



wwPDB EM Validation Summary Report ⓘ

Mar 11, 2025 – 11:55 PM EDT

PDB ID : 7N31
EMDB ID : EMD-24136
Title : Elongating 70S ribosome complex in a post-translocation (POST) conformation
Authors : Rundlet, E.J.; Holm, M.; Schacherl, M.; Natchiar, K.S.; Altman, R.B.; Spahn, C.M.T.; Myasnikov, A.G.; Blanchard, S.C.
Deposited on : 2021-05-31
Resolution : 2.69 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.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

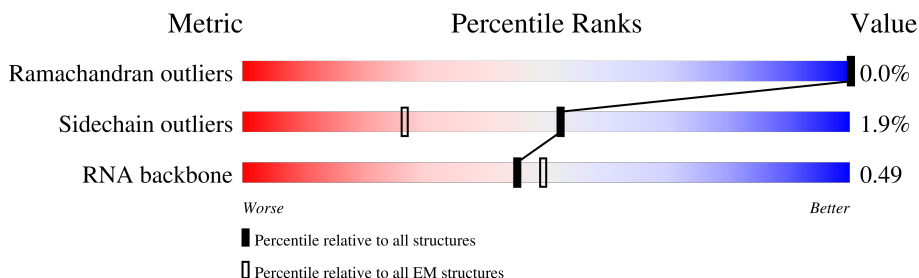
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.69 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	16	1534	<div> <div>6%</div> <div>81%</div> <div>19%</div> </div>
2	SB	241	<div> <div>32%</div> <div>94%</div> <div>5%</div> </div>
3	SC	233	<div> <div>16%</div> <div>91%</div> <div>9%</div> </div>
4	SD	206	<div> <div>18%</div> <div>99%</div> </div>
5	SE	167	<div> <div>6%</div> <div>92%</div> <div>7%</div> </div>
6	SF	135	<div> <div>16%</div> <div>77%</div> <div>21%</div> </div>
7	SG	179	<div> <div>25%</div> <div>84%</div> <div>14%</div> </div>
8	SH	130	<div> <div>5%</div> <div>98%</div> </div>

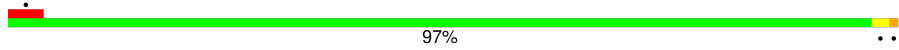
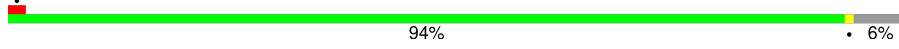
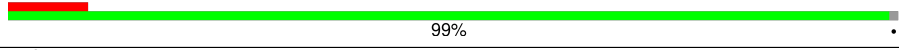
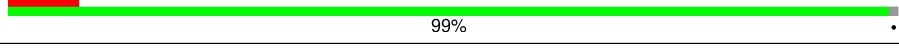
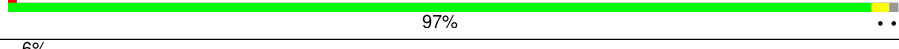
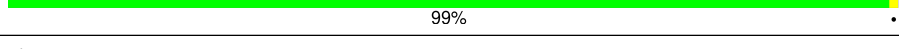
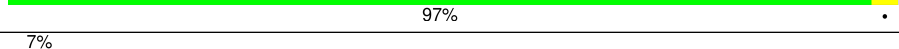
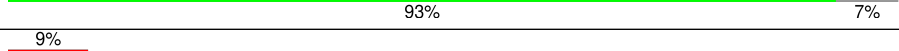
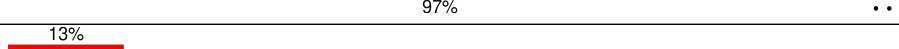
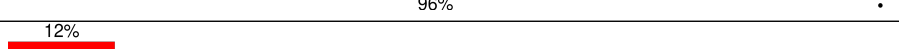
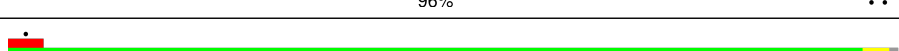
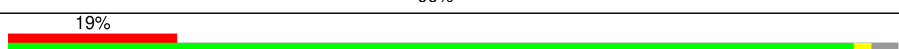


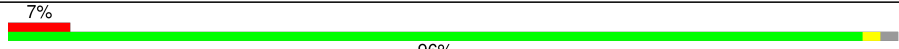
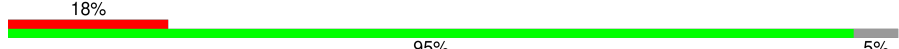
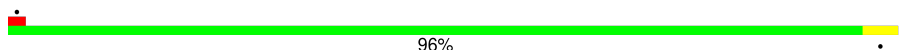
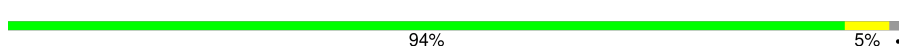
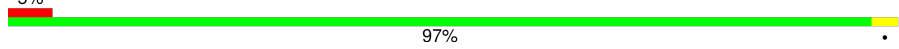

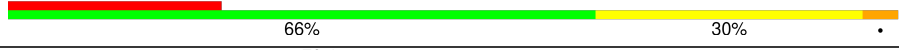


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Mol	Chain	Length	Quality of chain
9	SI	130	
10	SJ	103	
11	SK	129	
12	SL	124	
13	SM	118	
14	SN	101	
15	SO	89	
16	SP	82	
17	SQ	84	
18	SR	75	
19	SS	92	
20	ST	87	
21	SU	71	
22	mR	60	
23	23	2904	
24	5	120	
25	LB	273	
26	LC	209	
27	LD	201	
28	LE	179	
29	LF	177	
30	LI	149	
31	LM	142	
32	LN	123	
33	LO	144	

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

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 146546 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	1533	Total	C	N	O	P	0	0
			32908	14684	6036	10655	1533		

- 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
			1786	1129	320	329	8		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SE	156	Total	C	N	O	S	0	0
			1152	717	217	212	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	154	Total	C	N	O	S	0	0
			1214	756	235	219	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
			1021	634	206	178	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SJ	100	Total	C	N	O	S	0	0
			803	502	154	146	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	0	0
			877	540	174	160	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	115	Total	C	N	O	S	0	0
			891	552	179	157	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
			804	499	164	138	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SO	88	Total	C	N	O	S	0	0
			713	439	144	129	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
			669	414	138	114	3		

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

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	mR	12	Total	C	N	O	P	0	0
			252	113	41	86	12		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LF	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 L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LM	142	Total	C	N	O	S	0	0
			1128	714	212	198	4		

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LN	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

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

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LP	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 35 is a protein called 50S ribosomal protein L17.

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

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LR	116	Total	C	N	O		0	0
			891	552	178	161			

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LU	103	Total	C	N	O	S	0	0
			815	516	153	144	2		

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LV	110	Total	C	N	O	S	0	0
			856	532	166	155	3		

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

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

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	La	84	Total	C	N	O	S		
			634	391	129	113	1	0	0

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lb	77	Total	C	N	O	S		
			624	388	129	105	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lc	61	Total	C	N	O	S		
			495	305	97	92	1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Le	66	Total	C	N	O	S		
			522	323	99	94	6	0	0

- Molecule 49 is a protein called 50S ribosomal protein L32.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L34.

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

- Molecule 52 is a protein called 50S ribosomal protein L35.

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

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Lj	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 54 is a protein called Polypeptide.

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

- Molecule 55 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Pt	76	Total	C	N	O	P S	0	0
			1636	734	284	541	76 1		

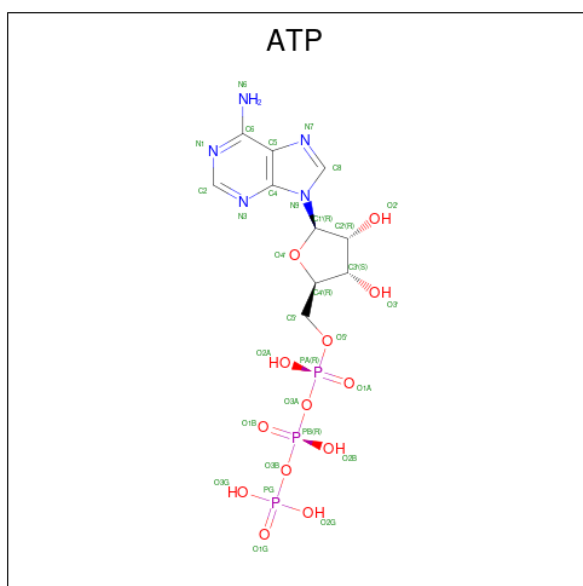
- Molecule 56 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	Dt	76	Total	C	N	O	P	S	0	0
			1634	734	291	532	75	2		

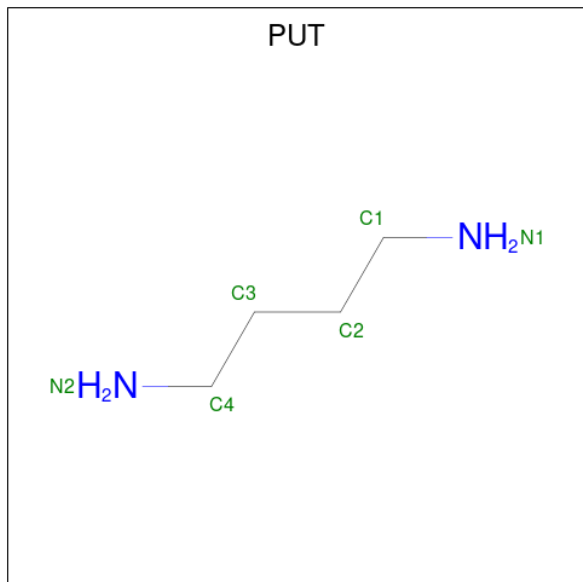
- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
57	16	57	Total	Mg	0
			57	57	
57	23	146	Total	Mg	0
			146	146	
57	5	3	Total	Mg	0
			3	3	
57	LC	1	Total	Mg	0
			1	1	
57	LD	1	Total	Mg	0
			1	1	
57	Lf	1	Total	Mg	0
			1	1	

- Molecule 58 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

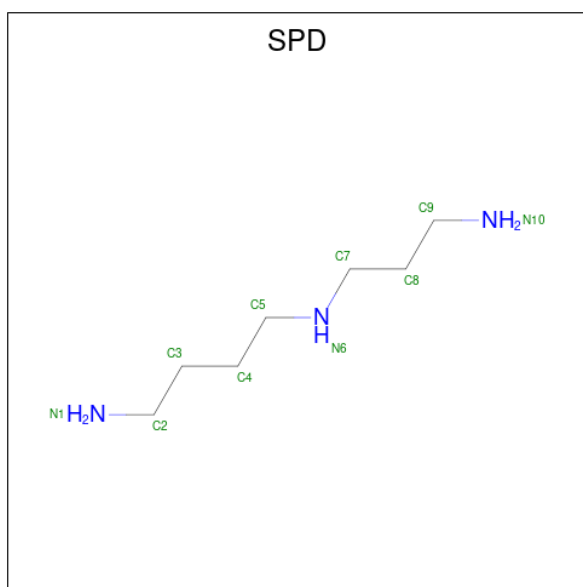


- Molecule 59 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
59	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 SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
60	23	1	Total	C	N	0
			10	7	3	
60	23	1	Total	C	N	0
			10	7	3	
60	23	1	Total	C	N	0
			10	7	3	
60	23	1	Total	C	N	0
			10	7	3	

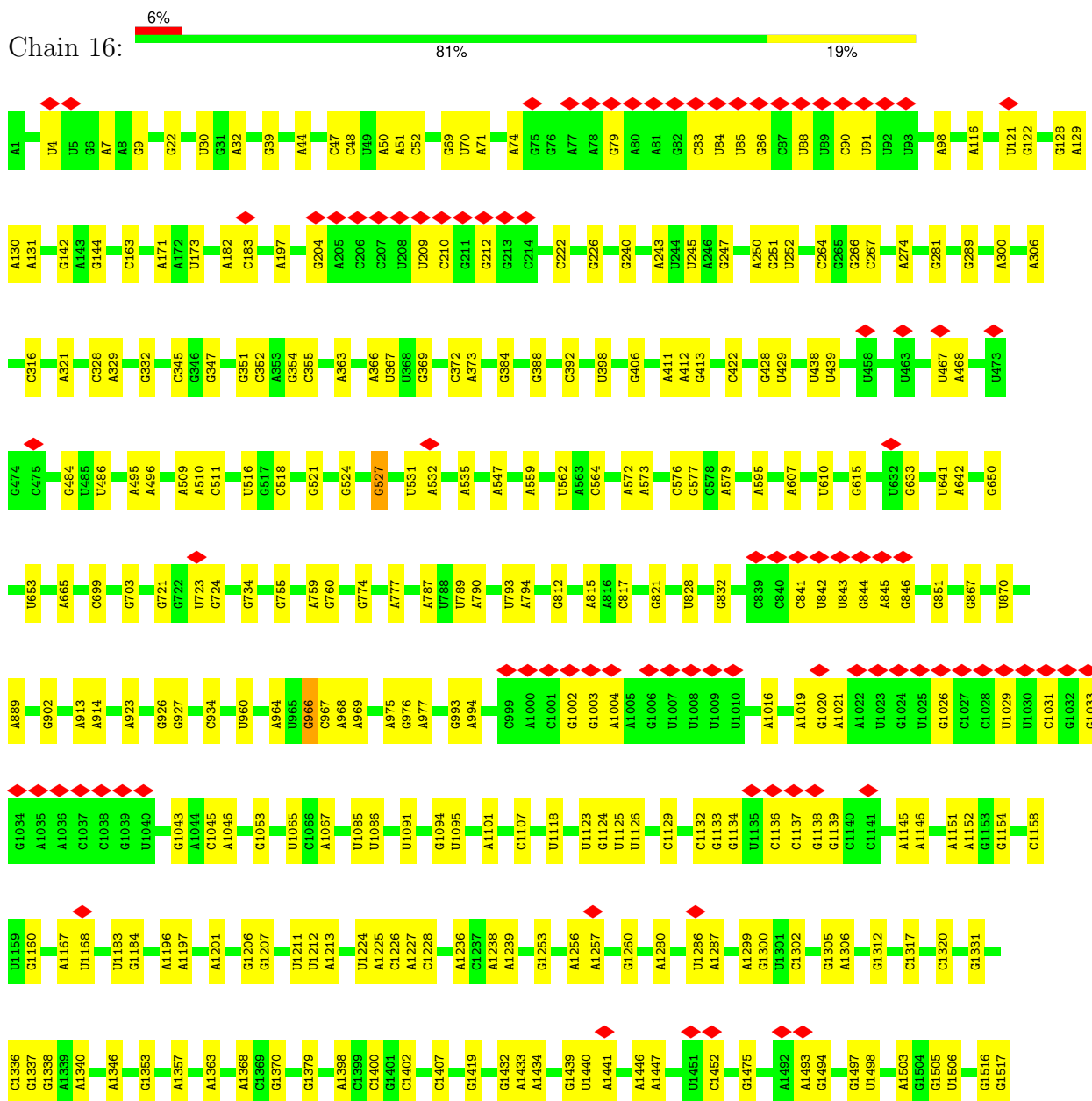
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots

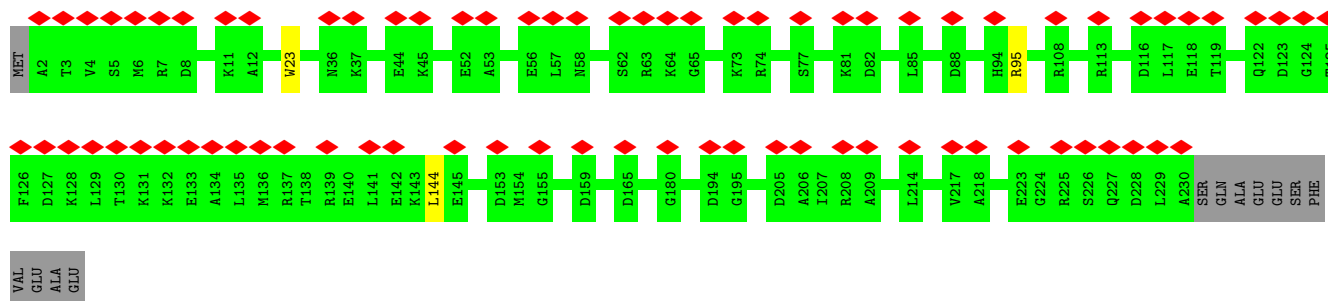
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S rRNA

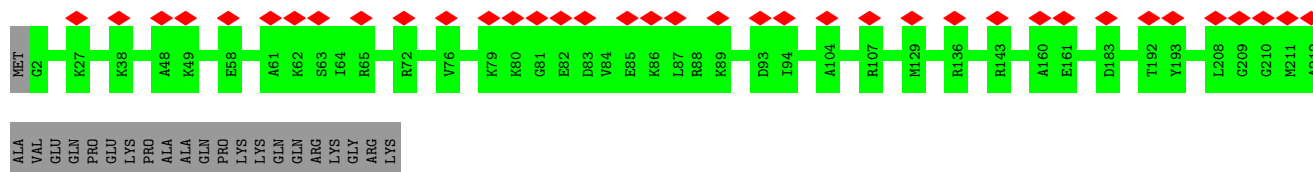




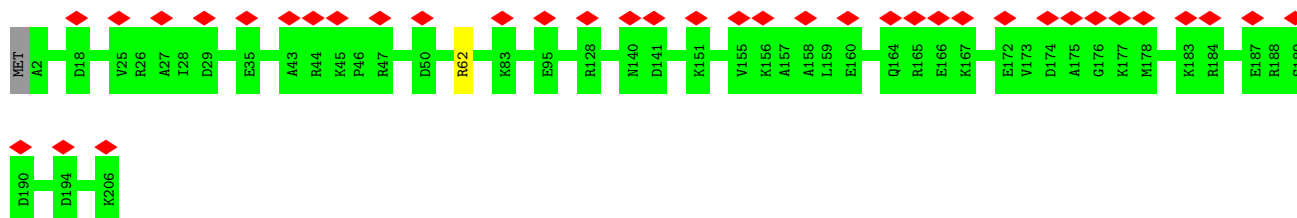
- Molecule 2: 30S ribosomal protein S2



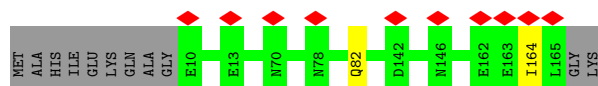
- Molecule 3: 30S ribosomal protein S3



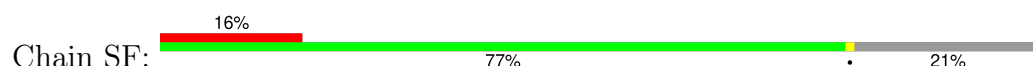
- Molecule 4: 30S ribosomal protein S4

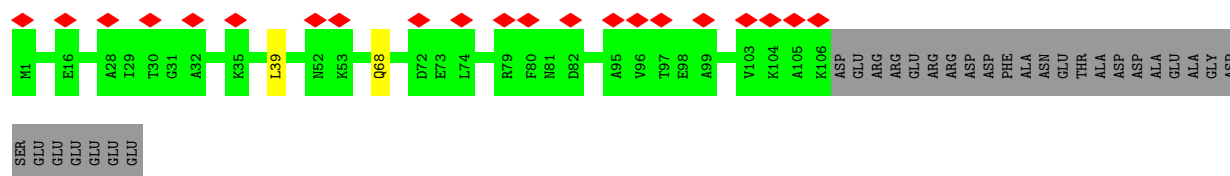


- Molecule 5: 30S ribosomal protein S5

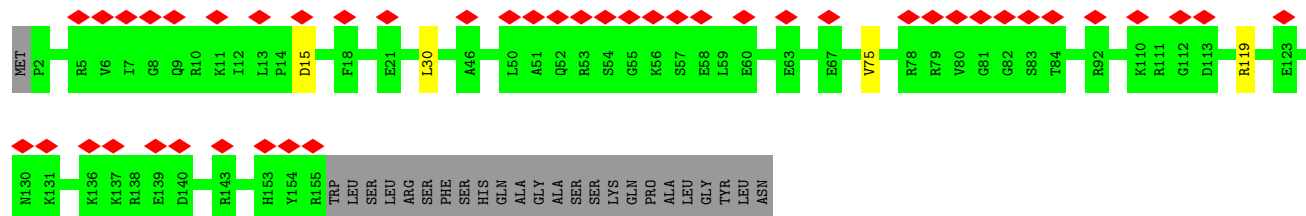
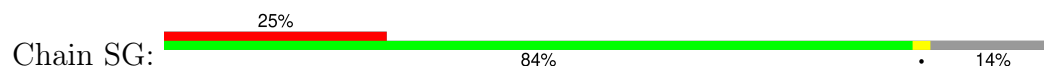


- Molecule 6: 30S ribosomal protein S6

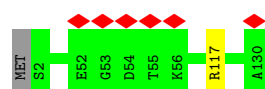




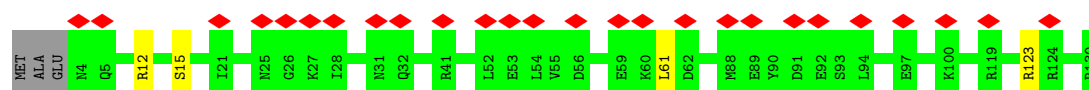
• Molecule 7: 30S ribosomal protein S7



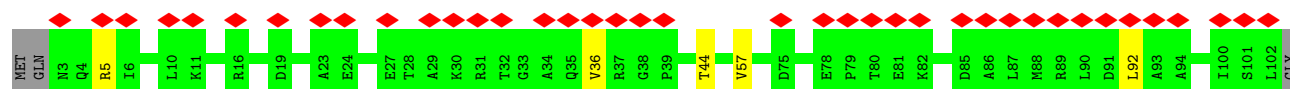
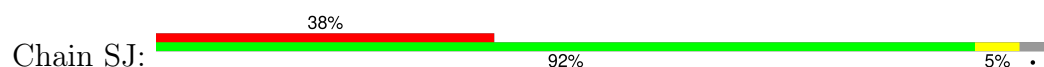
• Molecule 8: 30S ribosomal protein S8



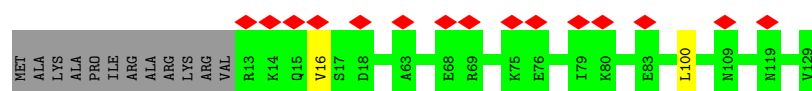
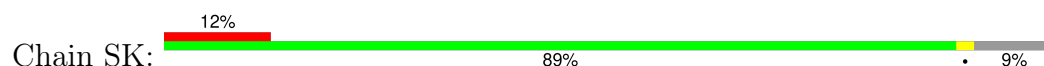
• Molecule 9: 30S ribosomal protein S9



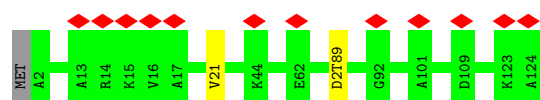
• Molecule 10: 30S ribosomal protein S10



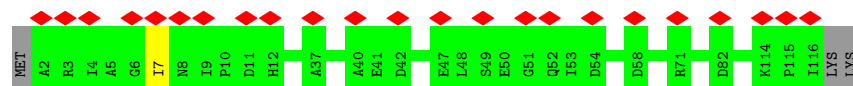
• Molecule 11: 30S ribosomal protein S11



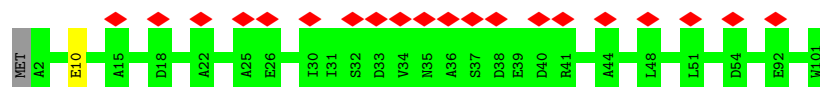
• Molecule 12: 30S ribosomal protein S12



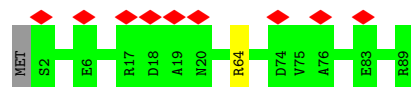
- Molecule 13: 30S ribosomal protein S13



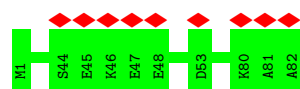
- Molecule 14: 30S ribosomal protein S14



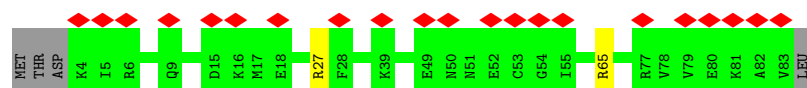
- Molecule 15: 30S ribosomal protein S15



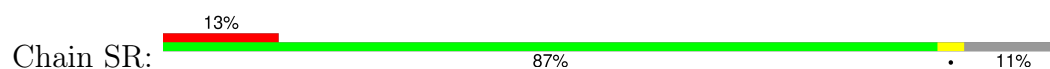
- Molecule 16: 30S ribosomal protein S16

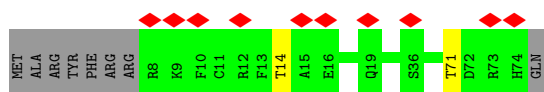


- Molecule 17: 30S ribosomal protein S17

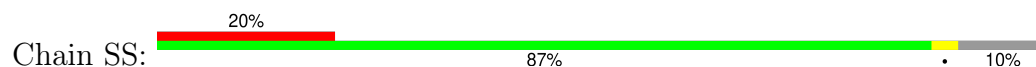


- Molecule 18: 30S ribosomal protein S18

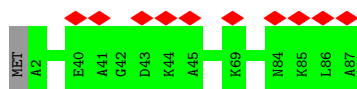




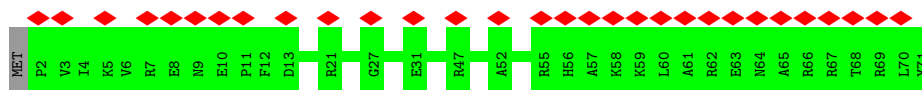
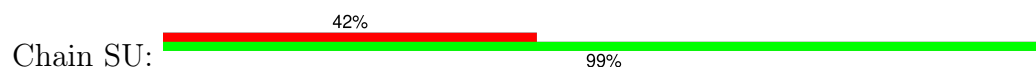
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



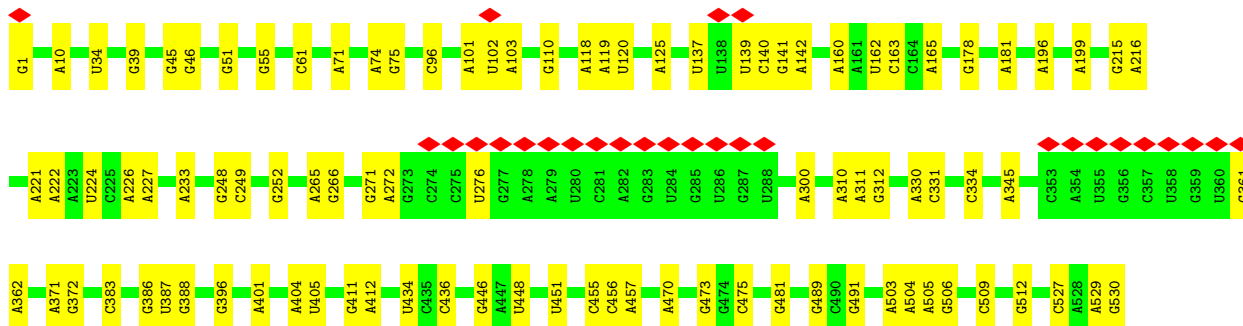
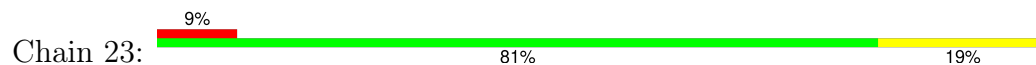
- Molecule 21: 30S ribosomal protein S21



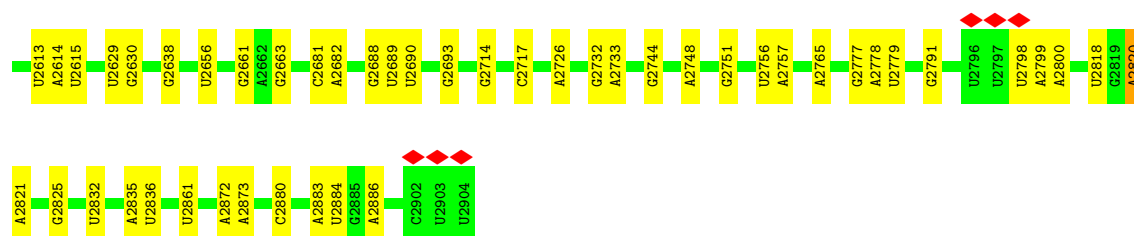
- Molecule 22: mRNA



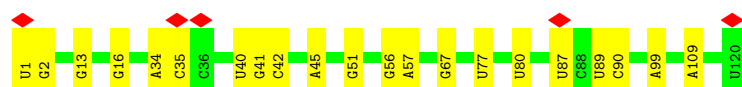
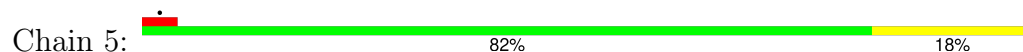
- Molecule 23: 23S rRNA



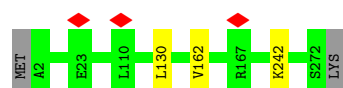




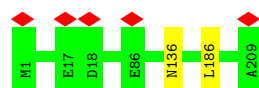
• Molecule 24: 5S rRNA



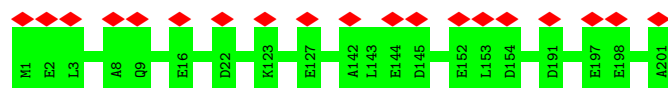
• Molecule 25: 50S ribosomal protein L2



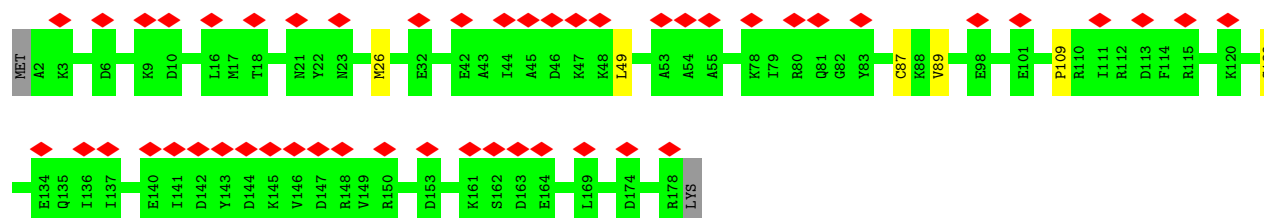
• Molecule 26: 50S ribosomal protein L3



• Molecule 27: 50S ribosomal protein L4

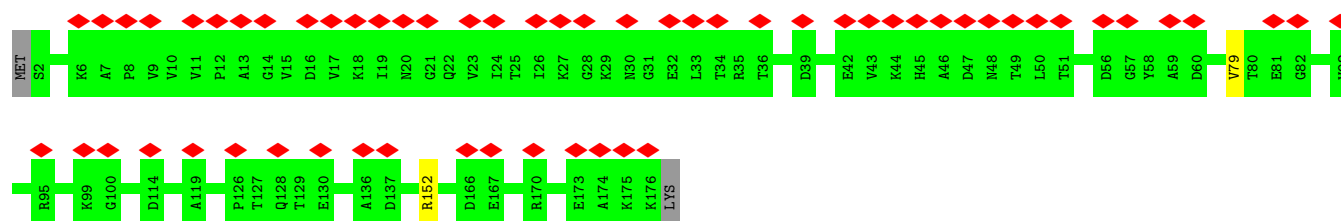


• Molecule 28: 50S ribosomal protein L5

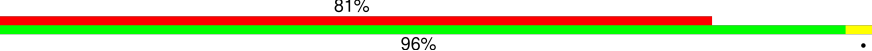


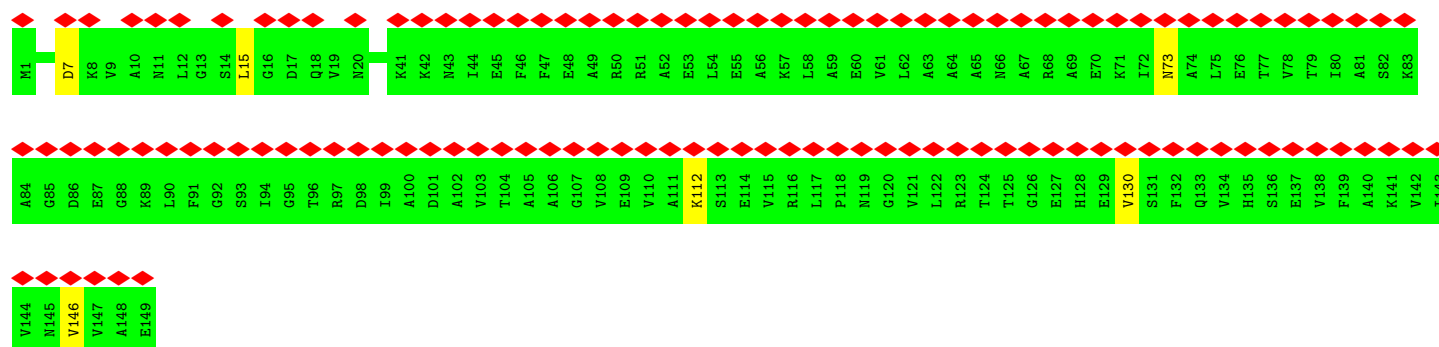
• Molecule 29: 50S ribosomal protein L6

Chain LF: 



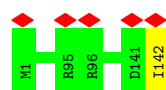
- Molecule 30: 50S ribosomal protein L9

Chain LI: 



- Molecule 31: 50S ribosomal protein L13

Chain LM: 



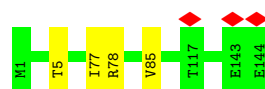
- Molecule 32: 50S ribosomal protein L14

Chain LN: 



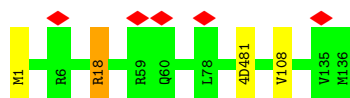
- Molecule 33: 50S ribosomal protein L15

Chain LO: 

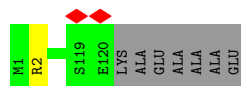


- Molecule 34: 50S ribosomal protein L16

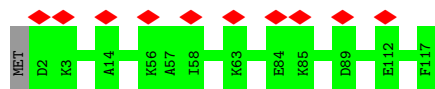
Chain LP: 



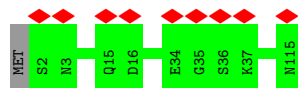
- Molecule 35: 50S ribosomal protein L17



- Molecule 36: 50S ribosomal protein L18



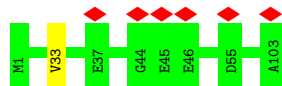
- Molecule 37: 50S ribosomal protein L19



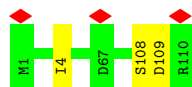
- Molecule 38: 50S ribosomal protein L20



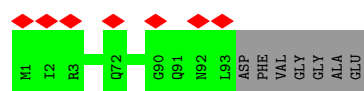
- Molecule 39: 50S ribosomal protein L21



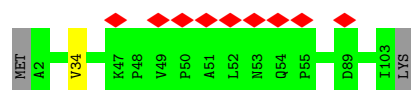
- Molecule 40: 50S ribosomal protein L22



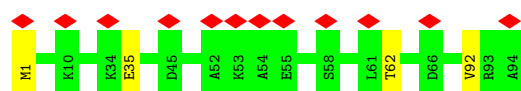
- Molecule 41: 50S ribosomal protein L23



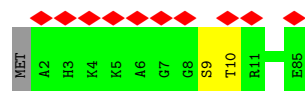
- Molecule 42: 50S ribosomal protein L24



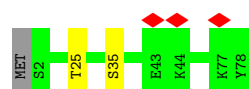
- Molecule 43: 50S ribosomal protein L25



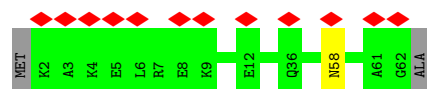
- Molecule 44: 50S ribosomal protein L27



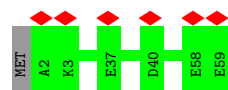
- Molecule 45: 50S ribosomal protein L28



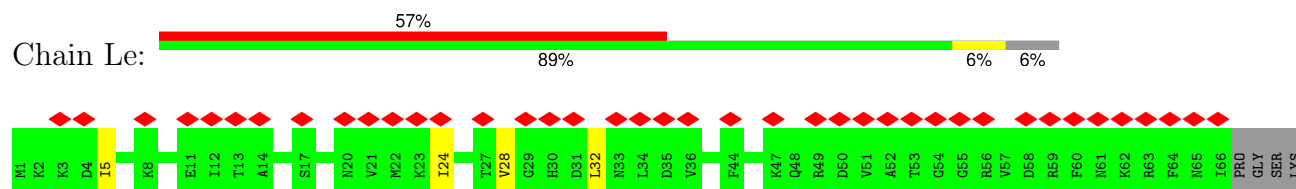
- Molecule 46: 50S ribosomal protein L29



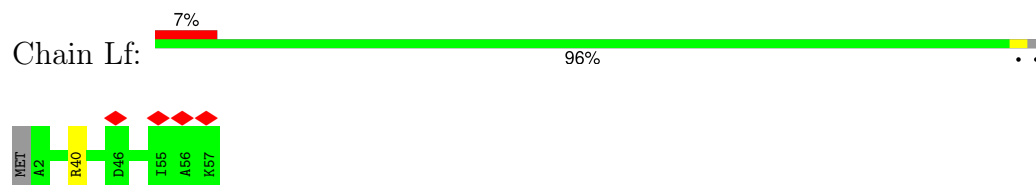
- Molecule 47: 50S ribosomal protein L30



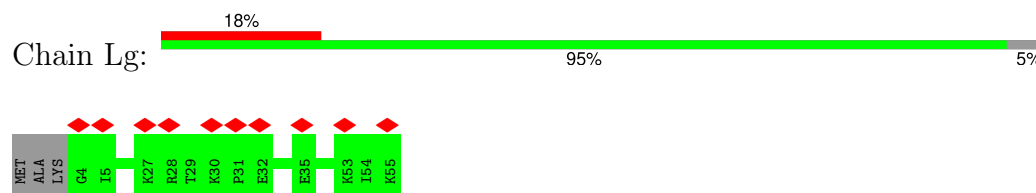
- Molecule 48: 50S ribosomal protein L31



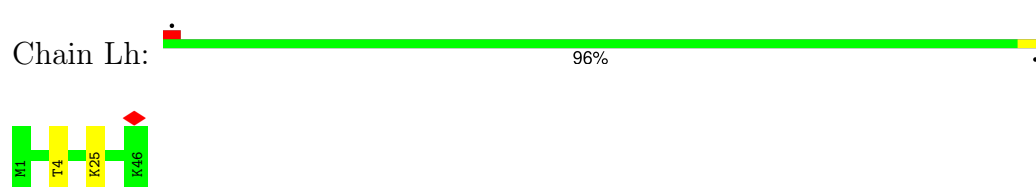
- Molecule 49: 50S ribosomal protein L32



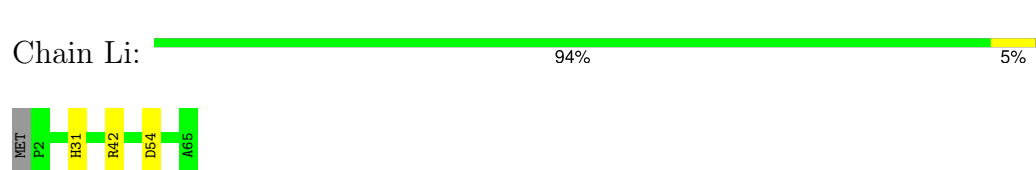
- Molecule 50: 50S ribosomal protein L33



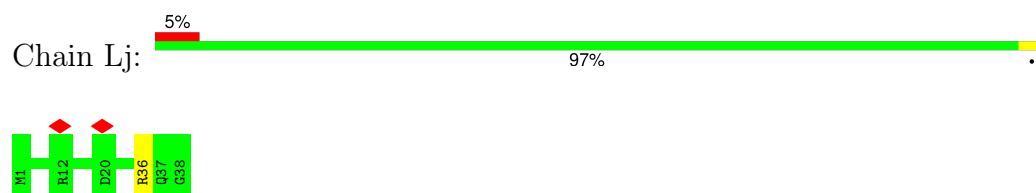
- Molecule 51: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L35

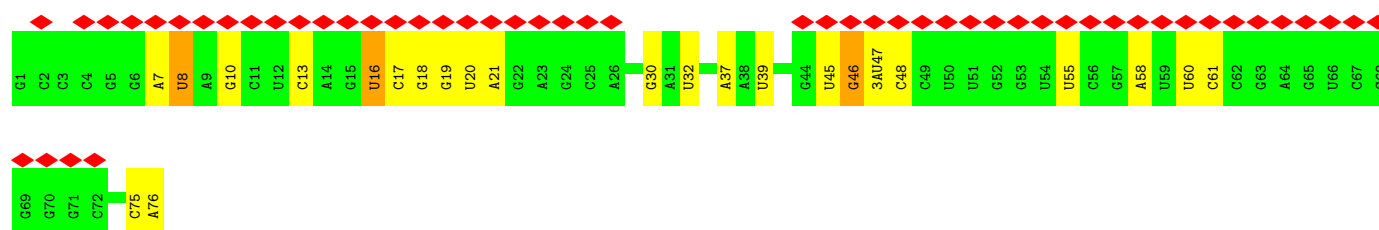


- Molecule 53: 50S ribosomal protein L36



- Molecule 54: Polypeptide





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34170	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	0.199	Depositor
Minimum map value	-0.103	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.025	Depositor
Map size (\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 (\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: D2T, 7MG, 4SU, SPD, 2MG, 2MA, 3TD, OMG, H2U, T6A, 5MU, 6MZ, 4D4, OMU, 5MC, MIA, MG, 4OC, PUT, 1MG, OMC, ZN, U8U, PSU, UR3, ATP, MA6, 3AU

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	0/36568	0.70	0/57042
2	SB	0.43	0/1817	0.62	0/2449
3	SC	0.43	0/1680	0.61	0/2263
4	SD	0.44	0/1665	0.64	0/2227
5	SE	0.45	0/1165	0.68	0/1568
6	SF	0.40	0/881	0.63	0/1189
7	SG	0.45	0/1230	0.67	0/1649
8	SH	0.45	0/989	0.64	0/1326
9	SI	0.49	0/1033	0.70	0/1375
10	SJ	0.50	0/813	0.73	0/1100
11	SK	0.47	0/893	0.68	0/1205
12	SL	0.46	0/960	0.70	0/1286
13	SM	0.47	0/900	0.73	0/1204
14	SN	0.42	0/816	0.61	0/1088
15	SO	0.40	0/721	0.60	0/964
16	SP	0.44	0/659	0.68	0/884
17	SQ	0.50	0/657	0.66	0/881
18	SR	0.45	0/564	0.66	0/756
19	SS	0.48	0/680	0.66	0/915
20	ST	0.46	0/675	0.63	0/895
21	SU	0.46	0/597	0.62	0/792
22	mR	0.29	0/280	0.58	0/433
23	23	0.46	2/69306 (0.0%)	0.71	4/108116 (0.0%)
24	5	0.47	1/2873 (0.0%)	0.72	0/4478
25	LB	0.51	0/2121	0.78	0/2852
26	LC	0.48	0/1586	0.77	1/2134 (0.0%)
27	LD	0.41	0/1571	0.67	0/2113
28	LE	0.49	0/1434	0.67	0/1926
29	LF	0.35	0/1333	0.58	0/1805
30	LI	0.48	0/1122	0.67	0/1515
31	LM	0.47	0/1151	0.67	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LN	0.47	0/956	0.73	0/1279
33	LO	0.49	0/1062	0.76	0/1413
34	LP	0.48	0/1080	0.74	1/1443 (0.1%)
35	LQ	0.44	0/973	0.70	0/1301
36	LR	0.41	0/901	0.63	0/1209
37	LS	0.46	0/929	0.67	0/1242
38	LT	0.49	0/960	0.78	0/1278
39	LU	0.45	0/828	0.70	0/1107
40	LV	0.45	0/863	0.69	0/1156
41	LW	0.46	0/744	0.67	0/994
42	LX	0.47	0/787	0.73	0/1051
43	LY	0.38	0/766	0.59	0/1025
44	La	0.42	0/642	0.66	0/848
45	Lb	0.48	0/634	0.74	0/848
46	Lc	0.49	0/496	0.61	0/660
47	Ld	0.43	0/453	0.69	0/605
48	Le	0.56	0/531	0.69	0/709
49	Lf	0.51	0/450	0.72	0/599
50	Lg	0.38	0/434	0.61	0/576
51	Lh	0.45	0/380	0.79	0/498
52	Li	0.46	0/513	0.75	0/676
53	Lj	0.45	0/302	0.72	0/397
54	Pp	0.49	0/28	1.75	1/34 (2.9%)
55	Pt	0.37	1/1595 (0.1%)	0.70	0/2479
56	Dt	0.33	0/1624	0.65	0/2527
All	All	0.44	4/157671 (0.0%)	0.70	7/235935 (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
33	LO	0	2
54	Pp	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	1	U	OP3-P	-10.62	1.48	1.61
23	23	1	G	OP3-P	-10.19	1.49	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	2074	U	O3'-P	-5.08	1.55	1.61
55	Pt	20	U	C1'-N1	5.04	1.56	1.48

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	2820	A	C2'-C3'-O3'	6.69	124.41	113.70
23	23	1079	C	O4'-C1'-N1	-5.73	103.62	108.20
54	Pp	2	PHE	C-N-CA	-5.66	107.56	121.70
34	LP	18	ARG	CB-CA-C	5.63	121.66	110.40
23	23	2178	C	C2-N1-C1'	5.21	124.53	118.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	LO	77	ILE	Mainchain
33	LO	78	ARG	Mainchain
54	Pp	1	MET	Mainchain

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%)	216 (95%)	10 (4%)	1 (0%)	30	55
3	SC	209/233 (90%)	204 (98%)	5 (2%)	0	100	100
4	SD	203/206 (98%)	201 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	SE	154/167 (92%)	148 (96%)	6 (4%)	0	100	100
6	SF	104/135 (77%)	103 (99%)	1 (1%)	0	100	100
7	SG	152/179 (85%)	148 (97%)	4 (3%)	0	100	100
8	SH	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
9	SI	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
10	SJ	98/103 (95%)	94 (96%)	3 (3%)	1 (1%)	13	33
11	SK	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
12	SL	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
13	SM	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
14	SN	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
15	SO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	SP	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
17	SQ	78/84 (93%)	71 (91%)	7 (9%)	0	100	100
18	SR	65/75 (87%)	63 (97%)	2 (3%)	0	100	100
19	SS	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
20	ST	84/87 (97%)	84 (100%)	0	0	100	100
21	SU	68/71 (96%)	68 (100%)	0	0	100	100
25	LB	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
26	LC	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
27	LD	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
28	LE	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
29	LF	173/177 (98%)	166 (96%)	7 (4%)	0	100	100
30	LI	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
31	LM	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
32	LN	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
33	LO	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
34	LP	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
35	LQ	118/127 (93%)	116 (98%)	2 (2%)	0	100	100
36	LR	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
37	LS	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
38	LT	115/118 (98%)	115 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	LU	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
40	LV	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
41	LW	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
42	LX	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
43	LY	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
44	La	82/85 (96%)	78 (95%)	4 (5%)	0	100	100
45	Lb	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
46	Lc	59/63 (94%)	59 (100%)	0	0	100	100
47	Ld	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
48	Le	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
49	Lf	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
50	Lg	50/55 (91%)	49 (98%)	1 (2%)	0	100	100
51	Lh	44/46 (96%)	44 (100%)	0	0	100	100
52	Li	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
53	Lj	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
54	Pp	1/3 (33%)	0	1 (100%)	0	100	100
All	All	5627/5916 (95%)	5459 (97%)	166 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	SJ	57	VAL
2	SB	95	ARG

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	189/199 (95%)	187 (99%)	2 (1%)	70	87
3	SC	172/190 (90%)	172 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	SD	172/173 (99%)	171 (99%)	1 (1%)	84	94
5	SE	119/126 (94%)	117 (98%)	2 (2%)	56	81
6	SF	92/116 (79%)	90 (98%)	2 (2%)	47	76
7	SG	127/147 (86%)	123 (97%)	4 (3%)	35	64
8	SH	104/105 (99%)	103 (99%)	1 (1%)	73	89
9	SI	105/107 (98%)	101 (96%)	4 (4%)	28	56
10	SJ	88/90 (98%)	84 (96%)	4 (4%)	23	50
11	SK	90/99 (91%)	88 (98%)	2 (2%)	47	76
12	SL	102/103 (99%)	101 (99%)	1 (1%)	73	89
13	SM	93/96 (97%)	92 (99%)	1 (1%)	70	87
14	SN	83/84 (99%)	82 (99%)	1 (1%)	67	86
15	SO	76/77 (99%)	75 (99%)	1 (1%)	65	85
16	SP	65/65 (100%)	65 (100%)	0	100	100
17	SQ	74/78 (95%)	72 (97%)	2 (3%)	40	69
18	SR	58/65 (89%)	56 (97%)	2 (3%)	32	61
19	SS	72/79 (91%)	69 (96%)	3 (4%)	25	53
20	ST	65/66 (98%)	65 (100%)	0	100	100
21	SU	60/61 (98%)	60 (100%)	0	100	100
25	LB	216/218 (99%)	213 (99%)	3 (1%)	62	84
26	LC	164/164 (100%)	163 (99%)	1 (1%)	84	94
27	LD	165/165 (100%)	165 (100%)	0	100	100
28	LE	148/150 (99%)	142 (96%)	6 (4%)	26	54
29	LF	136/138 (99%)	134 (98%)	2 (2%)	60	83
30	LI	114/114 (100%)	108 (95%)	6 (5%)	19	43
31	LM	116/116 (100%)	115 (99%)	1 (1%)	75	90
32	LN	104/104 (100%)	102 (98%)	2 (2%)	52	79
33	LO	103/103 (100%)	101 (98%)	2 (2%)	52	79
34	LP	108/108 (100%)	105 (97%)	3 (3%)	38	68
35	LQ	100/103 (97%)	99 (99%)	1 (1%)	73	89
36	LR	86/87 (99%)	86 (100%)	0	100	100
37	LS	99/100 (99%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	LT	89/90 (99%)	87 (98%)	2 (2%)	47	76
39	LU	84/84 (100%)	83 (99%)	1 (1%)	67	86
40	LV	93/93 (100%)	90 (97%)	3 (3%)	34	63
41	LW	80/84 (95%)	80 (100%)	0	100	100
42	LX	83/85 (98%)	82 (99%)	1 (1%)	67	86
43	LY	78/78 (100%)	74 (95%)	4 (5%)	20	45
44	La	62/63 (98%)	60 (97%)	2 (3%)	34	63
45	Lb	67/68 (98%)	65 (97%)	2 (3%)	36	65
46	Lc	54/55 (98%)	53 (98%)	1 (2%)	52	79
47	Ld	48/49 (98%)	48 (100%)	0	100	100
48	Le	59/62 (95%)	55 (93%)	4 (7%)	13	32
49	Lf	47/48 (98%)	46 (98%)	1 (2%)	48	76
50	Lg	47/49 (96%)	47 (100%)	0	100	100
51	Lh	38/38 (100%)	36 (95%)	2 (5%)	19	43
52	Li	51/52 (98%)	48 (94%)	3 (6%)	16	38
53	Lj	34/34 (100%)	33 (97%)	1 (3%)	37	67
54	Pp	3/3 (100%)	1 (33%)	2 (67%)	0	0
All	All	4682/4831 (97%)	4593 (98%)	89 (2%)	52	79

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	LP	18	ARG
44	La	9	SER
35	LQ	2	ARG
40	LV	109	ASP
46	Lc	58	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
20	ST	52	ASN
25	LB	243	HIS
44	La	50	ASN
21	SU	9	ASN

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Mol	Chain	Res	Type
30	LI	43	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1529/1534 (99%)	284 (18%)	21 (1%)
22	mR	11/60 (18%)	2 (18%)	0
23	23	2899/2904 (99%)	508 (17%)	60 (2%)
24	5	119/120 (99%)	18 (15%)	2 (1%)
55	Pt	73/76 (96%)	19 (26%)	0
56	Dt	73/76 (96%)	19 (26%)	0
All	All	4704/4770 (98%)	850 (18%)	83 (1%)

5 of 850 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	4	U
1	16	7	A
1	16	9	G
1	16	22	G
1	16	30	U

5 of 83 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	23	1286	A
23	23	2307	G
23	23	1451	C
23	23	1818	U
23	23	2681	C

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
1	5MC	16	967	1	19,22,23	1.51	3 (15%)	26,32,35	1.25	4 (15%)
34	4D4	LP	81	34	9,11,12	2.16	2 (22%)	7,13,15	2.04	3 (42%)
23	PSU	23	2457	23	18,21,22	1.72	4 (22%)	21,30,33	2.31	6 (28%)
55	PSU	Pt	55	55	18,21,22	1.42	3 (16%)	21,30,33	2.14	4 (19%)
55	PSU	Pt	39	55	18,21,22	1.57	5 (27%)	21,30,33	2.13	3 (14%)
23	2MG	23	2445	23	18,26,27	1.03	1 (5%)	16,38,41	1.81	5 (31%)
55	H2U	Pt	16	55	18,21,22	1.00	2 (11%)	19,30,33	1.47	4 (21%)
1	5MC	16	1407	1	19,22,23	1.42	3 (15%)	26,32,35	1.37	3 (11%)
1	2MG	16	966	1	18,26,27	1.02	1 (5%)	16,38,41	1.73	6 (37%)
23	PSU	23	2504	23	18,21,22	1.42	3 (16%)	21,30,33	2.06	4 (19%)
12	D2T	SL	89	12	8,9,10	1.65	2 (25%)	6,11,13	1.51	2 (33%)
55	3AU	Pt	47	55	24,28,29	1.04	1 (4%)	30,40,43	1.44	4 (13%)
1	PSU	16	516	1	18,21,22	1.63	5 (27%)	21,30,33	2.28	4 (19%)
23	H2U	23	2449	23	18,21,22	1.27	2 (11%)	19,30,33	1.13	1 (5%)
1	2MG	16	1207	1	18,26,27	1.04	1 (5%)	16,38,41	1.69	6 (37%)
23	2MA	23	2503	57,23	18,25,26	0.71	0	20,37,40	2.03	4 (20%)
23	5MU	23	747	23	19,22,23	1.44	6 (31%)	27,32,35	2.20	6 (22%)
55	7MG	Pt	46	55	23,26,27	1.36	3 (13%)	27,39,42	2.59	8 (29%)
23	5MC	23	1962	23	19,22,23	1.60	3 (15%)	26,32,35	1.10	2 (7%)
23	OMC	23	2498	57,23	19,22,23	0.88	0	25,31,34	1.14	1 (4%)
56	4SU	Dt	8	56	18,21,22	1.94	4 (22%)	25,30,33	2.53	5 (20%)
56	PSU	Dt	55	56	18,21,22	1.37	2 (11%)	21,30,33	2.09	4 (19%)
1	2MG	16	1516	1	18,26,27	1.09	1 (5%)	16,38,41	1.63	5 (31%)
23	PSU	23	2605	23	18,21,22	1.66	4 (22%)	21,30,33	2.06	4 (19%)
1	UR3	16	1498	1	19,22,23	0.98	2 (10%)	26,32,35	2.08	4 (15%)
1	4OC	16	1402	1	20,23,24	0.86	0	25,32,35	1.14	2 (8%)
56	PSU	Dt	39	56	18,21,22	1.51	4 (22%)	21,30,33	2.11	4 (19%)
23	OMU	23	2552	23	19,22,23	1.40	3 (15%)	25,31,34	2.16	6 (24%)
1	MA6	16	1519	1	19,26,27	0.96	1 (5%)	18,38,41	2.52	8 (44%)
23	PSU	23	2604	23	18,21,22	1.57	4 (22%)	21,30,33	2.32	7 (33%)
56	MIA	Dt	37	56	24,31,32	2.23	2 (8%)	22,44,47	2.77	6 (27%)
23	6MZ	23	1618	23	17,25,26	0.89	1 (5%)	15,36,39	2.31	4 (26%)
23	1MG	23	745	23	19,26,27	0.77	0	18,39,42	1.39	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	7MG	23	2069	23	23,26,27	1.54	4 (17%)	27,39,42	2.59	8 (29%)
56	3AU	Dt	47	56	24,28,29	1.11	1 (4%)	30,40,43	1.48	4 (13%)
56	7MG	Dt	46	56	23,26,27	1.41	3 (13%)	27,39,42	2.59	7 (25%)
1	7MG	16	527	1	23,26,27	1.47	3 (13%)	27,39,42	2.74	8 (29%)
23	OMG	23	2251	55,23	19,26,27	1.00	1 (5%)	21,38,41	1.19	2 (9%)
1	MA6	16	1518	1	19,26,27	1.07	0	18,38,41	2.43	7 (38%)
23	3TD	23	1915	23	19,22,23	1.24	2 (10%)	23,32,35	2.10	3 (13%)
56	PSU	Dt	32	56	18,21,22	1.46	4 (22%)	21,30,33	2.08	3 (14%)
23	PSU	23	746	57,23	18,21,22	1.51	5 (27%)	21,30,33	2.08	5 (23%)
23	2MG	23	1835	23	18,26,27	0.88	1 (5%)	16,38,41	1.33	4 (25%)
23	PSU	23	955	23	18,21,22	1.61	5 (27%)	21,30,33	2.33	5 (23%)
55	H2U	Pt	17	55	18,21,22	1.10	3 (16%)	19,30,33	1.11	1 (5%)
23	PSU	23	2580	23	18,21,22	1.50	4 (22%)	21,30,33	2.15	4 (19%)
55	U8U	Pt	34	22,55	20,24,25	1.89	4 (20%)	22,34,37	1.35	3 (13%)
55	T6A	Pt	37	55	26,34,35	0.99	1 (3%)	28,49,52	2.17	6 (21%)
23	6MZ	23	2030	23	17,25,26	0.87	1 (5%)	15,36,39	2.58	4 (26%)
56	H2U	Dt	16	56	18,21,22	1.19	3 (16%)	19,30,33	1.14	2 (10%)
55	5MU	Pt	54	55	19,22,23	1.46	6 (31%)	27,32,35	2.12	8 (29%)
23	5MU	23	1939	23	19,22,23	1.56	4 (21%)	27,32,35	2.29	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
34	4D4	LP	81	34	-	3/11/12/14	-
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
55	PSU	Pt	55	55	-	0/7/25/26	0/2/2/2
55	PSU	Pt	39	55	-	0/7/25/26	0/2/2/2
23	2MG	23	2445	23	-	0/5/27/28	0/3/3/3
55	H2U	Pt	16	55	-	6/7/38/39	0/2/2/2
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	16	966	1	-	2/5/27/28	0/3/3/3
23	PSU	23	2504	23	-	2/7/25/26	0/2/2/2
12	D2T	SL	89	12	-	3/7/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	3AU	Pt	47	55	-	6/16/34/35	0/2/2/2
1	PSU	16	516	1	-	0/7/25/26	0/2/2/2
23	H2U	23	2449	23	-	1/7/38/39	0/2/2/2
1	2MG	16	1207	1	-	1/5/27/28	0/3/3/3
23	2MA	23	2503	57,23	-	2/3/25/26	0/3/3/3
23	5MU	23	747	23	-	0/7/25/26	0/2/2/2
55	7MG	Pt	46	55	-	1/7/37/38	0/3/3/3
23	5MC	23	1962	23	-	2/7/25/26	0/2/2/2
23	OMC	23	2498	57,23	-	0/9/27/28	0/2/2/2
56	4SU	Dt	8	56	-	2/7/25/26	0/2/2/2
56	PSU	Dt	55	56	-	0/7/25/26	0/2/2/2
1	2MG	16	1516	1	-	0/5/27/28	0/3/3/3
23	PSU	23	2605	23	-	0/7/25/26	0/2/2/2
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
1	4OC	16	1402	1	-	1/9/29/30	0/2/2/2
56	PSU	Dt	39	56	-	0/7/25/26	0/2/2/2
23	OMU	23	2552	23	-	0/9/27/28	0/2/2/2
1	MA6	16	1519	1	-	1/7/29/30	0/3/3/3
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
56	MIA	Dt	37	56	-	5/11/33/34	0/3/3/3
23	6MZ	23	1618	23	-	2/5/27/28	0/3/3/3
23	1MG	23	745	23	-	0/3/25/26	0/3/3/3
23	7MG	23	2069	23	-	1/7/37/38	0/3/3/3
56	3AU	Dt	47	56	-	8/16/34/35	0/2/2/2
56	7MG	Dt	46	56	-	1/7/37/38	0/3/3/3
1	7MG	16	527	1	-	2/7/37/38	0/3/3/3
23	OMG	23	2251	55,23	-	1/5/27/28	0/3/3/3
1	MA6	16	1518	1	-	0/7/29/30	0/3/3/3
23	3TD	23	1915	23	-	2/7/25/26	0/2/2/2
56	PSU	Dt	32	56	-	0/7/25/26	0/2/2/2
23	PSU	23	746	57,23	-	0/7/25/26	0/2/2/2
23	2MG	23	1835	23	-	0/5/27/28	0/3/3/3
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
55	H2U	Pt	17	55	-	5/7/38/39	0/2/2/2
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
55	U8U	Pt	34	22,55	-	0/10/28/29	0/2/2/2
55	T6A	Pt	37	55	-	6/19/41/42	0/3/3/3
23	6MZ	23	2030	23	-	2/5/27/28	0/3/3/3
56	H2U	Dt	16	56	-	3/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	Pt	54	55	-	0/7/25/26	0/2/2/2
23	5MU	23	1939	23	-	0/7/25/26	0/2/2/2

The worst 5 of 133 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Dt	37	MIA	C2-S10	-7.35	1.69	1.75
56	Dt	37	MIA	C13-C14	6.76	1.52	1.32
55	Pt	34	U8U	C2-S2	-5.84	1.58	1.67
23	23	1962	5MC	C5-C4	5.83	1.48	1.44
56	Dt	8	4SU	C4-S4	-5.17	1.59	1.68

The worst 5 of 232 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Dt	37	MIA	C12-C13-C14	-10.51	108.14	127.01
55	Pt	46	7MG	N9-C4-N3	8.24	137.53	125.46
1	16	527	7MG	N9-C4-N3	8.10	137.33	125.46
1	16	1498	UR3	C4-N3-C2	-7.96	118.18	124.58
56	Dt	46	7MG	N9-C4-N3	7.90	137.04	125.46

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	527	7MG	O4'-C4'-C5'-O5'
12	SL	89	D2T	SB-CB-CG-OD2
23	23	1618	6MZ	O4'-C4'-C5'-O5'
55	Pt	16	H2U	O4'-C1'-N1-C2
55	Pt	16	H2U	O4'-C1'-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 226 ligands modelled in this entry, 211 are monoatomic - leaving 15 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	3003	-	5,5,5	0.14	0	4,4,4	0.27	0
59	PUT	23	3005	-	5,5,5	0.13	0	4,4,4	0.25	0
59	PUT	23	3007	-	5,5,5	0.12	0	4,4,4	0.25	0
60	SPD	23	3013	-	9,9,9	0.16	0	8,8,8	0.28	0
60	SPD	23	3014	-	9,9,9	0.17	0	8,8,8	0.30	0
60	SPD	23	3015	-	9,9,9	0.16	0	8,8,8	0.27	0
60	SPD	23	3012	-	9,9,9	0.17	0	8,8,8	0.19	0
59	PUT	23	3009	-	5,5,5	0.10	0	4,4,4	0.13	0
59	PUT	23	3010	-	5,5,5	0.13	0	4,4,4	0.15	0
58	ATP	23	3002	-	28,33,33	0.64	0	34,52,52	0.60	1 (2%)
58	ATP	23	3001	-	28,33,33	0.76	0	34,52,52	0.76	1 (2%)
59	PUT	23	3011	-	5,5,5	0.10	0	4,4,4	0.13	0
59	PUT	23	3006	-	5,5,5	0.12	0	4,4,4	0.23	0
59	PUT	23	3004	-	5,5,5	0.11	0	4,4,4	0.14	0
59	PUT	23	3008	-	5,5,5	0.14	0	4,4,4	0.29	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	3003	-	-	1/3/3/3	-
59	PUT	23	3005	-	-	0/3/3/3	-
59	PUT	23	3007	-	-	1/3/3/3	-
60	SPD	23	3013	-	-	3/7/7/7	-
60	SPD	23	3014	-	-	2/7/7/7	-
60	SPD	23	3015	-	-	0/7/7/7	-
60	SPD	23	3012	-	-	3/7/7/7	-
59	PUT	23	3009	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PUT	23	3010	-	-	1/3/3/3	-
58	ATP	23	3002	-	-	10/18/38/38	0/3/3/3
58	ATP	23	3001	-	-	0/18/38/38	0/3/3/3
59	PUT	23	3011	-	-	0/3/3/3	-
59	PUT	23	3006	-	-	0/3/3/3	-
59	PUT	23	3004	-	-	0/3/3/3	-
59	PUT	23	3008	-	-	0/3/3/3	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	23	3002	ATP	C5-C6-N6	2.36	123.90	120.31
58	23	3001	ATP	C5-C6-N6	2.27	123.76	120.31

There are no chirality outliers.

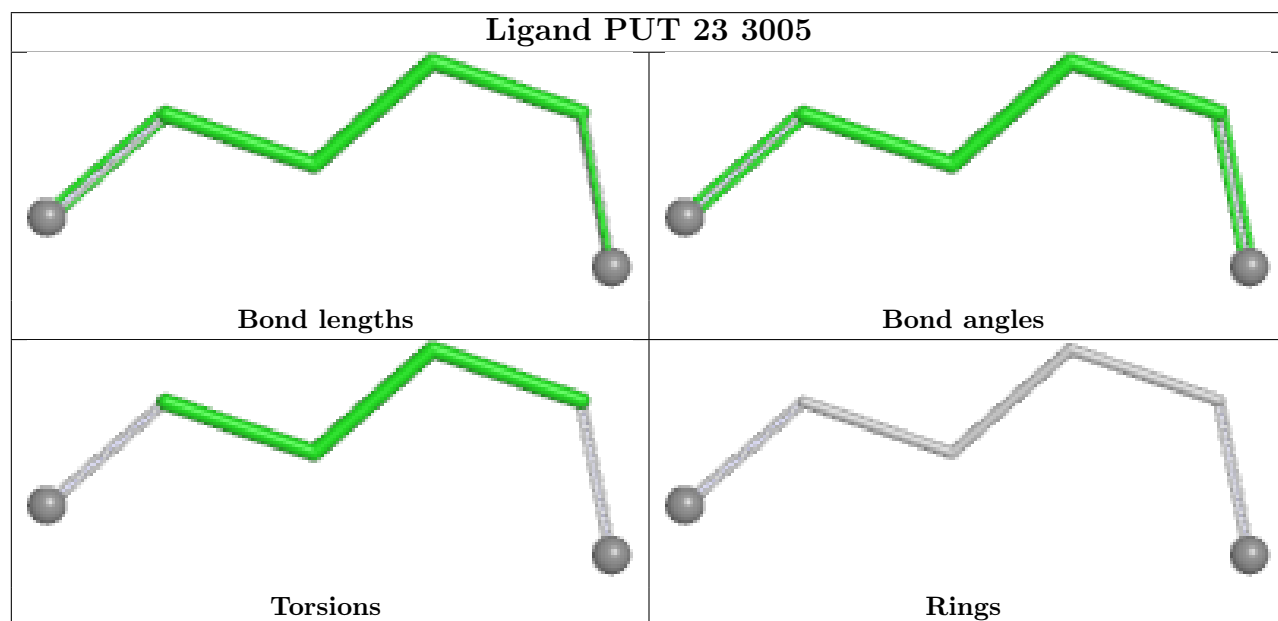
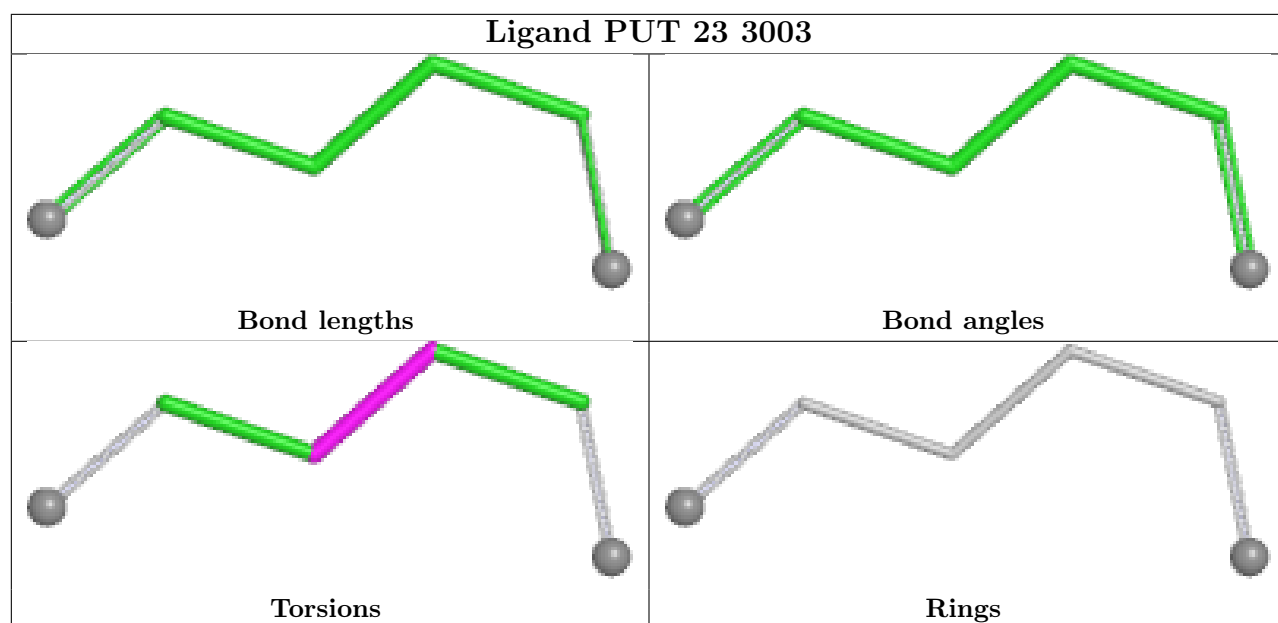
5 of 21 torsion outliers are listed below:

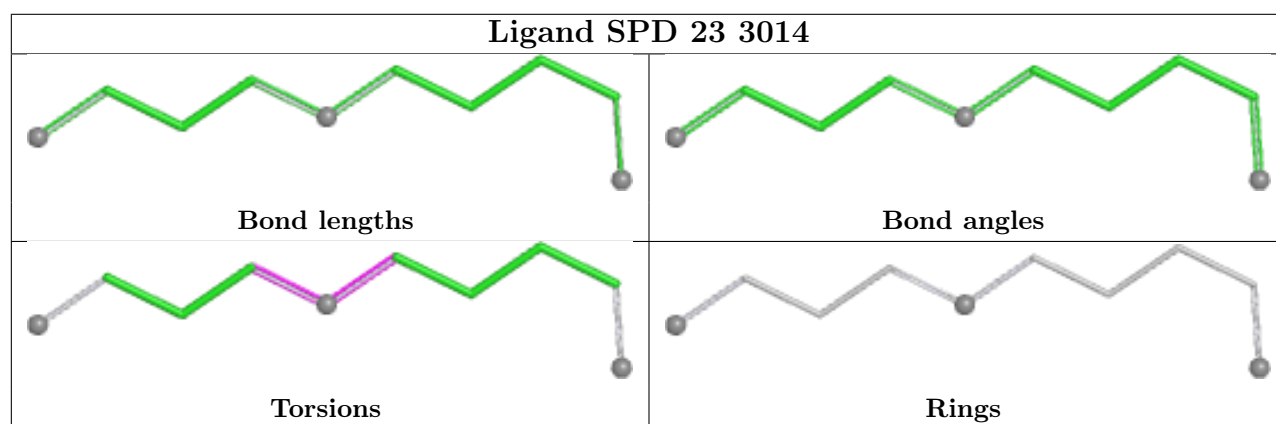
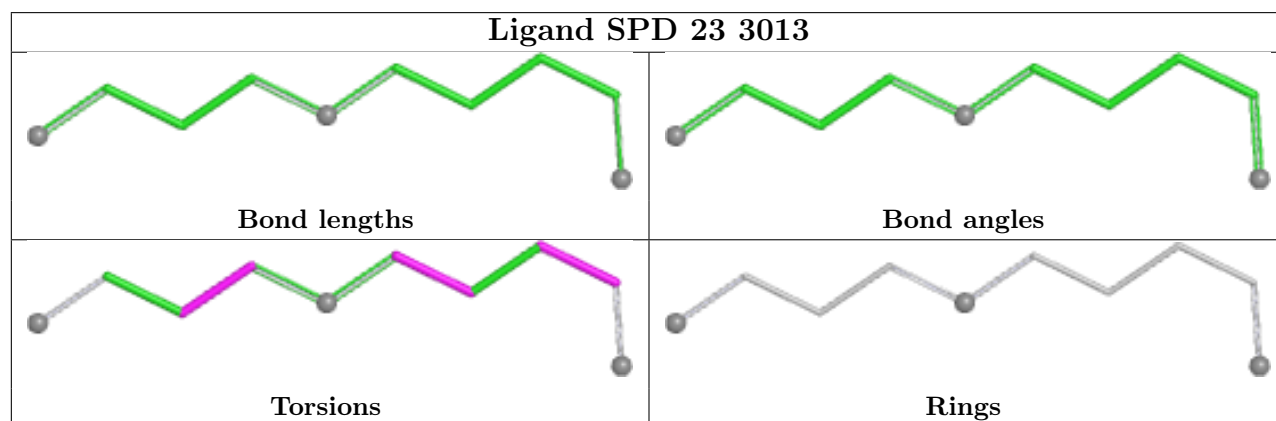
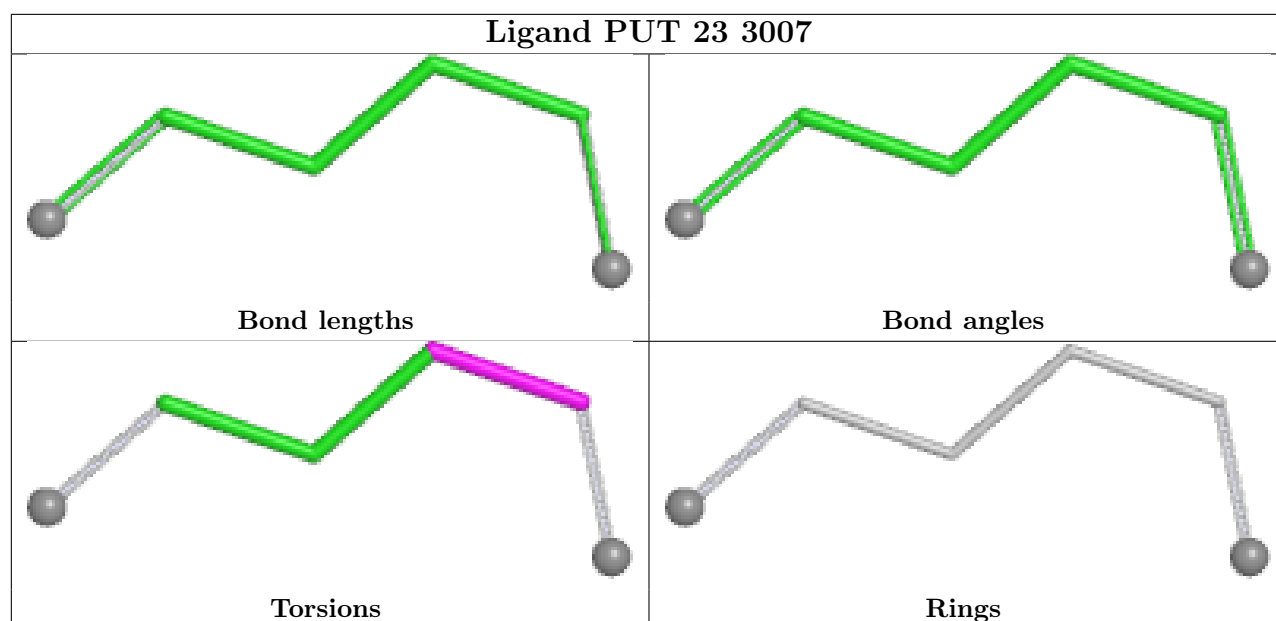
Mol	Chain	Res	Type	Atoms
58	23	3002	ATP	PB-O3B-PG-O2G
58	23	3002	ATP	C5'-O5'-PA-O2A
58	23	3002	ATP	C5'-O5'-PA-O3A
58	23	3002	ATP	O4'-C4'-C5'-O5'
60	23	3013	SPD	N6-C7-C8-C9

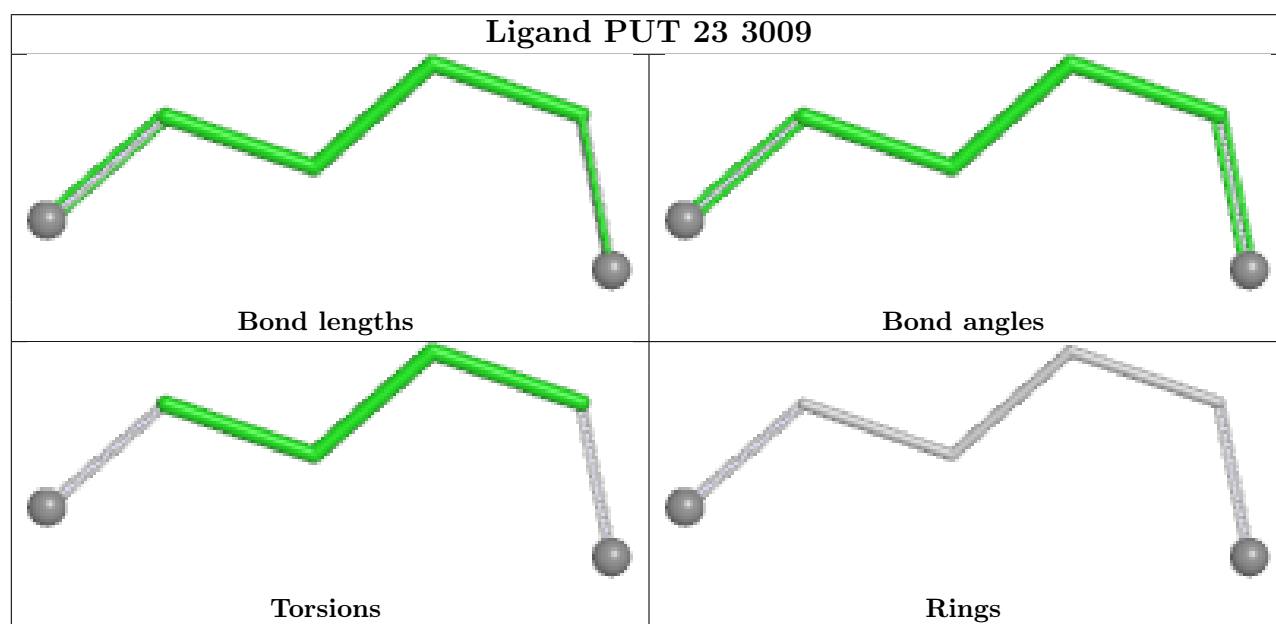
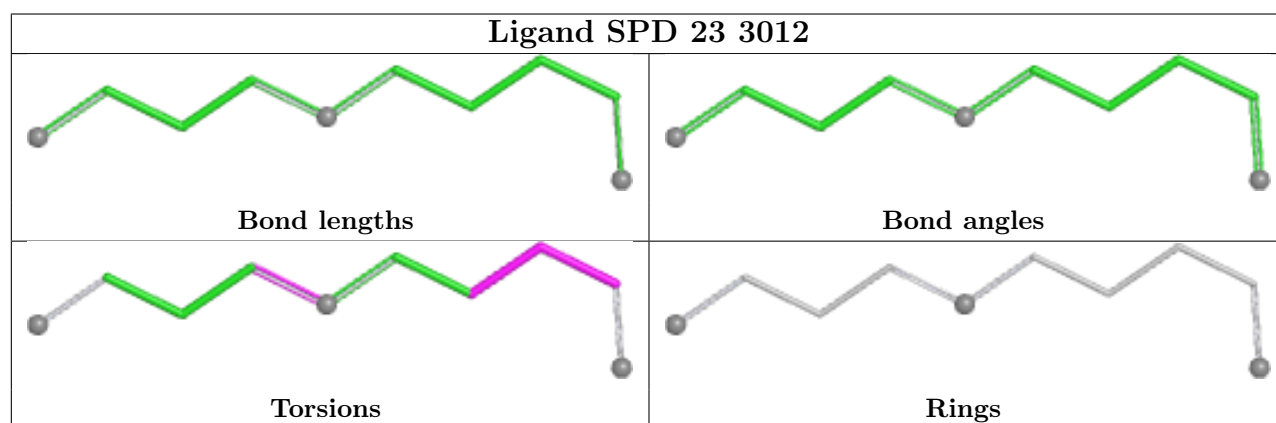
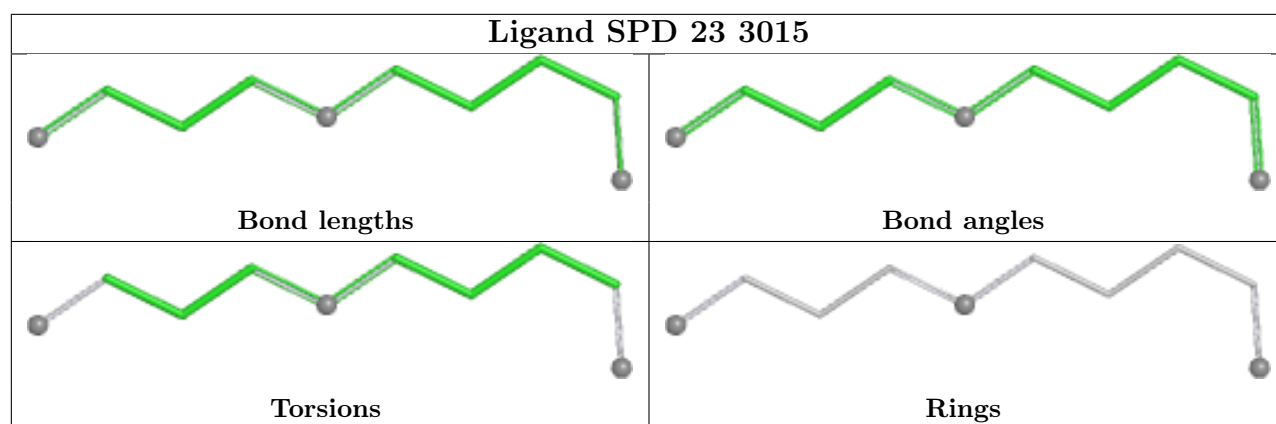
There are no ring outliers.

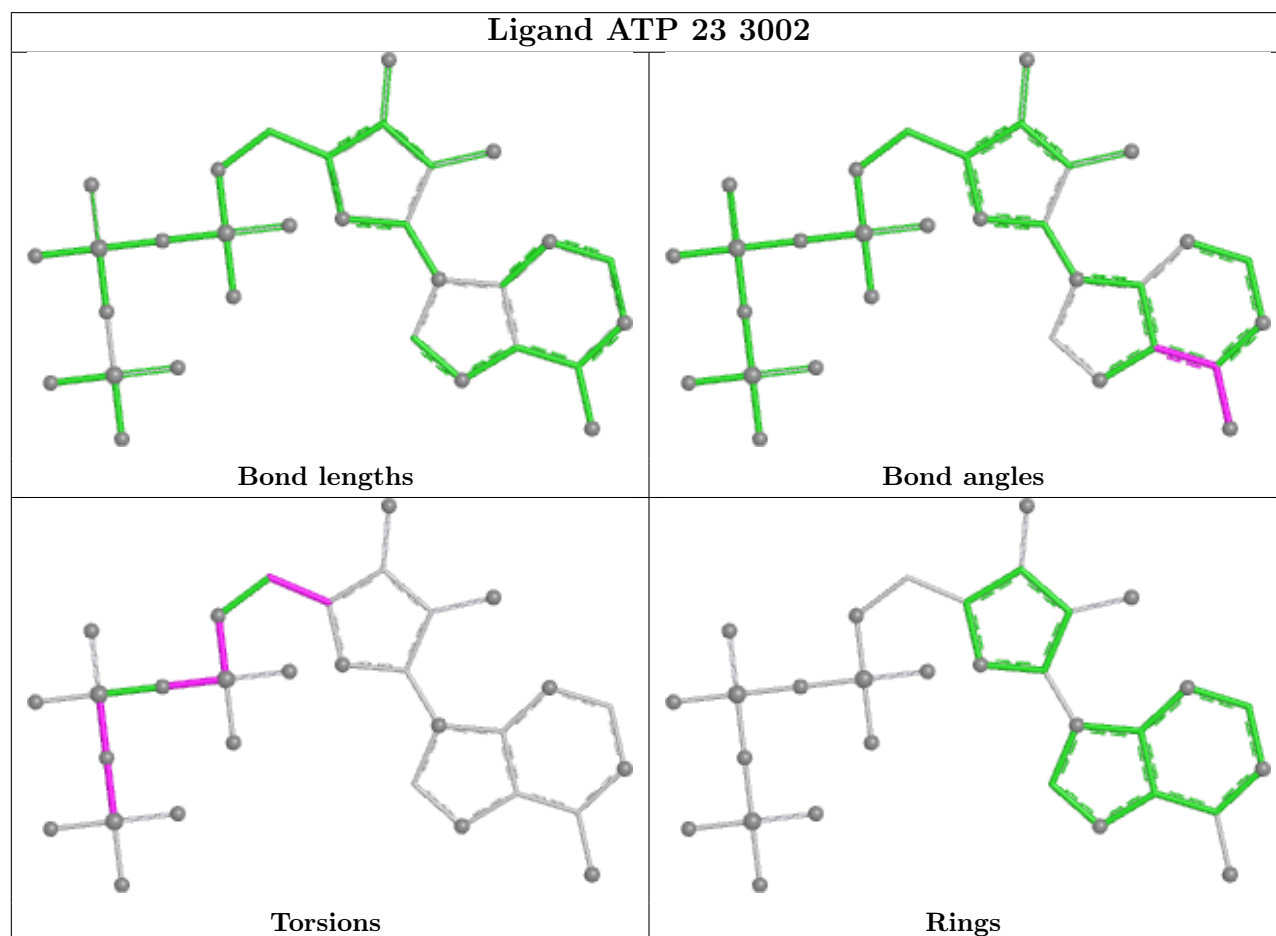
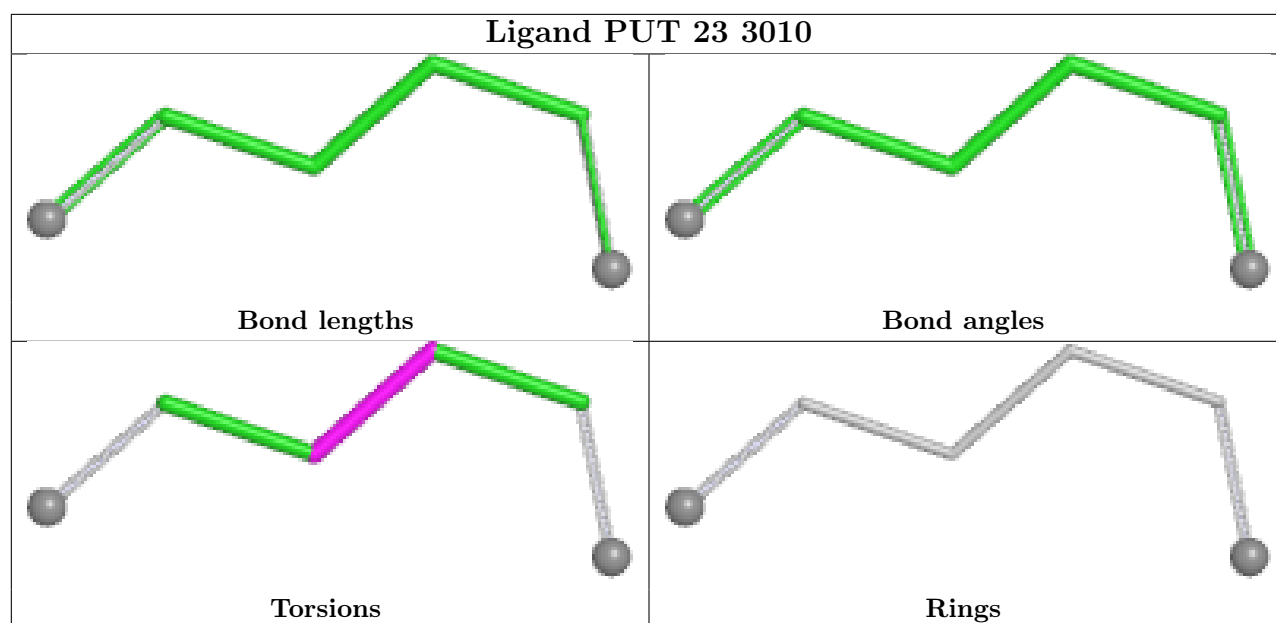
No monomer is involved in short contacts.

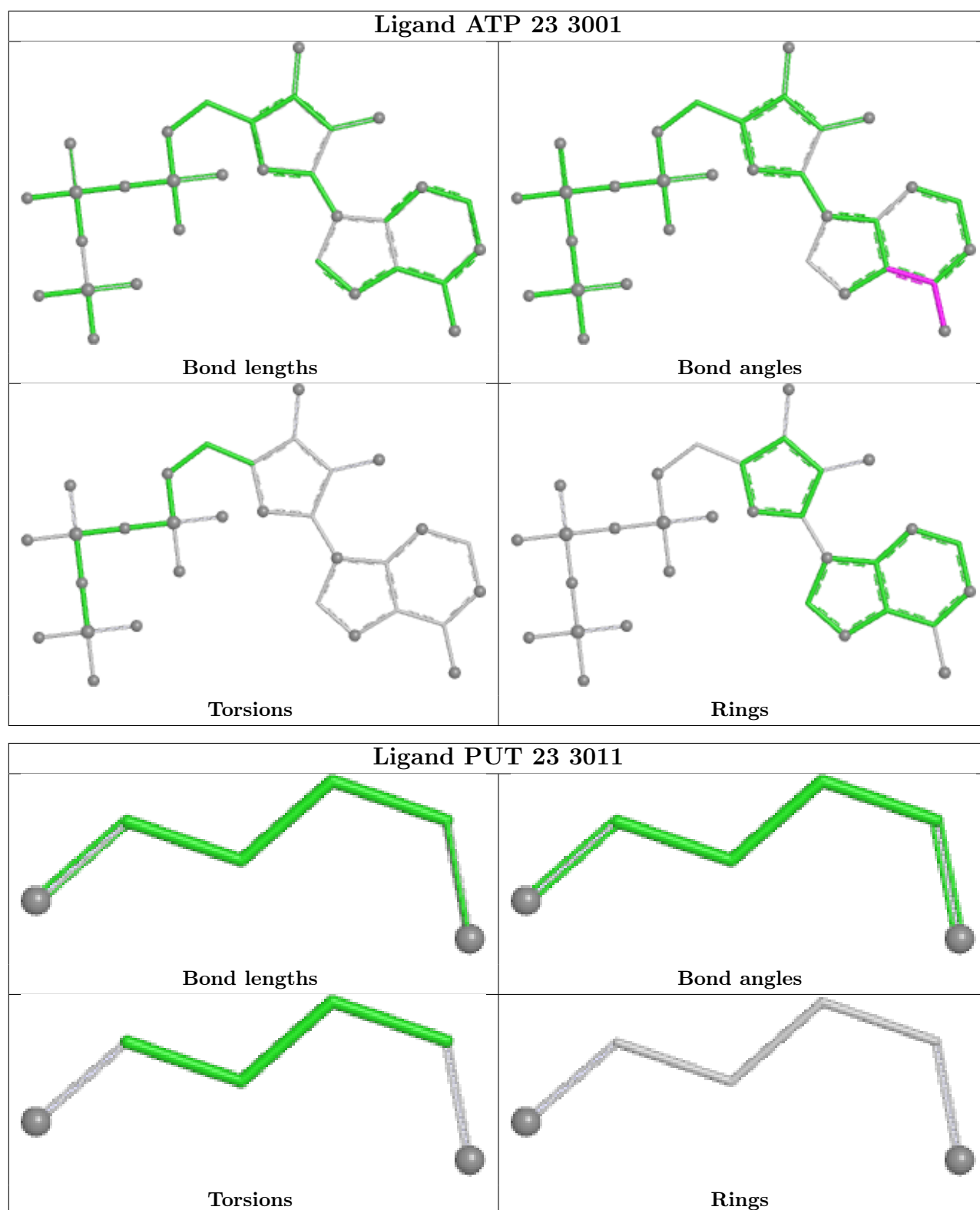
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

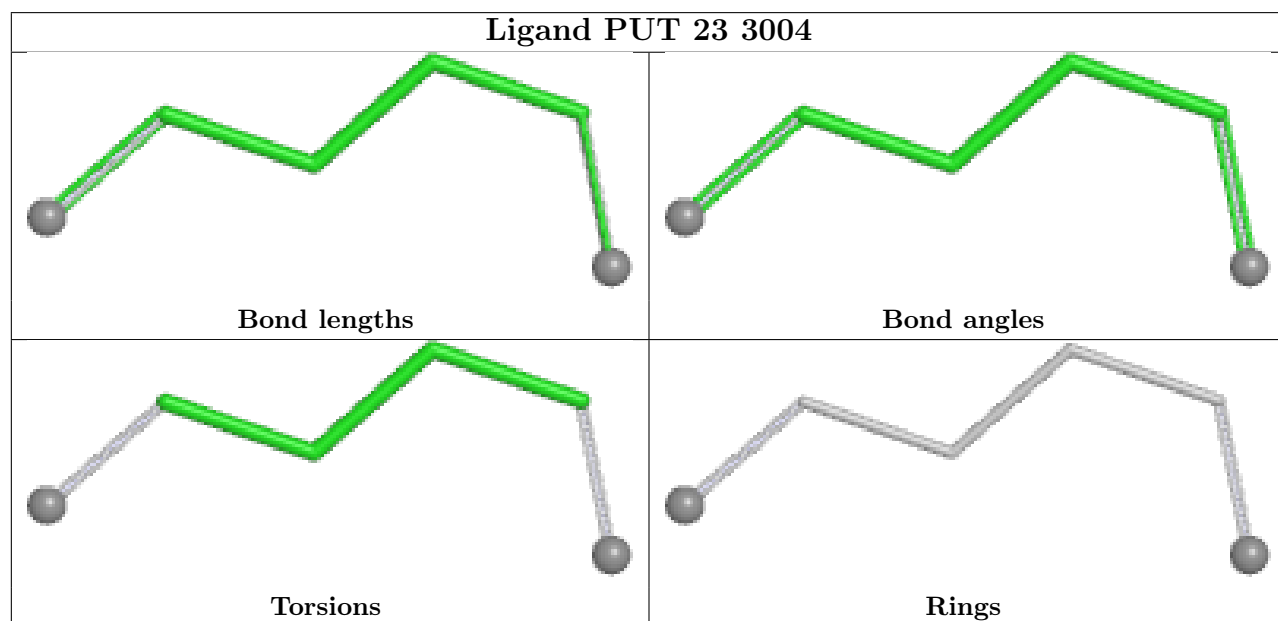
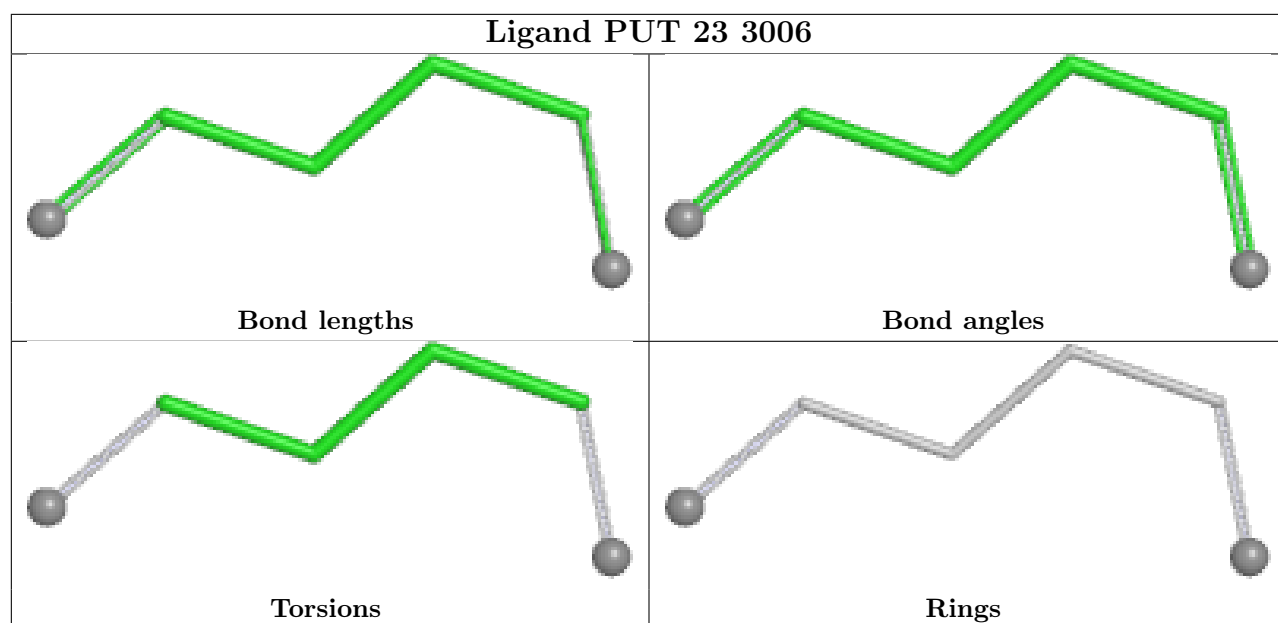


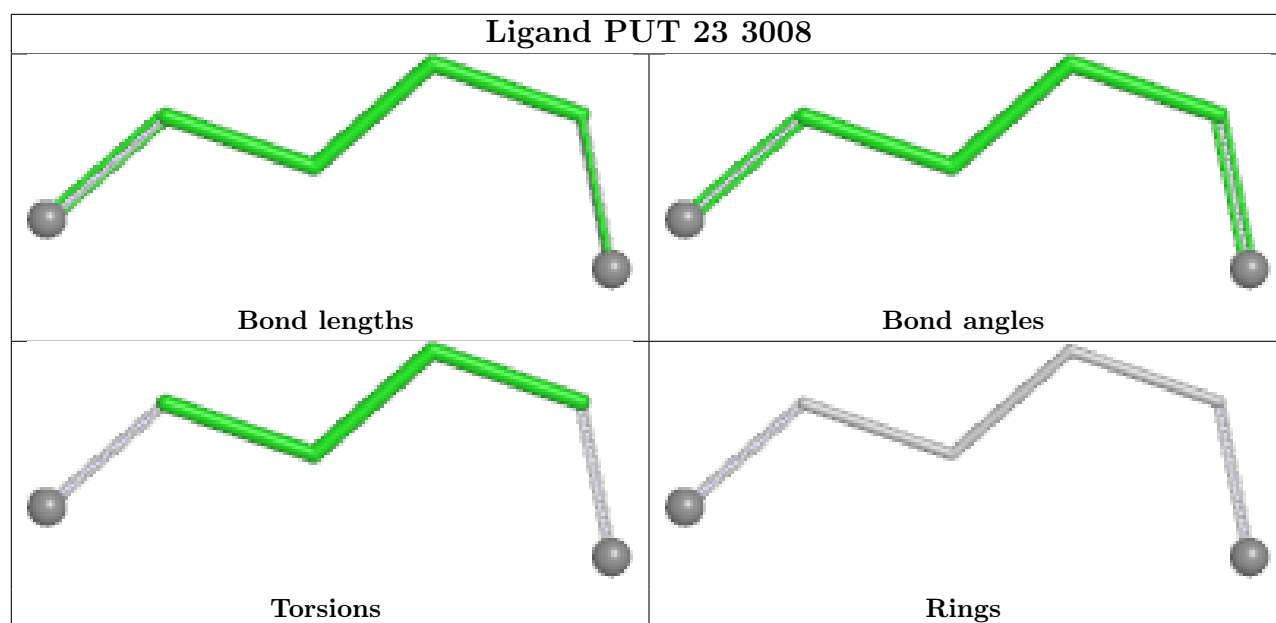












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

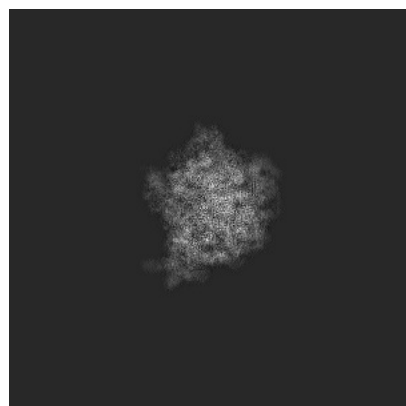
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24136. These allow visual inspection of the internal detail of the map and identification of artifacts.

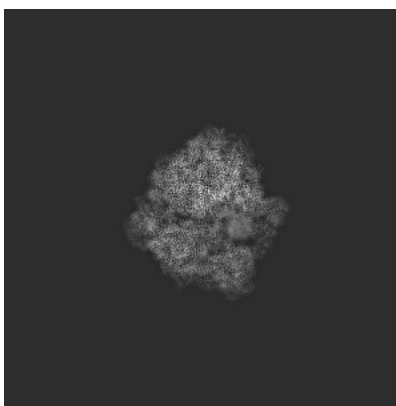
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

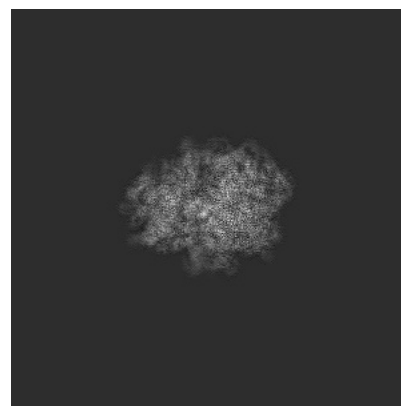
6.1.1 Primary map



X

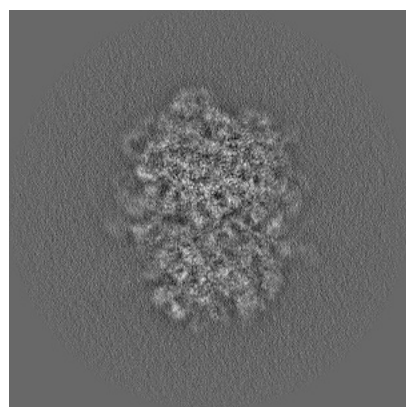


Y

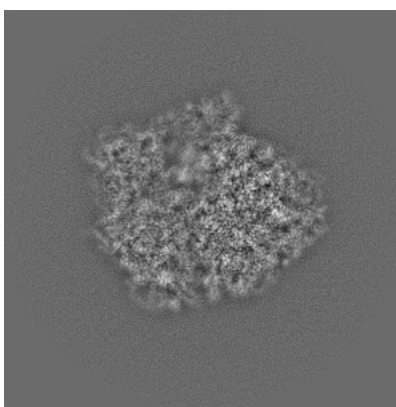


Z

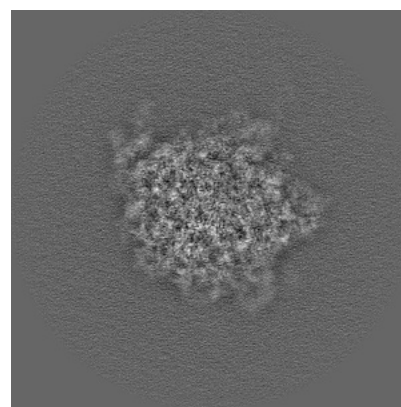
6.1.2 Raw map



X



Y

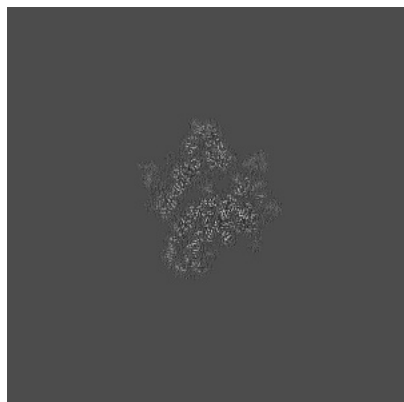


Z

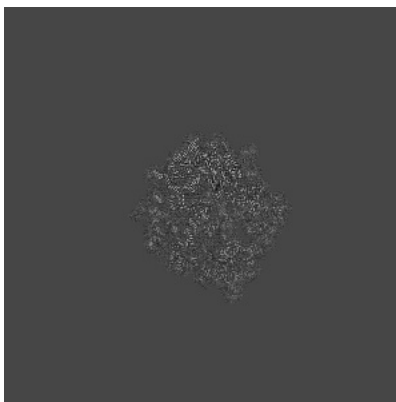
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

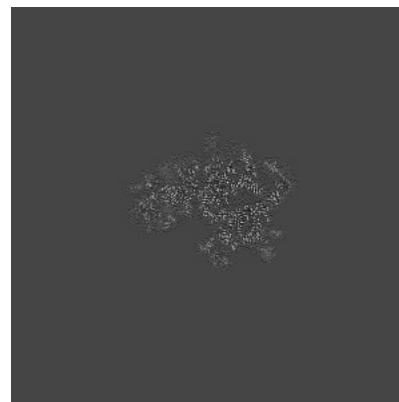
6.2.1 Primary map



X Index: 288

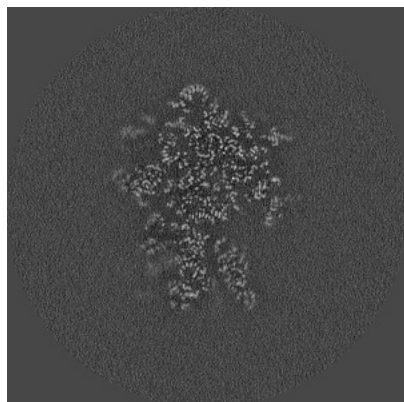


Y Index: 288

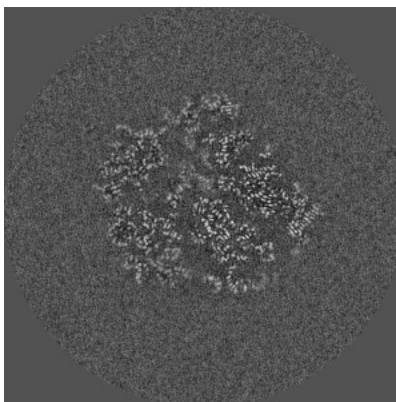


Z Index: 288

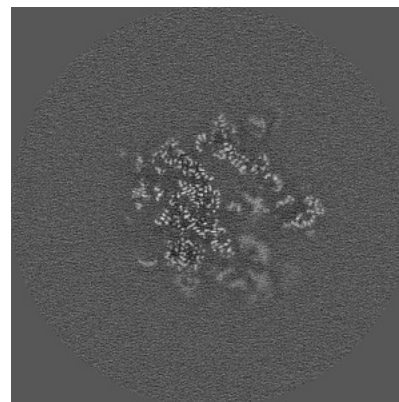
6.2.2 Raw map



X Index: 256



Y Index: 256

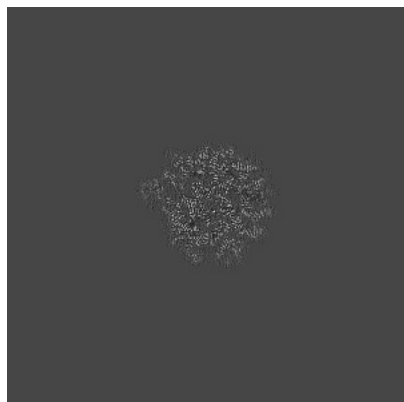


Z Index: 256

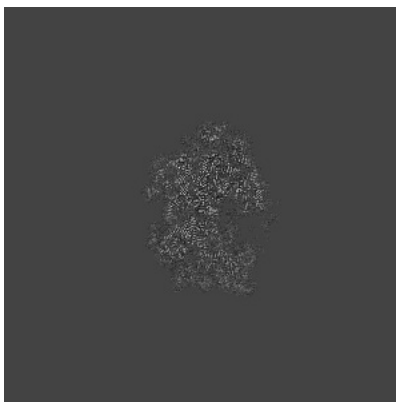
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

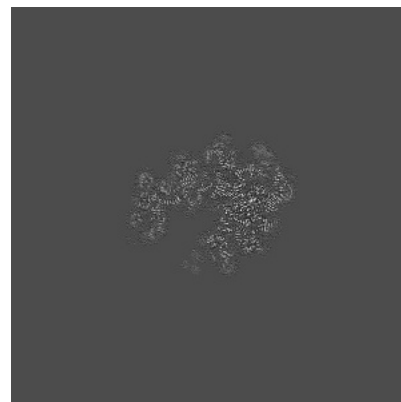
6.3.1 Primary map



X Index: 316

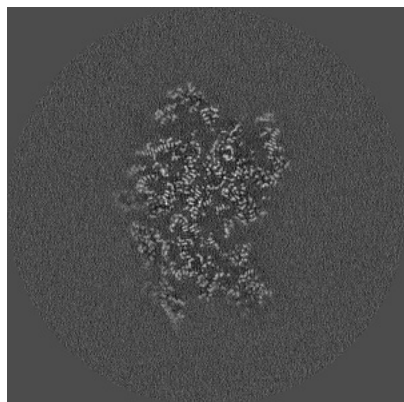


Y Index: 315

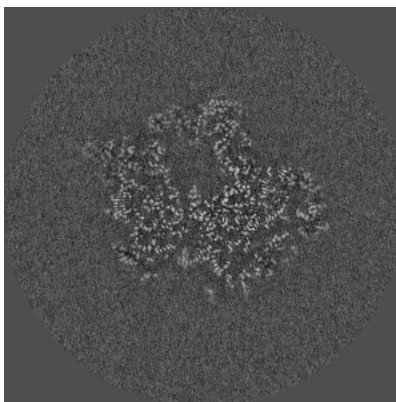


Z Index: 304

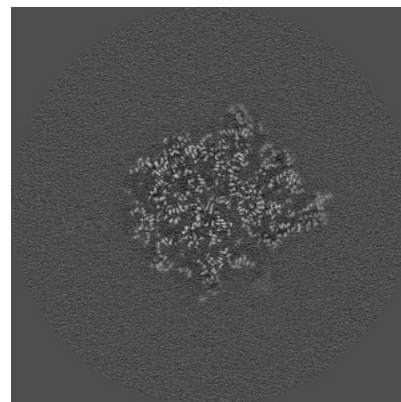
6.3.2 Raw map



X Index: 228



Y Index: 234

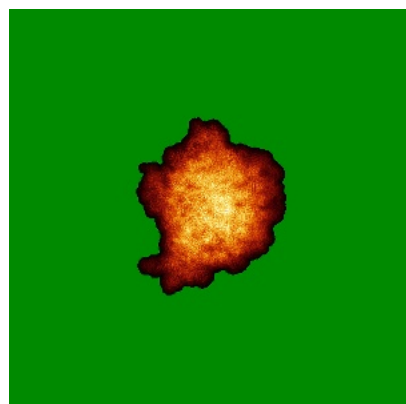


Z Index: 284

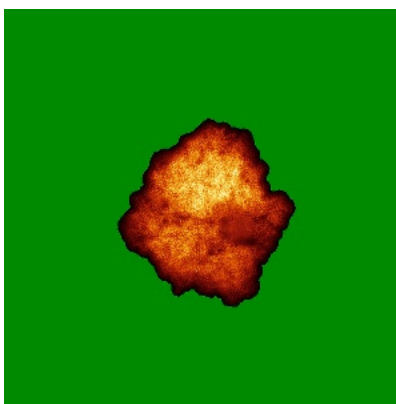
The images above show the largest variance slices of the map in three orthogonal directions.

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

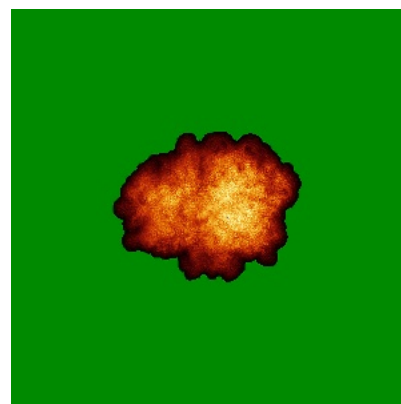
6.4.1 Primary map



X

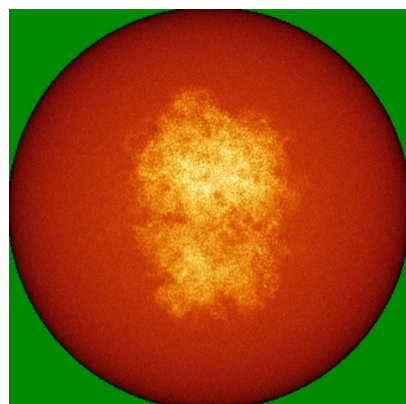


Y

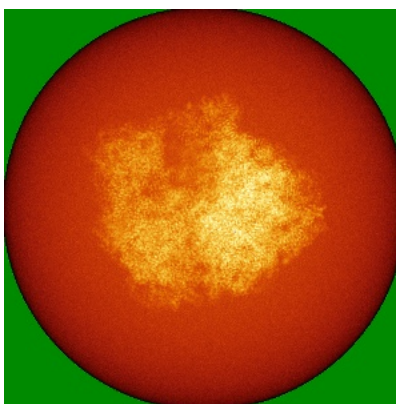


Z

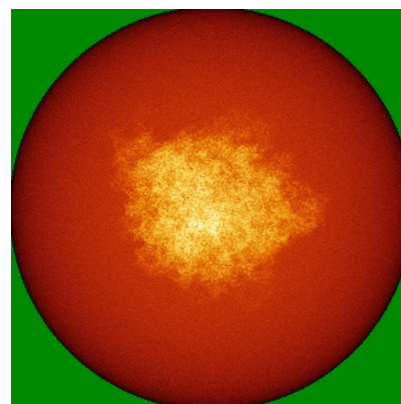
6.4.2 Raw map



X



Y

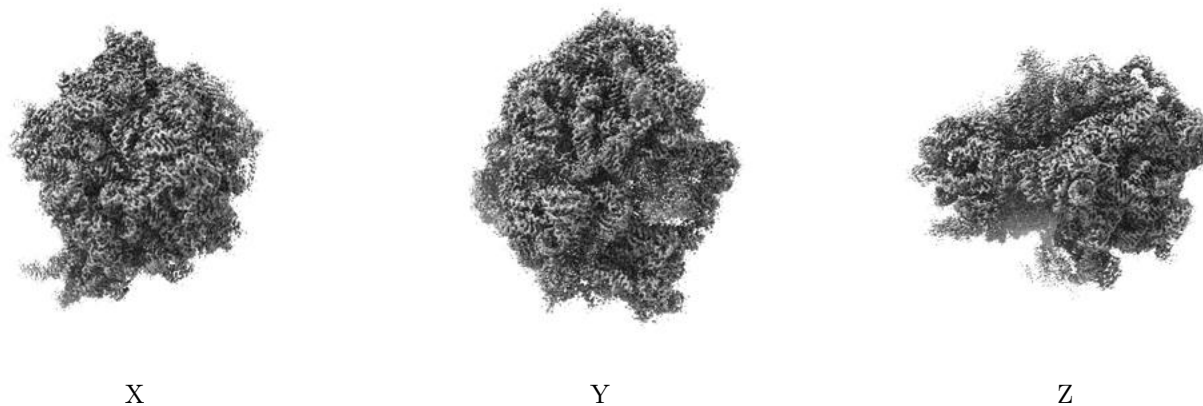


Z

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.

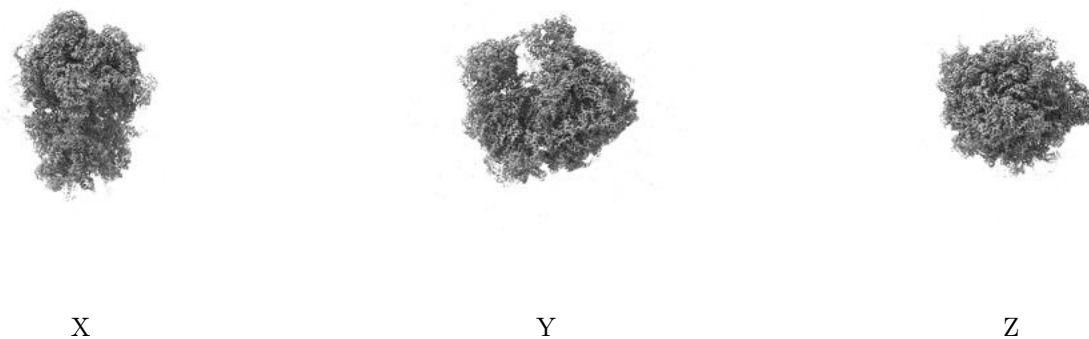
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

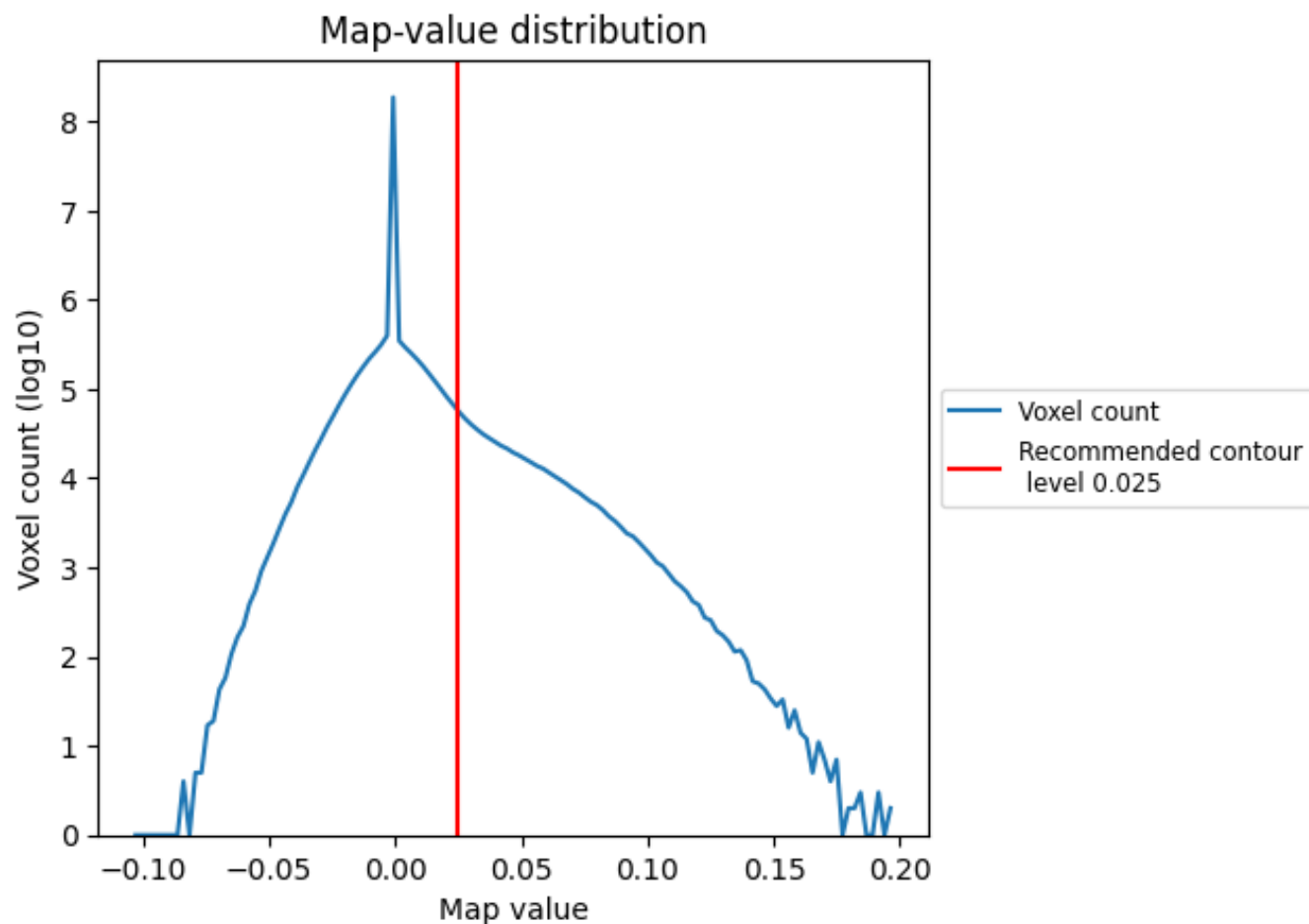
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

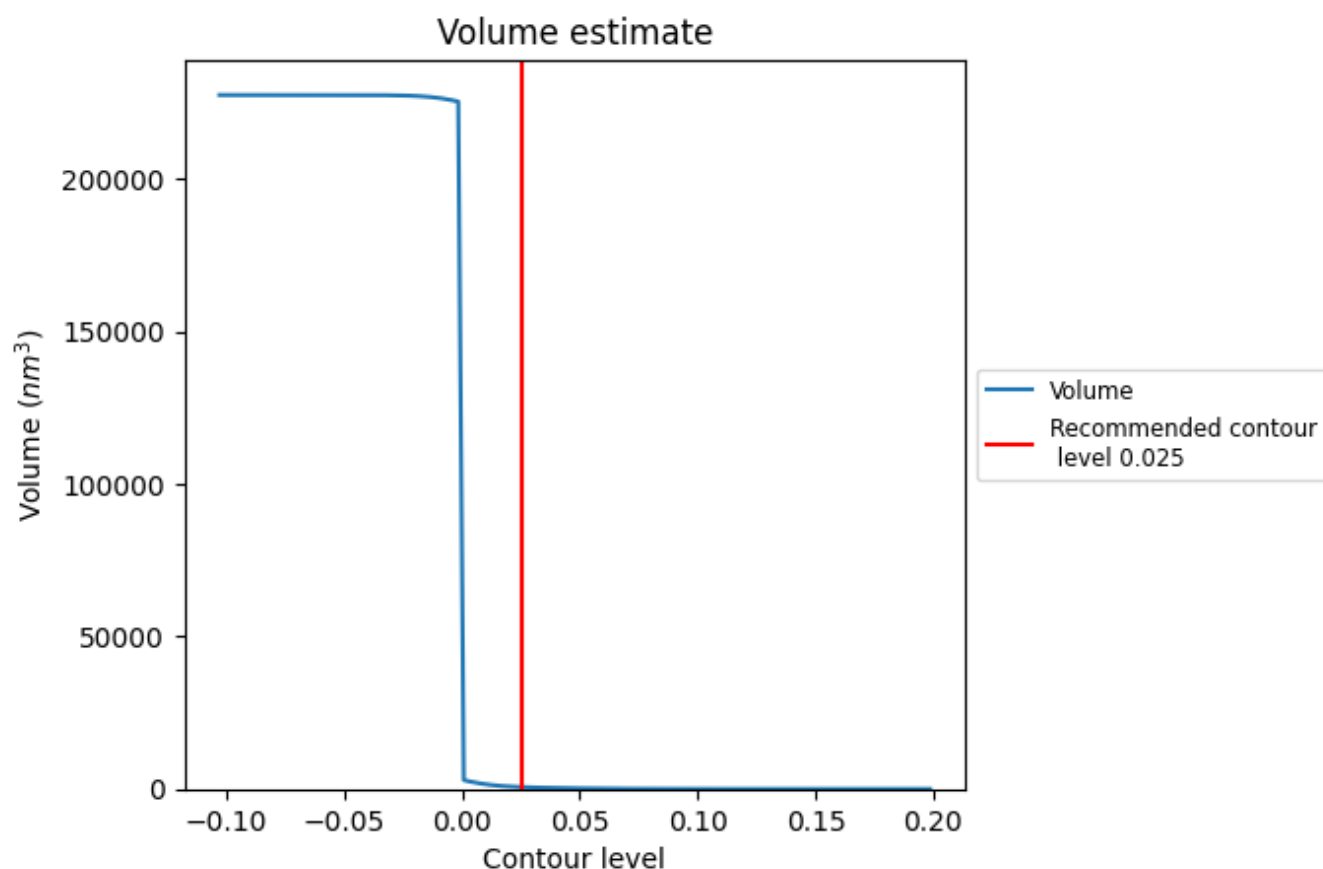
This section contains the results of statistical analysis of the map.

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.

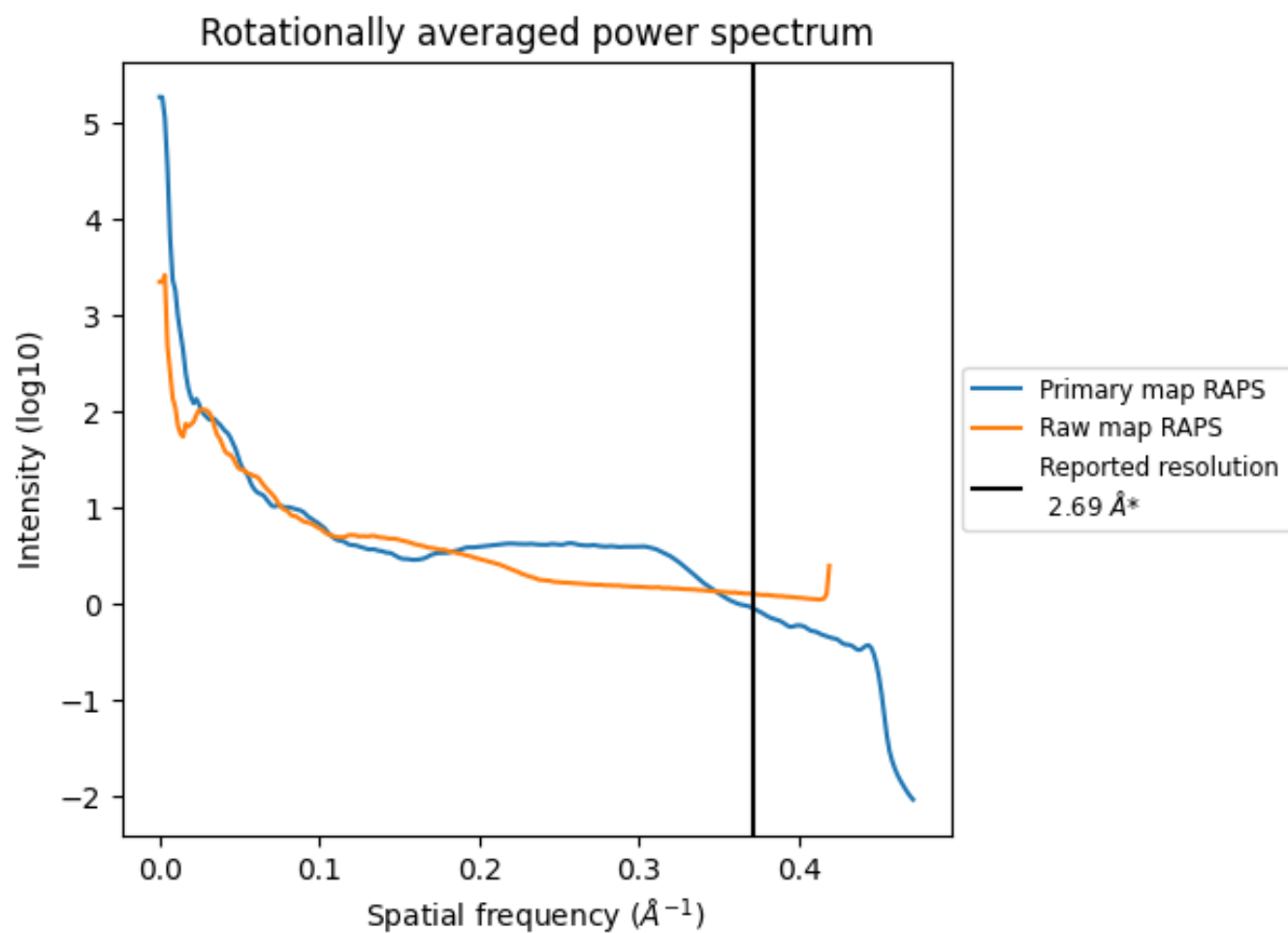
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 613 nm^3 ; this corresponds to an approximate mass of 553 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 ⓘ

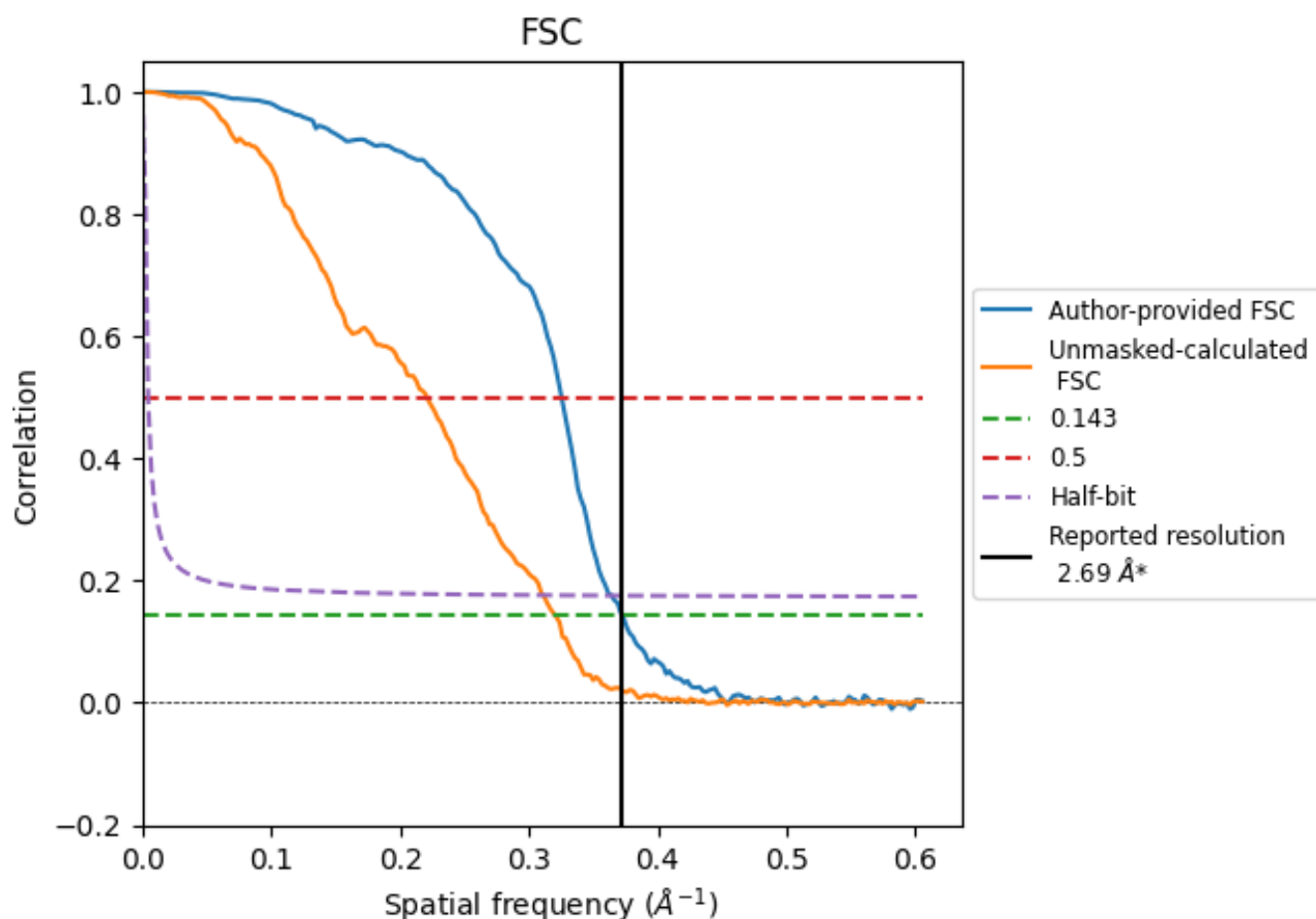


*Reported resolution corresponds to spatial frequency of 0.372 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.372 Å⁻¹

8.2 Resolution estimates [i](#)

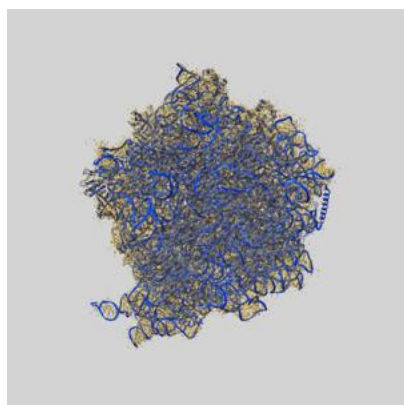
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.69	-	-
Author-provided FSC curve	2.68	3.07	2.74
Unmasked-calculated*	3.12	4.52	3.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.69 by more than 10 %

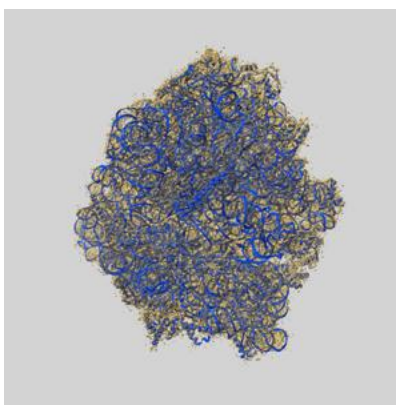
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24136 and PDB model 7N31. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

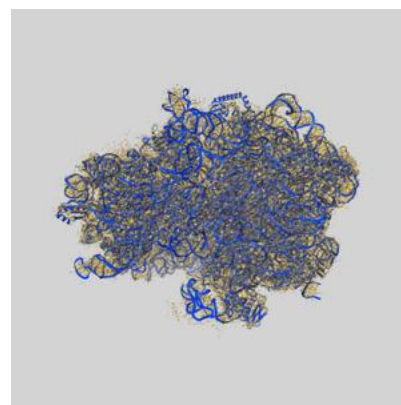
9.1 Map-model overlay [i](#)



X



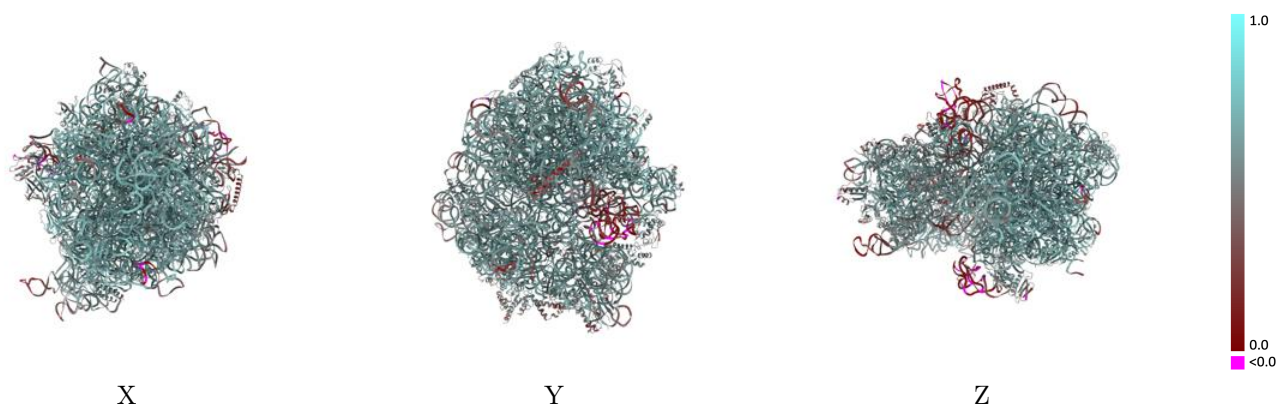
Y



Z

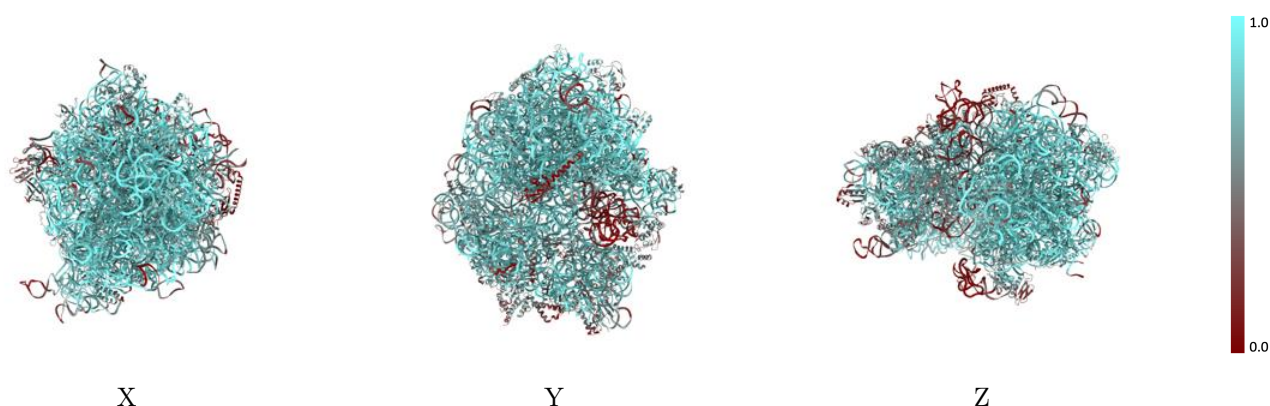
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



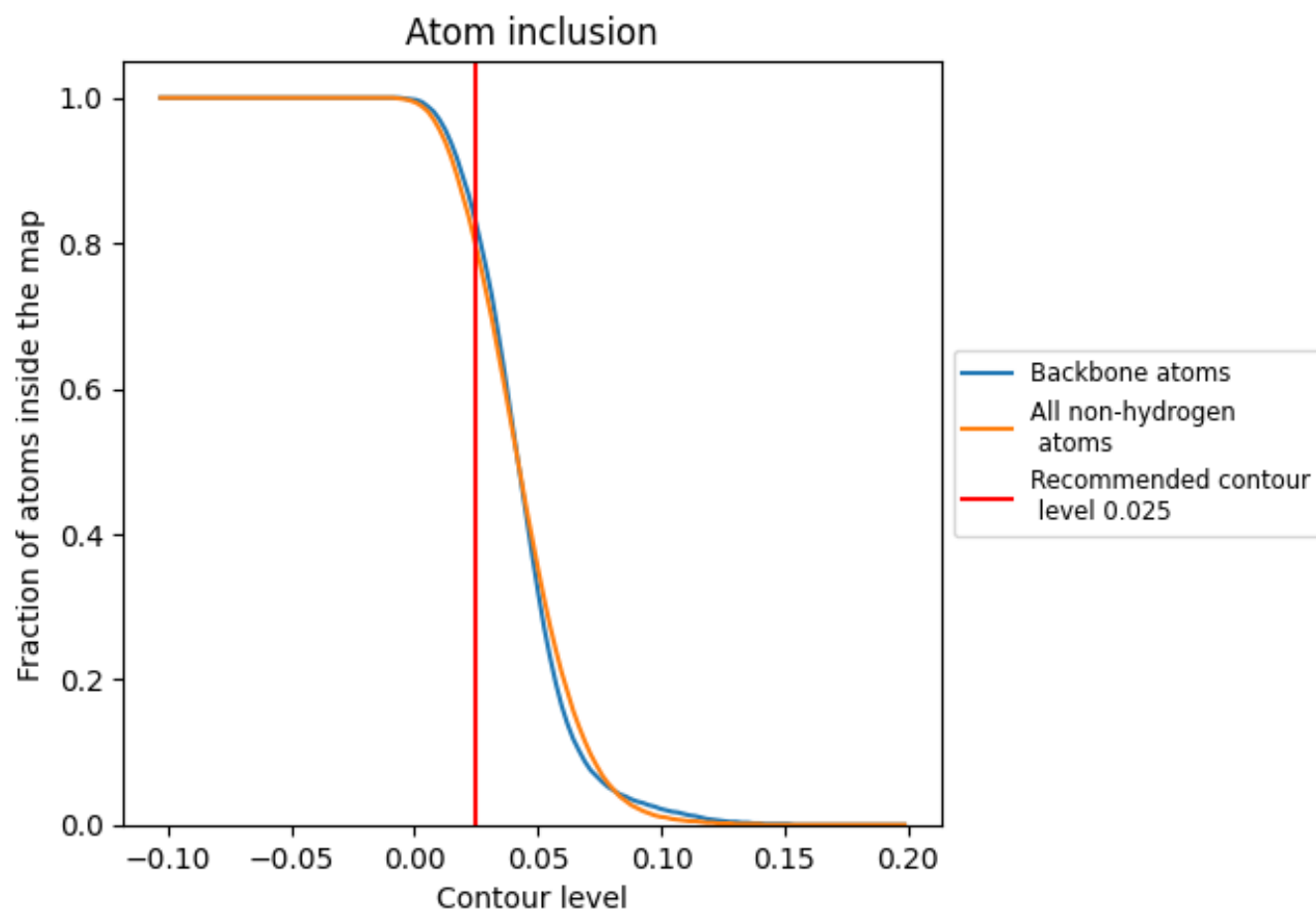
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 79% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7940	 0.5990
16	 0.8440	 0.6050
23	 0.8590	 0.6130
5	 0.8460	 0.6090
Dt	 0.2990	 0.3540
LB	 0.8580	 0.6630
LC	 0.8490	 0.6590
LD	 0.7550	 0.6130
LE	 0.5610	 0.5320
LF	 0.5190	 0.5070
LI	 0.2180	 0.3510
LM	 0.8380	 0.6520
LN	 0.7950	 0.6440
LO	 0.8020	 0.6340
LP	 0.8160	 0.6380
LQ	 0.8890	 0.6690
LR	 0.7090	 0.5970
LS	 0.7920	 0.6270
LT	 0.8940	 0.6750
LU	 0.7740	 0.6240
LV	 0.8160	 0.6480
LW	 0.7440	 0.6180
LX	 0.6920	 0.5740
LY	 0.6860	 0.5690
La	 0.7670	 0.6280
Lb	 0.8230	 0.6490
Lc	 0.6190	 0.5630
Ld	 0.7870	 0.6240
Le	 0.3910	 0.4480
Lf	 0.8160	 0.6480
Lg	 0.6540	 0.5920
Lh	 0.9100	 0.6840
Li	 0.8860	 0.6780
Lj	 0.8050	 0.6350
Pp	 0.2860	 0.5340



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Chain	Atom inclusion	Q-score
Pt	 0.5760	 0.5120
SB	 0.5090	 0.5030
SC	 0.6380	 0.5620
SD	 0.6220	 0.5650
SE	 0.7570	 0.6120
SF	 0.5670	 0.5280
SG	 0.5540	 0.5280
SH	 0.7430	 0.6060
SI	 0.6180	 0.5450
SJ	 0.4880	 0.4920
SK	 0.6790	 0.5870
SL	 0.7120	 0.6020
SM	 0.6080	 0.5510
SN	 0.6530	 0.5790
SO	 0.6910	 0.5890
SP	 0.7080	 0.5920
SQ	 0.5980	 0.5560
SR	 0.6730	 0.5720
SS	 0.5840	 0.5400
ST	 0.6800	 0.5940
SU	 0.4650	 0.4850
mR	 0.5240	 0.4920