



wwPDB EM Validation Summary Report ⓘ

Jun 25, 2026 – 01:28 PM EDT

PDB ID : 7N1P / pdb_00007n1p
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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

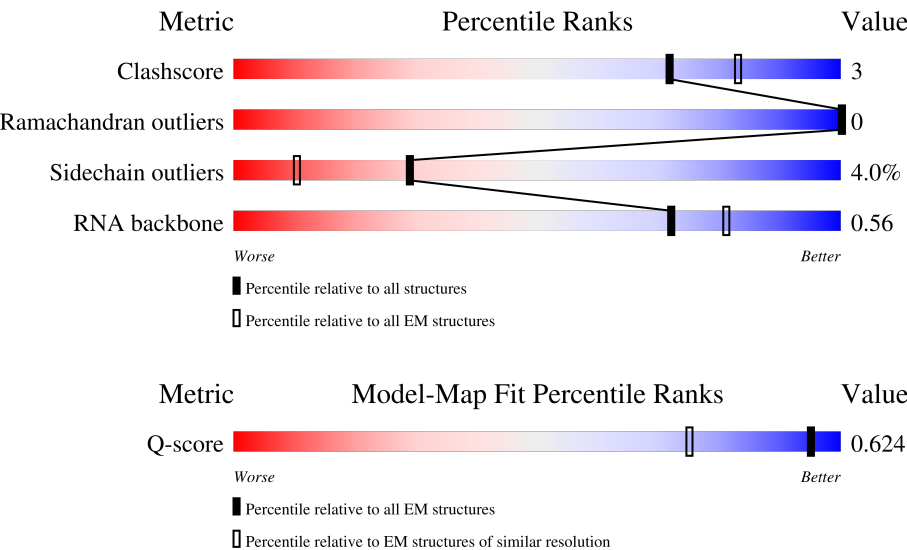
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4434 (1.83 - 2.83)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	16	1542	5% 75% 23% •
2	SB	241	20% 79% 15% • 5%
3	SC	233	7% 75% 15% • 9%

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Mol	Chain	Length	Quality of chain
4	SD	206	
5	SE	167	
6	SF	135	
7	SG	179	
8	SH	130	
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	

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Mol	Chain	Length	Quality of chain
29	LF	177	
30	LI	149	
31	LJ	165	
32	LK	142	
33	LM	142	
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	

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Mol	Chain	Length	Quality of chain
54	Li	65	91% 8%
55	Lj	38	5% 87% 13%
56	Pt	76	12% 63% 28% 5%
57	Pp	3	67% 33%
58	Dt	76	7% 38% 41% 17%

2 Entry composition

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
1	16	1542	Total	C	N	O	P	0	0
			33092	14767	6064	10719	1542		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SG	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	S	0	0
			427	275	78	74			

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

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

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

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

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

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

- Molecule 56 is a 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		

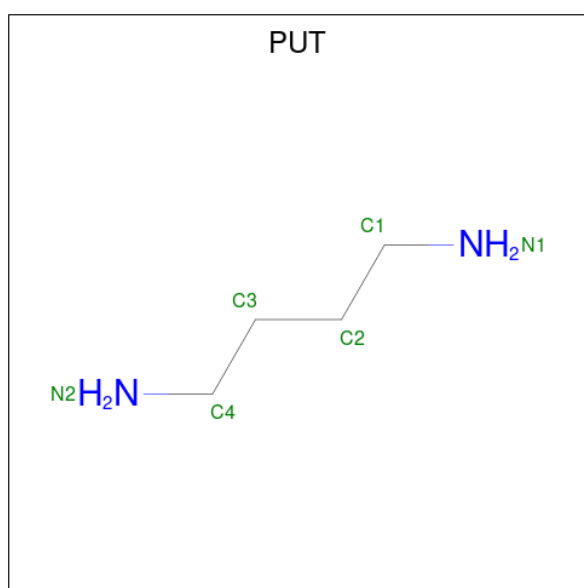
- Molecule 57 is a protein called Chains: Pp.

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-DIAMINOBTANE (CCD ID: 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	0
			6	4	2	
59	23	1	Total	C	N	0
			6	4	2	
59	23	1	Total	C	N	0
			6	4	2	
59	23	1	Total	C	N	0
			6	4	2	
59	23	1	Total	C	N	0
			6	4	2	
59	23	1	Total	C	N	0
			6	4	2	
59	23	1	Total	C	N	0
			6	4	2	
59	23	1	Total	C	N	0
			6	4	2	
59	23	1	Total	C	N	0
			6	4	2	
59	23	1	Total	C	N	0
			6	4	2	
59	23	1	Total	C	N	0
			6	4	2	

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

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

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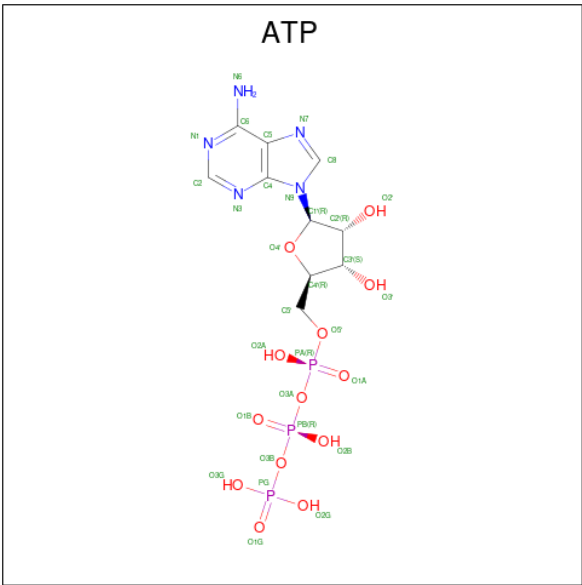
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Mol	Chain	Residues	Atoms		AltConf
60	LB	1	Total 1	Mg 1	0
60	LC	1	Total 1	Mg 1	0
60	LD	1	Total 1	Mg 1	0
60	LE	1	Total 1	Mg 1	0
60	Ld	1	Total 1	Mg 1	0
60	Lf	1	Total 1	Mg 1	0
60	Pt	1	Total 1	Mg 1	0
60	Dt	3	Total 3	Mg 3	0

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

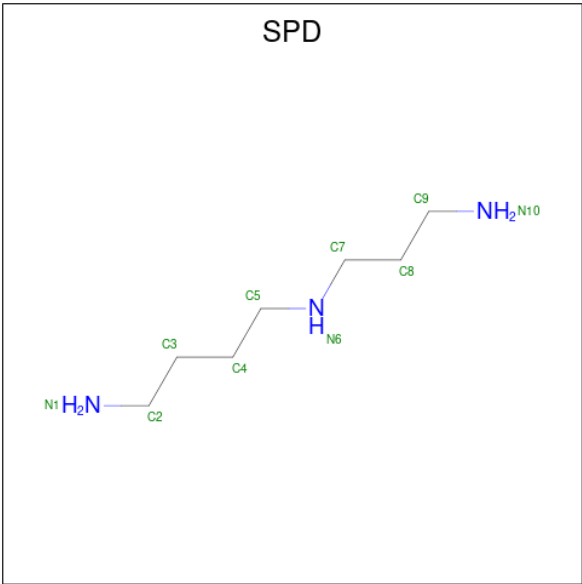
Mol	Chain	Residues	Atoms		AltConf
61	SB	1	Total 1	Zn 1	0
61	Le	1	Total 1	Zn 1	0
61	Lj	1	Total 1	Zn 1	0

- Molecule 62 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (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 (CCD ID: SPD) (formula: C₇H₁₉N₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 64 is water.

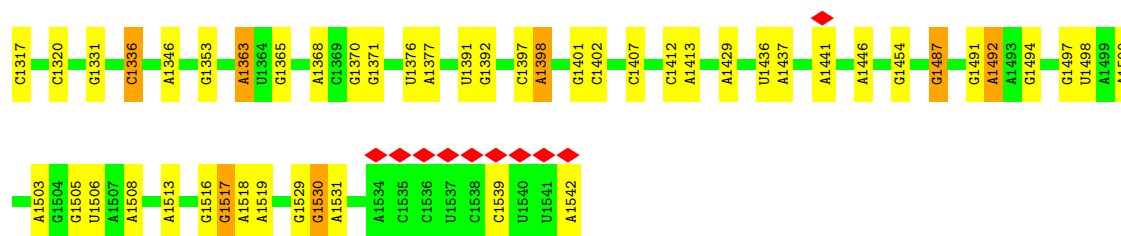
Mol	Chain	Residues	Atoms		AltConf
64	16	3	Total	O	0
			3	3	
64	23	41	Total	O	0
			41	41	
64	LB	3	Total	O	0
			3	3	
64	LC	1	Total	O	0
			1	1	
64	LT	1	Total	O	0
			1	1	
64	LY	1	Total	O	0
			1	1	

3 Residue-property plots [i](#)

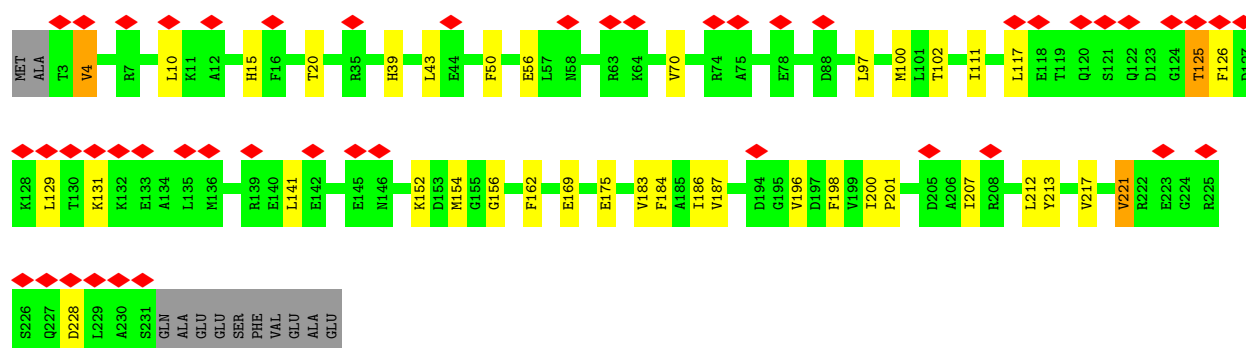
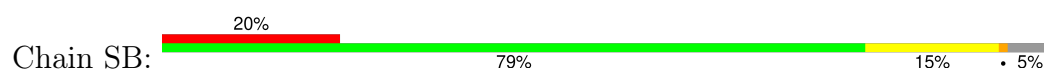
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

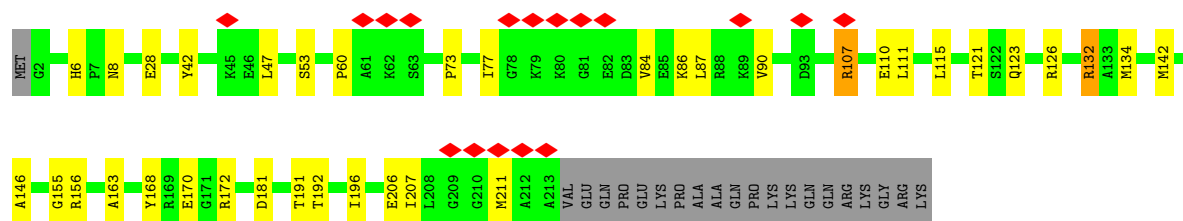
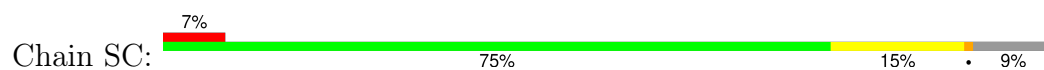




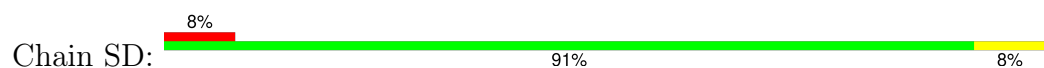
• Molecule 2: 30S ribosomal protein S2



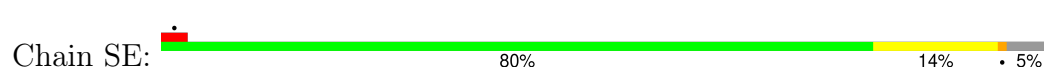
• Molecule 3: 30S ribosomal protein S3



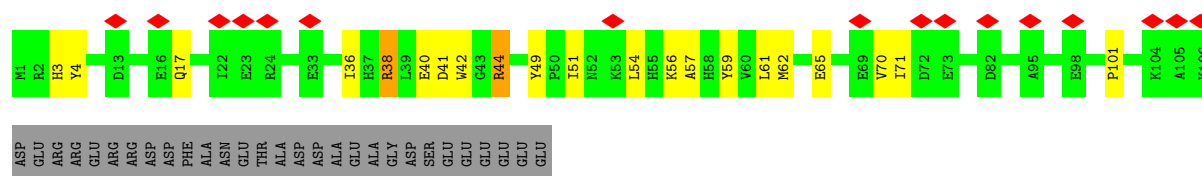
• Molecule 4: 30S ribosomal protein S4



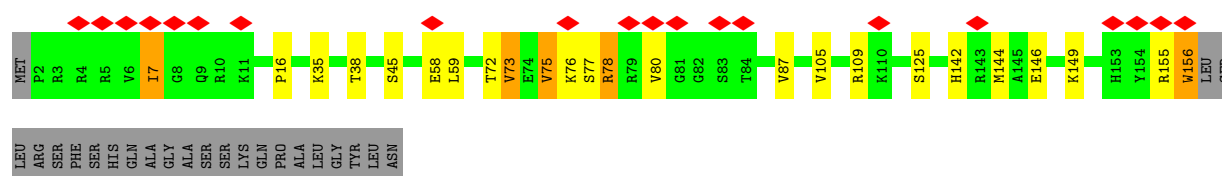
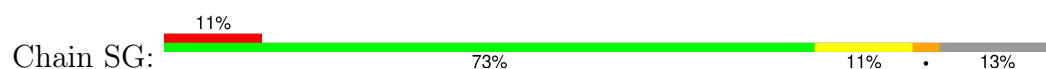
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6



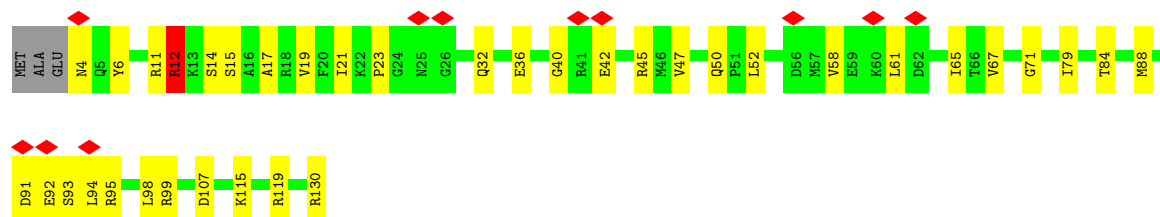
- Molecule 7: 30S ribosomal protein S7



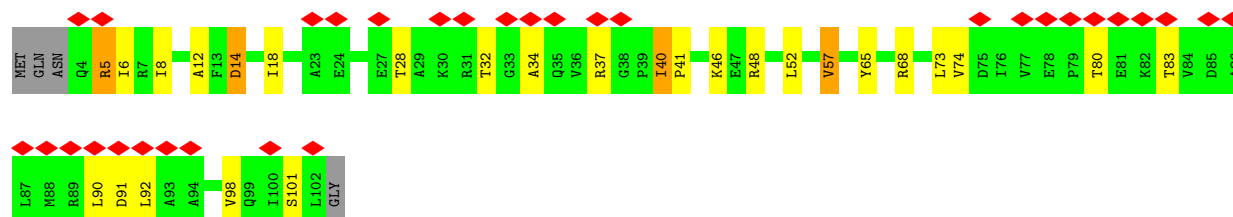
- Molecule 8: 30S ribosomal protein S8



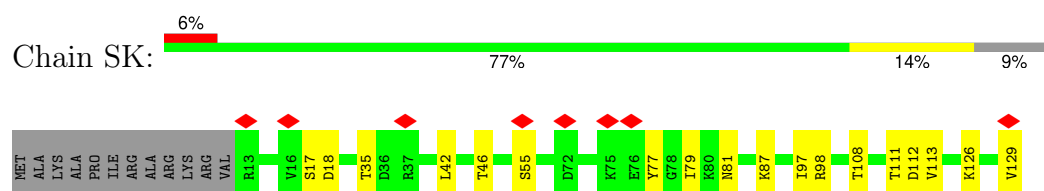
- Molecule 9: 30S ribosomal protein S9



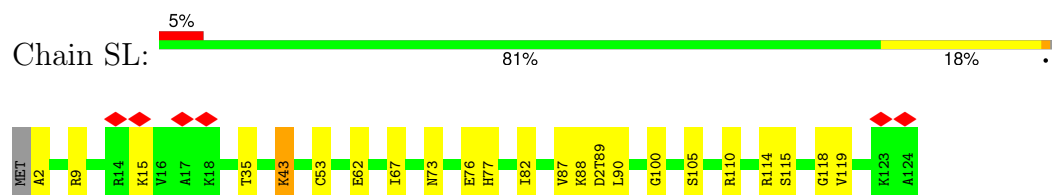
- Molecule 10: 30S ribosomal protein S10



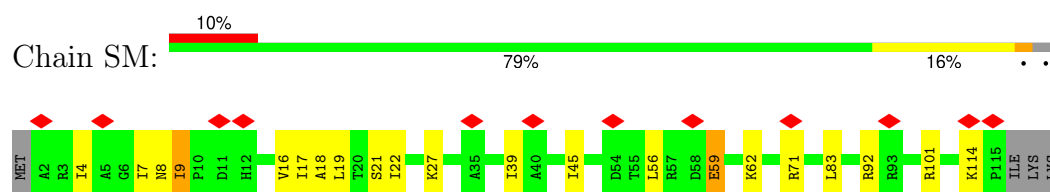
- Molecule 11: 30S ribosomal protein S11



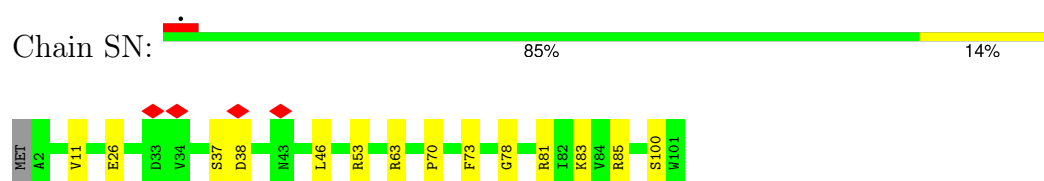
- Molecule 12: 30S ribosomal protein S12



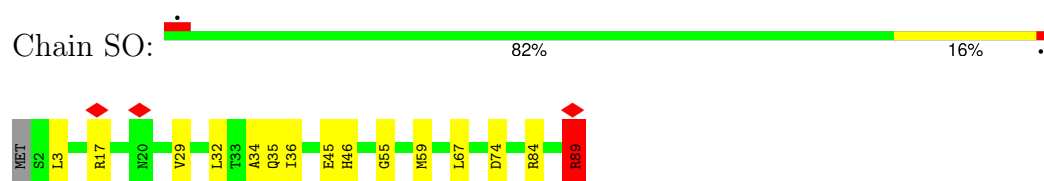
- Molecule 13: 30S ribosomal protein S13



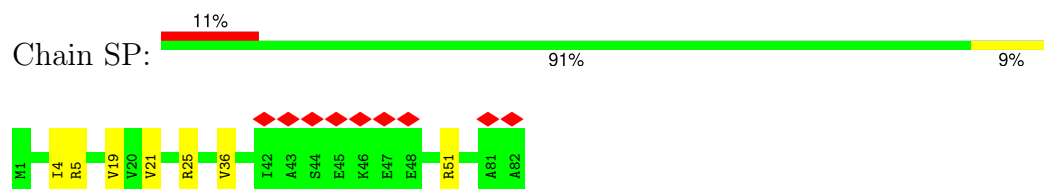
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

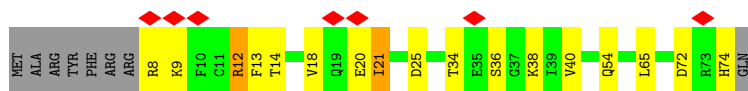


- Molecule 17: 30S ribosomal protein S17

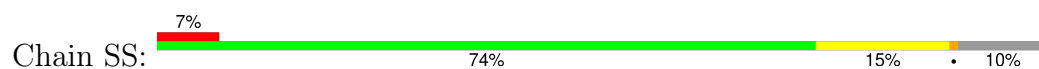




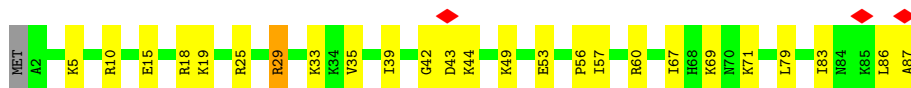
- Molecule 18: 30S ribosomal protein S18



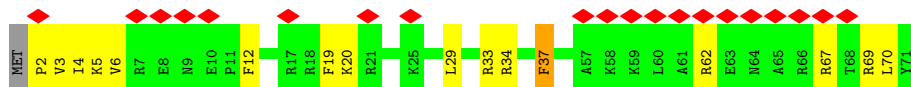
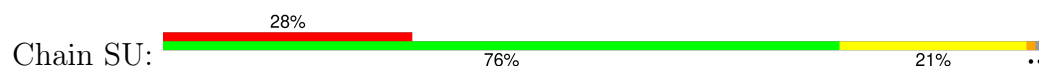
- Molecule 19: 30S ribosomal protein S19



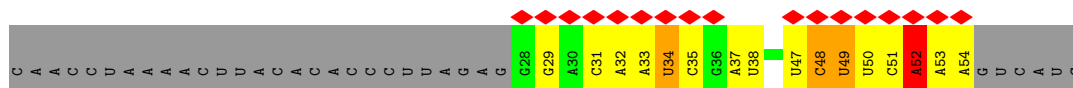
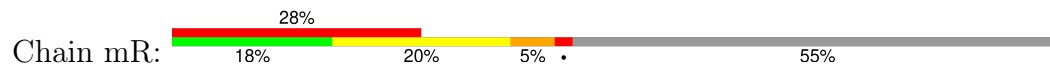
- Molecule 20: 30S ribosomal protein S20



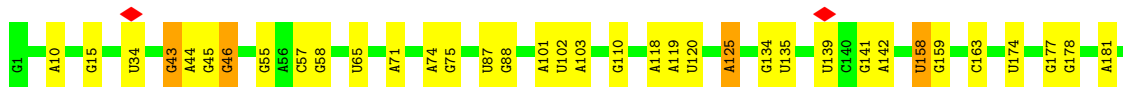
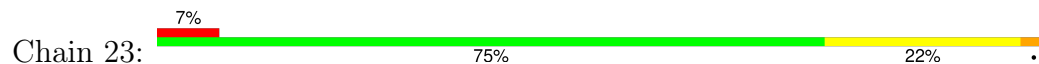
- Molecule 21: 30S ribosomal protein S21



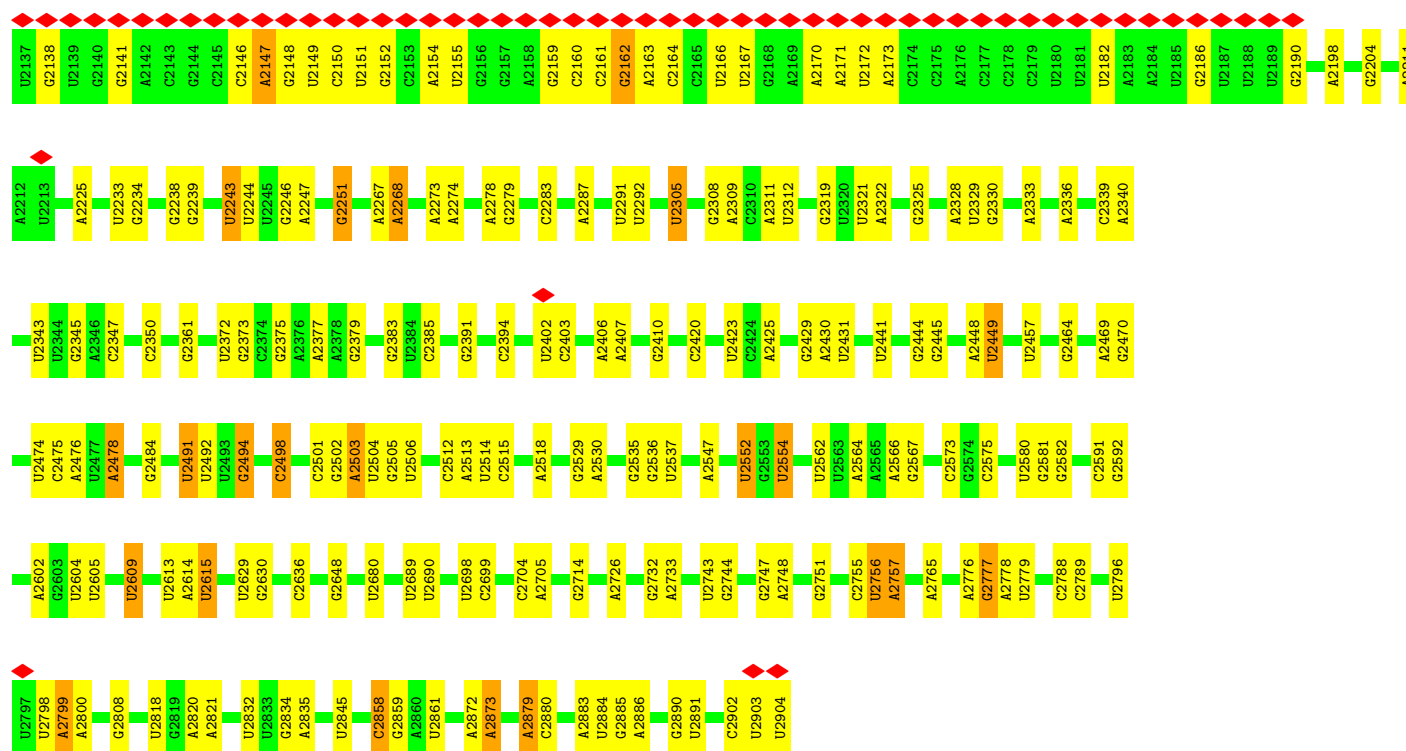
- Molecule 22: mRNA



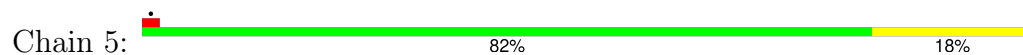
- Molecule 23: 23S rRNA



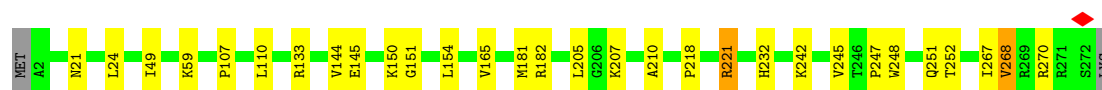
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C2043	G1873	C1704	A1509	U1173	G1074	U955	C840	A706	A547	G361	C841	C192
A2051	U1880	U1720	G1513	U1175	C1075	C961	A845	C717	G548	A371	A196	
C2055	G1906	G1721	A1515	U1176	A1077	G962	U846	A721	G549	G372	A199	
G2056	G1907	C1727	G1524	G1177	U1078	U967	U847	A722	U554	G386	C207	
A2060	A1912	U1729	C1531	G1178	C1079	C968	G858	G725	G555	U387	C208	
G2061	3TD1915	C1730	A1532	U1180	A1080	G971	G859	G726	G563	G388		
A2062	A1919	G1731	C1533	U1181	U1082	A972	U870	G729	U566	U395	G215	
G2069	U1949	G1738	U1534	A1395	U1083	G974	U871	A730	U567	G396	A216	
U2086	G1929	A1744	A1535	U1396	A1084	A983	U872	A742	U568	G400	A221	
G2087	G1930	A1745	C1536	U1405	A1085	A984	G869	A743	G570	A401	A222	
A2088	U1939	U1746	G1537	U1406	A1086	A996	G876	U744	A573	A404	C228	
G2093	U1940	U1747	U1539	G1238	G1087	A999	G877	G745	A574	U405	G248	
U2098	G1954	C1760	G1540	A1416	A1088	U999	G880	U746	A575	C249		
U2099	U1955	C1764	C1541	G1417	A1089	C1005	G881	U747	A576			
A2100	A1960	A1773	G1542	A1418	A1090	G1010	G882	A753	A577	A412		
G2102	C1961	C1773	G1543	G1419	G1091	A1010	G883	U754	A582	C413		
C2103	U1782	U1782	A1548	A1549	C1428	G1011	U884	A764	A586	C455	G271	
C2104	A1966	A1783	A1549	G1256	G1432	U1012	C885	C765	C456	A272	A272	
U2105	C1967	A1784	A1566	G1256	G1432	C1013	A886	G775	A457			
G2106	G1968	A1785	G1567	A1262	A1095	G1026	U887	G776	C595	C275		
U2107	A1969	A1786	G1568	U1263	A1096	A1027	C888	U779	C595	U276		
C2108	A1970	A1789	A1569	U1266	U1097	A1028	C889	A603	G469	G277		
U2109	C1790	C1790	U1578	U1267	A1098	U1033	C890	A613	A470	A278		
G2110	G1975	A1791	A1583	G1271	G1099	C1044	G891	A614	G473	A279		
C2111	U1982	C1795	U1584	U1272	C1100	G1045	A892	G784	G476	U280		
G2112	U1991	U1796	A1597	A1273	U1101	A1046	C893	G785		C281		
U2113	U1991	G1797	A1598	U1273	C1102	G1047	U895	A788	A479	A282		
A2114	G1992	U1798	A1598	C1278	A1103	U1047	A896	A789	A480	C283		
G2115	U1993	U1799	A1598	G1279	C1104	C1053	C897	C796	G481	U284		
C2116	C1997	A1800	A1603	G1279	U1105	A1054	C898	G797	A482	G285		
A2117	A2020	A1801	A1608	G1300	G1106	G1055	C902	C797	A483	U286		
U2118	C2021	G1807	A1609	A1301	A1111	G1056	G902	A802	G491	G287		
A2119	U2022	A1808	A1610	C1315	G1112	A1057	G907	A802	A492	U288		
G2120	C2023	A1810	A1614	A1321	G1125	U1058	A910	G805	G493	U296		
U2121	G2024	G1811	A1618	A1327	U1130	G1059	A917	G809	C494	C297		
U2122	C2025	C1816	A1637	A1328	G1131	U1060	A918	G809	A502	A311		
G2123	A2030	G1835	A1637	U1329	U1132	U1061	A919	C812	A503	A303		
C2124	C2031	A1847	G1645	C1330	U1133	G1062	U919	A819	A504	A330		
G2125	A2032	A1848	G1646	U1352	A1134	G1063	A927	A819	A505	A345		
A2126	C2033	A1848	U1647	U1352	C1135	G1064	A928	U827	C509	A352		
G2127	G2038	C1870	U1648	C1357	G1136	U1065	U931	U828	G669	C353		
U2128	U2039	A1871	G1649	G1358	G1136	U1066	U932	A833	A670	G354		
C2129			A1672	A1365	U1141	A1067	A941	G834	A532			
U2130			G1673		A1142	G1068	A945	G682				
U2131			G1674		G1149	A1069	C946					
U2132					C1153	A1070						
G2133						G1071						
A2134						C1072						
A2135												
G2136												



• Molecule 24: 5S rRNA



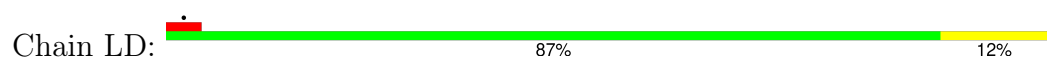
• Molecule 25: 50S ribosomal protein L2



• Molecule 26: 50S ribosomal protein L3

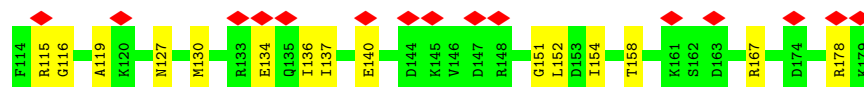
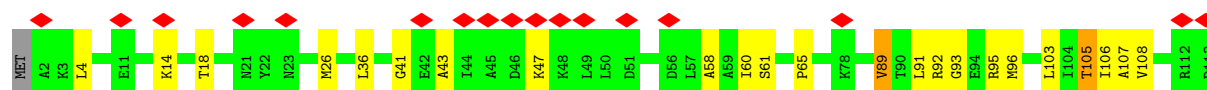
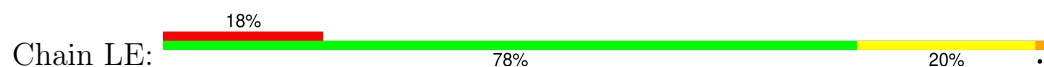


• Molecule 27: 50S ribosomal protein L4

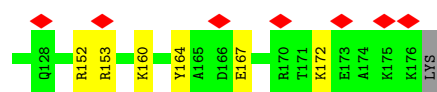
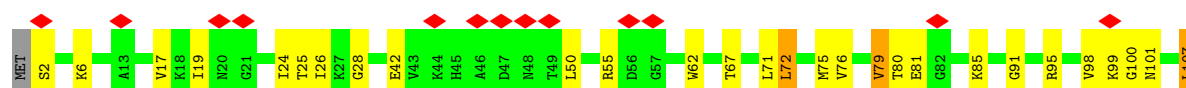
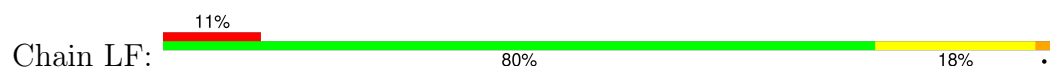




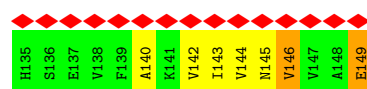
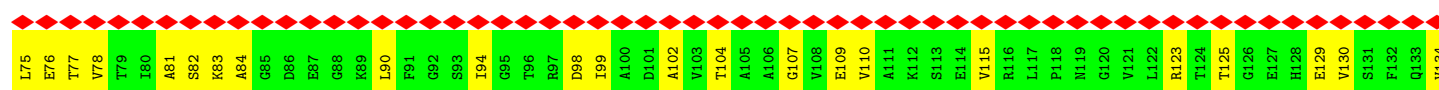
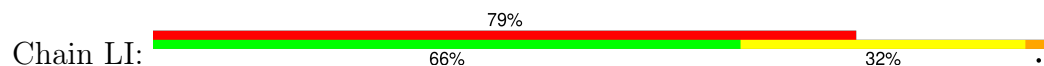
- Molecule 28: 50S ribosomal protein L5



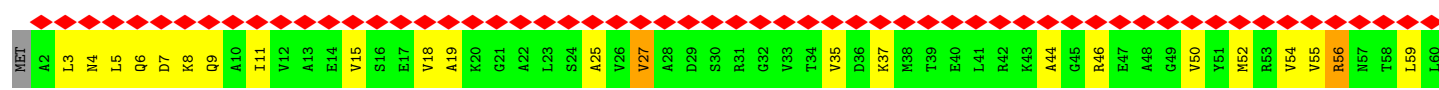
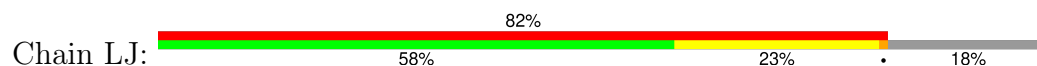
- Molecule 29: 50S ribosomal protein L6

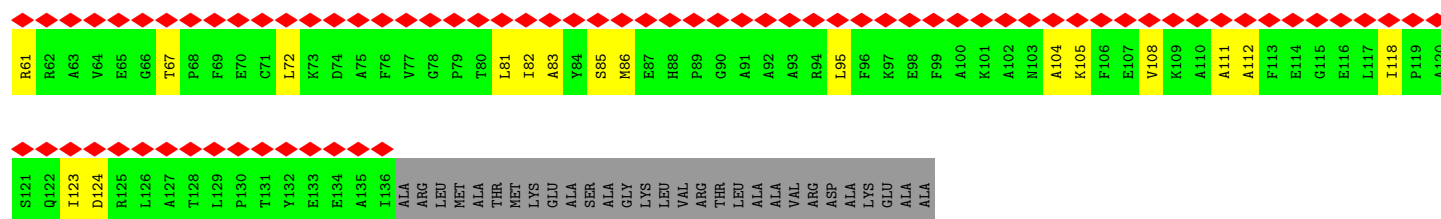


- Molecule 30: 50S ribosomal protein L9

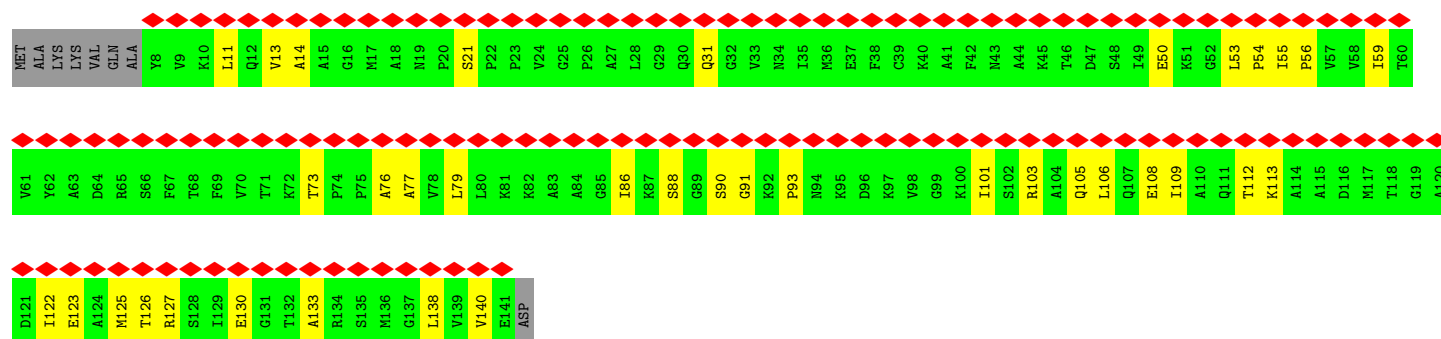


- Molecule 31: 50S ribosomal protein L10





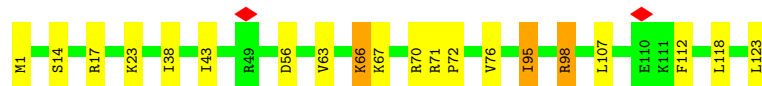
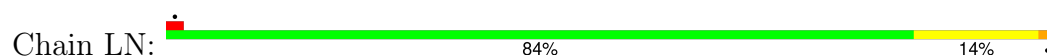
• Molecule 32: 50S ribosomal protein L11



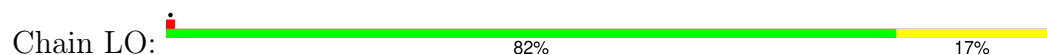
• Molecule 33: 50S ribosomal protein L13



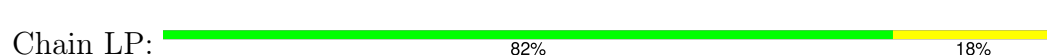
• Molecule 34: 50S ribosomal protein L14



• Molecule 35: 50S ribosomal protein L15

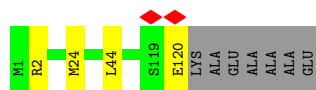


• Molecule 36: 50S ribosomal protein L16

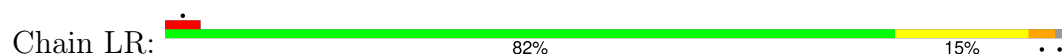




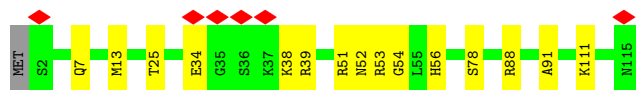
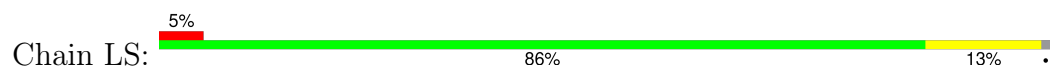
- Molecule 37: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L18



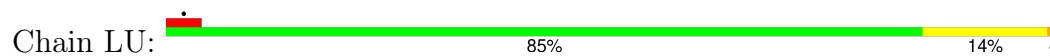
- Molecule 39: 50S ribosomal protein L19



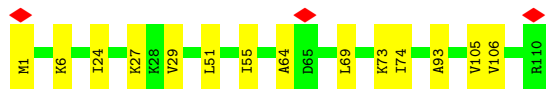
- Molecule 40: 50S ribosomal protein L20



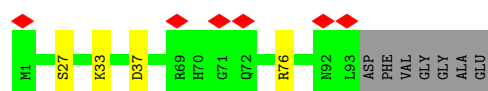
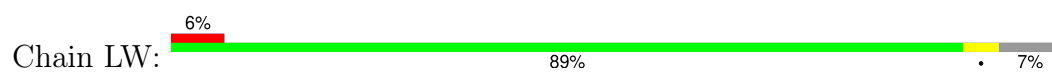
- Molecule 41: 50S ribosomal protein L21



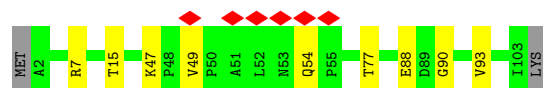
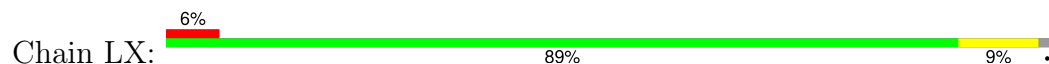
- Molecule 42: 50S ribosomal protein L22



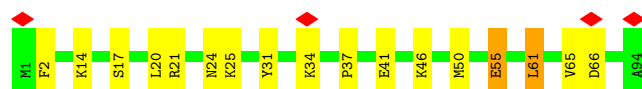
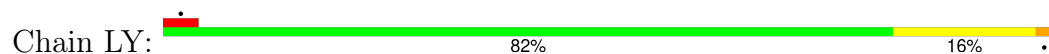
- Molecule 43: 50S ribosomal protein L23



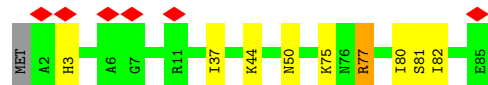
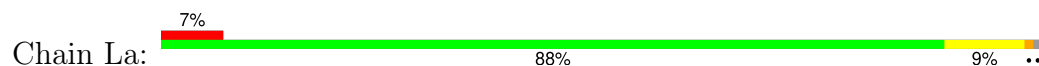
- Molecule 44: 50S ribosomal protein L24



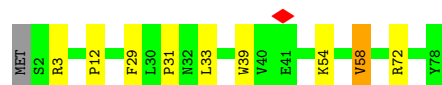
- Molecule 45: 50S ribosomal protein L25



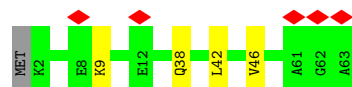
- Molecule 46: 50S ribosomal protein L27



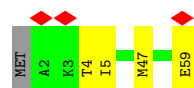
- Molecule 47: 50S ribosomal protein L28



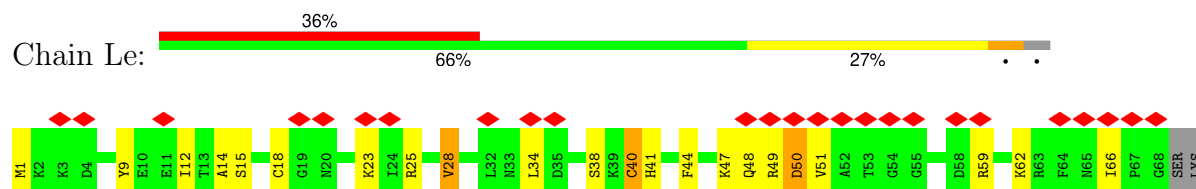
- Molecule 48: 50S ribosomal protein L29



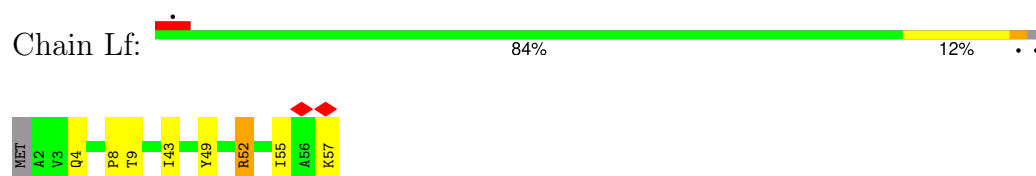
- Molecule 49: 50S ribosomal protein L30



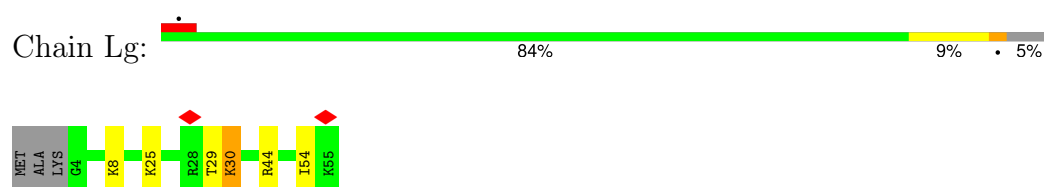
- Molecule 50: 50S ribosomal protein L31



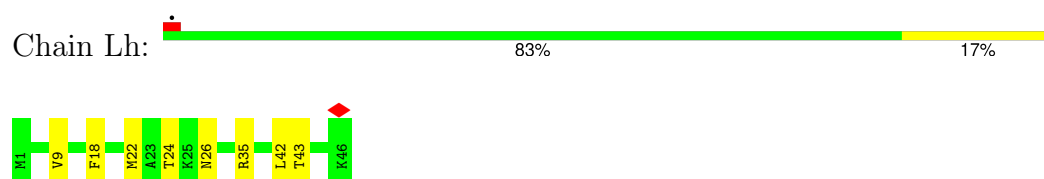
- Molecule 51: 50S ribosomal protein L32



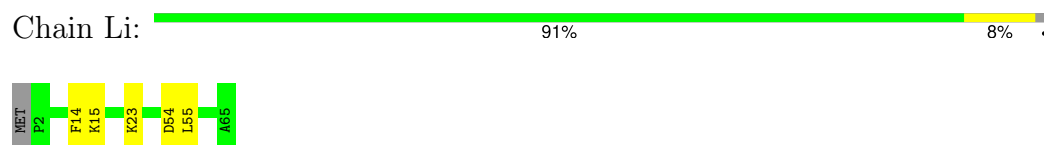
- Molecule 52: 50S ribosomal protein L33



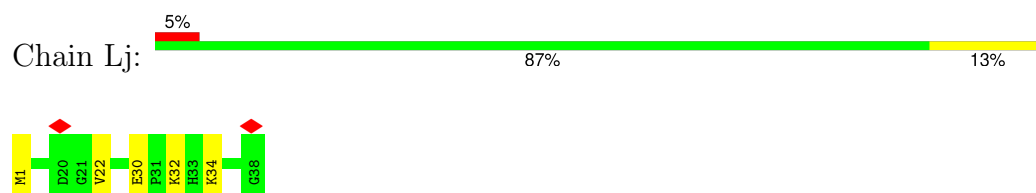
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35

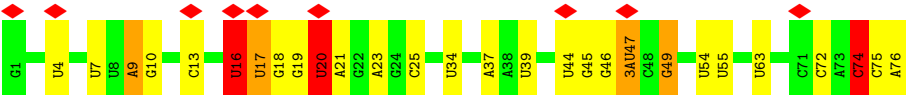


- Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA

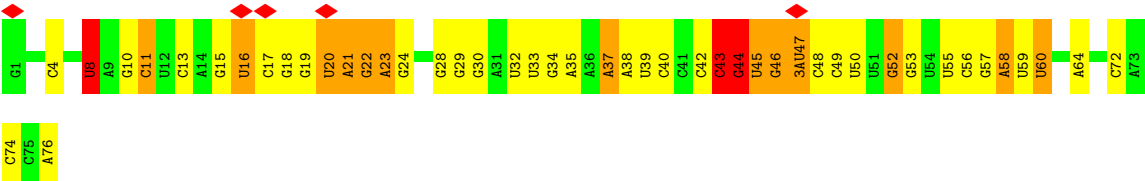




• Molecule 57: Chains: Pp



• Molecule 58: tRNA



4 Experimental information

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 ($e^-/\text{\AA}^2$)	87	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.235	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 ($\text{\AA}$)	610.55994, 610.55994, 610.55994	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, ZN, ATP, PUT, 4SU, G7M, OMU, U8U, OMC, 5MC, PSU, 4OC, MIA, MA6, 3AU, 2MA, T6A, 4D4, 3TD, D2T, MG, 2MG, H2U, SPD, 1MG, 5MU, OMG, UR3

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	0.23	0/36772	0.30	3/57358 (0.0%)
2	SB	0.43	0/1818	0.73	0/2450
3	SC	0.51	2/1696 (0.1%)	0.74	7/2284 (0.3%)
4	SD	0.33	0/1665	0.58	0/2227
5	SE	0.38	0/1179	0.55	0/1584
6	SF	0.30	0/881	0.52	0/1189
7	SG	0.72	2/1257 (0.2%)	0.93	3/1686 (0.2%)
8	SH	0.30	0/989	0.55	0/1326
9	SI	0.46	0/1034	0.84	4/1375 (0.3%)
10	SJ	0.53	0/805	0.86	1/1089 (0.1%)
11	SK	0.36	0/904	0.54	0/1219
12	SL	0.42	0/960	0.64	0/1286
13	SM	0.57	0/892	0.92	0/1193
14	SN	0.38	0/817	0.61	0/1088
15	SO	0.32	0/740	0.64	0/986
16	SP	0.36	0/659	0.53	0/884
17	SQ	0.32	0/657	0.56	0/881
18	SR	0.67	2/564 (0.4%)	0.91	1/756 (0.1%)
19	SS	0.47	0/680	0.78	1/915 (0.1%)
20	ST	0.21	0/676	0.40	0/895
21	SU	0.78	4/610 (0.7%)	0.95	4/808 (0.5%)
22	mR	0.41	0/716	0.83	3/1113 (0.3%)
23	23	0.25	0/69305	0.31	11/108114 (0.0%)
24	5	0.22	0/2873	0.26	0/4478
25	LB	0.31	0/2121	0.47	1/2852 (0.0%)
26	LC	0.38	0/1586	0.60	0/2134
27	LD	0.32	0/1571	0.49	2/2113 (0.1%)
28	LE	0.44	0/1444	0.78	3/1937 (0.2%)
29	LF	0.21	0/1333	0.44	0/1805
30	LI	0.62	0/1122	1.01	1/1515 (0.1%)
31	LJ	0.52	0/1037	0.78	0/1400

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LK	0.57	0/993	0.82	1/1341 (0.1%)
33	LM	0.35	0/1152	0.52	0/1551
34	LN	0.42	0/956	0.63	0/1279
35	LO	0.29	0/1062	0.50	0/1413
36	LP	0.21	0/1092	0.32	0/1457
37	LQ	0.34	0/973	0.46	0/1301
38	LR	0.38	0/902	0.67	0/1209
39	LS	0.34	0/929	0.53	0/1242
40	LT	0.33	0/960	0.45	0/1278
41	LU	0.40	0/829	0.65	0/1107
42	LV	0.33	0/864	0.47	1/1156 (0.1%)
43	LW	0.38	0/744	0.60	0/994
44	LX	0.39	0/787	0.65	2/1051 (0.2%)
45	LY	0.38	0/766	0.60	0/1025
46	La	0.37	0/642	0.59	1/848 (0.1%)
47	Lb	0.30	0/646	0.50	0/863
48	Lc	0.42	0/502	0.73	2/667 (0.3%)
49	Ld	0.29	0/453	0.51	0/605
50	Le	0.65	0/543	1.07	1/726 (0.1%)
51	Lf	0.31	0/450	0.56	0/599
52	Lg	0.66	0/434	0.97	1/576 (0.2%)
53	Lh	0.31	0/380	0.46	0/498
54	Li	0.38	0/513	0.60	0/676
55	Lj	0.20	0/303	0.31	0/397
56	Pt	0.32	1/1599 (0.1%)	0.45	1/2486 (0.0%)
57	Pp	0.43	0/28	0.78	0/34
58	Dt	0.75	2/1628 (0.1%)	0.99	19/2531 (0.8%)
All	All	0.32	13/160493 (0.0%)	0.44	74/239850 (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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	SG	78[A]	ARG	C-O	11.55	1.37	1.24
7	SG	78[B]	ARG	C-O	11.55	1.37	1.24
3	SC	132[A]	ARG	C-O	8.81	1.34	1.24
3	SC	132[B]	ARG	C-O	8.81	1.34	1.24
21	SU	37[A]	PHE	C-O	8.70	1.35	1.23

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SC	132[A]	ARG	CA-C-O	11.16	132.38	120.55
3	SC	132[B]	ARG	CA-C-O	11.16	132.38	120.55
1	16	252	U	C2'-C3'-O3'	9.76	128.34	113.70
21	SU	37[A]	PHE	CA-C-O	9.41	131.74	121.11
21	SU	37[B]	PHE	CA-C-O	9.41	131.74	121.11

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	SC	107	ARG	Sidechain
4	SD	104	ARG	Sidechain
5	SE	54	ARG	Sidechain
10	SJ	37	ARG	Sidechain
10	SJ	48	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	16	33092	0	16676	126	0
2	SB	1787	0	1812	27	0
3	SC	1666	0	1745	22	0
4	SD	1643	0	1707	9	0
5	SE	1166	0	1212	16	0
6	SF	862	0	864	14	0
7	SG	1236	0	1290	9	0
8	SH	979	0	1031	9	0
9	SI	1022	0	1070	17	0
10	SJ	795	0	836	21	0
11	SK	888	0	899	10	0
12	SL	957	0	1017	10	0
13	SM	883	0	941	14	0
14	SN	805	0	844	8	0
15	SO	730	0	759	8	0
16	SP	649	0	666	4	0
17	SQ	648	0	691	0	0
18	SR	555	0	578	7	0
19	SS	663	0	688	10	0
20	ST	670	0	719	17	0
21	SU	598	0	638	12	0
22	mR	640	0	323	13	0
23	23	62354	0	31384	212	0
24	5	2570	0	1301	6	0
25	LB	2082	0	2154	20	0
26	LC	1565	0	1616	13	0
27	LD	1552	0	1619	21	0
28	LE	1420	0	1457	25	0
29	LF	1313	0	1358	20	0
30	LI	1111	0	1148	26	0
31	LJ	1023	0	1050	21	0
32	LK	979	0	1028	21	0
33	LM	1129	0	1162	8	0
34	LN	947	0	1023	14	0
35	LO	1053	0	1129	21	0
36	LP	1086	0	1167	15	0
37	LQ	960	0	1000	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	LR	892	0	923	11	0
39	LS	917	0	962	9	0
40	LT	947	0	1019	3	0
41	LU	816	0	839	8	0
42	LV	857	0	922	8	0
43	LW	738	0	807	2	0
44	LX	779	0	831	3	0
45	LY	753	0	780	11	0
46	La	634	0	653	4	0
47	Lb	632	0	659	5	0
48	Lc	501	0	531	1	0
49	Ld	449	0	488	3	0
50	Le	533	0	530	14	0
51	Lf	444	0	458	6	0
52	Lg	427	0	464	4	0
53	Lh	377	0	418	5	0
54	Li	504	0	572	4	0
55	Lj	302	0	340	3	0
56	Pt	1635	0	840	13	0
57	Pp	28	0	33	0	0
58	Dt	1638	0	844	8	0
59	16	18	0	36	0	0
59	23	90	0	180	0	0
60	16	113	0	0	0	0
60	23	275	0	0	0	0
60	5	5	0	0	0	0
60	Dt	3	0	0	0	0
60	LB	1	0	0	0	0
60	LC	1	0	0	0	0
60	LD	1	0	0	0	0
60	LE	1	0	0	0	0
60	Ld	1	0	0	0	0
60	Lf	1	0	0	0	0
60	Pt	1	0	0	0	0
60	SD	1	0	0	0	0
60	mR	1	0	0	0	0
61	Le	1	0	0	0	0
61	Lj	1	0	0	0	0
61	SB	1	0	0	0	0
62	23	93	0	36	0	0
63	23	50	0	95	2	0
64	16	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	23	41	0	0	0	0
64	LB	3	0	0	0	0
64	LC	1	0	0	0	0
64	LT	1	0	0	0	0
64	LY	1	0	0	0	0
All	All	149590	0	100862	843	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 843 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:Pt:20:H2U:H4'	56:Pt:20:H2U:OP1	1.56	1.05
56:Pt:25:C:H5''	56:Pt:25:C:H6	1.32	0.95
34:LN:123:LEU:HD12	34:LN:123:LEU:OXT	1.74	0.87
35:LO:92:LEU:HD21	35:LO:106:GLU:HA	1.60	0.83
23:23:2377:A:O2'	38:LR:117:PHE:OXT	1.97	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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 ⓘ

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%)	187 (98%)	3 (2%)	55	67
3	SC	173/190 (91%)	166 (96%)	7 (4%)	28	36
4	SD	172/173 (99%)	170 (99%)	2 (1%)	63	75
5	SE	120/126 (95%)	115 (96%)	5 (4%)	26	34
6	SF	92/116 (79%)	87 (95%)	5 (5%)	20	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	SG	129/147 (88%)	113 (88%)	16 (12%)	4	3
8	SH	104/105 (99%)	103 (99%)	1 (1%)	68	79
9	SI	105/107 (98%)	96 (91%)	9 (9%)	10	10
10	SJ	87/90 (97%)	83 (95%)	4 (5%)	24	31
11	SK	91/99 (92%)	85 (93%)	6 (7%)	15	17
12	SL	102/103 (99%)	95 (93%)	7 (7%)	14	15
13	SM	92/96 (96%)	85 (92%)	7 (8%)	12	13
14	SN	83/84 (99%)	79 (95%)	4 (5%)	23	29
15	SO	78/77 (101%)	75 (96%)	3 (4%)	29	38
16	SP	65/65 (100%)	65 (100%)	0	100	100
17	SQ	74/78 (95%)	72 (97%)	2 (3%)	39	51
18	SR	58/65 (89%)	51 (88%)	7 (12%)	5	4
19	SS	72/79 (91%)	71 (99%)	1 (1%)	59	71
20	ST	65/66 (98%)	64 (98%)	1 (2%)	57	69
21	SU	61/61 (100%)	55 (90%)	6 (10%)	7	7
25	LB	216/218 (99%)	214 (99%)	2 (1%)	70	80
26	LC	164/164 (100%)	161 (98%)	3 (2%)	51	64
27	LD	165/165 (100%)	160 (97%)	5 (3%)	36	47
28	LE	149/150 (99%)	146 (98%)	3 (2%)	48	61
29	LF	136/138 (99%)	130 (96%)	6 (4%)	25	33
30	LI	114/114 (100%)	96 (84%)	18 (16%)	2	2
31	LJ	103/123 (84%)	90 (87%)	13 (13%)	4	3
32	LK	104/110 (94%)	100 (96%)	4 (4%)	29	38
33	LM	116/116 (100%)	114 (98%)	2 (2%)	53	66
34	LN	104/104 (100%)	101 (97%)	3 (3%)	37	48
35	LO	103/103 (100%)	100 (97%)	3 (3%)	37	48
36	LP	109/108 (101%)	107 (98%)	2 (2%)	51	64
37	LQ	100/103 (97%)	98 (98%)	2 (2%)	48	61
38	LR	86/87 (99%)	80 (93%)	6 (7%)	14	15
39	LS	99/100 (99%)	96 (97%)	3 (3%)	36	47
40	LT	89/90 (99%)	88 (99%)	1 (1%)	65	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	LU	84/84 (100%)	80 (95%)	4 (5%)	23	29
42	LV	93/93 (100%)	92 (99%)	1 (1%)	65	77
43	LW	80/84 (95%)	77 (96%)	3 (4%)	29	38
44	LX	83/85 (98%)	82 (99%)	1 (1%)	63	75
45	LY	78/78 (100%)	74 (95%)	4 (5%)	21	26
46	La	62/63 (98%)	61 (98%)	1 (2%)	55	67
47	Lb	68/68 (100%)	66 (97%)	2 (3%)	37	48
48	Lc	54/55 (98%)	54 (100%)	0	100	100
49	Ld	48/49 (98%)	48 (100%)	0	100	100
50	Le	60/62 (97%)	55 (92%)	5 (8%)	10	11
51	Lf	47/48 (98%)	46 (98%)	1 (2%)	47	60
52	Lg	47/49 (96%)	46 (98%)	1 (2%)	47	60
53	Lh	38/38 (100%)	37 (97%)	1 (3%)	40	53
54	Li	51/52 (98%)	51 (100%)	0	100	100
55	Lj	34/34 (100%)	33 (97%)	1 (3%)	37	48
57	Pp	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	4900/5064 (97%)	4702 (96%)	198 (4%)	29	36

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	LI	21	VAL
31	LJ	56	ARG
30	LI	72	ILE
30	LI	145	ASN
33	LM	2	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
27	LD	9	GLN
47	Lb	36	HIS
29	LF	45	HIS
46	La	57	HIS
40	LT	44	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1541/1542 (99%)	224 (14%)	13 (0%)
22	mR	23/60 (38%)	12 (52%)	0
23	23	2903/2904 (99%)	447 (15%)	27 (0%)
24	5	119/120 (99%)	14 (11%)	1 (0%)
56	Pt	75/76 (98%)	16 (21%)	0
58	Dt	75/76 (98%)	31 (41%)	0
All	All	4736/4778 (99%)	744 (15%)	41 (0%)

5 of 744 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

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	23	1379	U
23	23	2491	U
23	23	1416	G
23	23	2116	G
23	23	2581	G

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

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
23	PSU	23	2504	23	18,21,22	1.42	3 (16%)	21,30,33	2.08	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	H2U	23	2449	23	18,21,22	4.32	13 (72%)	19,30,33	1.72	4 (21%)
23	OMG	23	2251	58,23	23,26,27	0.52	0	32,38,41	0.47	0
23	PSU	23	2604	23	18,21,22	1.84	6 (33%)	21,30,33	2.32	9 (42%)
58	PSU	Dt	39	58	18,21,22	2.79	7 (38%)	21,30,33	3.07	10 (47%)
56	H2U	Pt	16	56	18,21,22	1.10	2 (11%)	19,30,33	1.22	1 (5%)
58	G7M	Dt	46	58	23,26,27	2.34	5 (21%)	34,39,42	3.37	11 (32%)
56	3AU	Pt	47	56	24,28,29	1.04	0	30,40,43	1.62	4 (13%)
56	PSU	Pt	55	56	18,21,22	1.39	2 (11%)	21,30,33	2.08	4 (19%)
23	OMC	23	2498	23,60	19,22,23	1.01	2 (10%)	25,31,34	1.13	1 (4%)
23	3TD	23	1915	23	19,22,23	1.21	2 (10%)	23,32,35	2.10	3 (13%)
56	H2U	Pt	17	56	18,21,22	1.06	2 (11%)	19,30,33	1.15	2 (10%)
23	6MZ	23	1618	23	22,25,26	1.43	5 (22%)	29,36,39	2.19	10 (34%)
23	6MZ	23	2030	23	22,25,26	1.43	5 (22%)	29,36,39	2.39	10 (34%)
36	4D4	LP	81	36	9,11,12	2.16	2 (22%)	7,13,15	2.04	3 (42%)
12	D2T	SL	89	12	8,9,10	1.65	2 (25%)	6,11,13	1.52	2 (33%)
56	5MU	Pt	54	56	19,22,23	1.36	5 (26%)	27,32,35	2.11	7 (25%)
23	OMU	23	2552	23	19,22,23	4.23	13 (68%)	25,31,34	2.29	6 (24%)
58	PSU	Dt	32	58	18,21,22	3.22	9 (50%)	21,30,33	3.06	6 (28%)
1	PSU	16	516	60,1	18,21,22	1.41	3 (16%)	21,30,33	2.14	5 (23%)
1	2MG	16	1207	60,1	23,26,27	1.26	4 (17%)	33,38,41	2.18	6 (18%)
23	2MG	23	2445	23	23,26,27	1.24	3 (13%)	33,38,41	2.24	10 (30%)
1	5MC	16	967	1	19,22,23	1.55	3 (15%)	26,32,35	1.12	2 (7%)
23	PSU	23	2605	23	18,21,22	1.38	3 (16%)	21,30,33	2.07	4 (19%)
23	PSU	23	746	23,60	18,21,22	1.41	3 (16%)	21,30,33	1.98	4 (19%)
58	H2U	Dt	16	58	18,21,22	1.43	3 (16%)	19,30,33	1.86	4 (21%)
56	T6A	Pt	37	56	31,34,35	1.47	6 (19%)	43,49,52	2.10	12 (27%)
58	3AU	Dt	47	58	24,28,29	0.98	0	30,40,43	1.49	5 (16%)
23	5MC	23	1962	23	19,22,23	1.51	3 (15%)	26,32,35	1.11	2 (7%)
1	MA6	16	1518	1	23,26,27	1.48	5 (21%)	33,38,41	2.12	10 (30%)
1	UR3	16	1498	1	19,22,23	0.93	0	26,32,35	1.76	3 (11%)
23	PSU	23	955	23	18,21,22	1.38	3 (16%)	21,30,33	2.13	4 (19%)
1	2MG	16	1516	1	23,26,27	1.25	4 (17%)	33,38,41	2.23	9 (27%)
58	4SU	Dt	8	58	18,21,22	1.85	4 (22%)	25,30,33	2.30	5 (20%)
58	MIA	Dt	37	58	28,31,32	2.34	6 (21%)	38,44,47	3.25	19 (50%)
1	4OC	16	1402	60,1	20,23,24	0.74	0	25,32,35	0.93	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	16	966	1	23,26,27	1.25	4 (17%)	33,38,41	2.17	7 (21%)
23	5MU	23	1939	23	19,22,23	1.39	5 (26%)	27,32,35	2.14	6 (22%)
23	PSU	23	2580	23	18,21,22	1.42	4 (22%)	21,30,33	2.08	5 (23%)
1	MA6	16	1519	1	23,26,27	1.47	5 (21%)	33,38,41	2.11	10 (30%)
23	1MG	23	745	23	23,26,27	1.18	3 (13%)	33,39,42	1.68	5 (15%)
56	H2U	Pt	20	56	18,21,22	4.44	12 (66%)	19,30,33	1.63	5 (26%)
56	PSU	Pt	39	56	18,21,22	1.37	3 (16%)	21,30,33	2.09	4 (19%)
23	PSU	23	2457	23	18,21,22	1.41	3 (16%)	21,30,33	2.16	4 (19%)
23	2MA	23	2503	23,60	22,25,26	1.44	5 (22%)	32,37,40	2.29	9 (28%)
1	5MC	16	1407	1	19,22,23	1.52	3 (15%)	26,32,35	1.10	3 (11%)
23	G7M	23	2069	23	23,26,27	2.25	6 (26%)	34,39,42	3.19	17 (50%)
58	PSU	Dt	55	58	18,21,22	2.23	6 (33%)	21,30,33	2.93	9 (42%)
23	5MU	23	747	23	19,22,23	1.41	6 (31%)	27,32,35	2.11	6 (22%)
56	U8U	Pt	34	56,22	20,24,25	1.51	3 (15%)	22,34,37	1.06	3 (13%)
23	2MG	23	1835	23	23,26,27	1.27	3 (13%)	33,38,41	2.19	6 (18%)
1	G7M	16	527	1	23,26,27	2.37	5 (21%)	34,39,42	2.99	10 (29%)

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
23	PSU	23	2504	23	-	2/7/25/26	0/2/2/2
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2
23	OMG	23	2251	58,23	-	3/9/27/28	0/3/3/3
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
58	PSU	Dt	39	58	-	0/7/25/26	0/2/2/2
56	H2U	Pt	16	56	-	7/7/38/39	0/2/2/2
58	G7M	Dt	46	58	-	2/7/25/26	0/3/3/3
56	3AU	Pt	47	56	-	7/16/34/35	0/2/2/2
56	PSU	Pt	55	56	-	0/7/25/26	0/2/2/2
23	OMC	23	2498	23,60	-	2/9/27/28	0/2/2/2
23	3TD	23	1915	23	-	2/7/25/26	0/2/2/2
56	H2U	Pt	17	56	-	3/7/38/39	0/2/2/2
23	6MZ	23	1618	23	-	2/9/27/28	0/3/3/3
23	6MZ	23	2030	23	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	4D4	LP	81	36	-	3/11/12/14	-
12	D2T	SL	89	12	-	3/7/12/14	-
56	5MU	Pt	54	56	-	0/7/25/26	0/2/2/2
23	OMU	23	2552	23	-	1/9/27/28	0/2/2/2
58	PSU	Dt	32	58	-	0/7/25/26	0/2/2/2
1	PSU	16	516	60,1	-	0/7/25/26	0/2/2/2
1	2MG	16	1207	60,1	-	0/9/27/28	0/3/3/3
23	2MG	23	2445	23	-	1/9/27/28	0/3/3/3
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
23	PSU	23	2605	23	-	0/7/25/26	0/2/2/2
23	PSU	23	746	23,60	-	2/7/25/26	0/2/2/2
58	H2U	Dt	16	58	-	0/7/38/39	0/2/2/2
56	T6A	Pt	37	56	-	10/23/41/42	0/3/3/3
58	3AU	Dt	47	58	-	6/16/34/35	0/2/2/2
23	5MC	23	1962	23	-	0/7/25/26	0/2/2/2
1	MA6	16	1518	1	-	0/11/29/30	0/3/3/3
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
1	2MG	16	1516	1	-	0/9/27/28	0/3/3/3
58	4SU	Dt	8	58	-	2/7/25/26	0/2/2/2
58	MIA	Dt	37	58	-	8/15/33/34	0/3/3/3
1	4OC	16	1402	60,1	-	0/9/29/30	0/2/2/2
1	2MG	16	966	1	-	0/9/27/28	0/3/3/3
23	5MU	23	1939	23	-	0/7/25/26	0/2/2/2
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
1	MA6	16	1519	1	-	2/11/29/30	0/3/3/3
23	1MG	23	745	23	-	0/7/25/26	0/3/3/3
56	H2U	Pt	20	56	-	2/7/38/39	0/2/2/2
56	PSU	Pt	39	56	-	0/7/25/26	0/2/2/2
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
23	2MA	23	2503	23,60	-	2/7/25/26	0/3/3/3
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
23	G7M	23	2069	23	-	1/7/25/26	0/3/3/3
58	PSU	Dt	55	58	-	0/7/25/26	0/2/2/2
23	5MU	23	747	23	-	0/7/25/26	0/2/2/2
56	U8U	Pt	34	56,22	-	0/10/28/29	0/2/2/2
23	2MG	23	1835	23	-	0/9/27/28	0/3/3/3
1	G7M	16	527	1	-	2/7/25/26	0/3/3/3

The worst 5 of 214 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

The worst 5 of 311 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Dt	46	G7M	CN7-N7-C8	-9.39	110.57	124.79
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
23	23	2069	G7M	CN7-N7-C8	-8.58	111.80	124.79
23	23	2503	2MA	C5-C4-N3	-8.07	118.68	127.18

There are no chirality outliers.

5 of 77 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'
12	SL	89	D2T	SB-CB-CG-OD2
23	23	1618	6MZ	O4'-C4'-C5'-O5'
23	23	2251	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	23	2449	H2U	1	0
23	23	2251	OMG	1	0
56	Pt	16	H2U	1	0
23	23	2030	6MZ	2	0
23	23	2552	OMU	2	0
1	16	967	5MC	1	0
58	Dt	8	4SU	1	0
1	16	966	2MG	1	0
56	Pt	20	H2U	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	3011	-	5,5,5	0.09	0	4,4,4	0.13	0
59	PUT	23	3007	-	5,5,5	0.08	0	4,4,4	0.14	0
59	PUT	23	3008	-	5,5,5	0.09	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	1602	-	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
63	SPD	23	3023	-	9,9,9	0.31	0	8,8,8	0.92	0
63	SPD	23	3019	-	9,9,9	0.32	0	8,8,8	0.95	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
59	PUT	23	3005	-	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	3018	-	5,5,5	0.10	0	4,4,4	0.12	0
63	SPD	23	3021	-	9,9,9	0.31	0	8,8,8	0.87	0
59	PUT	23	3013	-	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
59	PUT	23	3014	-	5,5,5	0.11	0	4,4,4	0.13	0
62	ATP	23	3001	-	32,33,33	0.27	0	48,52,52	0.29	0
59	PUT	16	1601	-	5,5,5	0.09	0	4,4,4	0.13	0
62	ATP	23	3003	-	32,33,33	0.25	0	48,52,52	0.27	0
59	PUT	23	3012	-	5,5,5	0.10	0	4,4,4	0.12	0
59	PUT	23	3017	-	5,5,5	0.11	0	4,4,4	0.12	0
62	ATP	23	3002	-	32,33,33	0.54	0	48,52,52	0.57	0
63	SPD	23	3022	-	9,9,9	0.32	0	8,8,8	0.90	0
59	PUT	23	3015	-	5,5,5	0.10	0	4,4,4	0.13	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	3011	-	-	0/3/3/3	-
59	PUT	23	3007	-	-	1/3/3/3	-
59	PUT	23	3008	-	-	1/3/3/3	-
59	PUT	23	3009	-	-	3/3/3/3	-
59	PUT	16	1602	-	-	1/3/3/3	-
63	SPD	23	3020	-	-	2/7/7/7	-
59	PUT	23	3010	-	-	1/3/3/3	-
63	SPD	23	3023	-	-	3/7/7/7	-
63	SPD	23	3019	-	-	0/7/7/7	-
59	PUT	23	3004	-	-	1/3/3/3	-
59	PUT	23	3016	-	-	0/3/3/3	-
59	PUT	23	3005	-	-	0/3/3/3	-
59	PUT	16	1603	-	-	1/3/3/3	-
59	PUT	23	3018	-	-	0/3/3/3	-
63	SPD	23	3021	-	-	5/7/7/7	-
59	PUT	23	3013	-	-	0/3/3/3	-
59	PUT	23	3006	-	-	1/3/3/3	-
59	PUT	23	3014	-	-	0/3/3/3	-
62	ATP	23	3001	-	-	10/22/38/38	0/3/3/3
59	PUT	16	1601	-	-	0/3/3/3	-
62	ATP	23	3003	-	-	6/22/38/38	0/3/3/3
59	PUT	23	3012	-	-	0/3/3/3	-
59	PUT	23	3017	-	-	1/3/3/3	-
62	ATP	23	3002	-	-	4/22/38/38	0/3/3/3
63	SPD	23	3022	-	-	1/7/7/7	-
59	PUT	23	3015	-	-	1/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

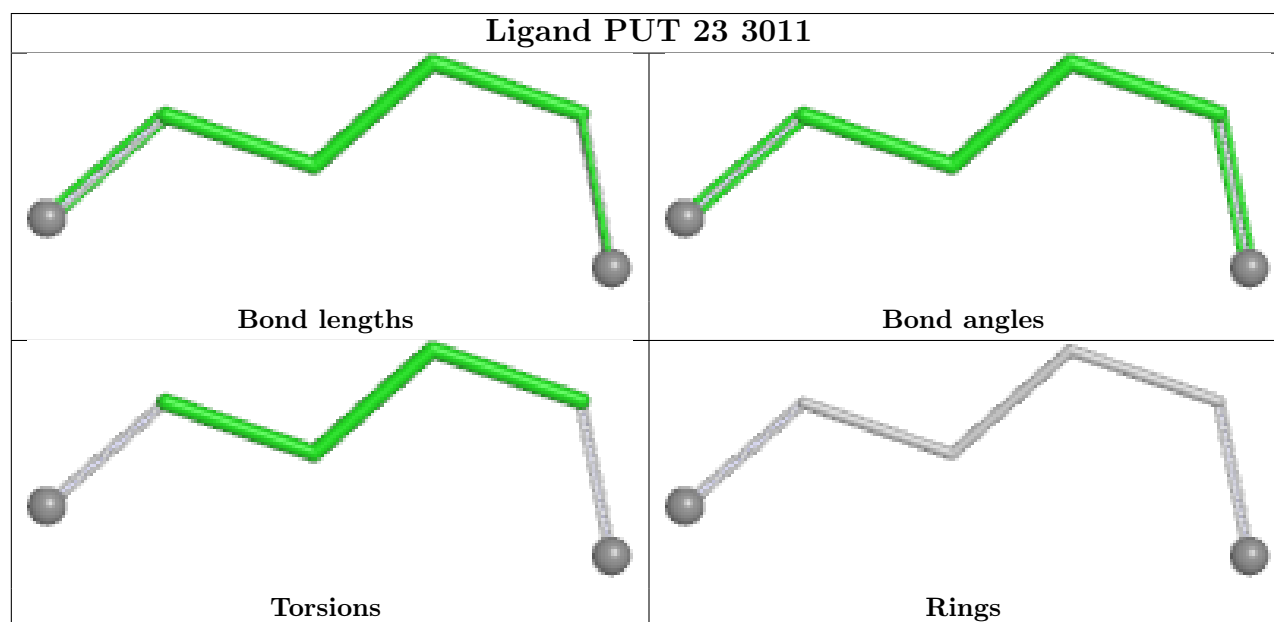
Mol	Chain	Res	Type	Atoms
62	23	3001	ATP	C5'-O5'-PA-O2A
62	23	3002	ATP	C5'-O5'-PA-O3A
62	23	3002	ATP	O4'-C4'-C5'-O5'
62	23	3003	ATP	C5'-O5'-PA-O1A
62	23	3003	ATP	C5'-O5'-PA-O2A

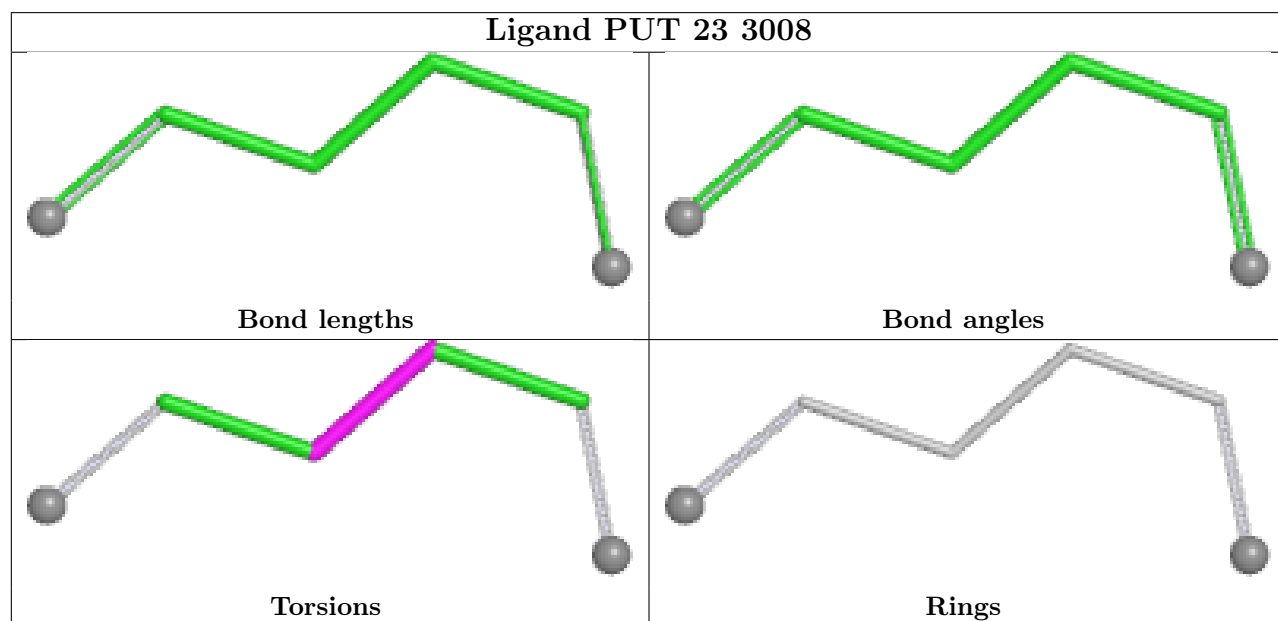
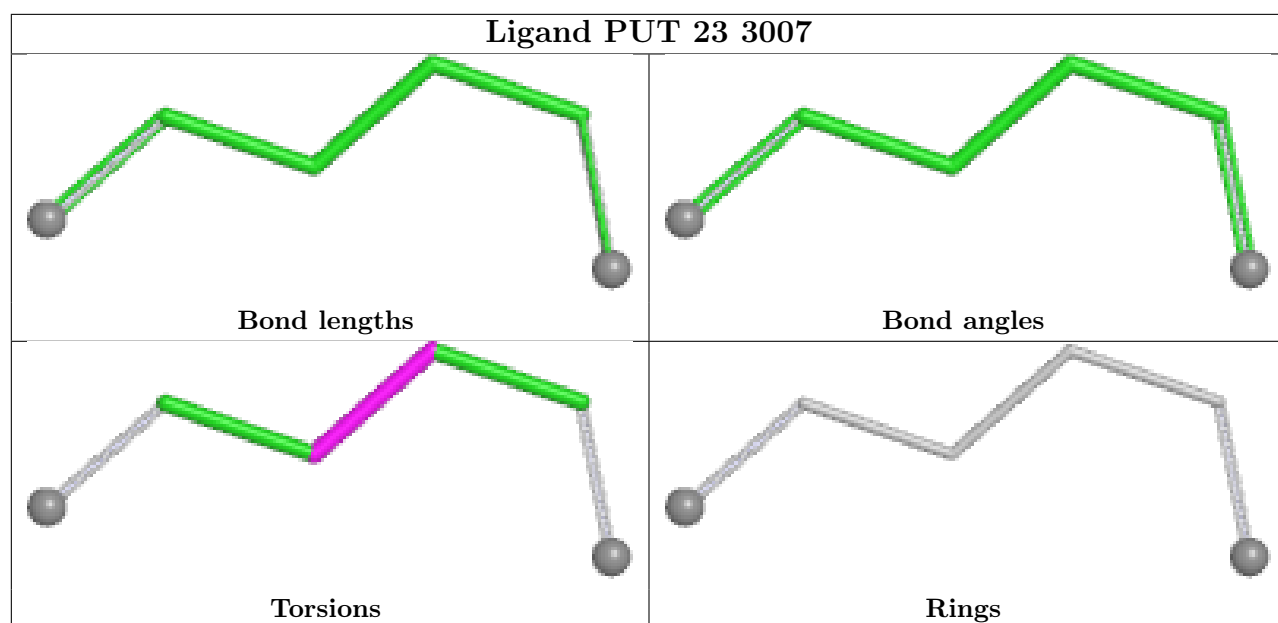
There are no ring outliers.

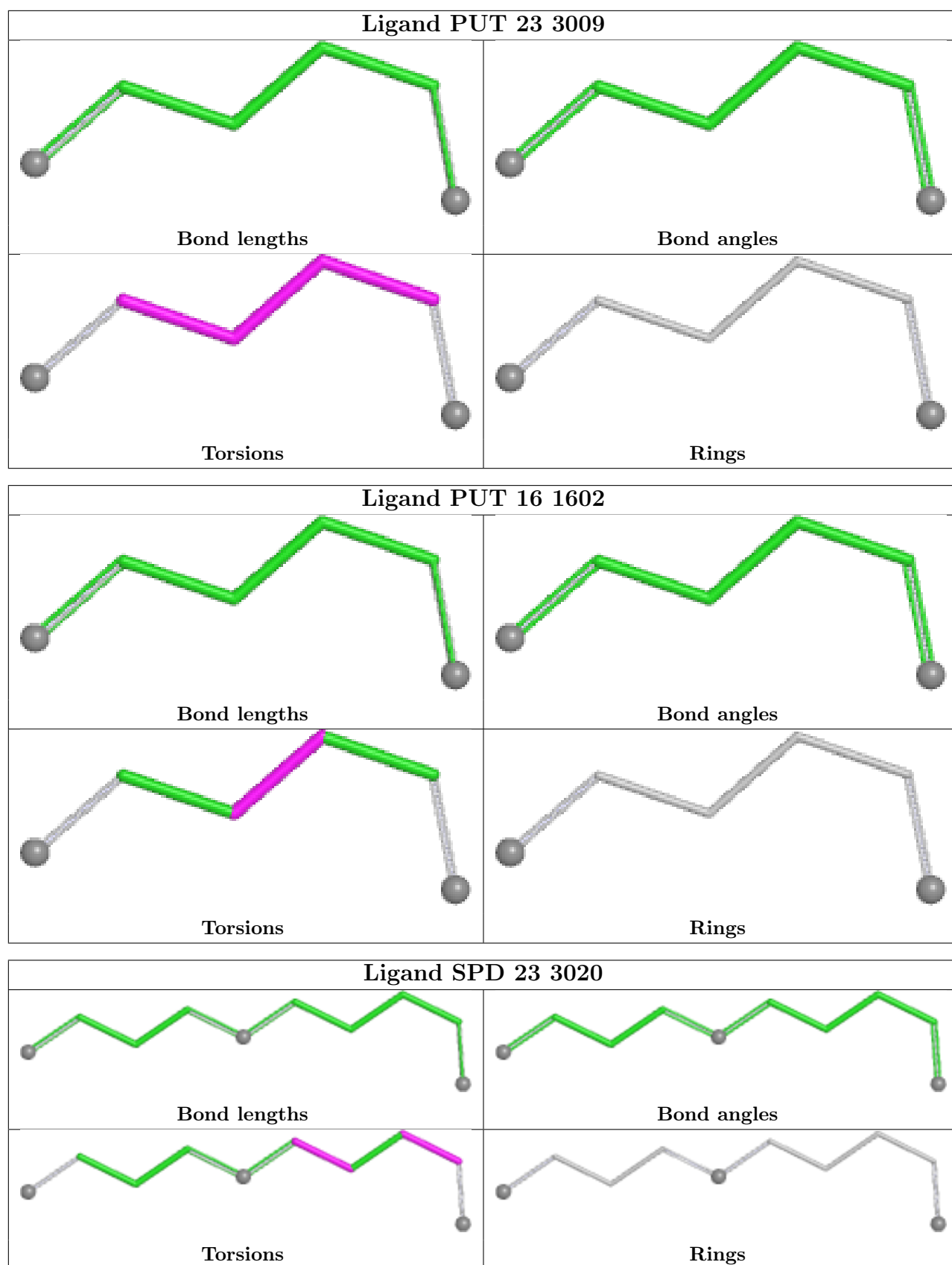
2 monomers are involved in 2 short contacts:

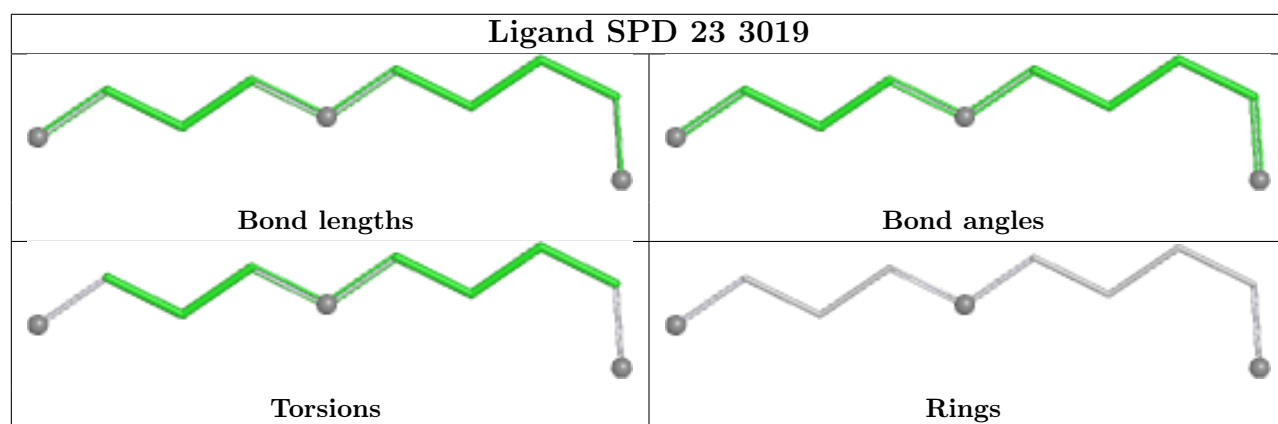
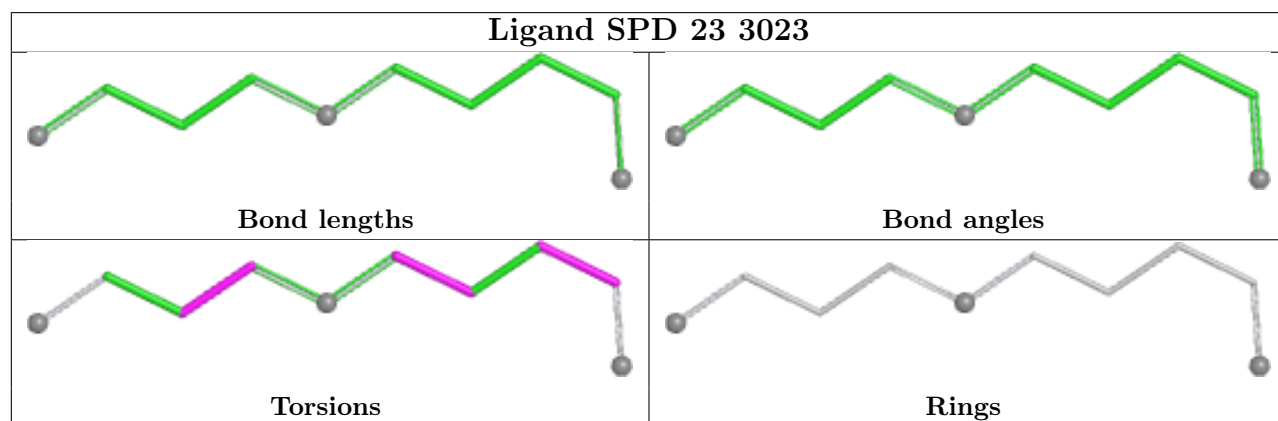
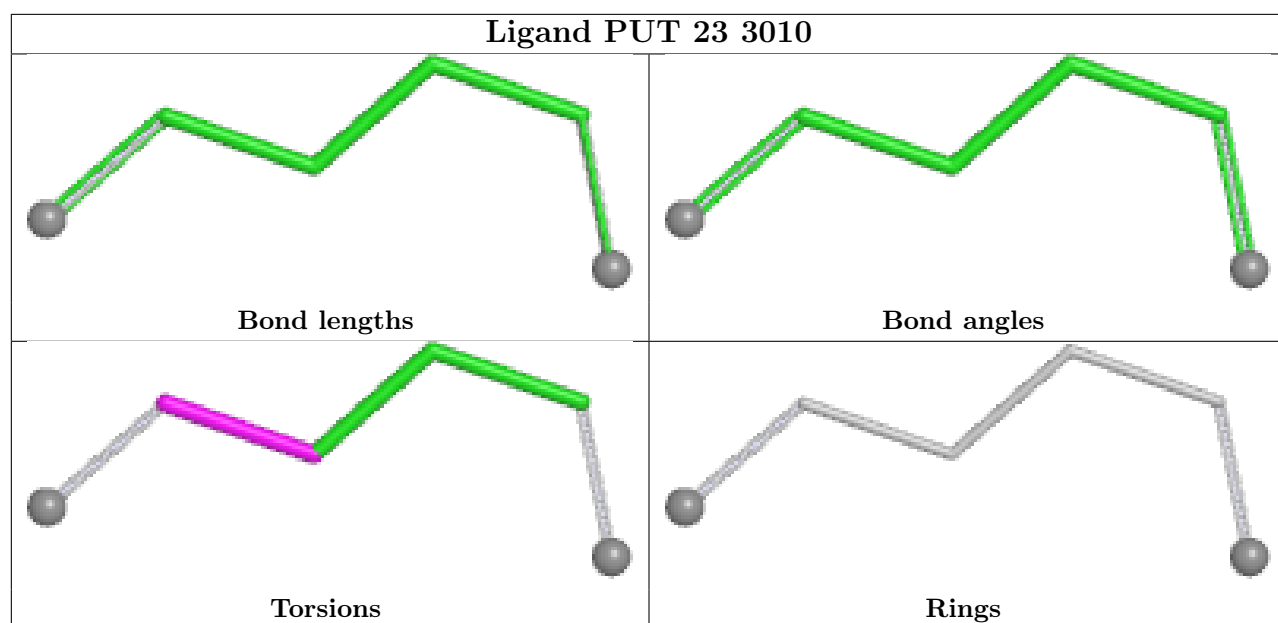
Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	23	3020	SPD	1	0
63	23	3019	SPD	1	0

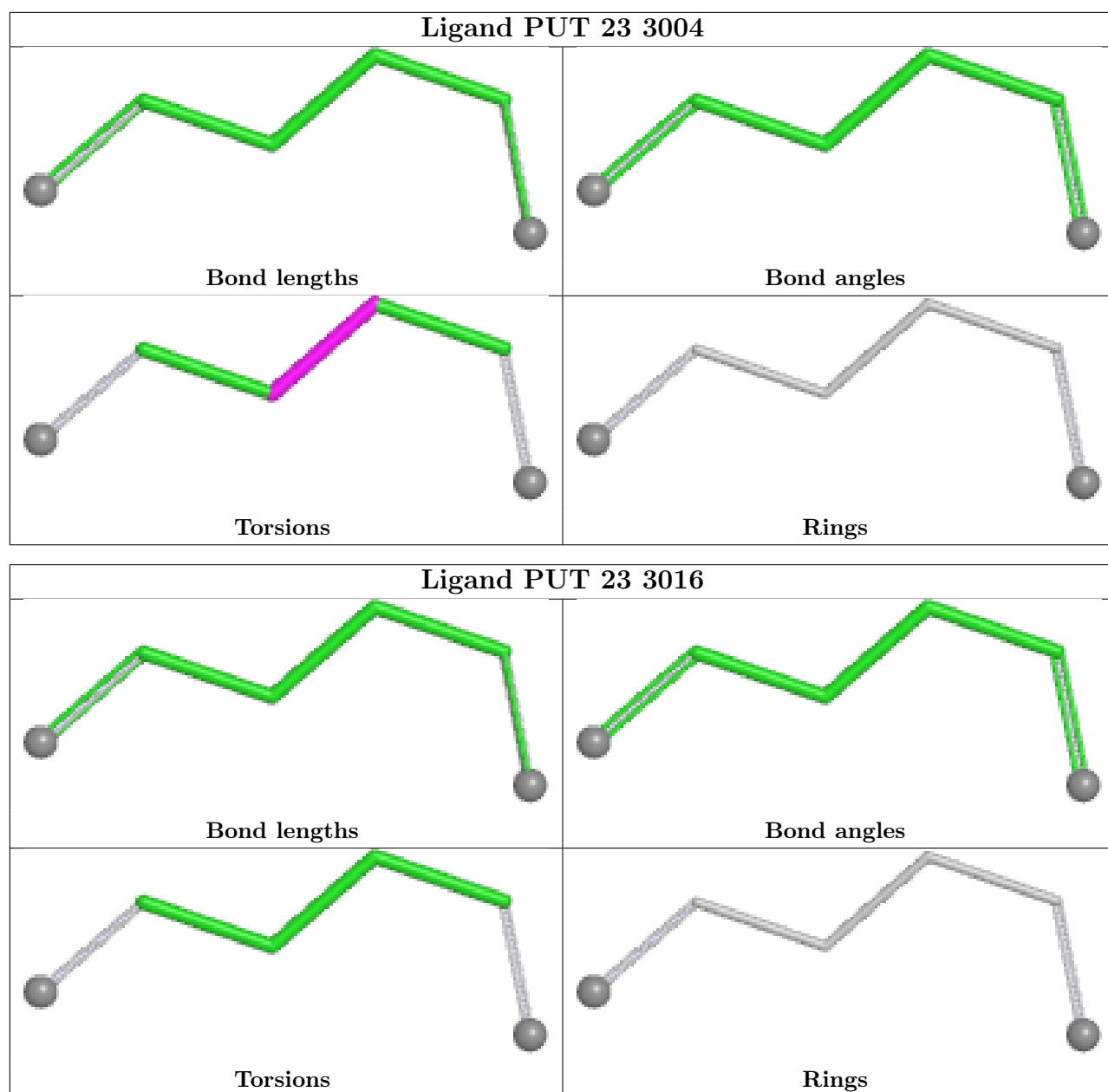
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

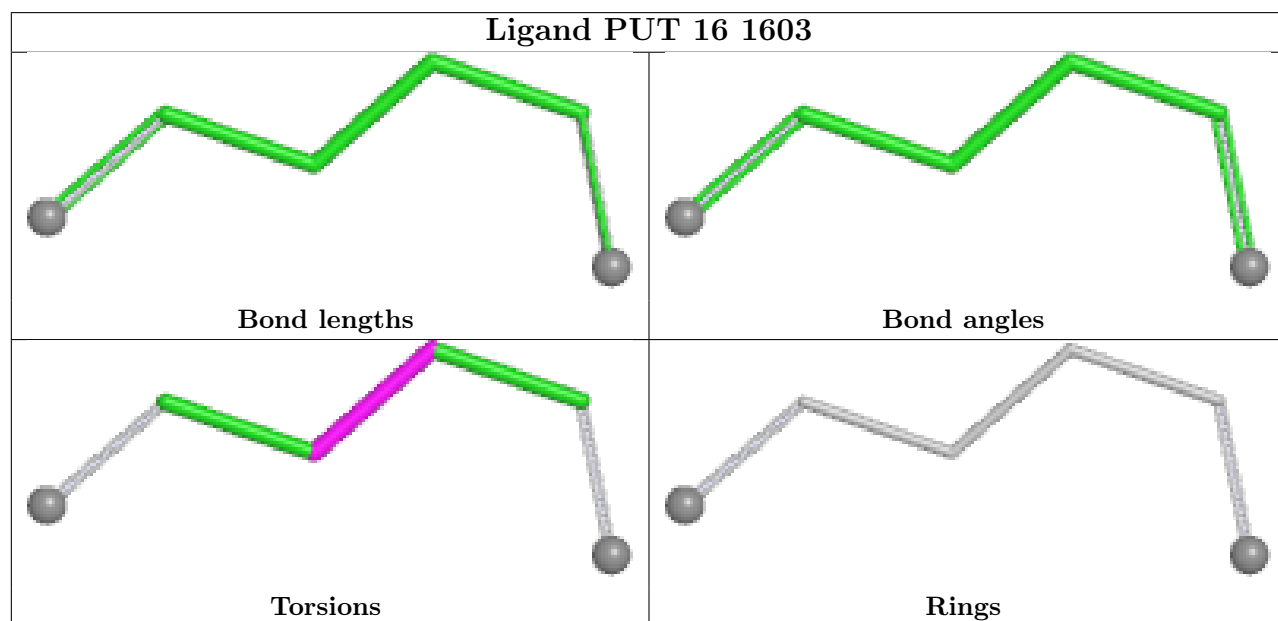
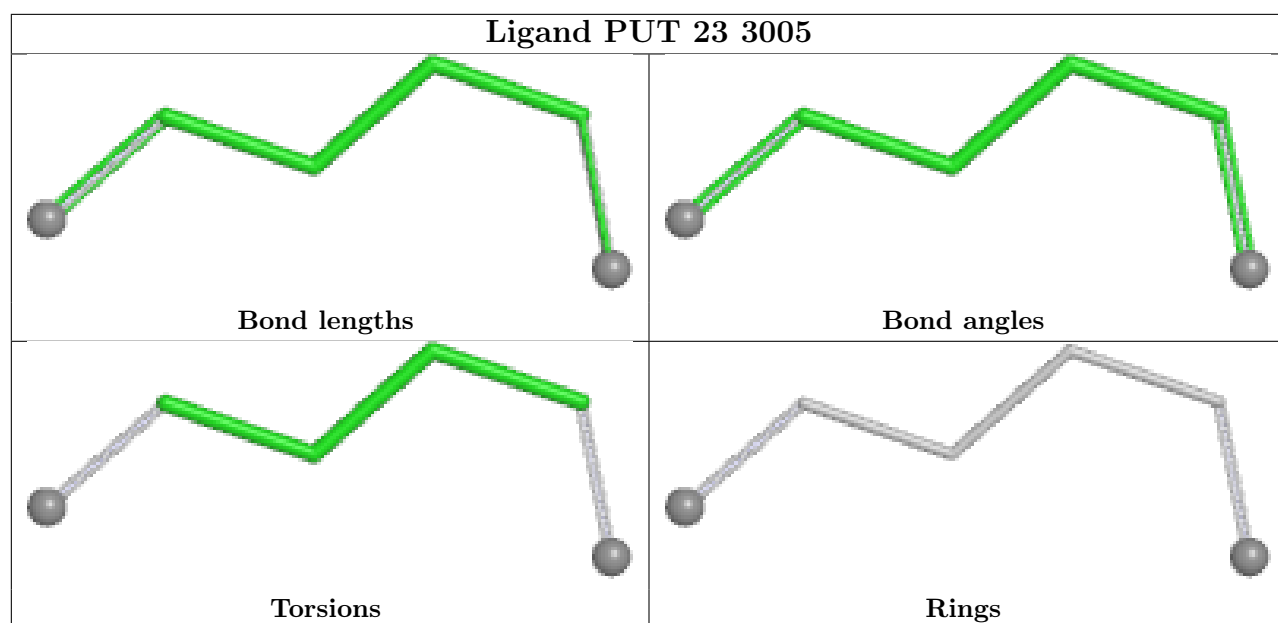


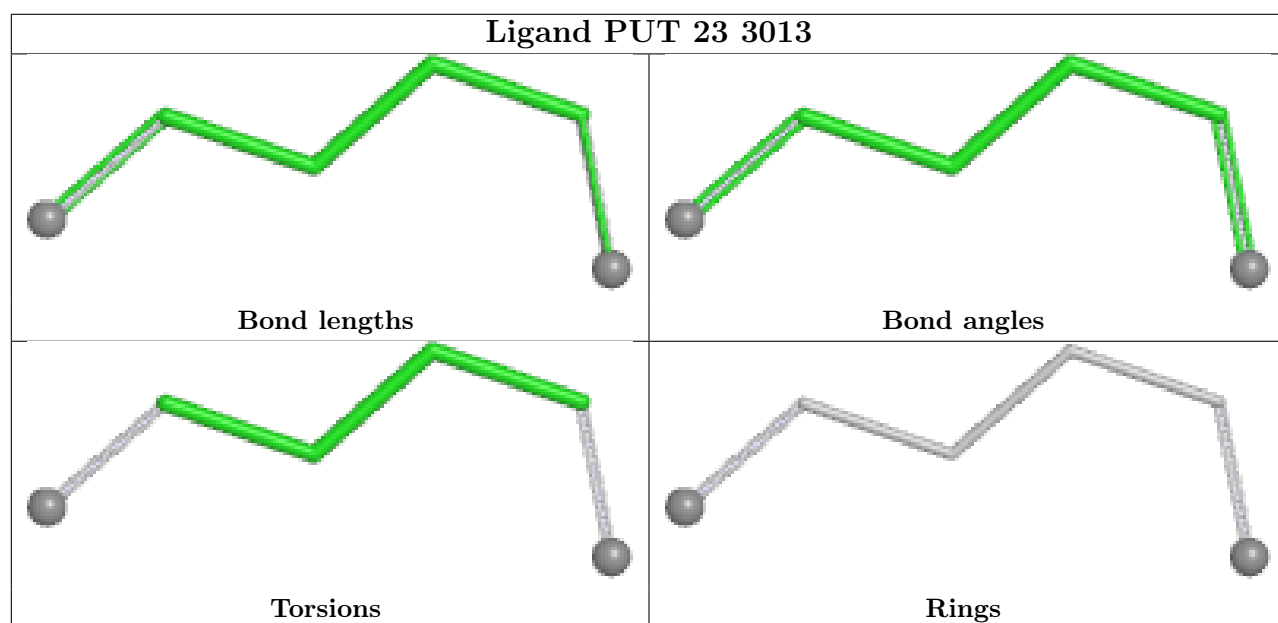
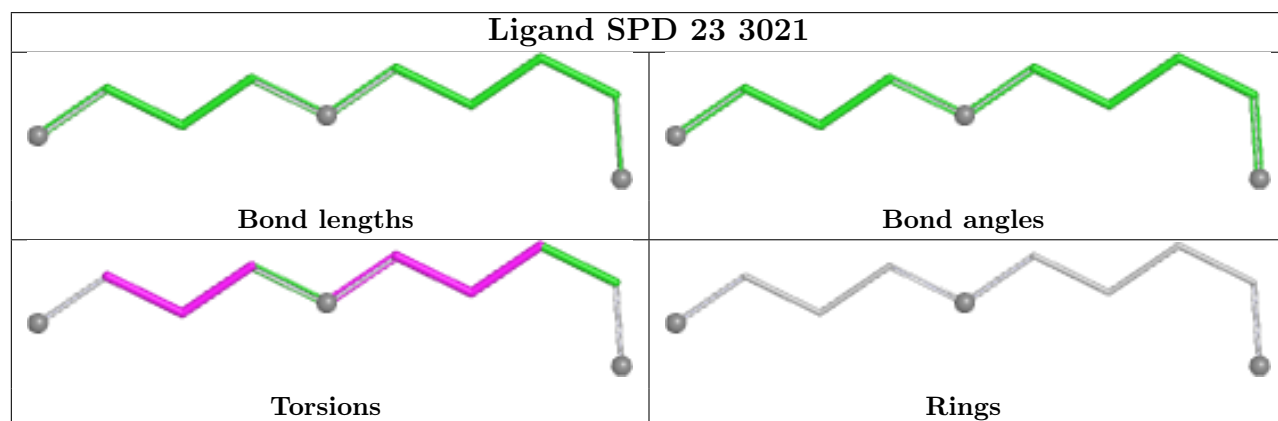
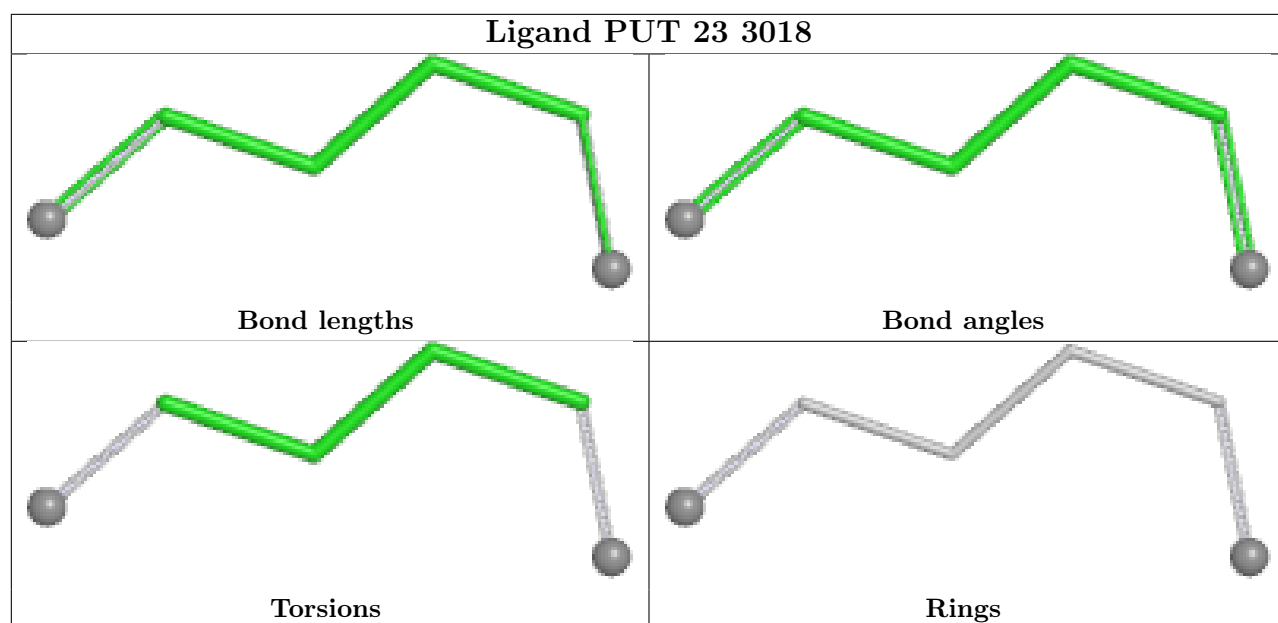


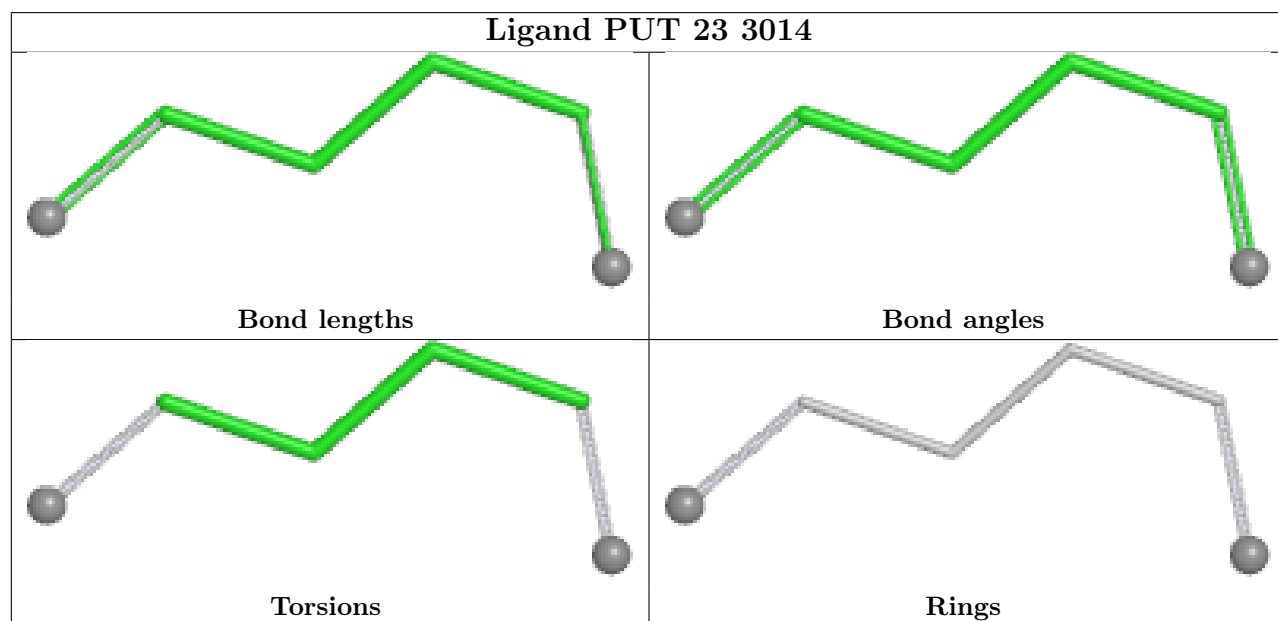
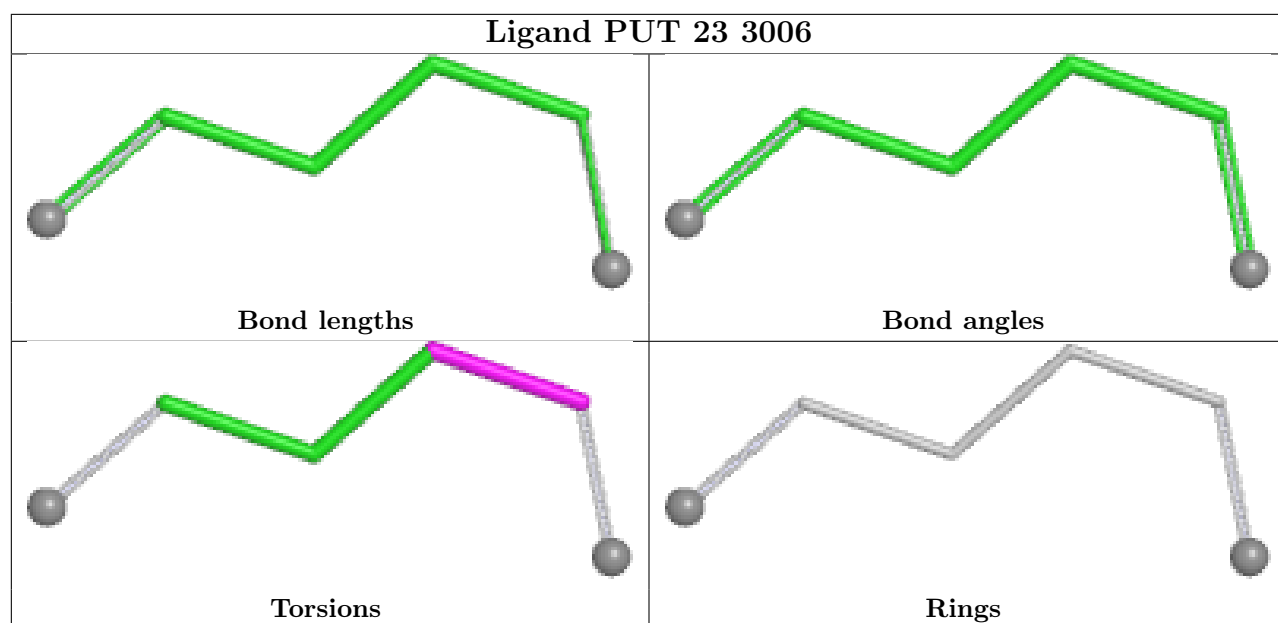




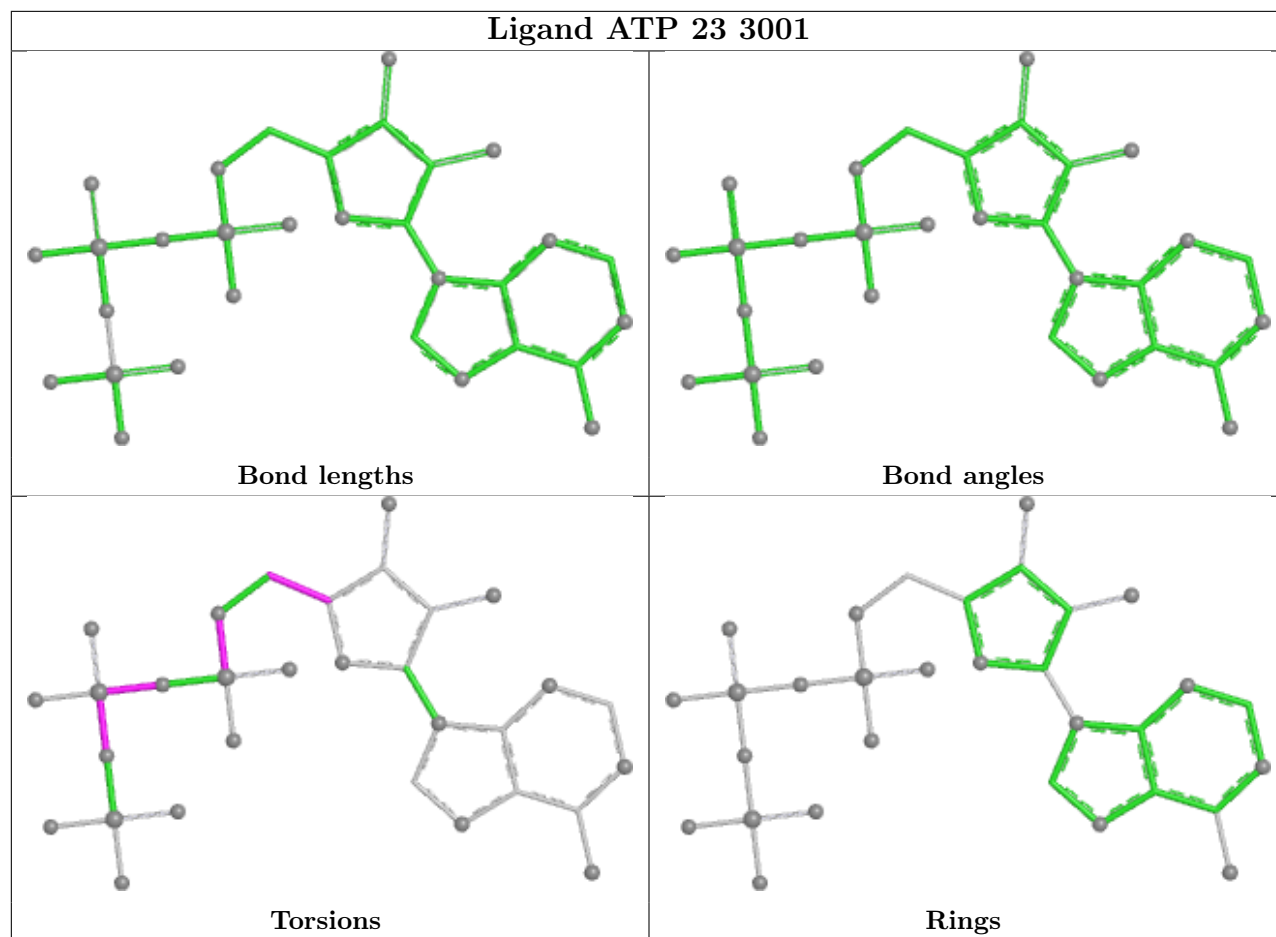




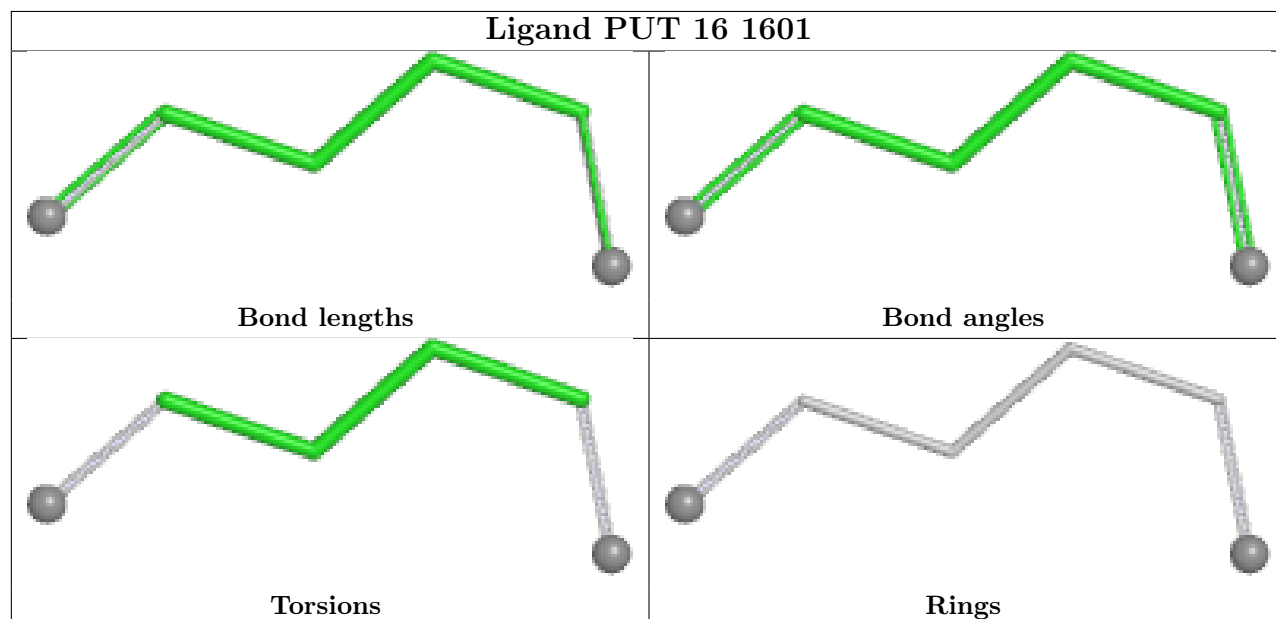




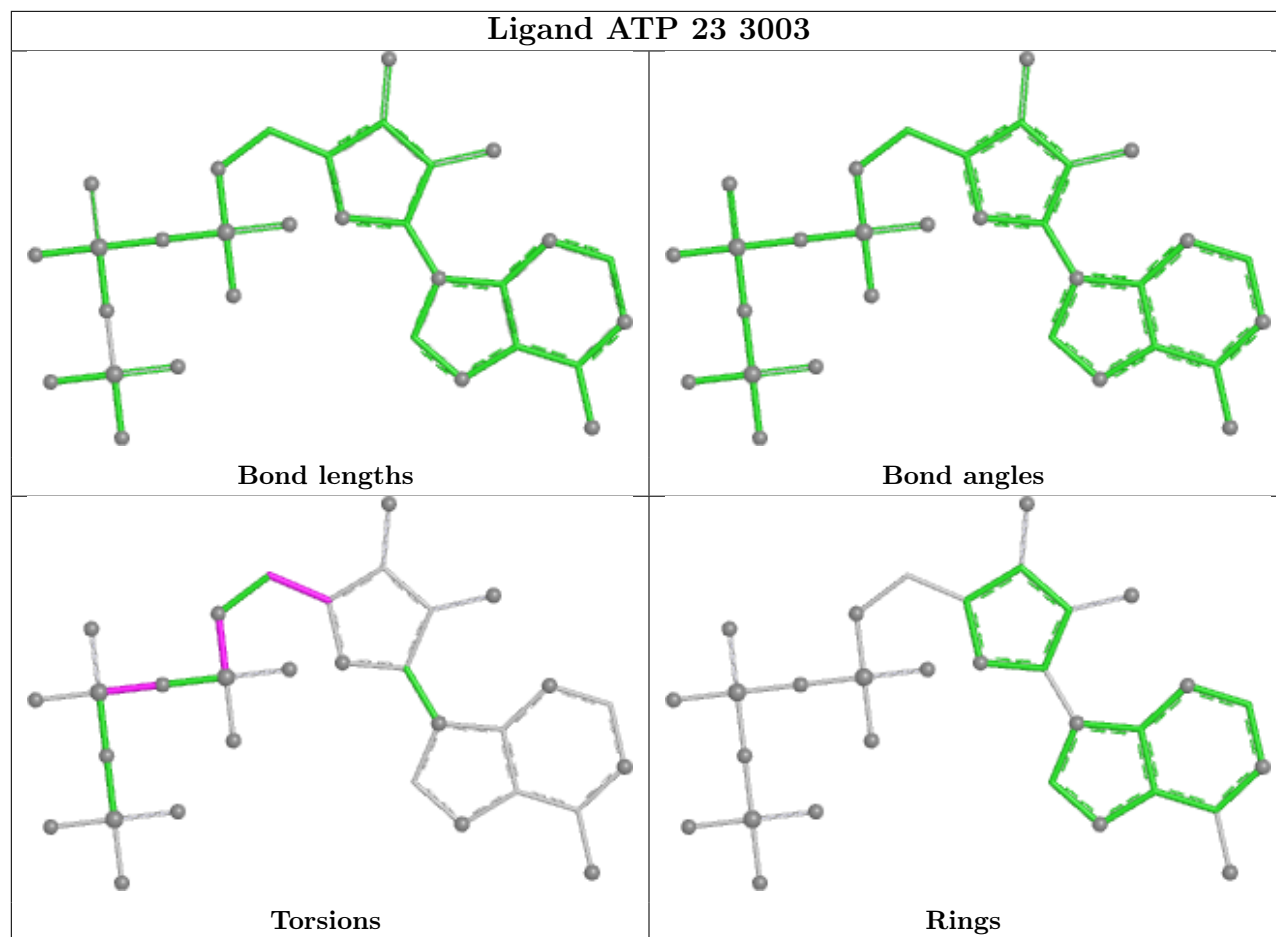
Ligand ATP 23 3001



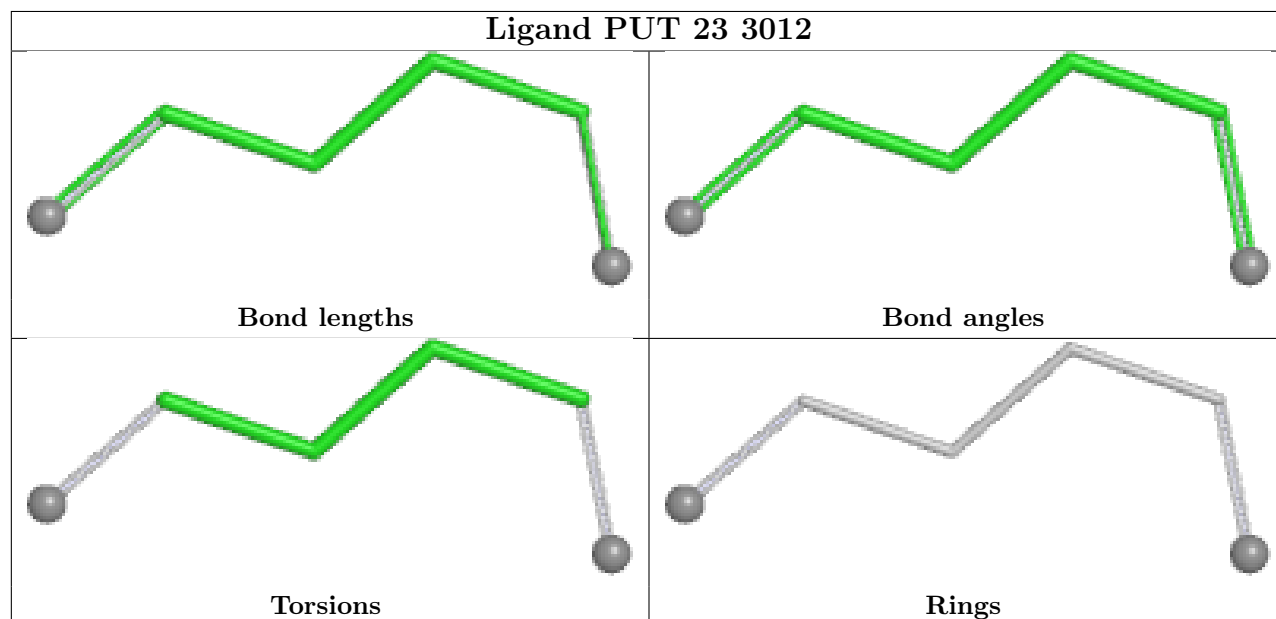
Ligand PUT 16 1601

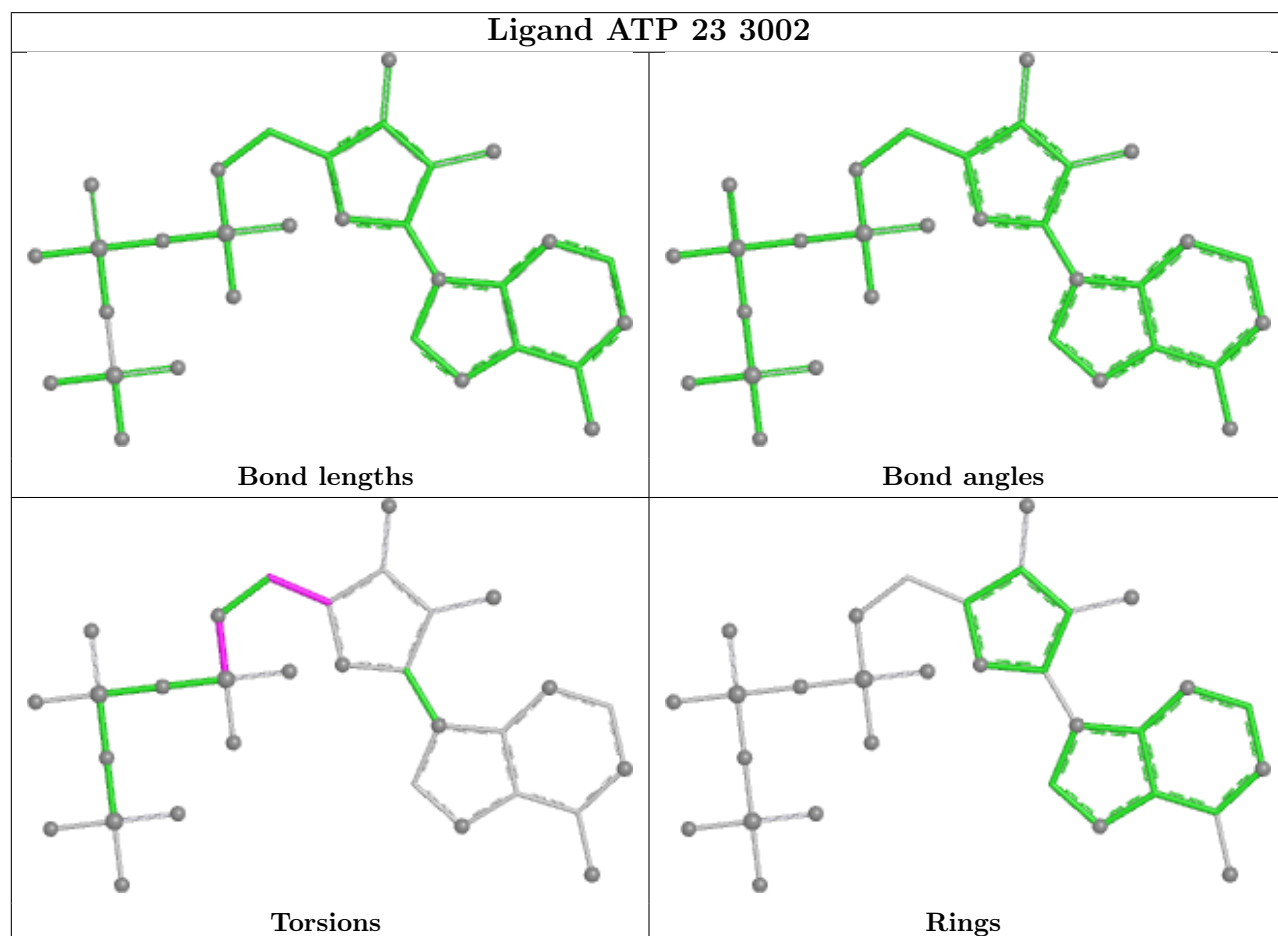
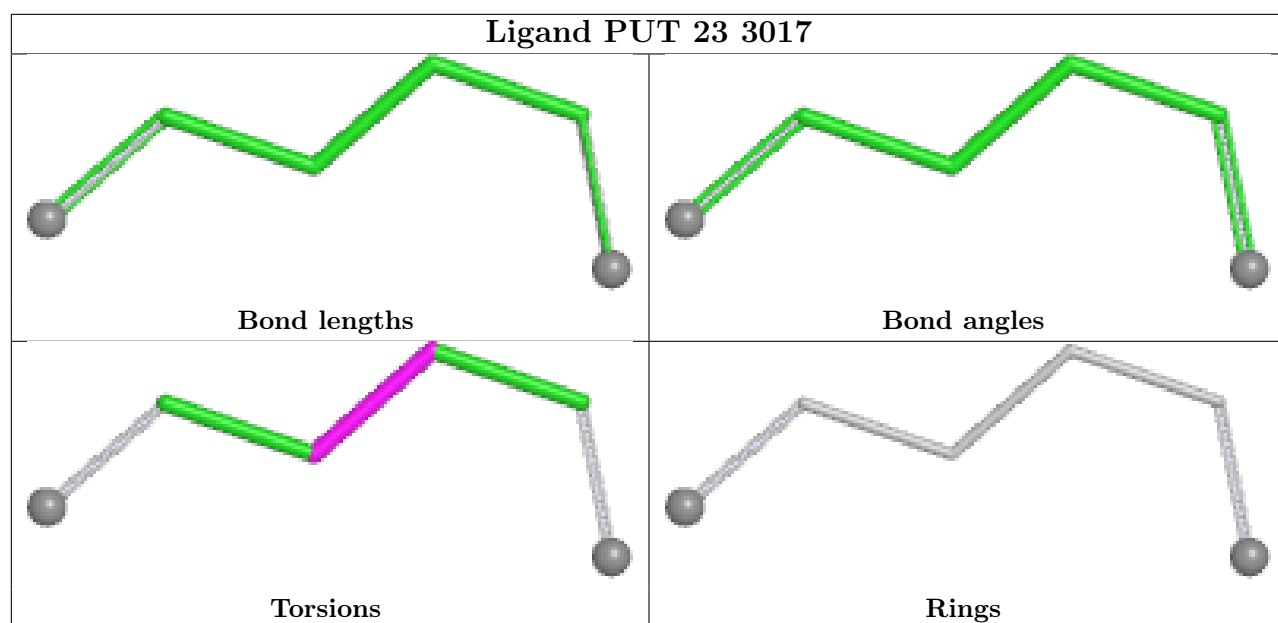


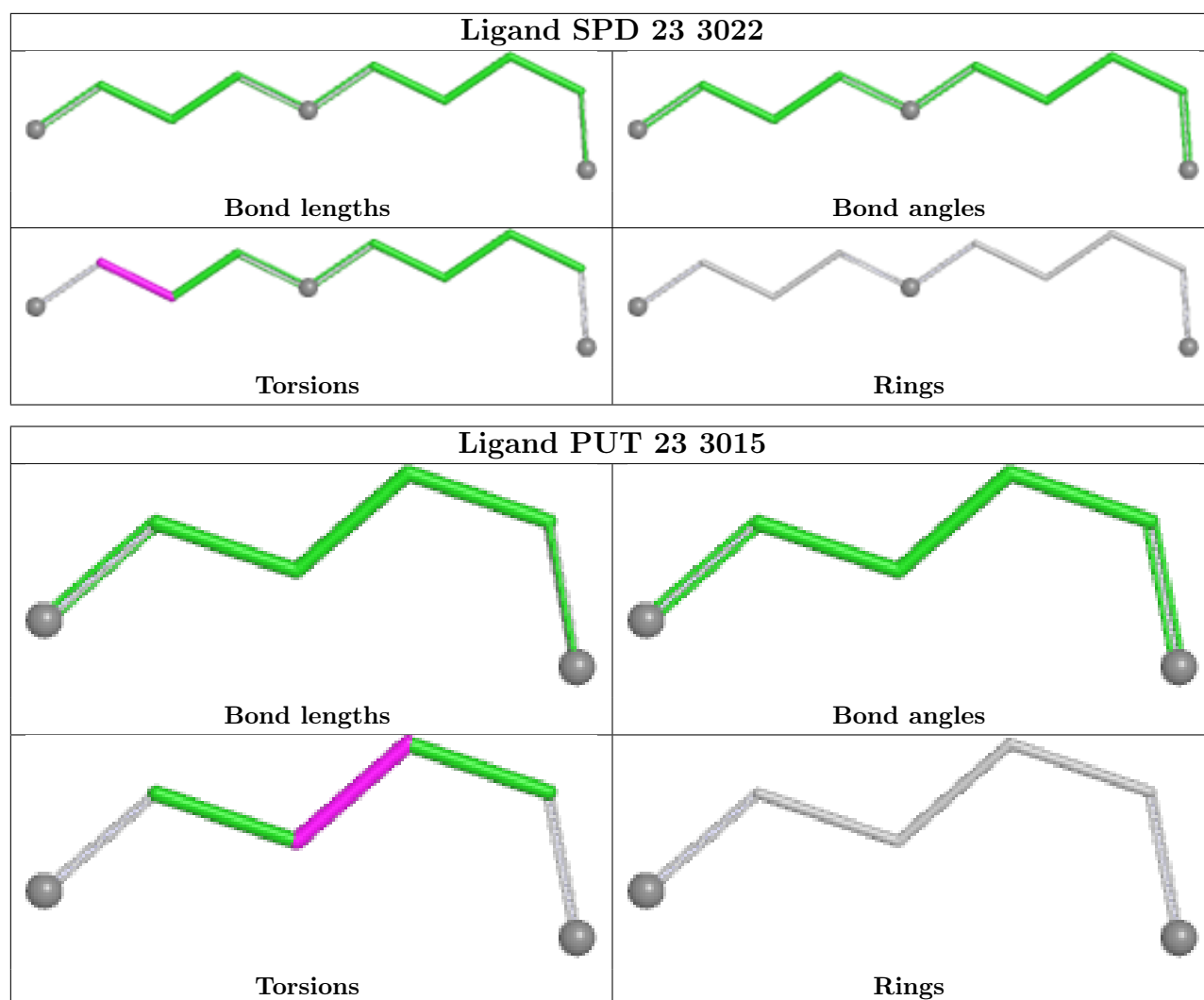
Ligand ATP 23 3003



Ligand PUT 23 3012







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.

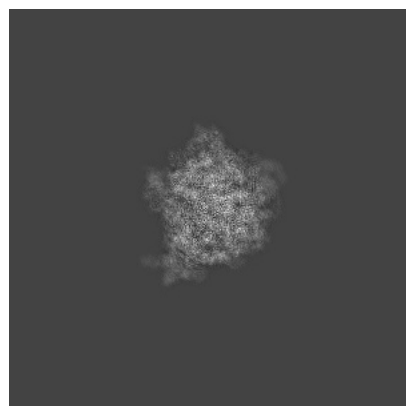
6 Map visualisation [i](#)

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.

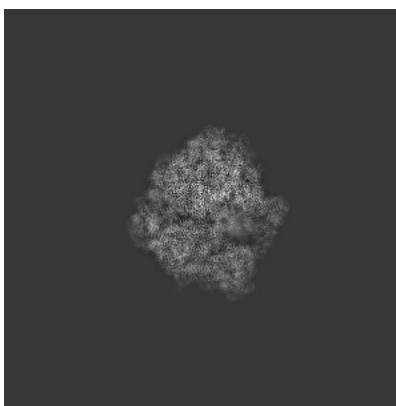
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

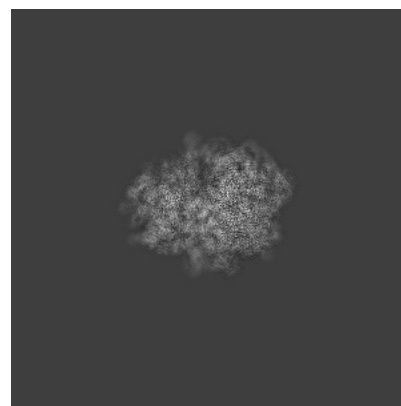
6.1.1 Primary map



X

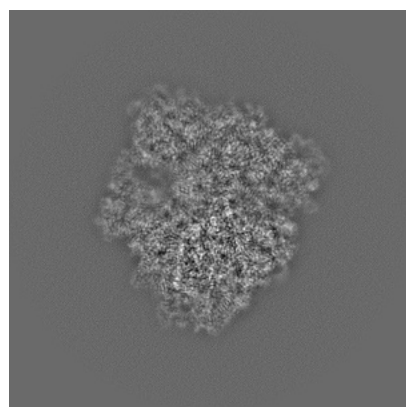


Y

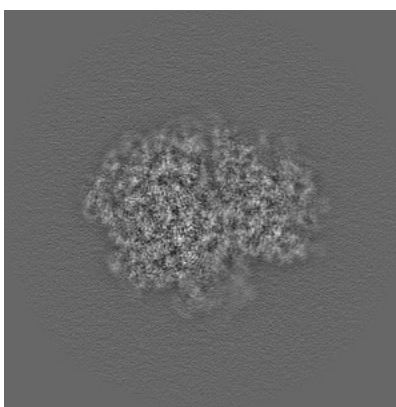


Z

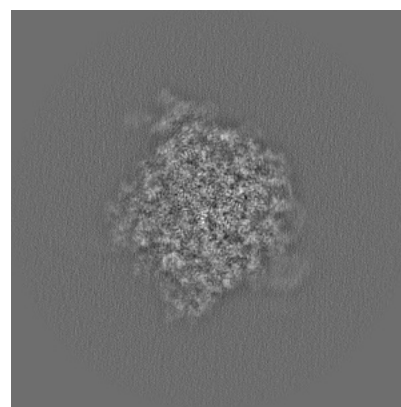
6.1.2 Raw map



X



Y



Z

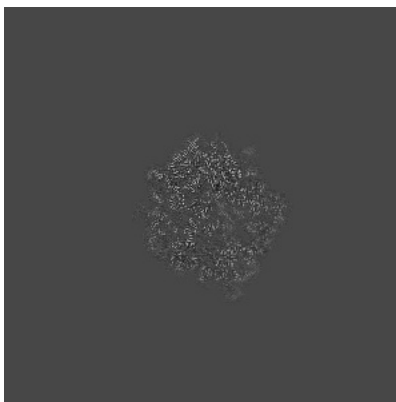
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

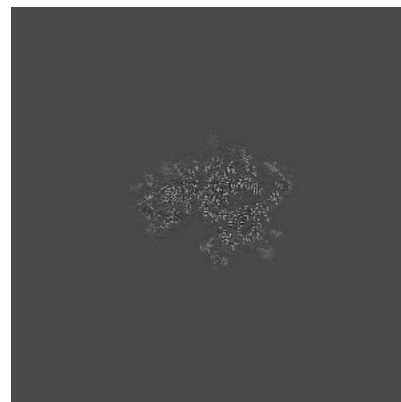
6.2.1 Primary map



X Index: 288

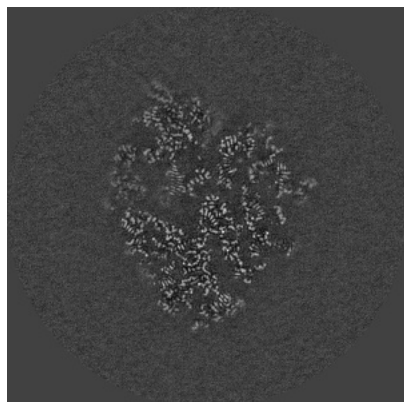


Y Index: 288

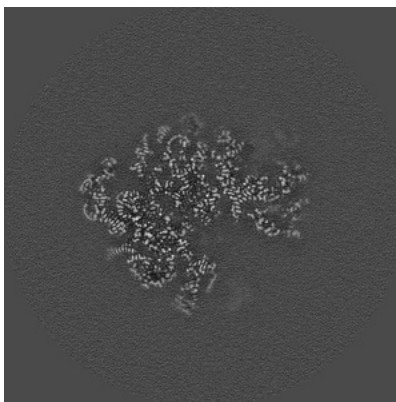


Z Index: 288

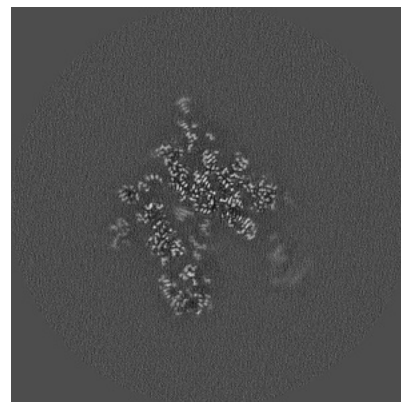
6.2.2 Raw map



X Index: 256



Y Index: 256

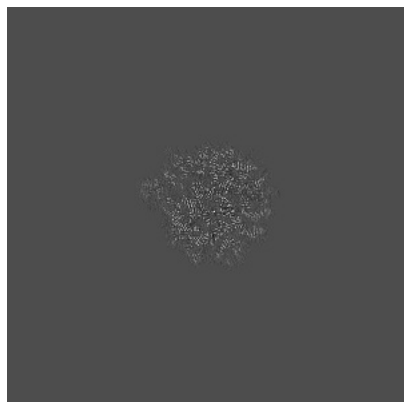


Z Index: 256

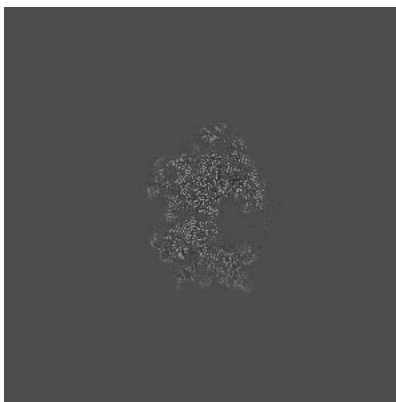
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

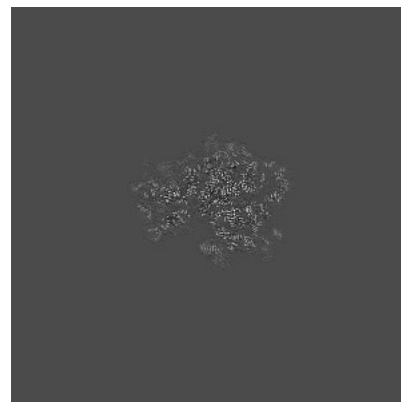
6.3.1 Primary map



X Index: 316

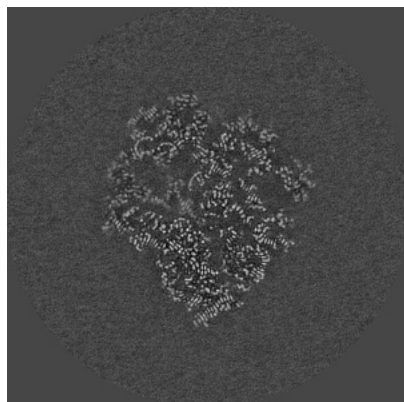


Y Index: 315

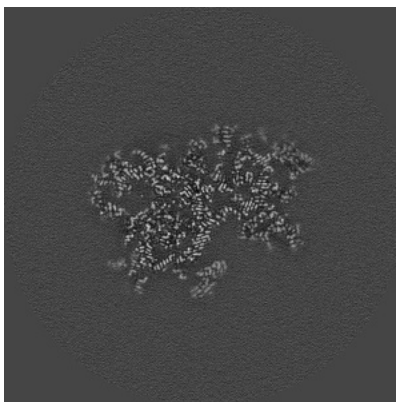


Z Index: 283

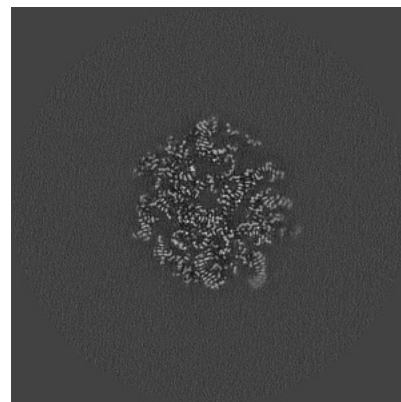
6.3.2 Raw map



X Index: 247



Y Index: 280

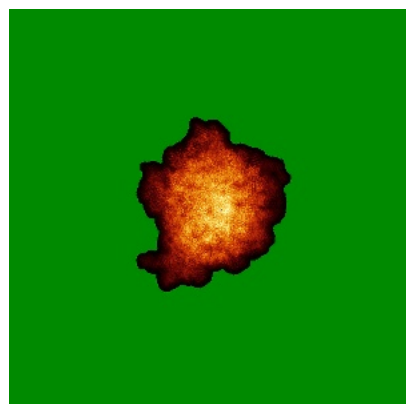


Z Index: 210

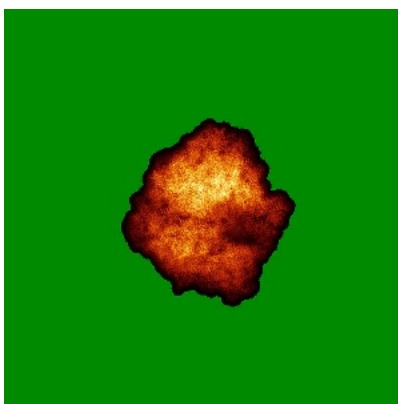
The images above show the largest variance slices of the map in three orthogonal directions.

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

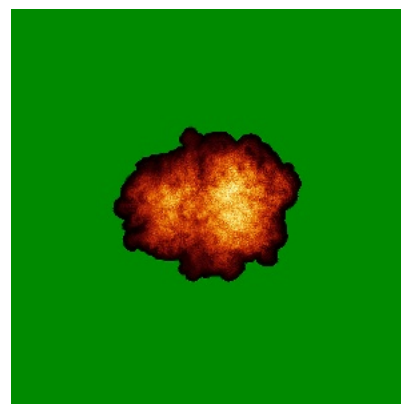
6.4.1 Primary map



X

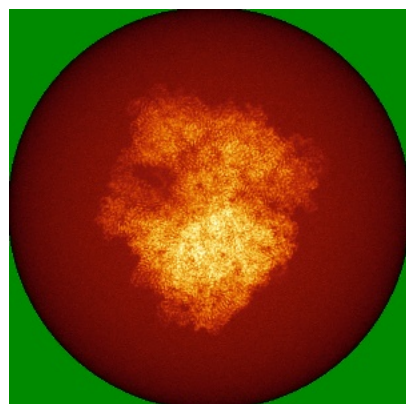


Y

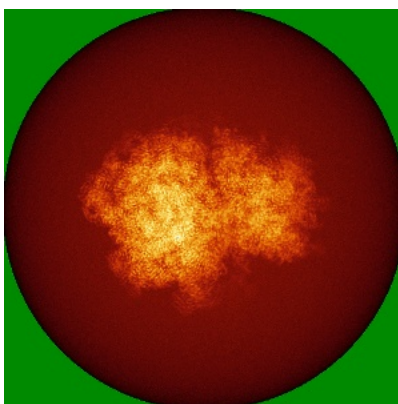


Z

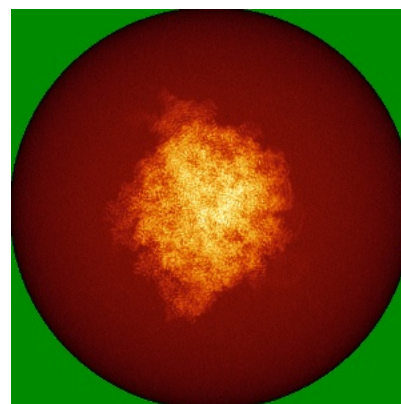
6.4.2 Raw map



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.

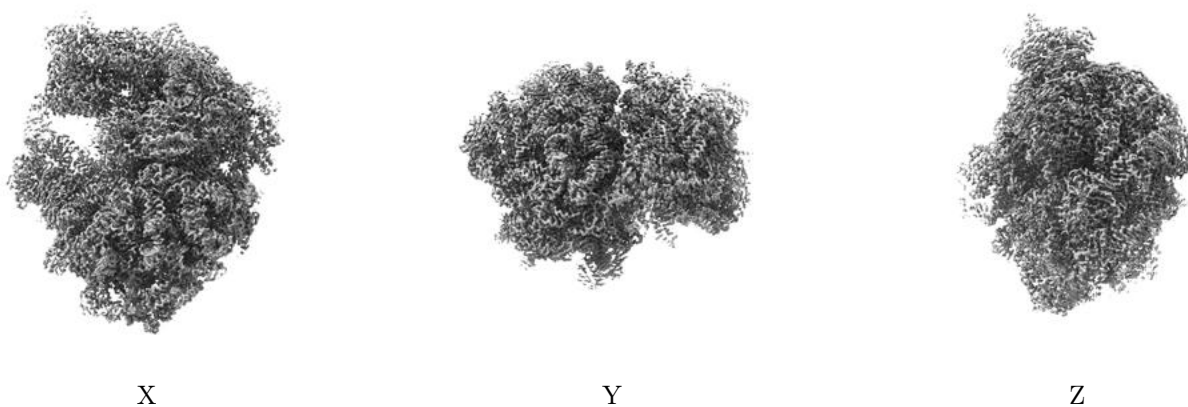
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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

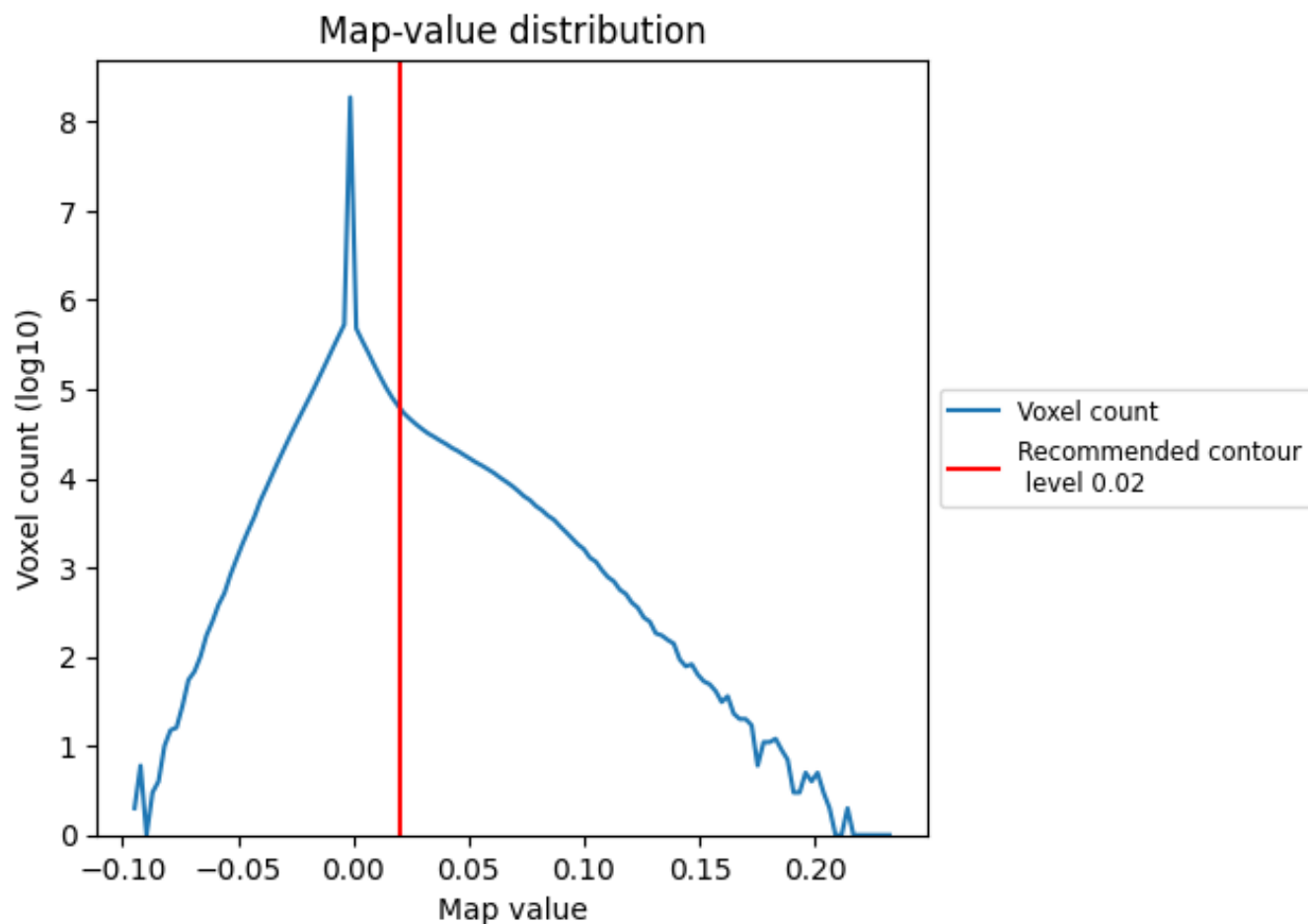
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

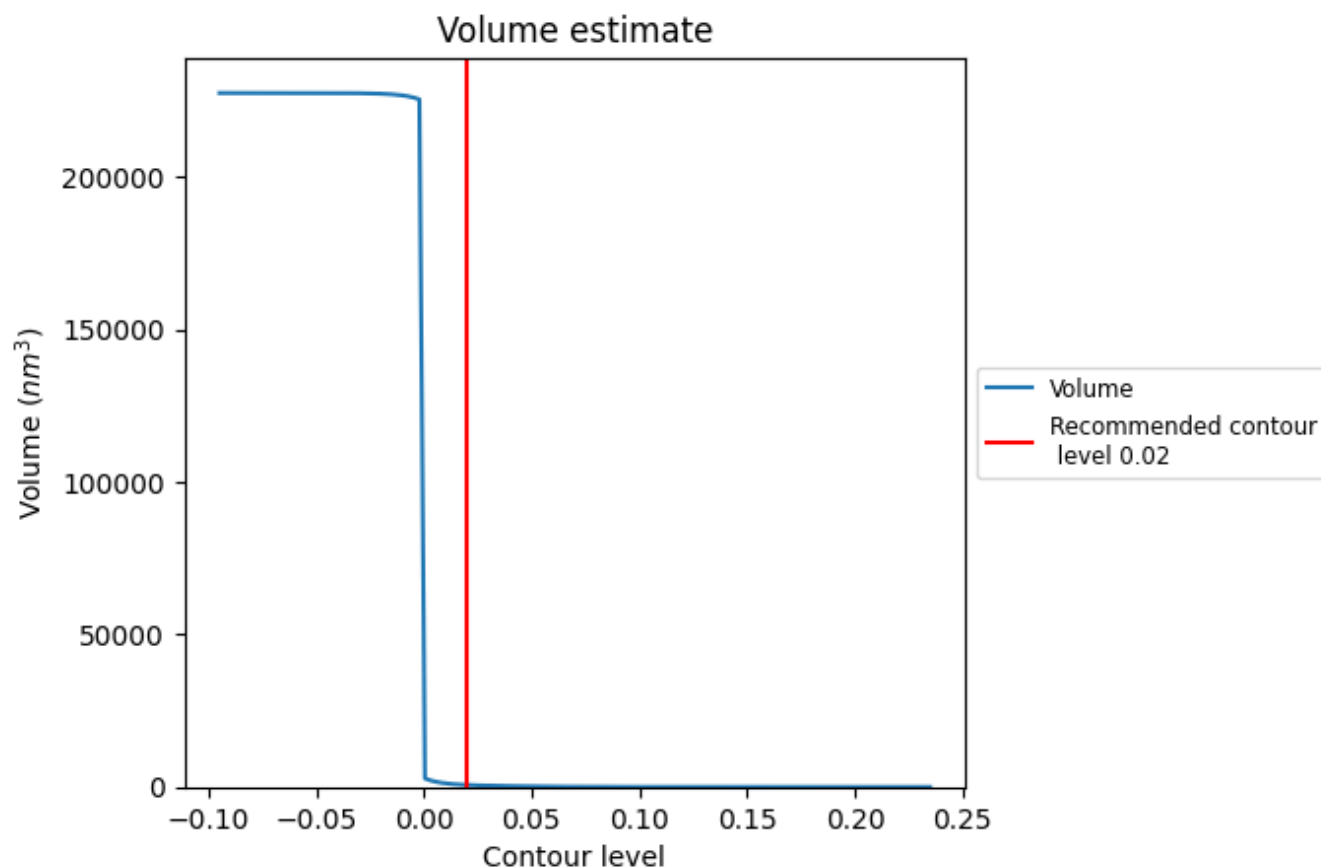
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

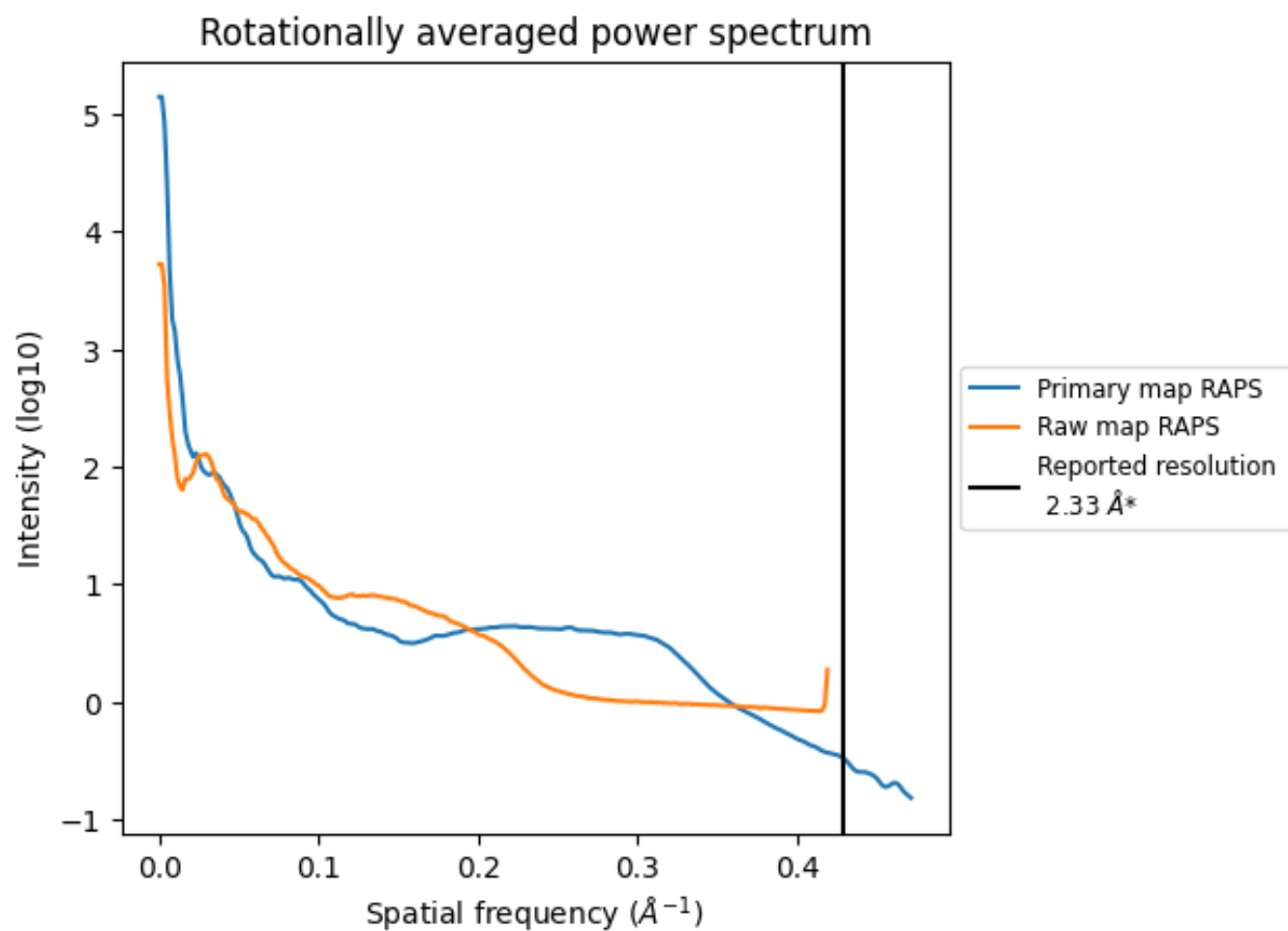
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

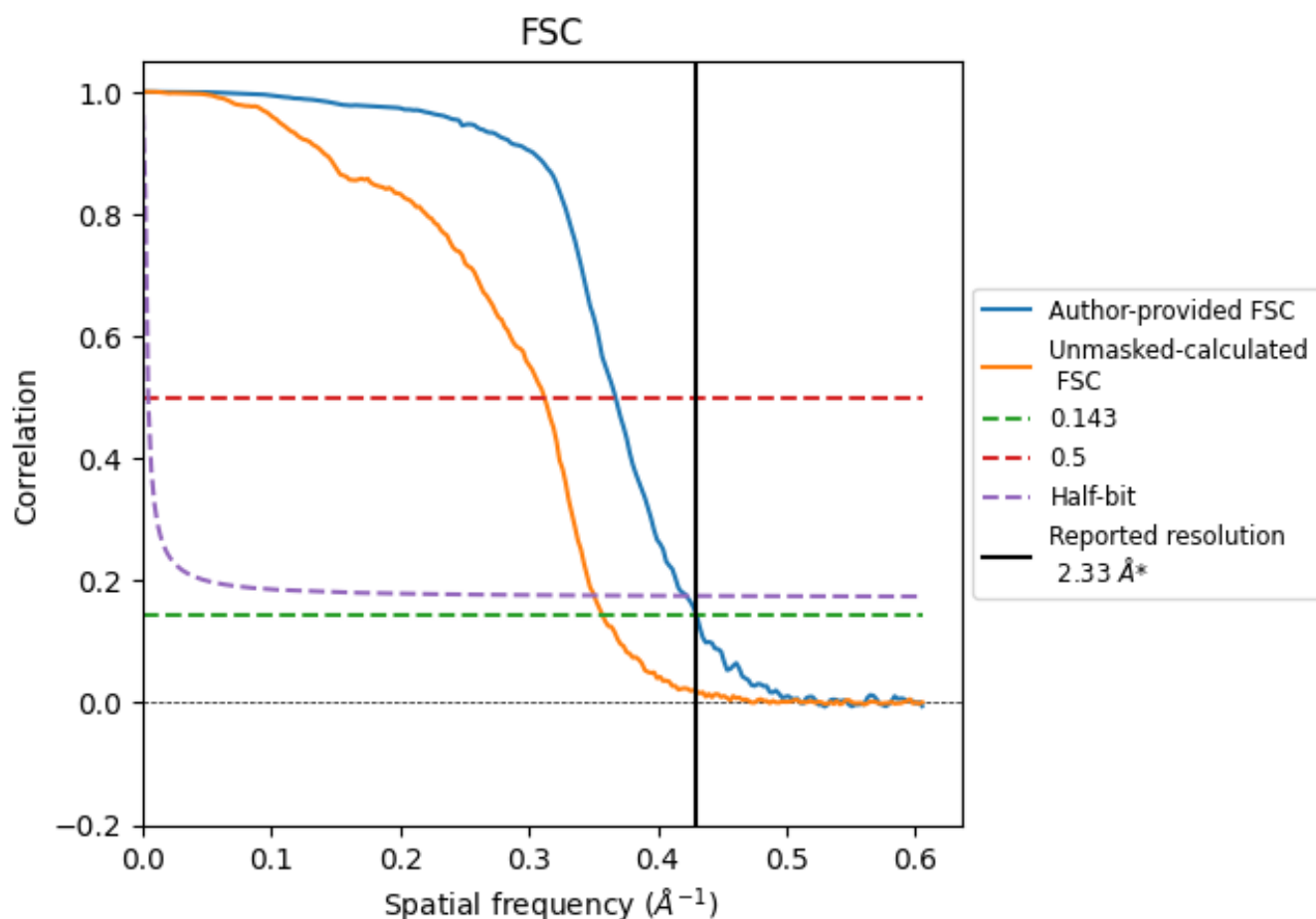


*Reported resolution corresponds to spatial frequency of 0.429 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.429 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

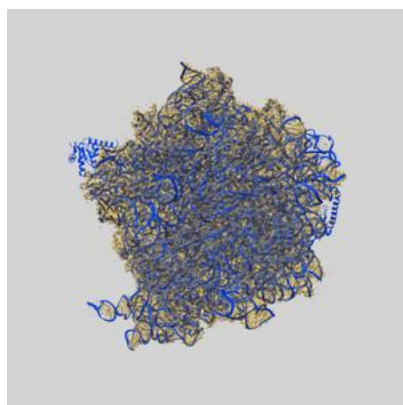
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.33	-	-
Author-provided FSC curve	2.32	2.72	2.37
Unmasked-calculated*	2.80	3.20	2.85

*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 %

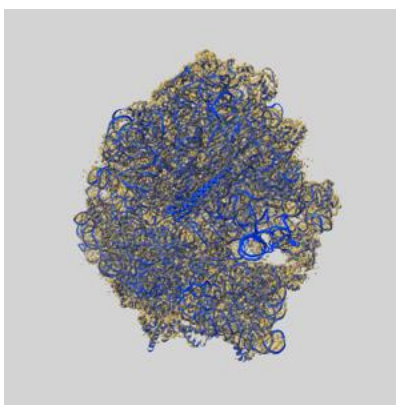
9 Map-model fit [i](#)

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 19.

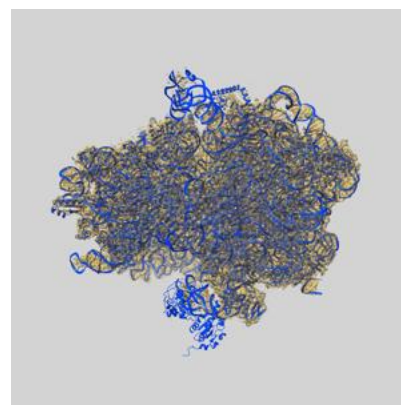
9.1 Map-model overlay [i](#)



X



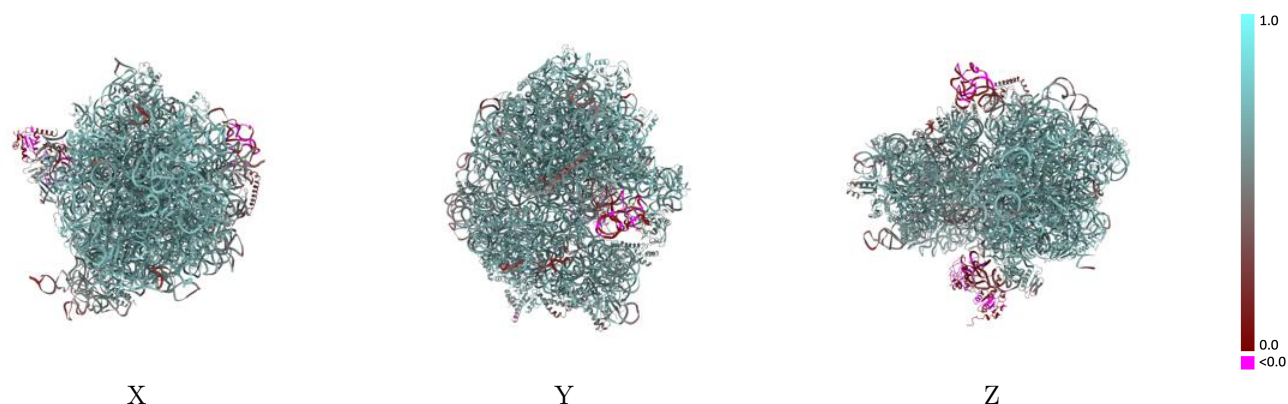
Y



Z

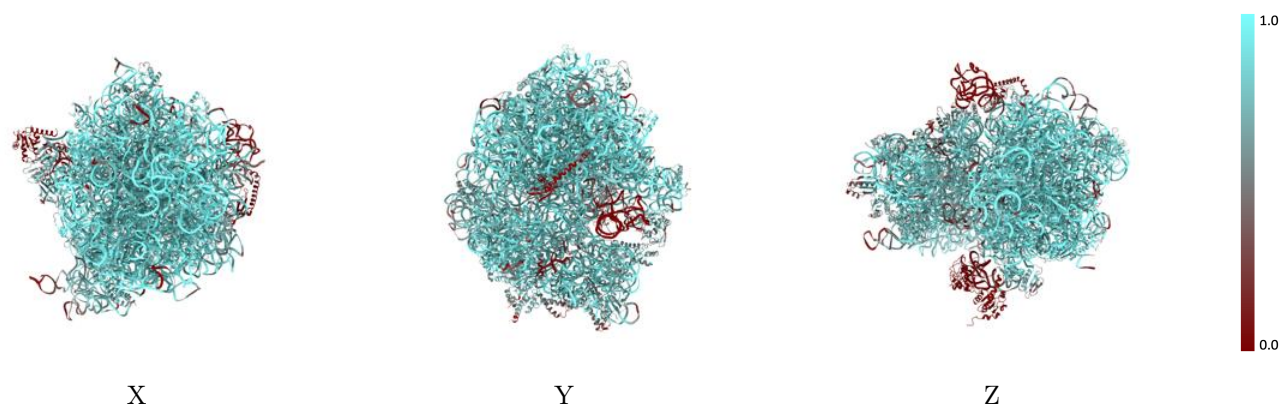
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



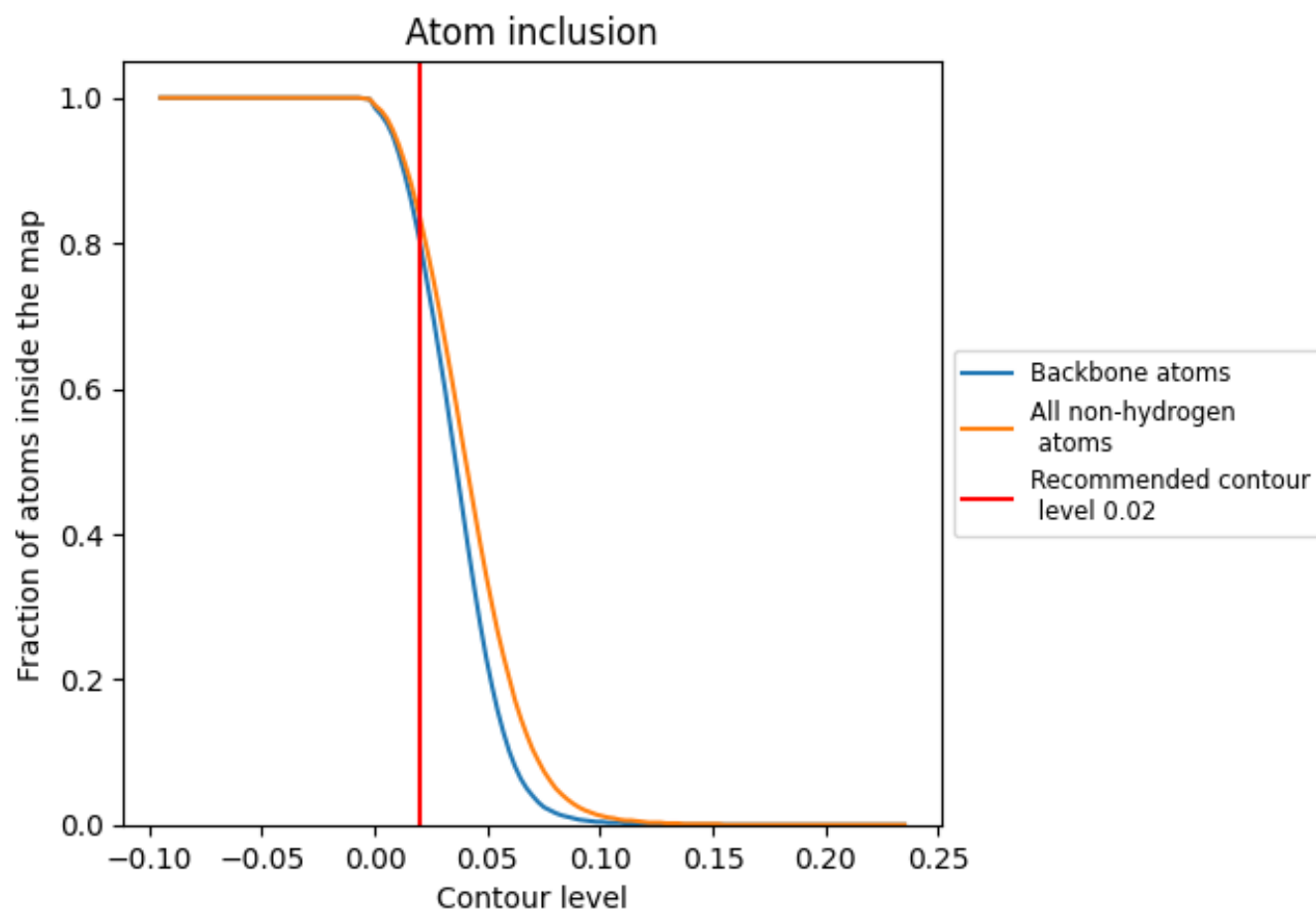
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

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



Continued on next page...

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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