



wwPDB EM Validation Summary Report ⓘ

Sep 16, 2026 – 10:28 PM EDT

PDB ID : 7N2V / pdb_00007n2v
EMDB ID : EMD-24134
Title : Elongating 70S ribosome complex in a spectinomycin-stalled intermediate state of translocation bound to EF-G in an active, GTP conformation (INT1)
Authors : Rundlet, E.J.; Holm, M.; Schacherl, M.; Natchiar, K.S.; Altman, R.B.; Spahn, C.M.T.; Myasnikov, A.G.; Blanchard, S.C.
Deposited on : 2021-05-29
Resolution : 2.54 Å(reported)

This is a 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:

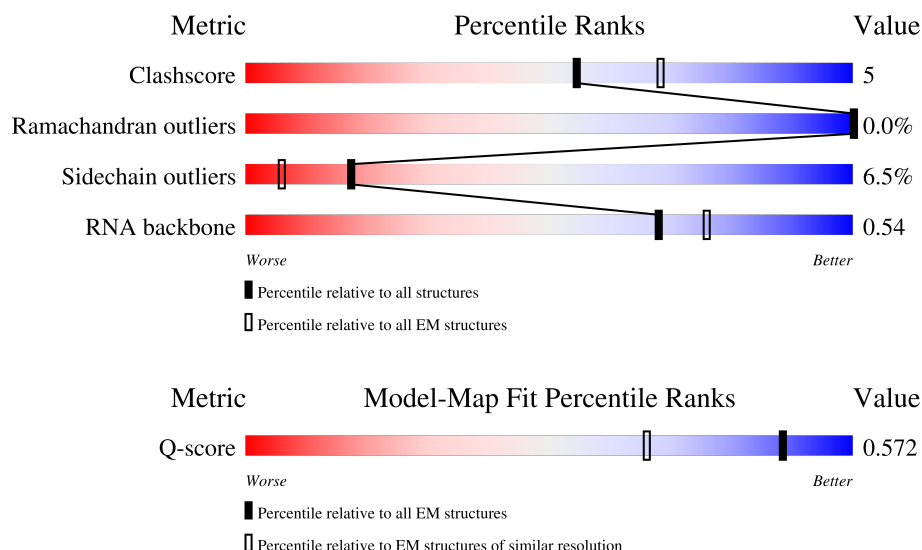
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.54 Å.

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



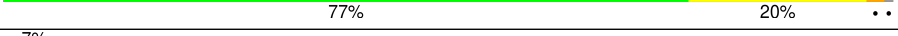
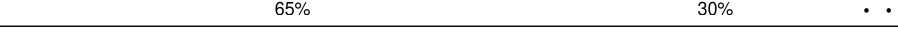
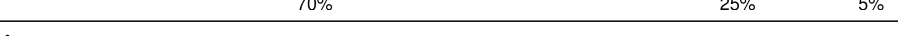
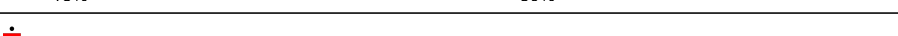
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7403 (2.04 - 3.04)

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	
2	SB	241	
3	SC	233	

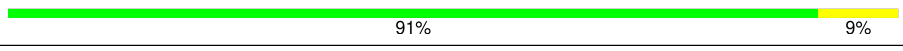
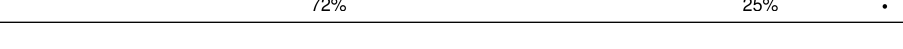
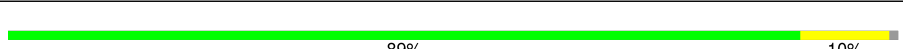
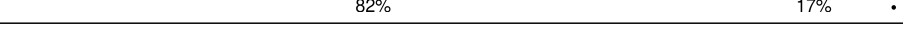
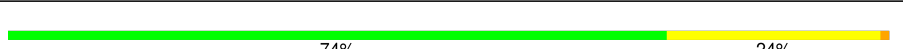
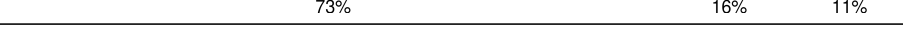
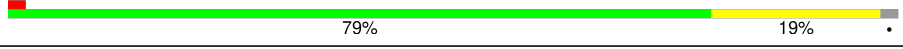
Continued on next page...

Continued from previous page...

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	

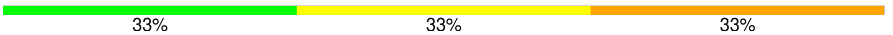
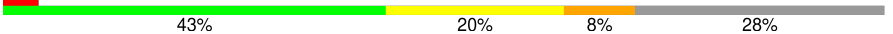
Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	Li	65	
55	Lj	38	
56	EF	704	
57	Pp	3	
58	Pt	106	
59	Dt	106	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
64	ATP	23	3003	X	-	-	-

2 Entry composition

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	16	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is a protein called Elongation factor G.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 57 is a protein called Nascent peptide.

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

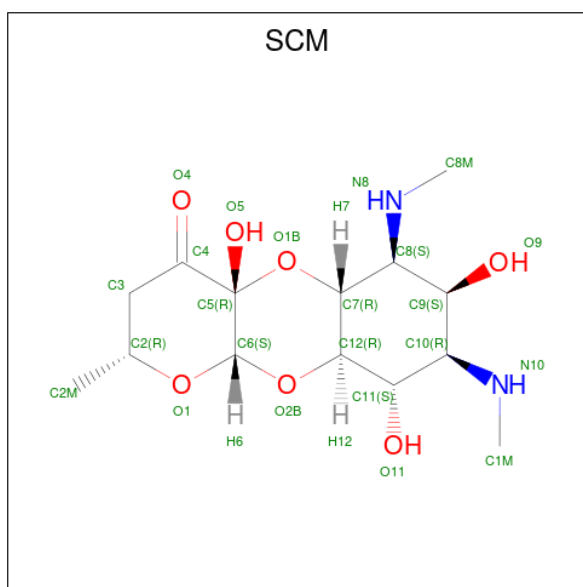
- Molecule 58 is a RNA chain called tRNA.

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

- Molecule 59 is a RNA chain called tRNA.

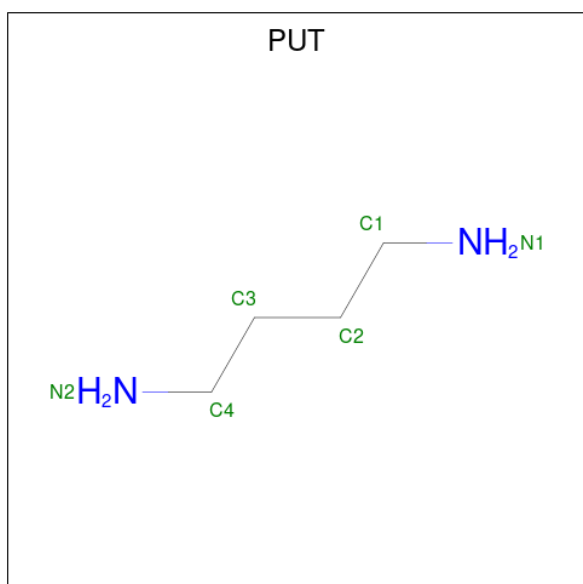
Mol	Chain	Residues	Atoms					AltConf	Trace
59	Dt	76	Total	C	N	O	P S	0	0
			1641	735	294	534	76 2		

- Molecule 60 is SPECTINOMYCIN (CCD ID: SCM) (formula: $C_{14}H_{24}N_2O_7$) (labeled as "Ligand of Interest" by depositor).



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

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



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

- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

Continued on next page...

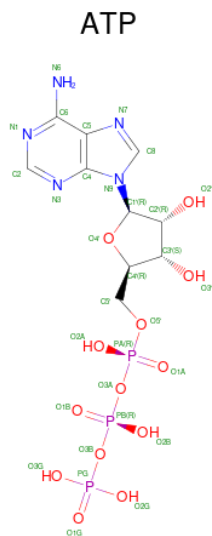
Continued from previous page...

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

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

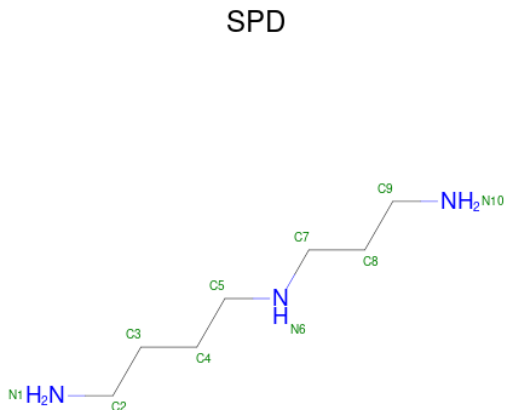
Mol	Chain	Residues	Atoms		AltConf
63	SB	1	Total 1	Zn 1	0
63	Le	1	Total 1	Zn 1	0
63	Lj	1	Total 1	Zn 1	0

- Molecule 64 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 65 is SPERMIDINE (CCD ID: SPD) (formula: $\text{C}_7\text{H}_{19}\text{N}_3$) (labeled as "Ligand of Interest" by depositor).



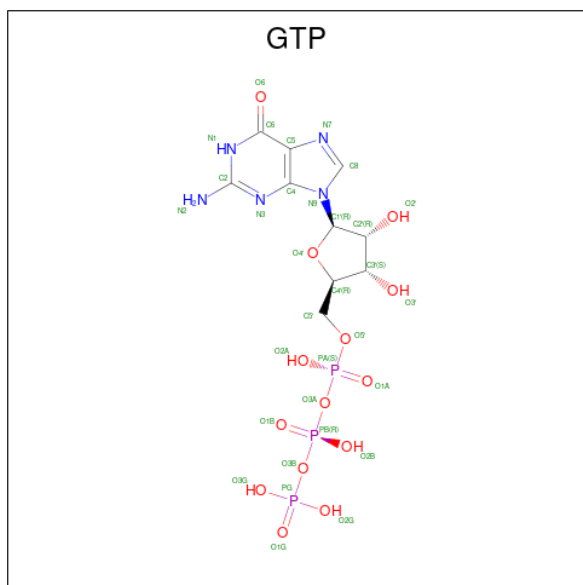
Mol	Chain	Residues	Atoms			AltConf
65	23	1	Total	C	N	0
			10	7	3	

Continued on next page...

Continued from previous page...

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

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



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

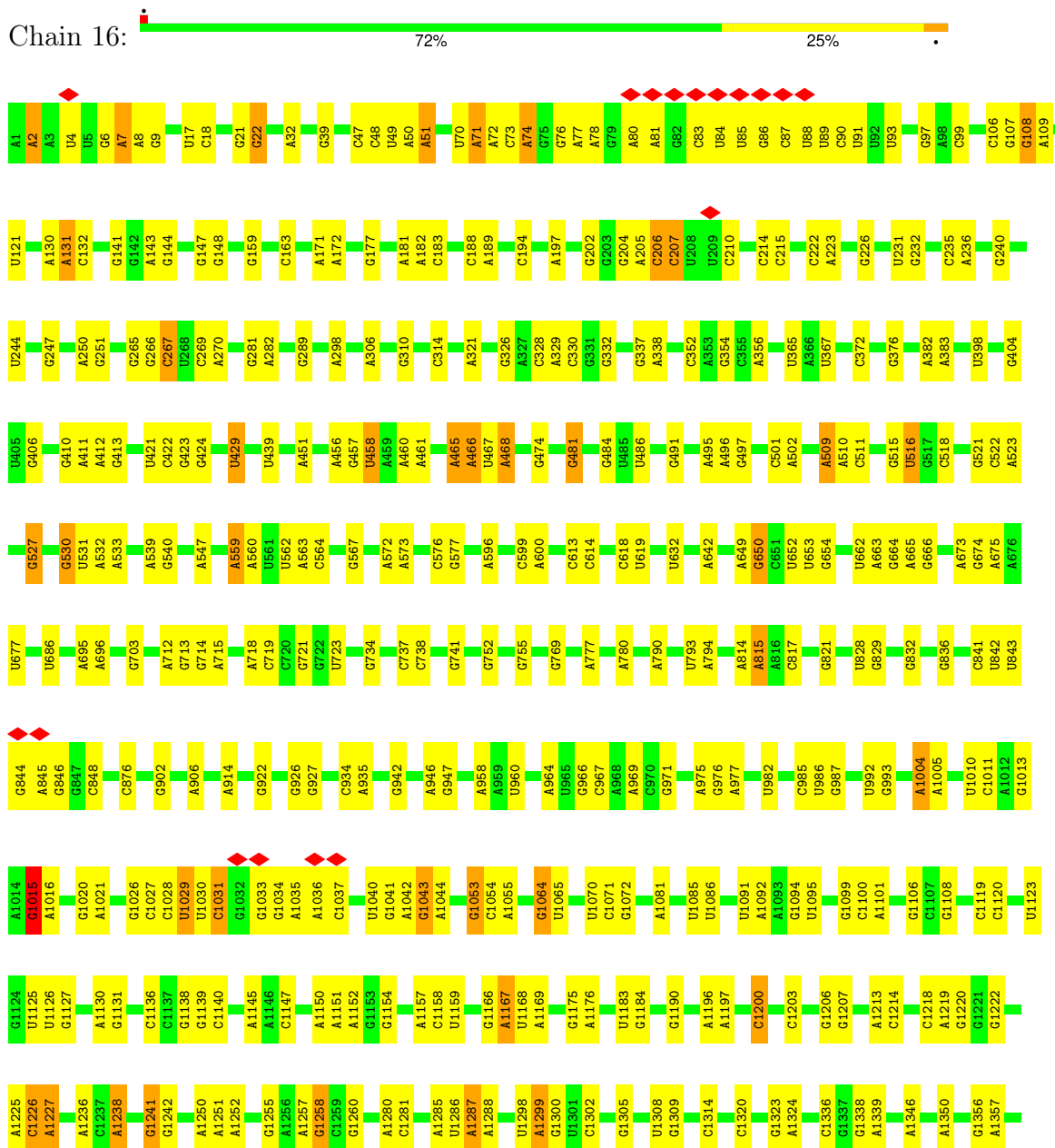
- Molecule 67 is water.

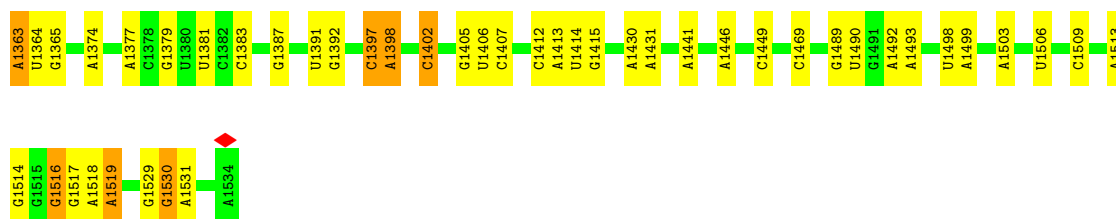
Mol	Chain	Residues	Atoms		AltConf
67	16	1	Total	O	0
			1	1	
67	SB	1	Total	O	0
			1	1	
67	23	22	Total	O	0
			22	22	
67	LB	1	Total	O	0
			1	1	
67	EF	1	Total	O	0
			1	1	

3 Residue-property plots

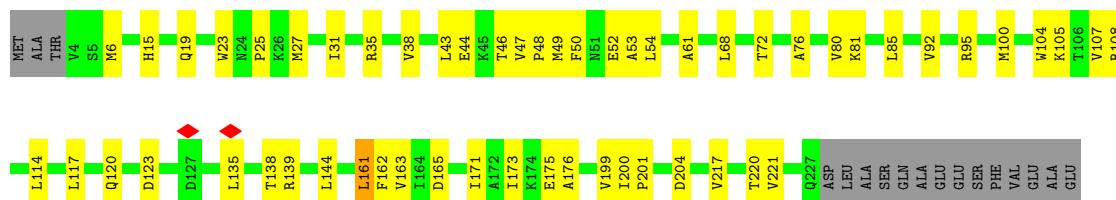
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

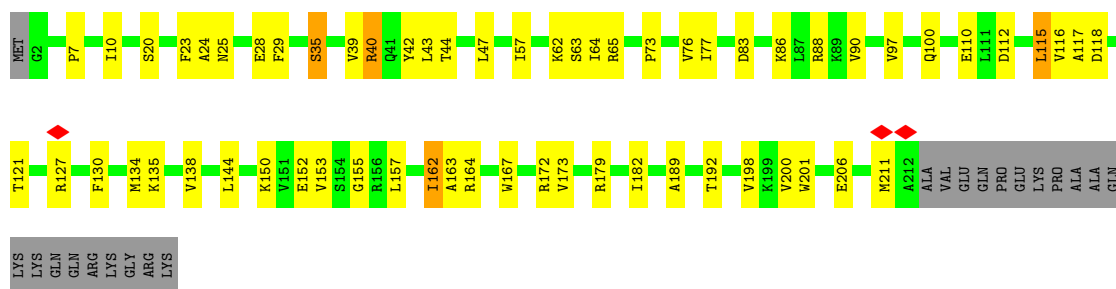




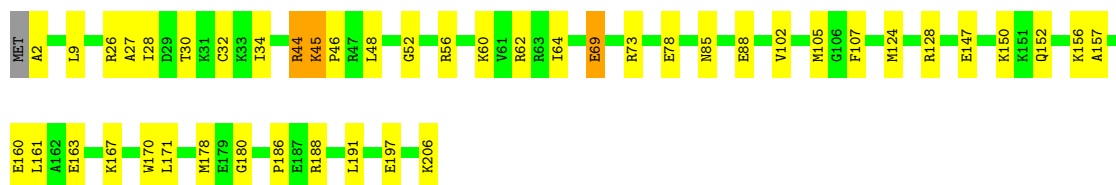
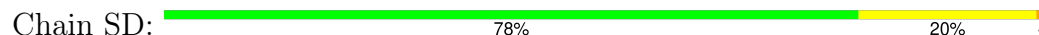
• Molecule 2: 30S ribosomal protein S2



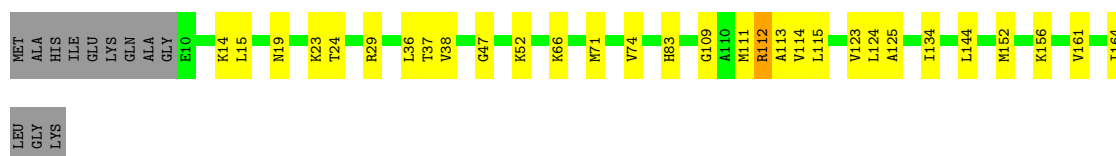
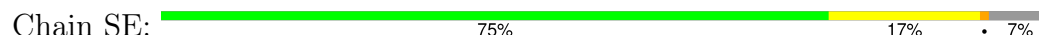
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5



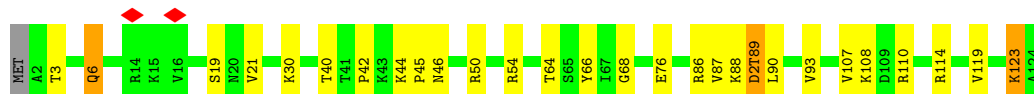
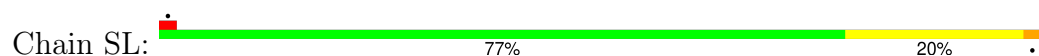
- | MET | GLN | ASN |
|-----|-----|-----|
| Q4 | | |
| R5 | | |
| I6 | | |
| R7 | | |
| I8 | | |
| R9 | | |
| L10 | | |
| K11 | | |
| D14 | | |
| H15 | | |
| R16 | | |
| L17 | | |
| I18 | | |
| D19 | | |
| Q20 | | |
| A21 | | |
| T22 | | |
| I25 | | |
| K30 | | |
| R31 | | |
| T32 | | |
| Q35 | | |
| G38 | | |
| P39 | | |
| L40 | | |
| P41 | | |
| L42 | | |
| P43 | | |
| R48 | | |
| V51 | | |
| L52 | | |
| H56 | | |
| V57 | | |
| R62 | | |
| T69 | | |
| H70 | | |
| L71 | | |
| R72 | | |
| L73 | | |
| V74 | | |
| E78 | | |
| F79 | | |
| T80 | | |
| E81 | | |
| K82 | | |



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14

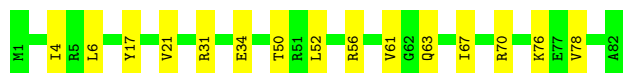


- Molecule 15: 30S ribosomal protein S15



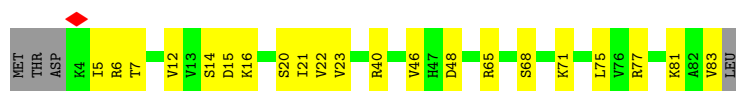
- Molecule 16: 30S ribosomal protein S16

Chain SP:  82% 18%



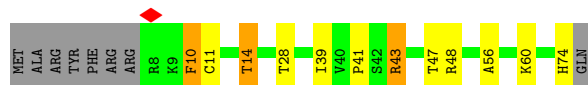
- Molecule 17: 30S ribosomal protein S17

Chain SQ:  70% 25% 5%



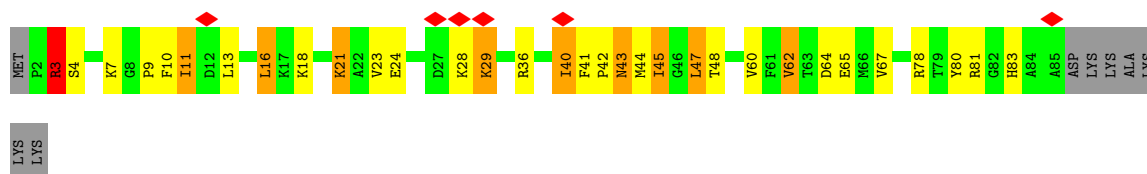
- Molecule 18: 30S ribosomal protein S18

Chain SR:  73% 12% 11%



- Molecule 19: 30S ribosomal protein S19

Chain SS:  7% 57% 24% 10% 9%



- Molecule 20: 30S ribosomal protein S20

Chain ST:  80% 16% ..



- Molecule 21: 30S ribosomal protein S21

Chain SU:  79% 18% ..

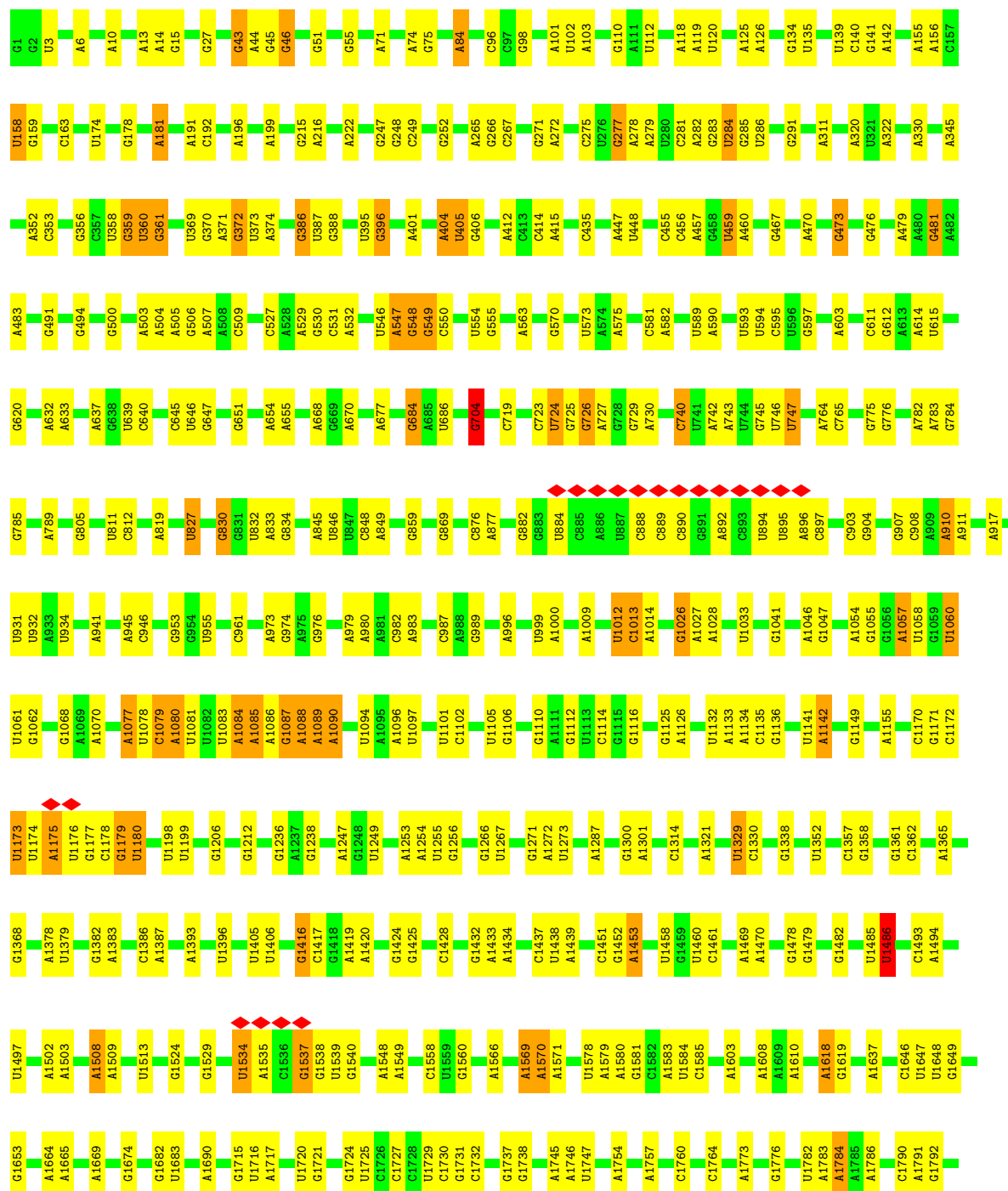
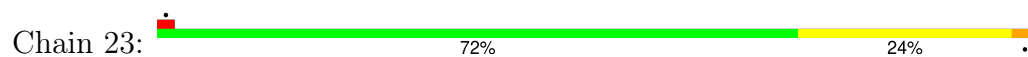


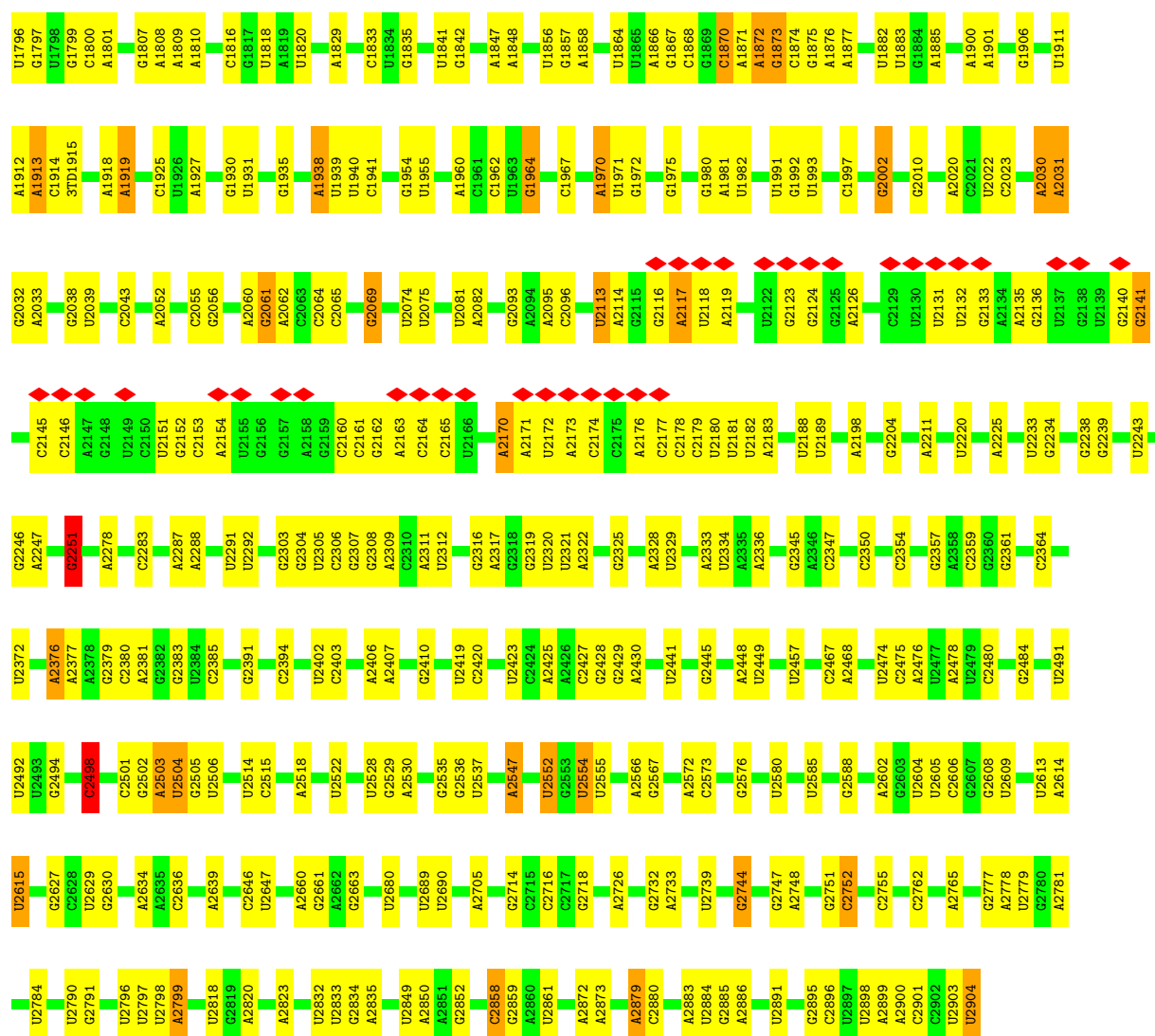
- Molecule 22: mRNA

Chain mR:  15% 80%



• Molecule 23: 23S rRNA





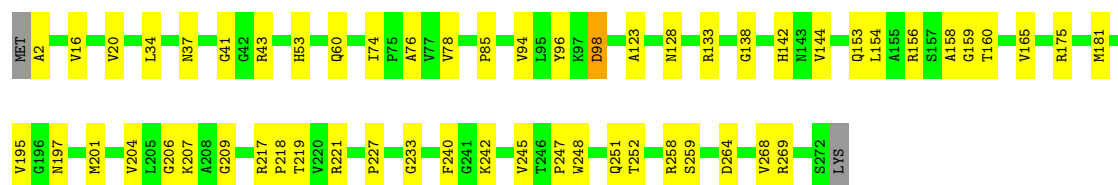
• Molecule 24: 5S rRNA

Chain 5: 79% 19%

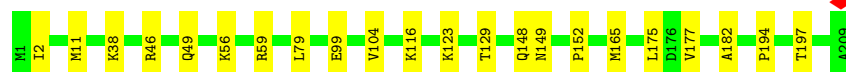


• Molecule 25: 50S ribosomal protein L2

Chain LB: 79% 20%

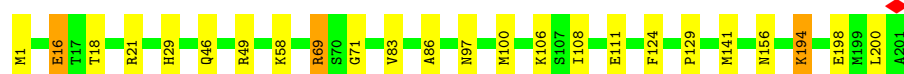


Chain LC:  89% 11%



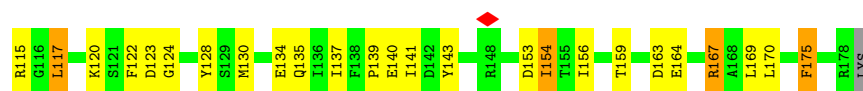
- Molecule 27: 50S ribosomal protein L4

Chain LD:  88% 10%



- Molecule 28: 50S ribosomal protein L5

Chain LE:  66% 27% 6%



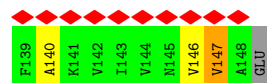
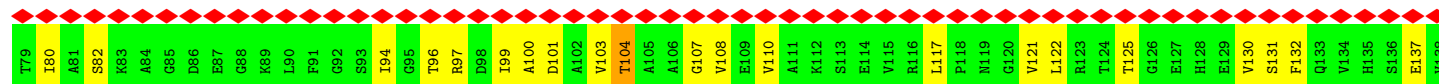
- Molecule 29: 50S ribosomal protein L6

Chain LF:  73% 25%

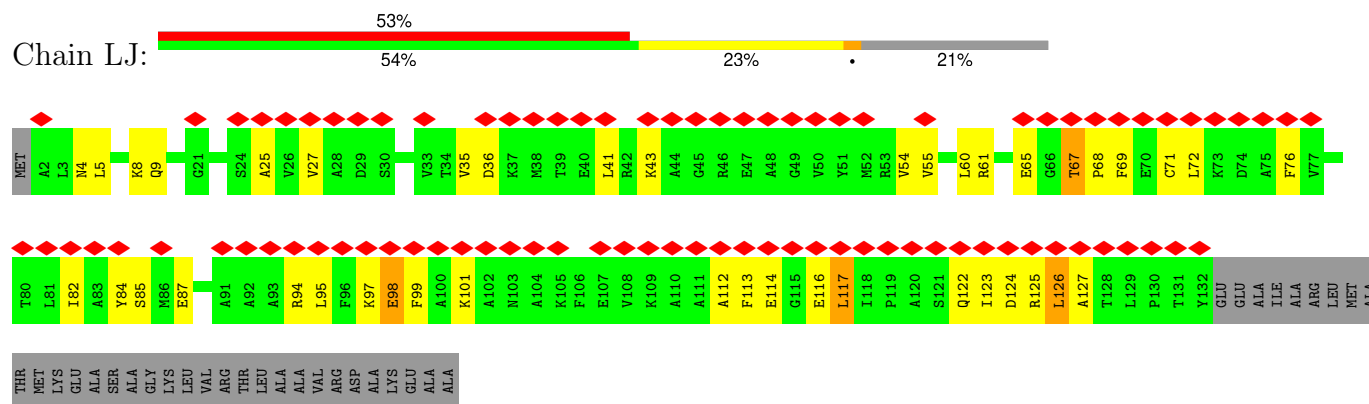


- Molecule 30: 50S ribosomal protein L9

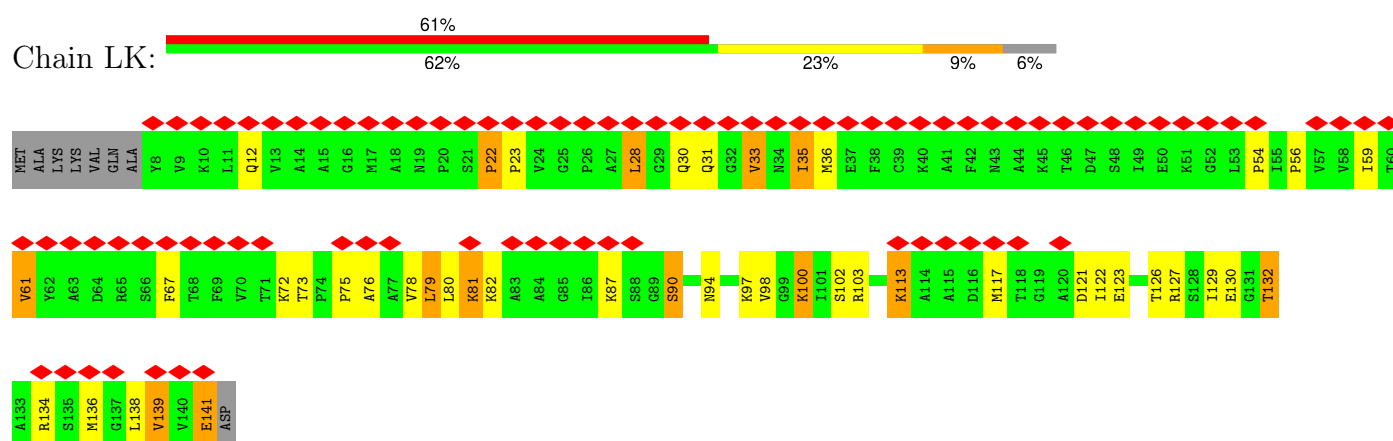
Chain LI:  66% 61% 36%



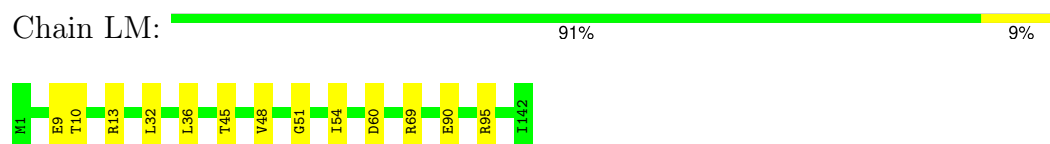
- Molecule 31: 50S ribosomal protein L10



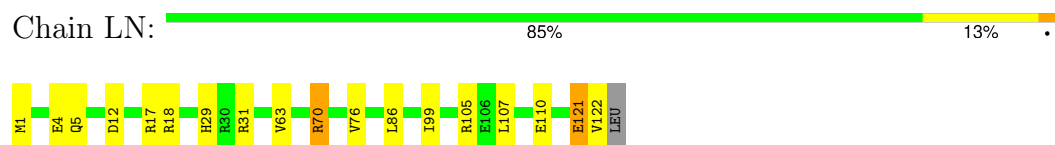
- Molecule 32: 50S ribosomal protein L11



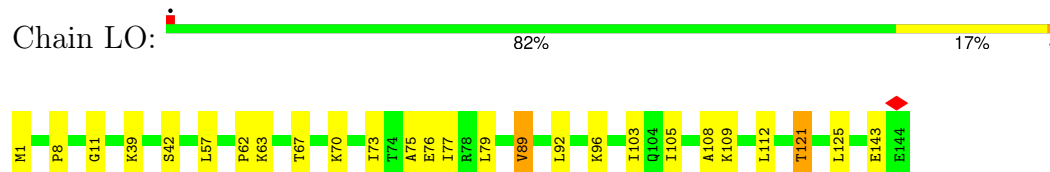
- Molecule 33: 50S ribosomal protein L13



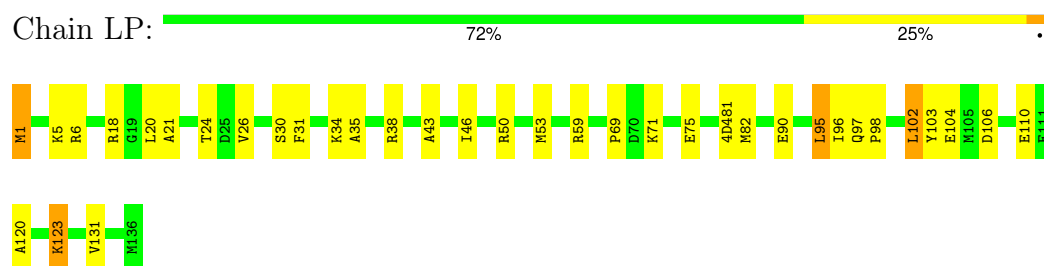
- Molecule 34: 50S ribosomal protein L14



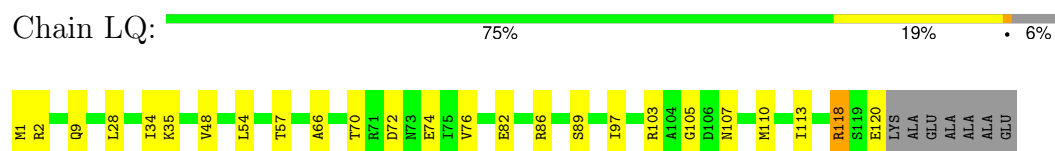
- Molecule 35: 50S ribosomal protein L15



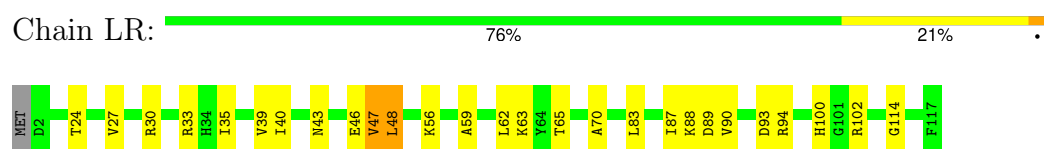
- Molecule 36: 50S ribosomal protein L16



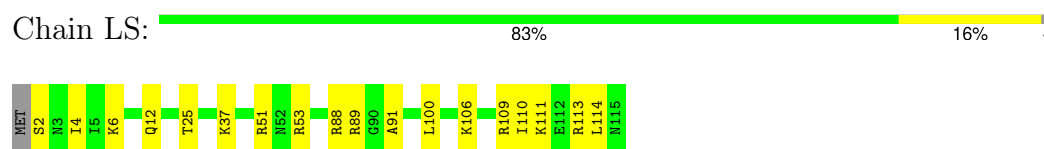
- Molecule 37: 50S ribosomal protein L17



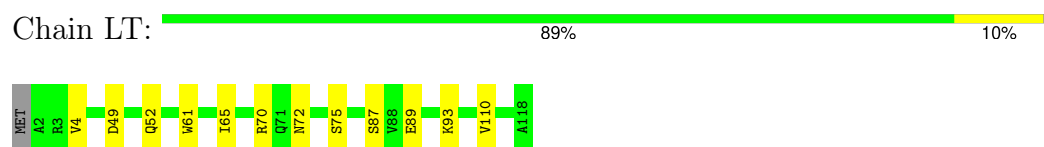
- Molecule 38: 50S ribosomal protein L18



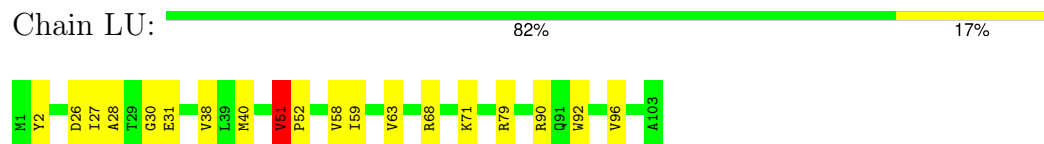
- Molecule 39: 50S ribosomal protein L19



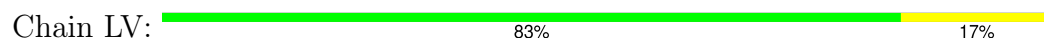
- Molecule 40: 50S ribosomal protein L20

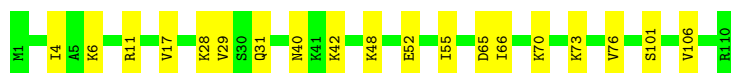


- Molecule 41: 50S ribosomal protein L21

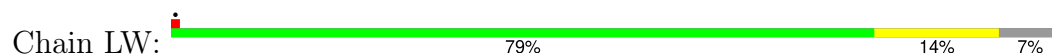


- Molecule 42: 50S ribosomal protein L22

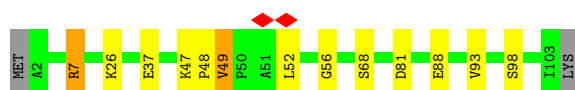
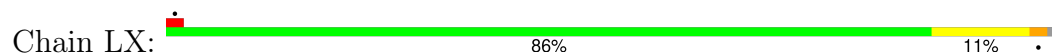




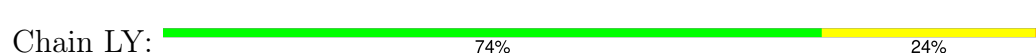
- Molecule 43: 50S ribosomal protein L23



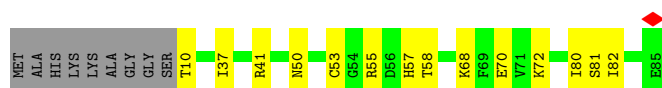
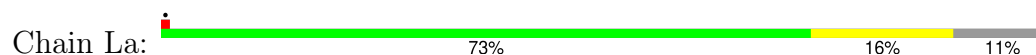
- Molecule 44: 50S ribosomal protein L24



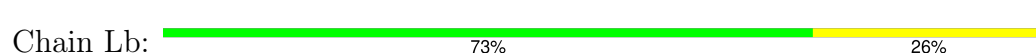
- Molecule 45: 50S ribosomal protein L25



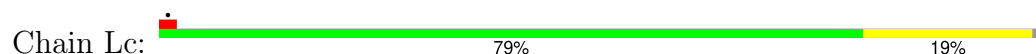
- Molecule 46: 50S ribosomal protein L27



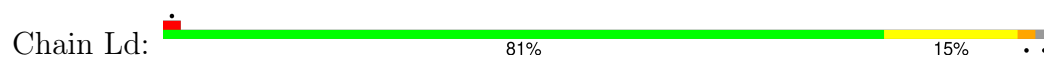
- Molecule 47: 50S ribosomal protein L28



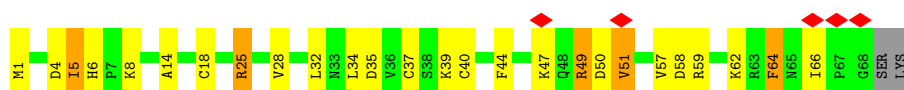
- Molecule 48: 50S ribosomal protein L29



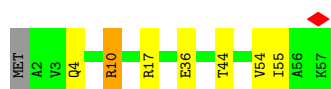
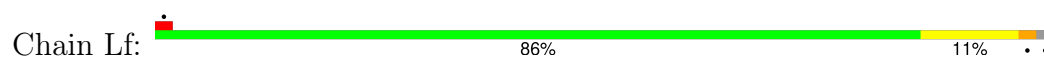
- Molecule 49: 50S ribosomal protein L30



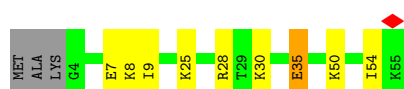
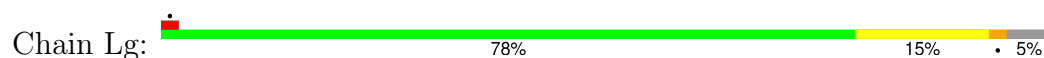
- Molecule 50: 50S ribosomal protein L31



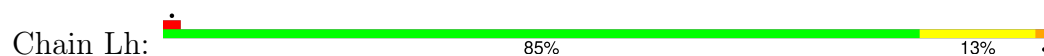
- Molecule 51: 50S ribosomal protein L32



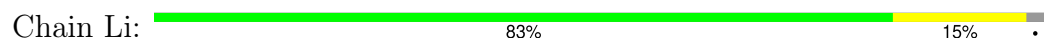
- Molecule 52: 50S ribosomal protein L33



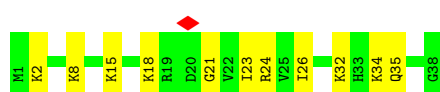
- Molecule 53: 50S ribosomal protein L34



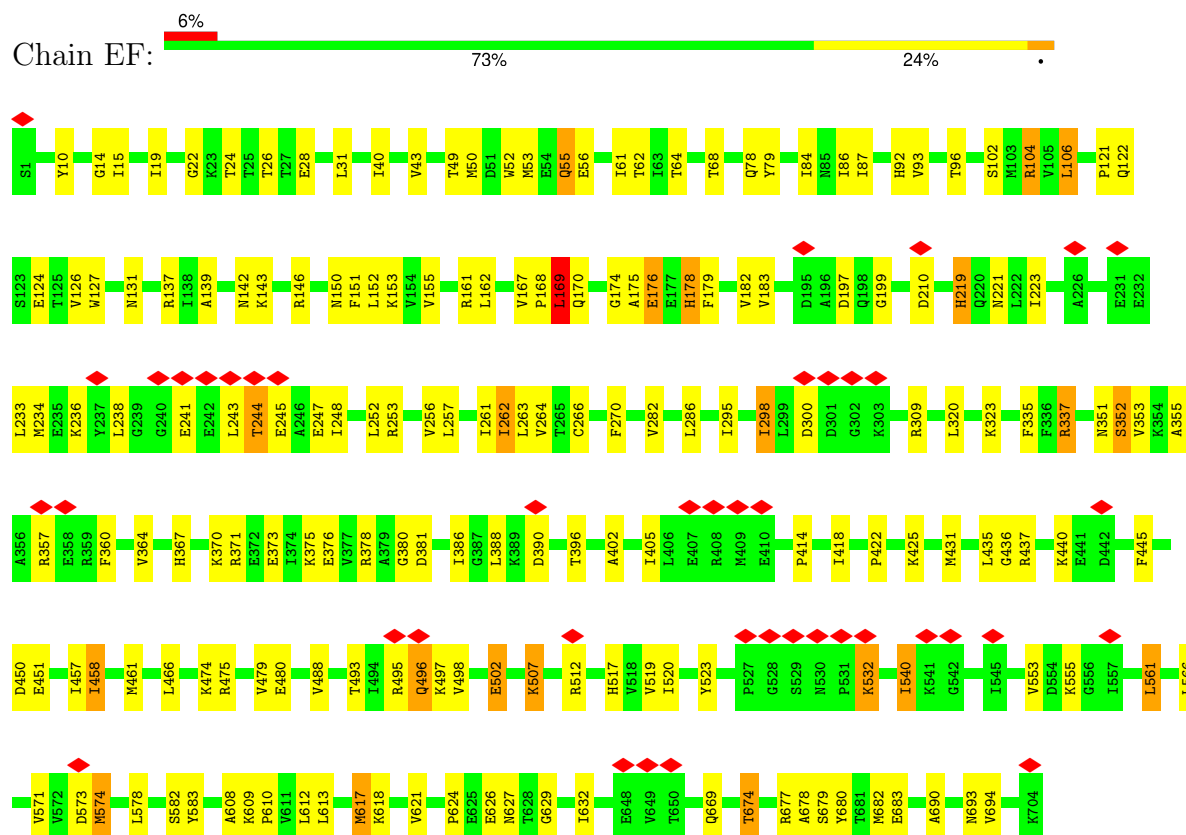
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



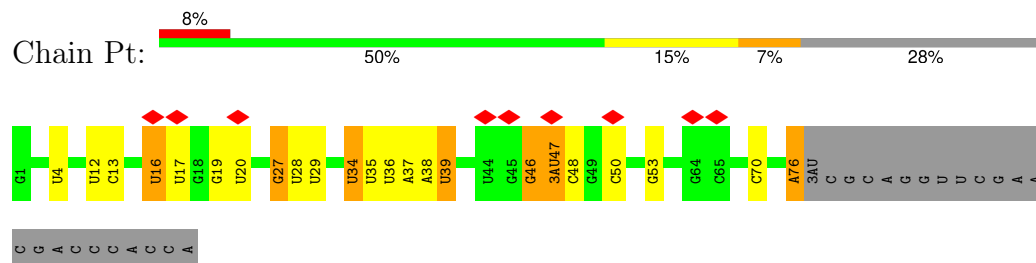
- Molecule 56: Elongation factor G



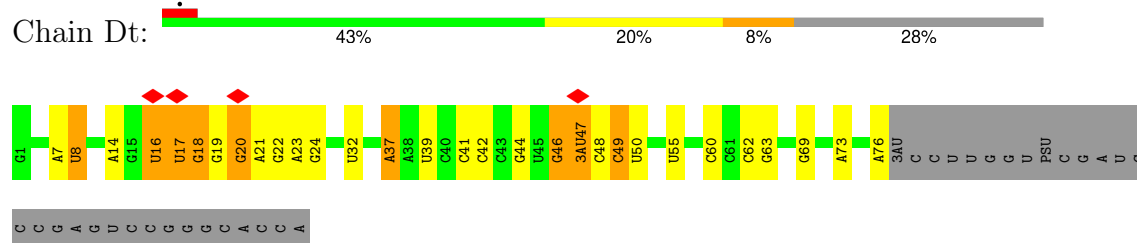
- Molecule 57: Nascent peptide



- Molecule 58: tRNA



- Molecule 59: tRNA



4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.34	0/36619	0.38	8/57122 (0.0%)
2	SB	0.44	0/1784	0.74	0/2403
3	SC	0.41	2/1680 (0.1%)	0.62	0/2263
4	SD	0.33	0/1665	0.52	0/2227
5	SE	0.37	0/1157	0.57	0/1557
6	SF	0.40	0/881	0.66	0/1189
7	SG	0.59	0/1195	1.08	4/1602 (0.2%)
8	SH	0.33	0/989	0.41	0/1326
9	SI	0.75	1/1034 (0.1%)	0.99	0/1375
10	SJ	0.46	0/805	0.78	1/1089 (0.1%)
11	SK	0.44	0/911	0.68	0/1229
12	SL	0.32	0/960	0.45	0/1286
13	SM	0.58	0/892	1.03	3/1193 (0.3%)
14	SN	0.53	0/817	1.15	4/1088 (0.4%)
15	SO	0.33	0/722	0.49	0/964
16	SP	0.36	0/659	0.51	0/884
17	SQ	0.39	0/657	0.64	0/881
18	SR	0.33	0/564	0.51	0/756
19	SS	0.66	0/685	0.97	2/922 (0.2%)
20	ST	0.33	0/670	0.54	0/888
21	SU	0.67	0/597	1.00	0/792
22	mR	0.30	0/283	0.39	0/438
23	23	0.40	0/69284	0.40	12/108082 (0.0%)
24	5	0.35	0/2873	0.36	1/4478 (0.0%)
25	LB	0.38	0/2121	0.48	0/2852
26	LC	0.38	0/1586	0.52	0/2134
27	LD	0.35	0/1571	0.46	0/2113
28	LE	0.61	1/1434 (0.1%)	0.90	3/1926 (0.2%)
29	LF	0.32	0/1343	0.54	0/1816
30	LI	0.35	0/1112	1.01	5/1503 (0.3%)
31	LJ	0.55	0/1006	0.85	2/1358 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LK	0.77	0/993	1.02	1/1341 (0.1%)
33	LM	0.37	0/1152	0.44	0/1551
34	LN	0.40	0/947	0.53	0/1268
35	LO	0.40	0/1062	0.56	0/1413
36	LP	0.37	0/1081	0.49	0/1443
37	LQ	0.34	0/973	0.40	0/1301
38	LR	0.40	1/902 (0.1%)	0.58	0/1209
39	LS	0.35	0/929	0.45	0/1242
40	LT	0.36	0/960	0.38	0/1278
41	LU	0.42	0/829	0.60	0/1107
42	LV	0.41	0/864	0.50	0/1156
43	LW	0.34	0/744	0.51	0/994
44	LX	0.42	0/787	0.61	0/1051
45	LY	0.32	0/766	0.47	0/1025
46	La	0.35	0/589	0.44	0/779
47	Lb	0.38	0/635	0.59	1/848 (0.1%)
48	Lc	0.54	0/502	0.81	0/667
49	Ld	0.47	0/453	0.63	0/605
50	Le	0.57	0/543	0.97	0/726
51	Lf	0.37	0/450	0.47	0/599
52	Lg	0.40	0/434	0.57	0/576
53	Lh	0.40	0/380	0.43	0/498
54	Li	0.36	0/513	0.50	0/676
55	Lj	0.35	0/303	0.46	0/397
56	EF	0.51	0/5490	0.74	2/7437 (0.0%)
57	Pp	0.58	0/28	1.61	0/34
58	Pt	0.38	2/1684 (0.1%)	0.44	0/2615
59	Dt	0.33	0/1654	0.46	0/2572
All	All	0.40	7/165203 (0.0%)	0.49	49/246144 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	SC	0	2
4	SD	0	3
5	SE	0	1
9	SI	0	3
10	SJ	0	2
12	SL	0	1

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	LE	93	GLY	C-N	-15.39	1.14	1.33
9	SI	41	ARG	C-O	7.29	1.32	1.24
38	LR	88	LYS	C-N	6.71	1.43	1.33
58	Pt	16	U	C1'-N1	6.67	1.58	1.48
3	SC	182	ILE	C-N	-5.92	1.25	1.33

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	SN	24	ARG	N-CA-C	19.09	131.78	110.97
30	LI	75	LEU	N-CA-C	18.30	131.34	111.03
14	SN	25	ALA	N-CA-CB	-14.51	88.78	110.12
1	16	1490	U	OP1-P-OP2	-13.48	79.15	119.60
13	SM	114	LYS	CB-CA-C	-13.02	88.58	108.63

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	SC	40	ARG	Sidechain
3	SC	88	ARG	Sidechain
4	SD	26	ARG	Sidechain
4	SD	44	ARG	Sidechain
4	SD	56	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	32929	0	16590	158	0
2	SB	1753	0	1780	36	0
3	SC	1653	0	1727	35	0
4	SD	1643	0	1707	27	0
5	SE	1144	0	1185	18	0
6	SF	862	0	864	16	0
7	SG	1181	0	1238	53	0
8	SH	979	0	1031	17	0
9	SI	1022	0	1070	29	0
10	SJ	795	0	836	40	0
11	SK	895	0	909	19	0
12	SL	957	0	1017	17	0
13	SM	883	0	941	25	0
14	SN	805	0	844	19	0
15	SO	714	0	734	5	0
16	SP	649	0	666	8	0
17	SQ	648	0	691	10	0
18	SR	555	0	578	8	0
19	SS	668	0	693	24	0
20	ST	664	0	714	9	0
21	SU	589	0	629	9	0
22	mR	254	0	129	2	0
23	23	62355	0	31382	238	0
24	5	2570	0	1301	7	0
25	LB	2082	0	2154	31	0
26	LC	1565	0	1616	13	0
27	LD	1552	0	1619	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	LE	1410	0	1443	46	0
29	LF	1323	0	1371	32	0
30	LI	1101	0	1141	34	0
31	LJ	992	0	1022	23	0
32	LK	979	0	1028	28	0
33	LM	1129	0	1162	7	0
34	LN	938	0	1012	12	0
35	LO	1053	0	1129	18	0
36	LP	1075	0	1155	22	0
37	LQ	960	0	1000	16	0
38	LR	892	0	923	11	0
39	LS	917	0	962	9	0
40	LT	947	0	1019	8	0
41	LU	816	0	839	10	0
42	LV	857	0	922	11	0
43	LW	738	0	807	8	0
44	LX	779	0	830	5	0
45	LY	753	0	780	14	0
46	La	582	0	599	6	0
47	Lb	625	0	652	12	0
48	Lc	501	0	531	10	0
49	Ld	449	0	488	5	0
50	Le	533	0	529	23	0
51	Lf	444	0	458	3	0
52	Lg	427	0	464	3	0
53	Lh	377	0	418	5	0
54	Li	504	0	572	10	0
55	Lj	302	0	340	7	0
56	EF	5388	0	5318	130	0
57	Pp	28	0	33	3	0
58	Pt	1636	0	836	9	0
59	Dt	1641	0	844	8	0
60	16	46	0	48	1	0
60	23	23	0	24	1	0
61	16	18	0	36	2	0
61	23	78	0	156	3	0
61	LC	6	0	10	1	0
62	16	63	0	0	0	0
62	23	264	0	0	0	0
62	5	6	0	0	0	0
62	EF	1	0	0	0	0
62	LB	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	LC	1	0	0	0	0
62	LD	1	0	0	0	0
62	LO	1	0	0	0	0
62	LQ	1	0	0	0	0
62	Lf	1	0	0	0	0
62	Pt	1	0	0	0	0
62	SK	1	0	0	0	0
62	SN	1	0	0	0	0
62	SR	1	0	0	0	0
63	Le	1	0	0	0	0
63	Lj	1	0	0	0	0
63	SB	1	0	0	0	0
64	23	62	0	24	0	0
65	23	20	0	38	6	0
66	EF	32	0	11	7	0
67	16	1	0	0	0	0
67	23	22	0	0	0	0
67	EF	1	0	0	0	0
67	LB	1	0	0	0	0
67	SB	1	0	0	0	0
All	All	154120	0	105619	1312	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 5.

The worst 5 of 1312 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)
7:SG:62:PHE:CZ	7:SG:124:LEU:HD22	1.09	1.59
7:SG:62:PHE:CZ	7:SG:124:LEU:CD2	1.90	1.49
57:Pp:3:LYS:C	58:Pt:76:A:O3'	1.67	1.35
7:SG:62:PHE:CE1	7:SG:124:LEU:HD22	1.73	1.23
7:SG:62:PHE:HZ	7:SG:124:LEU:CD2	1.31	1.18

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SB	222/241 (92%)	210 (95%)	12 (5%)	0	100	100
3	SC	209/233 (90%)	200 (96%)	9 (4%)	0	100	100
4	SD	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
5	SE	153/167 (92%)	150 (98%)	3 (2%)	0	100	100
6	SF	104/135 (77%)	101 (97%)	3 (3%)	0	100	100
7	SG	149/179 (83%)	141 (95%)	8 (5%)	0	100	100
8	SH	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
9	SI	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
10	SJ	97/103 (94%)	91 (94%)	6 (6%)	0	100	100
11	SK	117/129 (91%)	111 (95%)	6 (5%)	0	100	100
12	SL	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
13	SM	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
14	SN	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
15	SO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	SP	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
17	SQ	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
18	SR	65/75 (87%)	60 (92%)	5 (8%)	0	100	100
19	SS	82/92 (89%)	75 (92%)	7 (8%)	0	100	100
20	ST	83/87 (95%)	83 (100%)	0	0	100	100
21	SU	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
25	LB	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
26	LC	207/209 (99%)	198 (96%)	8 (4%)	1 (0%)	24	34
27	LD	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
28	LE	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
29	LF	174/177 (98%)	169 (97%)	5 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	LI	146/149 (98%)	129 (88%)	17 (12%)	0	100	100
31	LJ	129/165 (78%)	121 (94%)	8 (6%)	0	100	100
32	LK	132/142 (93%)	121 (92%)	11 (8%)	0	100	100
33	LM	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
34	LN	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
35	LO	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
36	LP	133/136 (98%)	133 (100%)	0	0	100	100
37	LQ	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
38	LR	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
39	LS	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
40	LT	115/118 (98%)	115 (100%)	0	0	100	100
41	LU	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
42	LV	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
43	LW	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
44	LX	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
45	LY	92/94 (98%)	92 (100%)	0	0	100	100
46	La	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
47	Lb	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
48	Lc	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
49	Ld	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	Le	66/70 (94%)	58 (88%)	8 (12%)	0	100	100
51	Lf	54/57 (95%)	54 (100%)	0	0	100	100
52	Lg	50/55 (91%)	49 (98%)	1 (2%)	0	100	100
53	Lh	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	Li	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
55	Lj	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
56	EF	702/704 (100%)	664 (95%)	38 (5%)	0	100	100
57	Pp	1/3 (33%)	1 (100%)	0	0	100	100
All	All	6575/6927 (95%)	6304 (96%)	270 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	LC	149	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SB	186/199 (94%)	181 (97%)	5 (3%)	39	58
3	SC	172/190 (90%)	162 (94%)	10 (6%)	18	27
4	SD	172/173 (99%)	165 (96%)	7 (4%)	27	41
5	SE	118/126 (94%)	115 (98%)	3 (2%)	42	60
6	SF	92/116 (79%)	86 (94%)	6 (6%)	15	22
7	SG	124/147 (84%)	100 (81%)	24 (19%)	1	1
8	SH	104/105 (99%)	100 (96%)	4 (4%)	29	44
9	SI	105/107 (98%)	95 (90%)	10 (10%)	8	9
10	SJ	87/90 (97%)	75 (86%)	12 (14%)	3	3
11	SK	92/99 (93%)	88 (96%)	4 (4%)	26	39
12	SL	102/103 (99%)	96 (94%)	6 (6%)	18	27
13	SM	92/96 (96%)	78 (85%)	14 (15%)	3	2
14	SN	83/84 (99%)	74 (89%)	9 (11%)	6	7
15	SO	76/77 (99%)	70 (92%)	6 (8%)	11	16
16	SP	65/65 (100%)	63 (97%)	2 (3%)	35	53
17	SQ	74/78 (95%)	69 (93%)	5 (7%)	14	20
18	SR	58/65 (89%)	54 (93%)	4 (7%)	14	20
19	SS	72/79 (91%)	56 (78%)	16 (22%)	1	1
20	ST	65/66 (98%)	59 (91%)	6 (9%)	8	10
21	SU	60/61 (98%)	57 (95%)	3 (5%)	22	33
25	LB	216/218 (99%)	208 (96%)	8 (4%)	30	45
26	LC	164/164 (100%)	161 (98%)	3 (2%)	51	70
27	LD	165/165 (100%)	161 (98%)	4 (2%)	43	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	LE	148/150 (99%)	133 (90%)	15 (10%)	7	8
29	LF	137/138 (99%)	132 (96%)	5 (4%)	31	46
30	LI	113/114 (99%)	104 (92%)	9 (8%)	11	15
31	LJ	100/123 (81%)	86 (86%)	14 (14%)	3	3
32	LK	104/110 (94%)	85 (82%)	19 (18%)	2	1
33	LM	116/116 (100%)	114 (98%)	2 (2%)	53	72
34	LN	103/104 (99%)	99 (96%)	4 (4%)	28	43
35	LO	103/103 (100%)	96 (93%)	7 (7%)	14	20
36	LP	108/108 (100%)	103 (95%)	5 (5%)	24	36
37	LQ	100/103 (97%)	98 (98%)	2 (2%)	48	67
38	LR	86/87 (99%)	78 (91%)	8 (9%)	8	10
39	LS	99/100 (99%)	96 (97%)	3 (3%)	36	53
40	LT	89/90 (99%)	88 (99%)	1 (1%)	65	79
41	LU	84/84 (100%)	81 (96%)	3 (4%)	31	46
42	LV	93/93 (100%)	89 (96%)	4 (4%)	26	39
43	LW	80/84 (95%)	78 (98%)	2 (2%)	42	60
44	LX	83/85 (98%)	78 (94%)	5 (6%)	17	26
45	LY	78/78 (100%)	77 (99%)	1 (1%)	61	76
46	La	58/63 (92%)	54 (93%)	4 (7%)	14	20
47	Lb	67/68 (98%)	66 (98%)	1 (2%)	57	74
48	Lc	54/55 (98%)	53 (98%)	1 (2%)	50	69
49	Ld	48/49 (98%)	44 (92%)	4 (8%)	10	14
50	Le	60/62 (97%)	50 (83%)	10 (17%)	2	2
51	Lf	47/48 (98%)	46 (98%)	1 (2%)	47	66
52	Lg	47/49 (96%)	42 (89%)	5 (11%)	6	7
53	Lh	38/38 (100%)	36 (95%)	2 (5%)	20	31
54	Li	51/52 (98%)	51 (100%)	0	100	100
55	Lj	34/34 (100%)	32 (94%)	2 (6%)	18	27
56	EF	561/578 (97%)	520 (93%)	41 (7%)	13	18
57	Pp	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	5436/5642 (96%)	5084 (94%)	352 (6%)	17	22

5 of 352 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	LK	139	VAL
49	Ld	5	ILE
34	LN	121	GLU
38	LR	94	ARG
51	Lf	10	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
50	Le	61	ASN
56	EF	560	GLN
56	EF	55	GLN
56	EF	344	ASN
26	LC	173	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1533/1534 (99%)	236 (15%)	10 (0%)
22	mR	11/60 (18%)	2 (18%)	0
23	23	2903/2904 (99%)	524 (18%)	28 (0%)
24	5	119/120 (99%)	16 (13%)	1 (0%)
58	Pt	75/106 (70%)	13 (17%)	0
59	Dt	75/106 (70%)	18 (24%)	0
All	All	4716/4830 (97%)	809 (17%)	39 (0%)

5 of 809 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	2	A
1	16	4	U
1	16	7	A
1	16	9	G
1	16	22	G

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	23	1508	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	23	2536	G
23	23	1570	A
23	23	2145	C
23	23	2858	C

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

47 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	16	1516	1	23,26,27	2.80	9 (39%)	33,38,41	2.30	13 (39%)
1	5MC	16	1407	1	19,22,23	3.66	8 (42%)	26,32,35	1.03	2 (7%)
59	MIA	Dt	37	59	28,31,32	2.35	6 (21%)	38,44,47	2.92	15 (39%)
23	OMG	23	2251	23,58	23,26,27	2.29	9 (39%)	32,38,41	1.94	8 (25%)
58	PSU	Pt	39	58	18,21,22	4.32	7 (38%)	21,30,33	2.09	5 (23%)
23	5MU	23	1939	23	19,22,23	4.78	7 (36%)	27,32,35	3.81	9 (33%)
23	7MG	23	2069	23	23,26,27	1.38	3 (13%)	27,39,42	2.67	6 (22%)
1	UR3	16	1498	1	19,22,23	2.75	7 (36%)	26,32,35	1.61	3 (11%)
12	D2T	SL	89	12	8,9,10	2.40	1 (12%)	6,11,13	2.29	2 (33%)
23	2MG	23	2445	23	23,26,27	2.72	8 (34%)	33,38,41	2.33	11 (33%)
59	PSU	Dt	39	59	18,21,22	4.27	7 (38%)	21,30,33	2.06	5 (23%)
59	7MG	Dt	46	59	23,26,27	3.43	10 (43%)	27,39,42	2.14	9 (33%)
23	OMC	23	2498	62,23	19,22,23	2.84	8 (42%)	25,31,34	0.79	0
23	2MA	23	2503	62,23	22,25,26	3.79	11 (50%)	32,37,40	2.63	10 (31%)
58	3AU	Pt	47	58	24,28,29	1.02	1 (4%)	30,40,43	1.51	4 (13%)
1	MA6	16	1518	1	23,26,27	1.48	4 (17%)	33,38,41	3.20	11 (33%)
23	PSU	23	2604	23	18,21,22	4.13	7 (38%)	21,30,33	2.10	5 (23%)
59	PSU	Dt	55	59	18,21,22	4.43	7 (38%)	21,30,33	2.09	5 (23%)
23	5MC	23	1962	23	19,22,23	3.64	8 (42%)	26,32,35	0.97	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PSU	23	746	62,23	18,21,22	4.21	7 (38%)	21,30,33	1.84	5 (23%)
1	4OC	16	1402	62,1	20,23,24	3.01	8 (40%)	25,32,35	0.93	1 (4%)
23	6MZ	23	1618	23	22,25,26	2.40	5 (22%)	29,36,39	3.19	11 (37%)
23	PSU	23	2580	23	18,21,22	4.19	8 (44%)	21,30,33	2.11	6 (28%)
23	6MZ	23	2030	23	22,25,26	2.58	6 (27%)	29,36,39	3.25	12 (41%)
23	3TD	23	1915	23	19,22,23	4.34	6 (31%)	23,32,35	1.87	3 (13%)
1	7MG	16	527	1	23,26,27	1.37	3 (13%)	27,39,42	2.65	7 (25%)
36	4D4	LP	81	36	9,11,12	2.57	3 (33%)	7,13,15	0.93	0
23	1MG	23	745	23	23,26,27	3.13	8 (34%)	33,39,42	2.32	8 (24%)
23	H2U	23	2449	23	18,21,22	2.93	5 (27%)	19,30,33	1.53	4 (21%)
23	PSU	23	2605	23	18,21,22	4.20	8 (44%)	21,30,33	2.05	5 (23%)
23	5MU	23	747	23	19,22,23	4.78	7 (36%)	27,32,35	3.72	10 (37%)
23	2MG	23	1835	23	23,26,27	2.74	8 (34%)	33,38,41	2.35	11 (33%)
23	PSU	23	2504	23	18,21,22	4.17	7 (38%)	21,30,33	2.00	5 (23%)
59	PSU	Dt	32	59	18,21,22	4.29	7 (38%)	21,30,33	2.07	5 (23%)
1	2MG	16	966	1	23,26,27	2.78	9 (39%)	33,38,41	2.21	10 (30%)
23	PSU	23	1911	23	18,21,22	4.21	8 (44%)	21,30,33	1.89	4 (19%)
1	MA6	16	1519	1	23,26,27	1.66	4 (17%)	33,38,41	2.47	12 (36%)
23	PSU	23	2457	23	18,21,22	4.17	8 (44%)	21,30,33	2.33	5 (23%)
58	7MG	Pt	46	58	23,26,27	3.53	10 (43%)	27,39,42	2.25	9 (33%)
23	PSU	23	955	23	18,21,22	4.16	7 (38%)	21,30,33	2.19	5 (23%)
23	OMU	23	2552	23	19,22,23	2.88	8 (42%)	25,31,34	2.02	5 (20%)
58	U8U	Pt	34	22,58	20,24,25	1.63	4 (20%)	22,34,37	1.12	4 (18%)
59	4SU	Dt	8	59	18,21,22	4.29	8 (44%)	25,30,33	2.40	5 (20%)
1	5MC	16	967	1	19,22,23	3.66	8 (42%)	26,32,35	1.01	1 (3%)
1	PSU	16	516	1	18,21,22	4.23	7 (38%)	21,30,33	1.92	5 (23%)
59	3AU	Dt	47	59	24,28,29	1.06	1 (4%)	30,40,43	1.58	3 (10%)
58	T6A	Pt	37	58	31,34,35	1.76	7 (22%)	43,49,52	2.28	12 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	16	1516	1	-	0/9/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
59	MIA	Dt	37	59	-	6/15/33/34	0/3/3/3
23	OMG	23	2251	23,58	-	3/9/27/28	0/3/3/3
58	PSU	Pt	39	58	-	0/7/25/26	0/2/2/2
23	5MU	23	1939	23	-	0/7/25/26	0/2/2/2
23	7MG	23	2069	23	-	0/7/37/38	0/3/3/3
1	UR3	16	1498	1	-	2/7/25/26	0/2/2/2
12	D2T	SL	89	12	-	1/7/12/14	-
23	2MG	23	2445	23	-	0/9/27/28	0/3/3/3
59	PSU	Dt	39	59	-	0/7/25/26	0/2/2/2
59	7MG	Dt	46	59	-	2/7/37/38	0/3/3/3
23	OMC	23	2498	62,23	-	2/9/27/28	0/2/2/2
23	2MA	23	2503	62,23	-	2/7/25/26	0/3/3/3
58	3AU	Pt	47	58	-	10/16/34/35	0/2/2/2
1	MA6	16	1518	1	-	0/11/29/30	0/3/3/3
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
59	PSU	Dt	55	59	-	0/7/25/26	0/2/2/2
23	5MC	23	1962	23	-	2/7/25/26	0/2/2/2
23	PSU	23	746	62,23	-	2/7/25/26	0/2/2/2
1	4OC	16	1402	62,1	-	1/9/29/30	0/2/2/2
23	6MZ	23	1618	23	-	4/9/27/28	0/3/3/3
23	PSU	23	2580	23	-	1/7/25/26	0/2/2/2
23	6MZ	23	2030	23	-	2/9/27/28	0/3/3/3
23	3TD	23	1915	23	-	2/7/25/26	0/2/2/2
1	7MG	16	527	1	-	3/7/37/38	0/3/3/3
36	4D4	LP	81	36	-	1/11/12/14	-
23	1MG	23	745	23	-	0/7/25/26	0/3/3/3
23	H2U	23	2449	23	-	1/7/38/39	0/2/2/2
23	PSU	23	2605	23	-	0/7/25/26	0/2/2/2
23	5MU	23	747	23	-	1/7/25/26	0/2/2/2
23	2MG	23	1835	23	-	2/9/27/28	0/3/3/3
23	PSU	23	2504	23	-	0/7/25/26	0/2/2/2
59	PSU	Dt	32	59	-	0/7/25/26	0/2/2/2
1	2MG	16	966	1	-	0/9/27/28	0/3/3/3
23	PSU	23	1911	23	-	2/7/25/26	0/2/2/2
1	MA6	16	1519	1	-	6/11/29/30	0/3/3/3
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
58	7MG	Pt	46	58	-	4/7/37/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
23	OMU	23	2552	23	-	0/9/27/28	0/2/2/2
58	U8U	Pt	34	22,58	-	2/10/28/29	0/2/2/2
59	4SU	Dt	8	59	-	0/7/25/26	0/2/2/2
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
1	PSU	16	516	1	-	0/7/25/26	0/2/2/2
59	3AU	Dt	47	59	-	9/16/34/35	0/2/2/2
58	T6A	Pt	37	58	-	10/23/41/42	0/3/3/3

The worst 5 of 313 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	1915	3TD	C6-C5	13.19	1.49	1.35
59	Dt	55	PSU	C6-C5	11.60	1.48	1.35
58	Pt	39	PSU	C6-C5	11.39	1.47	1.35
23	23	2503	2MA	C4-N3	11.38	1.49	1.34
59	Dt	39	PSU	C6-C5	11.24	1.47	1.35

The worst 5 of 297 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	1939	5MU	C5-C4-N3	12.60	126.27	115.32
23	23	747	5MU	C5-C4-N3	12.05	125.80	115.32
1	16	1518	MA6	N1-C6-N6	-11.49	102.86	116.86
23	23	1939	5MU	C5-C6-N1	-10.26	112.17	123.31
23	23	747	5MU	C5-C6-N1	-10.12	112.31	123.31

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	1519	MA6	O4'-C4'-C5'-O5'
1	16	1519	MA6	C3'-C4'-C5'-O5'
1	16	1519	MA6	C5-C6-N6-C10
23	23	1618	6MZ	C5-C6-N6-C9
23	23	1618	6MZ	N1-C6-N6-C9

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	16	1516	2MG	2	0
23	23	2251	OMG	1	0
58	Pt	39	PSU	1	0
12	SL	89	D2T	2	0
23	23	2498	OMC	1	0
1	16	1402	4OC	1	0
23	23	2030	6MZ	2	0
23	23	2504	PSU	1	0
23	23	2552	OMU	1	0
58	Pt	34	U8U	2	0
1	16	516	PSU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 372 ligands modelled in this entry, 347 are monoatomic - leaving 25 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	PUT	23	3013	-	5,5,5	0.15	0	4,4,4	0.60	0
61	PUT	23	3012	-	5,5,5	0.22	0	4,4,4	0.47	0
65	SPD	23	3018	-	9,9,9	0.31	0	8,8,8	0.95	0
61	PUT	16	1604	-	5,5,5	0.16	0	4,4,4	0.22	0
60	SCM	23	3001	-	23,25,25	1.38	4 (17%)	27,39,39	1.65	5 (18%)
61	PUT	23	3015	-	5,5,5	0.23	0	4,4,4	0.41	0
66	GTP	EF	901	62	33,34,34	3.63	18 (54%)	50,54,54	1.79	12 (24%)
61	PUT	23	3007	-	5,5,5	0.14	0	4,4,4	0.22	0
61	PUT	23	3005	-	5,5,5	0.23	0	4,4,4	0.42	0
61	PUT	23	3014	-	5,5,5	0.20	0	4,4,4	0.41	0
61	PUT	23	3008	-	5,5,5	0.22	0	4,4,4	0.49	0
61	PUT	LC	301	-	5,5,5	0.22	0	4,4,4	0.76	0
61	PUT	23	3006	-	5,5,5	0.21	0	4,4,4	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	PUT	23	3009	-	5,5,5	0.22	0	4,4,4	0.48	0
61	PUT	16	1605	-	5,5,5	0.15	0	4,4,4	0.23	0
61	PUT	23	3010	-	5,5,5	0.20	0	4,4,4	0.54	0
61	PUT	23	3011	-	5,5,5	0.23	0	4,4,4	0.44	0
61	PUT	16	1603	-	5,5,5	0.23	0	4,4,4	0.47	0
65	SPD	23	3017	-	9,9,9	0.31	0	8,8,8	0.91	0
61	PUT	23	3004	-	5,5,5	0.18	0	4,4,4	0.54	0
60	SCM	16	1602	-	23,25,25	1.37	3 (13%)	27,39,39	1.43	3 (11%)
64	ATP	23	3002	-	32,33,33	0.56	0	48,52,52	0.57	0
61	PUT	23	3016	-	5,5,5	0.22	0	4,4,4	0.47	0
64	ATP	23	3003	-	32,33,33	0.54	0	48,52,52	0.55	0
60	SCM	16	1601	-	23,25,25	1.35	3 (13%)	27,39,39	1.50	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PUT	23	3013	-	-	2/3/3/3	-
61	PUT	23	3012	-	-	2/3/3/3	-
65	SPD	23	3018	-	-	0/7/7/7	-
61	PUT	16	1604	-	-	0/3/3/3	-
60	SCM	23	3001	-	-	0/4/57/57	0/3/3/3
61	PUT	23	3015	-	-	2/3/3/3	-
66	GTP	EF	901	62	-	2/22/38/38	0/3/3/3
61	PUT	23	3007	-	-	2/3/3/3	-
61	PUT	23	3005	-	-	0/3/3/3	-
61	PUT	23	3014	-	-	1/3/3/3	-
61	PUT	23	3008	-	-	0/3/3/3	-
61	PUT	LC	301	-	-	1/3/3/3	-
61	PUT	23	3006	-	-	1/3/3/3	-
61	PUT	23	3009	-	-	1/3/3/3	-
61	PUT	16	1605	-	-	3/3/3/3	-
61	PUT	23	3010	-	-	1/3/3/3	-
61	PUT	23	3011	-	-	1/3/3/3	-
61	PUT	16	1603	-	-	0/3/3/3	-
65	SPD	23	3017	-	-	4/7/7/7	-
61	PUT	23	3004	-	-	2/3/3/3	-
60	SCM	16	1602	-	-	0/4/57/57	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	ATP	23	3003	-	1/1/7/7	7/22/38/38	0/3/3/3
61	PUT	23	3016	-	-	1/3/3/3	-
64	ATP	23	3002	-	-	3/22/38/38	0/3/3/3
60	SCM	16	1601	-	-	2/4/57/57	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	EF	901	GTP	O4'-C1'	8.31	1.61	1.42
66	EF	901	GTP	C2'-C1'	-8.03	1.28	1.53
66	EF	901	GTP	PB-O3B	7.21	1.67	1.59
66	EF	901	GTP	O4'-C4'	-6.51	1.30	1.45
66	EF	901	GTP	C4-N3	6.34	1.48	1.34

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	EF	901	GTP	C5-C4-N3	-5.27	120.00	128.39
60	16	1601	SCM	C8M-N8-C8	-4.74	108.11	114.23
66	EF	901	GTP	C2-N3-C4	4.45	119.97	112.30
60	23	3001	SCM	C1M-N10-C10	-3.79	109.34	114.23
60	16	1601	SCM	C1M-N10-C10	-3.70	109.46	114.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
64	23	3003	ATP	C4'

5 of 38 torsion outliers are listed below:

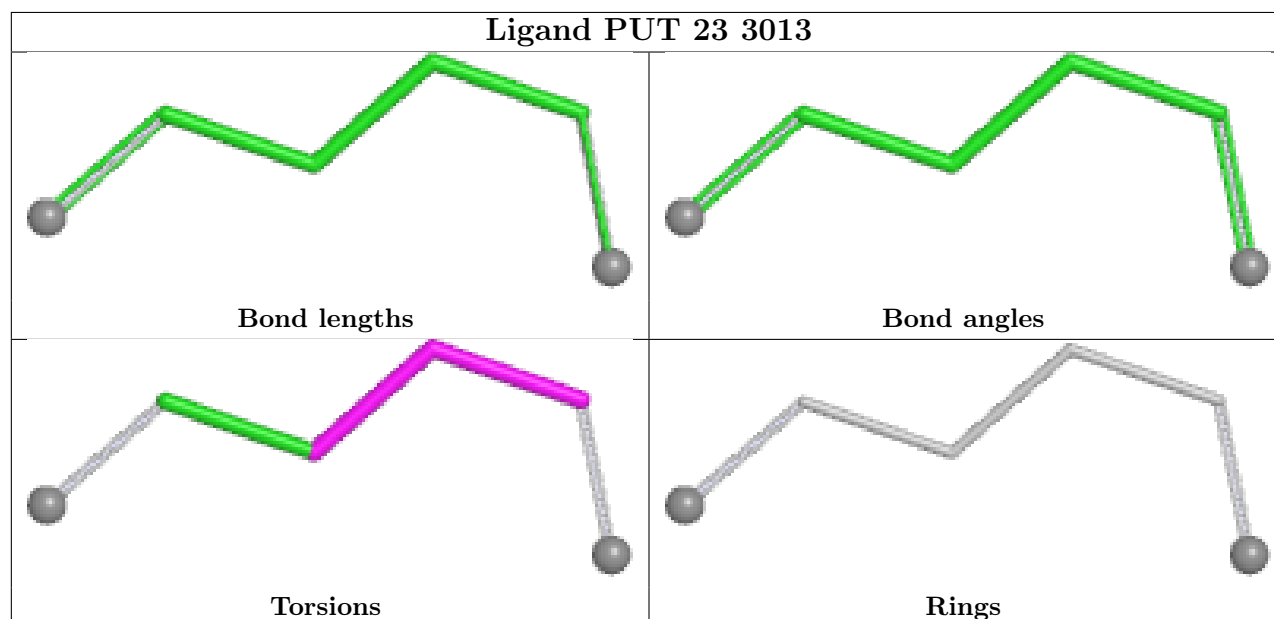
Mol	Chain	Res	Type	Atoms
64	23	3002	ATP	PB-O3B-PG-O3G
64	23	3002	ATP	O4'-C4'-C5'-O5'
64	23	3003	ATP	C5'-O5'-PA-O1A
64	23	3003	ATP	C5'-O5'-PA-O3A
66	EF	901	GTP	C5'-O5'-PA-O3A

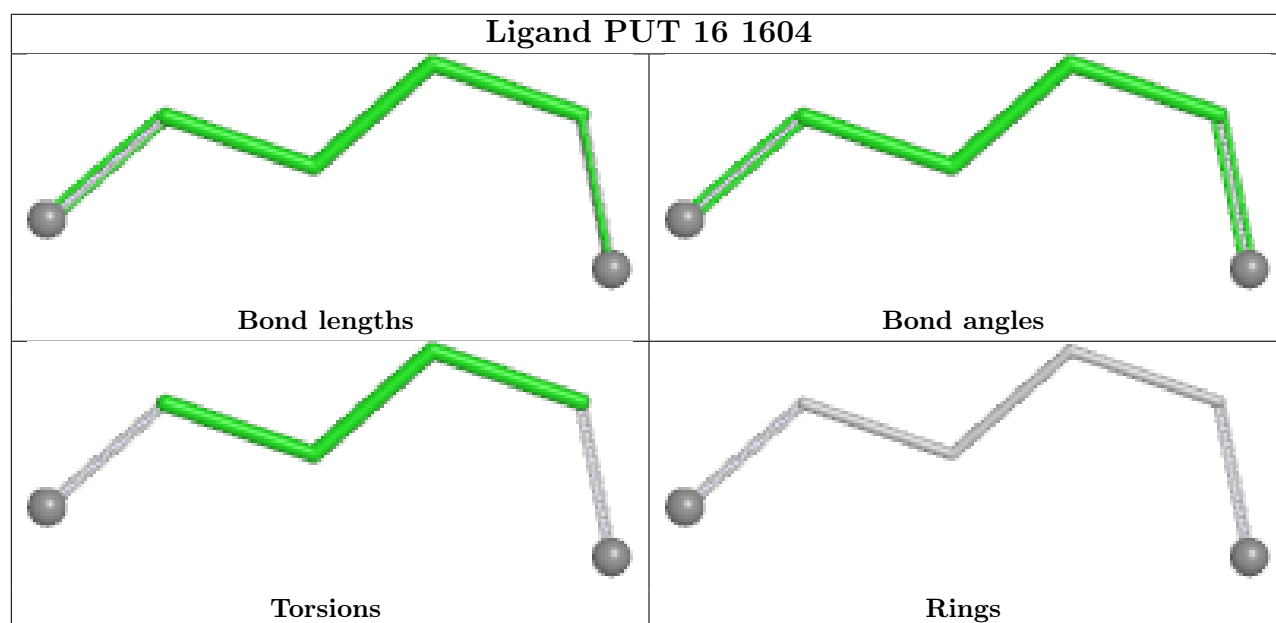
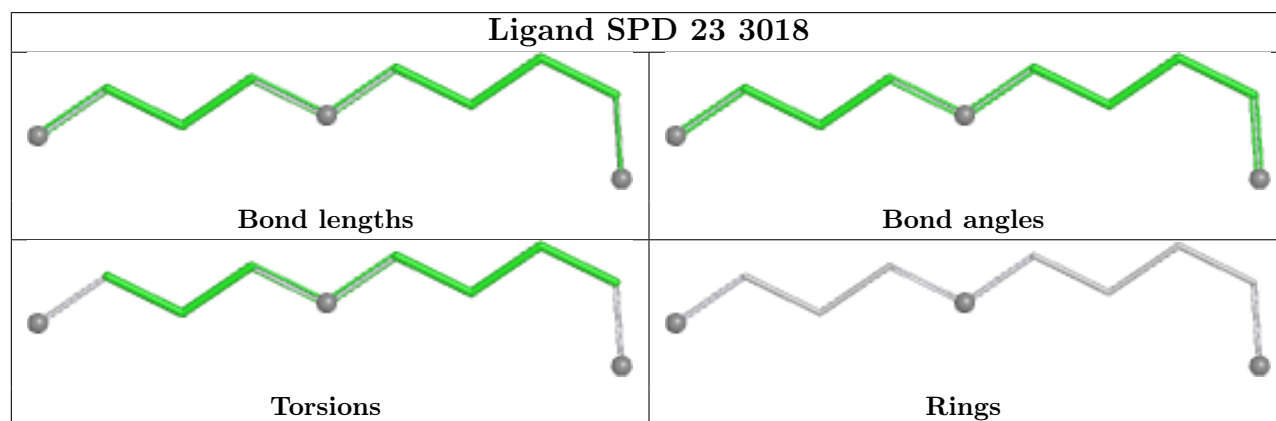
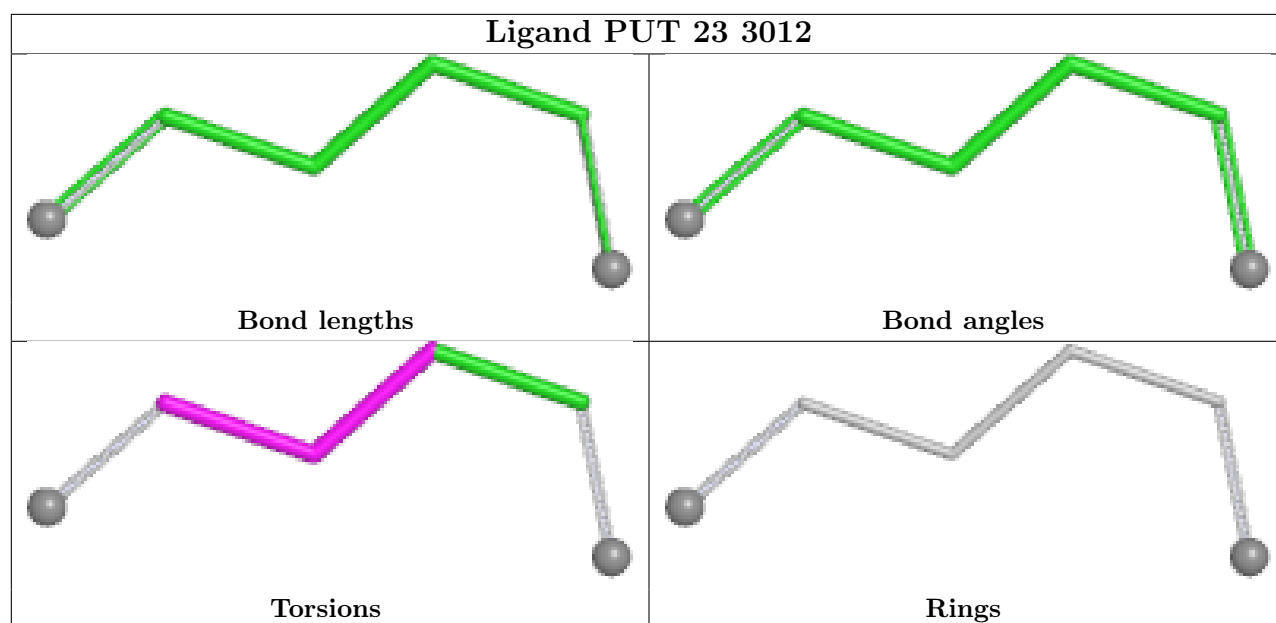
There are no ring outliers.

10 monomers are involved in 21 short contacts:

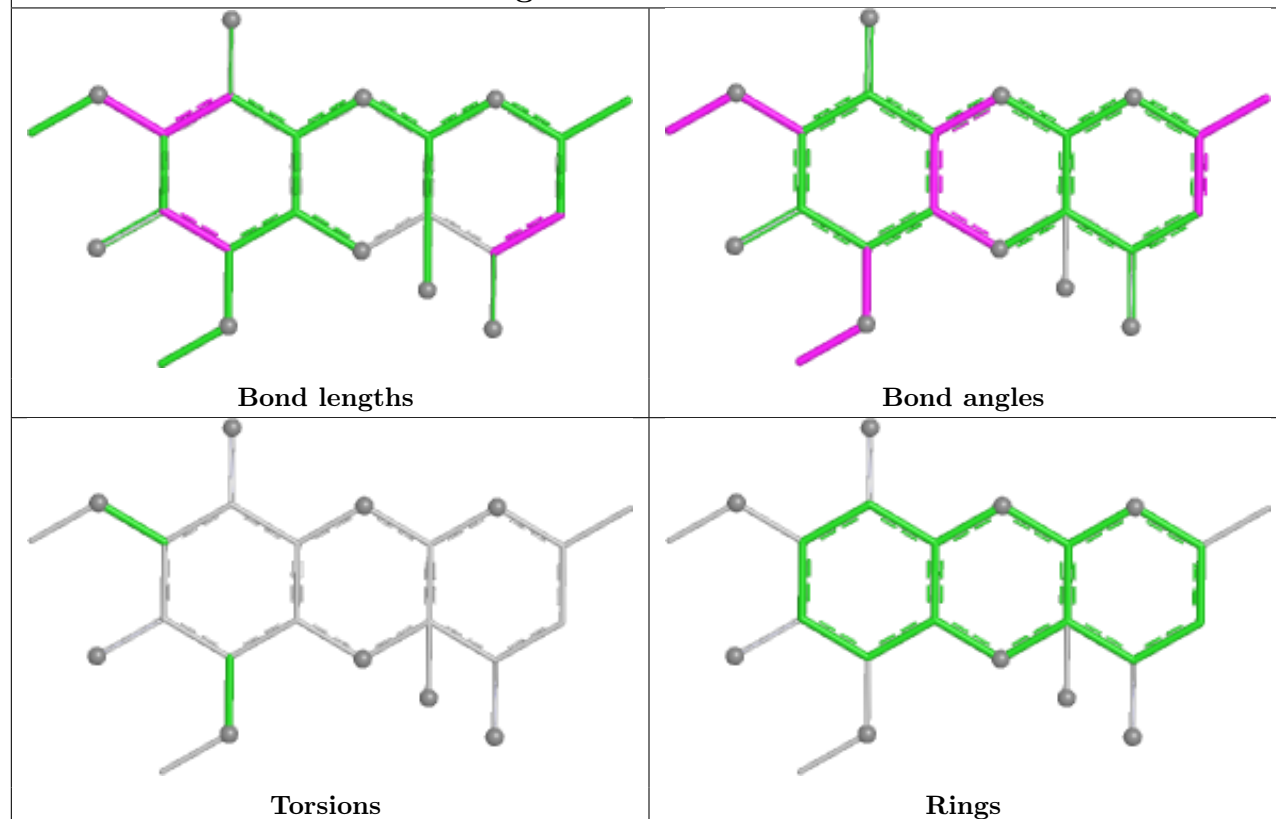
Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	23	3012	PUT	1	0
65	23	3018	SPD	1	0
60	23	3001	SCM	1	0
61	23	3015	PUT	1	0
66	EF	901	GTP	7	0
61	23	3007	PUT	1	0
61	LC	301	PUT	1	0
61	16	1603	PUT	2	0
65	23	3017	SPD	5	0
60	16	1601	SCM	1	0

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.

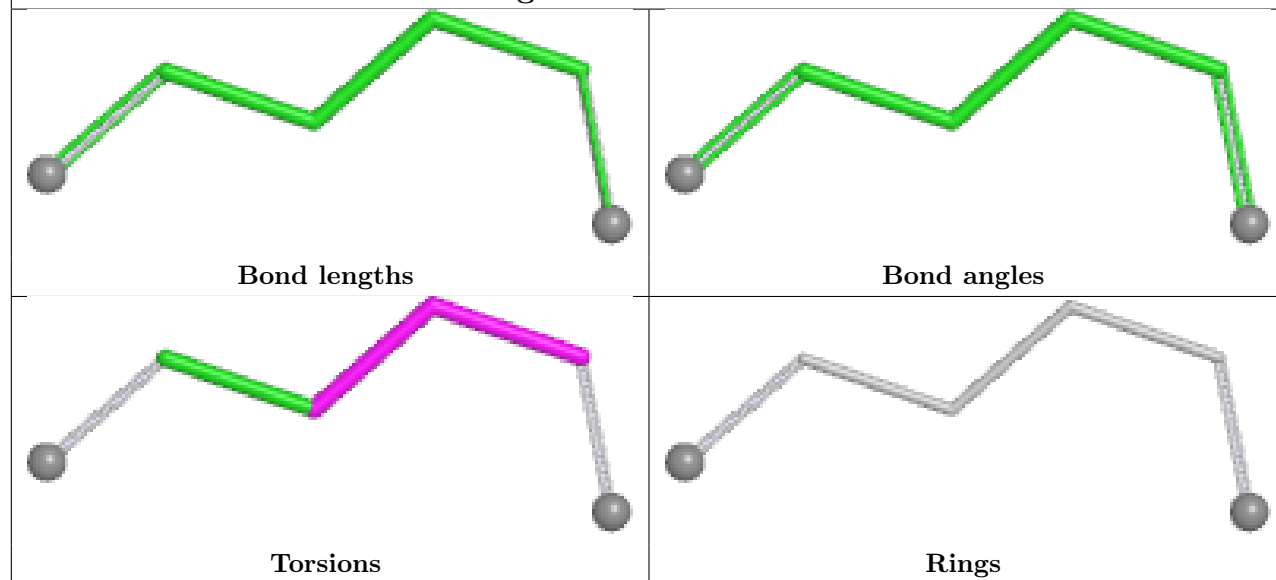


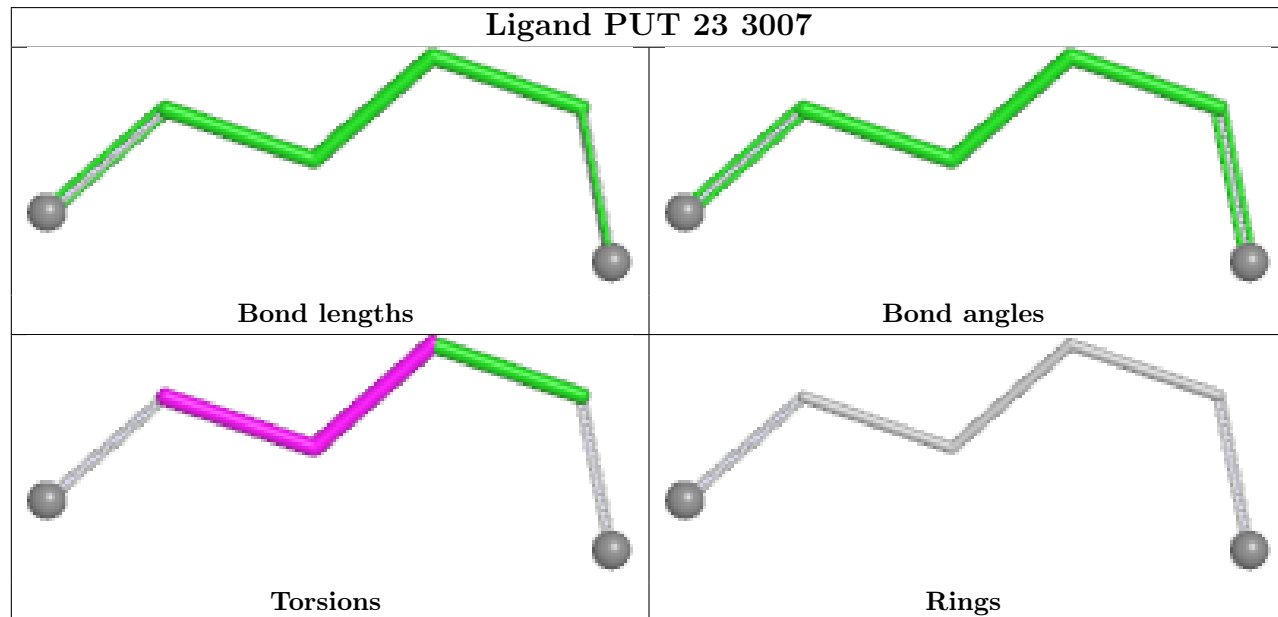
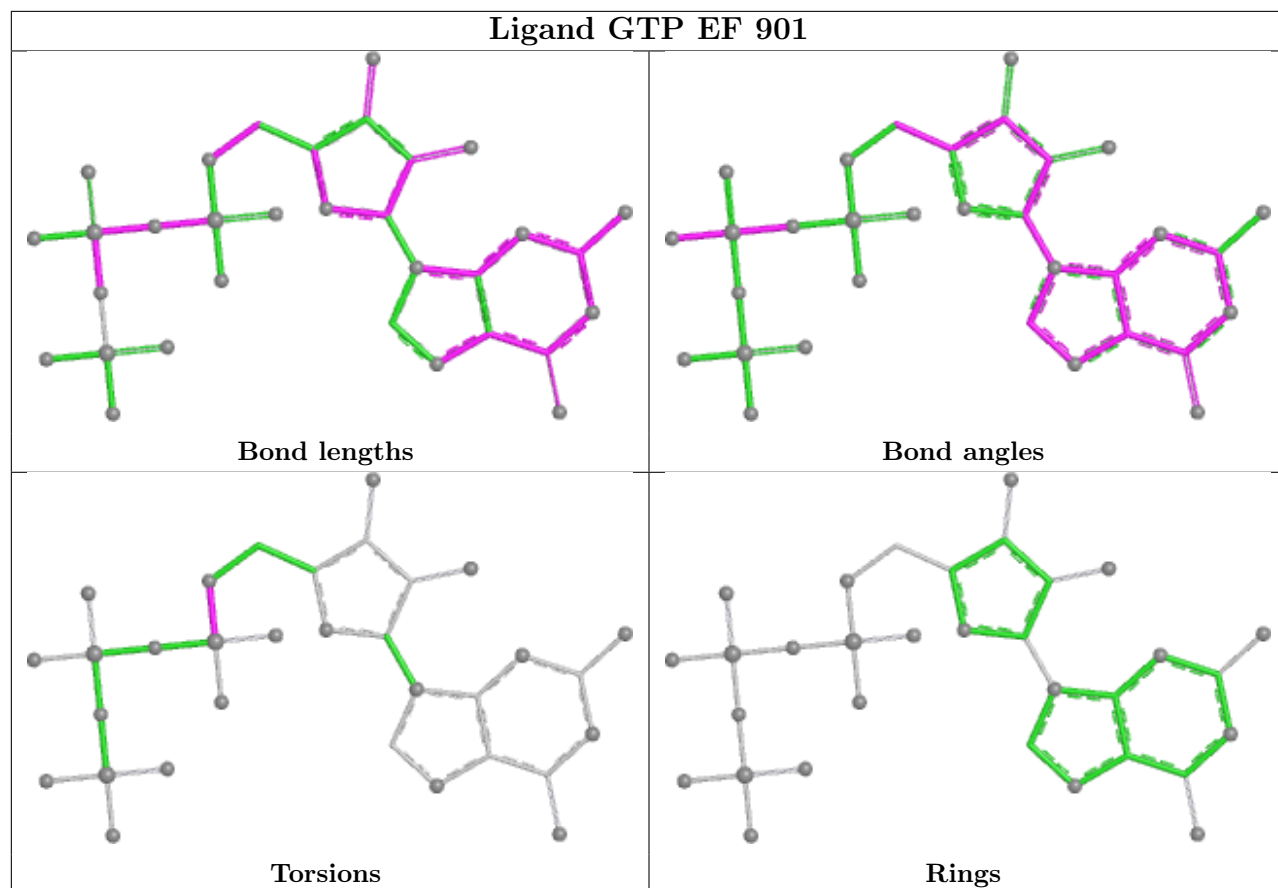


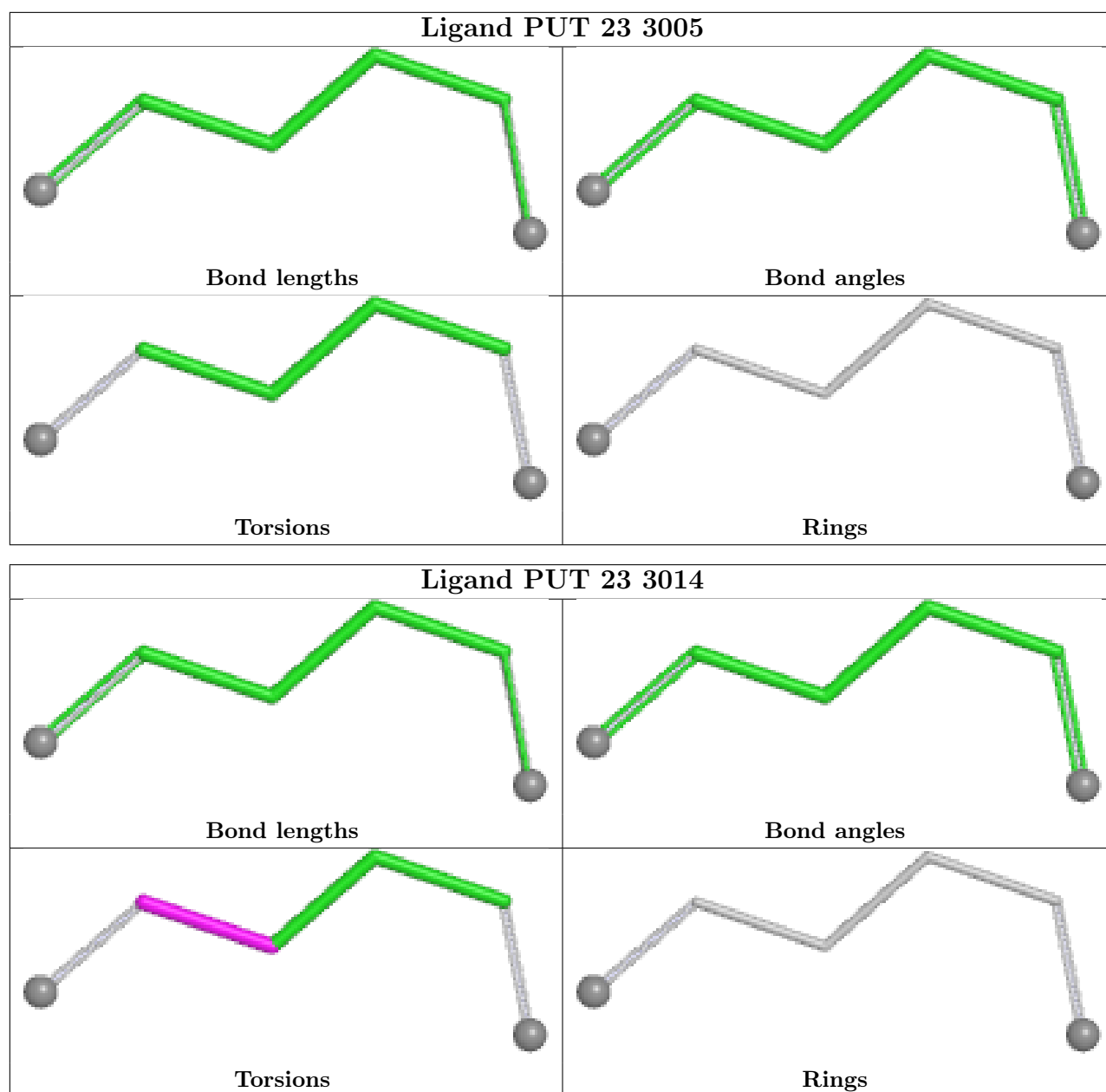
Ligand SCM 23 3001

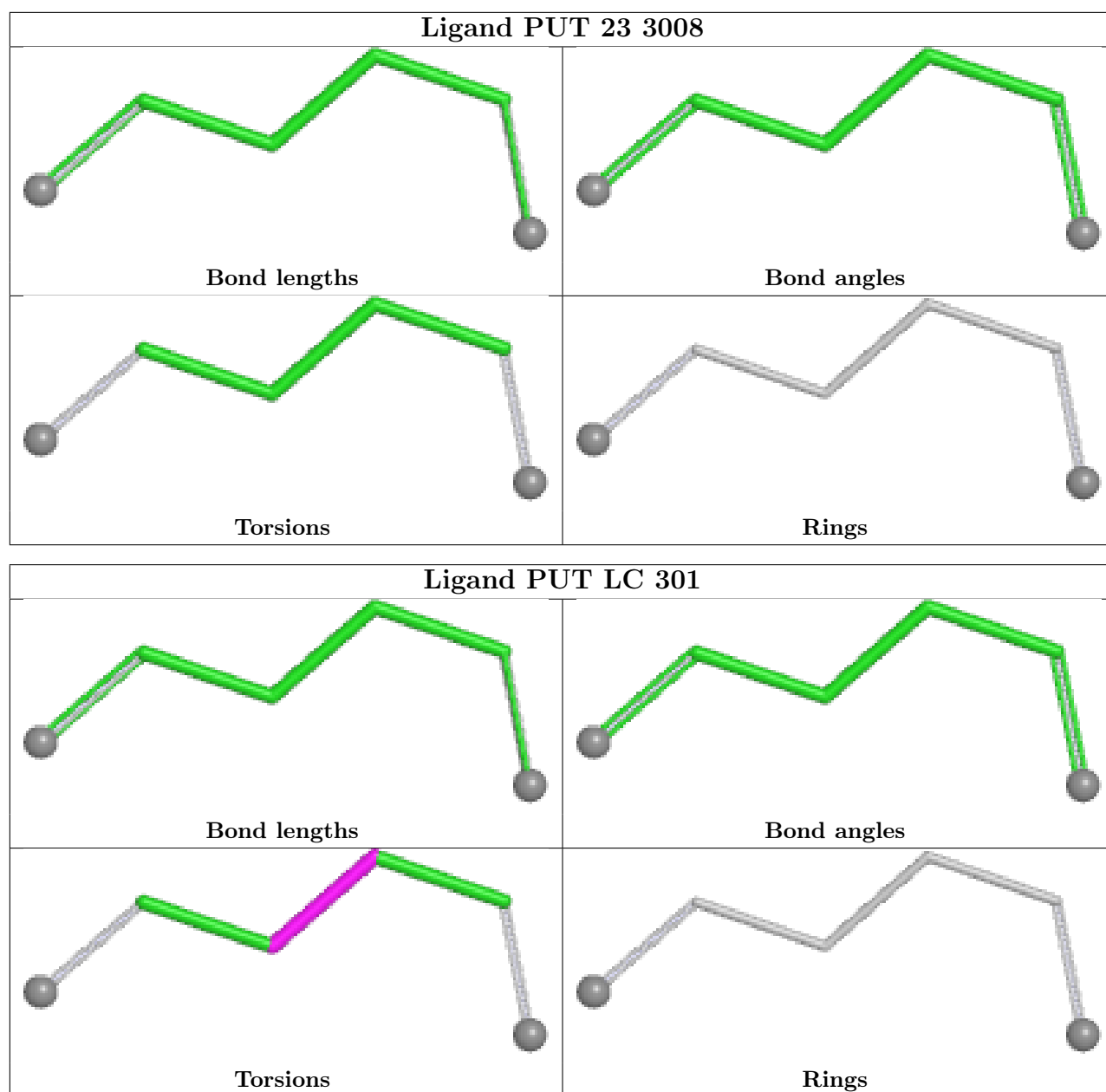


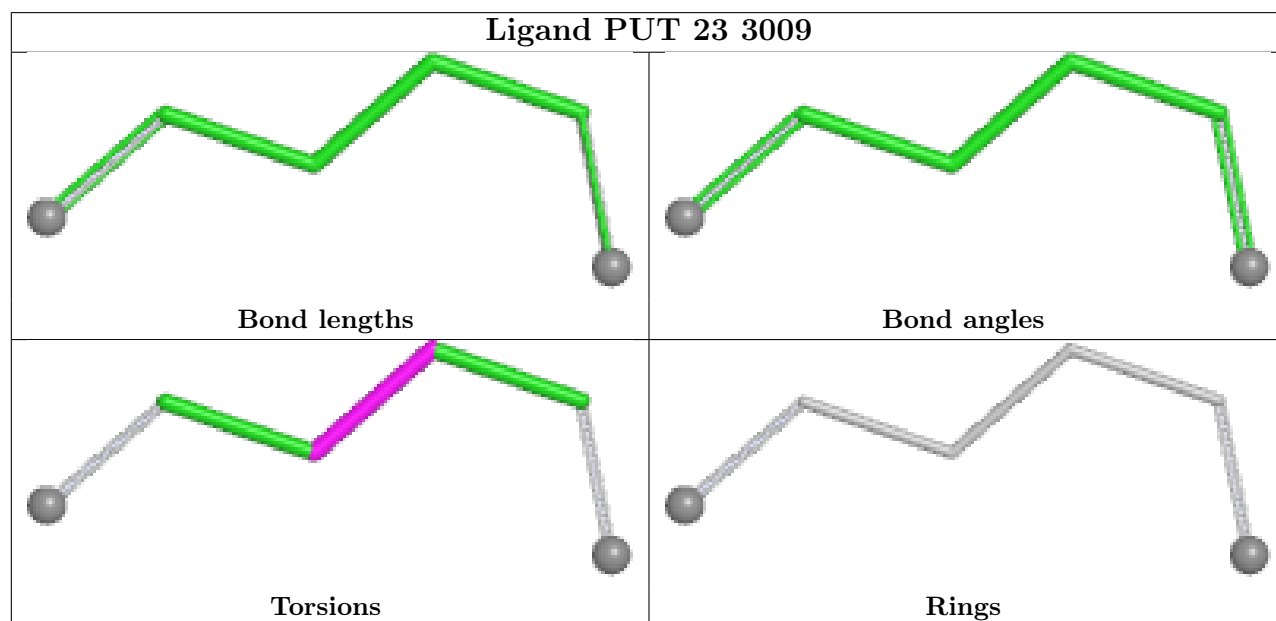
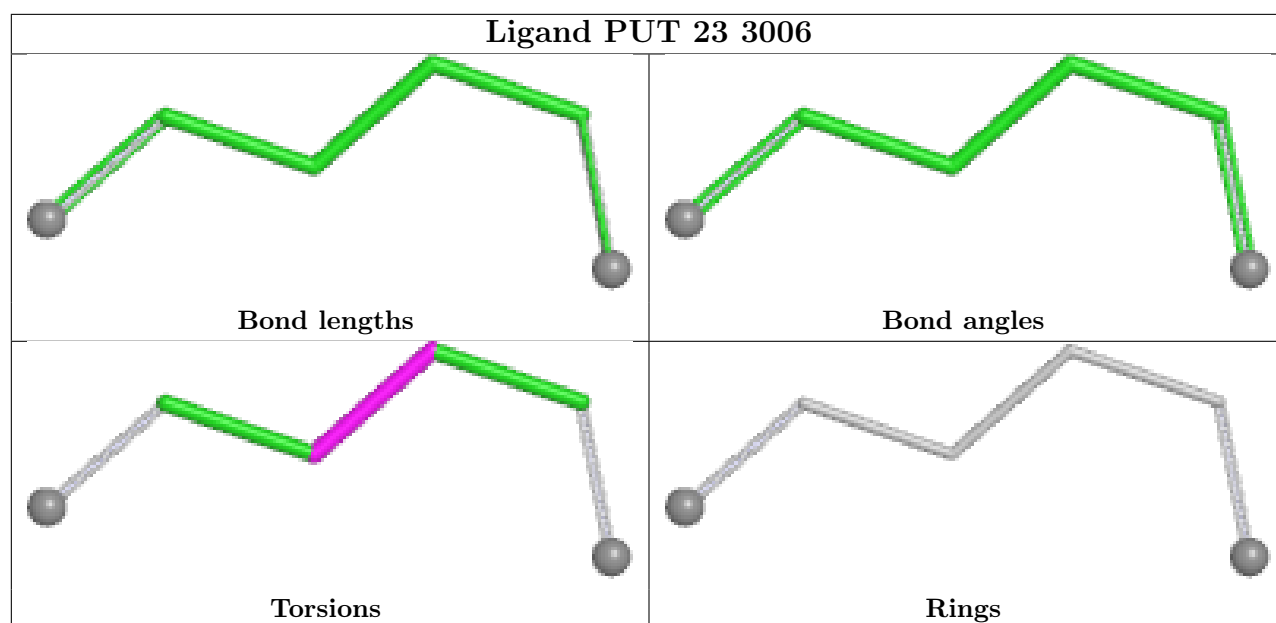
Ligand PUT 23 3015

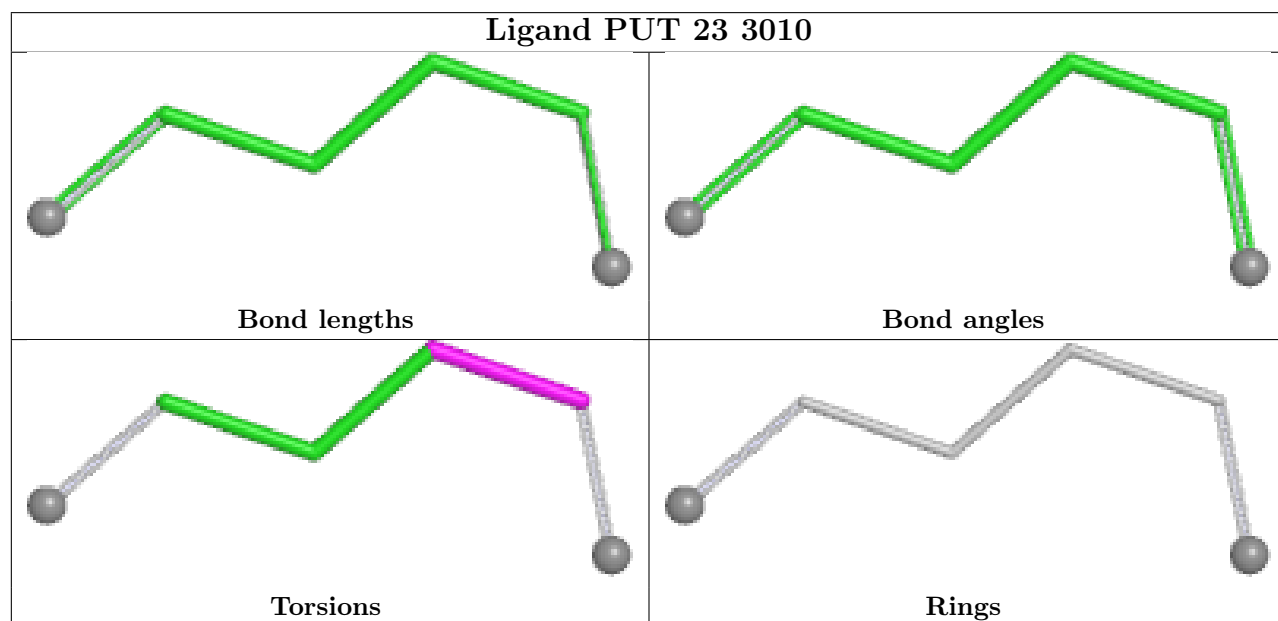
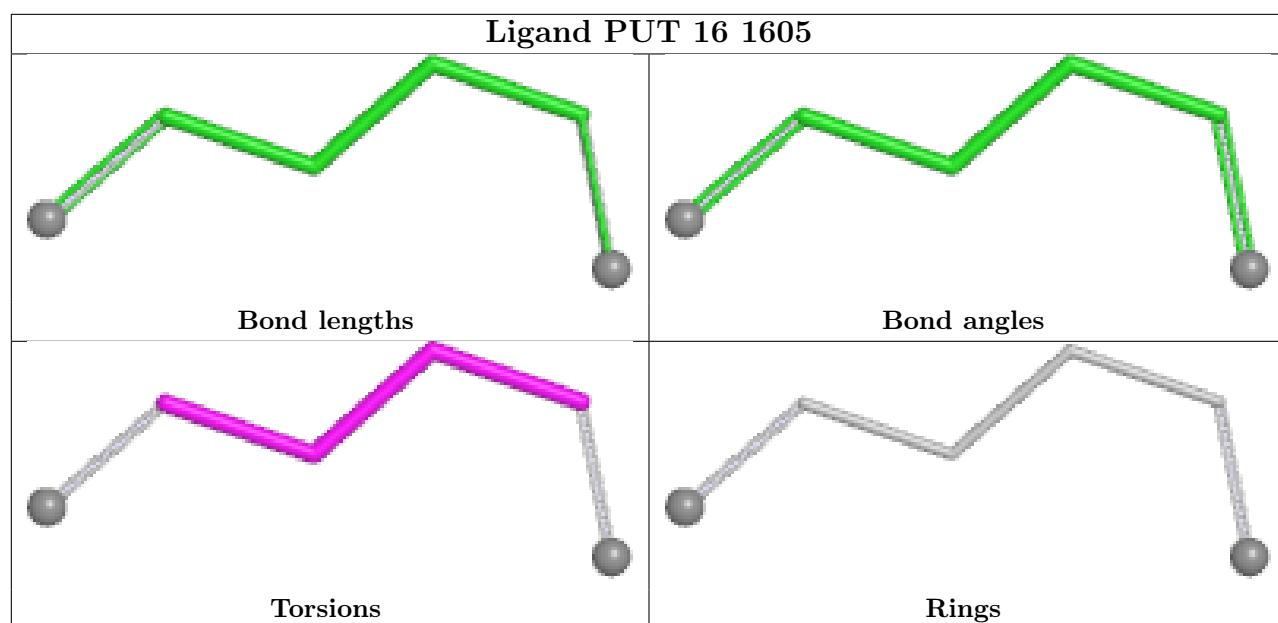


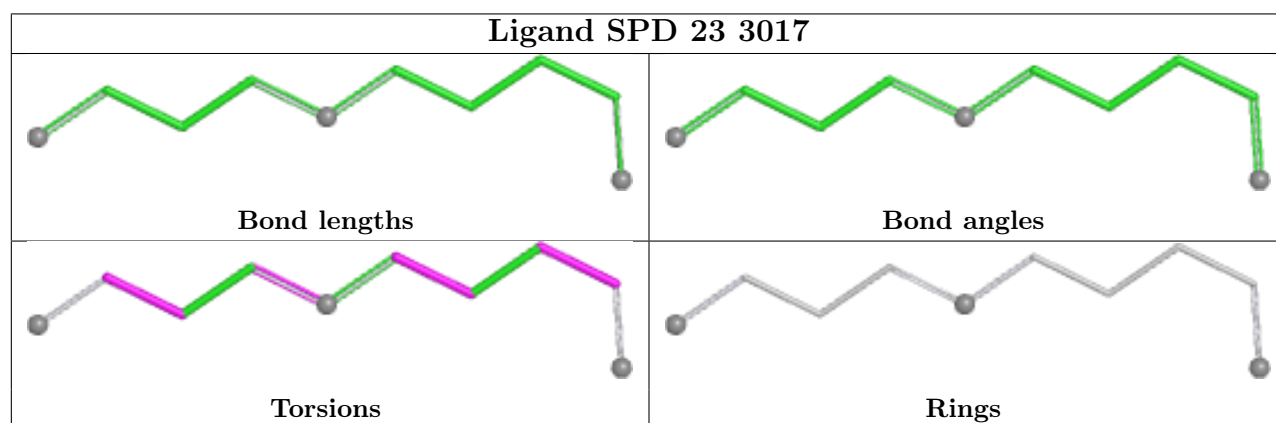
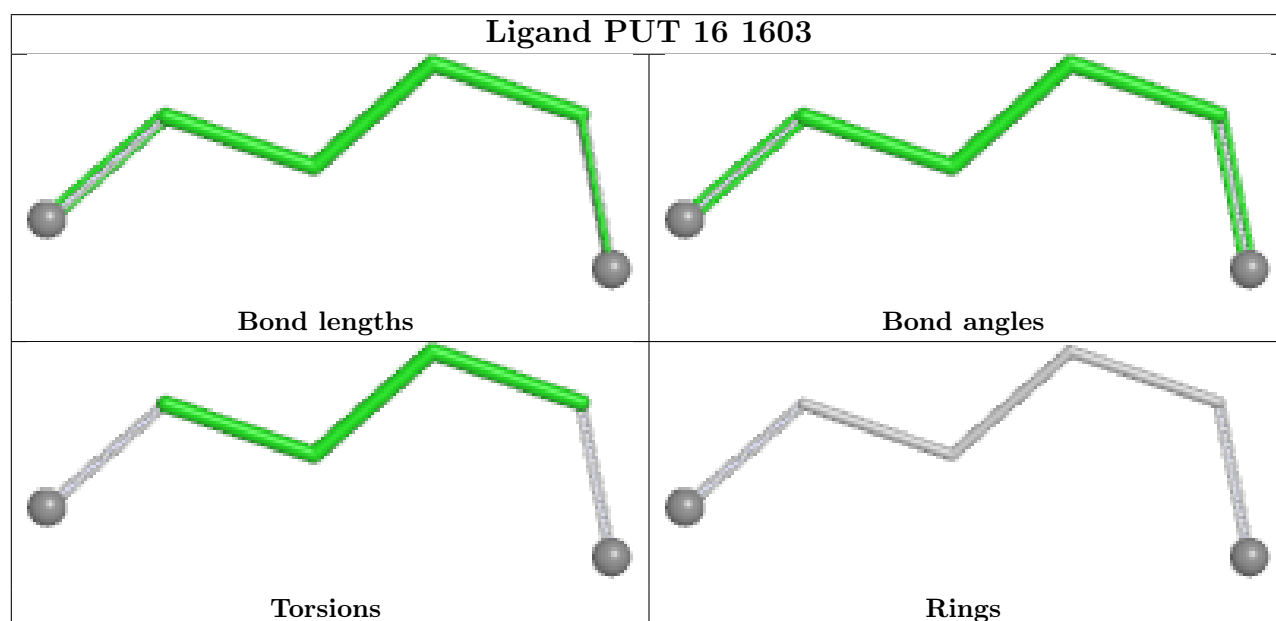
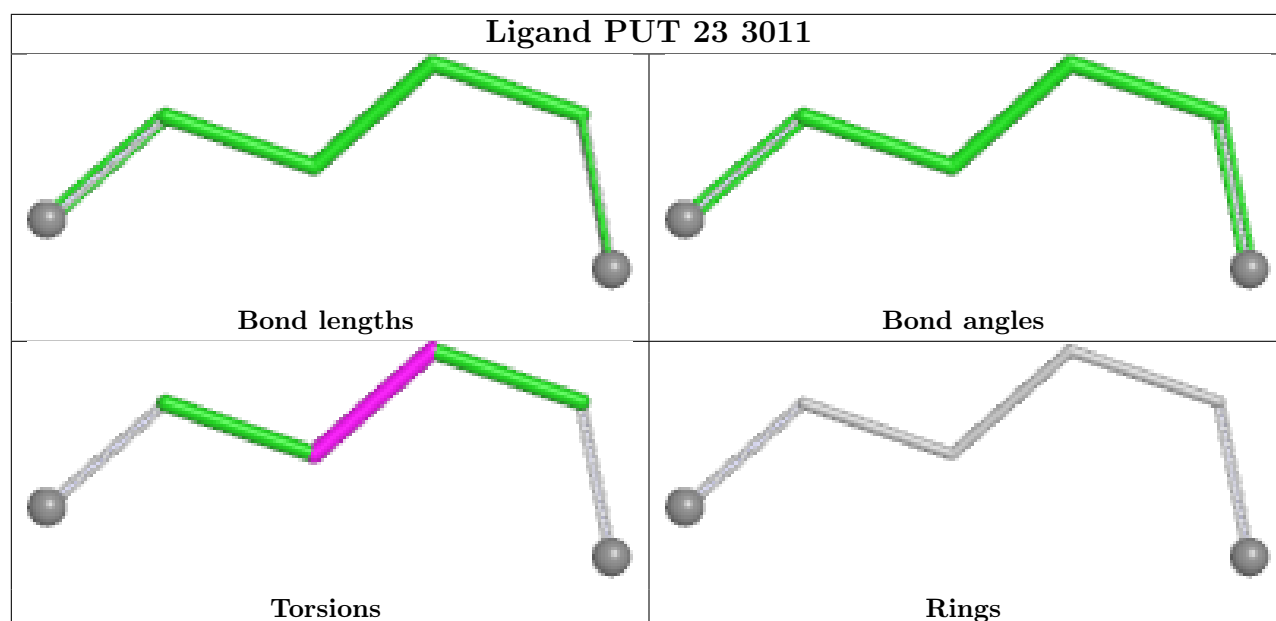


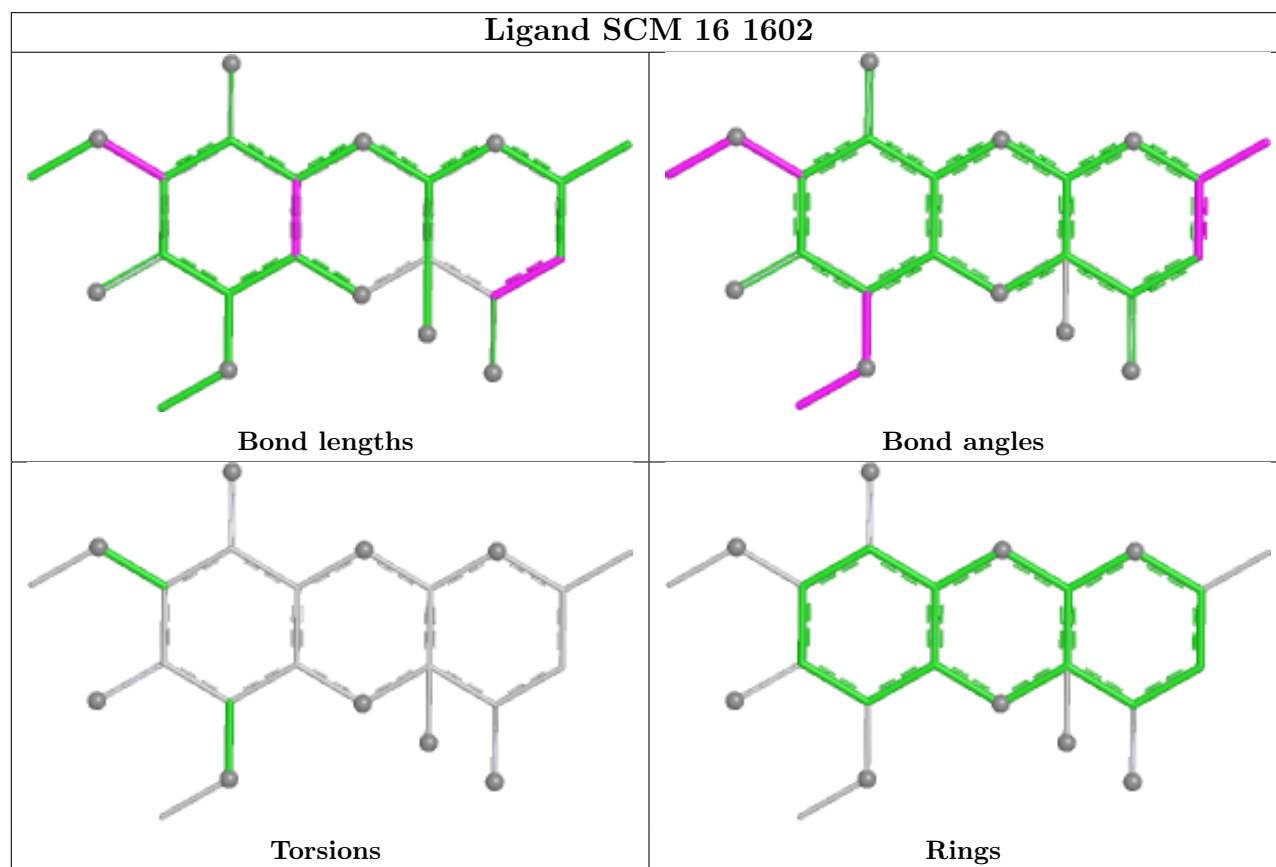
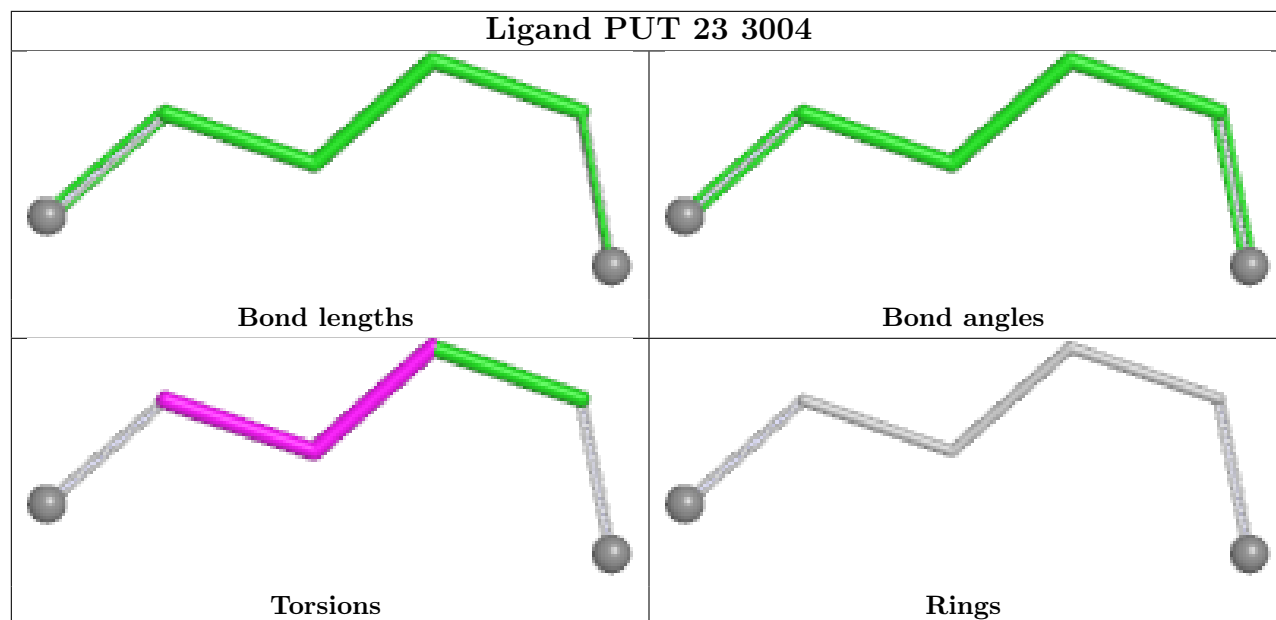


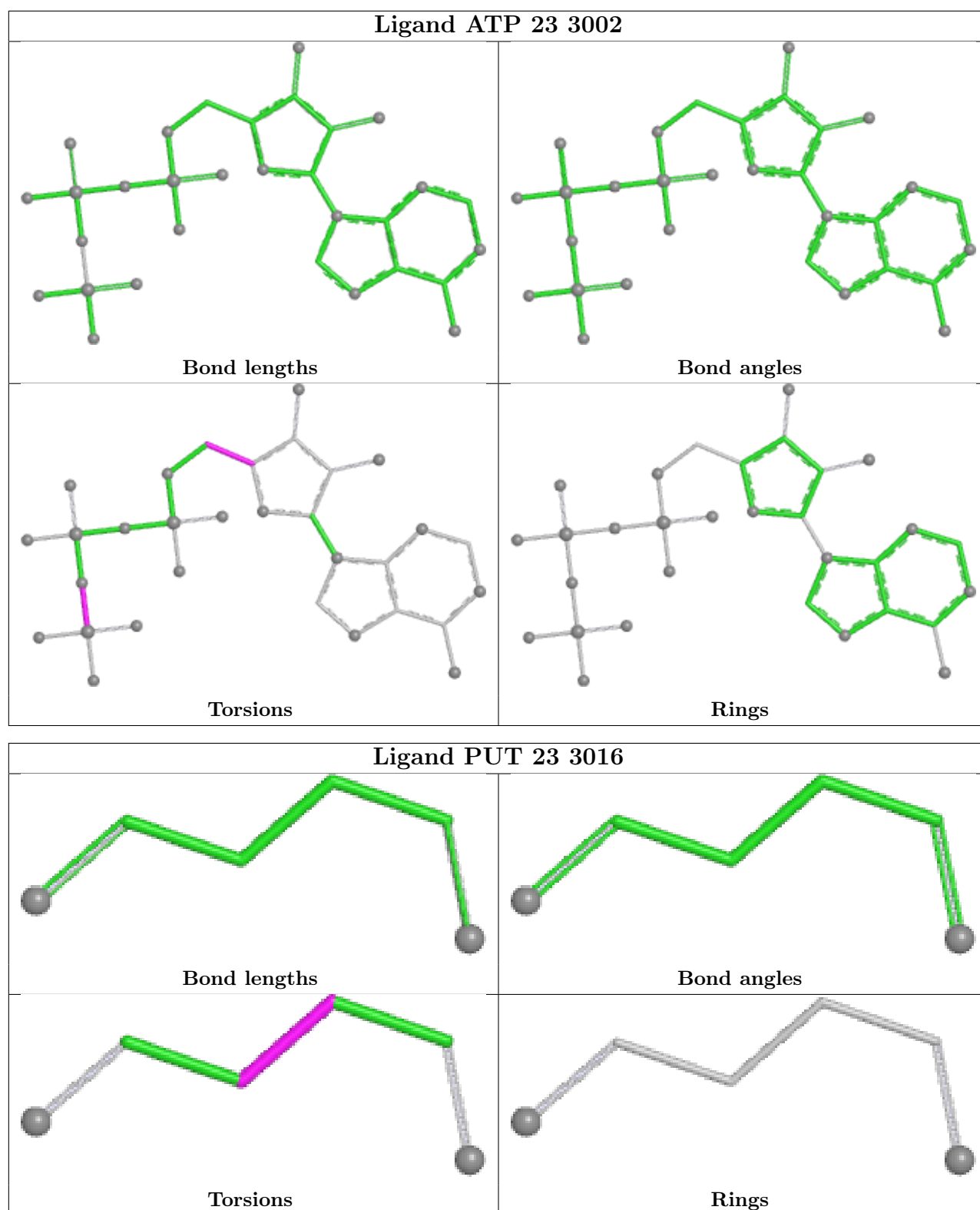




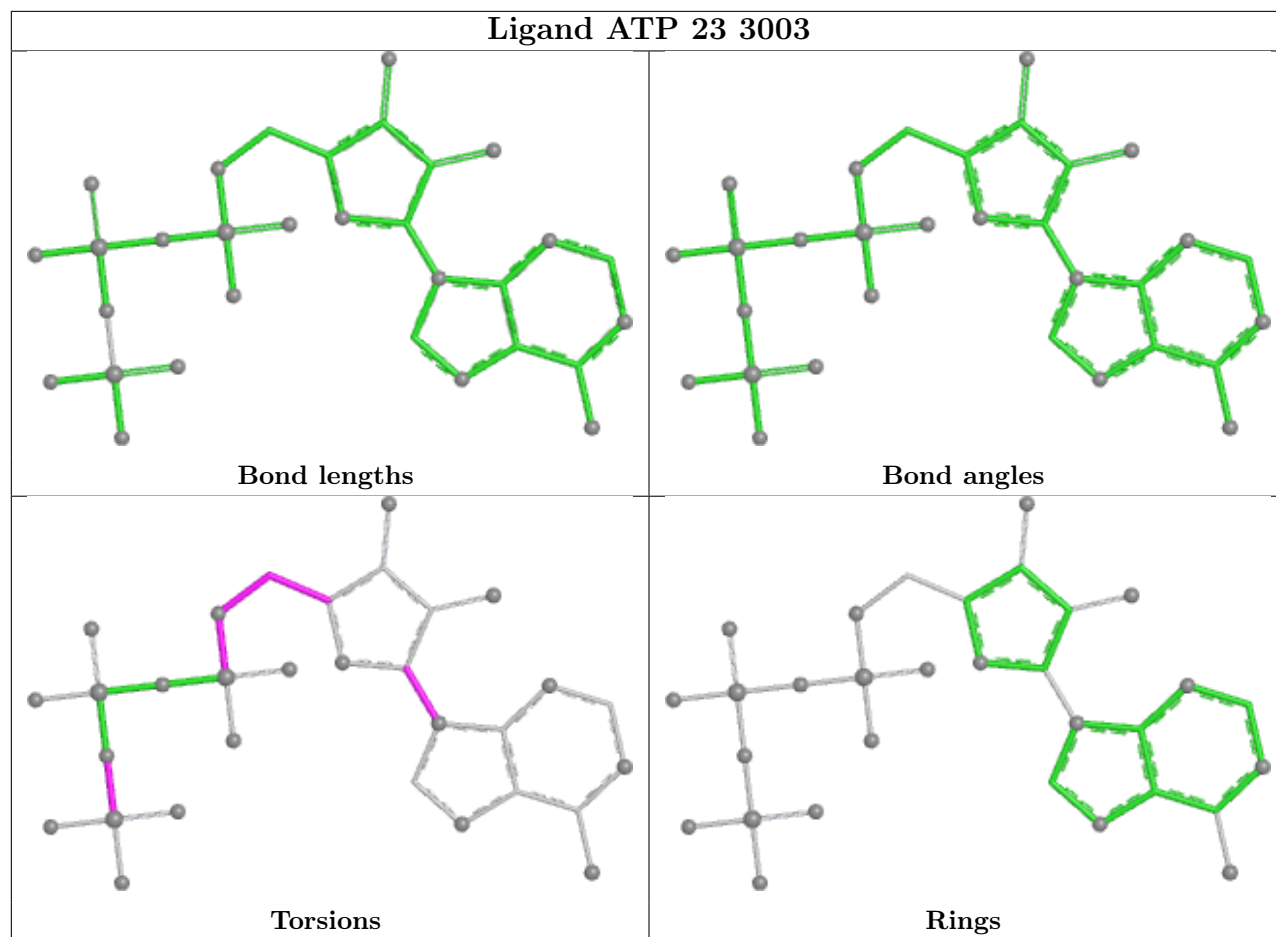




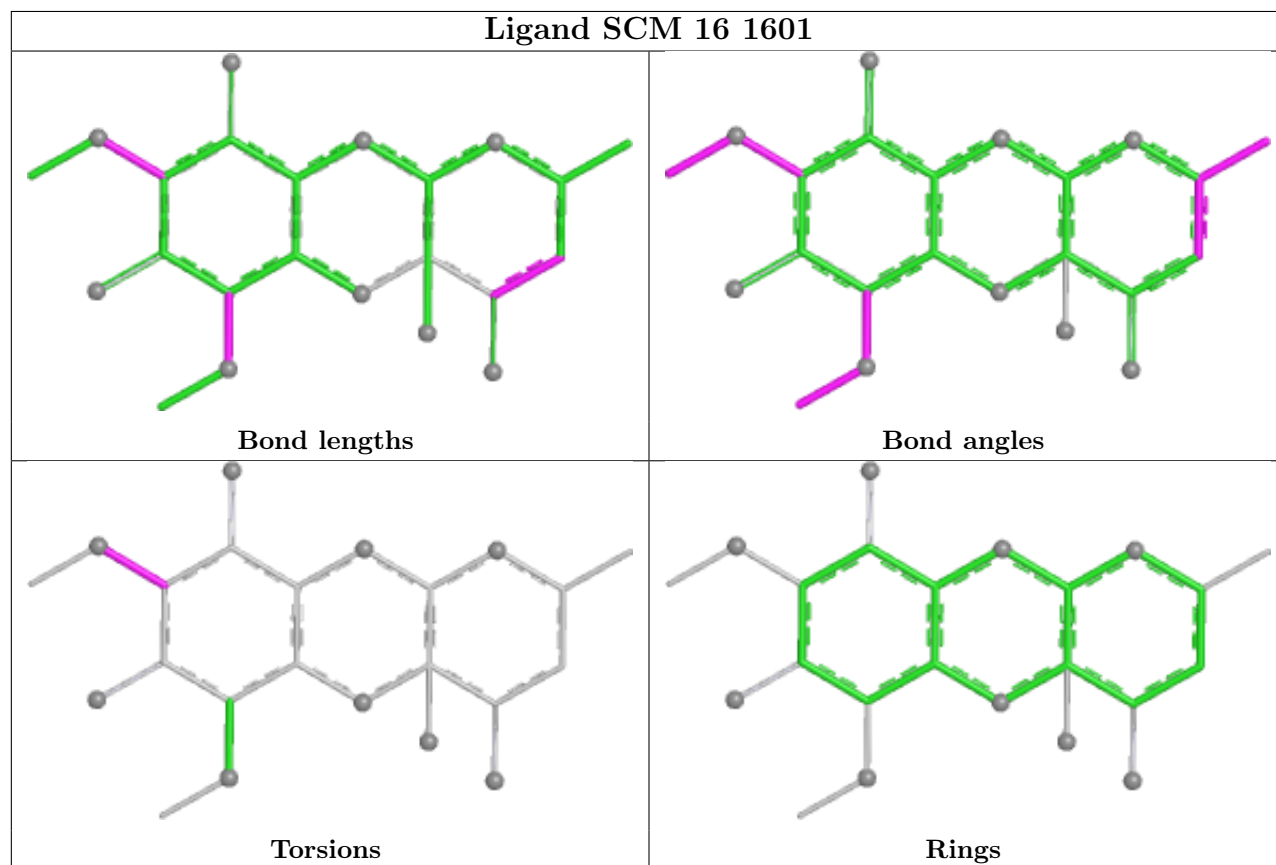




Ligand ATP 23 3003



Ligand SCM 16 1601



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
28	LE	1

All chain breaks are listed below:

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

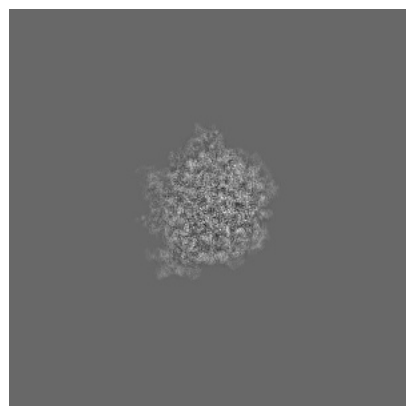
6 Map visualisation [i](#)

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

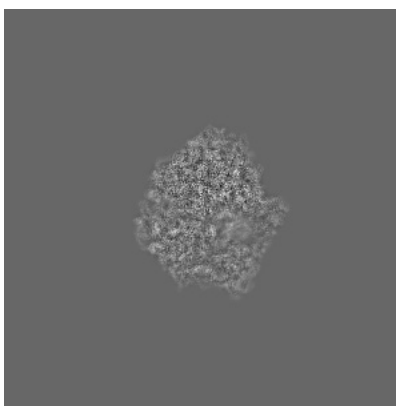
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

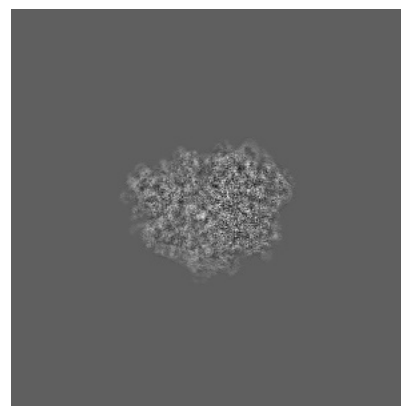
6.1.1 Primary map



X

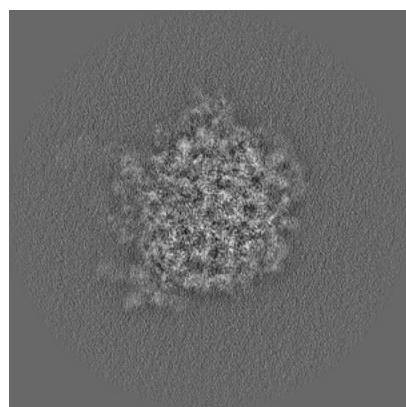


Y

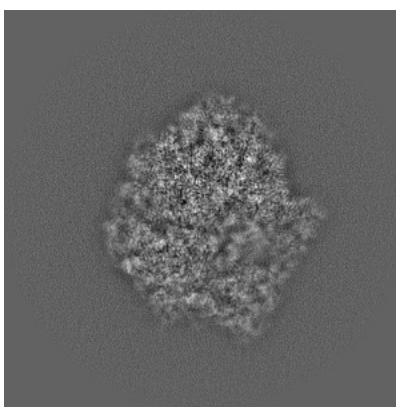


Z

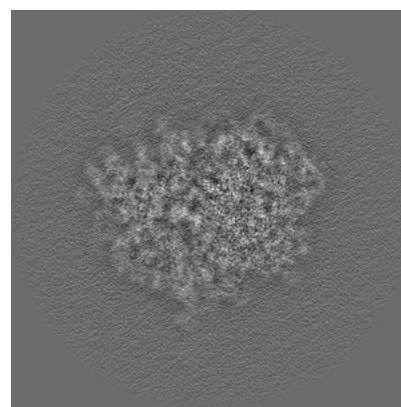
6.1.2 Raw map



X



Y

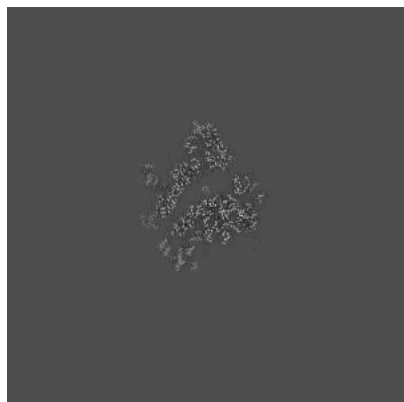


Z

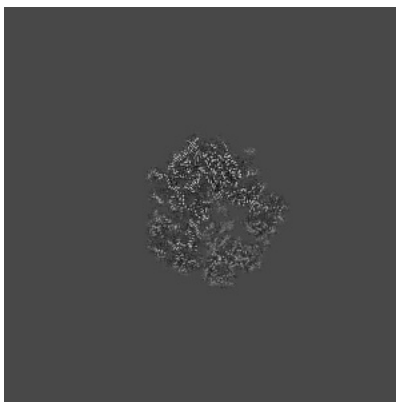
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

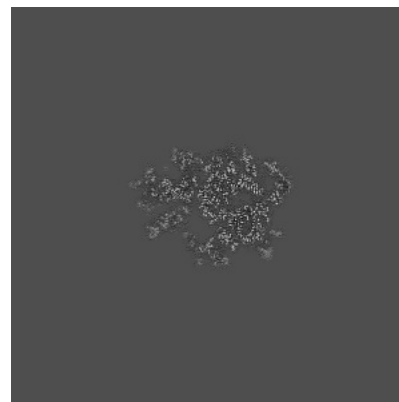
6.2.1 Primary map



X Index: 288

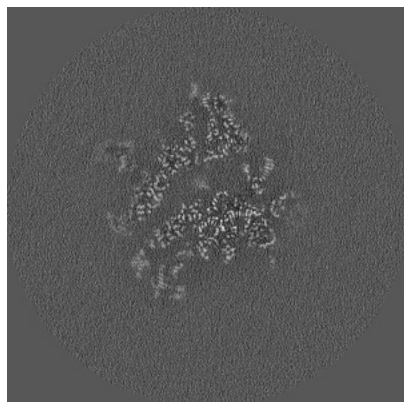


Y Index: 288

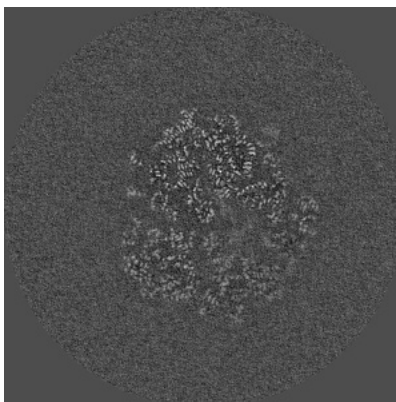


Z Index: 288

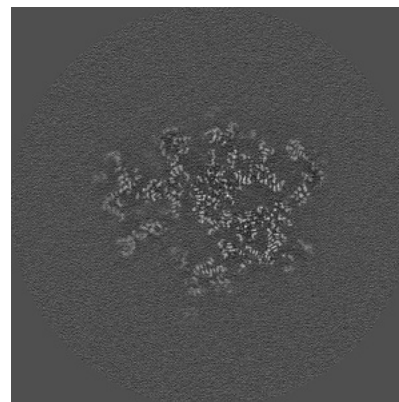
6.2.2 Raw map



X Index: 256



Y Index: 256

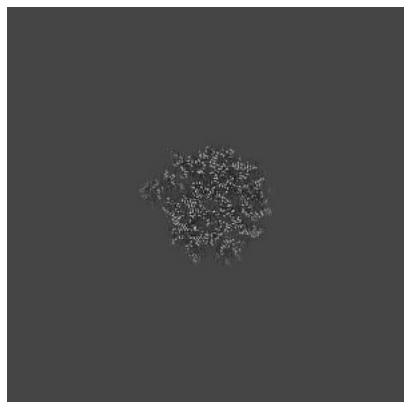


Z Index: 256

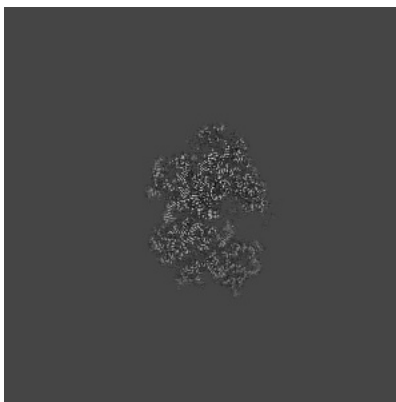
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

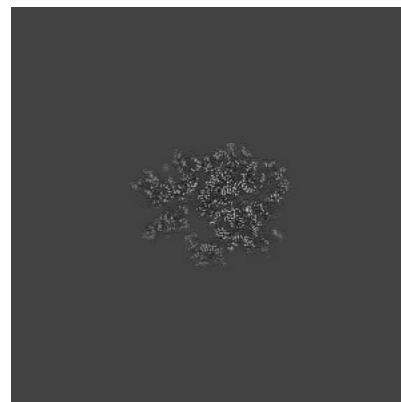
6.3.1 Primary map



X Index: 316

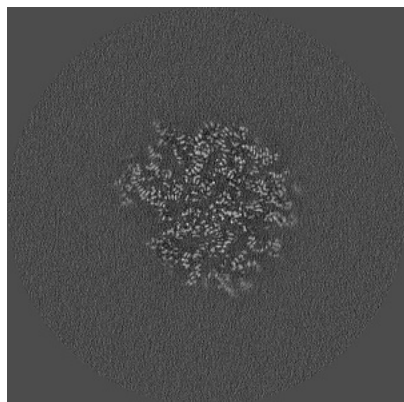


Y Index: 313

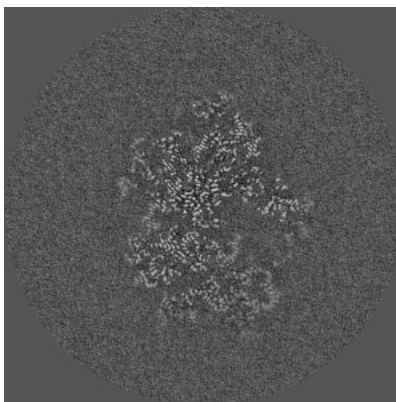


Z Index: 283

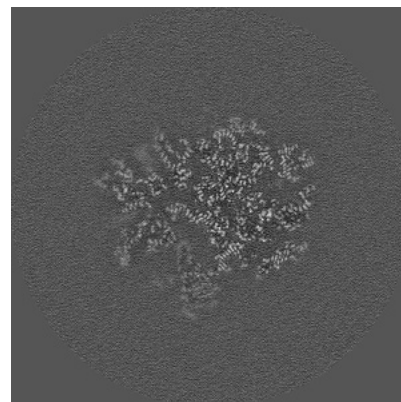
6.3.2 Raw map



X Index: 284



Y Index: 283

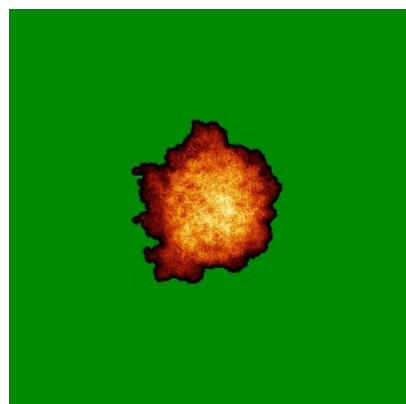


Z Index: 241

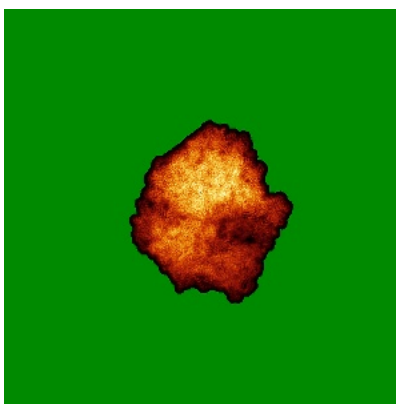
The images above show the largest variance slices of the map in three orthogonal directions.

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

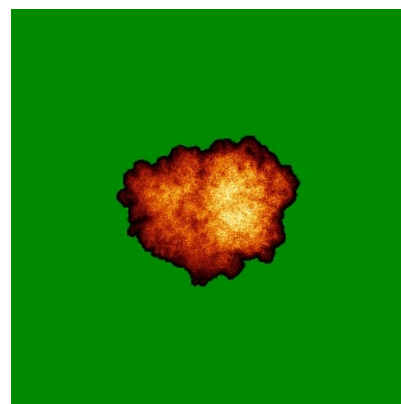
6.4.1 Primary map



X

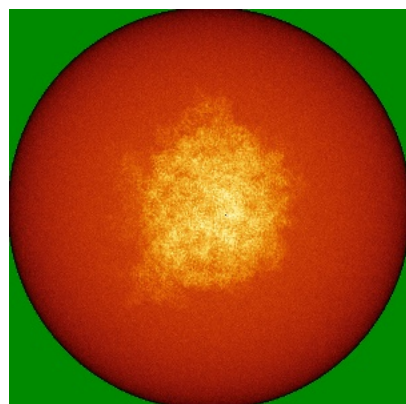


Y

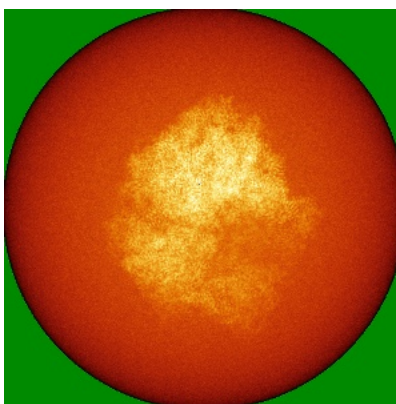


Z

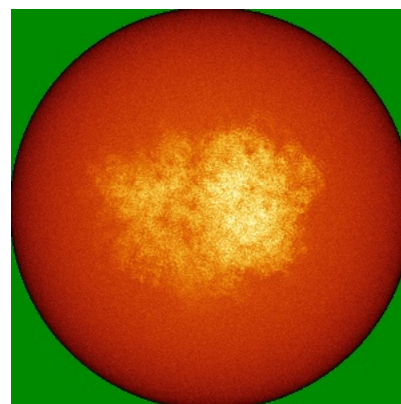
6.4.2 Raw map



X



Y

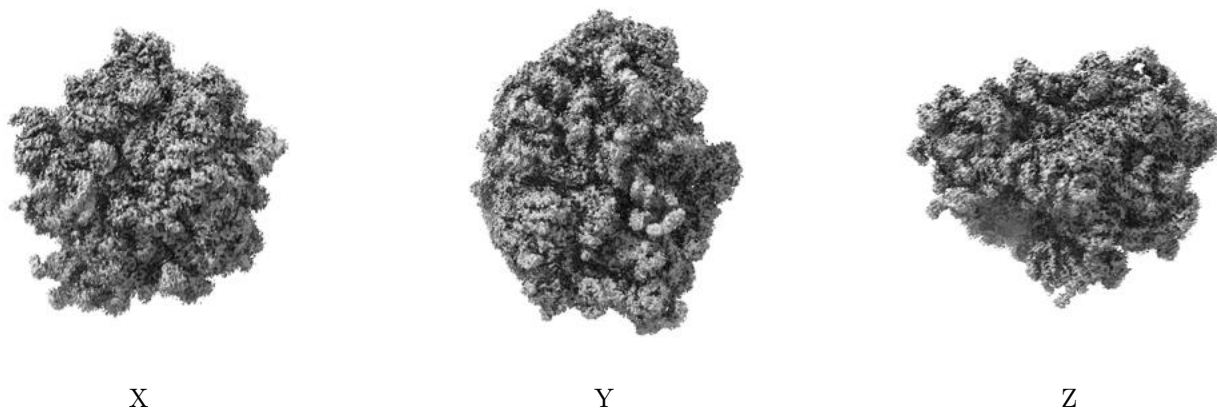


Z

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

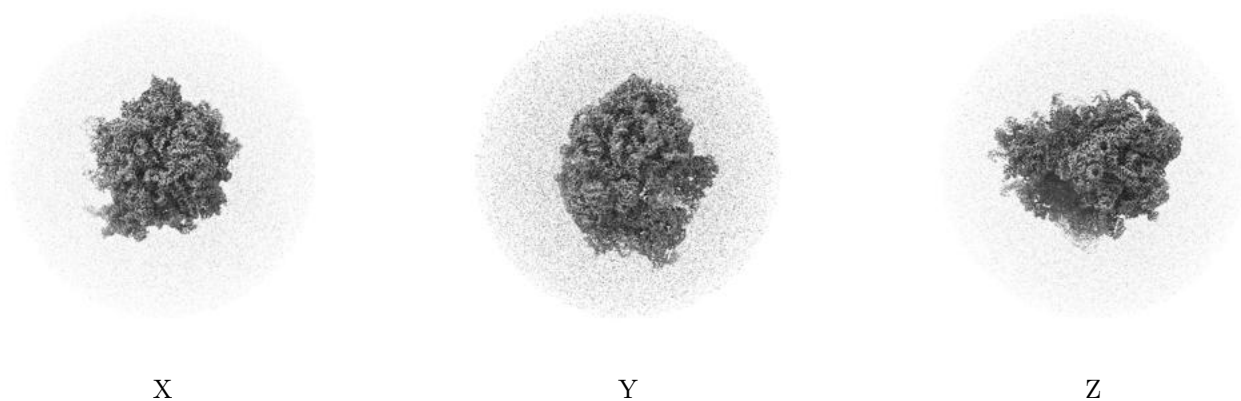
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

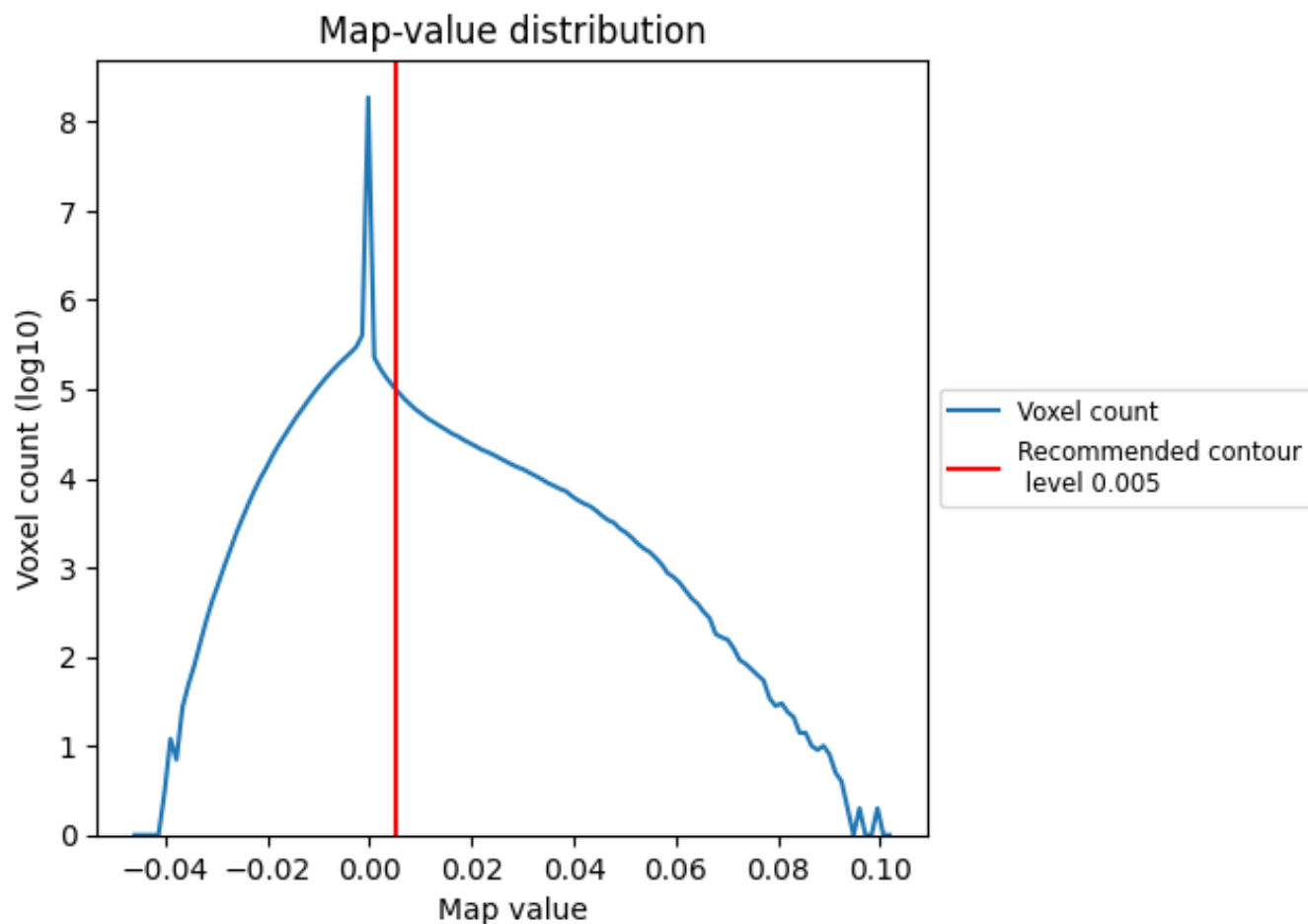
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

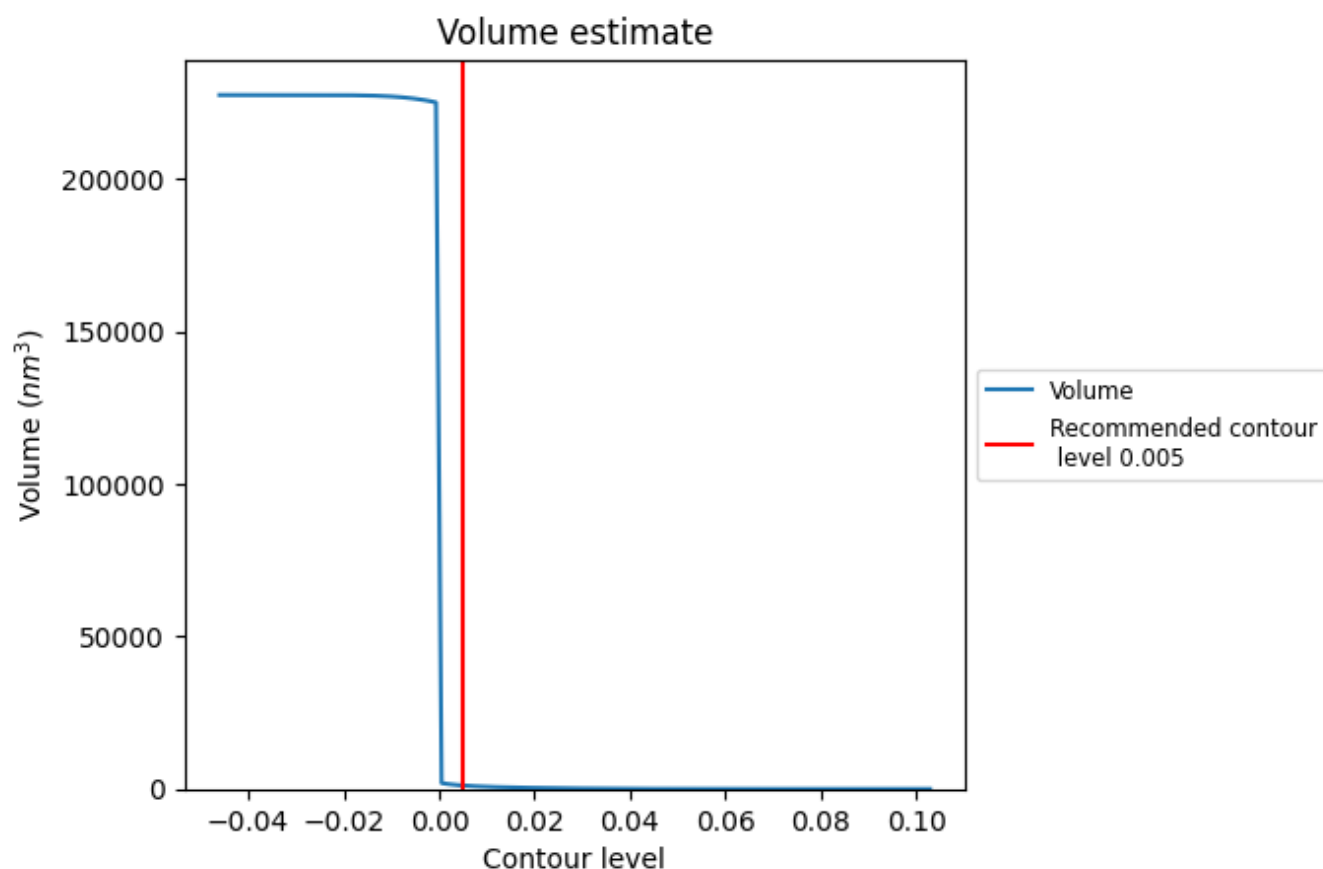
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

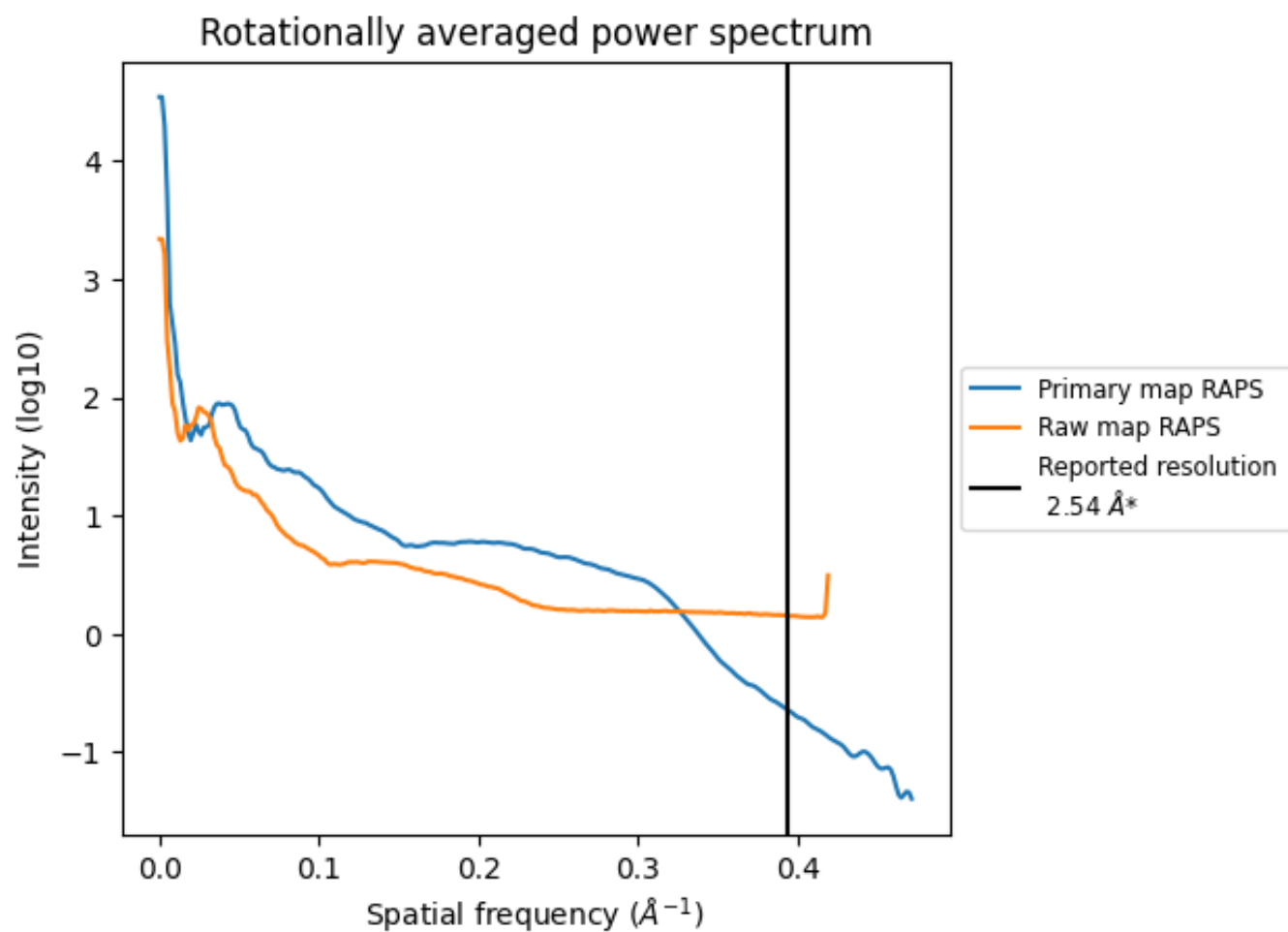
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

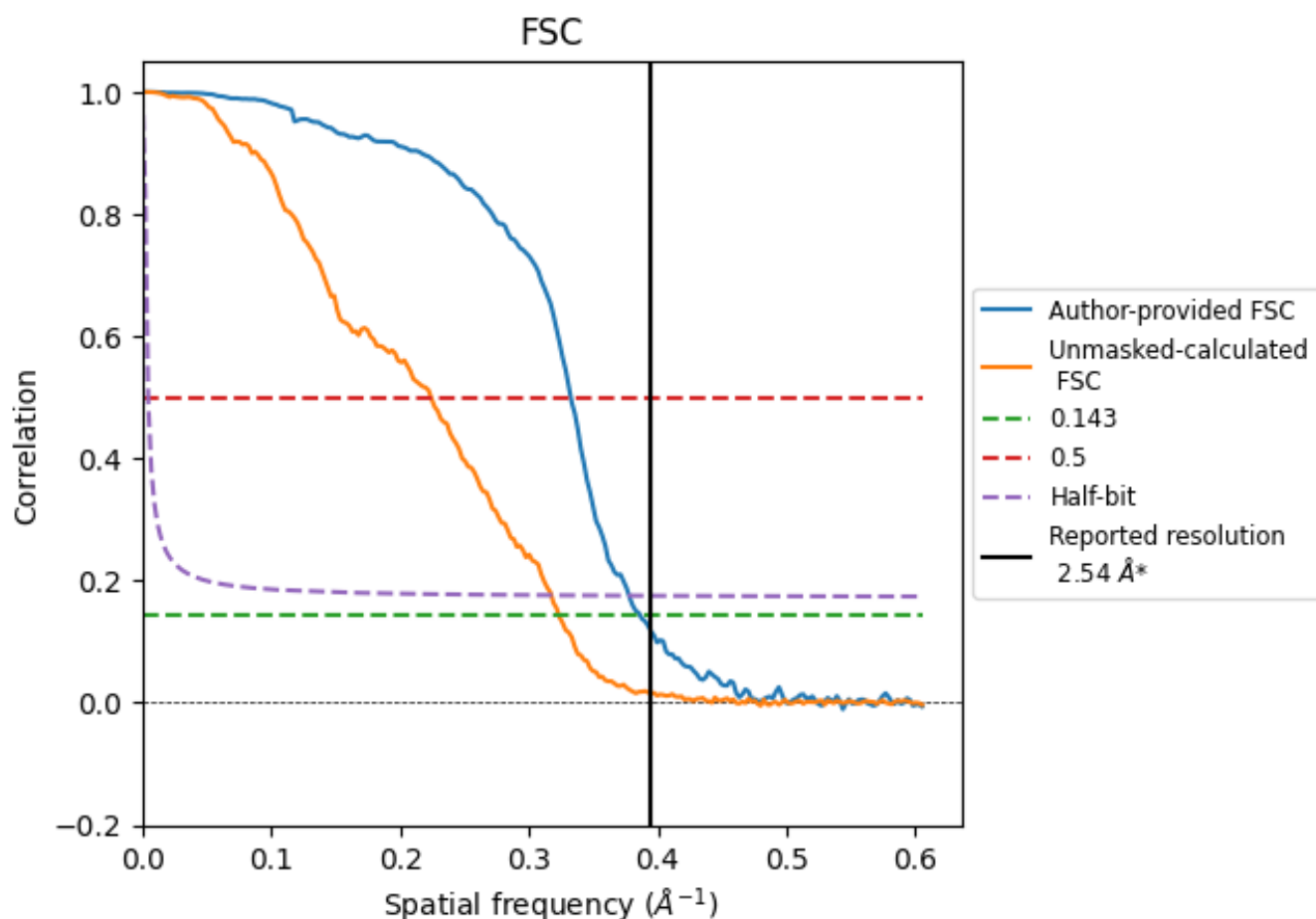


*Reported resolution corresponds to spatial frequency of 0.394 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

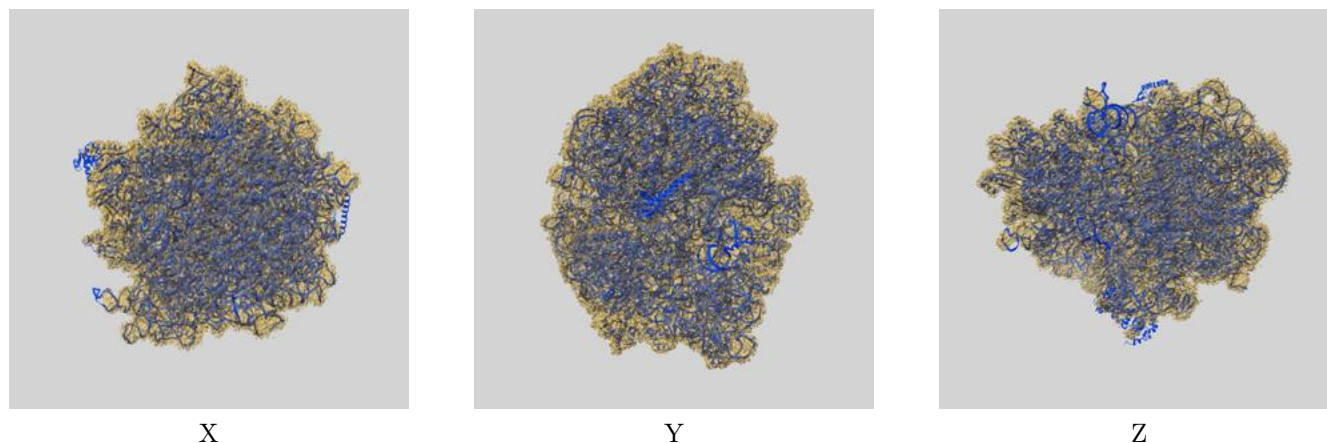
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.59	3.01	2.65
Unmasked-calculated*	3.09	4.46	3.15

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

9 Map-model fit [i](#)

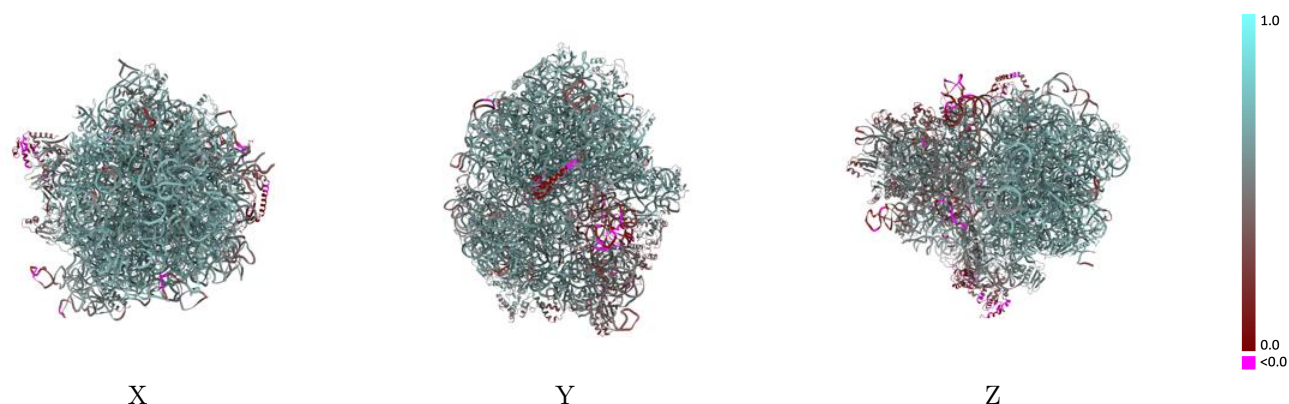
This section contains information regarding the fit between EMDB map EMD-24134 and PDB model 7N2V. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



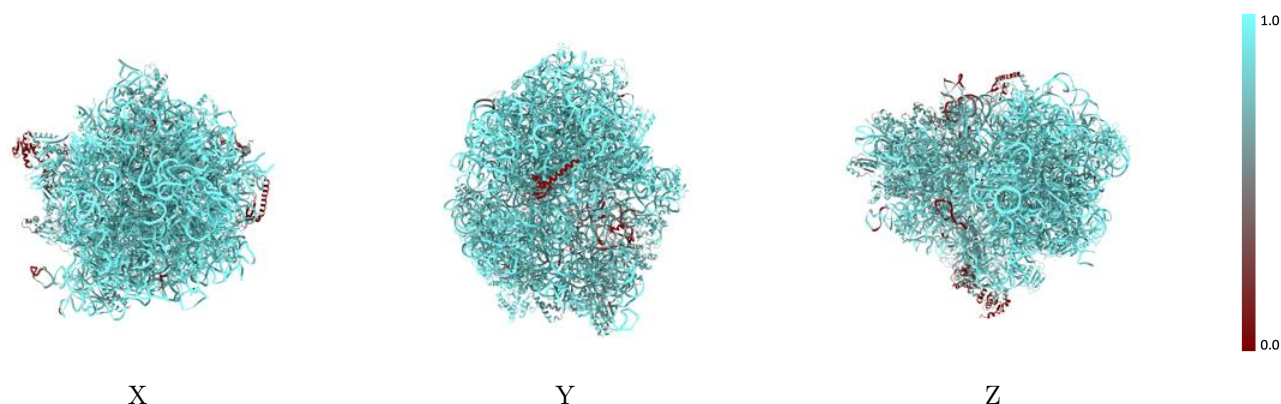
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



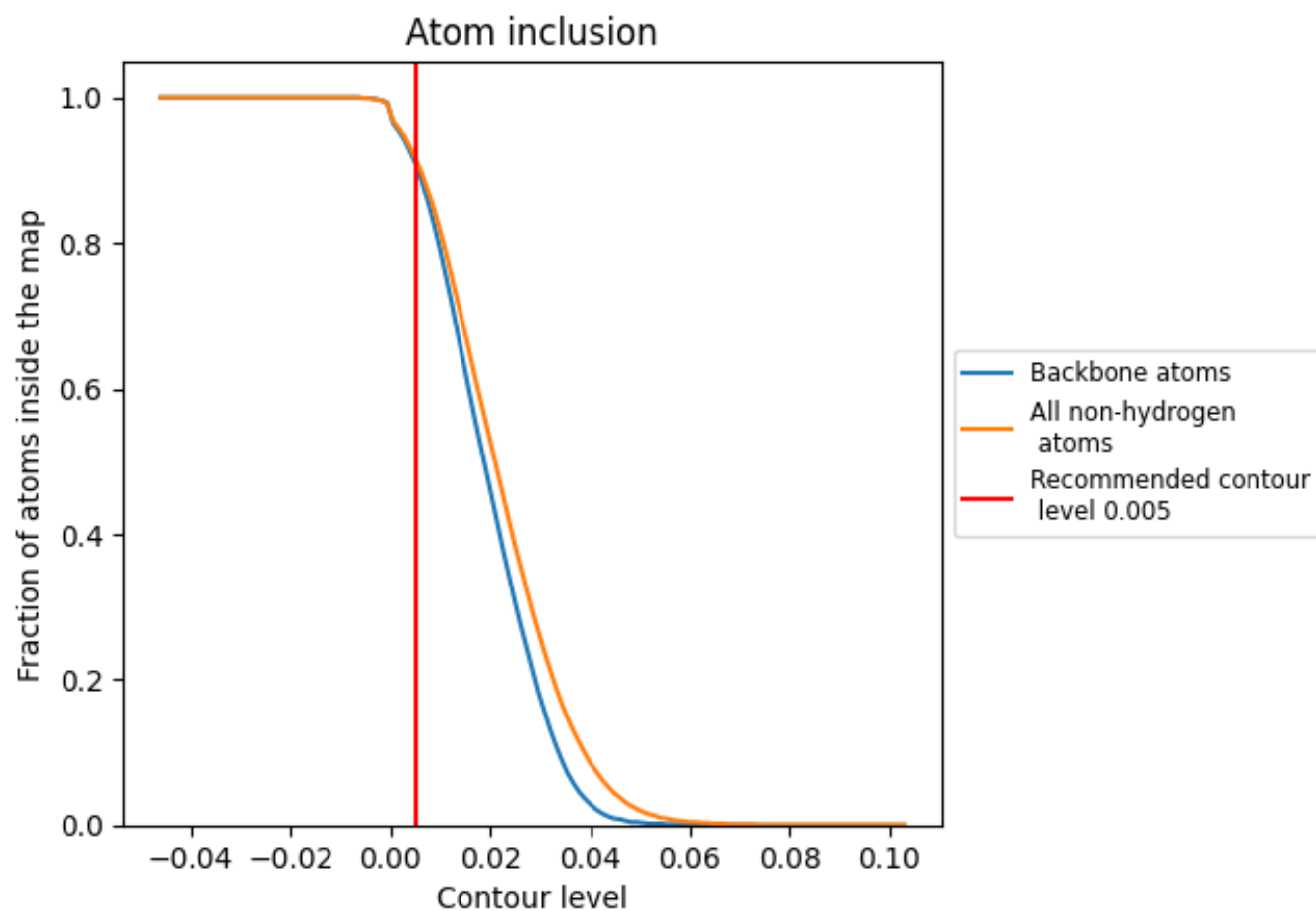
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion ⓘ



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

9.5 Map-model fit summary ⓘ

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

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



Continued on next page...

Continued from previous page...

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