Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 03:13 AM EDT

PDB ID	:	7N1P
EMDB ID	:	EMD-24120
Title	:	Elongating 70S ribosome complex in a classical pre-translocation (PRE-C) conformation
Authors	:	Rundlet, E.J.; Holm, M.; Schacherl, M.; Natchiar, S.K.; Altman, R.B.; Spahn, C.M.T.; Myasnikov, A.G.; Blanchard, S.C.
Deposited on	:	2021-05-28
Resolution	:	2.33 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*
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.

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

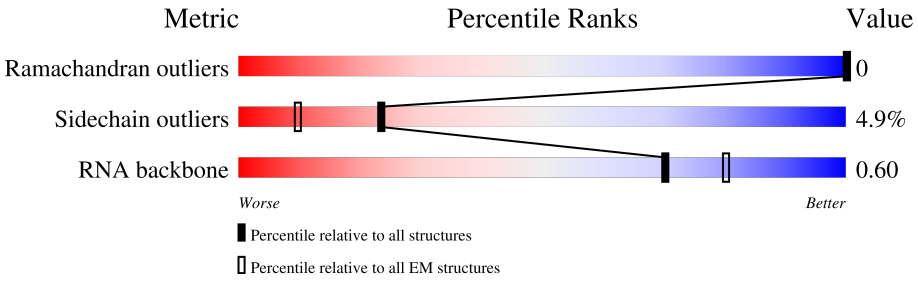
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.33 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 >=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 <=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	1542	5% 85% 15%
2	SB	241	20% 92% • 5%
3	SC	233	7% 87% • 9%
4	SD	206	8% 99% •
5	SE	167	• 89% 6% 5%
6	SF	135	12% 76% • 21%
7	SG	179	11% 77% 9% • 13%
8	SH	130	• 95% • •

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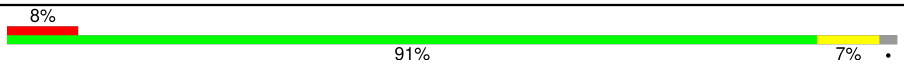
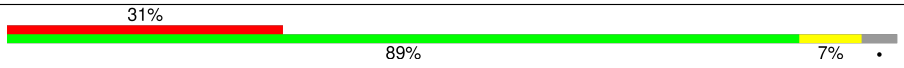
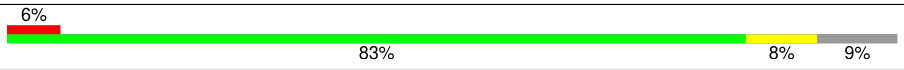
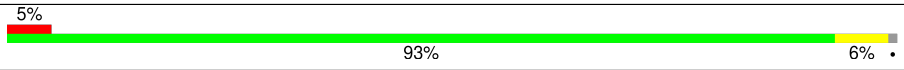
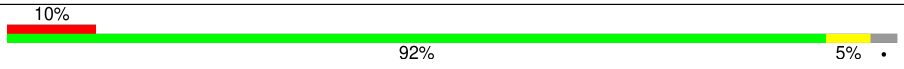
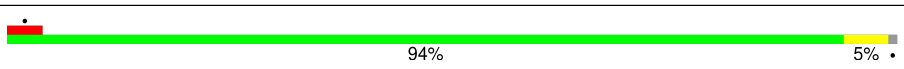
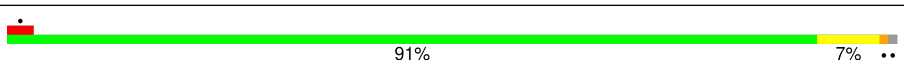
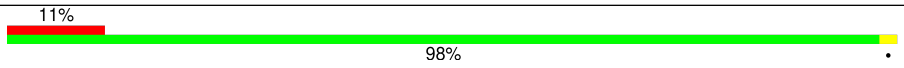
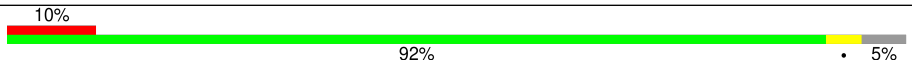
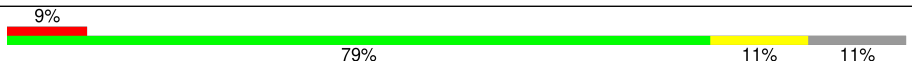
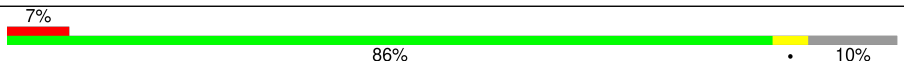
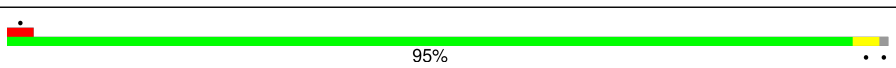
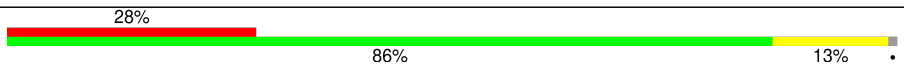
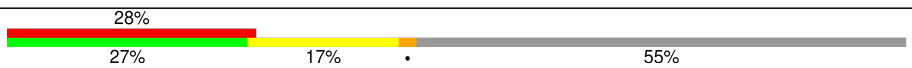
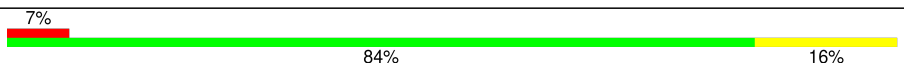
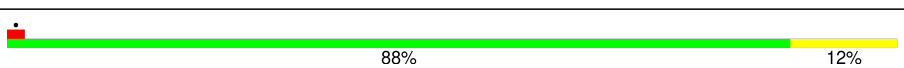
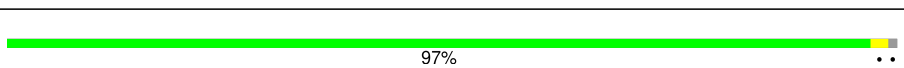
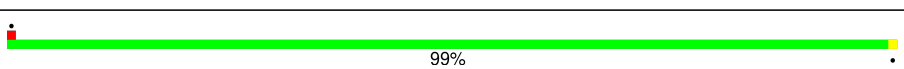
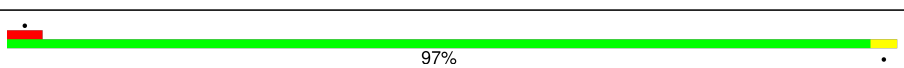
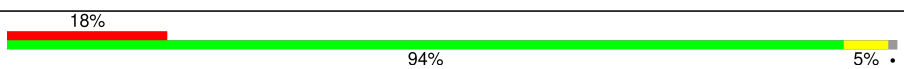
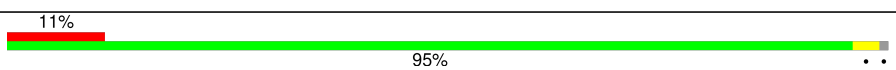
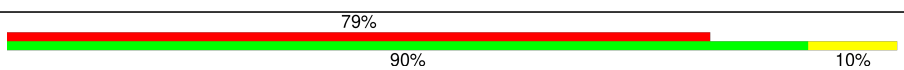
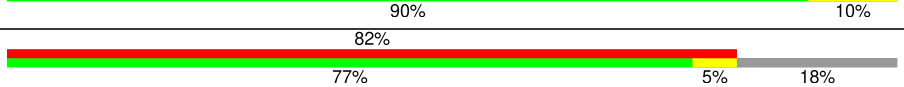
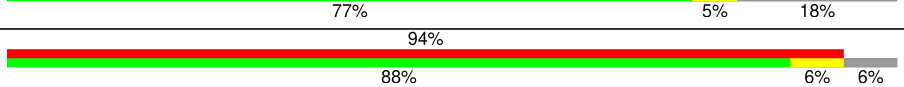
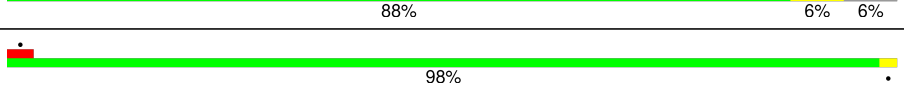
Mol	Chain	Length	Quality of chain
9	SI	130	
10	SJ	103	
11	SK	129	
12	SL	124	
13	SM	118	
14	SN	101	
15	SO	89	
16	SP	82	
17	SQ	84	
18	SR	75	
19	SS	92	
20	ST	87	
21	SU	71	
22	mR	60	
23	23	2904	
24	5	120	
25	LB	273	
26	LC	209	
27	LD	201	
28	LE	179	
29	LF	177	
30	LI	149	
31	LJ	165	
32	LK	142	
33	LM	142	

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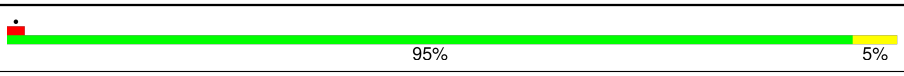
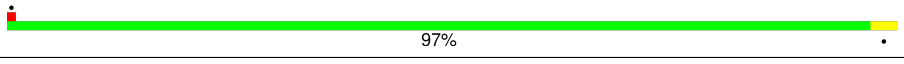
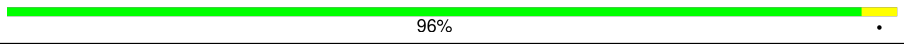
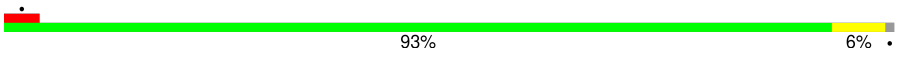
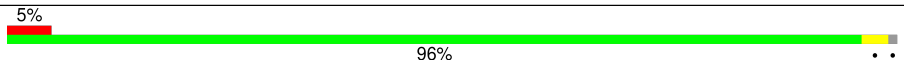
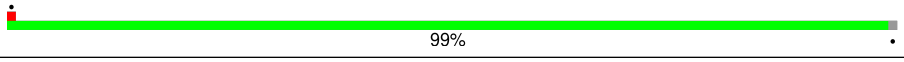
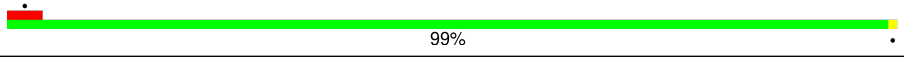
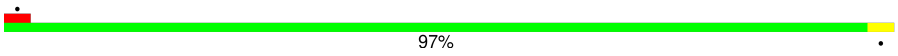
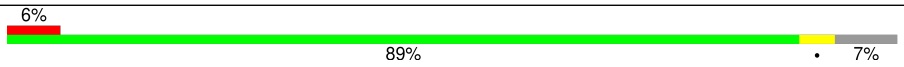
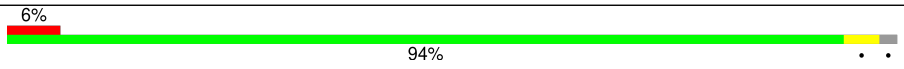
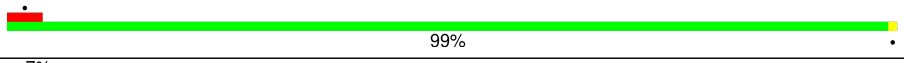
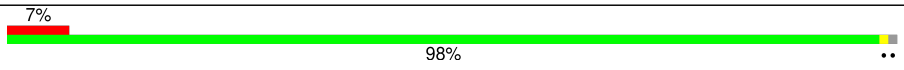
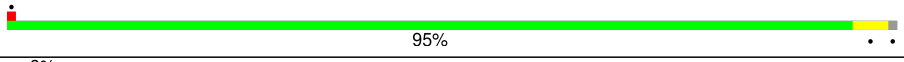
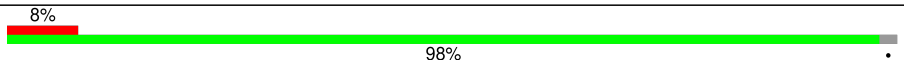
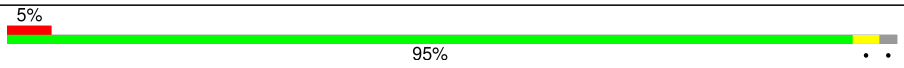
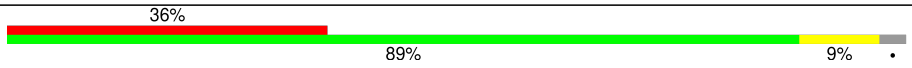
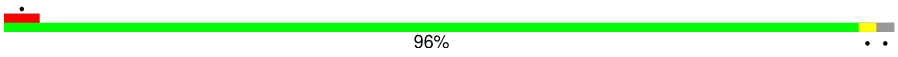
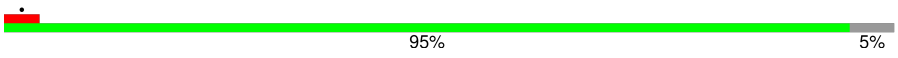
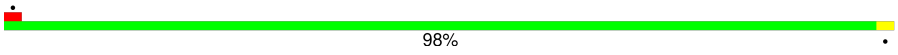
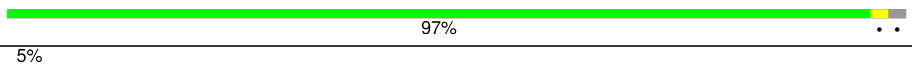
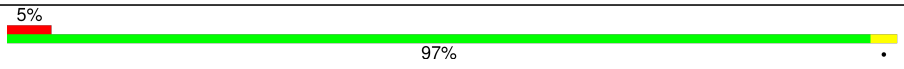
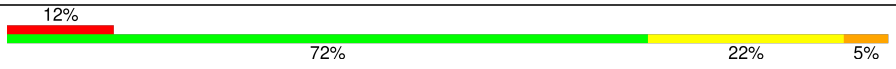
Mol	Chain	Length	Quality of chain
34	LN	123	
35	LO	144	
36	LP	136	
37	LQ	127	
38	LR	117	
39	LS	115	
40	LT	118	
41	LU	103	
42	LV	110	
43	LW	100	
44	LX	104	
45	LY	94	
46	La	85	
47	Lb	78	
48	Lc	63	
49	Ld	59	
50	Le	70	
51	Lf	57	
52	Lg	55	
53	Lh	46	
54	Li	65	
55	Lj	38	
56	Pt	76	
57	Pp	3	
58	Dt	76	

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 149590 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
			Total	C	N	O	P		
1	16	1542	33092	14767	6064	10719	1542	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SB	229	1787	1129	320	330	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SC	212	1666	1054	314	294	4	1	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SE	158	1166	725	220	215	6	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SG	155	Total	C	N	O	S	1	0
			1236	772	240	220	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	117	Total	C	N	O	S	1	0
			888	546	178	161	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	2	0
			730	450	149	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	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	ST	86	Total	C	N	O	S	0	0
			670	414	138	115	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	1	0
			598	374	125	98	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	mR	27	Total	C	N	O	P	3	0
			640	287	116	207	30		

- 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
			62354	27824	11469	20157	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	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LF	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LI	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LJ	135	Total	C	N	O	S	0	0
			1023	648	179	192	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	123	Total	C	N	O	S	0	0
			947	593	181	167	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	1	0
			1086	692	209	179	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	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	84	Total	C	N	O	S	0	0
			634	391	129	113	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	1	0
			632	393	131	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	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 RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	Pt	76	Total	C	N	O	P	S	0	0
			1635	733	284	541	76	1		

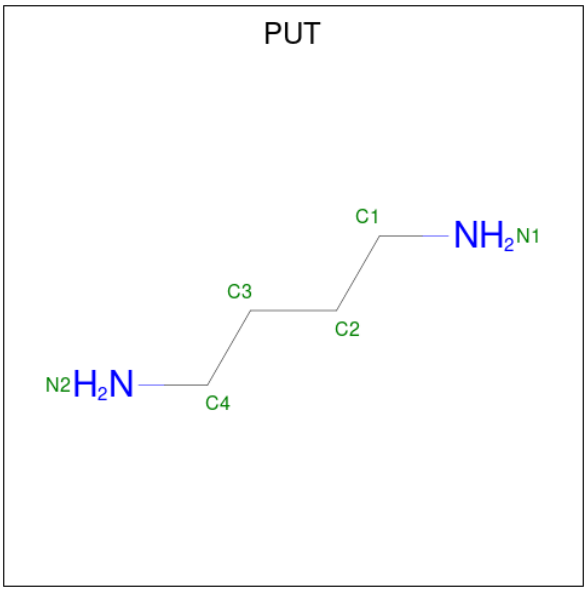
- Molecule 57 is a protein called Chains: Pp.

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	Dt	76	Total	C	N	O	P	S	0	0
			1638	734	291	535	76	2		

- Molecule 59 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
59	16	1	Total	C	N	0
			6	4	2	
59	16	1	Total	C	N	0
			6	4	2	
59	16	1	Total	C	N	0
			6	4	2	
59	23	1	Total	C	N	0
			6	4	2	

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Mol	Chain	Residues	Atoms	AltConf
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
60	16	113	Total Mg 113 113	0
60	SD	1	Total Mg 1 1	0
60	mR	1	Total Mg 1 1	0
60	23	275	Total Mg 275 275	0
60	5	5	Total Mg 5 5	0

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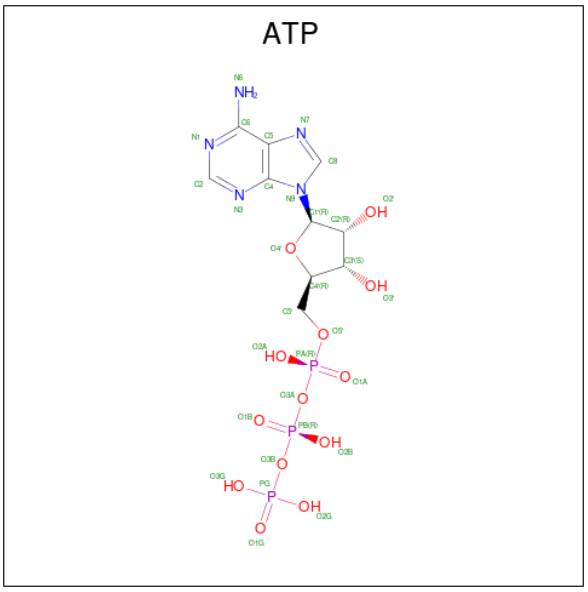
Mol	Chain	Residues	Atoms	AltConf
60	LB	1	Total Mg 1 1	0
60	LC	1	Total Mg 1 1	0
60	LD	1	Total Mg 1 1	0
60	LE	1	Total Mg 1 1	0
60	Ld	1	Total Mg 1 1	0
60	Lf	1	Total Mg 1 1	0
60	Pt	1	Total Mg 1 1	0
60	Dt	3	Total Mg 3 3	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

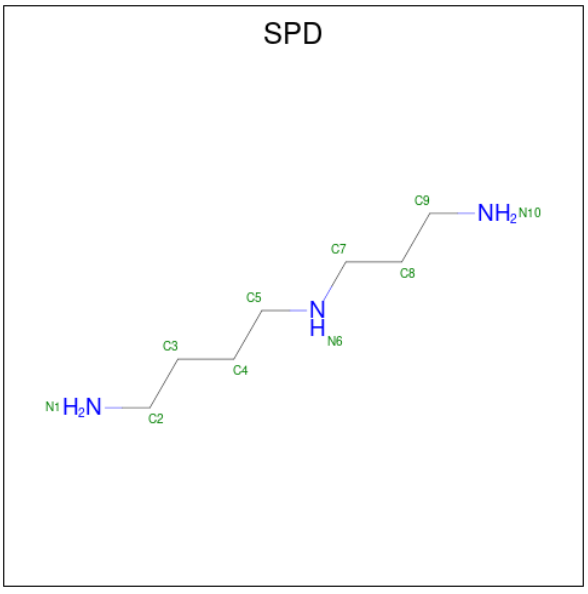
Mol	Chain	Residues	Atoms	AltConf
61	SB	1	Total Zn 1 1	0
61	Le	1	Total Zn 1 1	0
61	Lj	1	Total Zn 1 1	0

- Molecule 62 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
62	23	1	Total	C	N	O	P	0
			31	10	5	13	3	
62	23	1	Total	C	N	O	P	0
			31	10	5	13	3	
62	23	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 63 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
63	23	1	Total C N 10 7 3	0
63	23	1	Total C N 10 7 3	0
63	23	1	Total C N 10 7 3	0
63	23	1	Total C N 10 7 3	0
63	23	1	Total C N 10 7 3	0

- Molecule 64 is water.

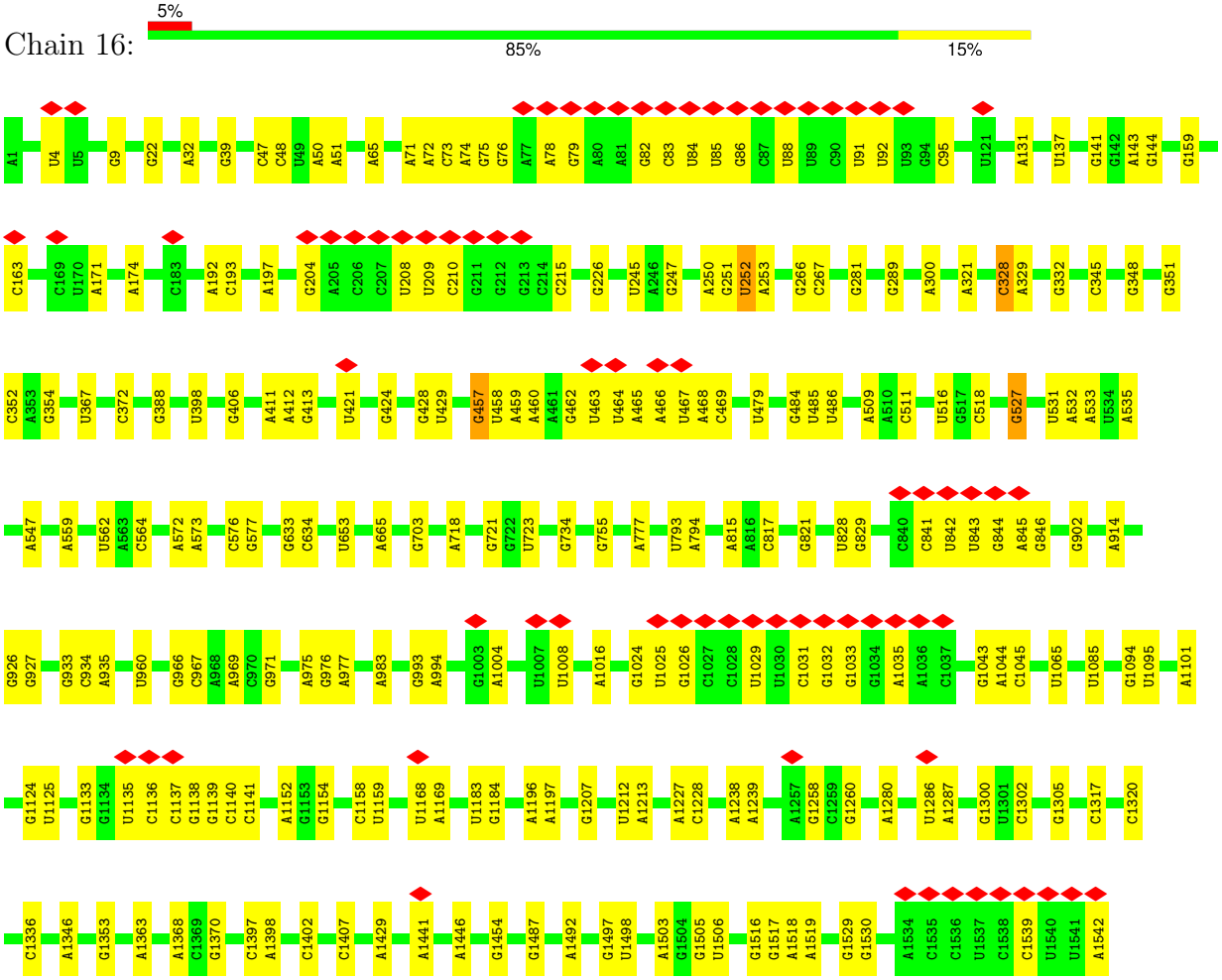
Mol	Chain	Residues	Atoms	AltConf
64	16	3	Total O 3 3	0
64	23	41	Total O 41 41	0
64	LB	3	Total O 3 3	0
64	LC	1	Total O 1 1	0
64	LT	1	Total O 1 1	0
64	LY	1	Total O 1 1	0

3 Residue-property plots (i)

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

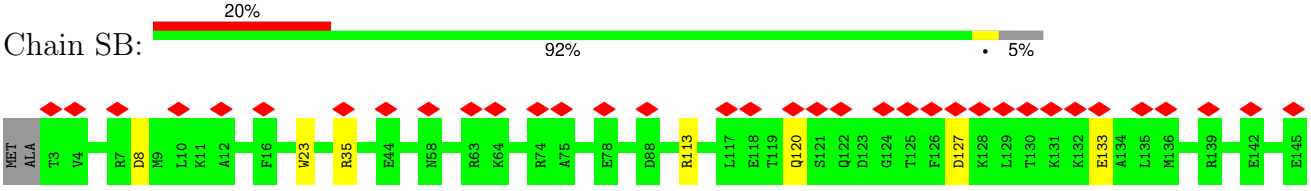
• Molecule 1: 16S rRNA

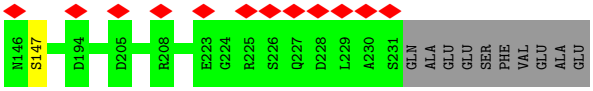
Chain 16:



• Molecule 2: 30S ribosomal protein S2

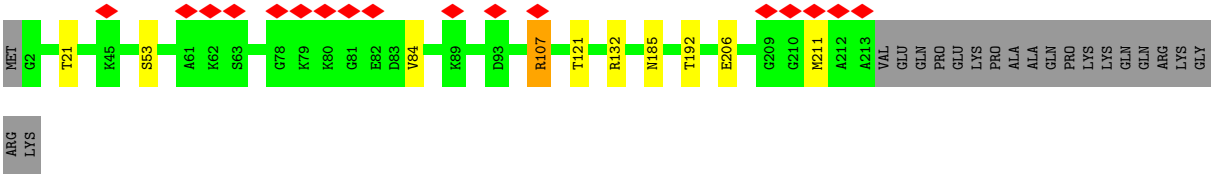
Chain SB:





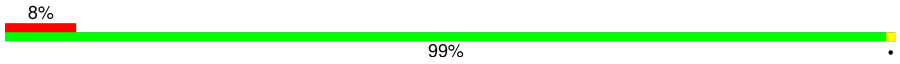
• Molecule 3: 30S ribosomal protein S3

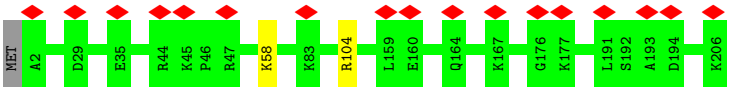
Chain SC:



• Molecule 4: 30S ribosomal protein S4

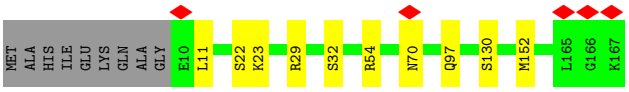
Chain SD:





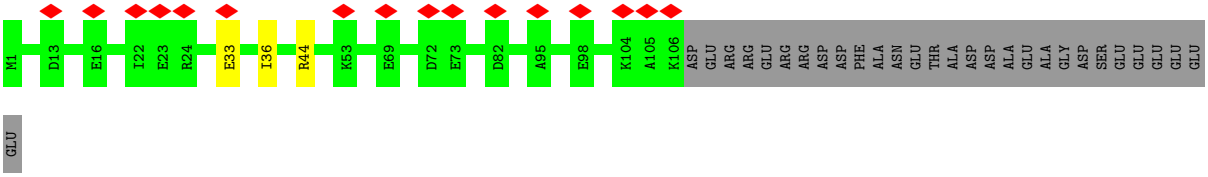
• Molecule 5: 30S ribosomal protein S5

Chain SE:



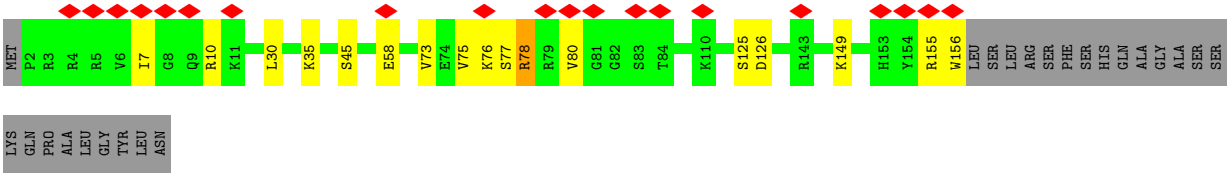
• Molecule 6: 30S ribosomal protein S6

Chain SF:



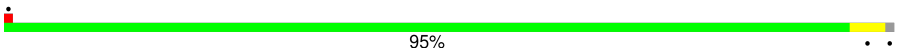
• Molecule 7: 30S ribosomal protein S7

Chain SG:



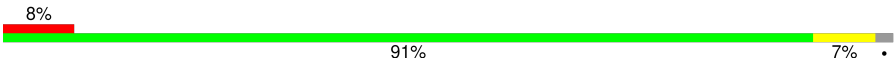
• Molecule 8: 30S ribosomal protein S8

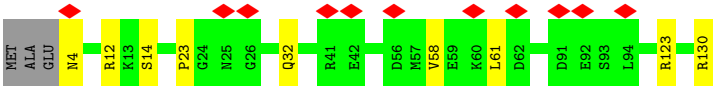
Chain SH:



• Molecule 9: 30S ribosomal protein S9

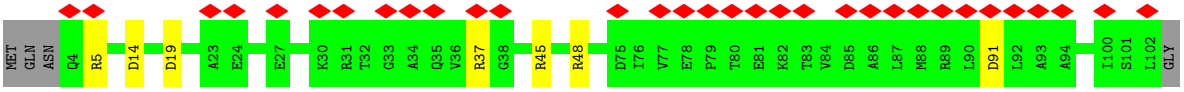
Chain SI:





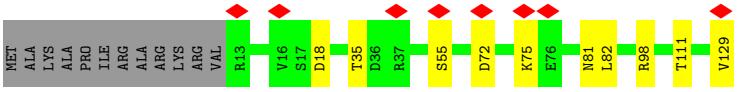
• Molecule 10: 30S ribosomal protein S10

Chain SJ:



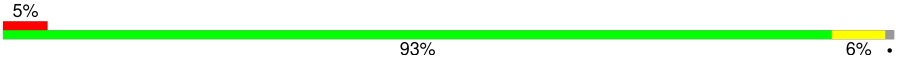
• Molecule 11: 30S ribosomal protein S11

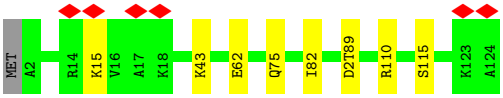
Chain SK:



• Molecule 12: 30S ribosomal protein S12

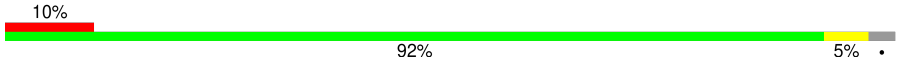
Chain SL:

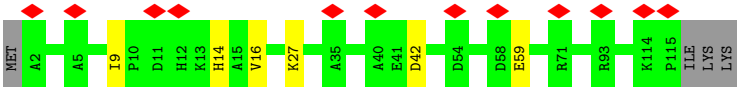




• Molecule 13: 30S ribosomal protein S13

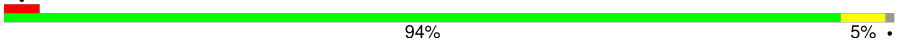
Chain SM:

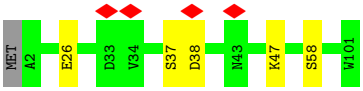




• Molecule 14: 30S ribosomal protein S14

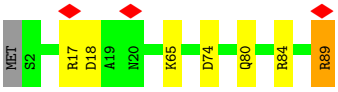
Chain SN:





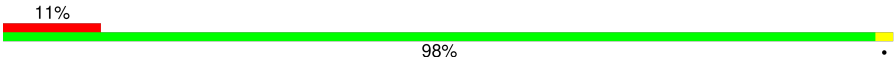
• Molecule 15: 30S ribosomal protein S15

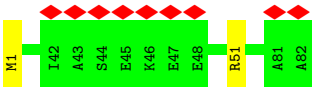
Chain SO:



• Molecule 16: 30S ribosomal protein S16

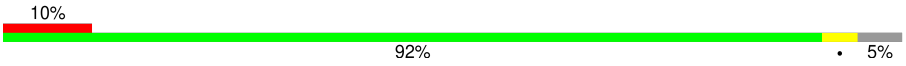
Chain SP:

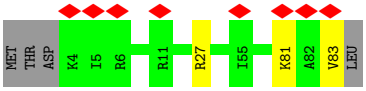




• Molecule 17: 30S ribosomal protein S17

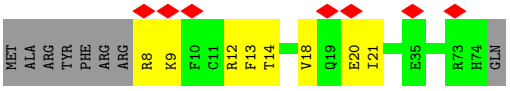
Chain SQ:





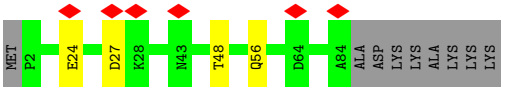
• Molecule 18: 30S ribosomal protein S18

Chain SR:



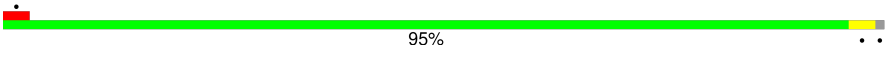
• Molecule 19: 30S ribosomal protein S19

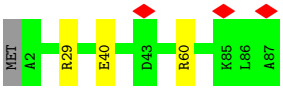
Chain SS:



• Molecule 20: 30S ribosomal protein S20

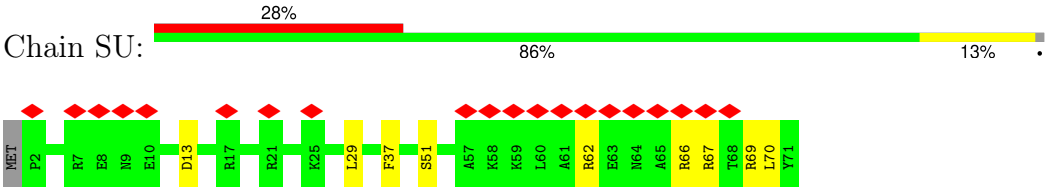
Chain ST:





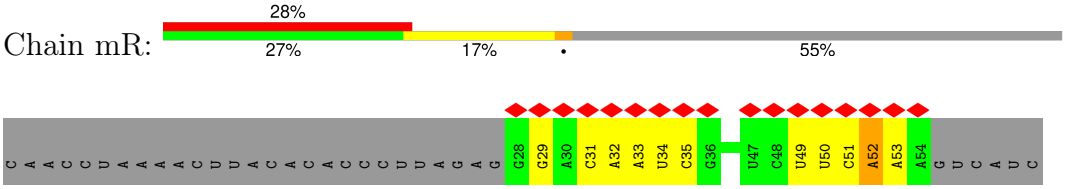
• Molecule 21: 30S ribosomal protein S21

Chain SU:



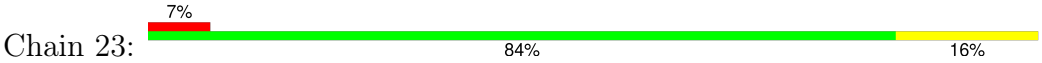
• Molecule 22: mRNA

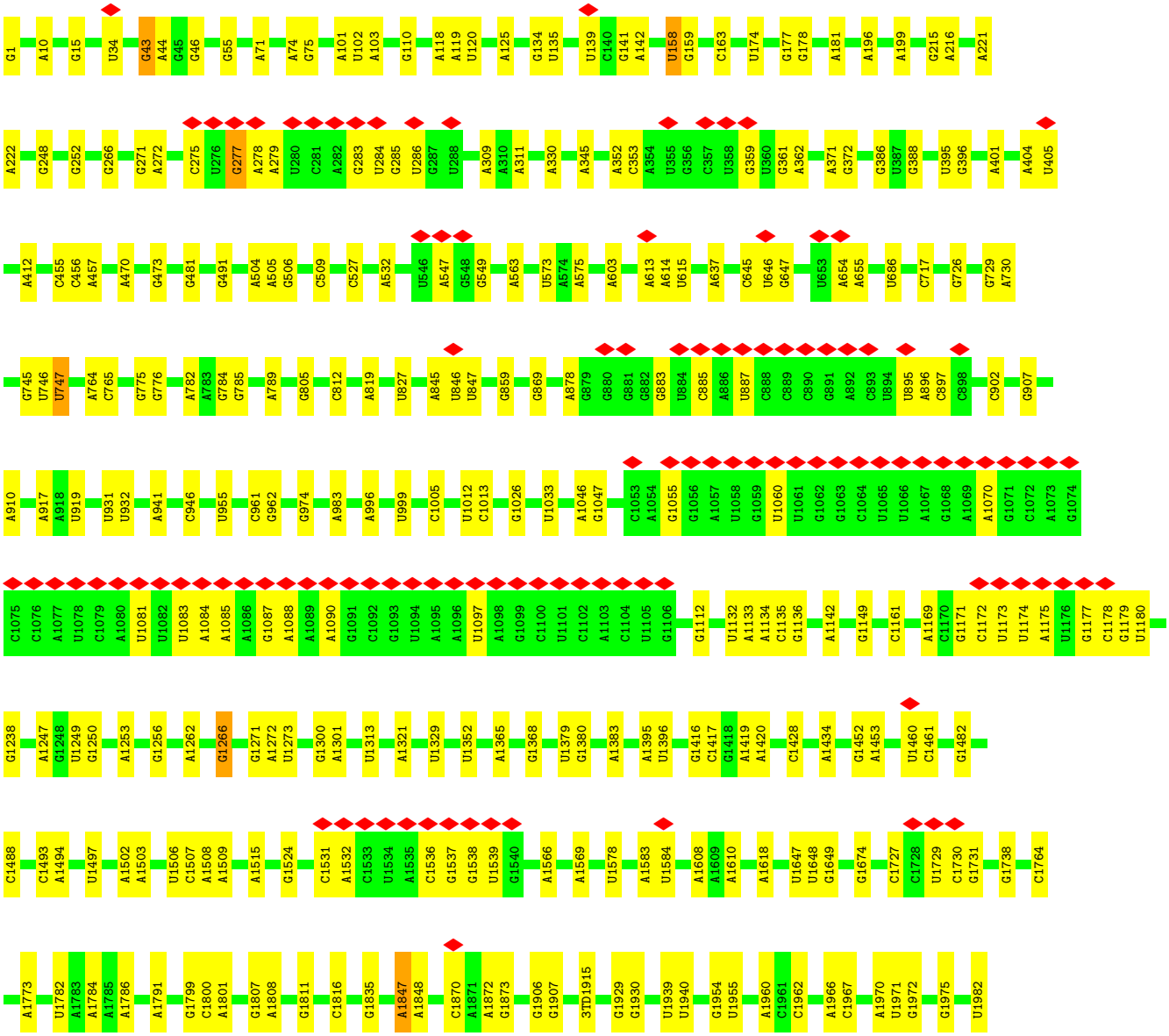
Chain mR:

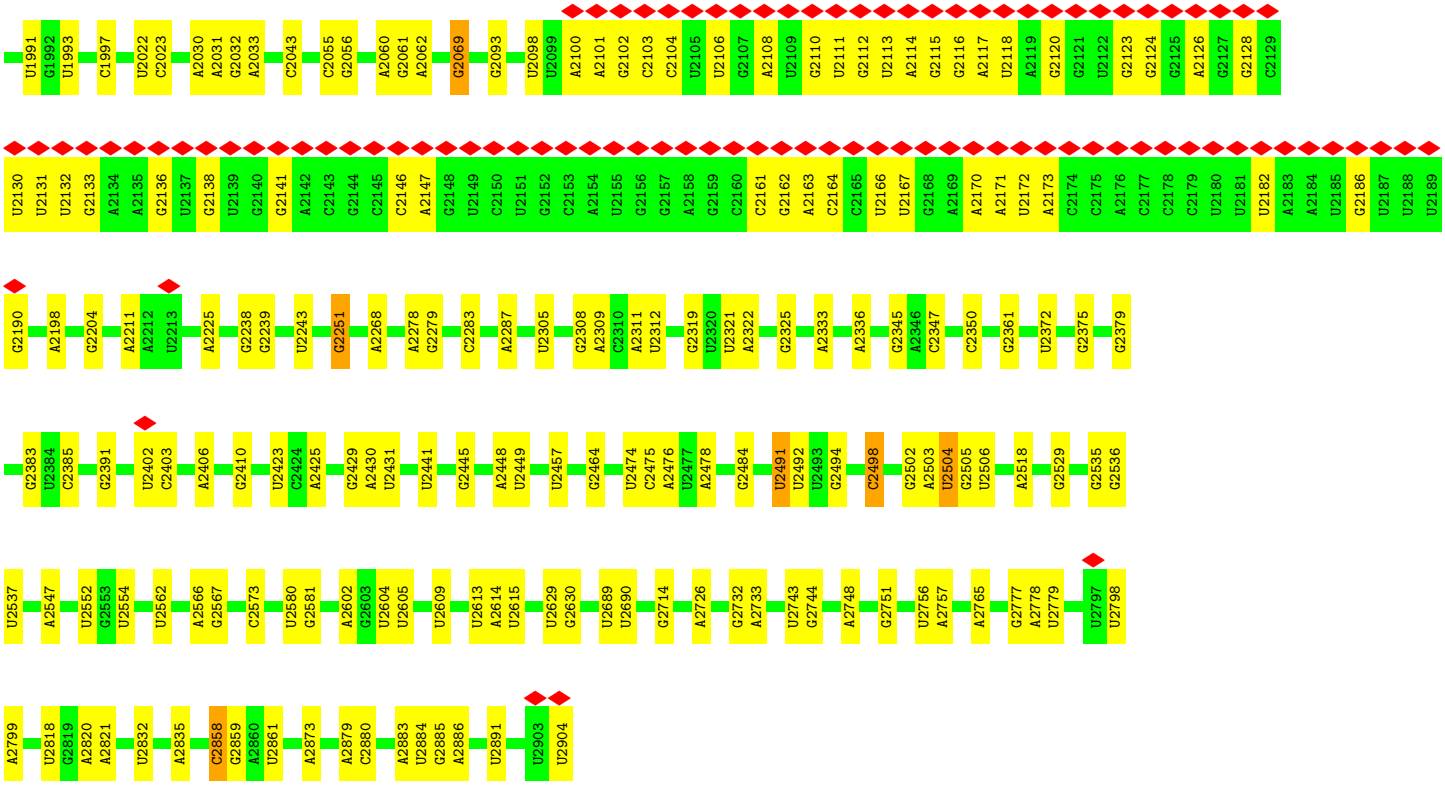


• Molecule 23: 23S rRNA

Chain 23:





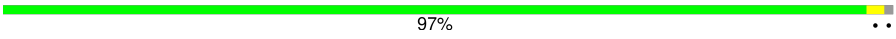


• Molecule 24: 5S rRNA

Chain 5:

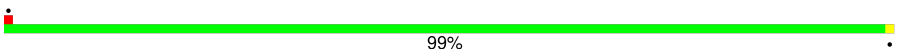
• Molecule 25: 50S ribosomal protein L2

Chain LB:



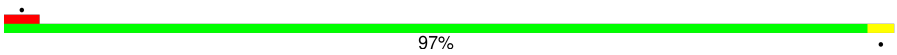
• Molecule 26: 50S ribosomal protein L3

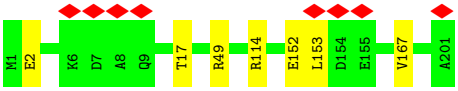
Chain LC:



• Molecule 27: 50S ribosomal protein L4

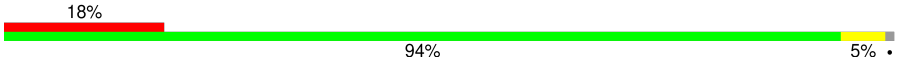
Chain LD:

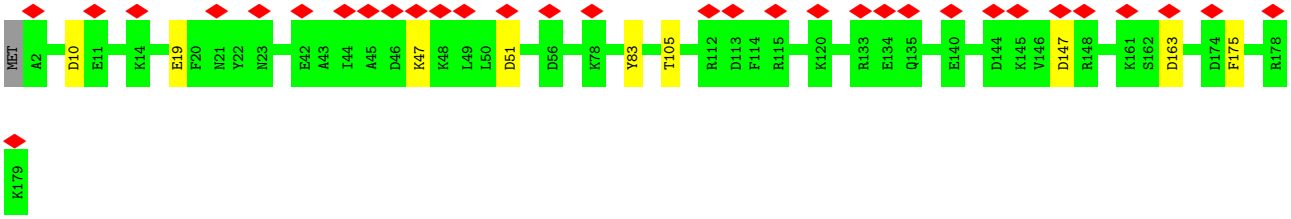




• Molecule 28: 50S ribosomal protein L5

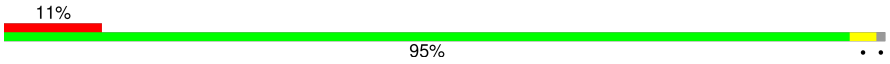
Chain LE:

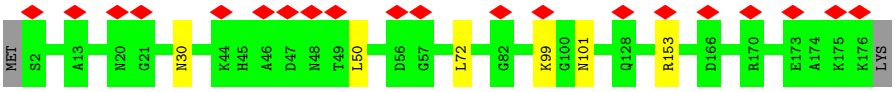




• Molecule 29: 50S ribosomal protein L6

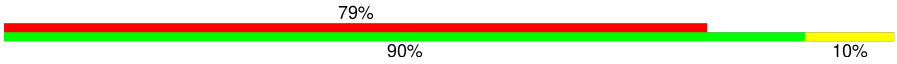
Chain LF:

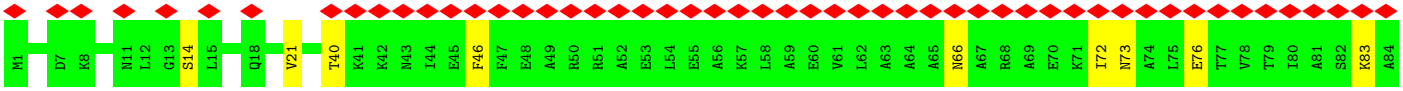


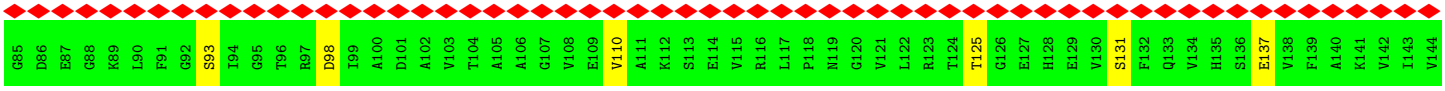


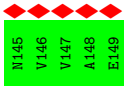
• Molecule 30: 50S ribosomal protein L9

Chain LI:



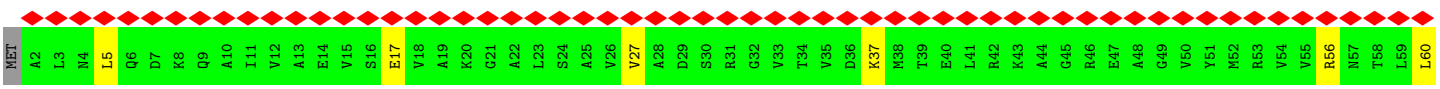


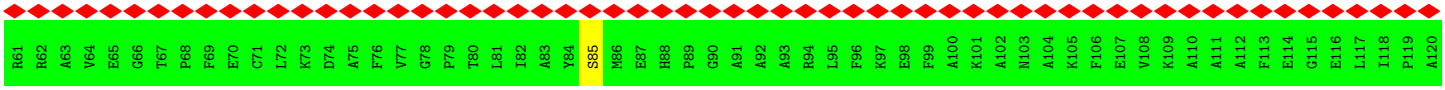


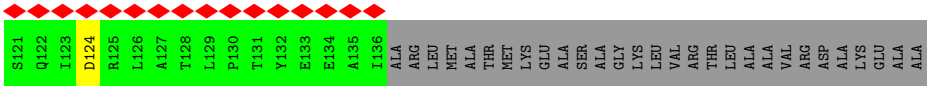


• Molecule 31: 50S ribosomal protein L10

Chain LJ:

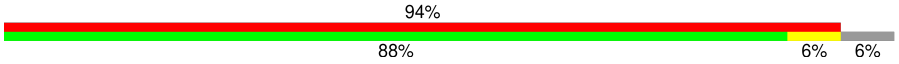


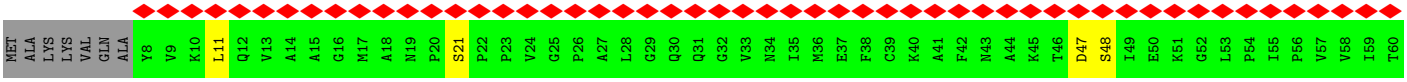


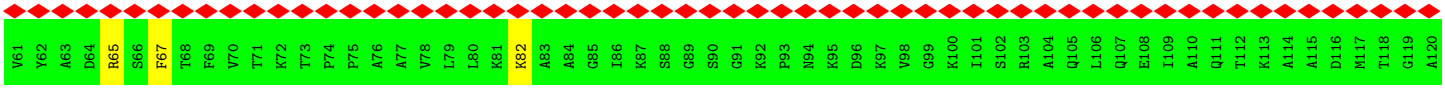


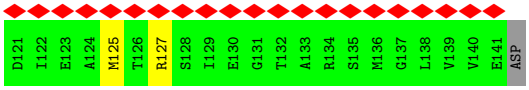
• Molecule 32: 50S ribosomal protein L11

Chain LK:



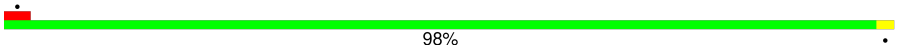


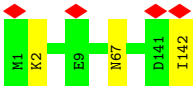




• Molecule 33: 50S ribosomal protein L13

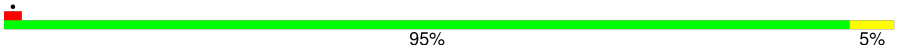
Chain LM:





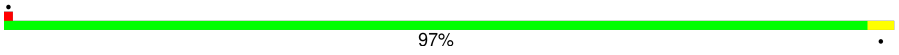
• Molecule 34: 50S ribosomal protein L14

Chain LN:



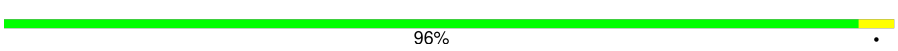
• Molecule 35: 50S ribosomal protein L15

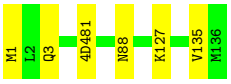
Chain LO:



• Molecule 36: 50S ribosomal protein L16

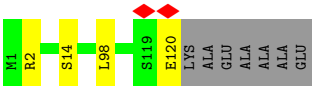
Chain LP:





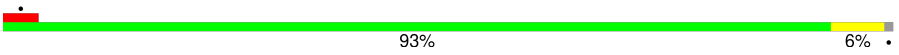
• Molecule 37: 50S ribosomal protein L17

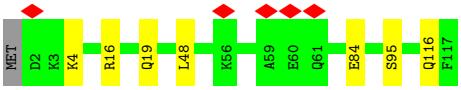
Chain LQ:



• Molecule 38: 50S ribosomal protein L18

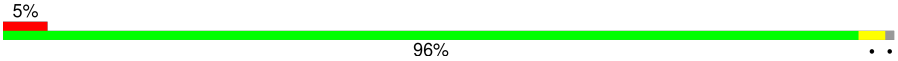
Chain LR:

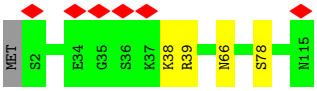




• Molecule 39: 50S ribosomal protein L19

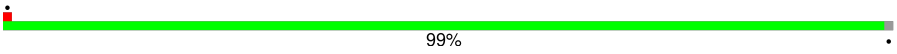
Chain LS:





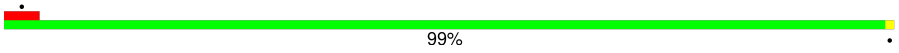
• Molecule 40: 50S ribosomal protein L20

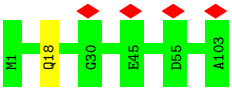
Chain LT:



• Molecule 41: 50S ribosomal protein L21

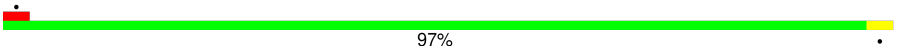
Chain LU:

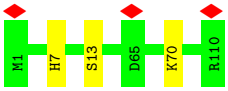




• Molecule 42: 50S ribosomal protein L22

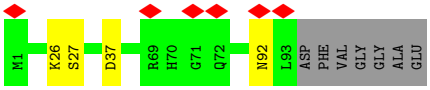
Chain LV:





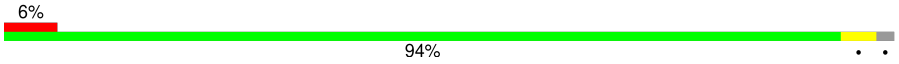
• Molecule 43: 50S ribosomal protein L23

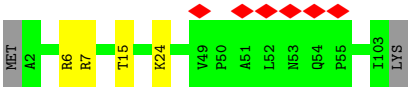
Chain LW:



• Molecule 44: 50S ribosomal protein L24

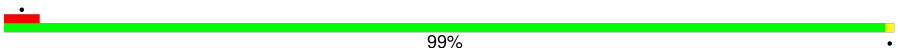
Chain LX:

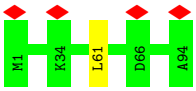




• Molecule 45: 50S ribosomal protein L25

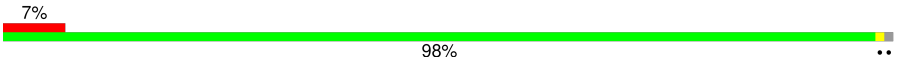
Chain LY:

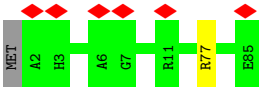




• Molecule 46: 50S ribosomal protein L27

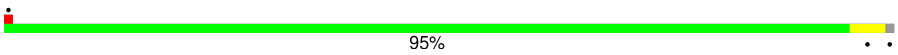
Chain La:

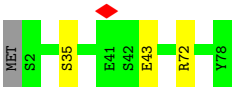




• Molecule 47: 50S ribosomal protein L28

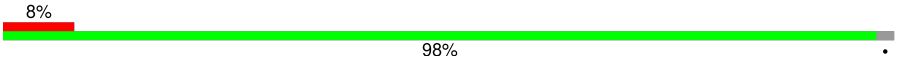
Chain Lb:

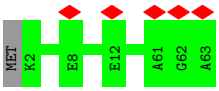




• Molecule 48: 50S ribosomal protein L29

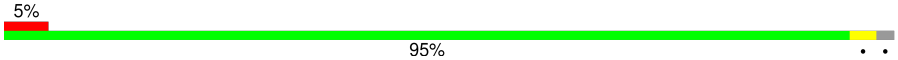
Chain Lc:

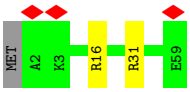




• Molecule 49: 50S ribosomal protein L30

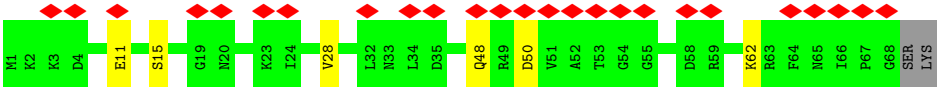
Chain Ld:





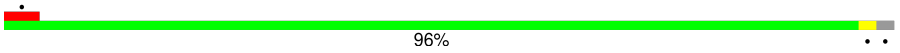
• Molecule 50: 50S ribosomal protein L31

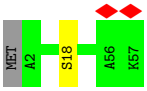
Chain Le:



• Molecule 51: 50S ribosomal protein L32

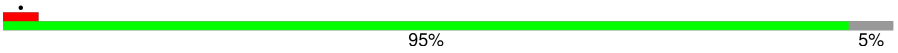
Chain Lf:

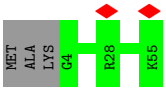




• Molecule 52: 50S ribosomal protein L33

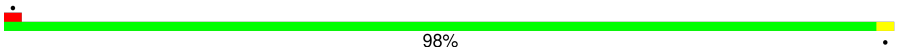
Chain Lg:

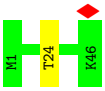




• Molecule 53: 50S ribosomal protein L34

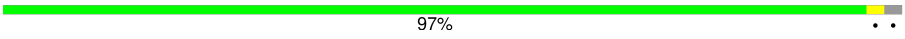
Chain Lh:

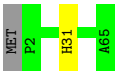




• Molecule 54: 50S ribosomal protein L35

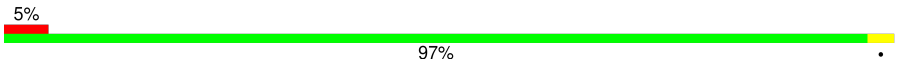
Chain Li:

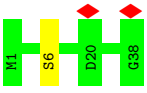




• Molecule 55: 50S ribosomal protein L36

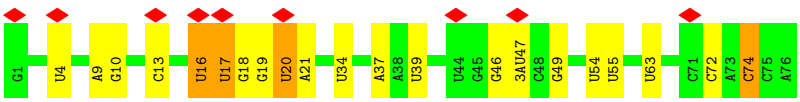
Chain Lj:





• Molecule 56: tRNA

Chain Pt:

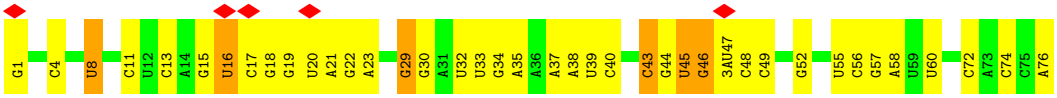


• Molecule 57: Chains: Pp

Chain Pp:

• Molecule 58: tRNA

Chain Dt:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109769	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 ($e^-/Å^2$)	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	0.235	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	610.55994, 610.55994, 610.55994	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: OMC, 2MG, MA6, 4OC, T6A, 3AU, SPD, 2MA, UR3, 1MG, 6MZ, U8U, MIA, 4SU, PSU, 5MC, MG, D2T, PUT, 3TD, H2U, OMU, OMG, 4D4, G7M, ATP, 5MU, ZN

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	0.39	0/36772	0.70	4/57358 (0.0%)
2	SB	0.36	0/1818	0.56	0/2450
3	SC	0.43	2/1696 (0.1%)	0.65	2/2284 (0.1%)
4	SD	0.33	0/1665	0.58	0/2227
5	SE	0.37	0/1179	0.57	0/1584
6	SF	0.31	0/881	0.54	0/1189
7	SG	0.51	2/1257 (0.2%)	0.70	2/1686 (0.1%)
8	SH	0.32	0/989	0.54	0/1326
9	SI	0.39	0/1034	0.68	1/1375 (0.1%)
10	SJ	0.43	0/805	0.73	1/1089 (0.1%)
11	SK	0.34	0/904	0.62	0/1219
12	SL	0.36	0/960	0.63	0/1286
13	SM	0.41	0/892	0.67	0/1193
14	SN	0.35	0/817	0.59	0/1088
15	SO	0.32	0/740	0.59	0/986
16	SP	0.35	0/659	0.61	0/884
17	SQ	0.31	0/657	0.58	0/881
18	SR	0.47	0/564	0.69	1/756 (0.1%)
19	SS	0.40	0/680	0.60	0/915
20	ST	0.27	0/676	0.54	0/895
21	SU	0.61	2/610 (0.3%)	0.78	2/808 (0.2%)
22	mR	0.41	0/716	0.87	2/1113 (0.2%)
23	23	0.44	1/69305 (0.0%)	0.72	9/108114 (0.0%)
24	5	0.43	1/2873 (0.0%)	0.70	0/4478
25	LB	0.33	0/2121	0.59	0/2852
26	LC	0.34	0/1586	0.58	0/2134
27	LD	0.33	0/1571	0.55	0/2113
28	LE	0.38	0/1444	0.61	0/1937
29	LF	0.31	0/1333	0.58	0/1805
30	LI	0.45	0/1122	0.68	0/1515
31	LJ	0.40	0/1037	0.59	0/1400

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LK	0.41	0/993	0.59	0/1341
33	LM	0.34	0/1152	0.54	0/1551
34	LN	0.38	0/956	0.61	0/1279
35	LO	0.31	0/1062	0.59	0/1413
36	LP	0.30	0/1092	0.54	0/1457
37	LQ	0.33	0/973	0.57	0/1301
38	LR	0.34	0/902	0.63	0/1209
39	LS	0.34	0/929	0.58	0/1242
40	LT	0.34	0/960	0.56	0/1278
41	LU	0.36	0/829	0.61	0/1107
42	LV	0.31	0/864	0.54	0/1156
43	LW	0.35	0/744	0.60	0/994
44	LX	0.35	0/787	0.57	0/1051
45	LY	0.35	0/766	0.56	0/1025
46	La	0.35	0/642	0.60	0/848
47	Lb	0.32	0/646	0.61	0/863
48	Lc	0.36	0/502	0.56	0/667
49	Ld	0.29	0/453	0.58	0/605
50	Le	0.48	0/543	0.73	0/726
51	Lf	0.32	0/450	0.60	0/599
52	Lg	0.46	0/434	0.63	0/576
53	Lh	0.33	0/380	0.67	0/498
54	Li	0.34	0/513	0.65	0/676
55	Lj	0.30	0/303	0.56	0/397
56	Pt	0.40	1/1599 (0.1%)	0.72	0/2486
57	Pp	0.46	0/28	0.77	0/34
58	Dt	0.96	7/1628 (0.4%)	0.92	9/2531 (0.4%)
All	All	0.42	16/160493 (0.0%)	0.69	33/239850 (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	1
4	SD	0	1
5	SE	0	1
10	SJ	0	2
11	SK	0	1
15	SO	0	4
16	SP	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
20	ST	0	2
25	LB	0	1
27	LD	0	1
29	LF	0	1
34	LN	0	1
35	LO	0	1
44	LX	0	1
46	La	0	1
50	Le	0	1
All	All	0	21

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	1	U	OP3-P	-10.71	1.48	1.61
23	23	1	G	OP3-P	-10.62	1.48	1.61
58	Dt	1	G	OP3-P	-10.18	1.49	1.61
58	Dt	34	G	O3'-P	-7.97	1.51	1.61
7	SG	78[A]	ARG	C-O	7.25	1.37	1.23
7	SG	78[B]	ARG	C-O	7.25	1.37	1.23
58	Dt	30	G	O3'-P	-6.97	1.52	1.61
21	SU	37[A]	PHE	C-O	6.24	1.35	1.23
21	SU	37[B]	PHE	C-O	6.24	1.35	1.23
3	SC	132[A]	ARG	C-O	5.83	1.34	1.23
3	SC	132[B]	ARG	C-O	5.83	1.34	1.23
58	Dt	35	A	P-OP2	-5.63	1.39	1.49
58	Dt	33	U	O3'-P	-5.61	1.54	1.61
58	Dt	29	G	O3'-P	-5.41	1.54	1.61
56	Pt	74	C	O3'-P	-5.28	1.54	1.61
58	Dt	35	A	O3'-P	-5.20	1.54	1.61

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	16	252	U	C2'-C3'-O3'	8.56	128.34	109.50
23	23	43	G	P-O3'-C3'	8.17	129.50	119.70
23	23	158	U	C2'-C3'-O3'	7.71	126.47	109.50
23	23	1847	A	C2'-C3'-O3'	7.37	125.70	109.50
58	Dt	43	C	C2'-C3'-O3'	7.30	125.56	109.50
23	23	2491	U	C2'-C3'-O3'	6.75	124.49	113.70
58	Dt	35	A	O5'-P-OP1	-6.72	99.65	105.70
1	16	457	G	P-O3'-C3'	6.68	127.72	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2858	C	C2'-C3'-O3'	6.65	124.33	113.70
58	Dt	45	U	C2'-C3'-O3'	6.50	124.10	113.70
21	SU	37[A]	PHE	CA-C-O	6.38	133.49	120.10
21	SU	37[B]	PHE	CA-C-O	6.38	133.49	120.10
58	Dt	45	U	C4'-C3'-O3'	6.37	125.74	113.00
23	23	1313	U	C2-N1-C1'	6.29	125.24	117.70
3	SC	132[A]	ARG	CA-C-O	5.85	132.38	120.10
3	SC	132[B]	ARG	CA-C-O	5.85	132.38	120.10
1	16	328	C	C2-N1-C1'	5.76	125.14	118.80
58	Dt	43	C	O4'-C4'-C3'	-5.65	98.35	104.00
58	Dt	38	A	O5'-P-OP2	-5.46	100.79	105.70
22	mR	52	A	N9-C1'-C2'	5.45	121.08	114.00
9	SI	23	PRO	N-CA-C	-5.43	97.97	112.10
1	16	328	C	N1-C2-O2	5.43	122.16	118.90
58	Dt	35	A	O5'-P-OP2	5.26	117.01	110.70
7	SG	78[A]	ARG	CA-C-O	5.21	131.03	120.10
7	SG	78[B]	ARG	CA-C-O	5.21	131.03	120.10
23	23	1266	G	O5'-P-OP1	-5.18	101.04	105.70
10	SJ	91	ASP	CB-CG-OD1	5.13	122.92	118.30
22	mR	52	A	C2'-C3'-O3'	-5.13	98.22	109.50
23	23	309	A	P-O3'-C3'	5.09	125.81	119.70
58	Dt	43	C	C4'-C3'-O3'	5.06	123.12	113.00
18	SR	13	PHE	CB-CA-C	5.05	120.50	110.40
58	Dt	45	U	O4'-C4'-C3'	-5.02	98.98	104.00
23	23	277	G	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	LB	221	ARG	Sidechain
27	LD	114	ARG	Sidechain
29	LF	153	ARG	Sidechain
34	LN	98	ARG	Sidechain
35	LO	69	ARG	Sidechain
44	LX	7	ARG	Sidechain
46	La	77	ARG	Sidechain
50	Le	62	LYS	Mainchain
3	SC	107	ARG	Sidechain
4	SD	104	ARG	Sidechain
5	SE	54	ARG	Sidechain
10	SJ	37	ARG	Sidechain

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Mol	Chain	Res	Type	Group
10	SJ	48	ARG	Sidechain
11	SK	98	ARG	Sidechain
15	SO	17	ARG	Sidechain
15	SO	84	ARG	Sidechain
15	SO	89[A]	ARG	Sidechain
15	SO	89[B]	ARG	Sidechain
16	SP	51	ARG	Sidechain
20	ST	29	ARG	Sidechain
20	ST	60	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	227/241 (94%)	217 (96%)	10 (4%)	0	100	100
3	SC	211/233 (91%)	208 (99%)	3 (1%)	0	100	100
4	SD	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
5	SE	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
6	SF	104/135 (77%)	102 (98%)	2 (2%)	0	100	100
7	SG	154/179 (86%)	150 (97%)	4 (3%)	0	100	100
8	SH	127/130 (98%)	127 (100%)	0	0	100	100
9	SI	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
10	SJ	97/103 (94%)	93 (96%)	4 (4%)	0	100	100
11	SK	116/129 (90%)	110 (95%)	6 (5%)	0	100	100
12	SL	120/124 (97%)	114 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	SM	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
14	SN	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	SO	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
16	SP	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
17	SQ	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
18	SR	65/75 (87%)	63 (97%)	2 (3%)	0	100	100
19	SS	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
20	ST	84/87 (97%)	84 (100%)	0	0	100	100
21	SU	69/71 (97%)	69 (100%)	0	0	100	100
25	LB	269/273 (98%)	265 (98%)	4 (2%)	0	100	100
26	LC	207/209 (99%)	205 (99%)	2 (1%)	0	100	100
27	LD	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
28	LE	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
29	LF	173/177 (98%)	169 (98%)	4 (2%)	0	100	100
30	LI	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
31	LJ	133/165 (81%)	123 (92%)	10 (8%)	0	100	100
32	LK	132/142 (93%)	123 (93%)	9 (7%)	0	100	100
33	LM	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
34	LN	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
35	LO	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
36	LP	134/136 (98%)	134 (100%)	0	0	100	100
37	LQ	118/127 (93%)	115 (98%)	3 (2%)	0	100	100
38	LR	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
39	LS	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
40	LT	115/118 (98%)	115 (100%)	0	0	100	100
41	LU	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
42	LV	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
43	LW	91/100 (91%)	89 (98%)	2 (2%)	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	82/85 (96%)	81 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	Lb	76/78 (97%)	74 (97%)	2 (3%)	0	100	100
48	Lc	60/63 (95%)	60 (100%)	0	0	100	100
49	Ld	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	Le	66/70 (94%)	61 (92%)	5 (8%)	0	100	100
51	Lf	54/57 (95%)	54 (100%)	0	0	100	100
52	Lg	50/55 (91%)	50 (100%)	0	0	100	100
53	Lh	44/46 (96%)	44 (100%)	0	0	100	100
54	Li	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
55	Lj	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
57	Pp	1/3 (33%)	1 (100%)	0	0	100	100
All	All	5905/6223 (95%)	5741 (97%)	164 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	190/199 (96%)	182 (96%)	8 (4%)	25	32
3	SC	173/190 (91%)	164 (95%)	9 (5%)	19	24
4	SD	172/173 (99%)	171 (99%)	1 (1%)	84	90
5	SE	120/126 (95%)	111 (92%)	9 (8%)	11	11
6	SF	92/116 (79%)	89 (97%)	3 (3%)	33	41
7	SG	129/147 (88%)	111 (86%)	18 (14%)	3	2
8	SH	104/105 (99%)	99 (95%)	5 (5%)	21	27
9	SI	105/107 (98%)	97 (92%)	8 (8%)	11	11
10	SJ	87/90 (97%)	83 (95%)	4 (5%)	23	28
11	SK	91/99 (92%)	82 (90%)	9 (10%)	6	5
12	SL	102/103 (99%)	95 (93%)	7 (7%)	13	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	SM	92/96 (96%)	86 (94%)	6 (6%)	14 15
14	SN	83/84 (99%)	78 (94%)	5 (6%)	16 18
15	SO	78/77 (101%)	72 (92%)	6 (8%)	10 10
16	SP	65/65 (100%)	64 (98%)	1 (2%)	60 72
17	SQ	74/78 (95%)	71 (96%)	3 (4%)	26 33
18	SR	58/65 (89%)	51 (88%)	7 (12%)	4 3
19	SS	72/79 (91%)	68 (94%)	4 (6%)	17 20
20	ST	65/66 (98%)	64 (98%)	1 (2%)	60 72
21	SU	61/61 (100%)	53 (87%)	8 (13%)	3 2
25	LB	216/218 (99%)	211 (98%)	5 (2%)	45 56
26	LC	164/164 (100%)	161 (98%)	3 (2%)	54 66
27	LD	165/165 (100%)	159 (96%)	6 (4%)	30 39
28	LE	149/150 (99%)	140 (94%)	9 (6%)	16 18
29	LF	136/138 (99%)	131 (96%)	5 (4%)	29 37
30	LI	114/114 (100%)	99 (87%)	15 (13%)	3 2
31	LJ	103/123 (84%)	95 (92%)	8 (8%)	10 10
32	LK	104/110 (94%)	95 (91%)	9 (9%)	8 7
33	LM	116/116 (100%)	113 (97%)	3 (3%)	41 51
34	LN	104/104 (100%)	99 (95%)	5 (5%)	21 27
35	LO	103/103 (100%)	100 (97%)	3 (3%)	37 47
36	LP	109/108 (101%)	104 (95%)	5 (5%)	23 28
37	LQ	100/103 (97%)	96 (96%)	4 (4%)	27 34
38	LR	86/87 (99%)	79 (92%)	7 (8%)	9 9
39	LS	99/100 (99%)	95 (96%)	4 (4%)	27 34
40	LT	89/90 (99%)	89 (100%)	0	100 100
41	LU	84/84 (100%)	83 (99%)	1 (1%)	67 79
42	LV	93/93 (100%)	90 (97%)	3 (3%)	34 42
43	LW	80/84 (95%)	76 (95%)	4 (5%)	20 25
44	LX	83/85 (98%)	80 (96%)	3 (4%)	30 39
45	LY	78/78 (100%)	77 (99%)	1 (1%)	65 77
46	La	62/63 (98%)	62 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	Lb	68/68 (100%)	65 (96%)	3 (4%)	24 30
48	Lc	54/55 (98%)	54 (100%)	0	100 100
49	Ld	48/49 (98%)	46 (96%)	2 (4%)	25 32
50	Le	60/62 (97%)	55 (92%)	5 (8%)	9 9
51	Lf	47/48 (98%)	46 (98%)	1 (2%)	48 60
52	Lg	47/49 (96%)	47 (100%)	0	100 100
53	Lh	38/38 (100%)	37 (97%)	1 (3%)	41 51
54	Li	51/52 (98%)	50 (98%)	1 (2%)	50 62
55	Lj	34/34 (100%)	33 (97%)	1 (3%)	37 47
57	Pp	3/3 (100%)	2 (67%)	1 (33%)	0 0
All	All	4900/5064 (97%)	4660 (95%)	240 (5%)	23 26

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	8	ASP
2	SB	23	TRP
2	SB	35	ARG
2	SB	113	ARG
2	SB	120	GLN
2	SB	127	ASP
2	SB	133	GLU
2	SB	147	SER
3	SC	21	THR
3	SC	53	SER
3	SC	84	VAL
3	SC	107	ARG
3	SC	121	THR
3	SC	185	ASN
3	SC	192	THR
3	SC	206	GLU
3	SC	211	MET
4	SD	58	LYS
5	SE	11	LEU
5	SE	22	SER
5	SE	23	LYS
5	SE	29	ARG
5	SE	32	SER

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Mol	Chain	Res	Type
5	SE	70	ASN
5	SE	97	GLN
5	SE	130	SER
5	SE	152	MET
6	SF	33	GLU
6	SF	36	ILE
6	SF	44	ARG
7	SG	7	ILE
7	SG	10	ARG
7	SG	30	LEU
7	SG	35	LYS
7	SG	45	SER
7	SG	58	GLU
7	SG	73	VAL
7	SG	75	VAL
7	SG	76	LYS
7	SG	77	SER
7	SG	78[A]	ARG
7	SG	78[B]	ARG
7	SG	80	VAL
7	SG	125	SER
7	SG	126	ASP
7	SG	149	LYS
7	SG	155	ARG
7	SG	156	TRP
8	SH	54	ASP
8	SH	55	THR
8	SH	60	GLU
8	SH	74	SER
8	SH	107	SER
9	SI	4	ASN
9	SI	12	ARG
9	SI	14	SER
9	SI	32	GLN
9	SI	58	VAL
9	SI	61	LEU
9	SI	123	ARG
9	SI	130	ARG
10	SJ	5	ARG
10	SJ	14	ASP
10	SJ	19	ASP
10	SJ	45	ARG

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Mol	Chain	Res	Type
11	SK	18	ASP
11	SK	35	THR
11	SK	55	SER
11	SK	72	ASP
11	SK	75	LYS
11	SK	81	ASN
11	SK	82	LEU
11	SK	111	THR
11	SK	129	VAL
12	SL	15	LYS
12	SL	43	LYS
12	SL	62	GLU
12	SL	75	GLN
12	SL	82	ILE
12	SL	110	ARG
12	SL	115	SER
13	SM	9	ILE
13	SM	14	HIS
13	SM	16	VAL
13	SM	27	LYS
13	SM	42	ASP
13	SM	59	GLU
14	SN	26	GLU
14	SN	37	SER
14	SN	38	ASP
14	SN	47	LYS
14	SN	58	SER
15	SO	18	ASP
15	SO	65	LYS
15	SO	74	ASP
15	SO	80	GLN
15	SO	89[A]	ARG
15	SO	89[B]	ARG
16	SP	1	MET
17	SQ	27	ARG
17	SQ	81	LYS
17	SQ	83	VAL
18	SR	8	ARG
18	SR	9	LYS
18	SR	12	ARG
18	SR	14	THR
18	SR	18	VAL

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Mol	Chain	Res	Type
18	SR	20	GLU
18	SR	21	ILE
19	SS	24	GLU
19	SS	27	ASP
19	SS	48	THR
19	SS	56	GLN
20	ST	40	GLU
21	SU	13	ASP
21	SU	29	LEU
21	SU	51	SER
21	SU	62	ARG
21	SU	66	ARG
21	SU	67	ARG
21	SU	69	ARG
21	SU	70	LEU
25	LB	108	LYS
25	LB	251	GLN
25	LB	252	THR
25	LB	268	VAL
25	LB	269	ARG
26	LC	18	ASP
26	LC	32	ASN
26	LC	95	SER
27	LD	2	GLU
27	LD	17	THR
27	LD	49	ARG
27	LD	152	GLU
27	LD	153	LEU
27	LD	167	VAL
28	LE	10	ASP
28	LE	19	GLU
28	LE	47	LYS
28	LE	51	ASP
28	LE	83	TYR
28	LE	105	THR
28	LE	147	ASP
28	LE	163	ASP
28	LE	175	PHE
29	LF	30	ASN
29	LF	50	LEU
29	LF	72	LEU
29	LF	99	LYS

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Mol	Chain	Res	Type
29	LF	101	ASN
30	LI	14	SER
30	LI	21	VAL
30	LI	40	THR
30	LI	46	PHE
30	LI	66	ASN
30	LI	72	ILE
30	LI	73	ASN
30	LI	76	GLU
30	LI	83	LYS
30	LI	93	SER
30	LI	98	ASP
30	LI	110	VAL
30	LI	125	THR
30	LI	131	SER
30	LI	137	GLU
31	LJ	5	LEU
31	LJ	17	GLU
31	LJ	27	VAL
31	LJ	37	LYS
31	LJ	56	ARG
31	LJ	60	LEU
31	LJ	85	SER
31	LJ	124	ASP
32	LK	11	LEU
32	LK	21	SER
32	LK	47	ASP
32	LK	48	SER
32	LK	65	ARG
32	LK	67	PHE
32	LK	82	LYS
32	LK	125	MET
32	LK	127	ARG
33	LM	2	LYS
33	LM	67	ASN
33	LM	142	ILE
34	LN	23	LYS
34	LN	66	LYS
34	LN	89	ASN
34	LN	95	ILE
34	LN	110	GLU
35	LO	1	MET

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Mol	Chain	Res	Type
35	LO	14	LYS
35	LO	121	THR
36	LP	1	MET
36	LP	3	GLN
36	LP	88	ASN
36	LP	127	LYS
36	LP	135	VAL
37	LQ	2	ARG
37	LQ	14	SER
37	LQ	98	LEU
37	LQ	120	GLU
38	LR	4	LYS
38	LR	16	ARG
38	LR	19	GLN
38	LR	48	LEU
38	LR	84	GLU
38	LR	95	SER
38	LR	116	GLN
39	LS	38	LYS
39	LS	39	ARG
39	LS	66	ASN
39	LS	78	SER
41	LU	18	GLN
42	LV	7	HIS
42	LV	13	SER
42	LV	70	LYS
43	LW	26	LYS
43	LW	27	SER
43	LW	37	ASP
43	LW	92	ASN
44	LX	6	ARG
44	LX	15	THR
44	LX	24	LYS
45	LY	61	LEU
47	Lb	35	SER
47	Lb	43	GLU
47	Lb	72	ARG
49	Ld	16	ARG
49	Ld	31	ARG
50	Le	11	GLU
50	Le	15	SER
50	Le	28	VAL

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Mol	Chain	Res	Type
50	Le	48	GLN
50	Le	50	ASP
51	Lf	18	SER
53	Lh	24	THR
54	Li	31	HIS
55	Lj	6	SER
57	Pp	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
4	SD	71	GLN
6	SF	68	GLN
7	SG	130	ASN
10	SJ	56	HIS
13	SM	8	ASN
15	SO	40	GLN
25	LB	134	ASN
26	LC	150	GLN
27	LD	163	ASN
28	LE	21	ASN
28	LE	63	GLN
28	LE	127	ASN
30	LI	33	GLN
30	LI	66	ASN
38	LR	38	GLN
39	LS	7	GLN
43	LW	59	ASN
44	LX	74	ASN
52	Lg	45	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1538/1542 (99%)	224 (14%)	13 (0%)
22	mR	23/60 (38%)	11 (47%)	0
23	23	2899/2904 (99%)	440 (15%)	27 (0%)
24	5	119/120 (99%)	13 (10%)	1 (0%)
56	Pt	73/76 (96%)	15 (20%)	0
58	Dt	73/76 (96%)	29 (39%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4725/4778 (98%)	732 (15%)	41 (0%)

All (732) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	4	U
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	65	A
1	16	71	A
1	16	72	A
1	16	73	C
1	16	74	A
1	16	75	G
1	16	76	G
1	16	78	A
1	16	79	G
1	16	82	G
1	16	83	C
1	16	84	U
1	16	85	U
1	16	86	G
1	16	88	U
1	16	91	U
1	16	92	U
1	16	95	C
1	16	131	A
1	16	137	U
1	16	141	G
1	16	143	A
1	16	144	G
1	16	159	G
1	16	163	C
1	16	171	A
1	16	174	A
1	16	192	A

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Mol	Chain	Res	Type
1	16	193	C
1	16	197	A
1	16	204	G
1	16	208	U
1	16	209	U
1	16	210	C
1	16	215	C
1	16	226	G
1	16	245	U
1	16	247	G
1	16	250	A
1	16	251	G
1	16	252	U
1	16	253	A
1	16	266	G
1	16	267	C
1	16	281	G
1	16	289	G
1	16	300	A
1	16	321	A
1	16	328	C
1	16	329	A
1	16	332	G
1	16	345	C
1	16	348	G
1	16	351	G
1	16	352	C
1	16	354	G
1	16	367	U
1	16	372	C
1	16	388	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	424	G
1	16	429	U
1	16	458	U
1	16	459	A
1	16	460	A

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Mol	Chain	Res	Type
1	16	462	G
1	16	463	U
1	16	464	U
1	16	465	A
1	16	466	A
1	16	467	U
1	16	468	A
1	16	469	C
1	16	479	U
1	16	484	G
1	16	485	U
1	16	486	U
1	16	509	A
1	16	511	C
1	16	518	C
1	16	527	G7M
1	16	531	U
1	16	532	A
1	16	533	A
1	16	535	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	633	G
1	16	634	C
1	16	653	U
1	16	665	A
1	16	703	G
1	16	718	A
1	16	721	G
1	16	723	U
1	16	734	G
1	16	755	G
1	16	777	A
1	16	793	U
1	16	794	A
1	16	815	A

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Mol	Chain	Res	Type
1	16	817	C
1	16	821	G
1	16	828	U
1	16	829	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	902	G
1	16	914	A
1	16	926	G
1	16	927	G
1	16	933	G
1	16	934	C
1	16	935	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	983	A
1	16	993	G
1	16	994	A
1	16	1004	A
1	16	1008	U
1	16	1016	A
1	16	1024	G
1	16	1026	G
1	16	1029	U
1	16	1031	C
1	16	1032	G
1	16	1033	G
1	16	1035	A
1	16	1043	G
1	16	1044	A
1	16	1045	C
1	16	1065	U
1	16	1085	U
1	16	1094	G

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Mol	Chain	Res	Type
1	16	1095	U
1	16	1101	A
1	16	1124	G
1	16	1125	U
1	16	1133	G
1	16	1135	U
1	16	1136	C
1	16	1137	C
1	16	1138	G
1	16	1139	G
1	16	1140	C
1	16	1141	C
1	16	1152	A
1	16	1154	G
1	16	1158	C
1	16	1159	U
1	16	1168	U
1	16	1169	A
1	16	1183	U
1	16	1184	G
1	16	1196	A
1	16	1197	A
1	16	1212	U
1	16	1213	A
1	16	1227	A
1	16	1228	C
1	16	1238	A
1	16	1239	A
1	16	1258	G
1	16	1260	G
1	16	1280	A
1	16	1286	U
1	16	1287	A
1	16	1300	G
1	16	1302	C
1	16	1305	G
1	16	1317	C
1	16	1320	C
1	16	1336	C
1	16	1346	A
1	16	1353	G
1	16	1363	A

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Mol	Chain	Res	Type
1	16	1368	A
1	16	1370	G
1	16	1397	C
1	16	1398	A
1	16	1429	A
1	16	1441	A
1	16	1446	A
1	16	1454	G
1	16	1487	G
1	16	1492	A
1	16	1497	G
1	16	1503	A
1	16	1505	G
1	16	1506	U
1	16	1517	G
1	16	1529	G
1	16	1530	G
1	16	1539	C
1	16	1542	A
22	mR	29	G
22	mR	31	C
22	mR	32	A
22	mR	33	A
22	mR	34	U
22	mR	35	C
22	mR	49	U
22	mR	50	U
22	mR	51	C
22	mR	52	A
22	mR	53	A
23	23	10	A
23	23	15	G
23	23	34	U
23	23	44	A
23	23	46	G
23	23	55	G
23	23	71	A
23	23	74	A
23	23	75	G
23	23	101	A
23	23	102	U
23	23	103	A

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Mol	Chain	Res	Type
23	23	110	G
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	141	G
23	23	142	A
23	23	159	G
23	23	163	C
23	23	174	U
23	23	177	G
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	221	A
23	23	222	A
23	23	248	G
23	23	252	G
23	23	266	G
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	283	G
23	23	284	U
23	23	285	G
23	23	286	U
23	23	311	A
23	23	330	A
23	23	345	A
23	23	353	C
23	23	359	G
23	23	361	G
23	23	362	A
23	23	371	A

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Mol	Chain	Res	Type
23	23	372	G
23	23	386	G
23	23	388	G
23	23	395	U
23	23	396	G
23	23	401	A
23	23	405	U
23	23	412	A
23	23	455	C
23	23	456	C
23	23	457	A
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	532	A
23	23	547	A
23	23	549	G
23	23	563	A
23	23	573	U
23	23	575	A
23	23	603	A
23	23	613	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	686	U
23	23	717	C
23	23	726	G
23	23	729	G
23	23	730	A
23	23	747	5MU

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Mol	Chain	Res	Type
23	23	764	A
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	812	C
23	23	819	A
23	23	827	U
23	23	845	A
23	23	846	U
23	23	847	U
23	23	859	G
23	23	869	G
23	23	878	A
23	23	883	G
23	23	885	C
23	23	887	U
23	23	895	U
23	23	896	A
23	23	897	C
23	23	902	C
23	23	907	G
23	23	910	A
23	23	917	A
23	23	919	U
23	23	931	U
23	23	932	U
23	23	941	A
23	23	946	C
23	23	961	C
23	23	962	G
23	23	974	G
23	23	983	A
23	23	996	A
23	23	999	U
23	23	1005	C
23	23	1012	U
23	23	1013	C

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Mol	Chain	Res	Type
23	23	1026	G
23	23	1033	U
23	23	1046	A
23	23	1047	G
23	23	1055	G
23	23	1060	U
23	23	1070	A
23	23	1081	U
23	23	1083	U
23	23	1084	A
23	23	1085	A
23	23	1087	G
23	23	1088	A
23	23	1090	A
23	23	1097	U
23	23	1112	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	1161	C
23	23	1169	A
23	23	1171	G
23	23	1172	C
23	23	1173	U
23	23	1174	U
23	23	1175	A
23	23	1177	G
23	23	1178	C
23	23	1179	G
23	23	1180	U
23	23	1238	G
23	23	1247	A
23	23	1249	U
23	23	1250	G
23	23	1253	A
23	23	1256	G
23	23	1262	A
23	23	1266	G

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Mol	Chain	Res	Type
23	23	1271	G
23	23	1272	A
23	23	1273	U
23	23	1300	G
23	23	1301	A
23	23	1321	A
23	23	1329	U
23	23	1352	U
23	23	1365	A
23	23	1368	G
23	23	1379	U
23	23	1380	G
23	23	1383	A
23	23	1395	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	1452	G
23	23	1453	A
23	23	1460	U
23	23	1461	C
23	23	1482	G
23	23	1488	C
23	23	1493	C
23	23	1494	A
23	23	1497	U
23	23	1502	A
23	23	1503	A
23	23	1506	U
23	23	1507	C
23	23	1508	A
23	23	1509	A
23	23	1515	A
23	23	1524	G
23	23	1531	C
23	23	1532	A
23	23	1536	C
23	23	1537	G

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Mol	Chain	Res	Type
23	23	1538	G
23	23	1539	U
23	23	1566	A
23	23	1569	A
23	23	1578	U
23	23	1583	A
23	23	1584	U
23	23	1608	A
23	23	1610	A
23	23	1647	U
23	23	1648	U
23	23	1649	G
23	23	1674	G
23	23	1727	C
23	23	1729	U
23	23	1730	C
23	23	1731	G
23	23	1738	G
23	23	1764	C
23	23	1773	A
23	23	1782	U
23	23	1784	A
23	23	1786	A
23	23	1791	A
23	23	1799	G
23	23	1800	C
23	23	1801	A
23	23	1807	G
23	23	1808	A
23	23	1811	G
23	23	1816	C
23	23	1848	A
23	23	1870	C
23	23	1872	A
23	23	1873	G
23	23	1906	G
23	23	1907	G
23	23	1929	G
23	23	1930	G
23	23	1940	U
23	23	1954	G
23	23	1955	U

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Mol	Chain	Res	Type
23	23	1960	A
23	23	1966	A
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	1993	U
23	23	1997	C
23	23	2022	U
23	23	2023	C
23	23	2031	A
23	23	2032	G
23	23	2033	A
23	23	2043	C
23	23	2055	C
23	23	2056	G
23	23	2060	A
23	23	2061	G
23	23	2062	A
23	23	2069	G7M
23	23	2093	G
23	23	2098	U
23	23	2100	A
23	23	2101	A
23	23	2102	G
23	23	2103	C
23	23	2104	C
23	23	2106	U
23	23	2108	A
23	23	2110	G
23	23	2111	U
23	23	2112	G
23	23	2113	U
23	23	2114	A
23	23	2115	G
23	23	2117	A
23	23	2118	U
23	23	2120	G
23	23	2123	G

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Mol	Chain	Res	Type
23	23	2124	G
23	23	2126	A
23	23	2128	G
23	23	2130	U
23	23	2131	U
23	23	2132	U
23	23	2133	G
23	23	2136	G
23	23	2138	G
23	23	2141	G
23	23	2146	C
23	23	2147	A
23	23	2161	C
23	23	2162	G
23	23	2163	A
23	23	2164	C
23	23	2166	U
23	23	2167	U
23	23	2170	A
23	23	2171	A
23	23	2172	U
23	23	2173	A
23	23	2182	U
23	23	2186	G
23	23	2190	G
23	23	2198	A
23	23	2204	G
23	23	2211	A
23	23	2225	A
23	23	2238	G
23	23	2239	G
23	23	2243	U
23	23	2251	OMG
23	23	2268	A
23	23	2278	A
23	23	2279	G
23	23	2283	C
23	23	2287	A
23	23	2305	U
23	23	2308	G
23	23	2309	A
23	23	2311	A

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Mol	Chain	Res	Type
23	23	2312	U
23	23	2319	G
23	23	2321	U
23	23	2322	A
23	23	2325	G
23	23	2333	A
23	23	2336	A
23	23	2345	G
23	23	2347	C
23	23	2350	C
23	23	2361	G
23	23	2372	U
23	23	2375	G
23	23	2379	G
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	2410	G
23	23	2423	U
23	23	2425	A
23	23	2429	G
23	23	2430	A
23	23	2431	U
23	23	2441	U
23	23	2448	A
23	23	2464	G
23	23	2475	C
23	23	2476	A
23	23	2478	A
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

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Mol	Chain	Res	Type
23	23	2529	G
23	23	2535	G
23	23	2537	U
23	23	2547	A
23	23	2554	U
23	23	2562	U
23	23	2566	A
23	23	2567	G
23	23	2573	C
23	23	2602	A
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	2689	U
23	23	2690	U
23	23	2714	G
23	23	2726	A
23	23	2732	G
23	23	2733	A
23	23	2743	U
23	23	2744	G
23	23	2748	A
23	23	2751	G
23	23	2757	A
23	23	2765	A
23	23	2777	G
23	23	2778	A
23	23	2779	U
23	23	2798	U
23	23	2799	A
23	23	2818	U
23	23	2820	A
23	23	2821	A
23	23	2832	U
23	23	2835	A
23	23	2858	C
23	23	2859	G
23	23	2861	U
23	23	2873	A

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Mol	Chain	Res	Type
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	2904	U
24	5	9	G
24	5	13	G
24	5	15	A
24	5	35	C
24	5	50	A
24	5	51	G
24	5	67	G
24	5	87	U
24	5	89	U
24	5	90	C
24	5	91	C
24	5	99	A
24	5	109	A
56	Pt	4	U
56	Pt	9	A
56	Pt	10	G
56	Pt	13	C
56	Pt	16	H2U
56	Pt	17	H2U
56	Pt	18	G
56	Pt	19	G
56	Pt	20	H2U
56	Pt	21	A
56	Pt	46	G
56	Pt	49	G
56	Pt	63	U
56	Pt	72	C
56	Pt	74	C
58	Dt	4	C
58	Dt	8	4SU
58	Dt	11	C
58	Dt	13	C
58	Dt	15	G
58	Dt	16	H2U

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Mol	Chain	Res	Type
58	Dt	17	C
58	Dt	18	G
58	Dt	19	G
58	Dt	20	U
58	Dt	21	A
58	Dt	22	G
58	Dt	23	A
58	Dt	29	G
58	Dt	40	C
58	Dt	43	C
58	Dt	44	G
58	Dt	45	U
58	Dt	46	G7M
58	Dt	48	C
58	Dt	49	C
58	Dt	52	G
58	Dt	56	C
58	Dt	57	G
58	Dt	58	A
58	Dt	60	U
58	Dt	72	C
58	Dt	74	C
58	Dt	76	A

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	16	72	A
1	16	84	U
1	16	85	U
1	16	251	G
1	16	252	U
1	16	428	G
1	16	457	G
1	16	633	G
1	16	845	A
1	16	1025	U
1	16	1124	G
1	16	1137	C
1	16	1505	G
23	23	43	G
23	23	134	G

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Mol	Chain	Res	Type
23	23	158	U
23	23	177	G
23	23	277	G
23	23	285	G
23	23	352	A
23	23	404	A
23	23	613	A
23	23	784	G
23	23	827	U
23	23	1046	A
23	23	1060	U
23	23	1087	G
23	23	1266	G
23	23	1379	U
23	23	1416	G
23	23	1506	U
23	23	1847	A
23	23	2116	G
23	23	2430	A
23	23	2474	U
23	23	2491	U
23	23	2536	G
23	23	2581	G
23	23	2756	U
23	23	2858	C
24	5	15	A

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

52 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	$\#\|Z\| > 2$
56	H2U	Pt	16	56	18,21,22	1.10	2 (11%)	19,30,33	1.22	1 (5%)
23	PSU	23	2580	23	18,21,22	1.42	4 (22%)	21,30,33	2.08	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	6MZ	23	1618	23	17,25,26	0.89	1 (5%)	15,36,39	2.31	4 (26%)
56	H2U	Pt	20	56	18,21,22	4.44	12 (66%)	19,30,33	1.63	5 (26%)
23	PSU	23	2504	23	18,21,22	1.42	3 (16%)	21,30,33	2.08	4 (19%)
56	3AU	Pt	47	56	24,28,29	1.04	0	30,40,43	1.62	4 (13%)
23	2MG	23	1835	23	18,26,27	0.91	1 (5%)	16,38,41	1.29	2 (12%)
1	2MG	16	966	1	18,26,27	0.88	1 (5%)	16,38,41	1.29	3 (18%)
23	H2U	23	2449	23	18,21,22	4.32	13 (72%)	19,30,33	1.72	4 (21%)
1	G7M	16	527	1	20,26,27	2.59	4 (20%)	16,39,42	0.93	1 (6%)
58	PSU	Dt	32	58	18,21,22	3.22	9 (50%)	21,30,33	3.06	6 (28%)
58	MIA	Dt	37	58	24,31,32	2.26	2 (8%)	22,44,47	3.15	11 (50%)
1	4OC	16	1402	1,60	20,23,24	0.74	0	25,32,35	0.93	1 (4%)
36	4D4	LP	81	36	9,11,12	2.16	2 (22%)	7,13,15	2.04	3 (42%)
23	PSU	23	746	60,23	18,21,22	1.41	3 (16%)	21,30,33	1.98	4 (19%)
58	3AU	Dt	47	58	24,28,29	0.98	0	30,40,43	1.49	5 (16%)
56	5MU	Pt	54	56	19,22,23	1.36	5 (26%)	27,32,35	2.11	7 (25%)
56	PSU	Pt	55	56	18,21,22	1.39	2 (11%)	21,30,33	2.08	4 (19%)
1	2MG	16	1207	1,60	18,26,27	0.91	1 (5%)	16,38,41	1.29	2 (12%)
23	PSU	23	2457	23	18,21,22	1.41	3 (16%)	21,30,33	2.16	4 (19%)
1	5MC	16	967	1	19,22,23	1.55	3 (15%)	26,32,35	1.12	2 (7%)
58	PSU	Dt	39	58	18,21,22	2.79	7 (38%)	21,30,33	3.07	10 (47%)
23	OMG	23	2251	23,58	19,26,27	1.19	2 (10%)	21,38,41	0.84	1 (4%)
23	6MZ	23	2030	23	17,25,26	0.87	1 (5%)	15,36,39	2.58	4 (26%)
1	MA6	16	1519	1	19,26,27	0.97	1 (5%)	18,38,41	1.97	3 (16%)
23	G7M	23	2069	23	20,26,27	2.45	4 (20%)	16,39,42	1.85	5 (31%)
56	U8U	Pt	34	56,22	20,24,25	1.51	3 (15%)	22,34,37	1.06	3 (13%)
23	2MG	23	2445	23	18,26,27	0.89	1 (5%)	16,38,41	1.43	5 (31%)
1	PSU	16	516	1,60	18,21,22	1.41	3 (16%)	21,30,33	2.14	5 (23%)
23	OMU	23	2552	23	19,22,23	4.23	13 (68%)	25,31,34	2.29	6 (24%)
56	PSU	Pt	39	56	18,21,22	1.37	3 (16%)	21,30,33	2.09	4 (19%)
23	PSU	23	2604	23	18,21,22	1.84	6 (33%)	21,30,33	2.32	9 (42%)
23	2MA	23	2503	60,23	18,25,26	0.68	0	20,37,40	2.01	4 (20%)
23	1MG	23	745	23	19,26,27	0.90	1 (5%)	18,39,42	1.12	2 (11%)
12	D2T	SL	89	12	8,9,10	1.65	2 (25%)	6,11,13	1.52	2 (33%)
1	UR3	16	1498	1	19,22,23	0.93	0	26,32,35	1.76	3 (11%)
23	OMC	23	2498	60,23	19,22,23	1.01	2 (10%)	25,31,34	1.13	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
58	PSU	Dt	55	58	18,21,22	2.23	6 (33%)	21,30,33	2.93	9 (42%)
23	5MU	23	1939	23	19,22,23	1.39	5 (26%)	27,32,35	2.14	6 (22%)
58	H2U	Dt	16	58	18,21,22	1.43	3 (16%)	19,30,33	1.86	4 (21%)
1	5MC	16	1407	1	19,22,23	1.52	3 (15%)	26,32,35	1.10	3 (11%)
23	3TD	23	1915	23	19,22,23	1.21	2 (10%)	23,32,35	2.10	3 (13%)
23	5MC	23	1962	23	19,22,23	1.51	3 (15%)	26,32,35	1.11	2 (7%)
58	4SU	Dt	8	58	18,21,22	1.85	4 (22%)	25,30,33	2.30	5 (20%)
56	T6A	Pt	37	56	26,34,35	1.05	1 (3%)	28,49,52	2.57	6 (21%)
23	5MU	23	747	23	19,22,23	1.41	6 (31%)	27,32,35	2.11	6 (22%)
23	PSU	23	955	23	18,21,22	1.38	3 (16%)	21,30,33	2.13	4 (19%)
58	G7M	Dt	46	58	20,26,27	2.52	4 (20%)	16,39,42	1.39	2 (12%)
1	MA6	16	1518	1	19,26,27	0.98	1 (5%)	18,38,41	1.92	3 (16%)
23	PSU	23	2605	23	18,21,22	1.38	3 (16%)	21,30,33	2.07	4 (19%)
56	H2U	Pt	17	56	18,21,22	1.06	2 (11%)	19,30,33	1.15	2 (10%)
1	2MG	16	1516	1	18,26,27	0.92	1 (5%)	16,38,41	1.44	4 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	H2U	Pt	16	56	-	7/7/38/39	0/2/2/2
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
23	6MZ	23	1618	23	-	2/5/27/28	0/3/3/3
56	H2U	Pt	20	56	-	2/7/38/39	0/2/2/2
23	PSU	23	2504	23	-	2/7/25/26	0/2/2/2
56	3AU	Pt	47	56	-	7/16/34/35	0/2/2/2
23	2MG	23	1835	23	-	0/5/27/28	0/3/3/3
1	2MG	16	966	1	-	0/5/27/28	0/3/3/3
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2
1	G7M	16	527	1	-	2/3/25/26	0/3/3/3
58	PSU	Dt	32	58	-	0/7/25/26	0/2/2/2
58	MIA	Dt	37	58	-	8/11/33/34	0/3/3/3
1	4OC	16	1402	1,60	-	0/9/29/30	0/2/2/2
36	4D4	LP	81	36	-	3/11/12/14	-
23	PSU	23	746	60,23	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	3AU	Dt	47	58	-	6/16/34/35	0/2/2/2
56	5MU	Pt	54	56	-	0/7/25/26	0/2/2/2
56	PSU	Pt	55	56	-	0/7/25/26	0/2/2/2
1	2MG	16	1207	1,60	-	0/5/27/28	0/3/3/3
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
58	PSU	Dt	39	58	-	0/7/25/26	0/2/2/2
23	OMG	23	2251	23,58	-	3/5/27/28	0/3/3/3
23	6MZ	23	2030	23	-	2/5/27/28	0/3/3/3
1	MA6	16	1519	1	-	3/7/29/30	0/3/3/3
23	G7M	23	2069	23	-	1/3/25/26	0/3/3/3
56	U8U	Pt	34	56,22	-	0/10/28/29	0/2/2/2
23	2MG	23	2445	23	-	1/5/27/28	0/3/3/3
1	PSU	16	516	1,60	-	0/7/25/26	0/2/2/2
23	OMU	23	2552	23	-	1/9/27/28	0/2/2/2
56	PSU	Pt	39	56	-	0/7/25/26	0/2/2/2
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
23	2MA	23	2503	60,23	-	2/3/25/26	0/3/3/3
23	1MG	23	745	23	-	0/3/25/26	0/3/3/3
12	D2T	SL	89	12	-	3/7/12/14	-
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
23	OMC	23	2498	60,23	-	2/9/27/28	0/2/2/2
58	PSU	Dt	55	58	-	0/7/25/26	0/2/2/2
23	5MU	23	1939	23	-	0/7/25/26	0/2/2/2
58	H2U	Dt	16	58	-	0/7/38/39	0/2/2/2
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
23	3TD	23	1915	23	-	2/7/25/26	0/2/2/2
23	5MC	23	1962	23	-	0/7/25/26	0/2/2/2
58	4SU	Dt	8	58	-	2/7/25/26	0/2/2/2
56	T6A	Pt	37	56	-	10/19/41/42	0/3/3/3
23	5MU	23	747	23	-	0/7/25/26	0/2/2/2
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
58	G7M	Dt	46	58	-	0/3/25/26	0/3/3/3
1	MA6	16	1518	1	-	0/7/29/30	0/3/3/3
23	PSU	23	2605	23	-	0/7/25/26	0/2/2/2
56	H2U	Pt	17	56	-	3/7/38/39	0/2/2/2
1	2MG	16	1516	1	-	0/5/27/28	0/3/3/3

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	2552	OMU	C3'-C2'	-10.60	1.29	1.53
23	23	2449	H2U	C2'-C3'	-10.18	1.25	1.53
56	Pt	20	H2U	C2'-C3'	-10.02	1.26	1.53
56	Pt	20	H2U	C2-N1	9.59	1.48	1.35
23	23	2449	H2U	C2-N1	8.93	1.48	1.35
58	Dt	37	MIA	C2-S10	-7.57	1.69	1.75
1	16	527	G7M	C8-N9	7.41	1.46	1.33
23	23	2069	G7M	C8-N9	7.09	1.46	1.33
58	Dt	46	G7M	C8-N9	7.04	1.46	1.33
1	16	527	G7M	C8-N7	7.04	1.46	1.33
58	Dt	37	MIA	C13-C14	6.58	1.52	1.32
23	23	2069	G7M	C8-N7	6.55	1.45	1.33
58	Dt	46	G7M	C8-N7	6.42	1.44	1.33
23	23	2552	OMU	C2-N1	6.01	1.47	1.38
58	Dt	32	PSU	C2-N1	-5.97	1.28	1.36
56	Pt	20	H2U	C2-N3	5.95	1.48	1.38
23	23	2552	OMU	C2-N3	5.80	1.48	1.38
58	Dt	32	PSU	C6-N1	-5.73	1.26	1.36
58	Dt	32	PSU	C4-N3	-5.64	1.28	1.38
23	23	2552	OMU	O4'-C1'	-5.60	1.29	1.42
56	Pt	20	H2U	C4-N3	5.50	1.46	1.37
1	16	967	5MC	C5-C4	5.50	1.48	1.44
58	Dt	39	PSU	C4-N3	-5.48	1.28	1.38
1	16	1407	5MC	C5-C4	5.36	1.48	1.44
23	23	1962	5MC	C5-C4	5.35	1.48	1.44
58	Dt	32	PSU	C2-N3	-5.34	1.28	1.37
23	23	2552	OMU	C6-C5	5.17	1.47	1.35
23	23	2449	H2U	C2-N3	5.16	1.46	1.38
58	Dt	8	4SU	C4-S4	-5.04	1.59	1.68
36	LP	81	4D4	CZ-NE	5.03	1.43	1.33
56	Pt	34	U8U	C2-S2	-4.97	1.59	1.67
58	Dt	39	PSU	C2-N3	-4.94	1.29	1.37
23	23	2449	H2U	O4'-C1'	-4.84	1.30	1.42
58	Dt	55	PSU	C2-N1	-4.82	1.30	1.36
58	Dt	55	PSU	C4-N3	-4.81	1.29	1.38
58	Dt	39	PSU	C2-N1	-4.80	1.30	1.36
58	Dt	39	PSU	C2'-C1'	-4.47	1.47	1.53
56	Pt	20	H2U	O4'-C1'	-4.46	1.31	1.42
23	23	2449	H2U	C4-N3	4.37	1.44	1.37
58	Dt	39	PSU	C6-N1	-4.29	1.29	1.36
1	16	527	G7M	C5-C4	4.10	1.47	1.39
58	Dt	46	G7M	C5-C4	4.03	1.47	1.39
23	23	2552	OMU	O4'-C4'	3.97	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	2449	H2U	C5'-C4'	-3.96	1.39	1.51
56	Pt	20	H2U	C5'-C4'	-3.92	1.39	1.51
23	23	2552	OMU	C5'-C4'	-3.92	1.39	1.51
58	Dt	55	PSU	C2-N3	-3.85	1.31	1.37
23	23	2449	H2U	O4-C4	-3.82	1.15	1.23
58	Dt	16	H2U	C2-N3	-3.71	1.31	1.38
23	23	2604	PSU	C4-N3	-3.69	1.31	1.38
23	23	2069	G7M	C5-C4	3.68	1.46	1.39
23	23	2552	OMU	O4-C4	-3.65	1.17	1.24
56	Pt	20	H2U	C2'-C1'	3.60	1.64	1.53
23	23	2552	OMU	O2-C2	-3.49	1.16	1.23
36	LP	81	4D4	CZ-NH2	3.42	1.44	1.32
58	Dt	32	PSU	C2'-C1'	-3.41	1.49	1.53
23	23	1915	3TD	C6-C5	3.40	1.39	1.35
23	23	2552	OMU	C4-N3	3.37	1.44	1.38
58	Dt	8	4SU	C4-N3	-3.36	1.34	1.37
23	23	2449	H2U	O2-C2	-3.33	1.17	1.23
58	Dt	32	PSU	O4'-C1'	-3.26	1.39	1.43
56	Pt	55	PSU	C6-C5	3.23	1.38	1.35
23	23	2504	PSU	C6-C5	3.19	1.38	1.35
23	23	2552	OMU	C2'-C1'	3.15	1.60	1.53
58	Dt	32	PSU	C1'-C5	-3.14	1.43	1.50
23	23	746	PSU	C6-C5	3.13	1.38	1.35
23	23	2457	PSU	C6-C5	3.12	1.38	1.35
23	23	2251	OMG	C8-N7	-3.11	1.30	1.34
23	23	2449	H2U	O3'-C3'	3.08	1.50	1.43
56	Pt	20	H2U	O3'-C3'	3.08	1.50	1.43
56	Pt	39	PSU	C6-C5	3.05	1.38	1.35
1	16	516	PSU	C6-C5	3.05	1.38	1.35
23	23	2604	PSU	C2'-C1'	-3.01	1.49	1.53
58	Dt	46	G7M	C6-N1	-2.98	1.33	1.37
23	23	2580	PSU	C6-C5	2.97	1.38	1.35
23	23	2605	PSU	C6-C5	2.95	1.38	1.35
23	23	2605	PSU	C4-N3	-2.93	1.33	1.38
56	Pt	16	H2U	C2-N3	-2.93	1.32	1.38
23	23	1939	5MU	C4-N3	-2.92	1.33	1.38
23	23	2604	PSU	C2-N3	-2.92	1.32	1.37
58	Dt	16	H2U	C4-N3	-2.92	1.32	1.37
23	23	2457	PSU	C4-N3	-2.92	1.33	1.38
23	23	2504	PSU	C4-N3	-2.92	1.33	1.38
23	23	2449	H2U	C2'-C1'	2.91	1.62	1.53
23	23	2580	PSU	C4-N3	-2.91	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Pt	20	H2U	O4-C4	-2.91	1.17	1.23
58	Dt	16	H2U	C2-N1	-2.90	1.31	1.35
12	SL	89	D2T	CB-CA	-2.88	1.53	1.54
56	Pt	17	H2U	C2-N3	-2.88	1.32	1.38
23	23	747	5MU	C4-N3	-2.87	1.33	1.38
58	Dt	8	4SU	C5-C4	-2.86	1.39	1.42
1	16	516	PSU	C4-N3	-2.86	1.33	1.38
23	23	955	PSU	C4-N3	-2.83	1.33	1.38
23	23	955	PSU	C6-C5	2.81	1.38	1.35
56	Pt	39	PSU	C4-N3	-2.81	1.33	1.38
23	23	2604	PSU	C2-N1	-2.79	1.33	1.36
58	Dt	55	PSU	C6-N1	-2.78	1.31	1.36
23	23	746	PSU	C4-N3	-2.78	1.33	1.38
56	Pt	55	PSU	C4-N3	-2.77	1.33	1.38
56	Pt	54	5MU	C4-N3	-2.77	1.33	1.38
56	Pt	34	U8U	C4-N3	-2.76	1.33	1.38
56	Pt	16	H2U	C4-N3	-2.66	1.33	1.37
58	Dt	39	PSU	C6-C5	-2.66	1.32	1.35
23	23	1835	2MG	C6-N1	-2.66	1.33	1.37
1	16	1518	MA6	C6-C5	2.62	1.48	1.44
1	16	967	5MC	C6-C5	2.60	1.38	1.34
23	23	2251	OMG	C5-C6	-2.60	1.42	1.47
23	23	1939	5MU	C6-C5	2.58	1.38	1.34
1	16	1519	MA6	C6-C5	2.58	1.48	1.44
56	Pt	20	H2U	O2-C2	-2.57	1.18	1.23
23	23	1962	5MC	C6-C5	2.56	1.38	1.34
58	Dt	32	PSU	C6-C5	-2.55	1.32	1.35
1	16	1207	2MG	C6-N1	-2.54	1.33	1.37
58	Dt	55	PSU	O4'-C1'	-2.53	1.40	1.43
1	16	1407	5MC	C6-C5	2.53	1.38	1.34
1	16	1516	2MG	C6-N1	-2.53	1.33	1.37
56	Pt	54	5MU	C6-C5	2.52	1.38	1.34
23	23	2604	PSU	C6-C5	2.51	1.38	1.35
23	23	747	5MU	C6-N1	-2.49	1.33	1.38
56	Pt	20	H2U	C3'-C4'	2.48	1.59	1.53
23	23	747	5MU	C6-C5	2.48	1.38	1.34
23	23	2445	2MG	C6-N1	-2.46	1.34	1.37
23	23	1939	5MU	C2-N3	-2.44	1.33	1.38
56	Pt	20	H2U	O4'-C4'	2.43	1.50	1.45
1	16	527	G7M	C6-N1	-2.43	1.34	1.37
23	23	1939	5MU	C6-N1	-2.43	1.33	1.38
56	Pt	34	U8U	C6-N1	-2.43	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Pt	17	H2U	C4-N3	-2.42	1.33	1.37
23	23	1915	3TD	C2-N1	-2.41	1.34	1.37
23	23	2552	OMU	O3'-C3'	2.40	1.48	1.43
1	16	966	2MG	C6-N1	-2.40	1.34	1.37
23	23	747	5MU	C2-N3	-2.40	1.33	1.38
1	16	967	5MC	C6-N1	-2.39	1.33	1.38
23	23	1962	5MC	C6-N1	-2.39	1.33	1.38
56	Pt	54	5MU	C6-N1	-2.38	1.34	1.38
1	16	1407	5MC	C6-N1	-2.36	1.34	1.38
23	23	745	1MG	C2-N1	2.33	1.41	1.37
23	23	2552	OMU	C6-N1	2.31	1.43	1.38
23	23	2449	H2U	O4'-C4'	2.25	1.50	1.45
23	23	2498	OMC	C6-N1	-2.21	1.32	1.38
58	Dt	8	4SU	C2-N3	-2.21	1.34	1.38
56	Pt	54	5MU	C2-N3	-2.18	1.34	1.38
23	23	2457	PSU	C2-N3	-2.17	1.33	1.37
23	23	2030	6MZ	C6-C5	2.16	1.48	1.44
23	23	2504	PSU	C2-N3	-2.16	1.33	1.37
58	Dt	39	PSU	O2'-C2'	-2.15	1.37	1.43
23	23	747	5MU	C4-C5	2.15	1.48	1.44
23	23	2449	H2U	C3'-C4'	2.14	1.58	1.53
23	23	2604	PSU	C6-N1	-2.13	1.32	1.36
56	Pt	54	5MU	C4-C5	2.11	1.48	1.44
23	23	955	PSU	C2-N3	-2.11	1.34	1.37
23	23	2580	PSU	O4'-C1'	-2.11	1.40	1.43
23	23	2498	OMC	C5-C4	-2.10	1.38	1.42
12	SL	89	D2T	CB1-SB	-2.10	1.75	1.79
58	Dt	32	PSU	C3'-C2'	-2.07	1.47	1.53
23	23	2605	PSU	C2-N3	-2.07	1.34	1.37
23	23	1939	5MU	C4-C5	2.07	1.48	1.44
23	23	746	PSU	C2-N3	-2.06	1.34	1.37
56	Pt	37	T6A	C10-N6	-2.05	1.32	1.37
23	23	2449	H2U	C1'-N1	-2.05	1.43	1.46
1	16	516	PSU	C2-N3	-2.04	1.34	1.37
23	23	1618	6MZ	C6-C5	2.04	1.48	1.44
58	Dt	55	PSU	C1'-C5	-2.04	1.45	1.50
56	Pt	39	PSU	C2-N3	-2.02	1.34	1.37
23	23	747	5MU	C2-N1	2.02	1.41	1.38
23	23	2069	G7M	C6-N1	-2.02	1.34	1.37
23	23	2580	PSU	C2-N3	-2.01	1.34	1.37

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	Dt	37	MIA	C12-C13-C14	-9.35	110.23	127.01
58	Dt	32	PSU	N1-C2-N3	9.22	124.89	115.17
56	Pt	37	T6A	C2-N1-C6	8.27	123.02	116.60
58	Dt	55	PSU	N1-C2-N3	7.71	123.31	115.17
23	23	1915	3TD	N1-C2-N3	7.21	121.37	116.13
58	Dt	32	PSU	C4-N3-C2	-7.19	116.47	126.37
23	23	2503	2MA	C2-N3-C4	7.12	121.21	115.46
58	Dt	8	4SU	C4-N3-C2	-6.98	120.62	127.31
1	16	1498	UR3	C4-N3-C2	-6.90	119.02	124.58
23	23	2604	PSU	N1-C2-N3	6.83	122.38	115.17
23	23	2457	PSU	N1-C2-N3	6.81	122.35	115.17
1	16	516	PSU	N1-C2-N3	6.68	122.22	115.17
23	23	955	PSU	N1-C2-N3	6.66	122.19	115.17
23	23	1618	6MZ	C2-N1-C6	6.62	121.74	116.60
23	23	2504	PSU	N1-C2-N3	6.58	122.11	115.17
23	23	2580	PSU	N1-C2-N3	6.56	122.09	115.17
23	23	2552	OMU	C4-N3-C2	-6.56	118.47	126.61
23	23	2030	6MZ	C2-N1-C6	6.52	121.66	116.60
56	Pt	39	PSU	N1-C2-N3	6.52	122.05	115.17
56	Pt	55	PSU	N1-C2-N3	6.49	122.02	115.17
23	23	2605	PSU	N1-C2-N3	6.43	121.96	115.17
58	Dt	39	PSU	N1-C2-N3	6.30	121.82	115.17
23	23	746	PSU	N1-C2-N3	6.30	121.81	115.17
58	Dt	39	PSU	O2-C2-N1	-6.24	116.36	122.79
58	Dt	37	MIA	C11-S10-C2	-6.03	97.72	102.25
56	Pt	37	T6A	N6-C6-N1	5.93	125.38	118.71
58	Dt	8	4SU	C5-C4-N3	5.83	120.17	114.75
1	16	1518	MA6	C2-N1-C6	5.73	122.45	116.84
1	16	1519	MA6	C2-N1-C6	5.70	122.43	116.84
58	Dt	39	PSU	C6-C5-C4	-5.70	114.33	118.17
56	Pt	47	3AU	C4-N3-C2	-5.69	117.98	124.66
58	Dt	55	PSU	C4-N3-C2	-5.69	118.54	126.37
23	23	1939	5MU	C4-N3-C2	-5.31	120.38	127.34
23	23	2030	6MZ	C9-N6-C6	-5.22	118.00	122.85
23	23	1939	5MU	N3-C2-N1	5.16	121.61	114.89
56	Pt	54	5MU	C4-N3-C2	-5.15	120.59	127.34
58	Dt	39	PSU	C4-N3-C2	-5.15	119.28	126.37
23	23	1915	3TD	C4-N3-C2	-5.13	119.18	124.61
23	23	747	5MU	C4-N3-C2	-5.10	120.65	127.34
58	Dt	55	PSU	O2-C2-N1	-5.05	117.58	122.79
23	23	747	5MU	N3-C2-N1	5.02	121.42	114.89
56	Pt	54	5MU	N3-C2-N1	5.00	121.41	114.89
58	Dt	47	3AU	C4-N3-C2	-4.82	119.00	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2069	G7M	O4'-C1'-N9	4.74	115.03	108.75
23	23	1939	5MU	C5-C4-N3	4.61	119.33	115.32
56	Pt	37	T6A	N6-C10-N11	4.61	120.10	113.77
56	Pt	37	T6A	N3-C2-N1	-4.57	122.47	128.67
56	Pt	54	5MU	C5-C4-N3	4.50	119.24	115.32
23	23	2457	PSU	C4-N3-C2	-4.41	120.30	126.37
58	Dt	16	H2U	C3'-C2'-C1'	4.40	109.78	101.46
23	23	747	5MU	C5-C4-N3	4.38	119.13	115.32
23	23	2552	OMU	C5-C4-N3	4.36	120.90	114.80
23	23	2552	OMU	N3-C2-N1	4.32	120.52	114.89
23	23	2552	OMU	C2'-C1'-N1	-4.30	106.07	114.24
1	16	516	PSU	C4-N3-C2	-4.30	120.45	126.37
23	23	955	PSU	C4-N3-C2	-4.29	120.47	126.37
56	Pt	39	PSU	C4-N3-C2	-4.24	120.53	126.37
23	23	2449	H2U	N3-C2-N1	4.23	120.90	116.65
23	23	2605	PSU	C4-N3-C2	-4.20	120.58	126.37
56	Pt	55	PSU	C4-N3-C2	-4.20	120.59	126.37
58	Dt	8	4SU	N3-C2-N1	4.20	120.35	114.89
23	23	2504	PSU	C4-N3-C2	-4.19	120.60	126.37
23	23	746	PSU	C4-N3-C2	-4.17	120.63	126.37
58	Dt	37	MIA	C16-C14-C13	-4.08	110.41	122.66
58	Dt	8	4SU	C5-C4-S4	-4.08	119.65	124.31
23	23	2498	OMC	C2'-C1'-N1	-4.07	106.51	114.24
23	23	2580	PSU	C4-N3-C2	-4.04	120.81	126.37
58	Dt	16	H2U	O3'-C3'-C2'	-4.03	98.89	111.82
23	23	2604	PSU	C4-N3-C2	-4.02	120.83	126.37
56	Pt	54	5MU	O4-C4-C5	-4.02	120.32	124.92
23	23	955	PSU	O2-C2-N1	-4.01	118.65	122.79
58	Dt	55	PSU	C2'-C3'-C4'	-4.01	94.87	102.61
58	Dt	37	MIA	C15-C14-C13	-4.00	110.66	122.66
1	16	1519	MA6	N3-C2-N1	-3.95	123.31	128.67
23	23	1939	5MU	C5-C6-N1	-3.92	119.06	123.31
23	23	1939	5MU	O4-C4-C5	-3.90	120.46	124.92
1	16	1518	MA6	N3-C2-N1	-3.89	123.39	128.67
58	Dt	32	PSU	O2-C2-N1	-3.89	118.77	122.79
23	23	747	5MU	O4-C4-C5	-3.87	120.50	124.92
1	16	516	PSU	O2-C2-N1	-3.84	118.83	122.79
23	23	1618	6MZ	N3-C2-N1	-3.80	123.52	128.67
23	23	2030	6MZ	N3-C2-N1	-3.79	123.52	128.67
56	Pt	55	PSU	O2-C2-N1	-3.70	118.97	122.79
58	Dt	39	PSU	C3'-C2'-C1'	3.70	106.05	101.69
23	23	2580	PSU	O2-C2-N1	-3.68	118.99	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2457	PSU	O2-C2-N1	-3.68	118.99	122.79
23	23	747	5MU	C5-C6-N1	-3.61	119.40	123.31
56	Pt	39	PSU	O2-C2-N1	-3.60	119.07	122.79
56	Pt	47	3AU	C10-N3-C2	3.59	122.94	117.64
36	LP	81	4D4	NE-CZ-NH2	-3.57	114.54	120.67
23	23	1618	6MZ	C9-N6-C6	-3.51	119.59	122.85
1	16	1498	UR3	C5-C4-N3	3.48	119.62	115.04
23	23	746	PSU	O2-C2-N1	-3.45	119.23	122.79
58	Dt	55	PSU	C5-C6-N1	-3.43	117.37	122.14
23	23	2605	PSU	O2-C2-N1	-3.43	119.25	122.79
23	23	2449	H2U	C5-C4-N3	3.42	120.32	116.69
56	Pt	54	5MU	C5-C6-N1	-3.41	119.61	123.31
23	23	1962	5MC	C5-C6-N1	-3.41	119.61	123.31
23	23	2504	PSU	O2-C2-N1	-3.40	119.28	122.79
1	16	967	5MC	C5-C6-N1	-3.39	119.63	123.31
56	Pt	20	H2U	N3-C2-N1	3.39	120.05	116.65
1	16	1519	MA6	C4-C5-N7	-3.38	105.77	109.34
56	Pt	47	3AU	C5-C4-N3	3.36	120.28	115.64
36	LP	81	4D4	NH1-CZ-NE	3.27	126.70	119.27
1	16	1518	MA6	C4-C5-N7	-3.21	105.95	109.34
58	Dt	32	PSU	C3'-C2'-C1'	3.16	105.42	101.69
23	23	2604	PSU	O2-C2-N1	-3.15	119.53	122.79
1	16	1407	5MC	C5-C6-N1	-3.14	119.90	123.31
58	Dt	32	PSU	O2-C2-N3	-3.12	116.31	121.86
56	Pt	37	T6A	C12-N11-C10	3.11	127.15	121.99
58	Dt	46	G7M	CN7-N7-C8	-3.09	110.57	125.43
58	Dt	39	PSU	C4'-O4'-C1'	3.04	116.06	108.44
58	Dt	32	PSU	C5-C6-N1	-3.04	117.92	122.14
56	Pt	20	H2U	C5-C4-N3	3.00	119.88	116.69
58	Dt	37	MIA	N3-C2-N1	-2.97	121.60	127.03
23	23	2552	OMU	O4-C4-C5	-2.97	120.05	125.16
23	23	2030	6MZ	C4-C5-N7	-2.96	106.21	109.34
23	23	2445	2MG	C8-N7-C5	2.96	107.58	102.55
56	Pt	37	T6A	O10-C10-N6	-2.93	118.43	123.64
23	23	2449	H2U	C5-C6-N1	2.93	120.37	111.52
58	Dt	37	MIA	O3'-C3'-C2'	-2.92	102.44	111.82
23	23	1915	3TD	C1'-C5-C4	2.91	122.02	117.61
23	23	1939	5MU	O2-C2-N1	-2.91	119.01	122.80
1	16	1207	2MG	C8-N7-C5	2.90	107.48	102.55
23	23	745	1MG	C8-N7-C5	2.90	107.48	102.55
1	16	1516	2MG	C8-N7-C5	2.86	107.41	102.55
23	23	2069	G7M	CN7-N7-C8	-2.83	111.80	125.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	16	966	2MG	C8-N7-C5	2.82	107.34	102.55
23	23	1835	2MG	C8-N7-C5	2.80	107.32	102.55
56	Pt	20	H2U	C5-C6-N1	2.79	119.97	111.52
56	Pt	20	H2U	O2-C2-N1	-2.76	119.79	123.10
58	Dt	47	3AU	C5-C4-N3	2.75	119.45	115.64
58	Dt	55	PSU	O4'-C4'-C3'	-2.72	99.75	105.15
23	23	2069	G7M	N2-C2-N1	2.69	122.44	116.76
56	Pt	16	H2U	C3'-C2'-C1'	2.68	106.54	101.46
58	Dt	46	G7M	O4'-C1'-N9	2.66	112.27	108.75
58	Dt	55	PSU	C3'-C2'-C1'	2.65	104.81	101.69
1	16	527	G7M	CN7-N7-C8	-2.64	112.73	125.43
58	Dt	39	PSU	O2'-C2'-C1'	-2.64	104.95	111.21
23	23	2503	2MA	C4-C5-N7	-2.63	106.56	109.34
1	16	1407	5MC	C5-C4-N3	-2.61	119.08	121.75
23	23	2503	2MA	C2-N1-C6	2.60	122.10	118.10
56	Pt	54	5MU	O2-C2-N1	-2.60	119.41	122.80
23	23	2604	PSU	O2'-C2'-C3'	-2.60	103.50	111.82
1	16	967	5MC	C5-C4-N3	-2.59	119.10	121.75
23	23	1962	5MC	C5-C4-N3	-2.59	119.10	121.75
58	Dt	37	MIA	O4'-C4'-C3'	-2.58	100.04	105.15
58	Dt	37	MIA	C2-N1-C6	2.57	121.99	117.42
23	23	2445	2MG	N1-C2-N2	2.54	119.15	116.56
23	23	2069	G7M	N2-C2-N3	-2.53	114.74	119.67
23	23	2251	OMG	O6-C6-C5	2.52	129.31	124.32
56	Pt	20	H2U	C3'-C2'-C1'	2.51	106.22	101.46
58	Dt	55	PSU	O2'-C2'-C3'	-2.51	103.78	111.82
58	Dt	39	PSU	O4'-C1'-C2'	-2.50	101.69	105.15
56	Pt	17	H2U	C5-C6-N1	-2.50	103.95	111.52
58	Dt	37	MIA	C4'-O4'-C1'	-2.49	107.64	109.92
56	Pt	34	U8U	O4-C4-C5	-2.49	120.53	124.71
56	Pt	34	U8U	C1'-N1-C6	-2.47	117.08	121.15
56	Pt	34	U8U	C5-C4-N3	2.46	118.96	115.21
23	23	745	1MG	C5-C6-N1	2.44	117.49	113.96
23	23	1618	6MZ	C4-C5-N7	-2.42	106.78	109.34
23	23	2457	PSU	C5-C6-N1	-2.39	118.83	122.14
58	Dt	37	MIA	C4-C5-N7	-2.35	106.86	109.34
23	23	2552	OMU	O2-C2-N1	-2.34	119.75	122.80
58	Dt	39	PSU	O4'-C4'-C3'	-2.34	100.51	105.15
23	23	2069	G7M	C5'-C4'-C3'	-2.34	106.80	115.21
58	Dt	55	PSU	O4'-C1'-C2'	-2.33	101.94	105.15
56	Pt	17	H2U	N3-C2-N1	-2.32	114.31	116.65
1	16	1402	4OC	C6-C5-C4	2.29	119.76	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	Dt	37	MIA	O4'-C1'-N9	2.27	111.75	108.75
23	23	747	5MU	O2-C2-N1	-2.26	119.86	122.80
23	23	2604	PSU	C3'-C2'-C1'	2.24	104.33	101.69
1	16	1516	2MG	N1-C2-N2	2.24	118.84	116.56
58	Dt	16	H2U	O4'-C1'-N1	2.22	112.33	109.30
58	Dt	8	4SU	O2-C2-N1	-2.21	119.92	122.80
1	16	516	PSU	C5-C6-N1	-2.21	119.08	122.14
23	23	2580	PSU	O4'-C1'-C2'	2.19	108.18	105.15
56	Pt	39	PSU	C5-C6-N1	-2.19	119.10	122.14
58	Dt	47	3AU	C2'-C3'-C4'	2.18	106.81	102.61
58	Dt	16	H2U	O2'-C2'-C3'	-2.17	104.85	111.82
1	16	516	PSU	O4'-C1'-C2'	2.16	108.14	105.15
58	Dt	47	3AU	C3'-C2'-C1'	2.15	105.54	101.46
1	16	1498	UR3	C1'-N1-C2	2.15	120.55	117.04
56	Pt	54	5MU	C5M-C5-C4	2.13	121.06	118.78
12	SL	89	D2T	CB-CA-N	2.13	113.42	109.10
23	23	2604	PSU	O4'-C4'-C3'	-2.13	100.92	105.15
23	23	2445	2MG	CM2-N2-C2	-2.13	119.07	123.65
1	16	1207	2MG	C5-C6-N1	2.13	118.13	114.07
23	23	2604	PSU	O2-C2-N3	-2.12	118.09	121.86
23	23	2605	PSU	C5-C6-N1	-2.12	119.20	122.14
23	23	2604	PSU	C5-C6-N1	-2.12	119.20	122.14
36	LP	81	4D4	O-C-CA	-2.12	119.32	124.77
23	23	1835	2MG	C5-C6-N1	2.12	118.11	114.07
23	23	2449	H2U	O2-C2-N1	-2.11	120.56	123.10
1	16	1516	2MG	C5-C6-N1	2.11	118.09	114.07
23	23	2503	2MA	C5-C6-N1	-2.11	118.35	120.84
58	Dt	47	3AU	C10-N3-C4	2.10	121.17	117.10
1	16	966	2MG	C5-C6-N1	2.10	118.08	114.07
23	23	2604	PSU	O2'-C2'-C1'	-2.10	106.22	111.21
1	16	1407	5MC	O2-C2-N3	-2.10	119.02	122.33
1	16	1516	2MG	CM2-N2-C2	-2.10	119.14	123.65
23	23	746	PSU	C5-C6-N1	-2.10	119.23	122.14
23	23	2445	2MG	C5-C6-N1	2.09	118.06	114.07
58	Dt	39	PSU	O4-C4-C5	-2.08	118.85	124.01
1	16	966	2MG	N1-C2-N2	2.07	118.68	116.56
56	Pt	55	PSU	C5-C6-N1	-2.06	119.28	122.14
23	23	2504	PSU	C5-C6-N1	-2.05	119.29	122.14
23	23	2445	2MG	N2-C2-N3	-2.05	117.89	120.51
56	Pt	47	3AU	O2-C2-N1	-2.05	118.21	122.78
23	23	955	PSU	C5-C6-N1	-2.04	119.31	122.14
12	SL	89	D2T	O-C-CA	-2.04	119.53	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2580	PSU	C5-C6-N1	-2.00	119.36	122.14

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	527	G7M	O4'-C4'-C5'-O5'
1	16	527	G7M	C3'-C4'-C5'-O5'
1	16	1519	MA6	C5-C6-N6-C9
12	SL	89	D2T	SB-CB-CG-OD2
23	23	1618	6MZ	O4'-C4'-C5'-O5'
23	23	2251	OMG	O4'-C4'-C5'-O5'
23	23	2251	OMG	C1'-C2'-O2'-CM2
56	Pt	16	H2U	O4'-C4'-C5'-O5'
56	Pt	16	H2U	O4'-C1'-N1-C2
56	Pt	16	H2U	O4'-C1'-N1-C6
56	Pt	20	H2U	C4'-C5'-O5'-P
58	Dt	37	MIA	O4'-C4'-C5'-O5'
58	Dt	37	MIA	C5-C6-N6-C12
58	Dt	37	MIA	N1-C2-S10-C11
58	Dt	37	MIA	N3-C2-S10-C11
58	Dt	37	MIA	C12-C13-C14-C16
1	16	1519	MA6	O4'-C4'-C5'-O5'
23	23	2251	OMG	C3'-C4'-C5'-O5'
23	23	2498	OMC	C3'-C4'-C5'-O5'
56	Pt	16	H2U	C3'-C4'-C5'-O5'
23	23	1915	3TD	C3'-C4'-C5'-O5'
23	23	1915	3TD	O4'-C4'-C5'-O5'
23	23	2030	6MZ	O4'-C4'-C5'-O5'
23	23	2498	OMC	O4'-C4'-C5'-O5'
23	23	2503	2MA	O4'-C4'-C5'-O5'
58	Dt	8	4SU	C3'-C4'-C5'-O5'
58	Dt	8	4SU	O4'-C4'-C5'-O5'
23	23	2030	6MZ	C3'-C4'-C5'-O5'
56	Pt	37	T6A	N11-C12-C14-O14
56	Pt	16	H2U	C2'-C1'-N1-C6
56	Pt	37	T6A	N11-C10-N6-C6
56	Pt	37	T6A	C14-C12-C13-ODA
23	23	1618	6MZ	C3'-C4'-C5'-O5'
23	23	2503	2MA	C3'-C4'-C5'-O5'
56	Pt	47	3AU	C3'-C4'-C5'-O5'
58	Dt	37	MIA	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
58	Dt	37	MIA	C12-C13-C14-C15
56	Pt	37	T6A	N11-C12-C13-ODA
1	16	1519	MA6	C3'-C4'-C5'-O5'
23	23	2504	PSU	O4'-C4'-C5'-O5'
56	Pt	47	3AU	O4'-C4'-C5'-O5'
58	Dt	37	MIA	N1-C6-N6-C12
56	Pt	17	H2U	C4'-C5'-O5'-P
56	Pt	37	T6A	C13-C12-C14-C15
56	Pt	47	3AU	C2'-C1'-N1-C6
58	Dt	47	3AU	C2'-C1'-N1-C6
56	Pt	37	T6A	C14-C12-C13-ODB
56	Pt	37	T6A	N11-C12-C13-ODB
56	Pt	16	H2U	C4'-C5'-O5'-P
23	23	2445	2MG	C3'-C4'-C5'-O5'
36	LP	81	4D4	OB-CB-CG-CD
58	Dt	47	3AU	O4'-C4'-C5'-O5'
56	Pt	16	H2U	C2'-C1'-N1-C2
36	LP	81	4D4	CA-CB-CG-CD
56	Pt	17	H2U	C2'-C1'-N1-C2
58	Dt	47	3AU	O4'-C1'-N1-C6
56	Pt	37	T6A	N11-C12-C14-C15
56	Pt	47	3AU	O4'-C1'-N1-C6
56	Pt	37	T6A	C13-C12-C14-O14
56	Pt	20	H2U	C3'-C4'-C5'-O5'
58	Dt	47	3AU	C3'-C4'-C5'-O5'
56	Pt	17	H2U	C2'-C1'-N1-C6
23	23	2552	OMU	C3'-C2'-O2'-CM2
56	Pt	47	3AU	C11-C10-N3-C4
23	23	2069	G7M	C4'-C5'-O5'-P
58	Dt	47	3AU	O4'-C1'-N1-C2
12	SL	89	D2T	CA-CB-SB-CB1
58	Dt	47	3AU	C2'-C1'-N1-C2
23	23	746	PSU	O4'-C1'-C5-C6
56	Pt	47	3AU	C2'-C1'-N1-C2
56	Pt	47	3AU	O4'-C1'-N1-C2
23	23	2504	PSU	C3'-C4'-C5'-O5'
12	SL	89	D2T	CG-CB-SB-CB1
23	23	746	PSU	C2'-C1'-C5-C6
56	Pt	37	T6A	O10-C10-N6-C6
36	LP	81	4D4	CG-CD-NE-CZ

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 434 ligands modelled in this entry, 408 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
59	PUT	23	3013	-	5,5,5	0.10	0	4,4,4	0.13	0
62	ATP	23	3002	-	28,33,33	0.76	0	34,52,52	0.75	1 (2%)
59	PUT	16	1601	-	5,5,5	0.09	0	4,4,4	0.13	0
59	PUT	23	3014	-	5,5,5	0.11	0	4,4,4	0.13	0
59	PUT	23	3015	-	5,5,5	0.10	0	4,4,4	0.13	0
59	PUT	23	3006	-	5,5,5	0.10	0	4,4,4	0.13	0
63	SPD	23	3020	-	9,9,9	0.31	0	8,8,8	0.91	0
59	PUT	23	3010	-	5,5,5	0.12	0	4,4,4	0.19	0
59	PUT	23	3017	-	5,5,5	0.11	0	4,4,4	0.12	0
59	PUT	23	3005	-	5,5,5	0.09	0	4,4,4	0.13	0
62	ATP	23	3001	-	28,33,33	0.63	0	34,52,52	0.60	1 (2%)
63	SPD	23	3022	-	9,9,9	0.32	0	8,8,8	0.90	0
59	PUT	23	3007	-	5,5,5	0.08	0	4,4,4	0.14	0
63	SPD	23	3021	-	9,9,9	0.31	0	8,8,8	0.87	0
59	PUT	23	3008	-	5,5,5	0.09	0	4,4,4	0.13	0
63	SPD	23	3023	-	9,9,9	0.31	0	8,8,8	0.92	0
59	PUT	16	1602	-	5,5,5	0.10	0	4,4,4	0.13	0
59	PUT	23	3009	-	5,5,5	0.09	0	4,4,4	0.13	0
59	PUT	16	1603	-	5,5,5	0.12	0	4,4,4	0.13	0
59	PUT	23	3012	-	5,5,5	0.10	0	4,4,4	0.12	0
62	ATP	23	3003	-	28,33,33	0.63	0	34,52,52	0.59	1 (2%)
59	PUT	23	3018	-	5,5,5	0.10	0	4,4,4	0.12	0
59	PUT	23	3004	-	5,5,5	0.11	0	4,4,4	0.12	0
59	PUT	23	3016	-	5,5,5	0.10	0	4,4,4	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
59	PUT	23	3011	-	5,5,5	0.09	0	4,4,4	0.13	0
63	SPD	23	3019	-	9,9,9	0.32	0	8,8,8	0.95	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
59	PUT	23	3013	-	-	0/3/3/3	-
62	ATP	23	3002	-	-	4/18/38/38	0/3/3/3
59	PUT	16	1601	-	-	0/3/3/3	-
59	PUT	23	3014	-	-	0/3/3/3	-
59	PUT	23	3015	-	-	1/3/3/3	-
59	PUT	23	3006	-	-	1/3/3/3	-
63	SPD	23	3020	-	-	2/7/7/7	-
59	PUT	23	3010	-	-	1/3/3/3	-
59	PUT	23	3017	-	-	1/3/3/3	-
59	PUT	23	3005	-	-	0/3/3/3	-
62	ATP	23	3001	-	-	10/18/38/38	0/3/3/3
63	SPD	23	3022	-	-	1/7/7/7	-
59	PUT	23	3007	-	-	1/3/3/3	-
63	SPD	23	3021	-	-	5/7/7/7	-
59	PUT	23	3008	-	-	1/3/3/3	-
63	SPD	23	3023	-	-	3/7/7/7	-
59	PUT	16	1602	-	-	1/3/3/3	-
59	PUT	23	3009	-	-	3/3/3/3	-
59	PUT	16	1603	-	-	1/3/3/3	-
59	PUT	23	3012	-	-	0/3/3/3	-
62	ATP	23	3003	-	-	6/18/38/38	0/3/3/3
59	PUT	23	3018	-	-	0/3/3/3	-
59	PUT	23	3004	-	-	1/3/3/3	-
59	PUT	23	3016	-	-	0/3/3/3	-
59	PUT	23	3011	-	-	0/3/3/3	-
63	SPD	23	3019	-	-	0/7/7/7	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	23	3001	ATP	C5-C6-N6	2.35	123.89	120.31
62	23	3003	ATP	C5-C6-N6	2.33	123.86	120.31
62	23	3002	ATP	C5-C6-N6	2.28	123.78	120.31

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	23	3001	ATP	C5'-O5'-PA-O2A
62	23	3002	ATP	C5'-O5'-PA-O3A
62	23	3002	ATP	O4'-C4'-C5'-O5'
62	23	3003	ATP	C5'-O5'-PA-O1A
62	23	3003	ATP	C5'-O5'-PA-O2A
62	23	3003	ATP	C5'-O5'-PA-O3A
62	23	3002	ATP	C3'-C4'-C5'-O5'
62	23	3003	ATP	O4'-C4'-C5'-O5'
62	23	3003	ATP	C3'-C4'-C5'-O5'
63	23	3021	SPD	N6-C7-C8-C9
63	23	3023	SPD	N6-C7-C8-C9
63	23	3023	SPD	C3-C4-C5-N6
63	23	3020	SPD	C3-C4-C5-N6
59	23	3007	PUT	C1-C2-C3-C4
62	23	3001	ATP	O4'-C4'-C5'-O5'
62	23	3001	ATP	C3'-C4'-C5'-O5'
59	23	3015	PUT	C1-C2-C3-C4
59	23	3009	PUT	C1-C2-C3-C4
63	23	3021	SPD	C3-C4-C5-N6
62	23	3001	ATP	PG-O3B-PB-O3A
59	23	3009	PUT	C2-C3-C4-N2
59	23	3009	PUT	N1-C1-C2-C3
63	23	3021	SPD	C2-C3-C4-C5
59	16	1603	PUT	C1-C2-C3-C4
62	23	3001	ATP	C5'-O5'-PA-O1A
62	23	3001	ATP	C5'-O5'-PA-O3A
62	23	3002	ATP	C5'-O5'-PA-O1A
63	23	3021	SPD	C7-C8-C9-N10
59	23	3006	PUT	C2-C3-C4-N2
63	23	3020	SPD	N1-C2-C3-C4
63	23	3023	SPD	N1-C2-C3-C4
63	23	3021	SPD	C4-C5-N6-C7
59	23	3004	PUT	C1-C2-C3-C4
59	23	3008	PUT	C1-C2-C3-C4
59	23	3017	PUT	C1-C2-C3-C4

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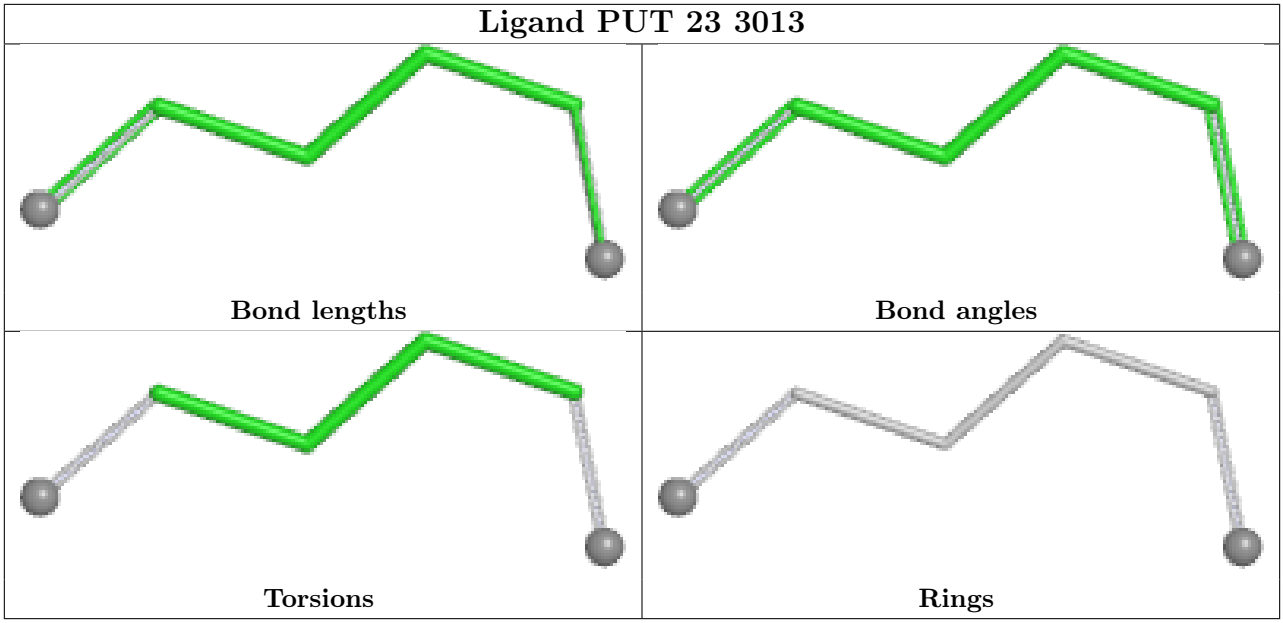
Mol	Chain	Res	Type	Atoms
59	16	1602	PUT	C1-C2-C3-C4
62	23	3001	ATP	PG-O3B-PB-O1B
62	23	3001	ATP	PA-O3A-PB-O1B
62	23	3001	ATP	PA-O3A-PB-O2B
62	23	3003	ATP	PA-O3A-PB-O2B
59	23	3010	PUT	N1-C1-C2-C3
63	23	3022	SPD	C7-C8-C9-N10
62	23	3001	ATP	PG-O3B-PB-O2B

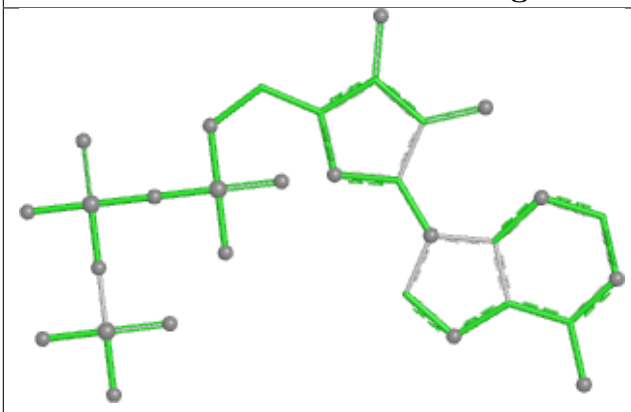
There are no ring outliers.

No monomer is involved in short contacts.

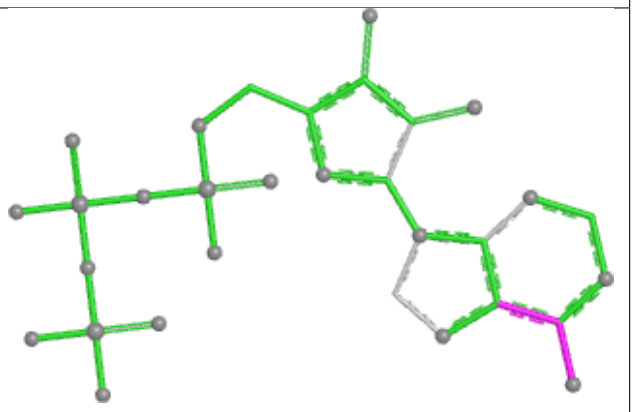
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



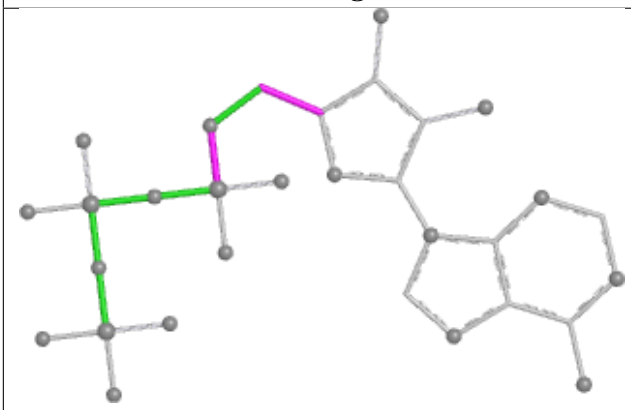
Ligand ATP 23 3002



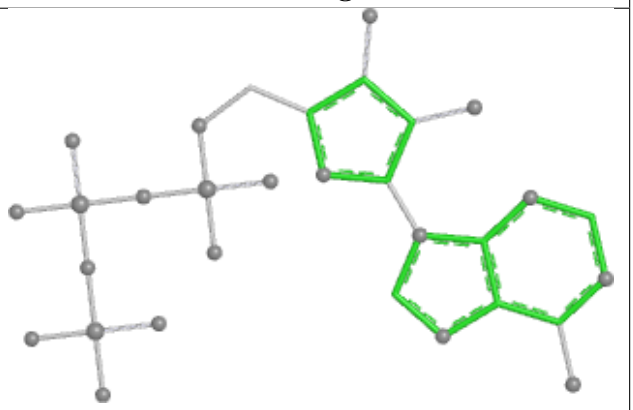
Bond lengths



Bond angles

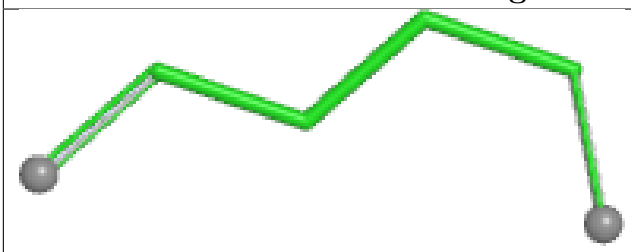


Torsions

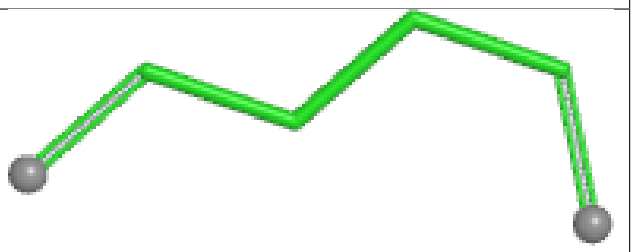


Rings

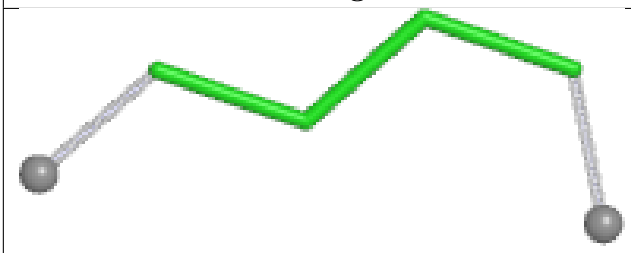
Ligand PUT 16 1601



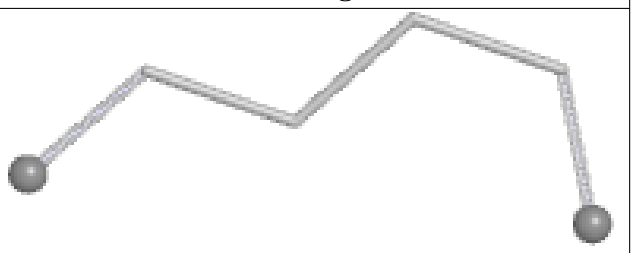
Bond lengths



Bond angles

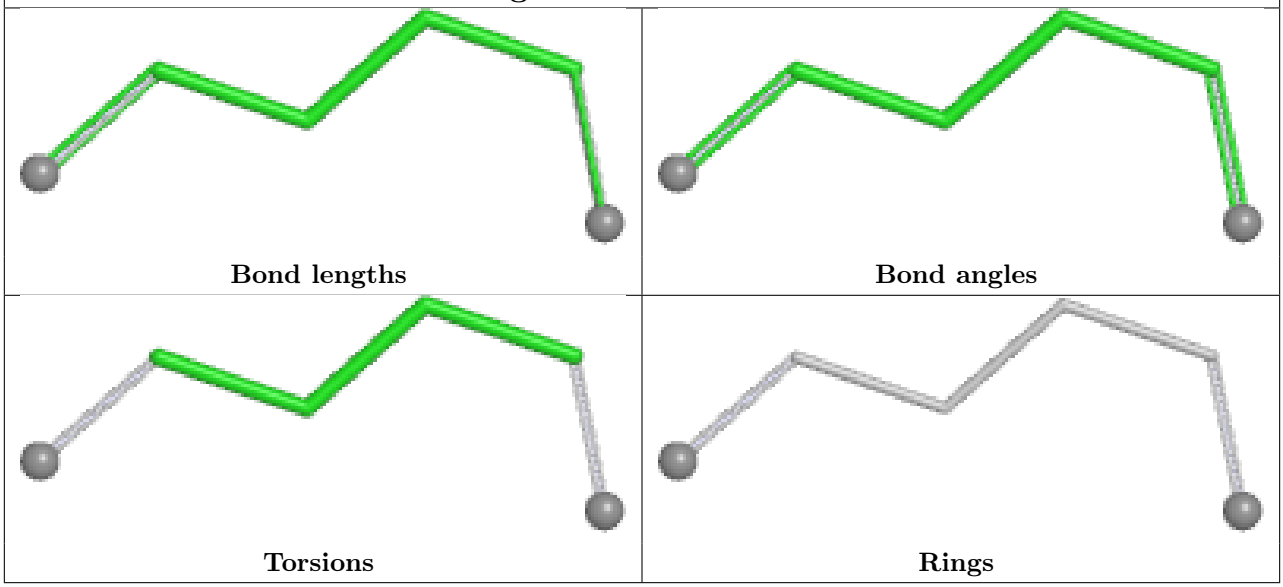


Torsions

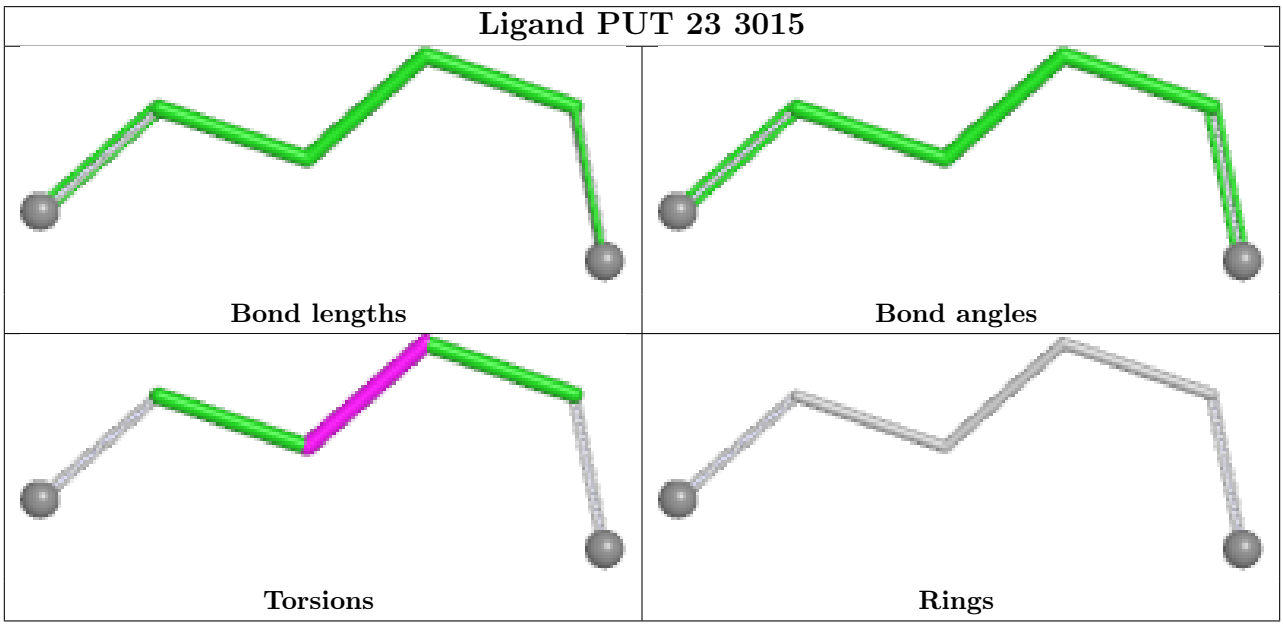


Rings

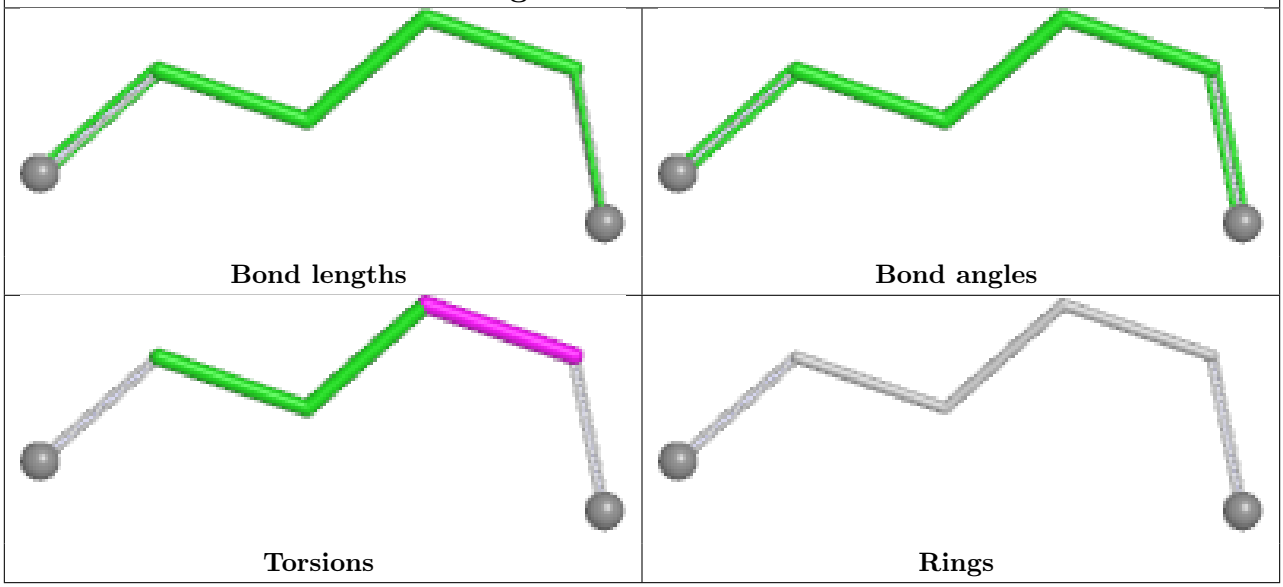
Ligand PUT 23 3014



Ligand PUT 23 3015



Ligand PUT 23 3006



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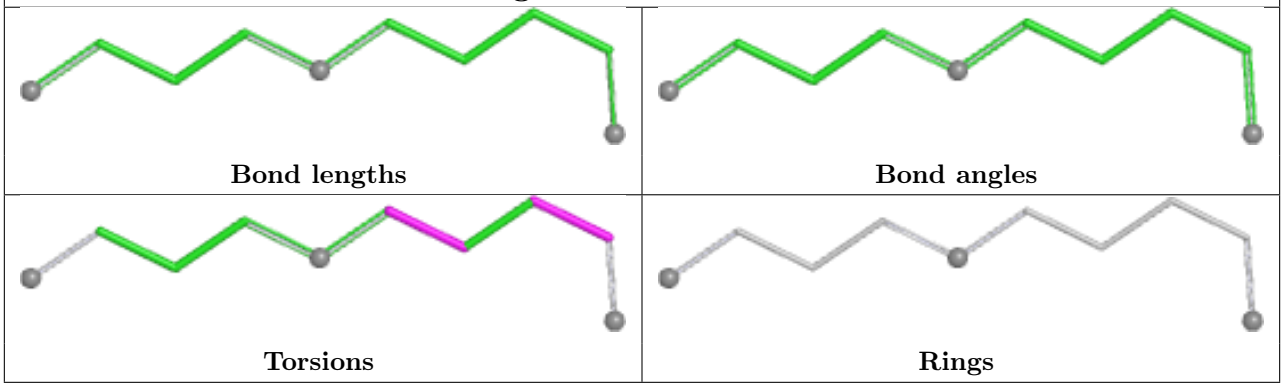

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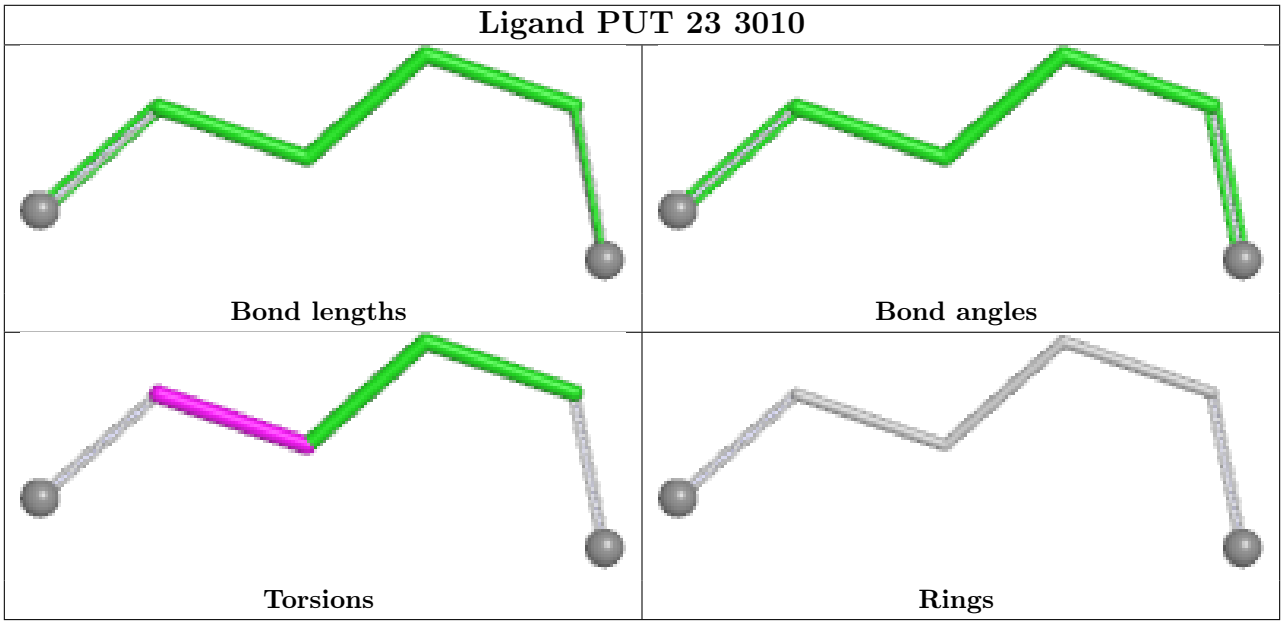

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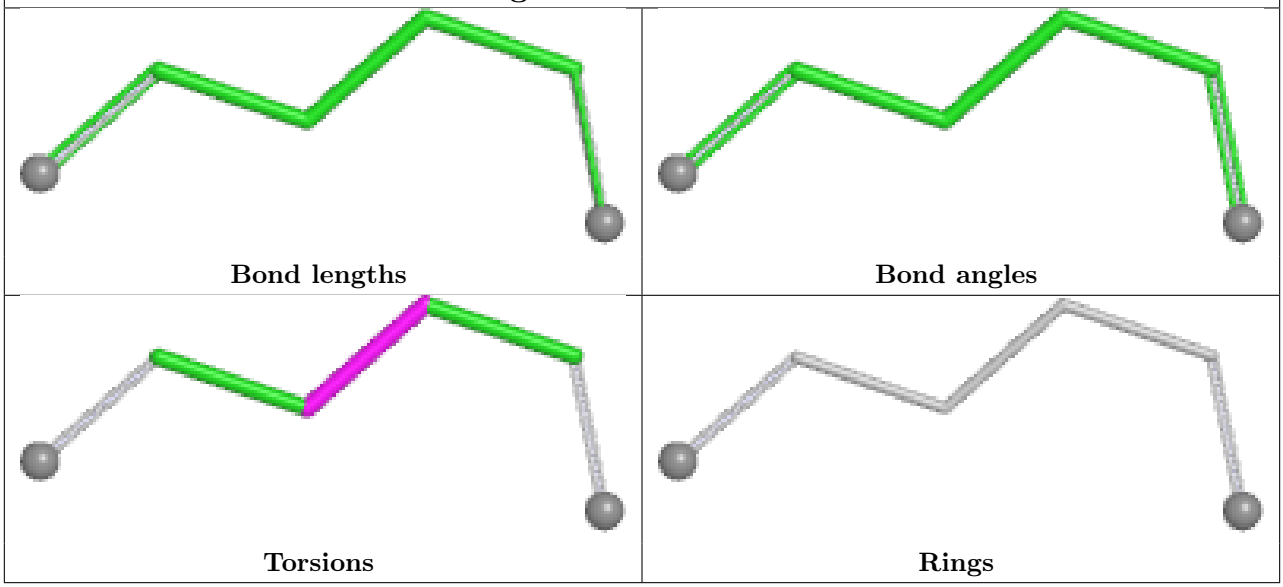
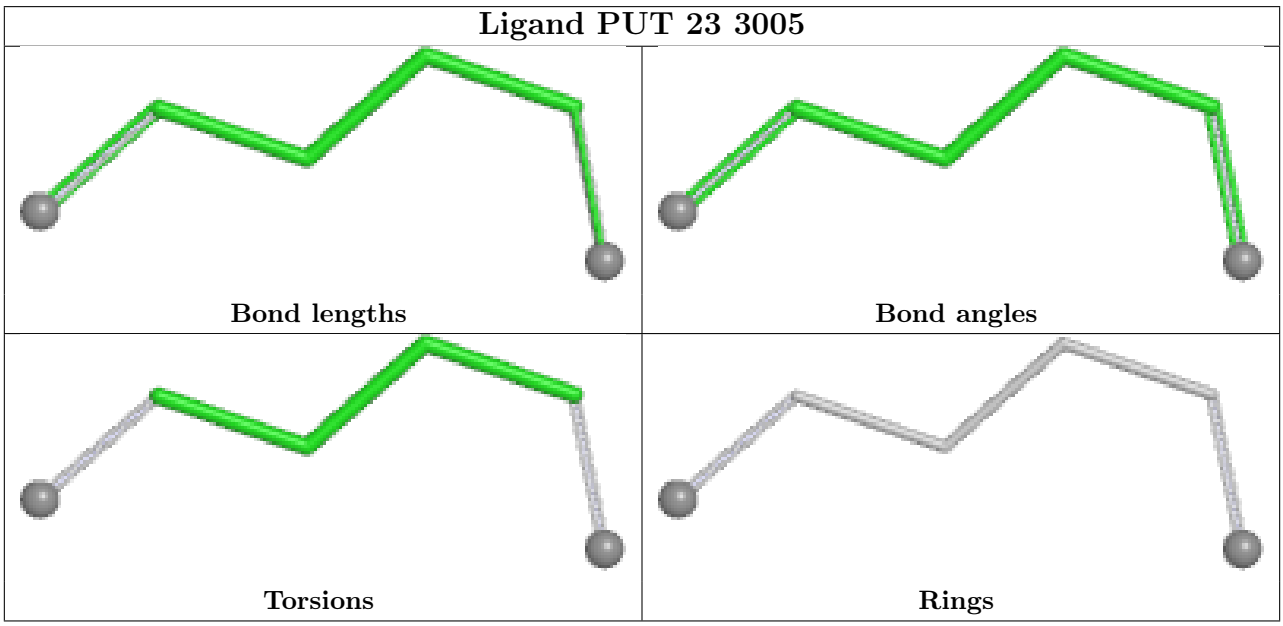
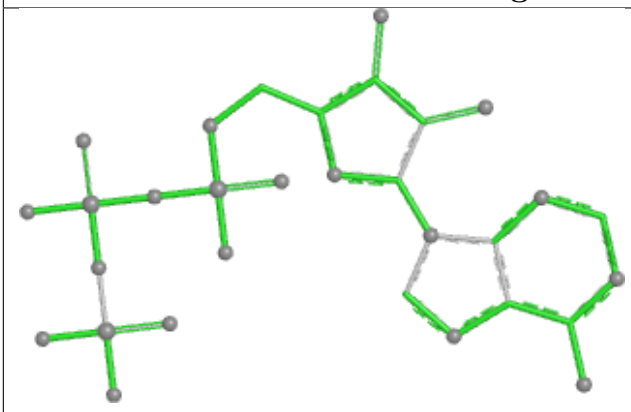


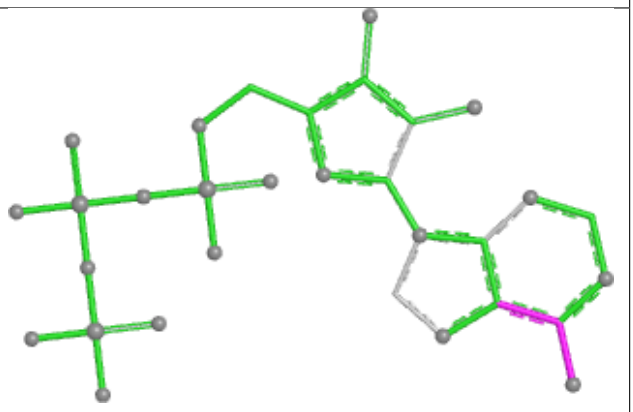
Ligand PUT 23 3005



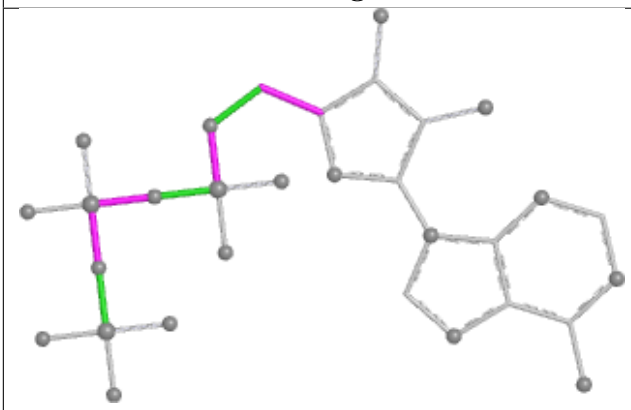
Ligand ATP 23 3001



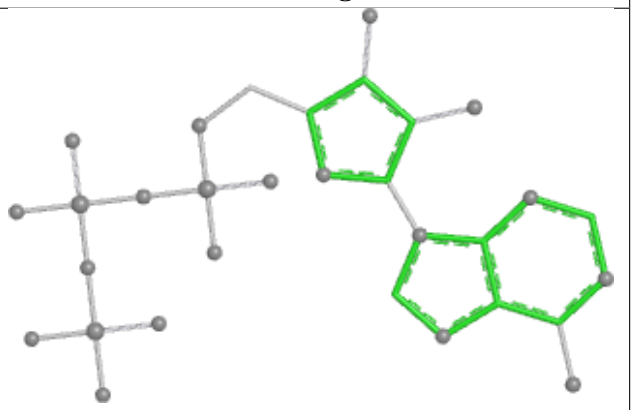
Bond lengths



Bond angles

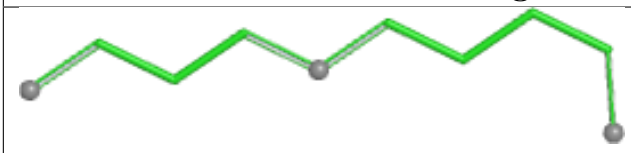


Torsions

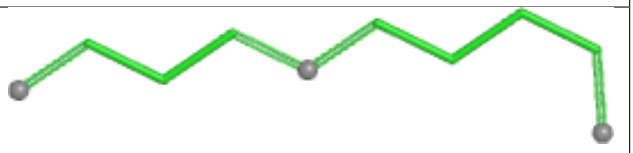


Rings

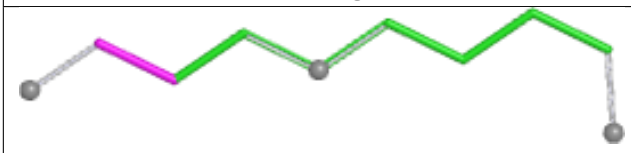
Ligand SPD 23 3022



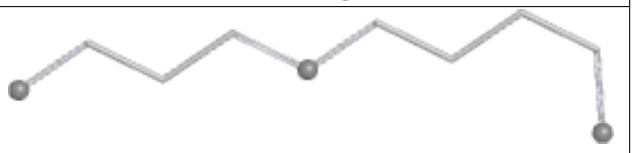
Bond lengths



Bond angles

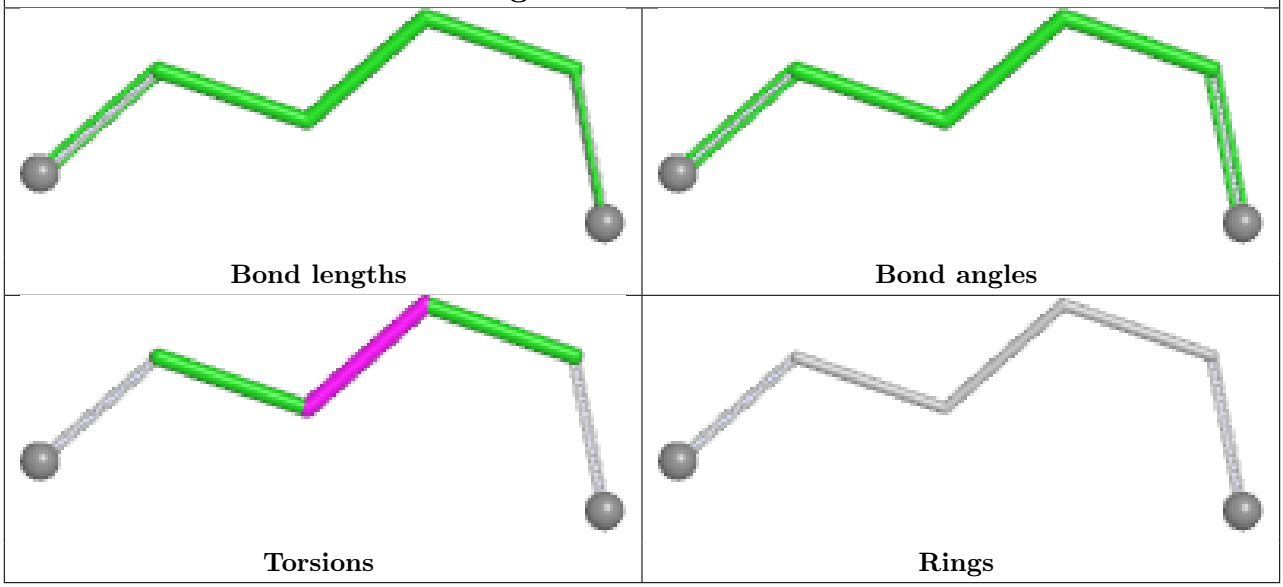


Torsions

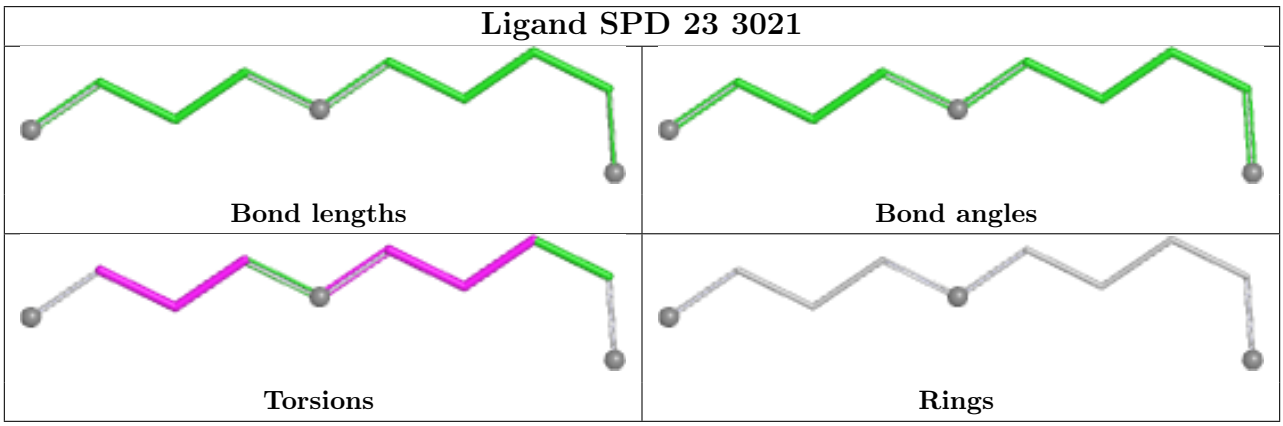


Rings

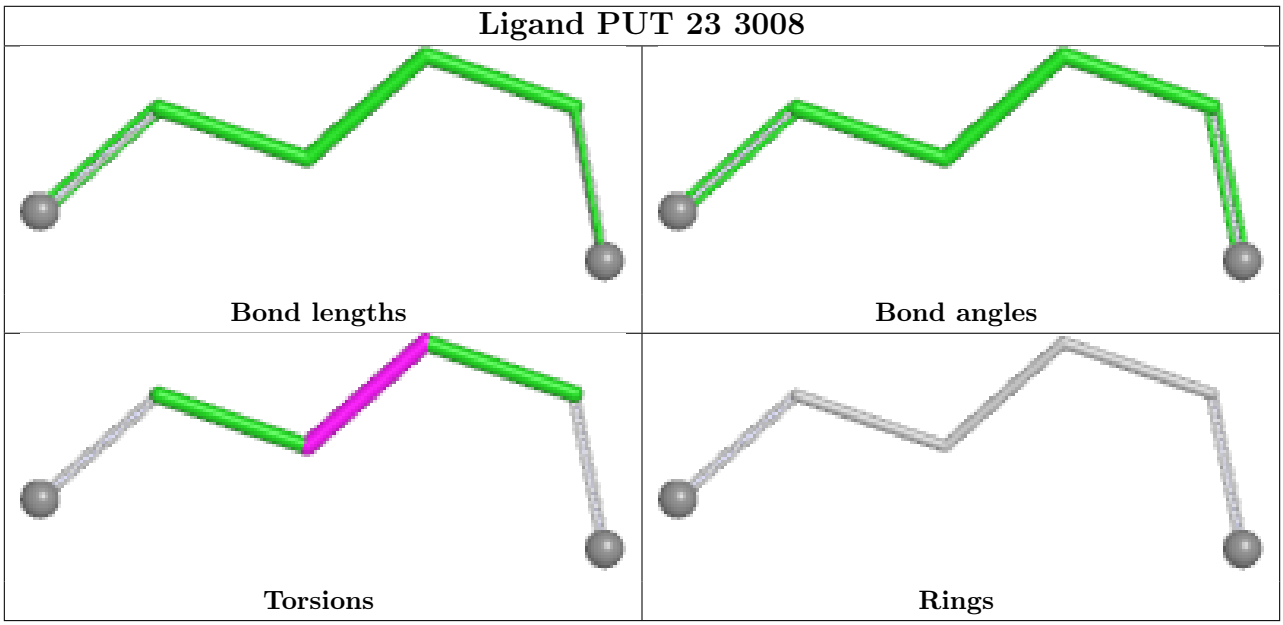
Ligand PUT 23 3007



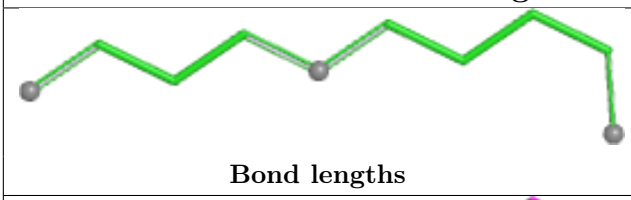
Ligand SPD 23 3021



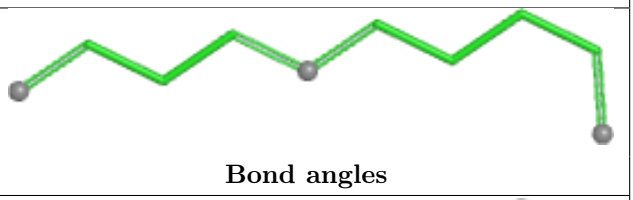
Ligand PUT 23 3008



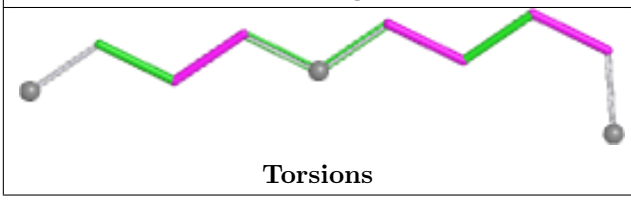
Ligand SPD 23 3023



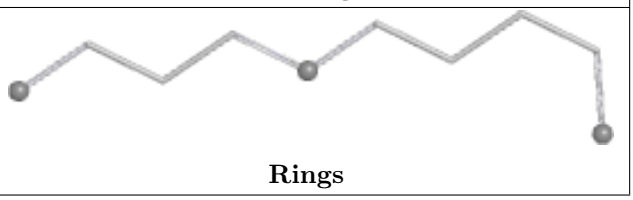
Bond lengths



Bond angles

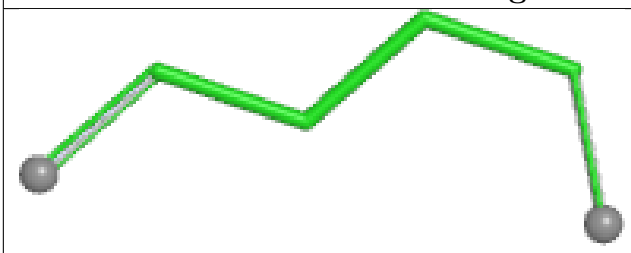


Torsions

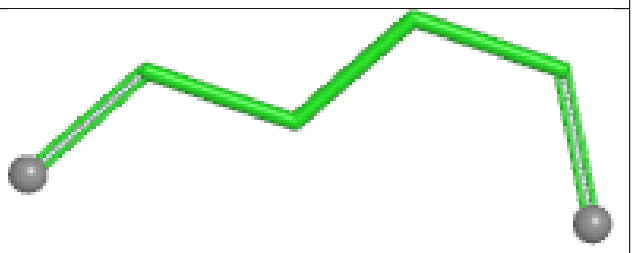


Rings

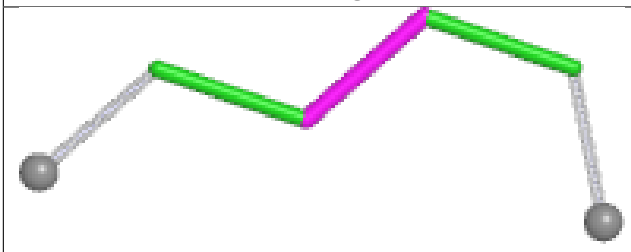
Ligand PUT 16 1602



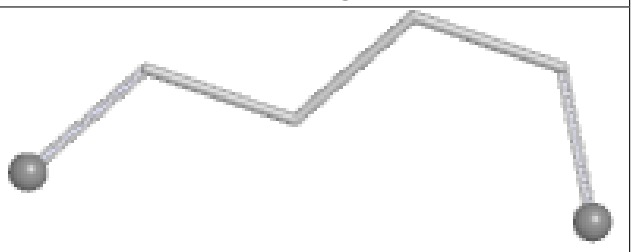
Bond lengths



Bond angles

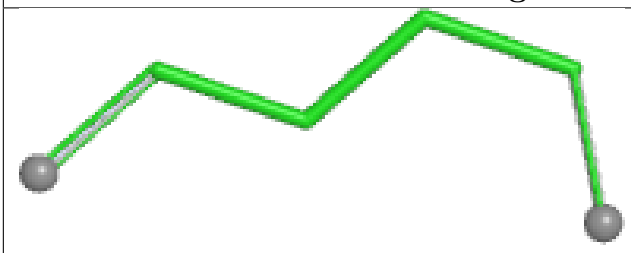


Torsions

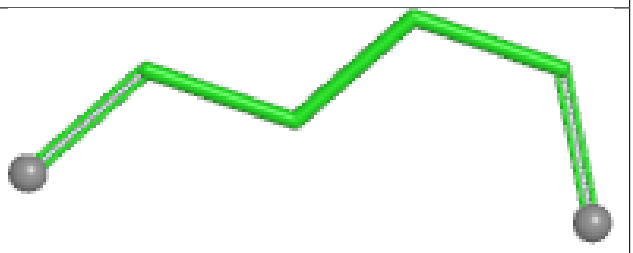


Rings

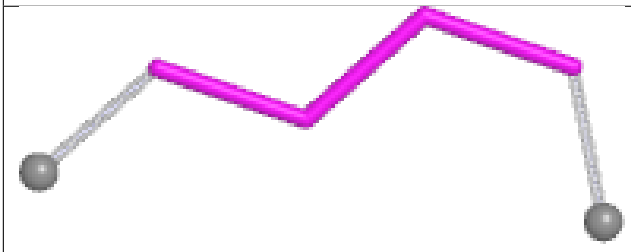
Ligand PUT 23 3009



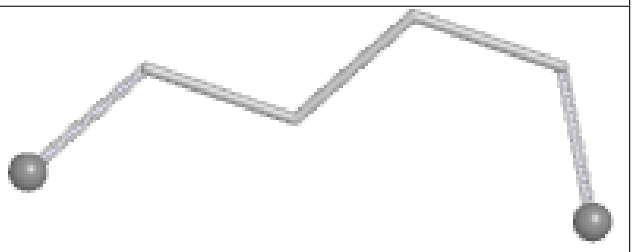
Bond lengths



Bond angles

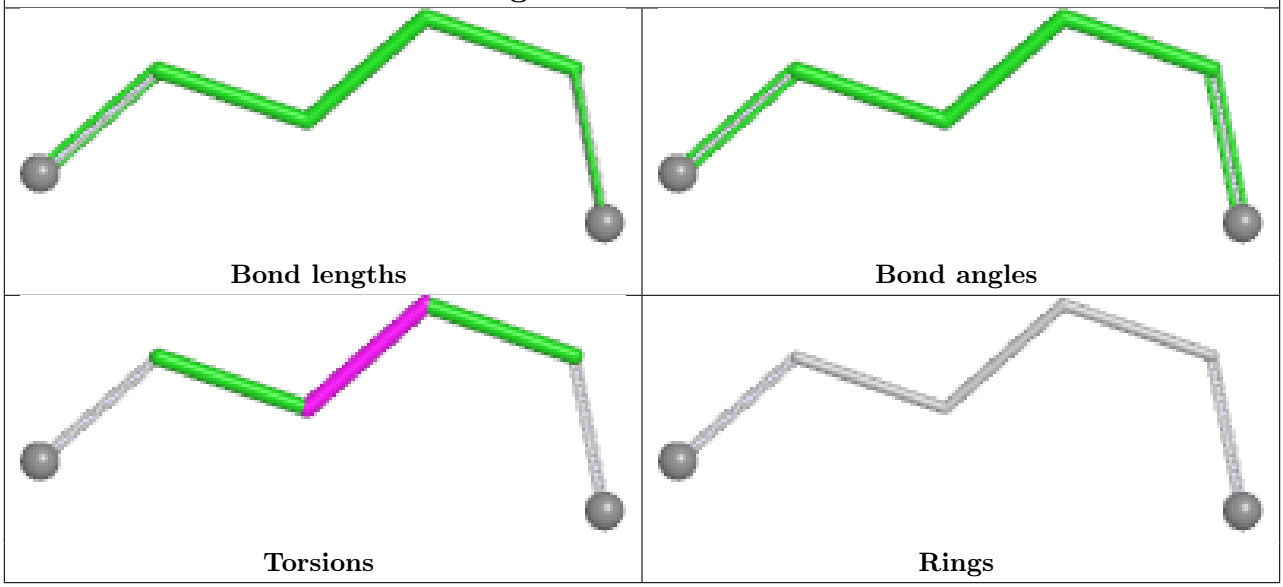


Torsions

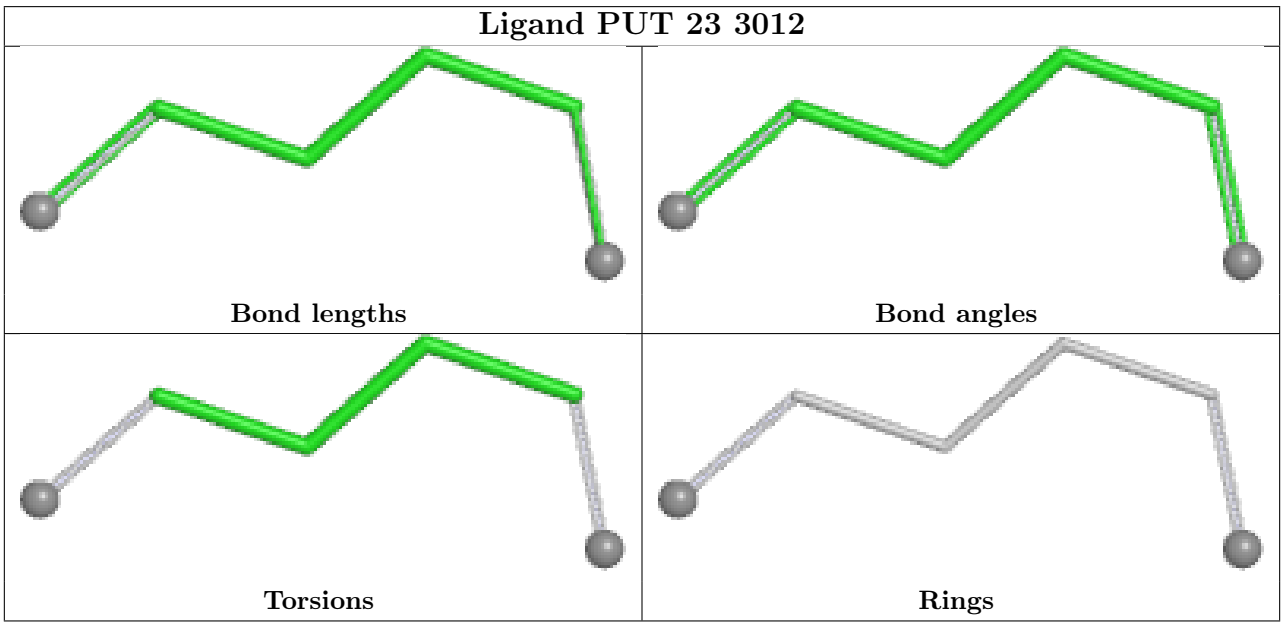


Rings

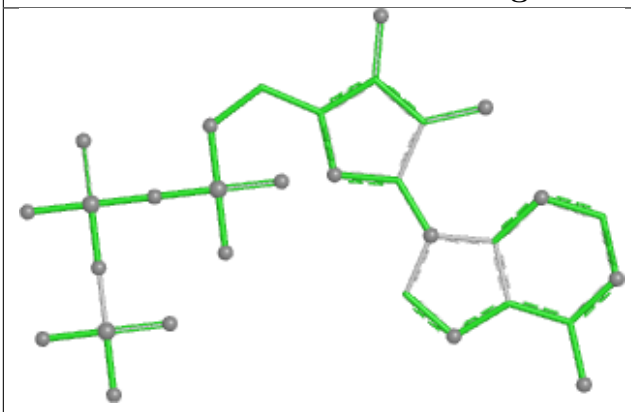
Ligand PUT 16 1603



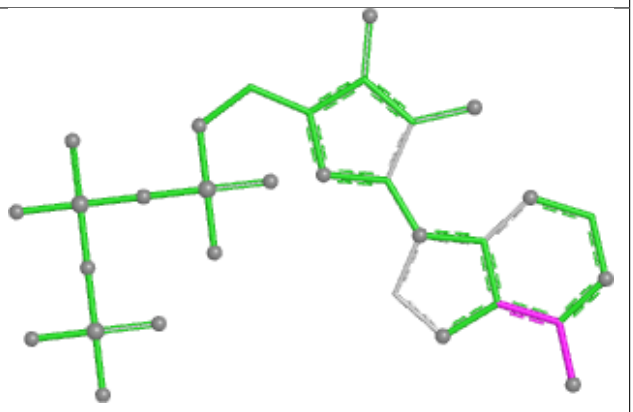
Ligand PUT 23 3012



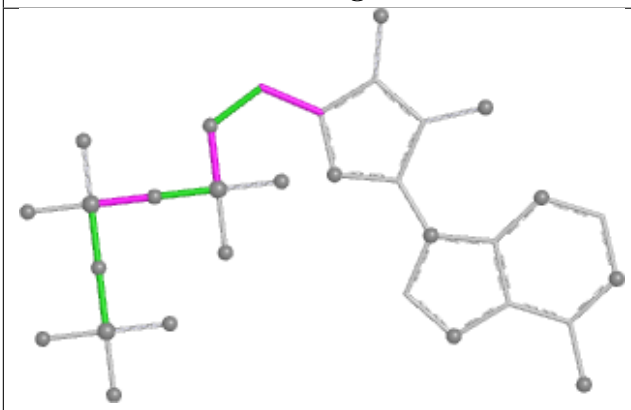
Ligand ATP 23 3003



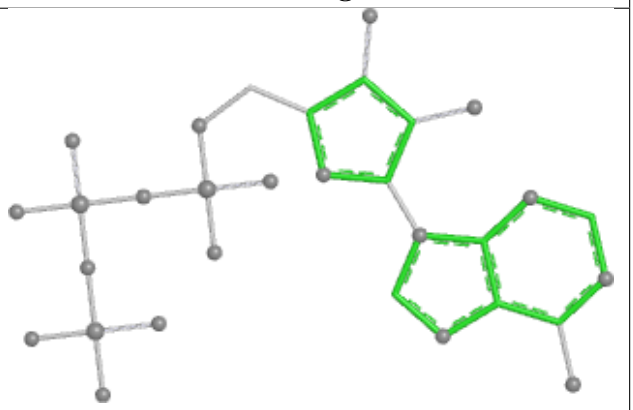
Bond lengths



Bond angles

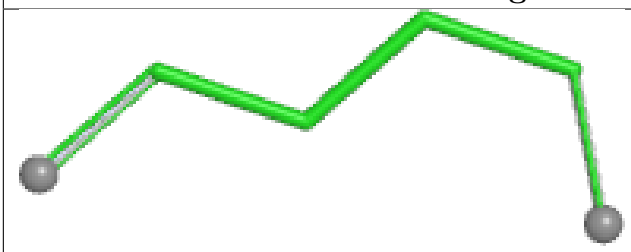


Torsions

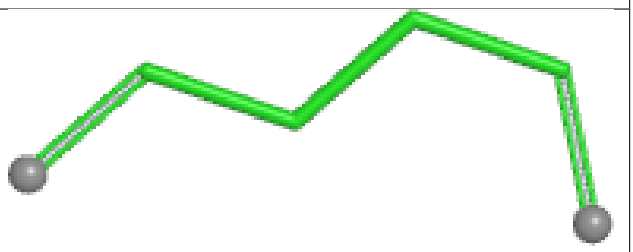


Rings

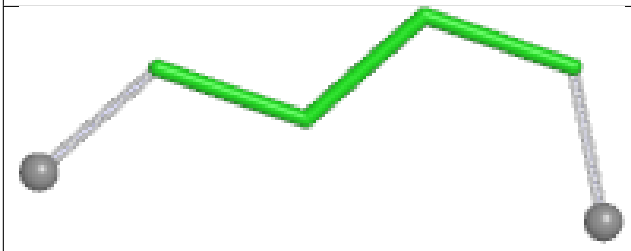
Ligand PUT 23 3018



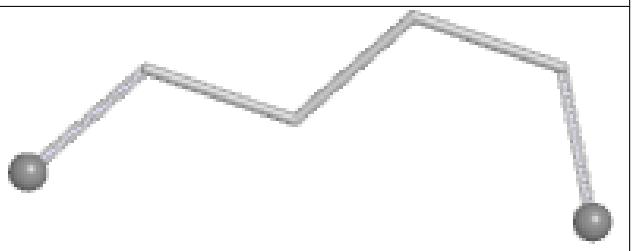
Bond lengths



Bond angles

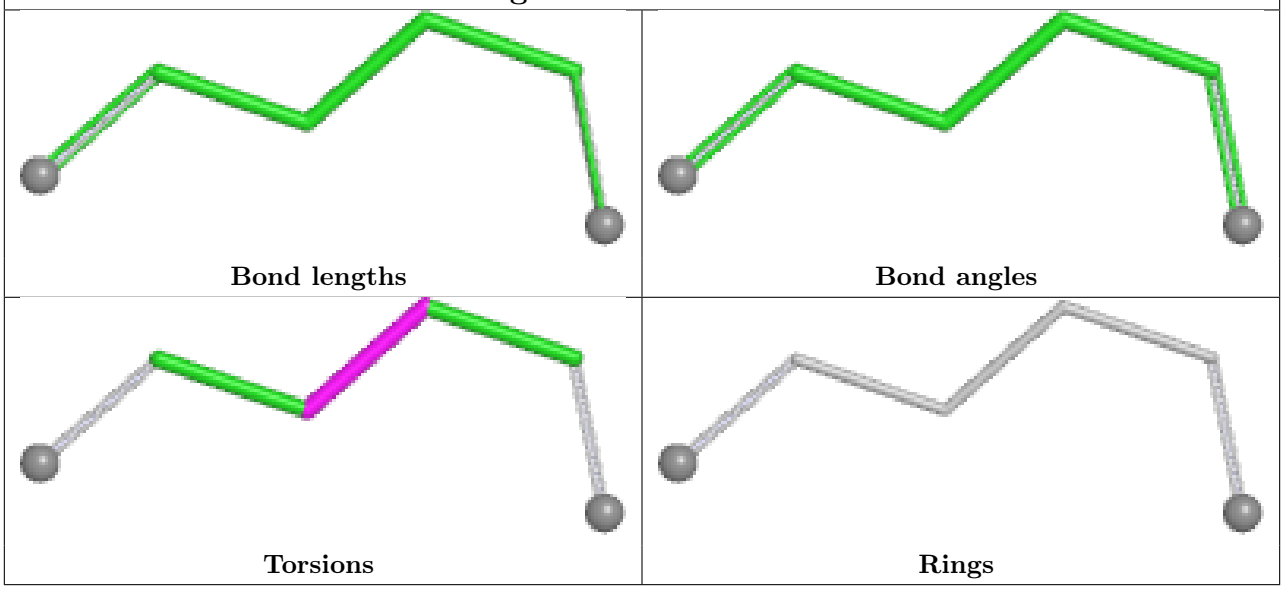


Torsions

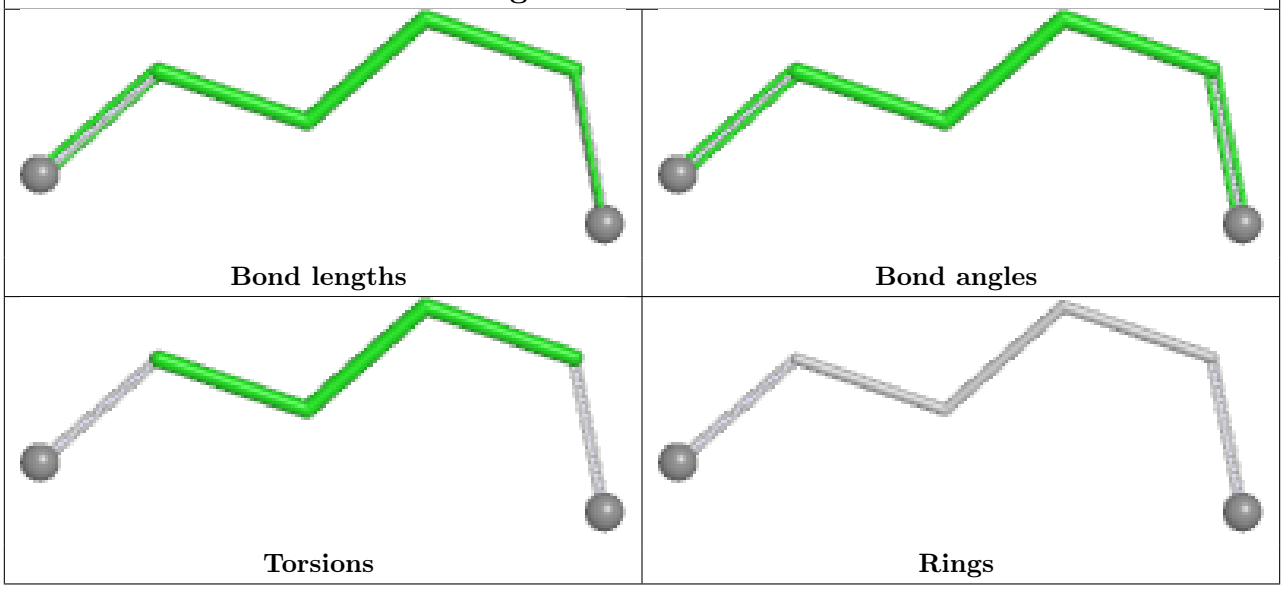


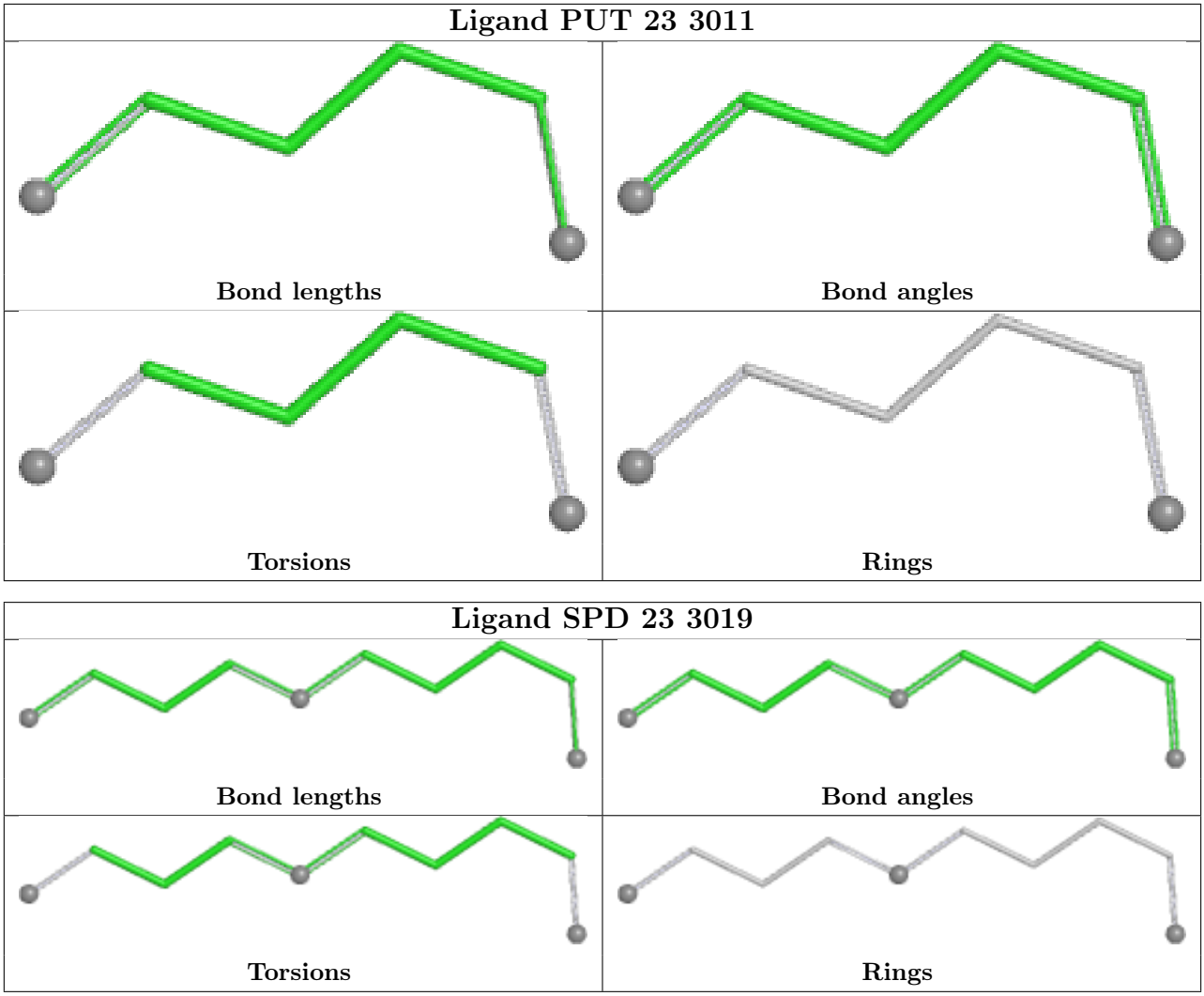
Rings

Ligand PUT 23 3004



Ligand PUT 23 3016





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

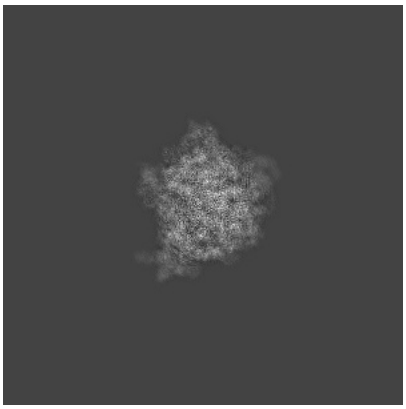
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24120. These allow visual inspection of the internal detail of the map and identification of artifacts.

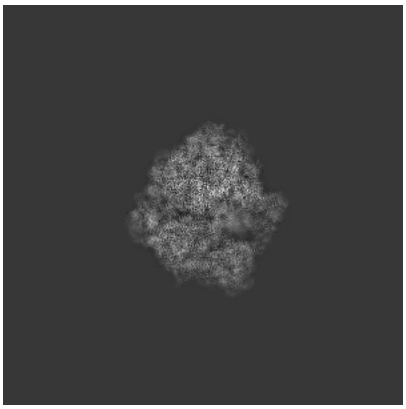
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

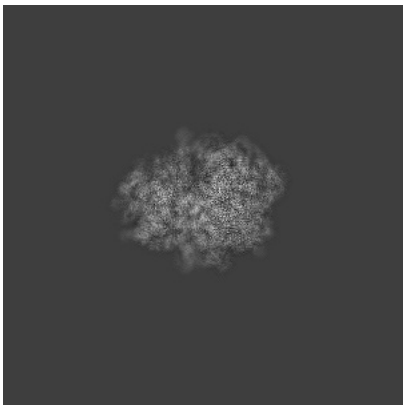
6.1.1 Primary map



X

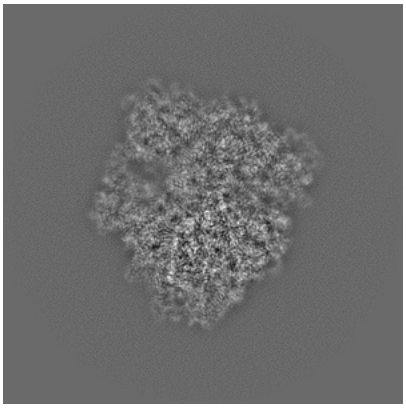


Y

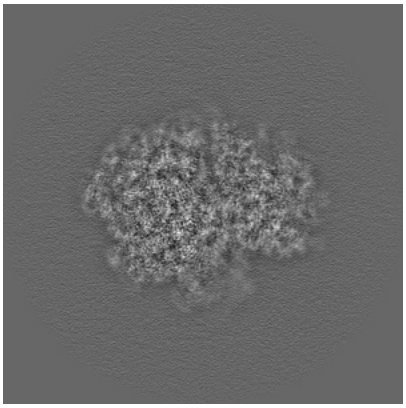


Z

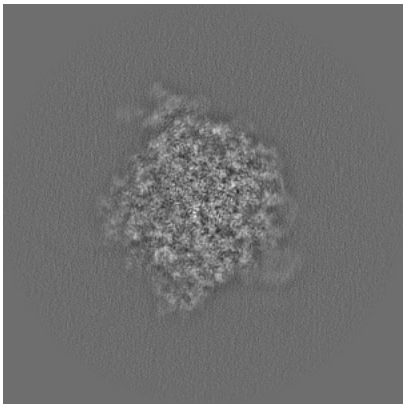
6.1.2 Raw map



X



Y

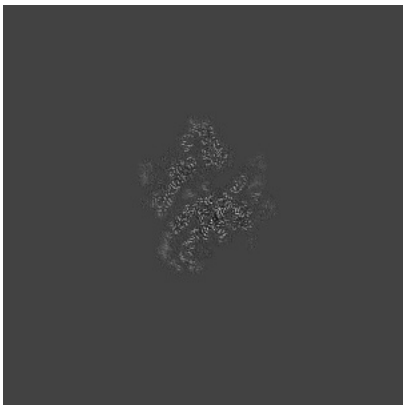


Z

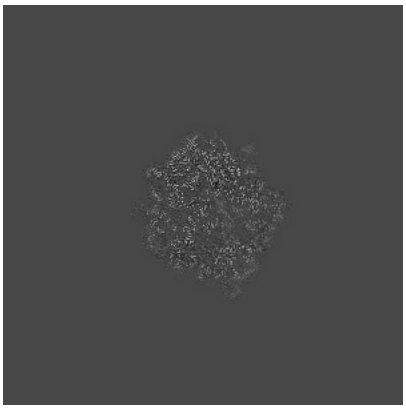
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

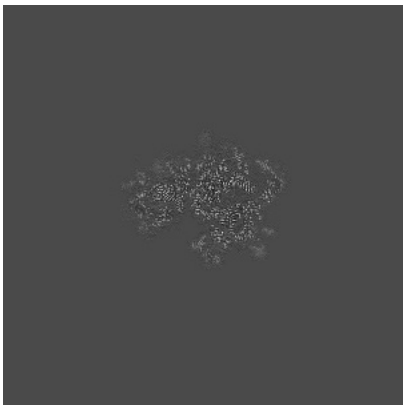
6.2.1 Primary map



X Index: 288

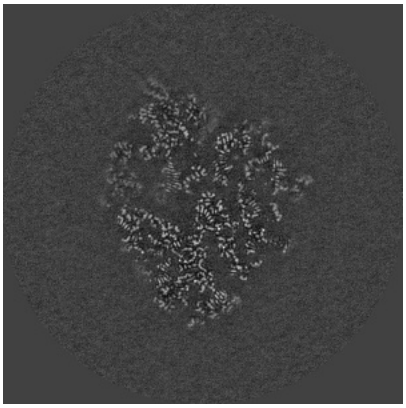


Y Index: 288

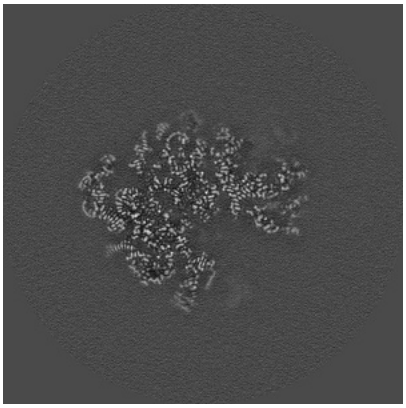


Z Index: 288

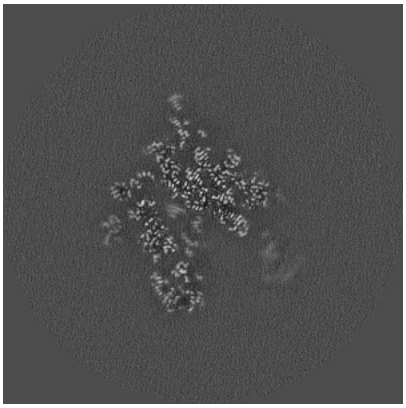
6.2.2 Raw map



X Index: 256



Y Index: 256

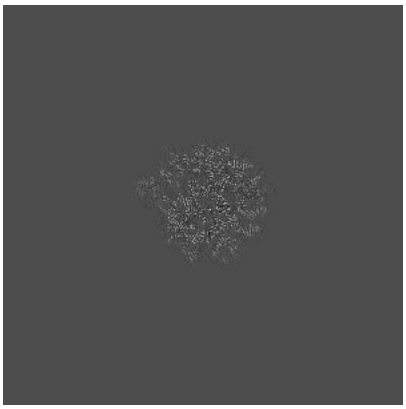


Z Index: 256

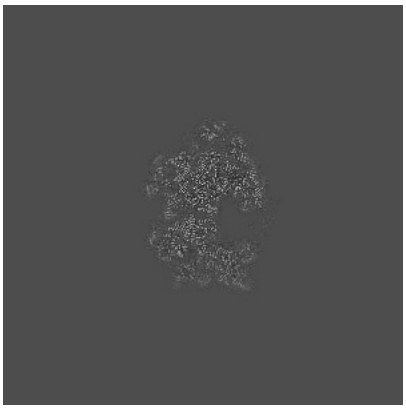
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

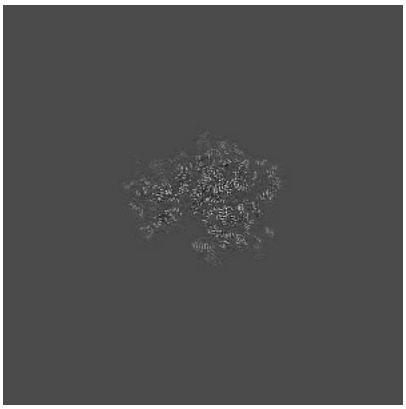
6.3.1 Primary map



X Index: 316

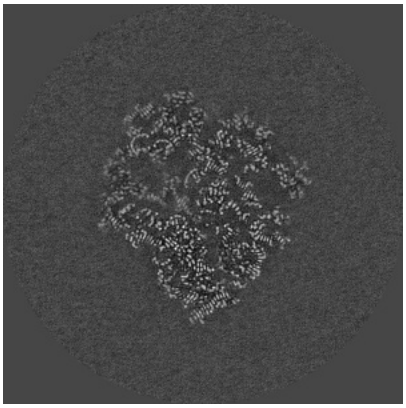


Y Index: 315

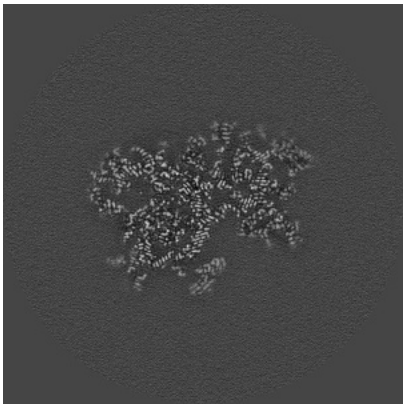


Z Index: 283

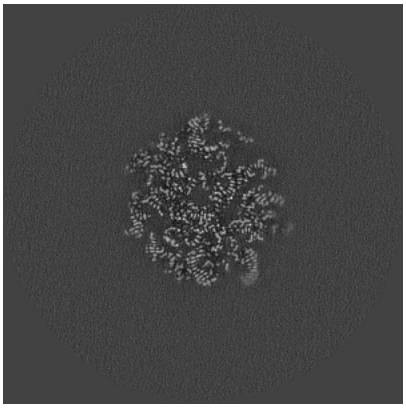
6.3.2 Raw map



X Index: 247



Y Index: 280

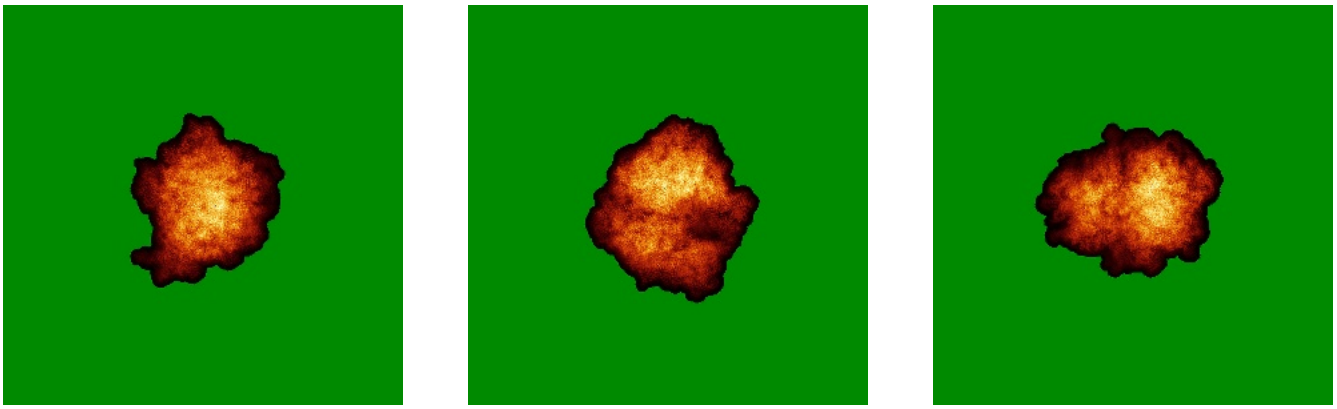


Z Index: 210

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

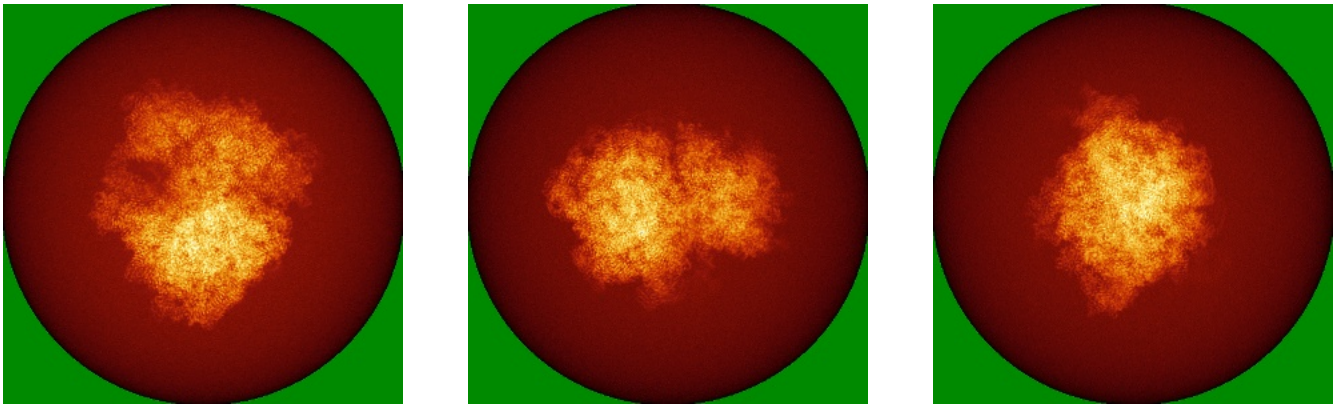
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

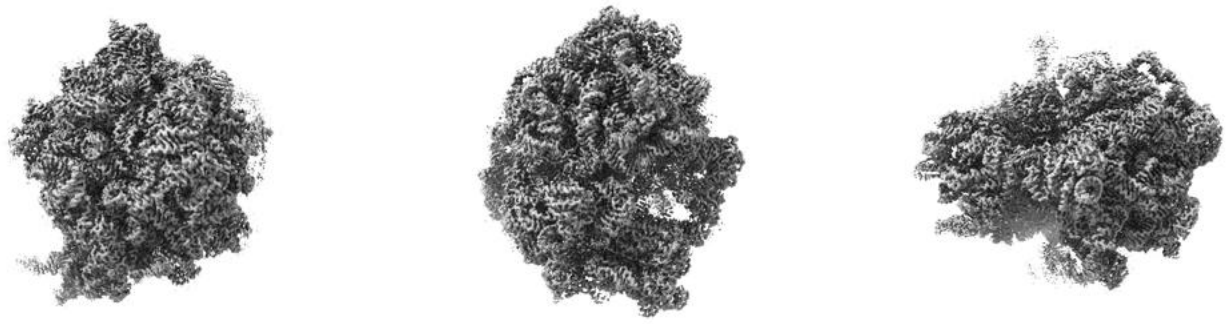


X Y Z

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)

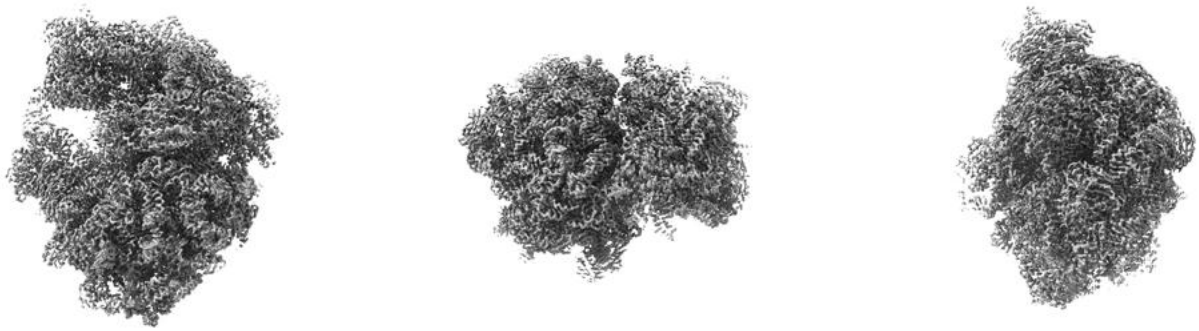
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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



X Y Z

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.

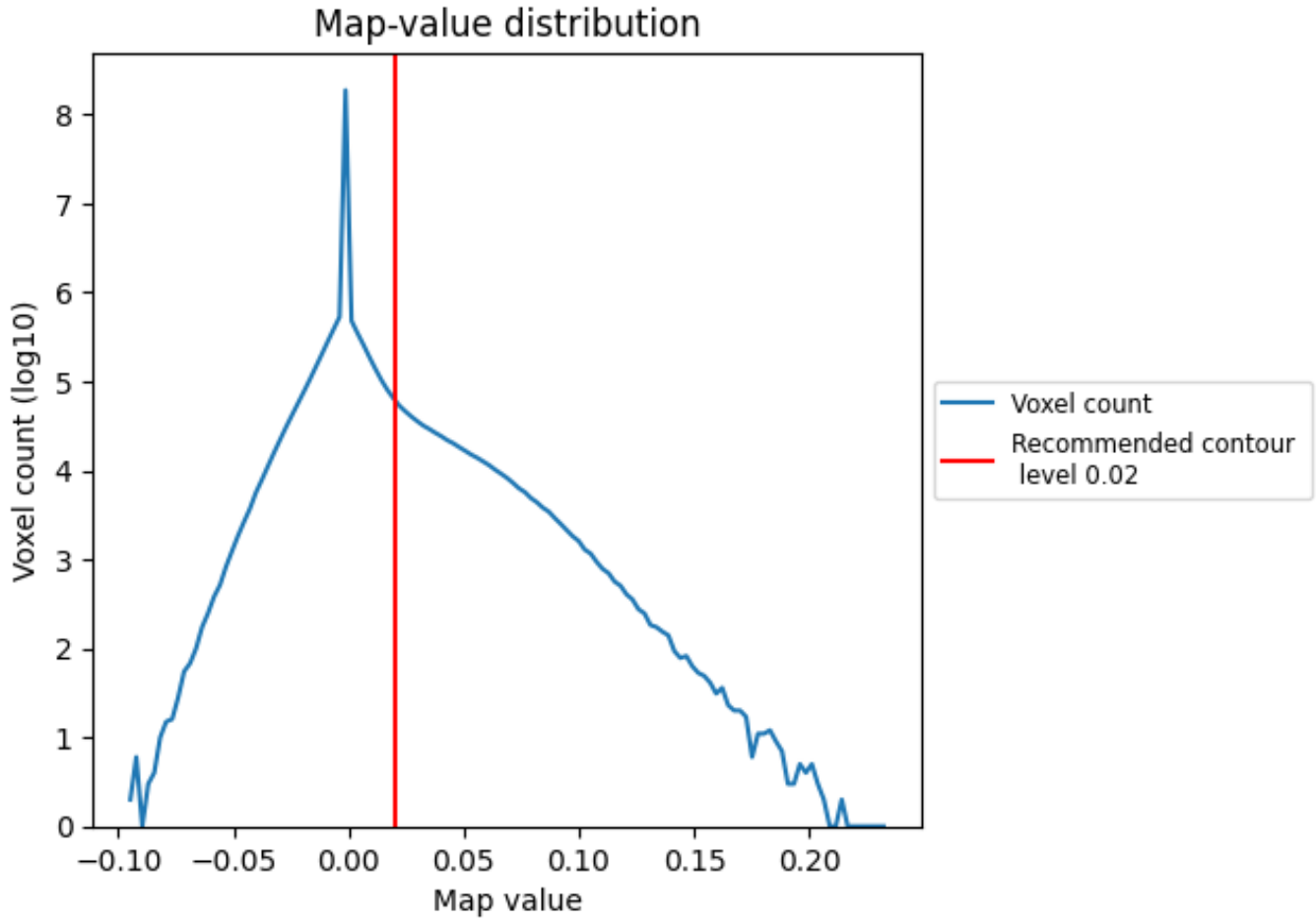
6.6 Mask visualisation (i)

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

7 Map analysis

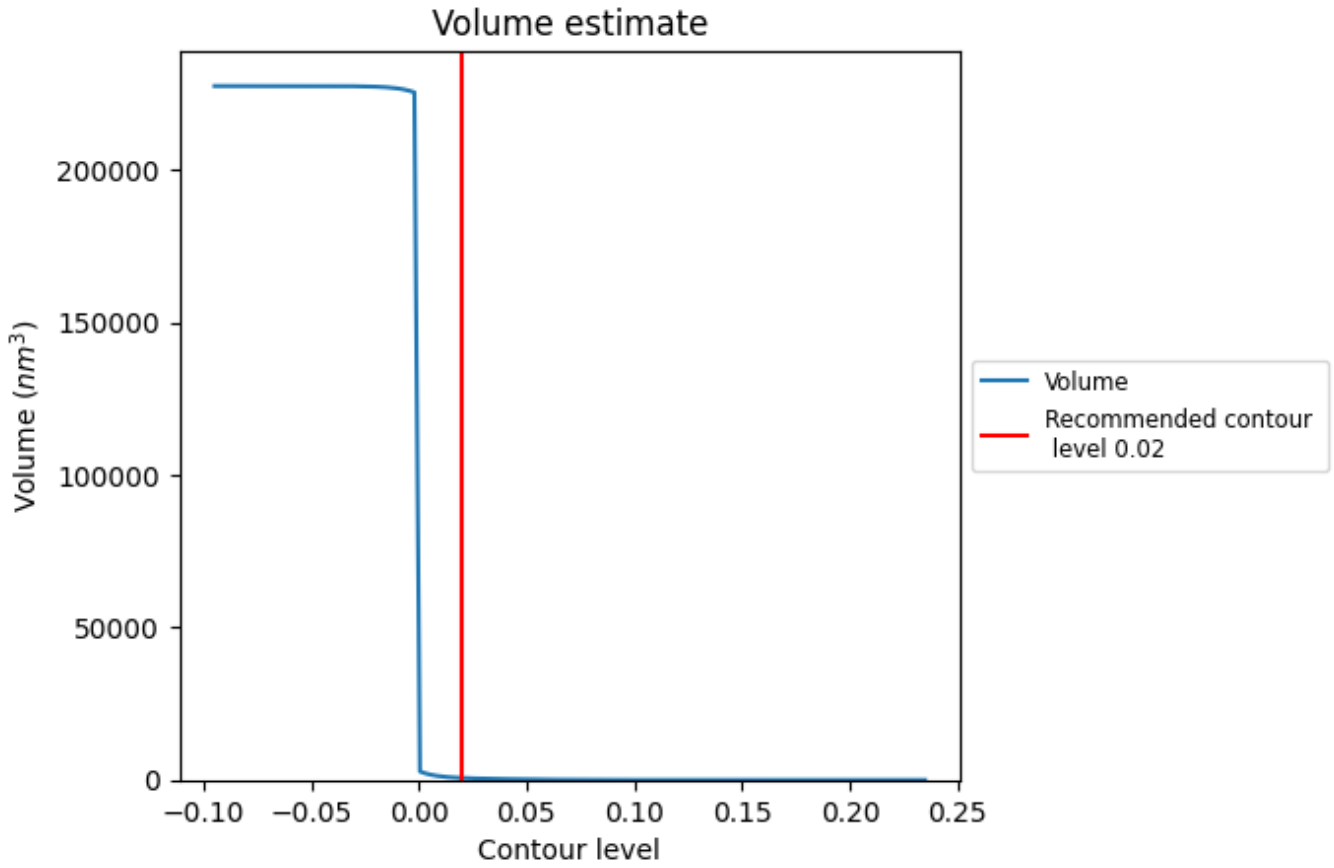
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

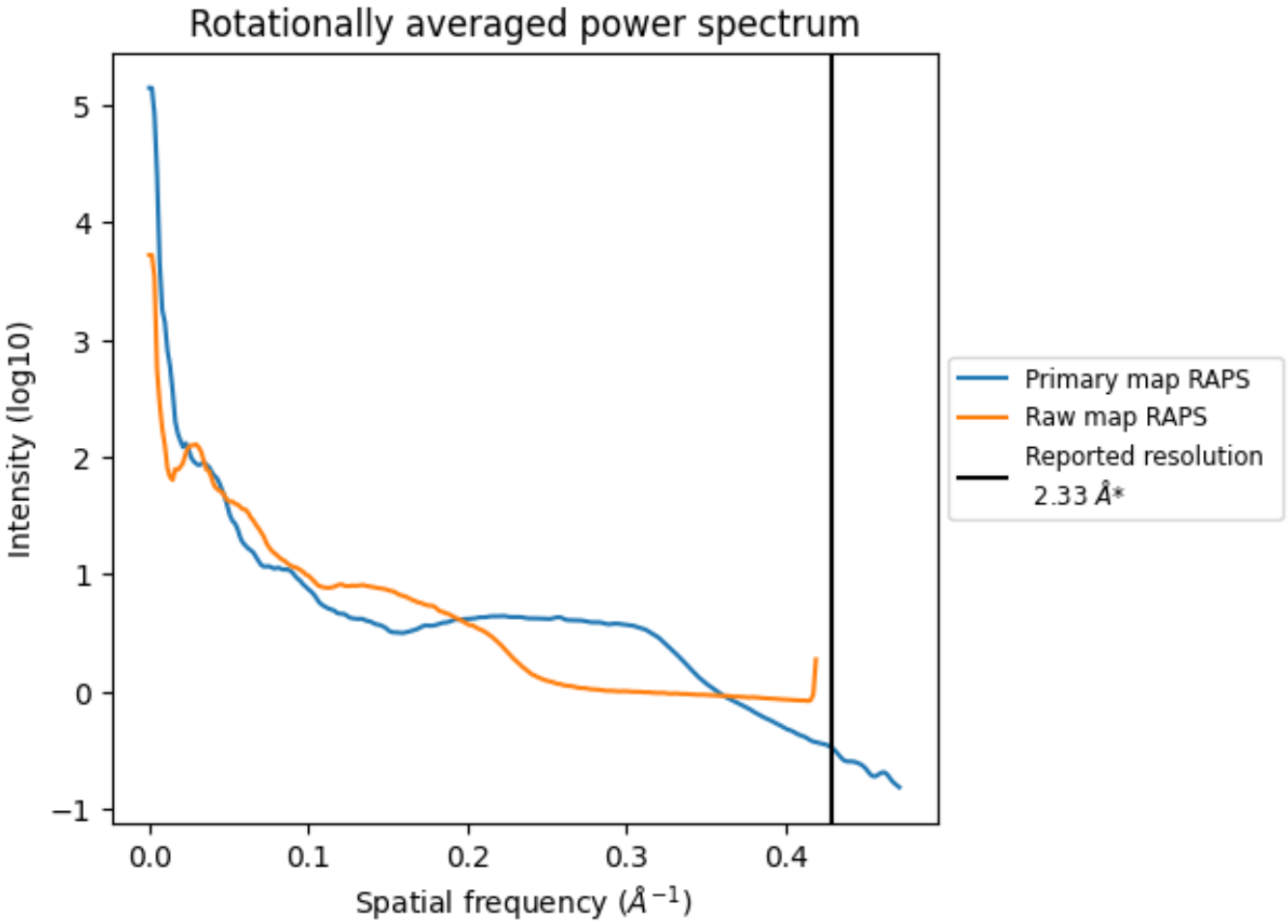
7.2 Volume estimate



The volume at the recommended contour level is 657 nm^3; this corresponds to an approximate mass of 593 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)

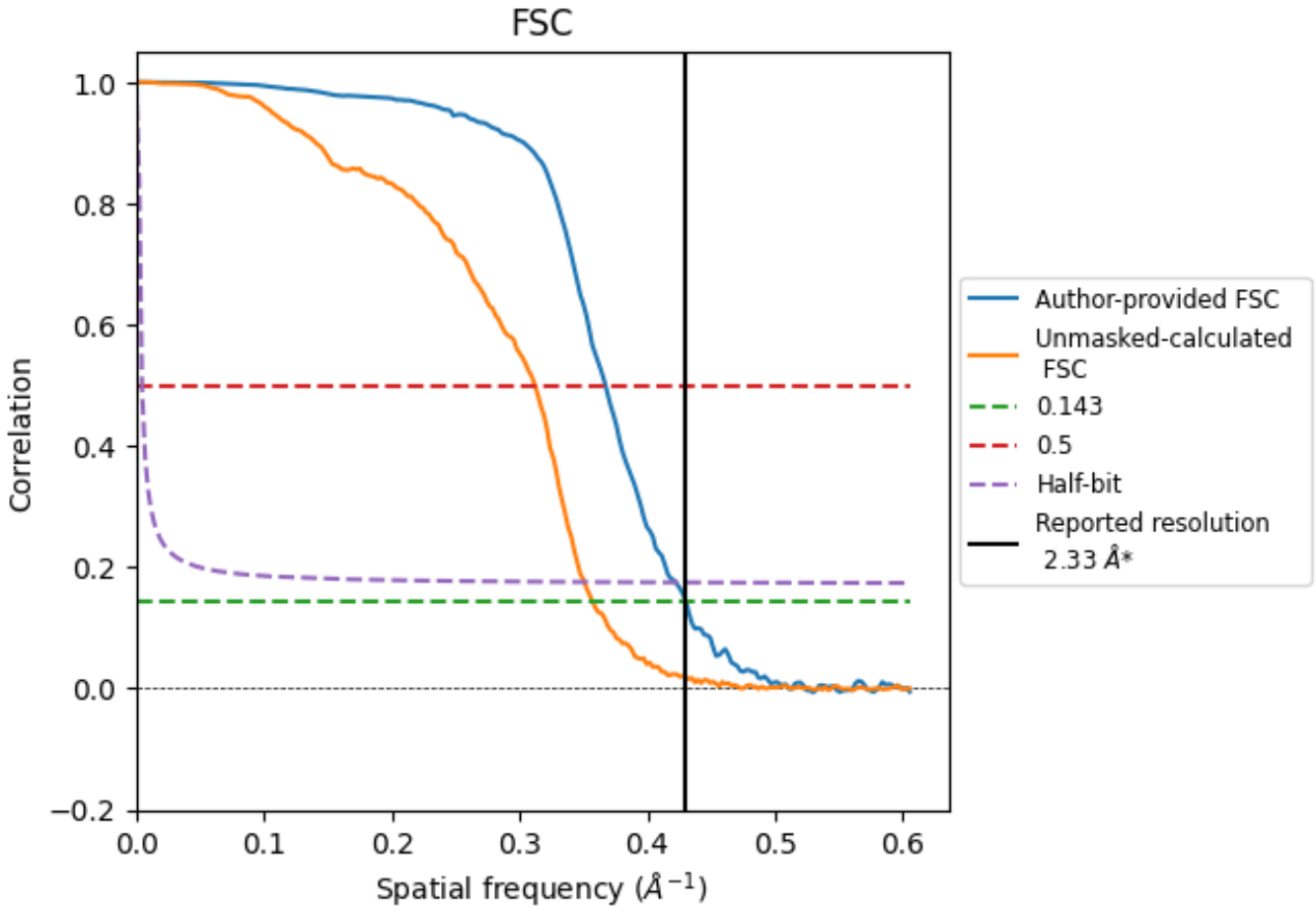


*Reported resolution corresponds to spatial frequency of 0.429 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.429 $Å^{-1}$

8.2 Resolution estimates (i)

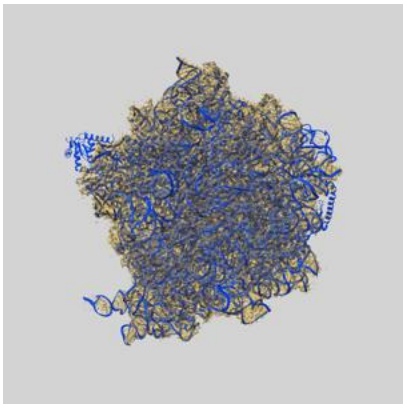
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.33	-	-
Author-provided FSC curve	2.32	2.72	2.37
Unmasked-calculated*	2.80	3.20	2.85

*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 2.80 differs from the reported value 2.33 by more than 10 %

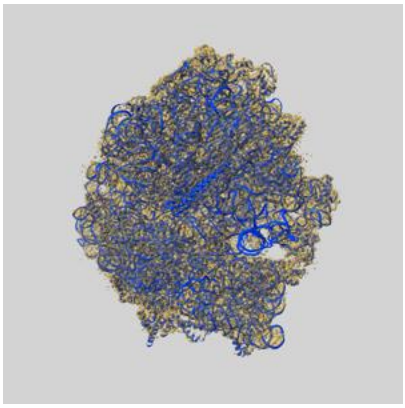
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24120 and PDB model 7N1P. Per-residue inclusion information can be found in section 3 on page 18.

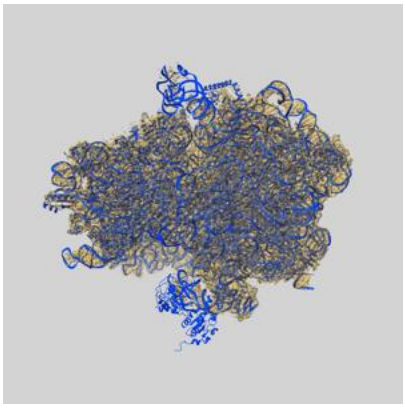
9.1 Map-model overlay



X



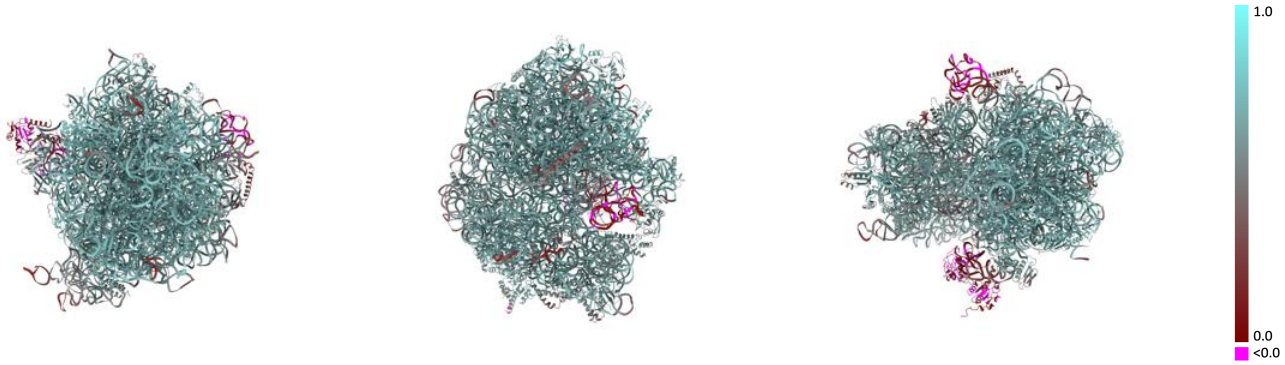
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

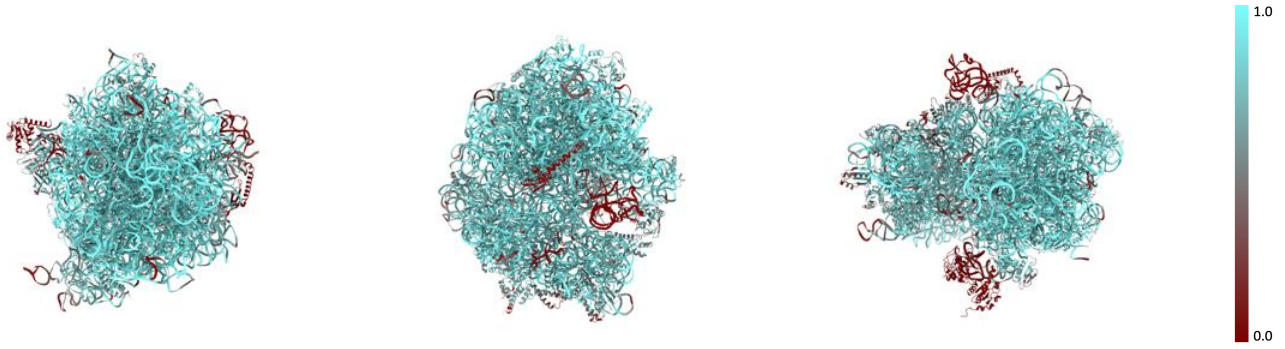
9.2 Q-score mapped to coordinate model



X Y Z

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.

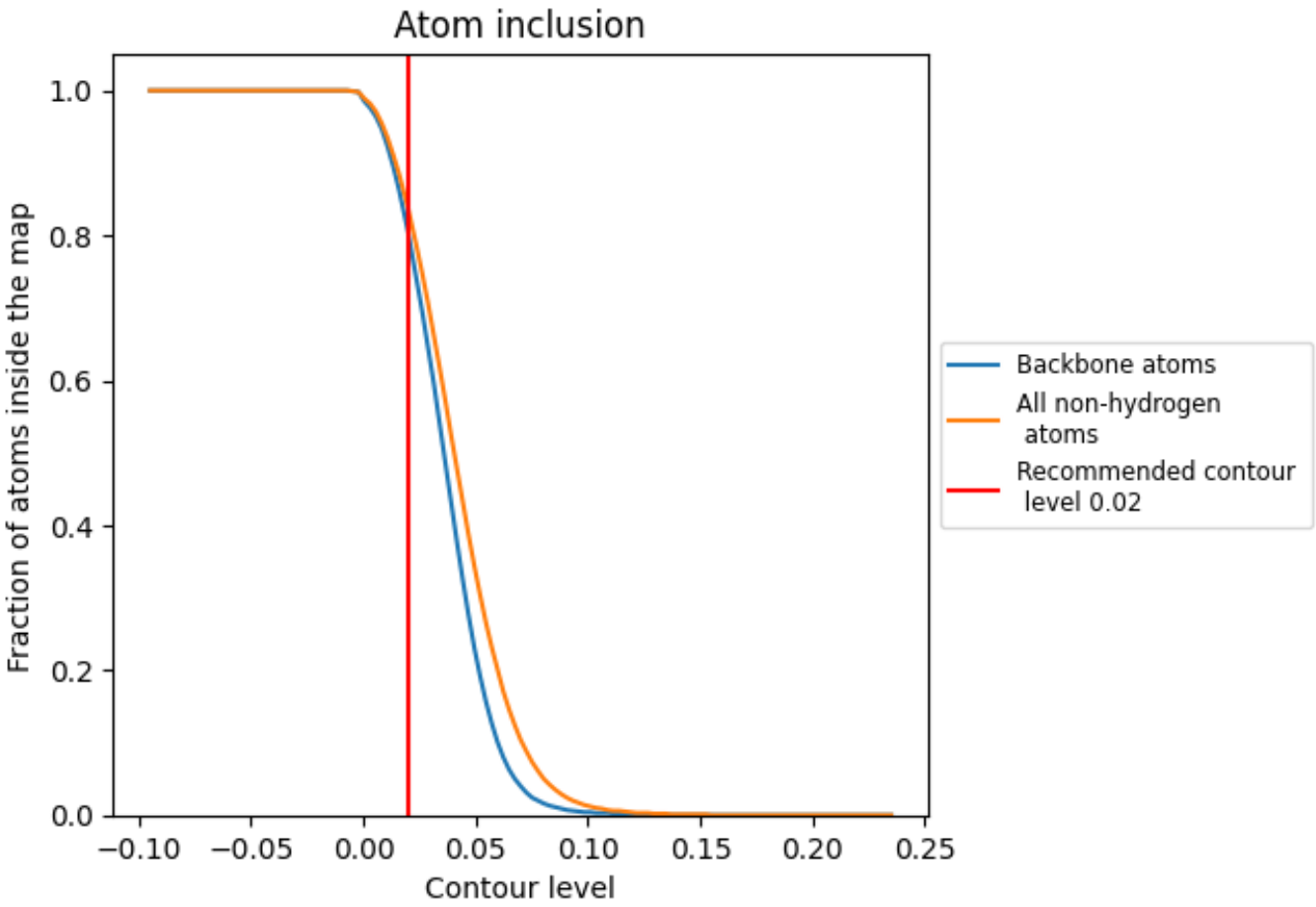
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 84% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8380	0.6240
16	0.8870	0.6290
23	0.8930	0.6400
5	0.9020	0.6400
Dt	0.7420	0.5980
LB	0.9210	0.6960
LC	0.9110	0.6790
LD	0.8380	0.6570
LE	0.6320	0.5760
LF	0.6830	0.5700
LI	0.2340	0.4160
LJ	0.0040	0.0320
LK	0.0010	0.0320
LM	0.9010	0.6870
LN	0.8660	0.6810
LO	0.9000	0.6740
LP	0.9100	0.6950
LQ	0.9340	0.7020
LR	0.7900	0.6220
LS	0.8550	0.6650
LT	0.9360	0.7080
LU	0.8290	0.6630
LV	0.8760	0.6790
LW	0.7880	0.6490
LX	0.7840	0.6170
LY	0.8270	0.6400
La	0.8590	0.6790
Lb	0.8850	0.6800
Lc	0.7120	0.6220
Ld	0.8580	0.6540
Le	0.5030	0.5010
Lf	0.8650	0.6800
Lg	0.8110	0.6540
Lh	0.9470	0.7100
Li	0.9490	0.7090

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Chain	Atom inclusion	Q-score
Lj	0.8800	0.6670
Pp	0.3210	0.4120
Pt	0.7090	0.5670
SB	0.6120	0.5660
SC	0.7470	0.6340
SD	0.7400	0.6140
SE	0.8610	0.6490
SF	0.6580	0.5790
SG	0.6700	0.5560
SH	0.8560	0.6560
SI	0.7300	0.6160
SJ	0.5810	0.5580
SK	0.7690	0.6220
SL	0.8600	0.6630
SM	0.7240	0.5910
SN	0.7620	0.6330
SO	0.7980	0.6360
SP	0.7540	0.5970
SQ	0.7930	0.6410
SR	0.7410	0.6090
SS	0.7250	0.5890
ST	0.7600	0.6130
SU	0.5320	0.5550
mR	0.3630	0.3990