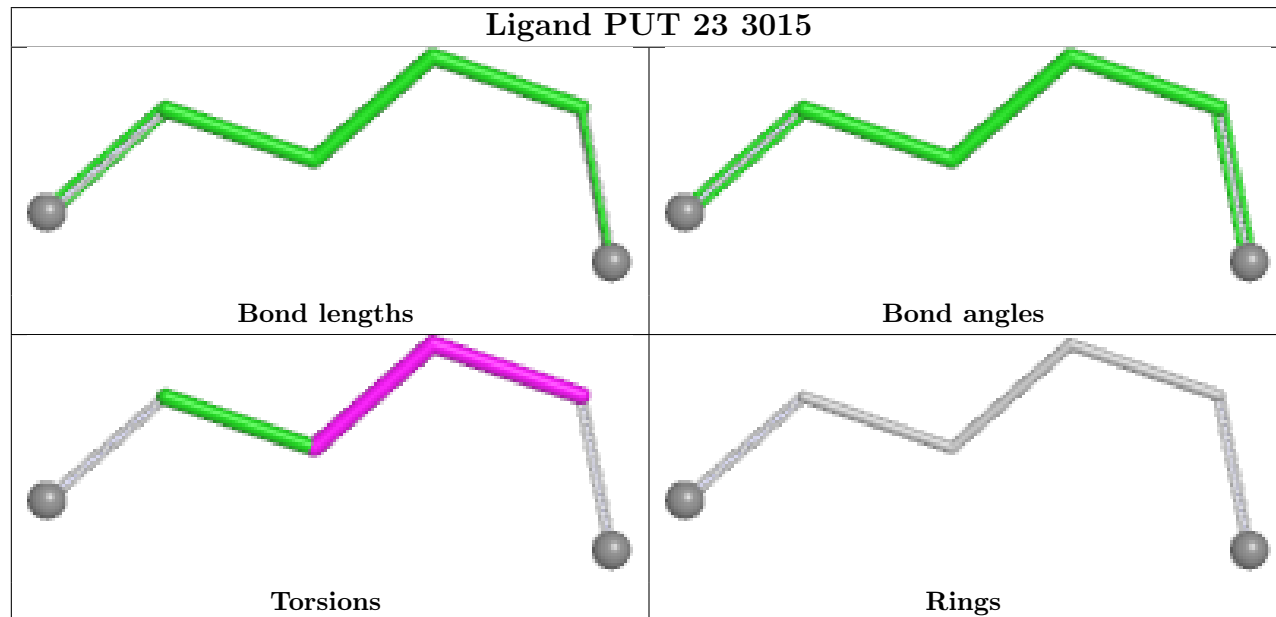
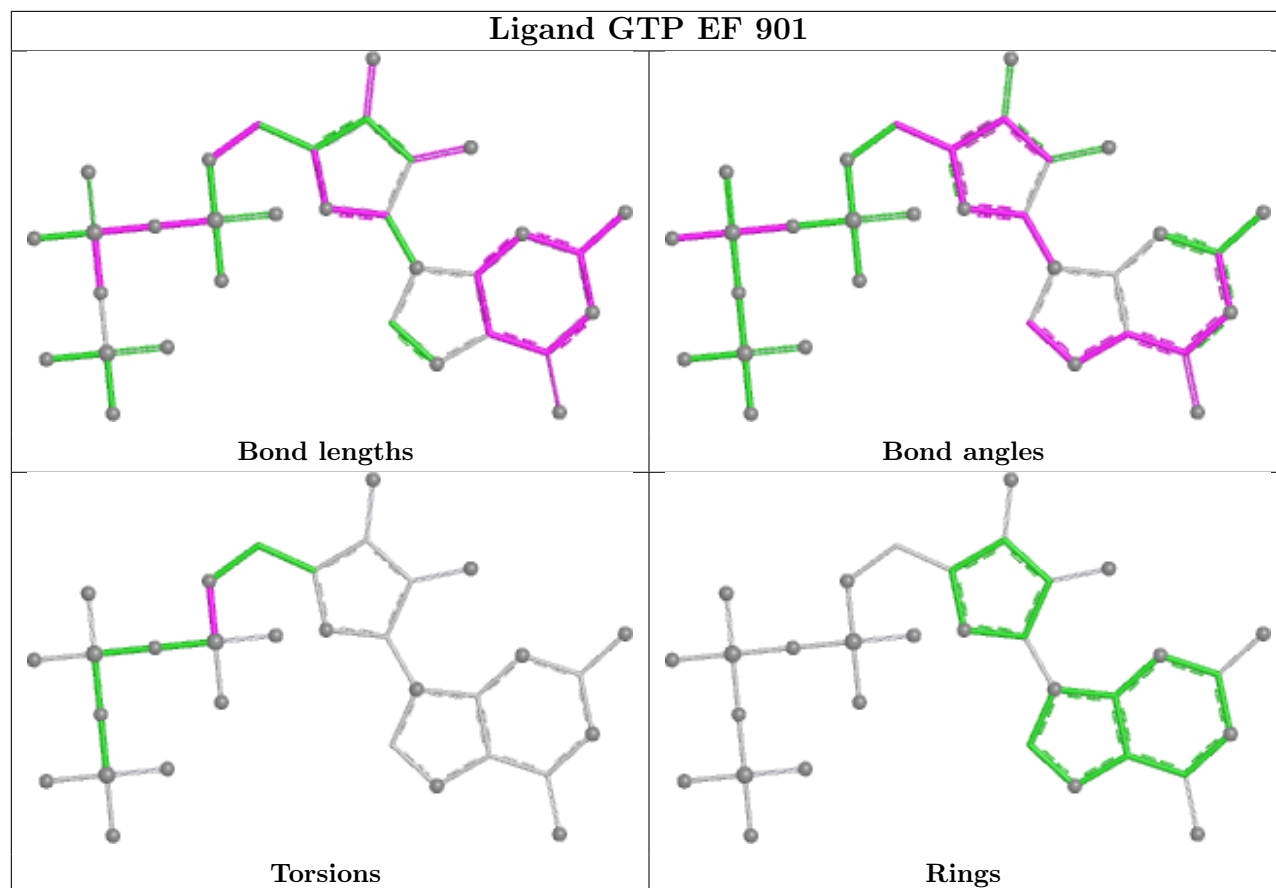
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

## Ligand PUT 23 3013

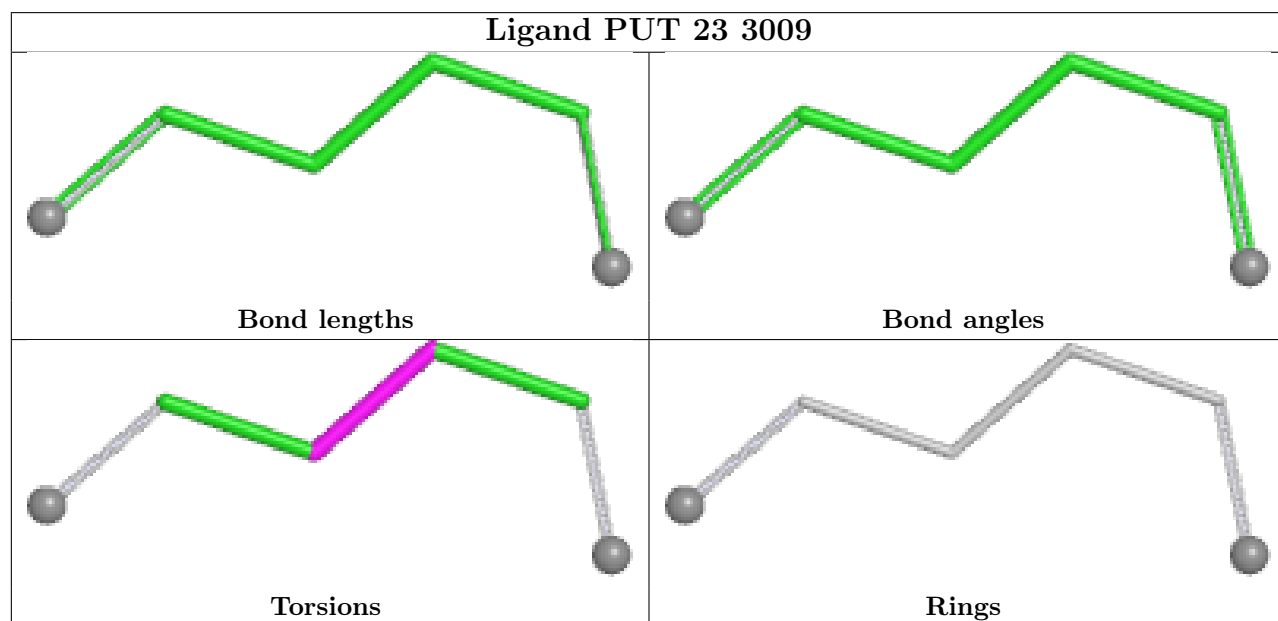
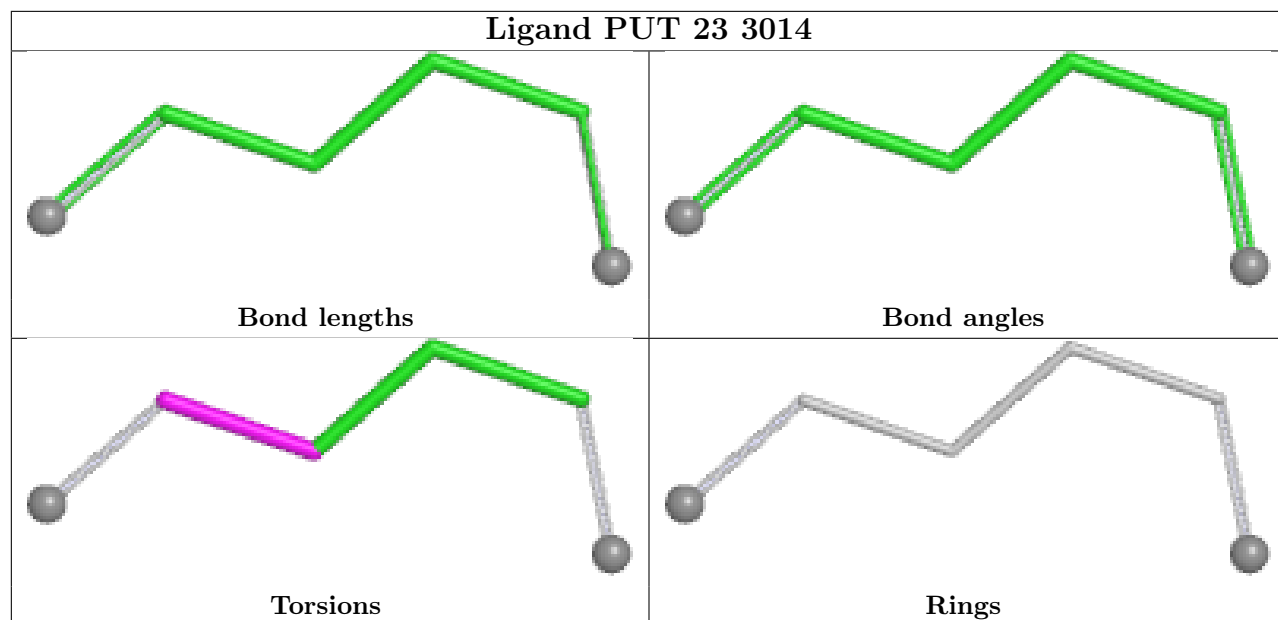


## Ligand SCM 16 1602

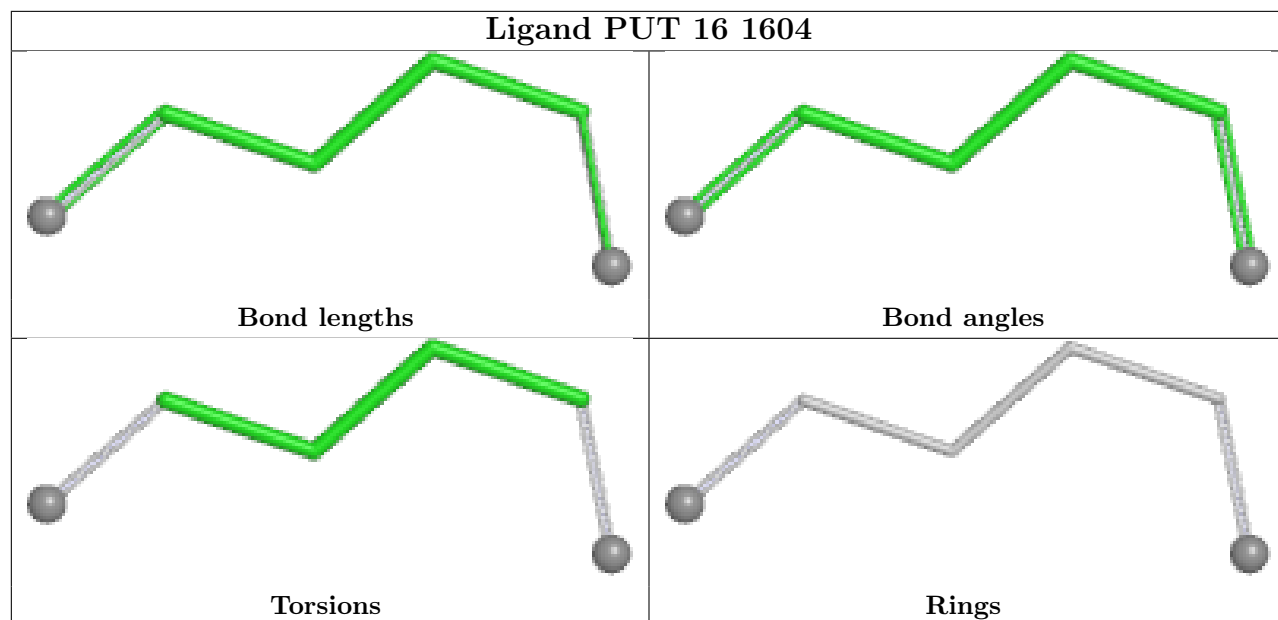




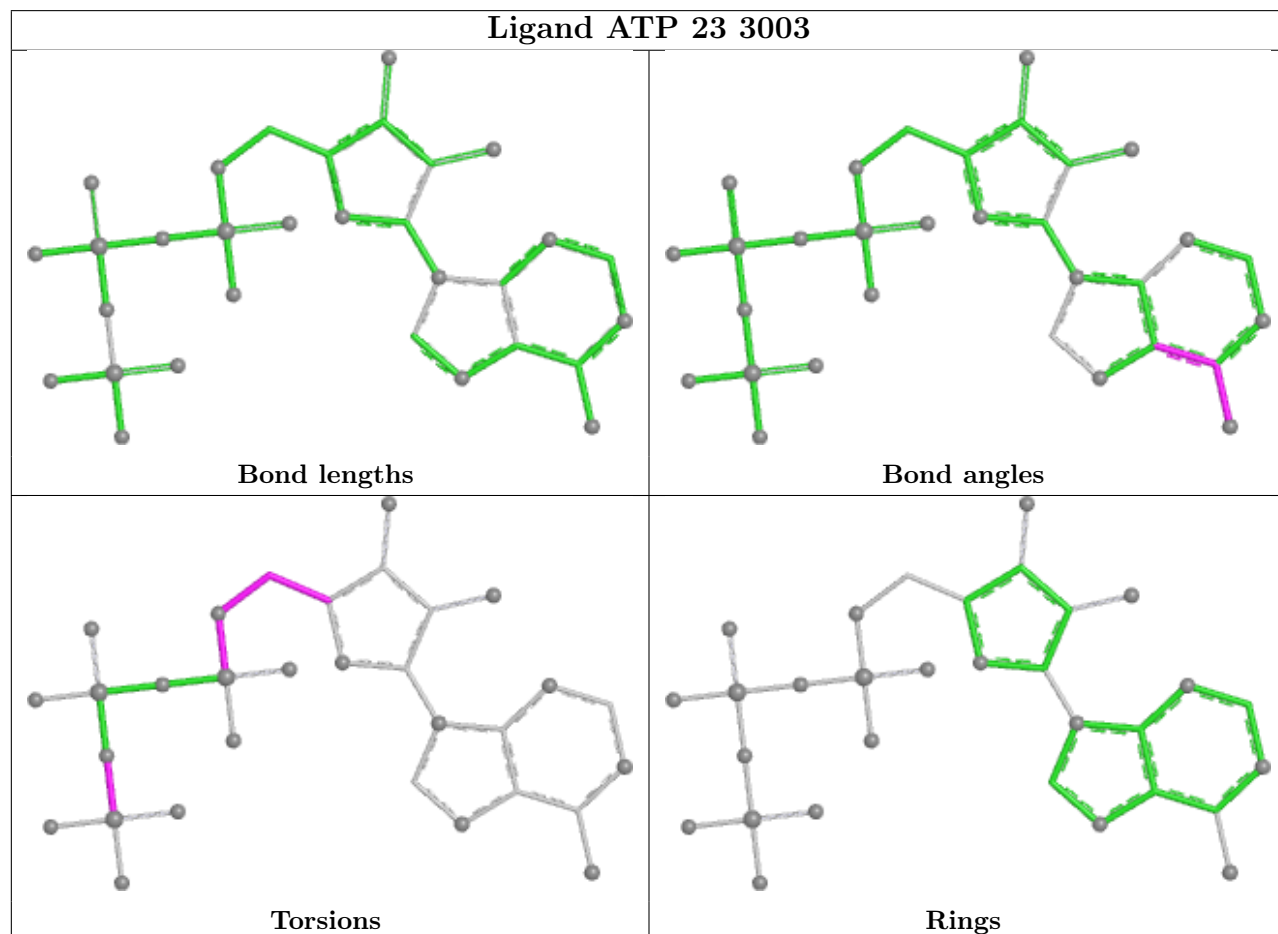




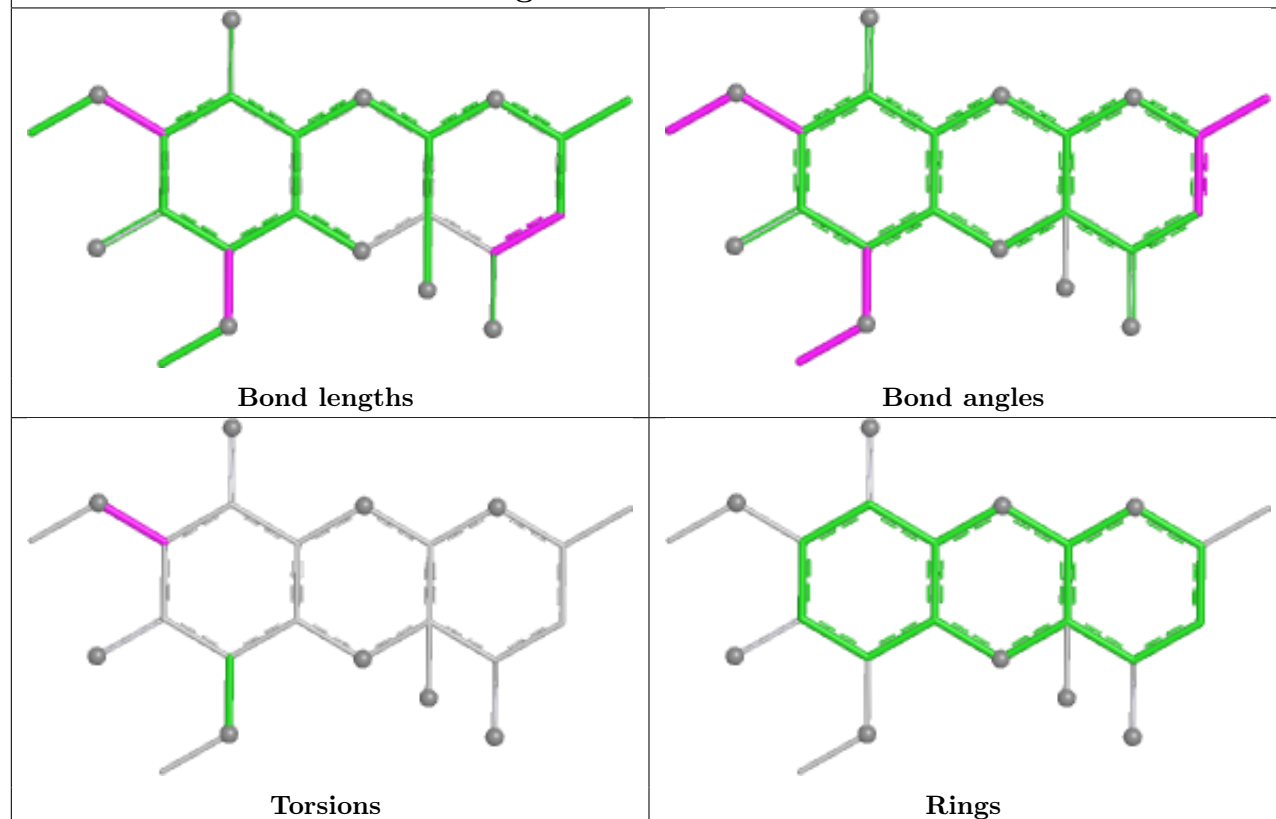
## Ligand PUT 16 1604



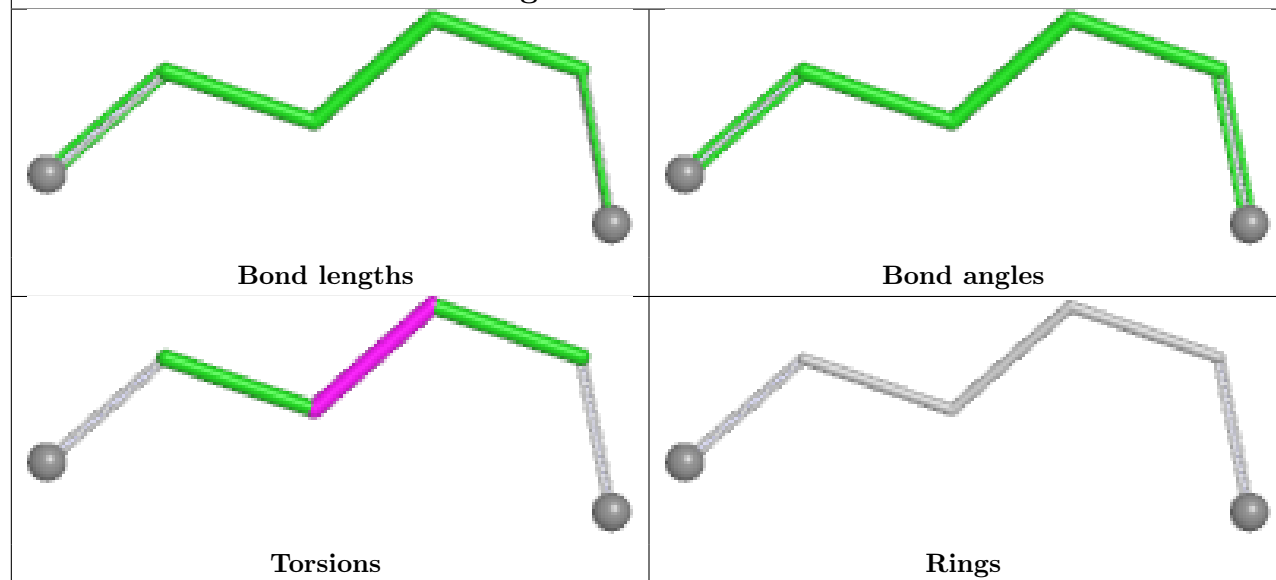
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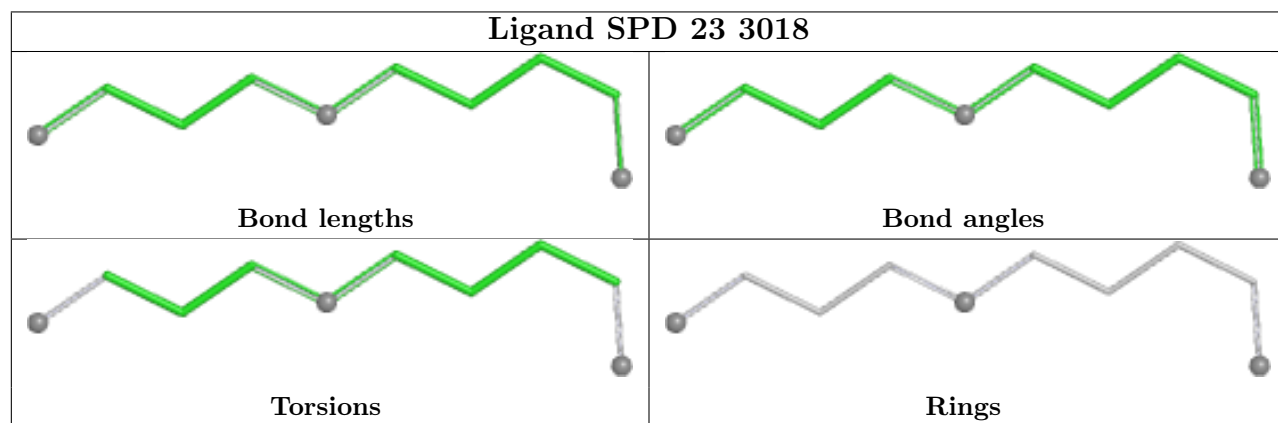
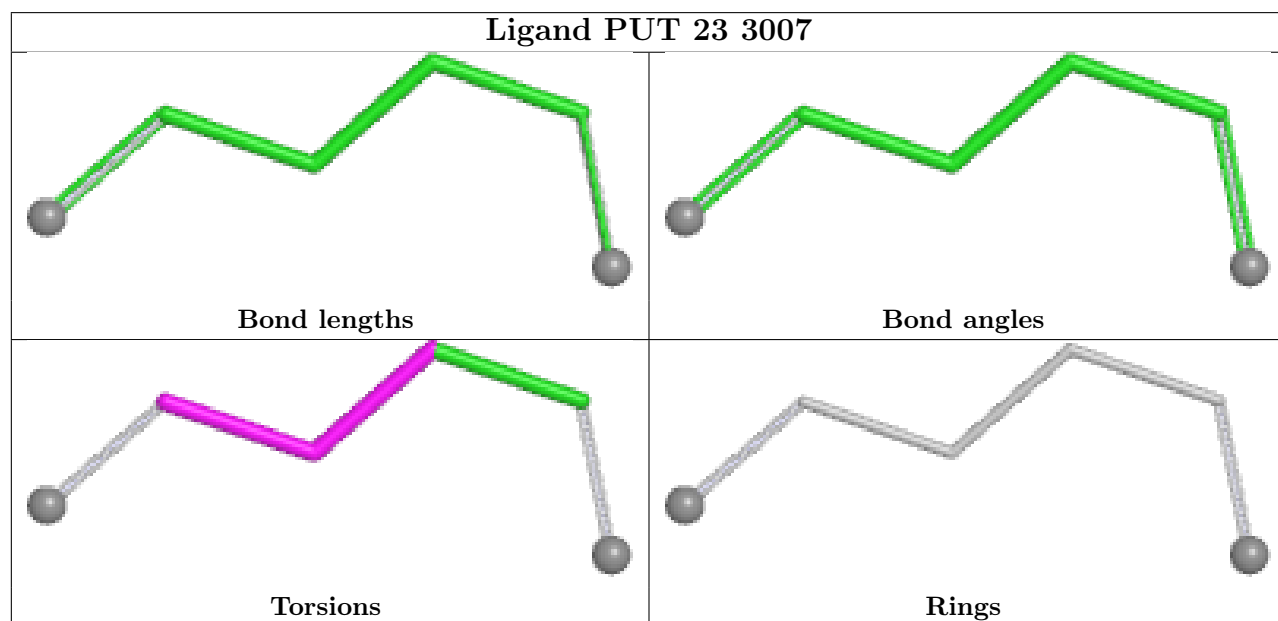
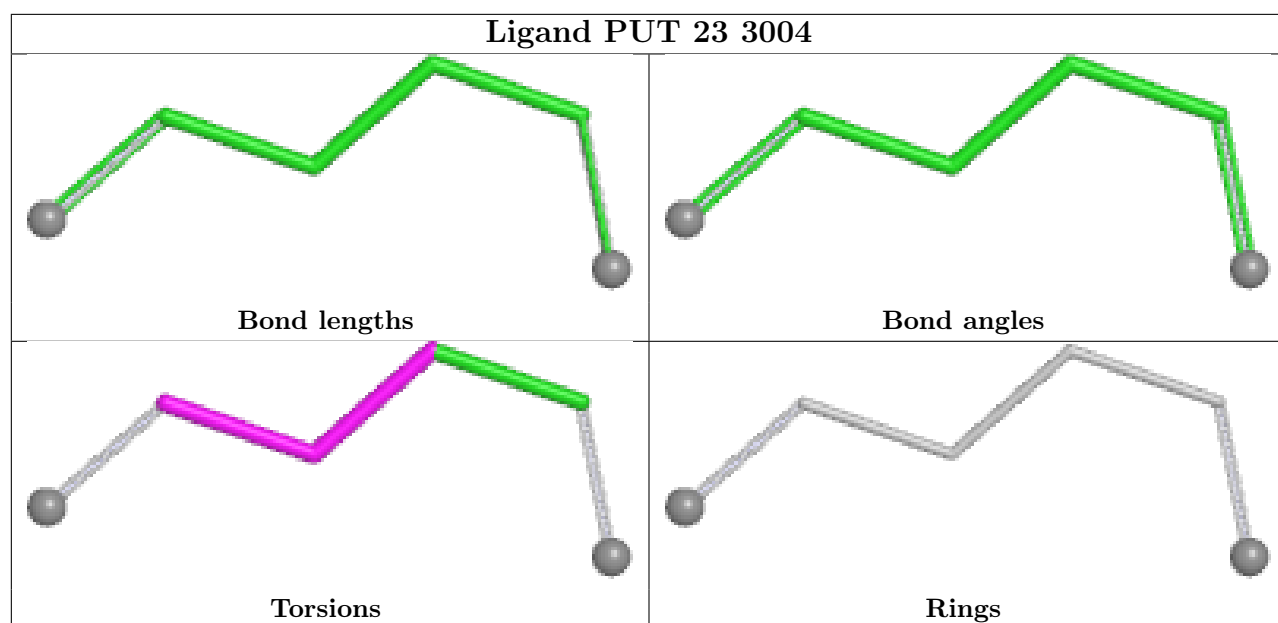


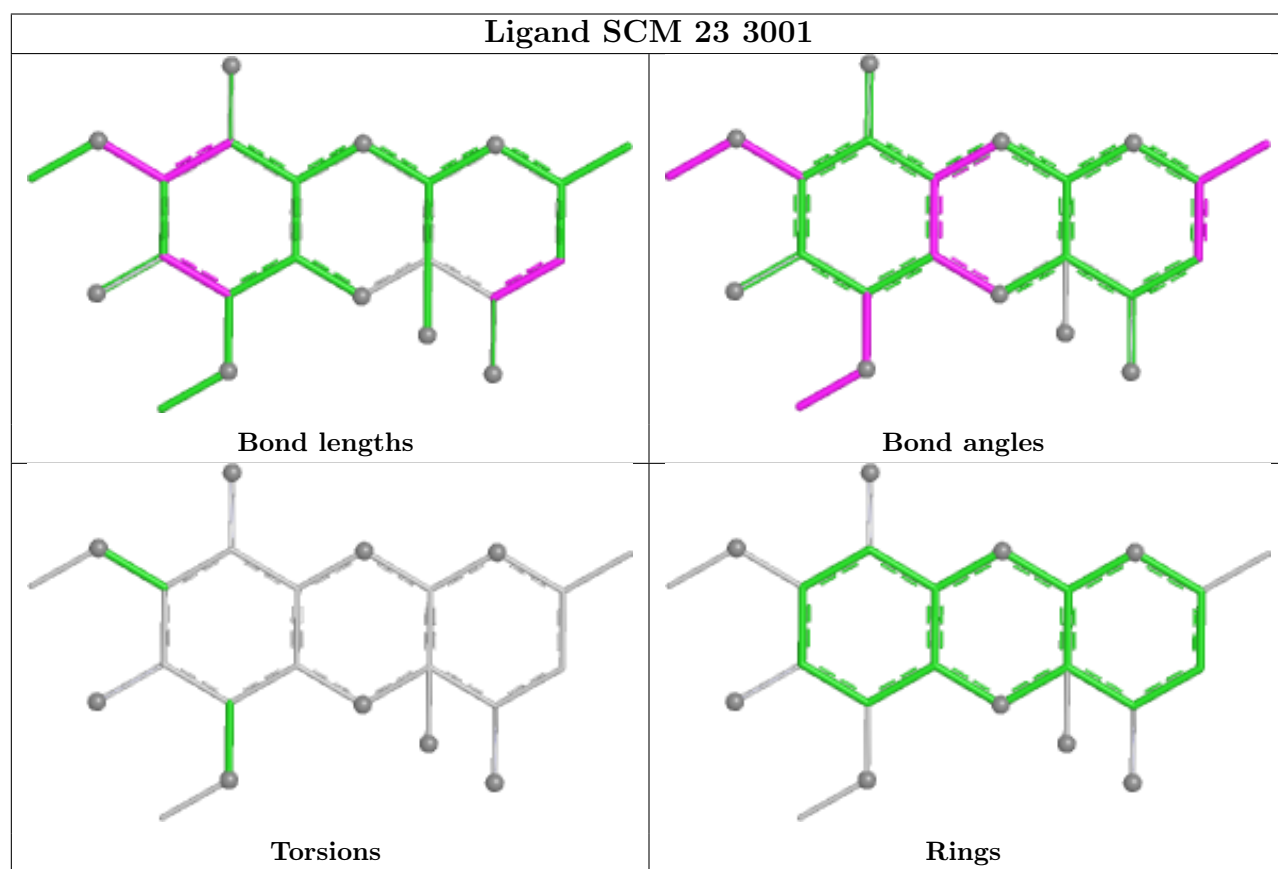
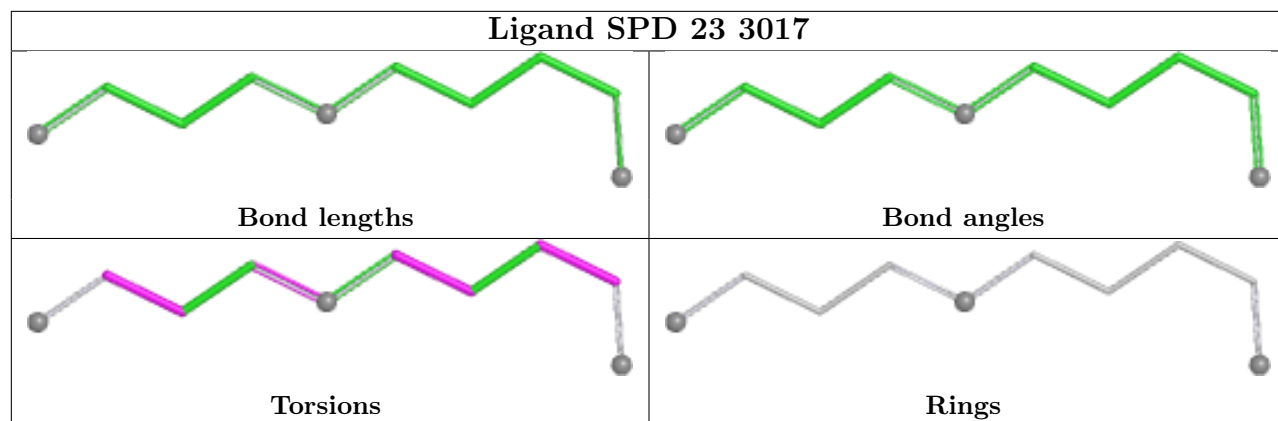
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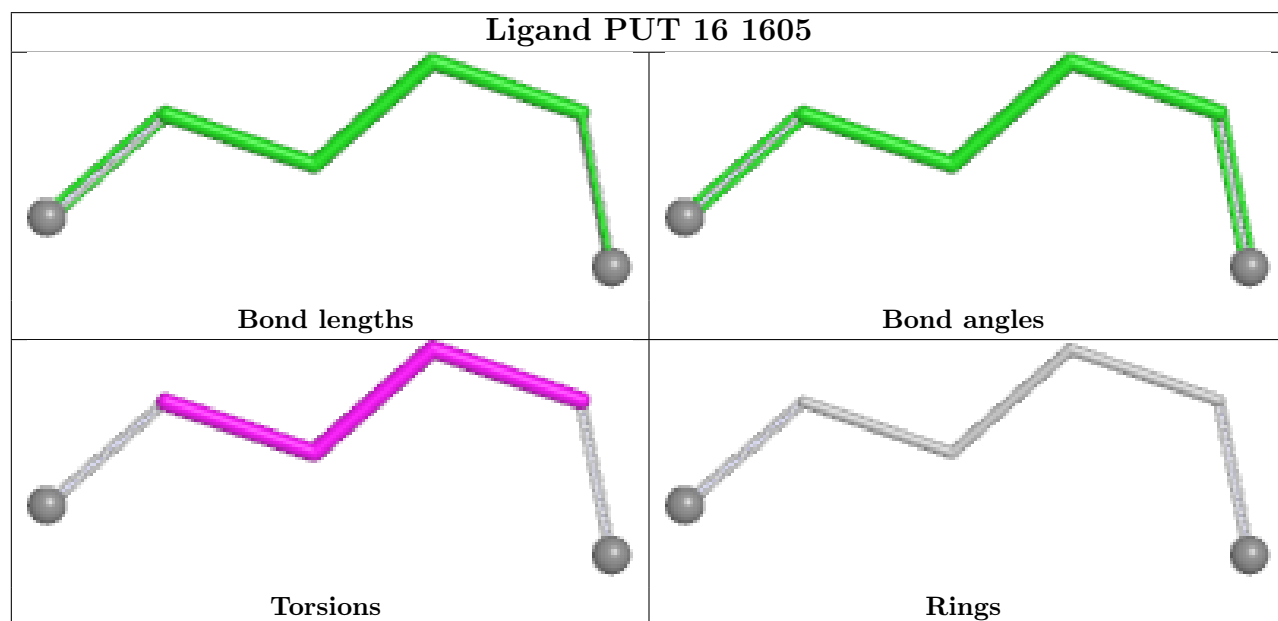
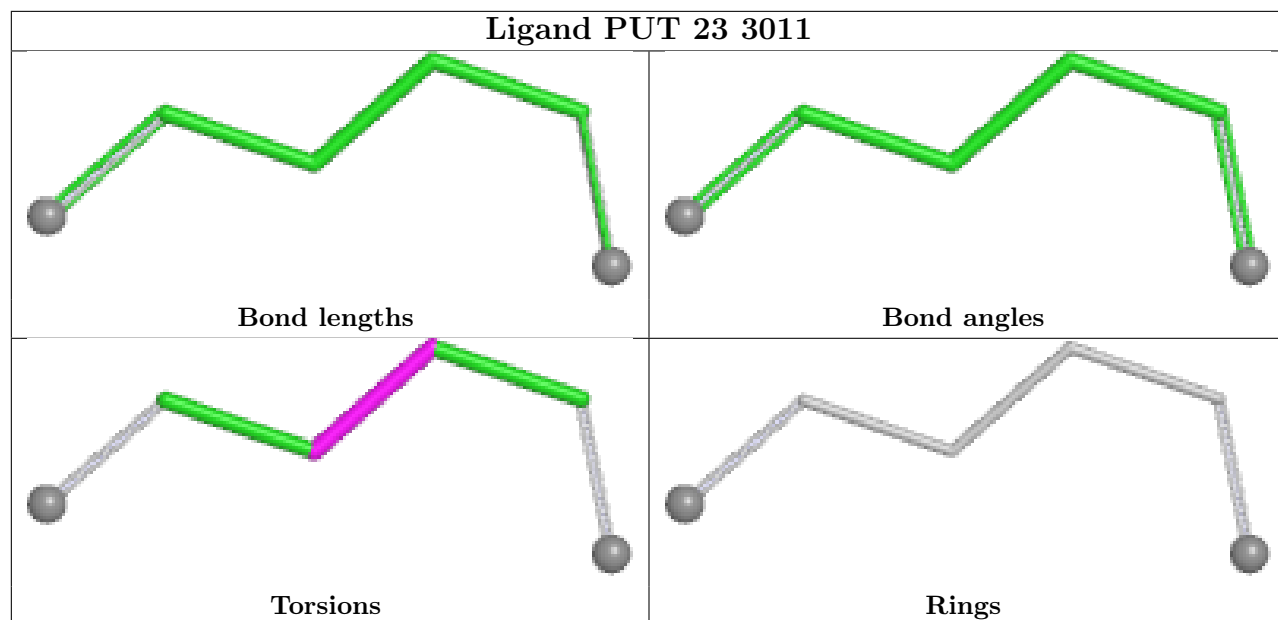


## Ligand PUT LC 301

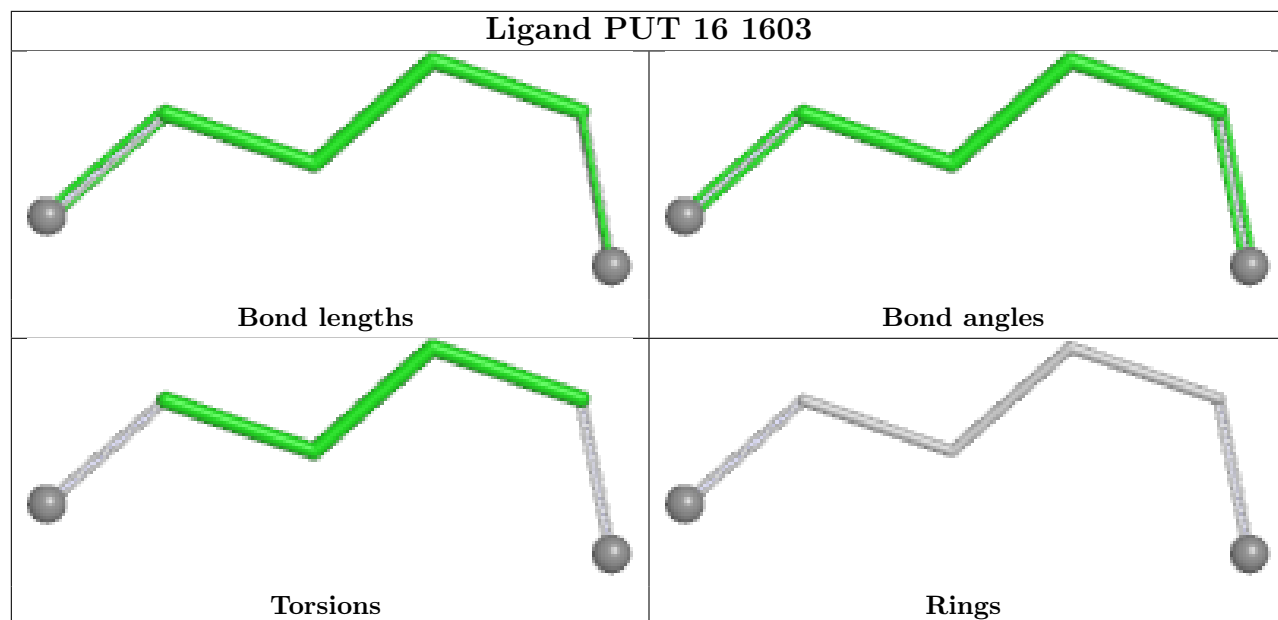




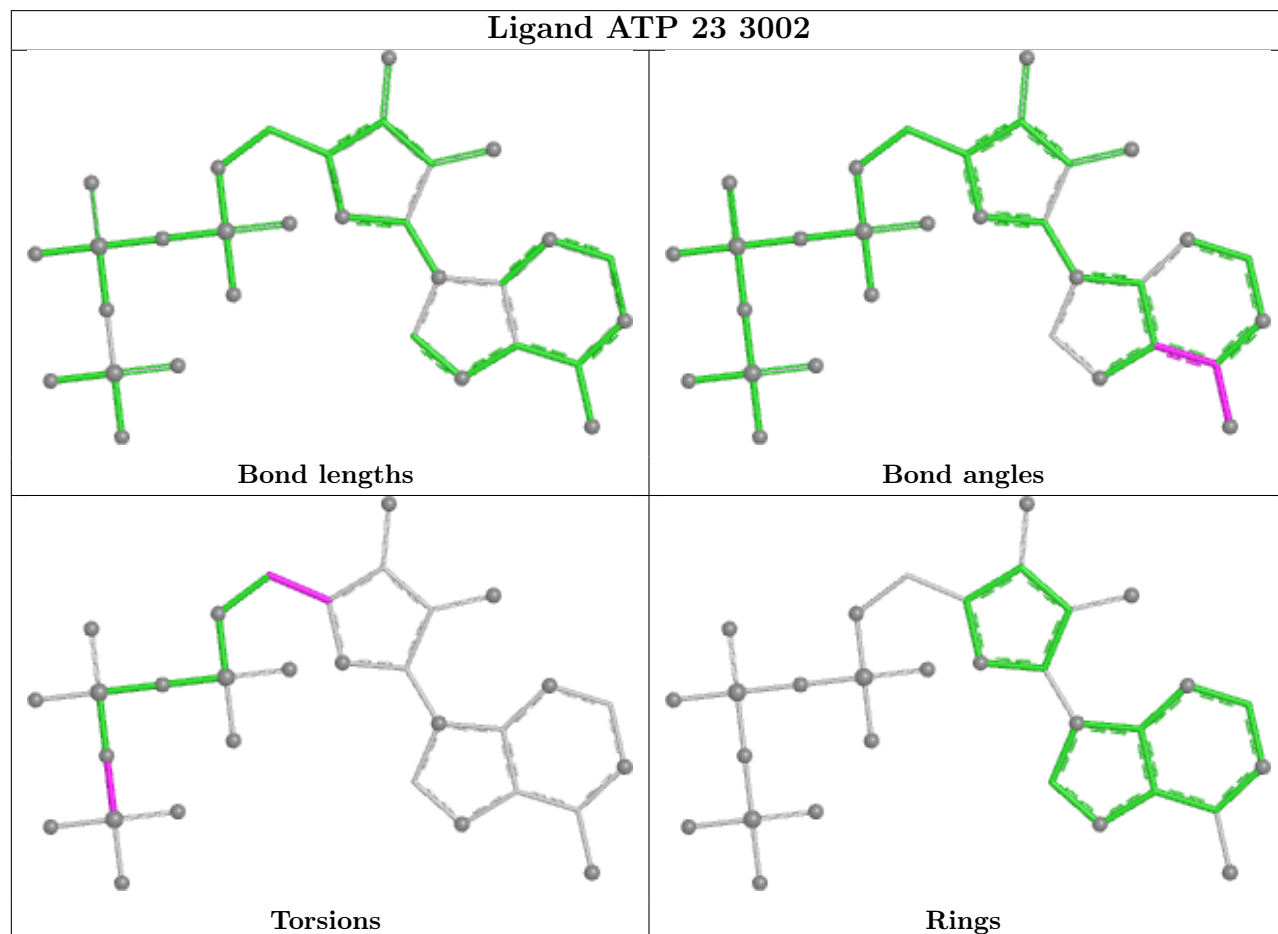


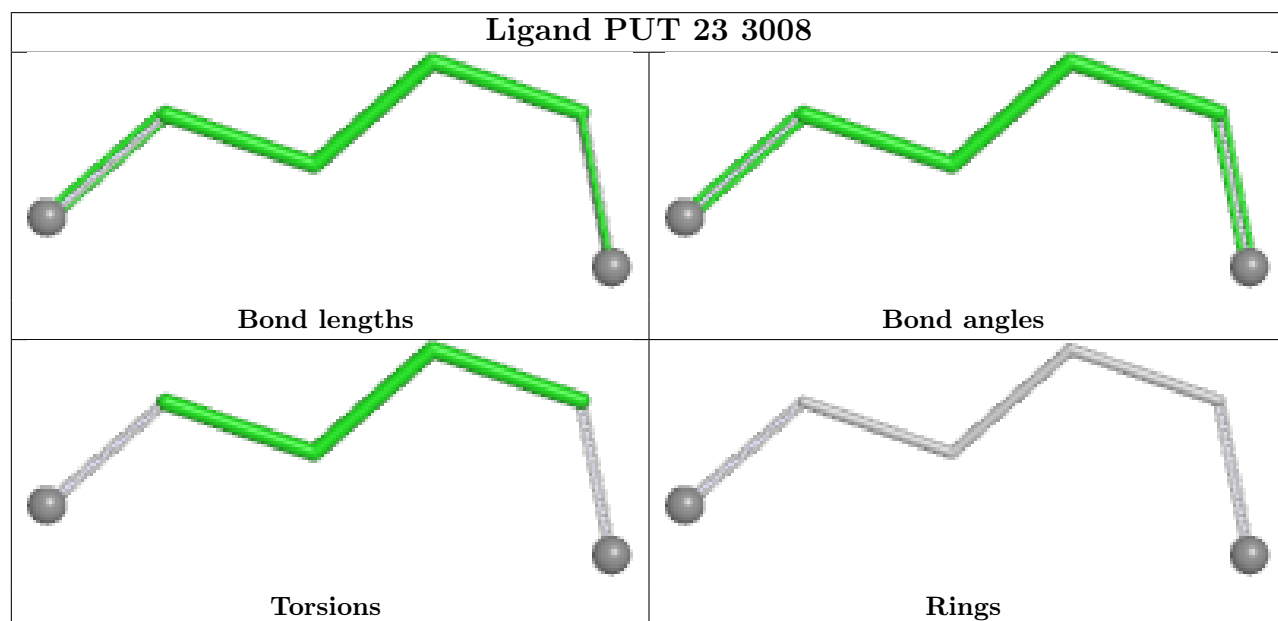
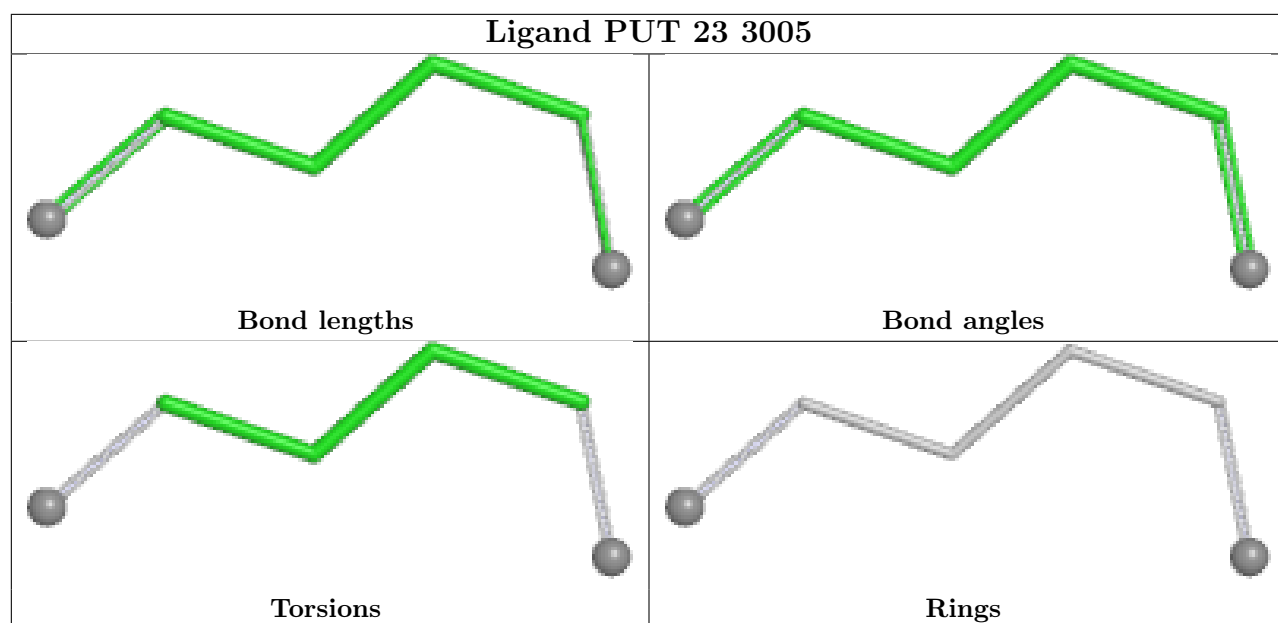


## Ligand PUT 16 1603

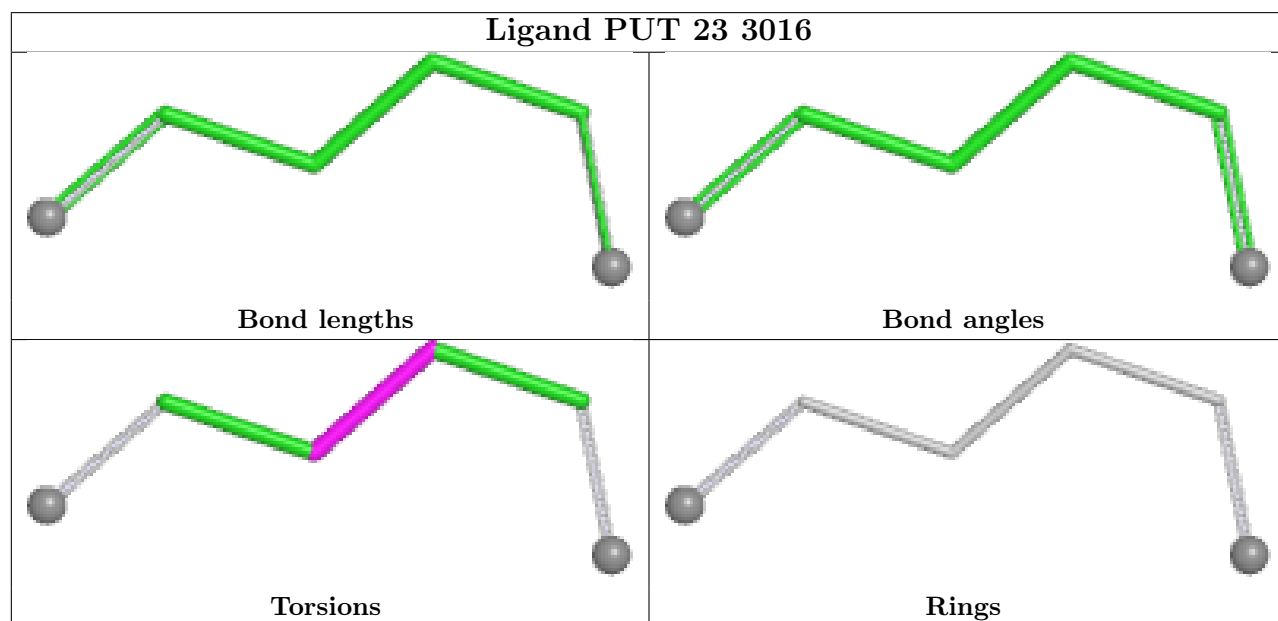
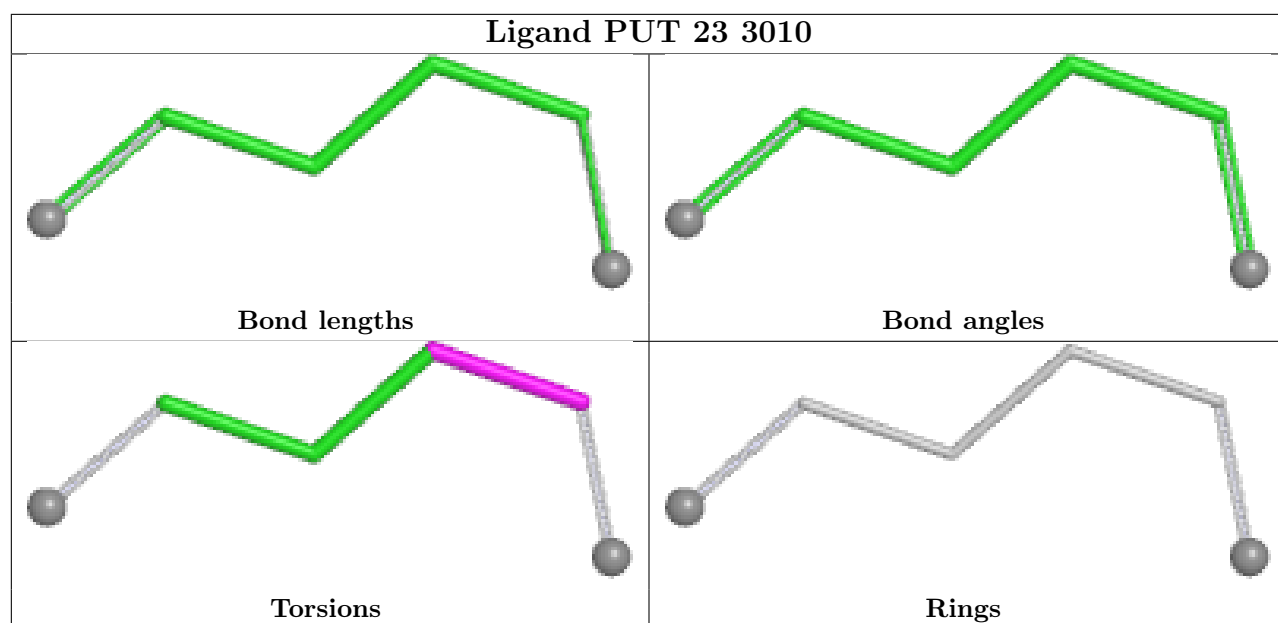


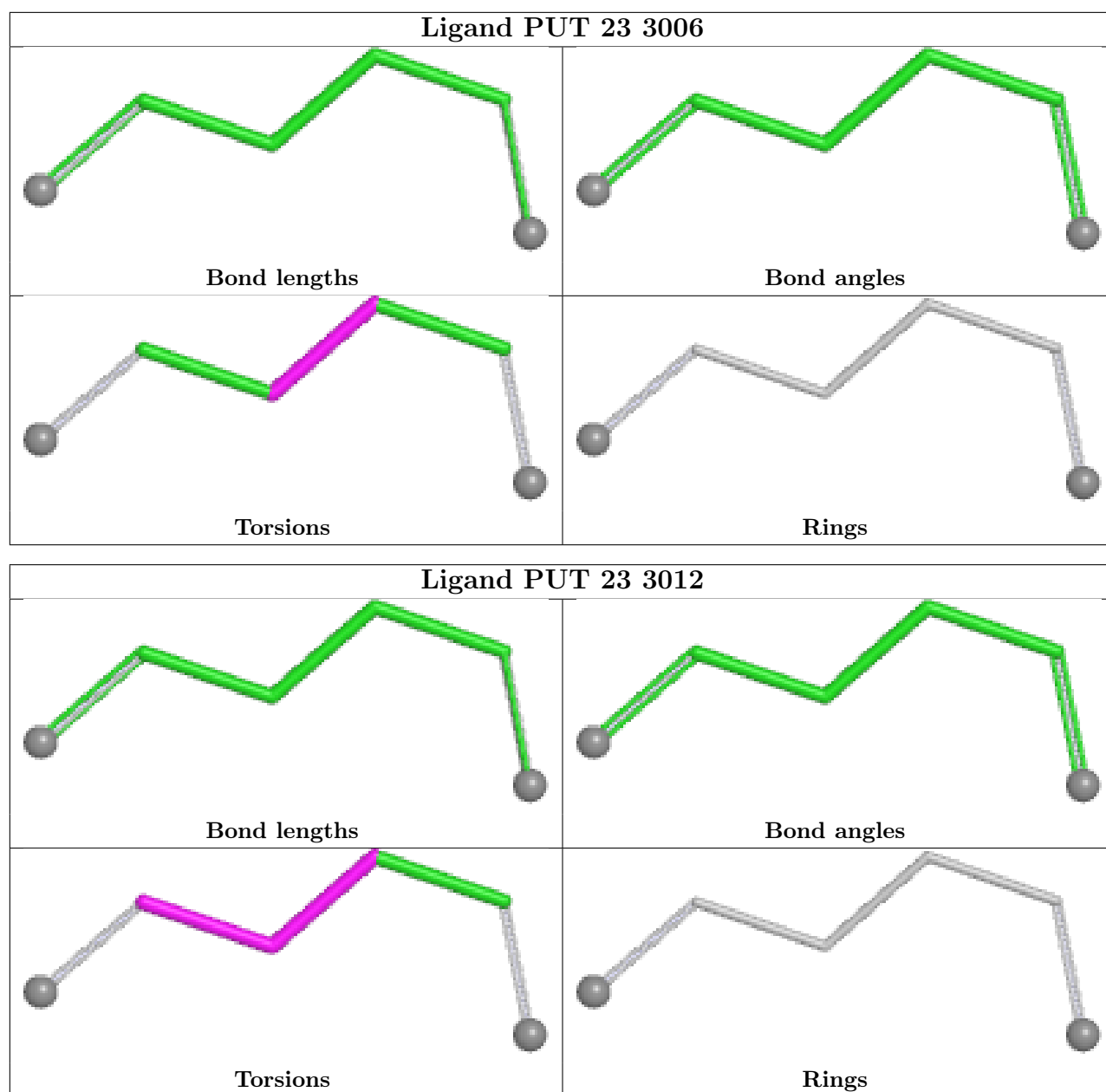
## Ligand ATP 23 3002











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
28	LE	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	LE	93:GLY	C	94:GLU	N	1.14

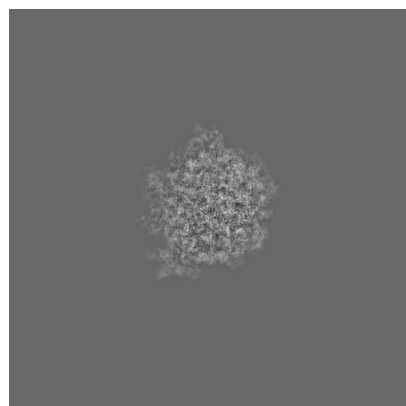
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24134. These allow visual inspection of the internal detail of the map and identification of artifacts.

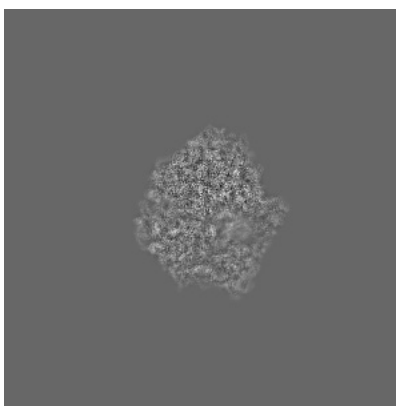
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

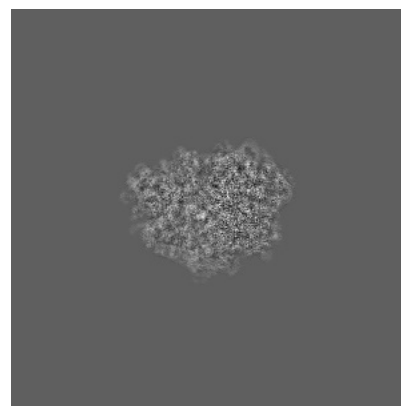
#### 6.1.1 Primary map



X

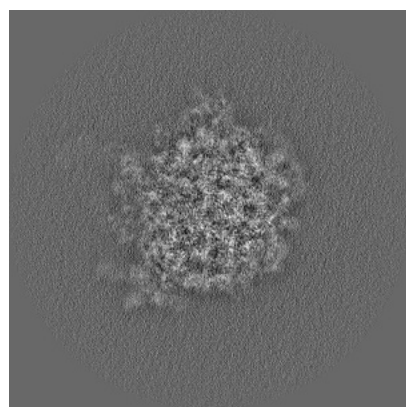


Y

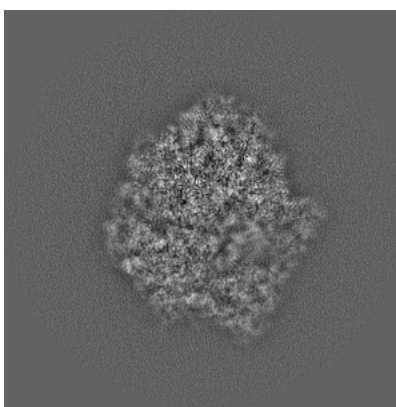


Z

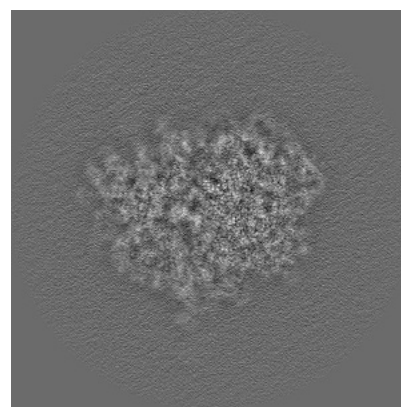
#### 6.1.2 Raw map



X



Y

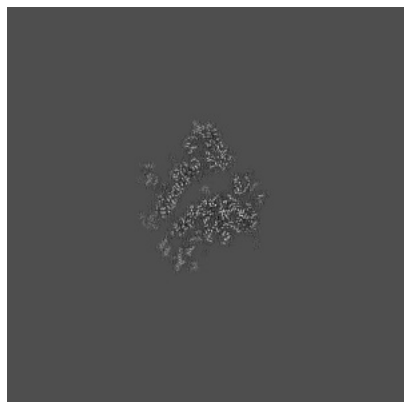


Z

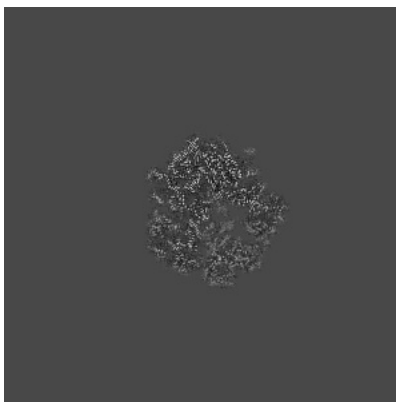
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

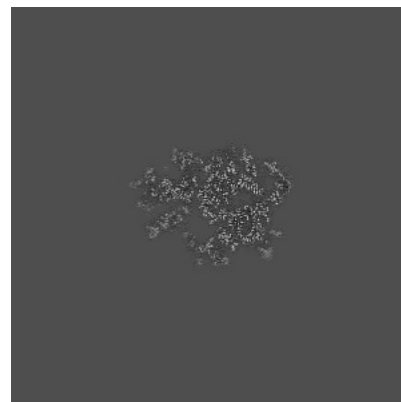
### 6.2.1 Primary map



X Index: 288

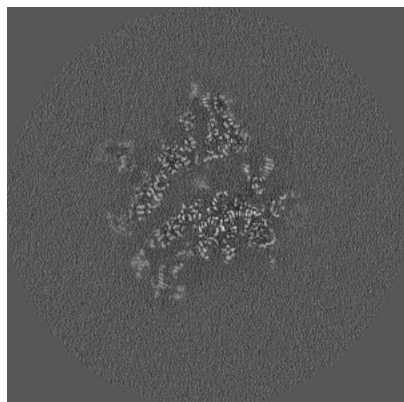


Y Index: 288

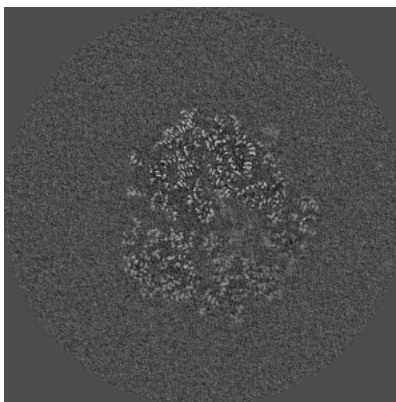


Z Index: 288

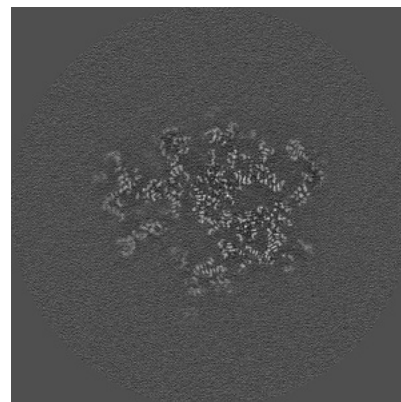
### 6.2.2 Raw map



X Index: 256



Y Index: 256

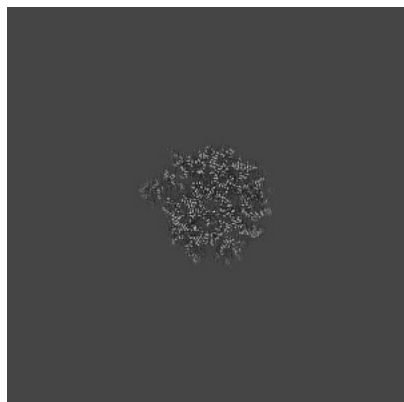


Z Index: 256

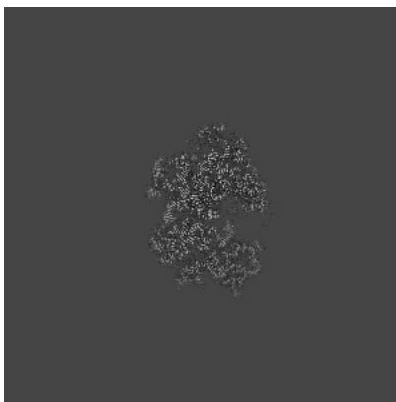
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 316

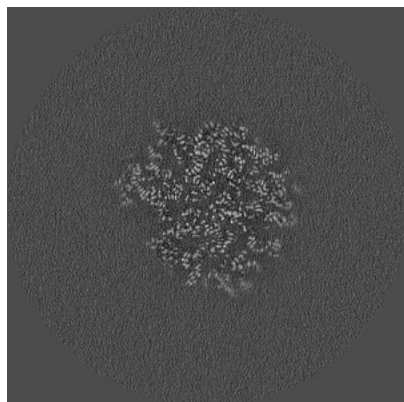


Y Index: 313

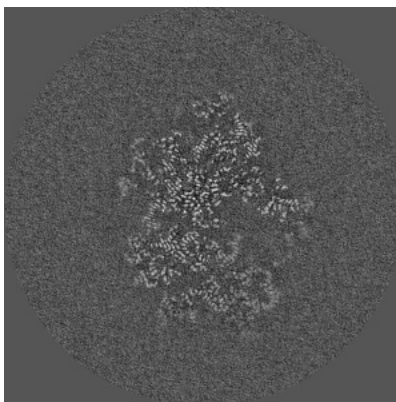


Z Index: 283

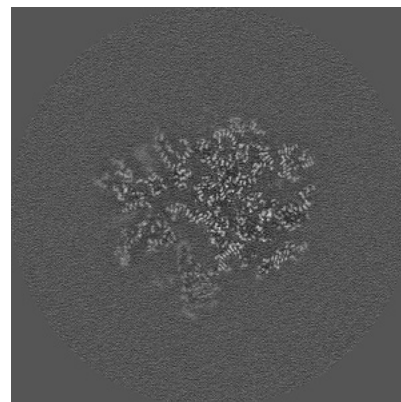
### 6.3.2 Raw map



X Index: 284



Y Index: 283

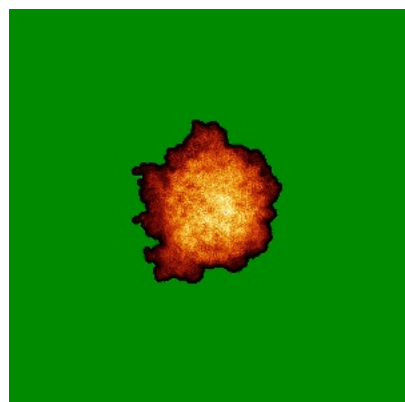


Z Index: 241

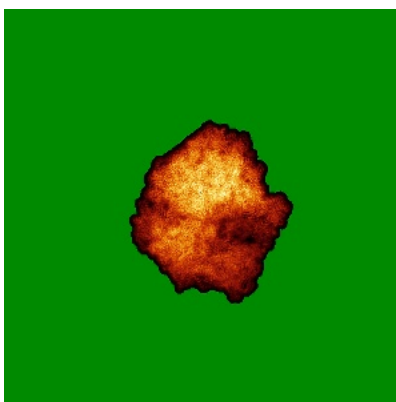
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

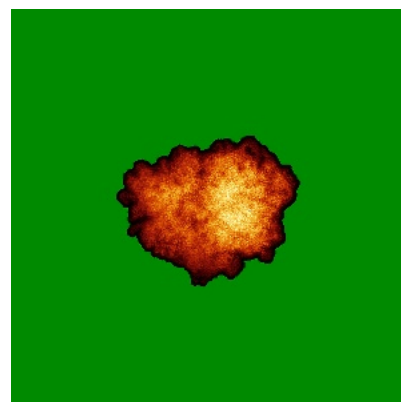
### 6.4.1 Primary map



X

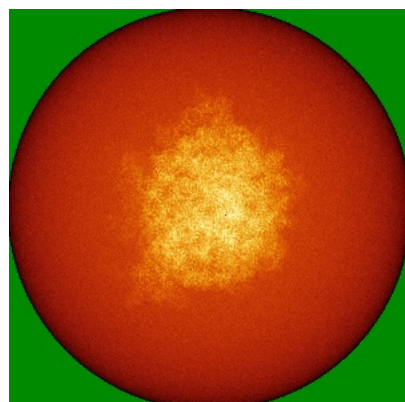


Y

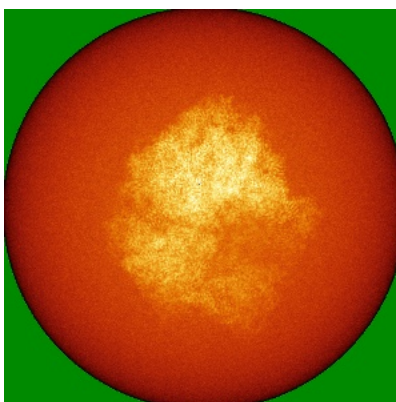


Z

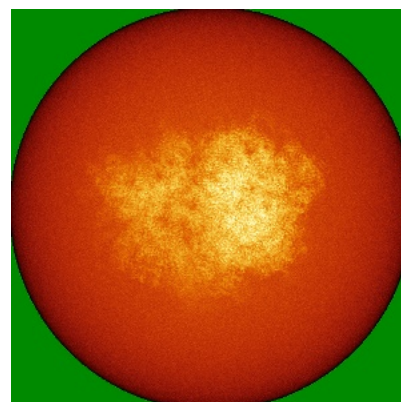
### 6.4.2 Raw map



X



Y



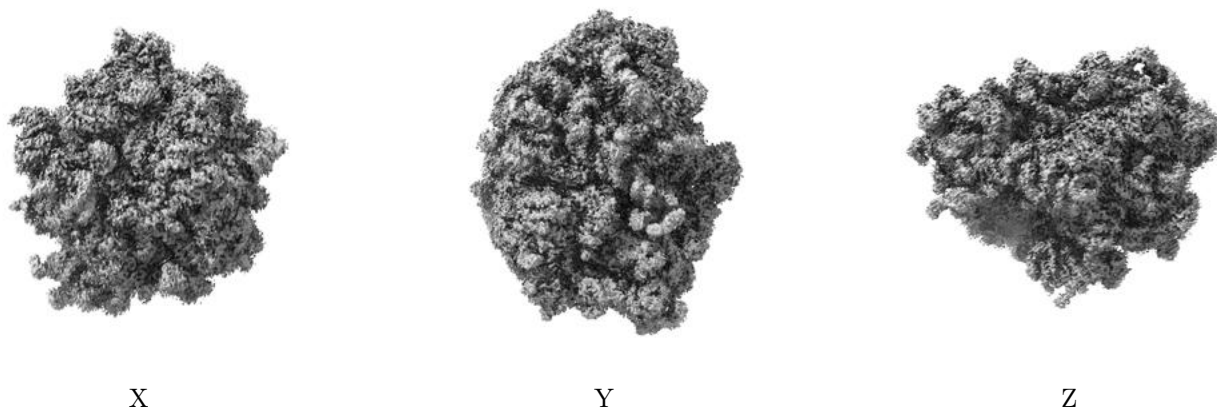
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



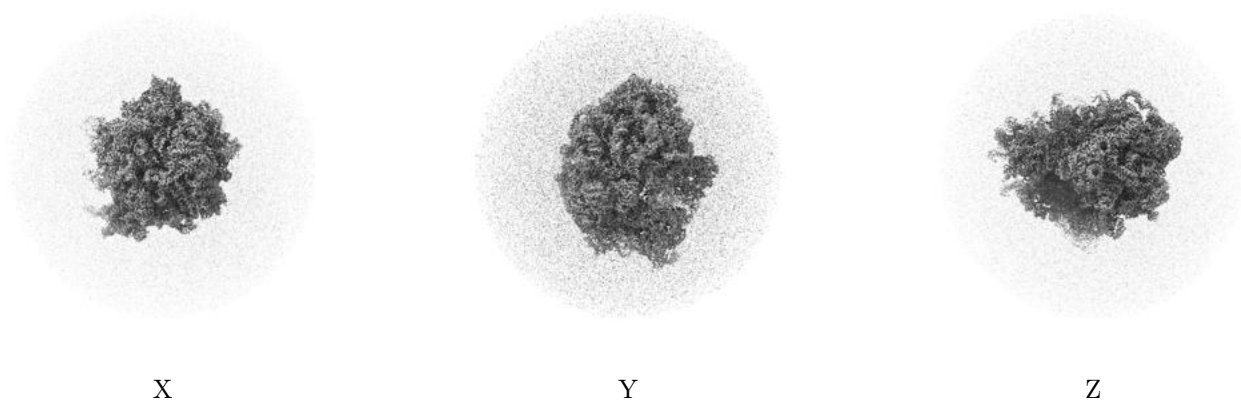
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

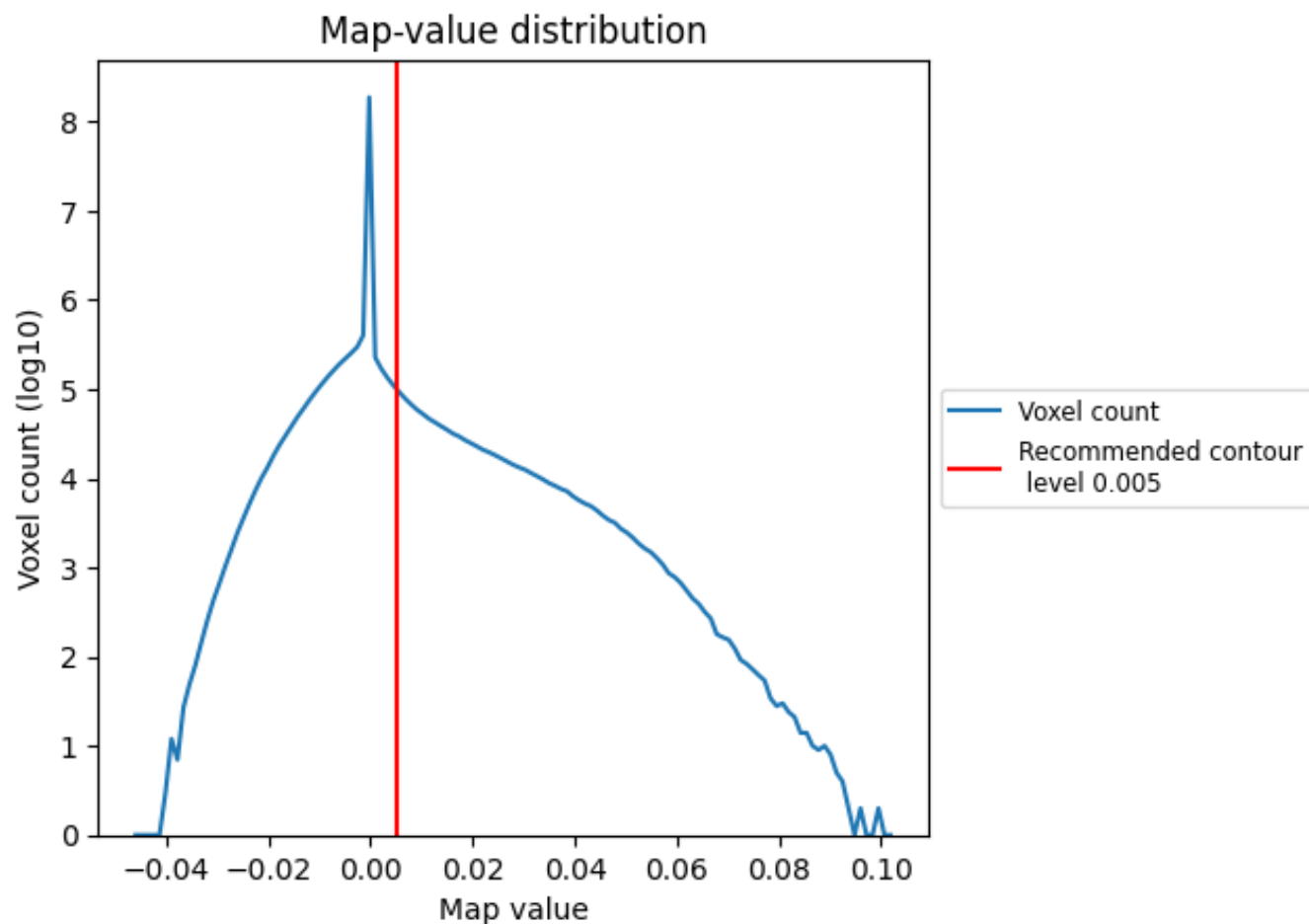
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

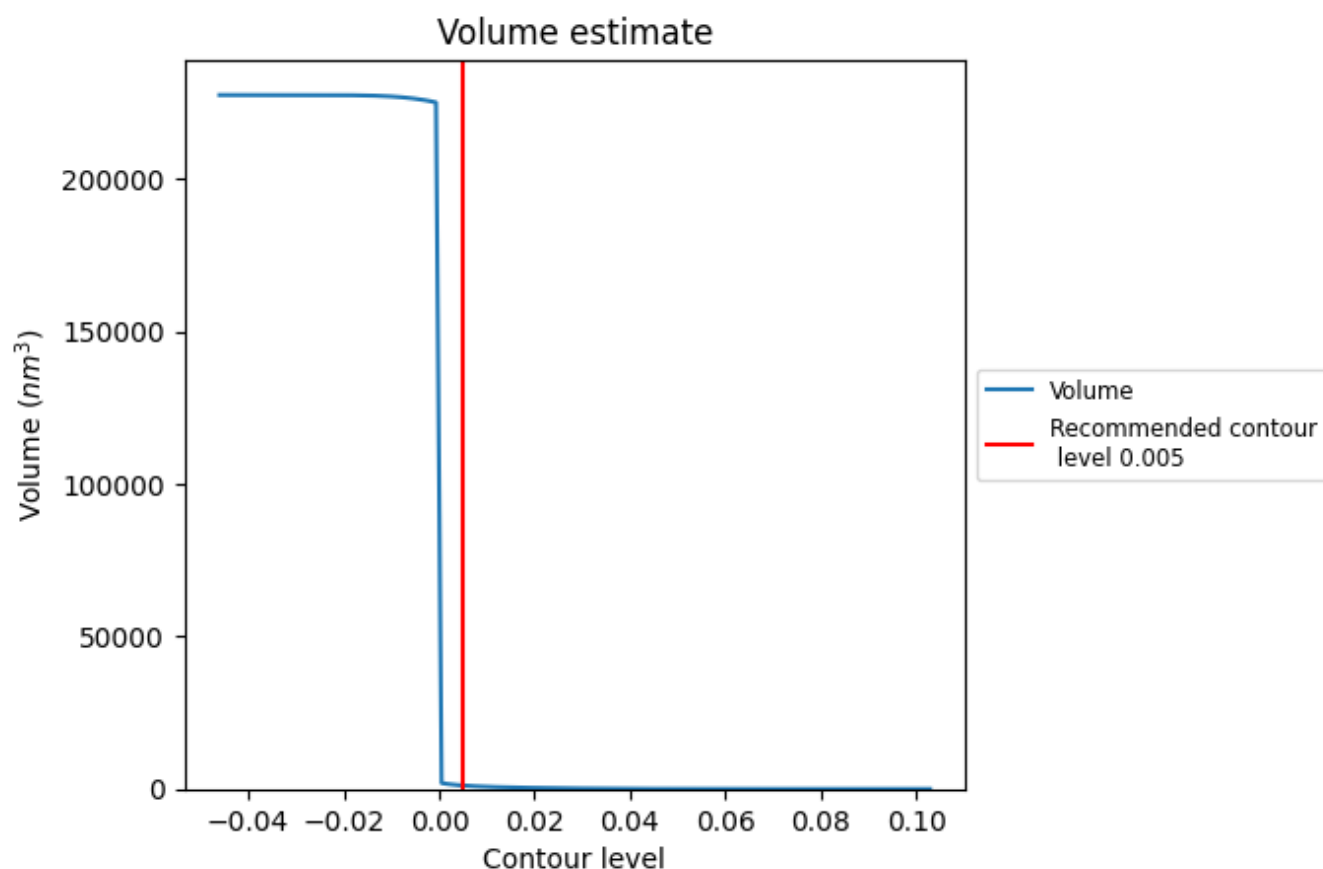
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

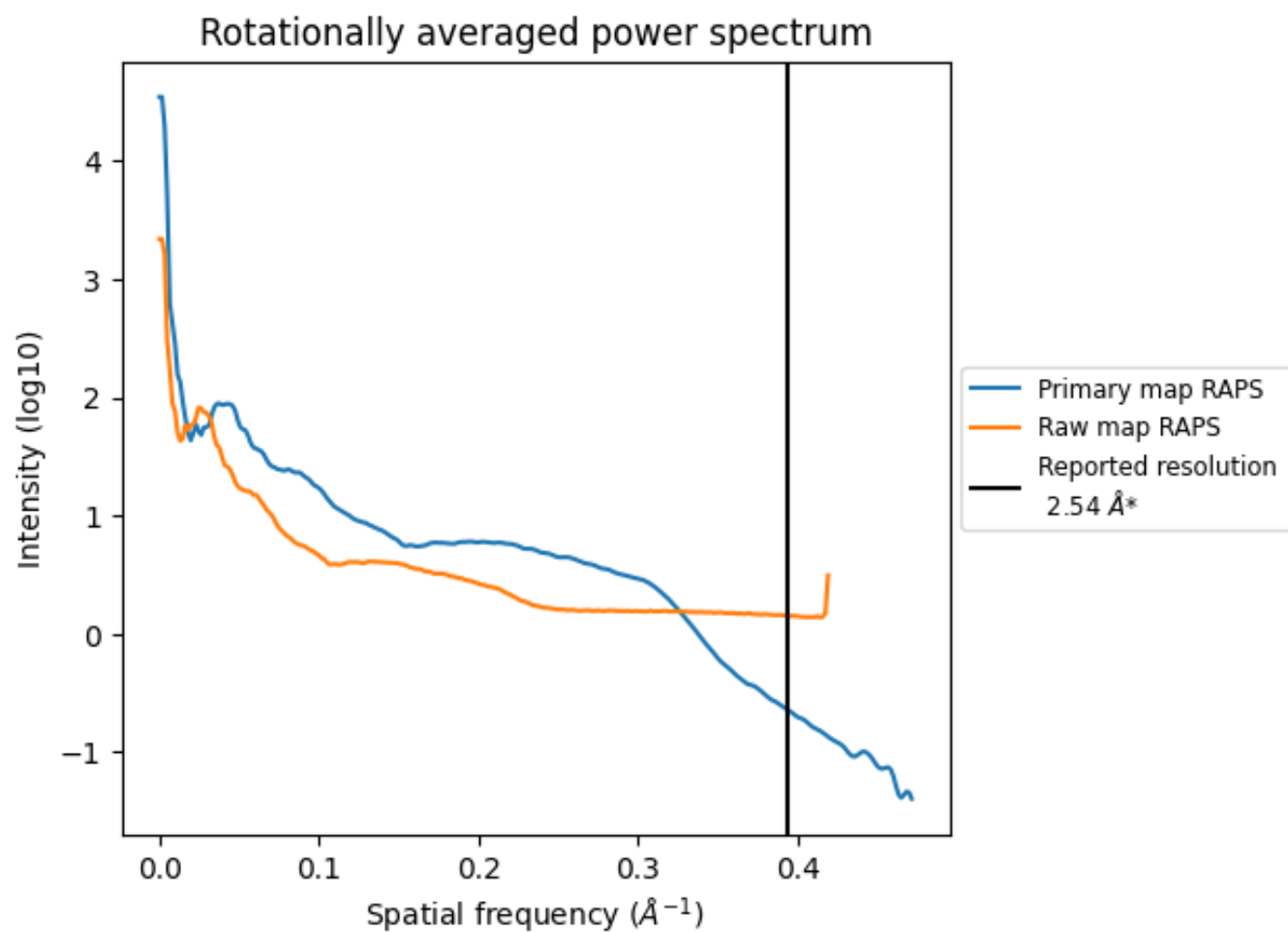
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1138 nm<sup>3</sup>; this corresponds to an approximate mass of 1028 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

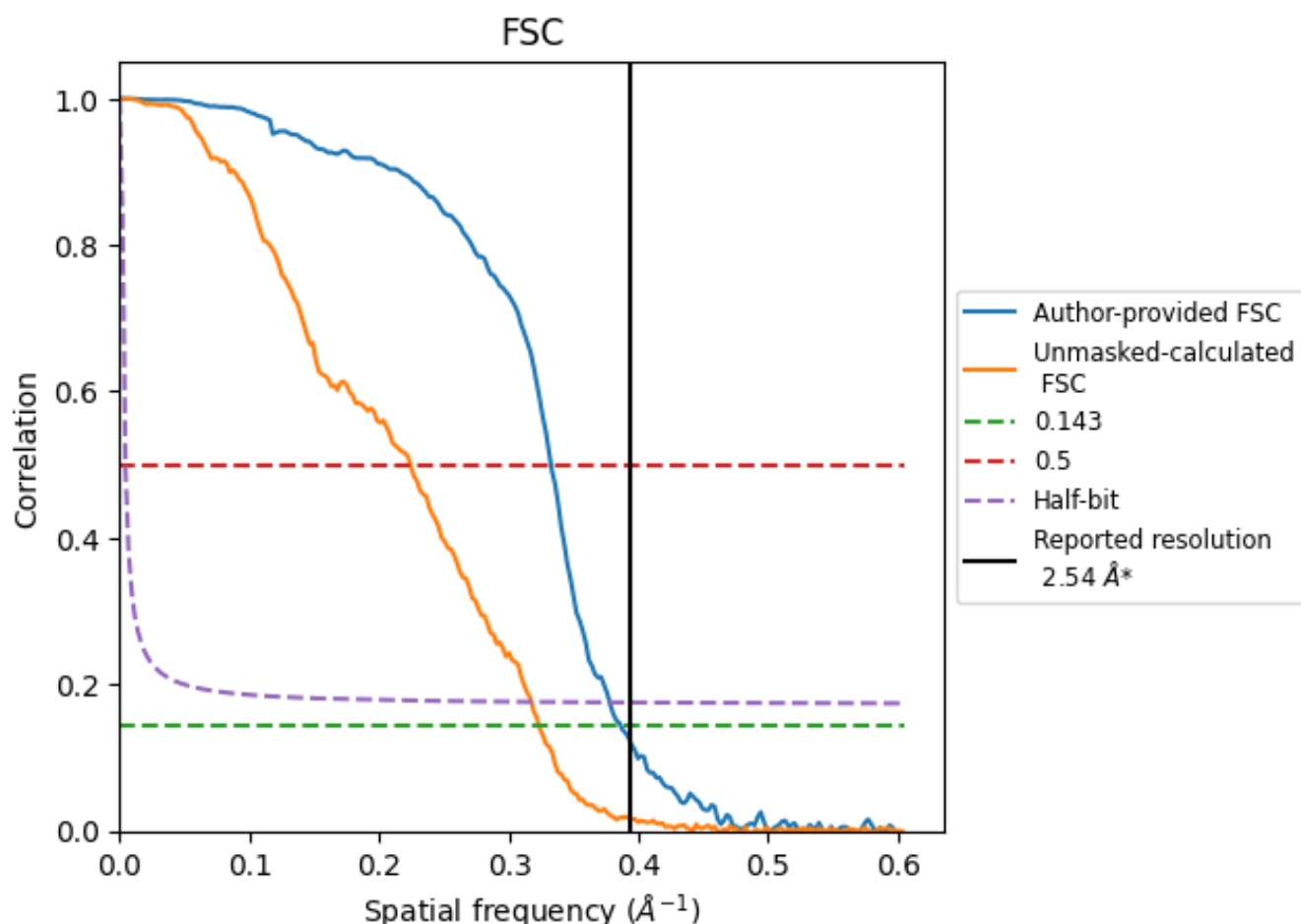


\*Reported resolution corresponds to spatial frequency of 0.394  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.394 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

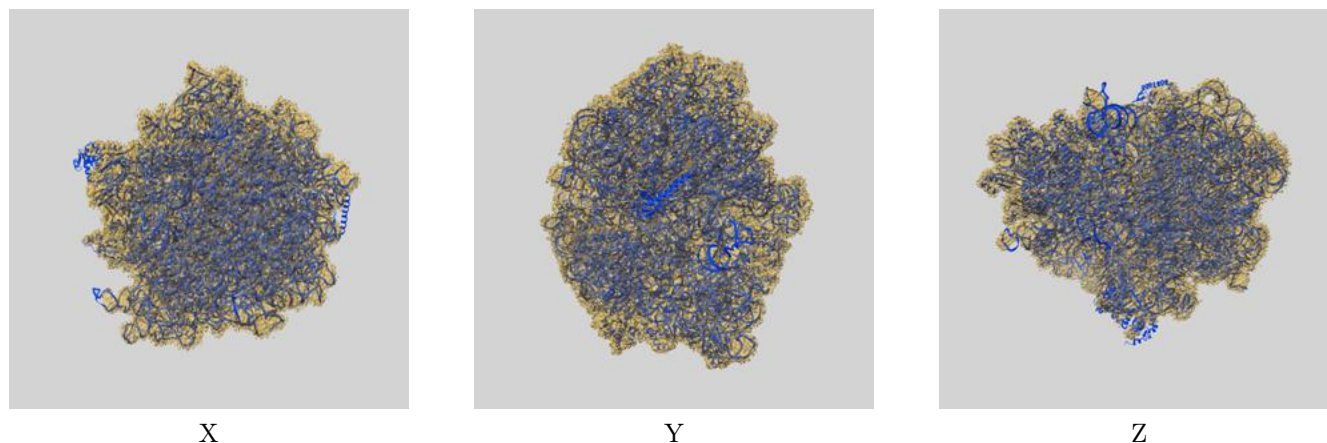
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.59	3.01	2.65
Unmasked-calculated*	3.09	4.46	3.15

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.54 by more than 10 %

## 9 Map-model fit [i](#)

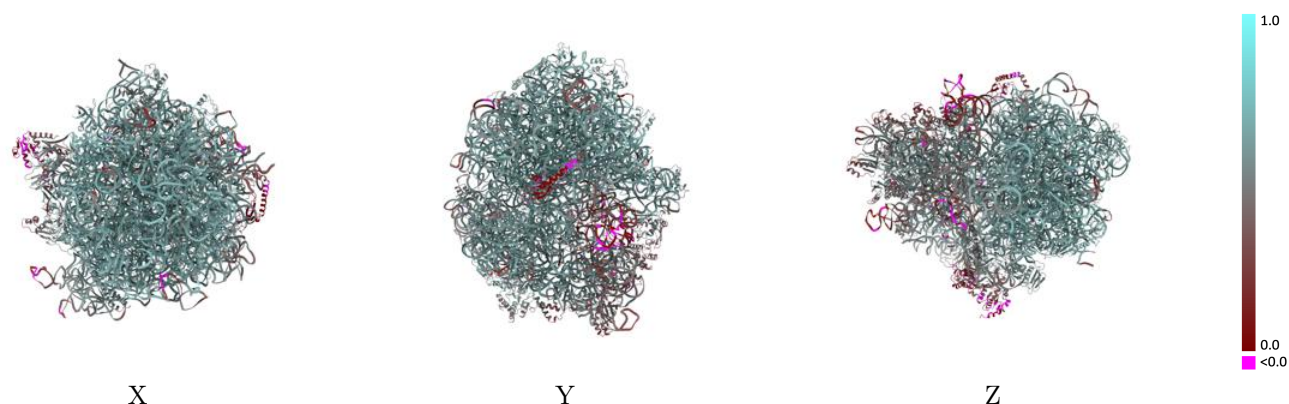
This section contains information regarding the fit between EMDB map EMD-24134 and PDB model 7N2V. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

### 9.1 Map-model overlay [i](#)



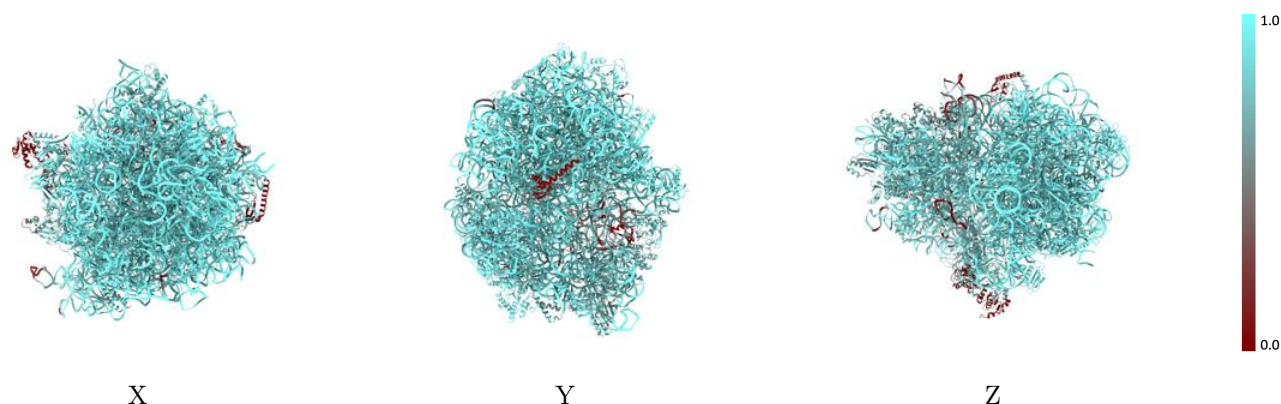
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



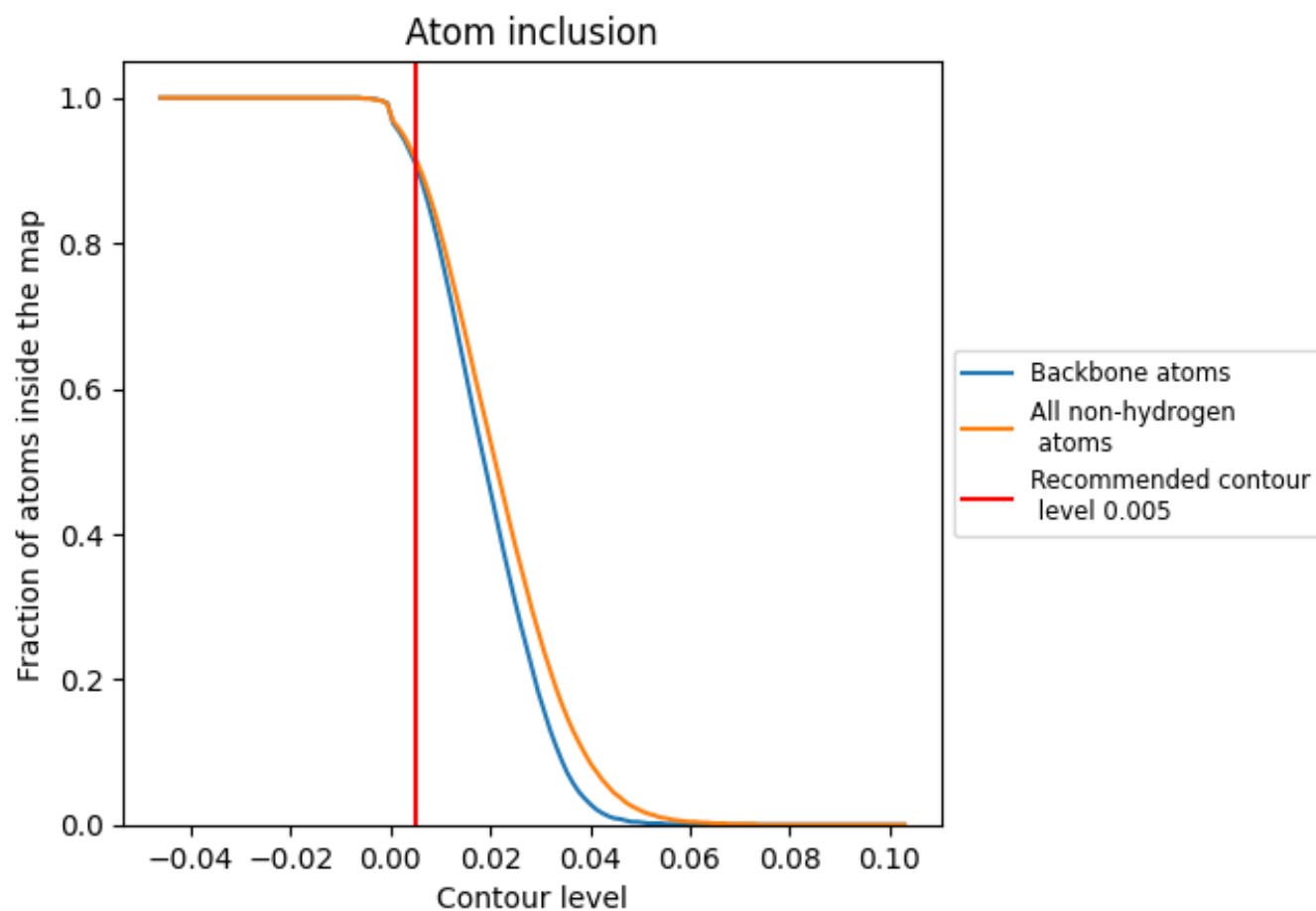
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

## 9.4 Atom inclusion ⓘ









































































At the recommended contour level, 91% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary ⓘ



















































The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9170	 0.5720
16	 0.9590	 0.5690
23	 0.9640	 0.6090
5	 0.9780	 0.6000
Dt	 0.8910	 0.4920
EF	 0.7830	 0.4930
LB	 0.9650	 0.6490
LC	 0.9550	 0.6400
LD	 0.9450	 0.6130
LE	 0.8080	 0.4680
LF	 0.9030	 0.5430
LI	 0.3000	 0.1740
LJ	 0.2670	 0.1690
LK	 0.2660	 0.1600
LM	 0.9600	 0.6430
LN	 0.9610	 0.6400
LO	 0.9560	 0.6290
LP	 0.9590	 0.6400
LQ	 0.9600	 0.6440
LR	 0.9110	 0.5740
LS	 0.9320	 0.6190
LT	 0.9710	 0.6620
LU	 0.9460	 0.6210
LV	 0.9450	 0.6390
LW	 0.9090	 0.5920
LX	 0.9260	 0.5800
LY	 0.9360	 0.5950
La	 0.9400	 0.6330
Lb	 0.9380	 0.6210
Lc	 0.8900	 0.5650
Ld	 0.9380	 0.6210
Le	 0.7840	 0.4100
Lf	 0.9390	 0.6280
Lg	 0.9040	 0.5960
Lh	 0.9470	 0.6590



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
Li	 0.9590	 0.6550
Lj	 0.9210	 0.6330
Pp	 0.7860	 0.5470
Pt	 0.6950	 0.3690
SB	 0.8530	 0.5020
SC	 0.8540	 0.5200
SD	 0.8650	 0.5320
SE	 0.9390	 0.6010
SF	 0.8910	 0.5170
SG	 0.6150	 0.3520
SH	 0.9460	 0.6090
SI	 0.7730	 0.4500
SJ	 0.7540	 0.4310
SK	 0.9130	 0.5740
SL	 0.9090	 0.5920
SM	 0.7760	 0.3940
SN	 0.8250	 0.4890
SO	 0.9190	 0.5860
SP	 0.8990	 0.5700
SQ	 0.8640	 0.5580
SR	 0.8740	 0.5590
SS	 0.7390	 0.4270
ST	 0.8780	 0.5560
SU	 0.8280	 0.5010
mR	 0.8780	 0.5250