



## wwPDB EM Validation Summary Report ⓘ

Mar 12, 2025 – 02:16 AM EDT

PDB ID : 7N2C  
EMDB ID : EMD-24132  
Title : Elongating 70S ribosome complex in a fusidic acid-stalled intermediate state of translocation bound to EF-G(GDP) (INT2)  
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 : 2021-05-28  
Resolution : 2.72 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

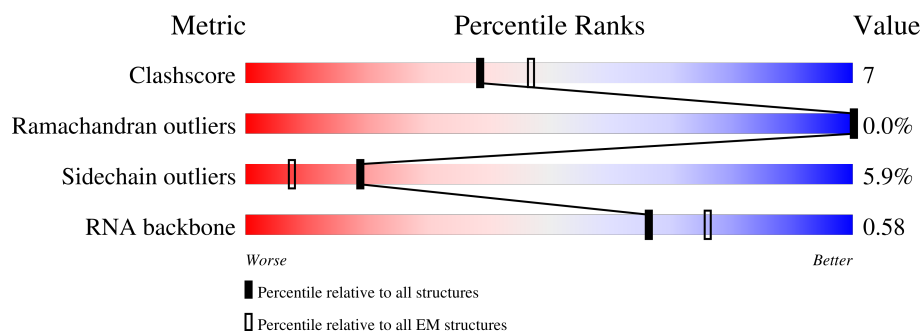
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.72 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

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





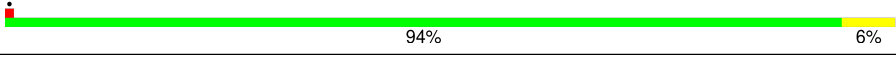










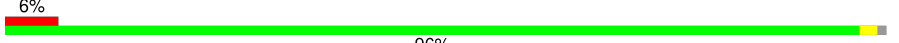
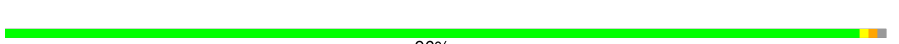






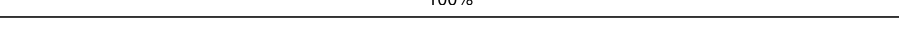
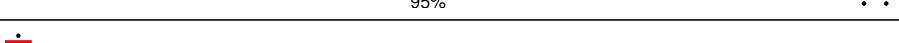
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Mol	Chain	Length	Quality of chain
8	SH	130	
9	SI	130	
10	SJ	103	
11	SK	129	
12	SL	124	
13	SM	118	
14	SN	101	
15	SO	89	
16	SP	82	
17	SQ	84	
18	SR	75	
19	SS	92	
20	ST	87	
21	SU	71	
22	mR	60	
23	23	2904	
24	5	120	
25	LA	234	
26	LB	273	
27	LC	209	
28	LD	201	
29	LE	179	
30	LF	177	
31	LG	121	
32	LI	149	

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Mol	Chain	Length	Quality of chain
33	LJ	165	
34	LK	142	
35	LM	142	
36	LN	123	
37	LO	144	
38	LP	136	
39	LQ	127	
40	LR	117	
41	LS	115	
42	LT	118	
43	LU	103	
44	LV	110	
45	LW	100	
46	LX	104	
47	LY	94	
48	La	85	
49	Lb	78	
50	Lc	63	
51	Ld	59	
52	Le	70	
53	Lf	57	
54	Lg	55	
55	Lh	46	
56	Li	65	
57	Lj	38	

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Mol	Chain	Length	Quality of chain
58	EF	704	<div><div></div><div>6%</div><div>75%</div><div>21%</div><div></div><div></div></div>
59	Pp	3	<div><div></div><div>67%</div><div>33%</div><div></div><div></div></div>
60	Pt	76	<div><div></div><div>5%</div><div>72%</div><div>24%</div><div></div><div></div></div>
61	Dt	76	<div><div></div><div>7%</div><div>63%</div><div>33%</div><div></div><div></div></div>

## 2 Entry composition

There are 68 unique types of molecules in this entry. The entry contains 155157 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	226	Total	C	N	O	S	0	0
			1769	1119	317	325	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SC	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- 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	156	Total	C	N	O	S	0	0
			1235	773	237	221	4		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SK	117	Total	C	N	O	S	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
			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	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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



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

- Molecule 22 is a RNA chain called Chains: mR.

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	2903	Total	C	N	O	P	0	0
			62334	27815	11467	20149	2903		

- 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 L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LA	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

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

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	LG	68	Total	C	N	O	0	0
			487	306	82	99		

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LJ	135	Total	C	N	O	S	0	0
			1023	648	179	192	4		

- Molecule 34 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LK	134	Total	C	N	O	S	0	0
			973	616	166	185	6		

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L17.

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

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

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

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Le	67	Total	C	N	O	S	0	0
			529	328	100	95	6		

- Molecule 53 is a protein called 50S ribosomal protein L32.

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

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	Lg	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 55 is a protein called 50S ribosomal protein L34.

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

- Molecule 56 is a protein called 50S ribosomal protein L35.

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

- Molecule 57 is a protein called 50S ribosomal protein L36.

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

- Molecule 58 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	EF	685	Total	C	N	O	S	0	0
			4999	3161	893	927	18		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EF	1	SER	MET	engineered mutation	UNP P0A6M8

- Molecule 59 is a protein called Polypeptide.

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

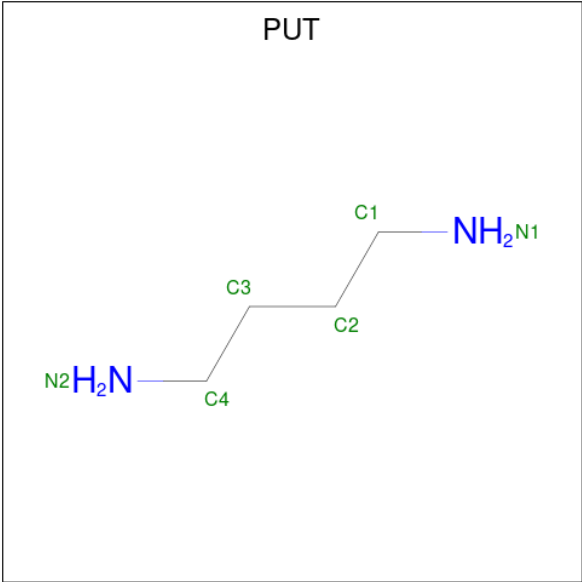
- Molecule 60 is a RNA chain called Chains: Pt.

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

- Molecule 61 is a RNA chain called tRNA.

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

- Molecule 62 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: C<sub>4</sub>H<sub>12</sub>N<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
62	16	1	Total	C	N	0
			6	4	2	
62	16	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	

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Mol	Chain	Residues	Atoms			AltConf
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	23	1	Total	C	N	0
			6	4	2	
62	LC	1	Total	C	N	0
			6	4	2	

- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
63	16	40	Total	Mg	0
			40	40	
63	SN	2	Total	Mg	0
			2	2	
63	23	144	Total	Mg	0
			144	144	
63	5	4	Total	Mg	0
			4	4	
63	LB	1	Total	Mg	0
			1	1	
63	LC	1	Total	Mg	0
			1	1	
63	LD	1	Total	Mg	0
			1	1	
63	LQ	1	Total	Mg	0
			1	1	
63	LW	1	Total	Mg	0
			1	1	
63	Lf	1	Total	Mg	0
			1	1	
63	EF	1	Total	Mg	0
			1	1	

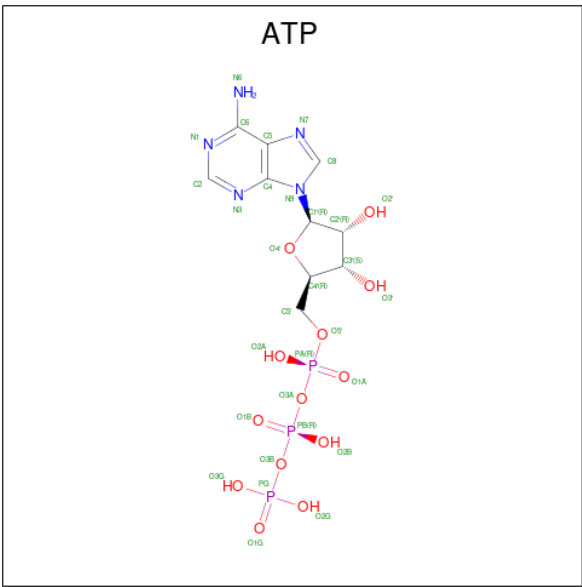
- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of



Interest" by depositor).

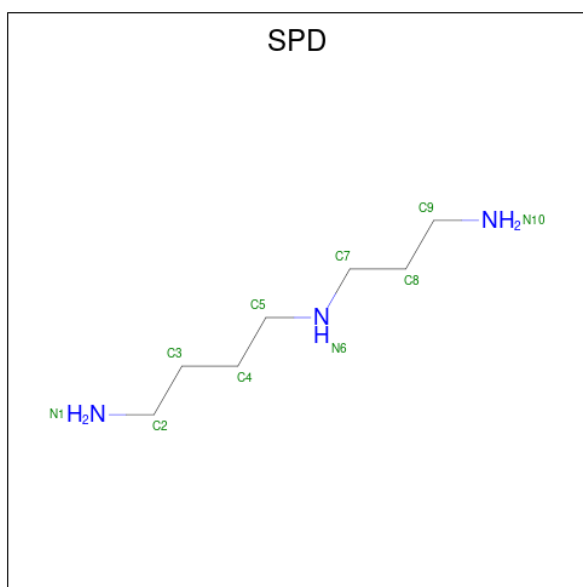
Mol	Chain	Residues	Atoms		AltConf
64	SB	1	Total	Zn	0
			1	1	
64	Le	1	Total	Zn	0
			1	1	
64	Lj	1	Total	Zn	0
			1	1	

- Molecule 65 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



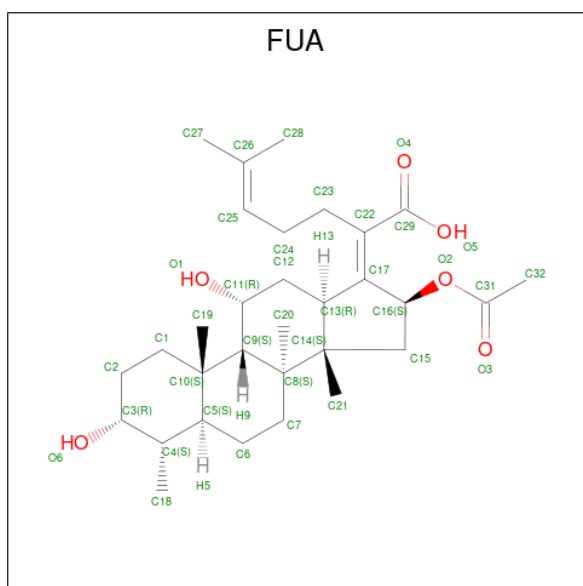
Mol	Chain	Residues	Atoms					AltConf
65	23	1	Total	C	N	O	P	0
			31	10	5	13	3	
65	23	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 66 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



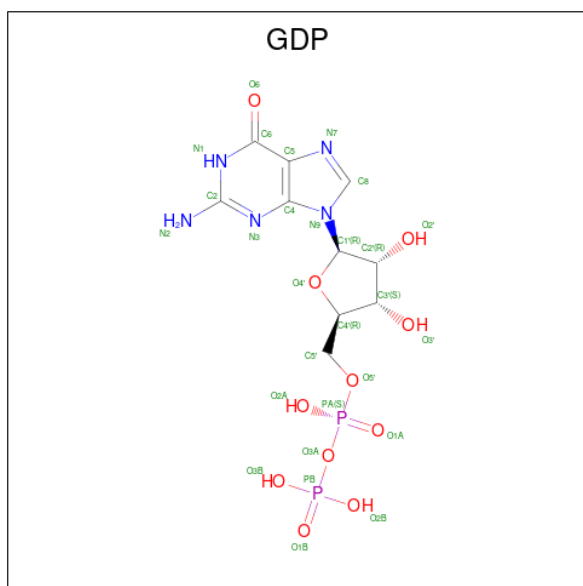
Mol	Chain	Residues	Atoms			AltConf
66	23	1	Total	C	N	0
			10	7	3	
66	23	1	Total	C	N	0
			10	7	3	
66	23	1	Total	C	N	0
			10	7	3	

- Molecule 67 is FUSIDIC ACID (three-letter code: FUA) (formula:  $C_{31}H_{48}O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
67	EF	1	Total	C	O	0
			37	31	6	

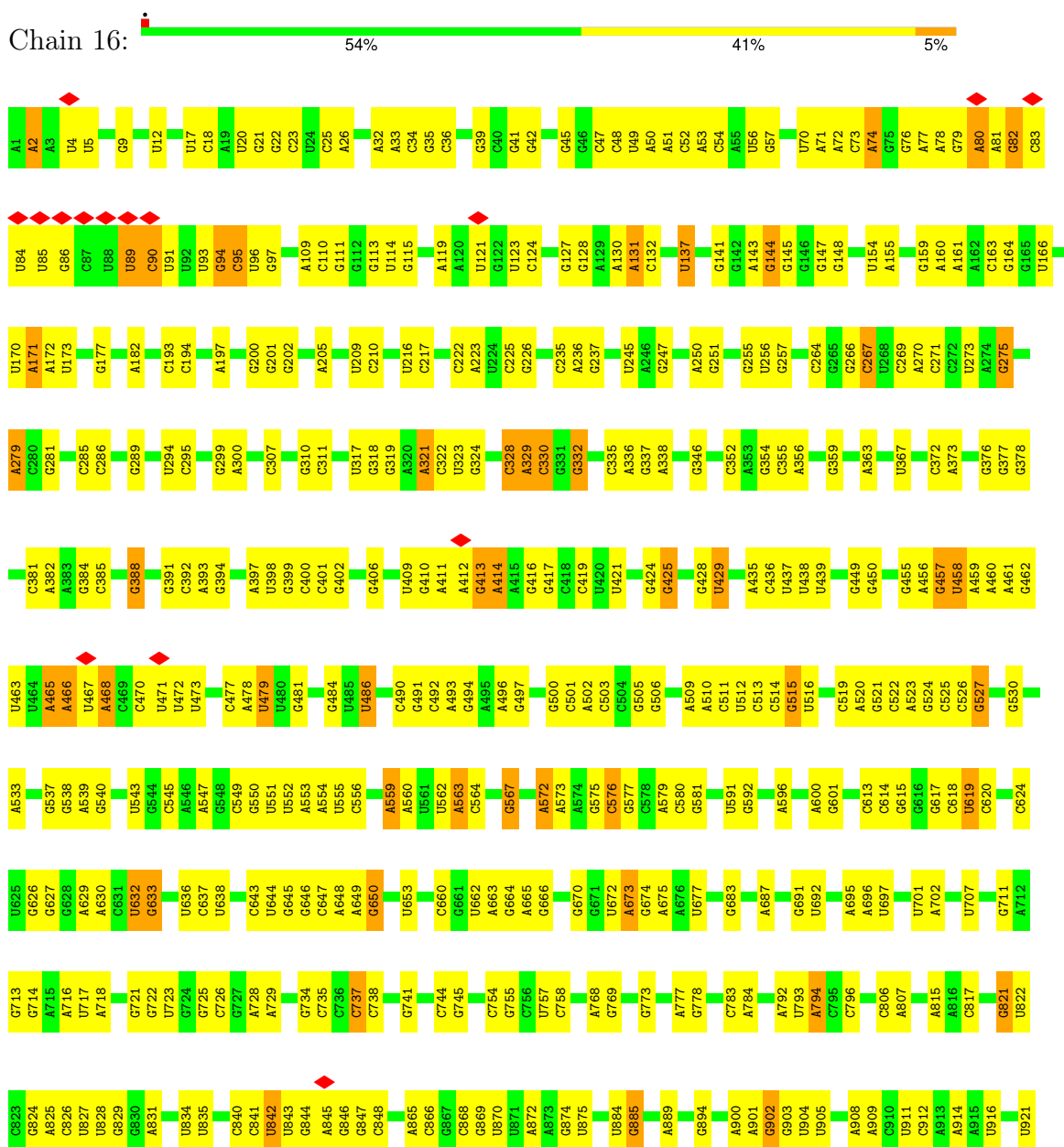
- Molecule 68 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ) (labeled as "Ligand of Interest" by depositor).

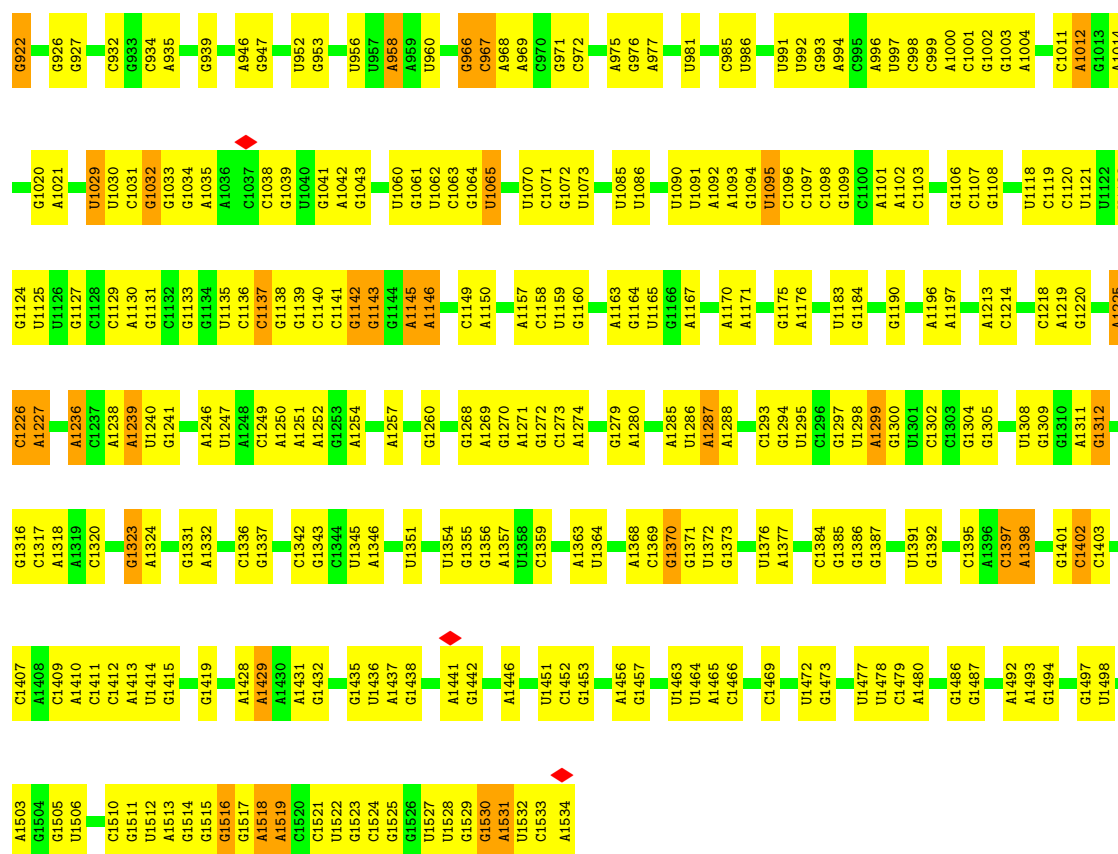


### 3 Residue-property plots

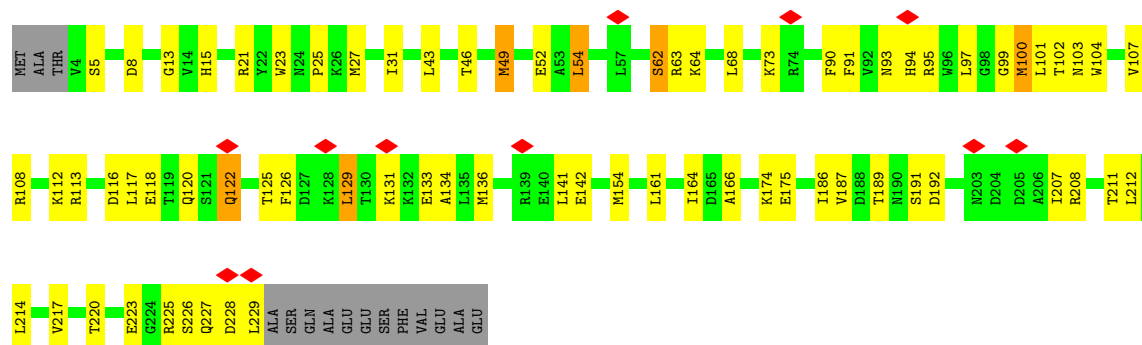
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

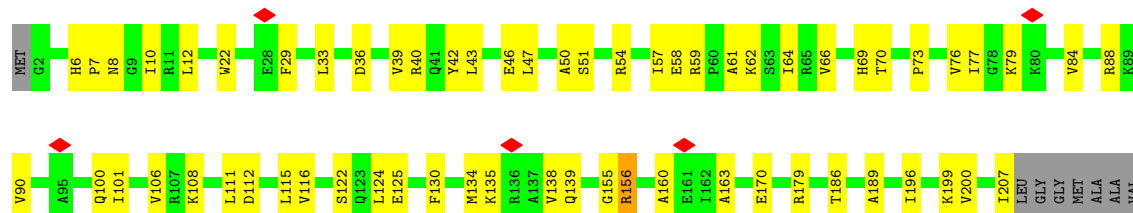




• Molecule 2: 30S ribosomal protein S2



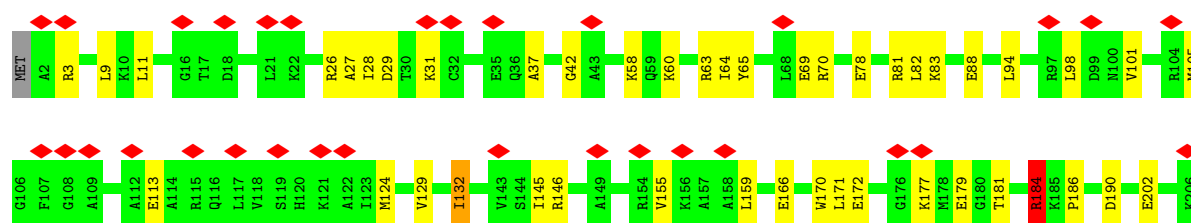
• Molecule 3: 30S ribosomal protein S3



GLU  
GLN  
PRO  
GLU  
LYS  
PRO  
ALA  
GLN  
PRO  
LYS  
LYS  
GLN  
GLN  
ARG  
LYS  
GLY  
ARG  
LYS

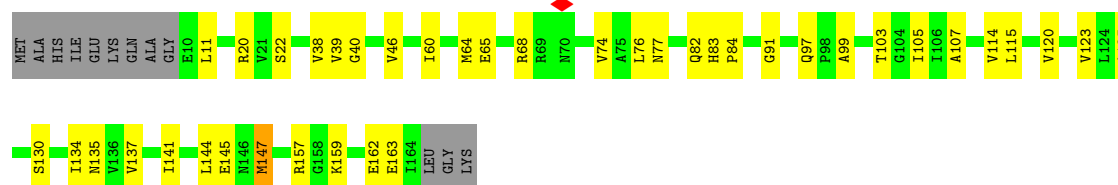
• Molecule 4: 30S ribosomal protein S4

Chain SD: 15% 78% 21%



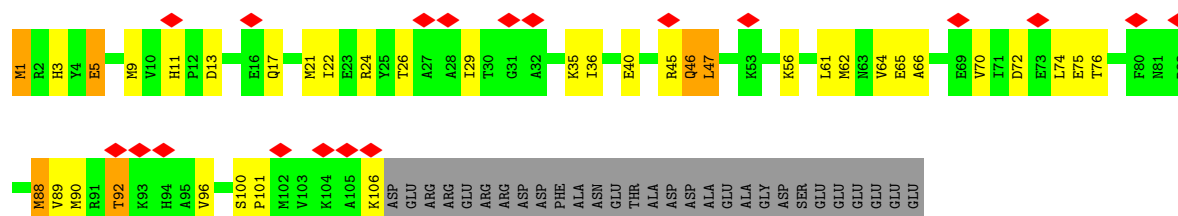
• Molecule 5: 30S ribosomal protein S5

Chain SE: 69% 23% 7%



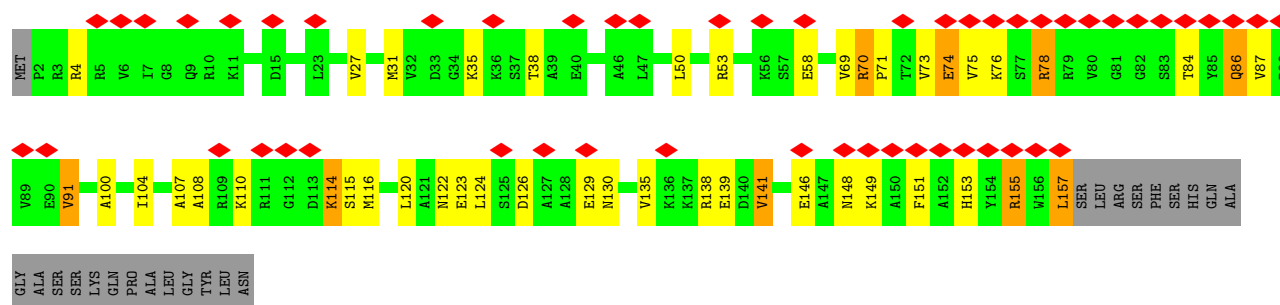
• Molecule 6: 30S ribosomal protein S6

Chain SF: 14% 51% 23% 21%



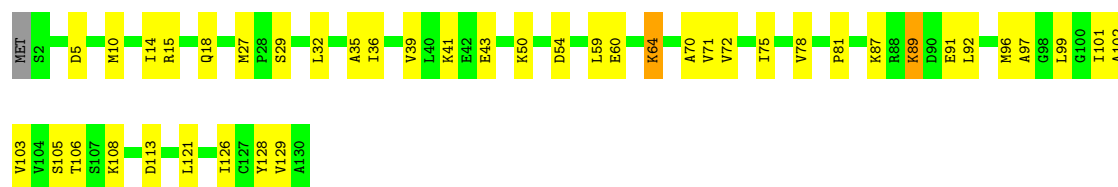
• Molecule 7: 30S ribosomal protein S7

Chain SG: 29% 61% 21% 5% 13%



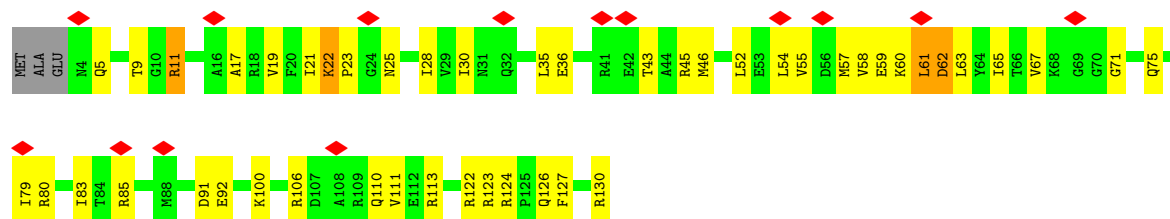
• Molecule 8: 30S ribosomal protein S8

Chain SH:  67% 31% ..



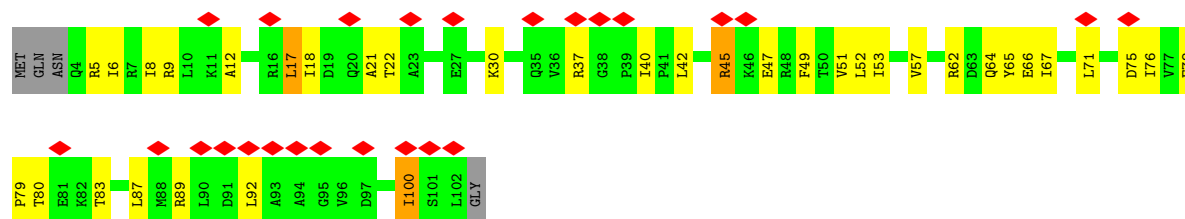
• Molecule 9: 30S ribosomal protein S9

Chain SI:  11% 62% 33% ..



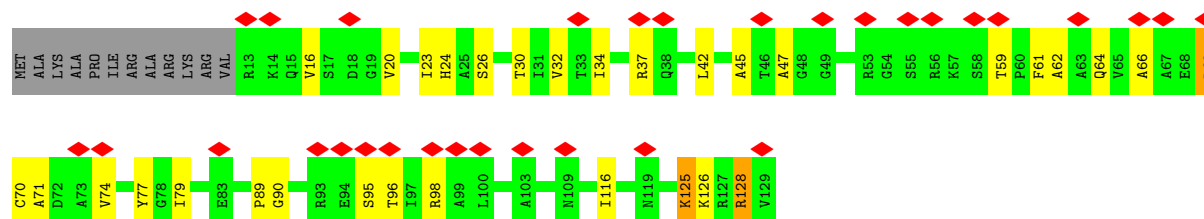
• Molecule 10: 30S ribosomal protein S10

Chain SJ:  24% 61% 32% ..




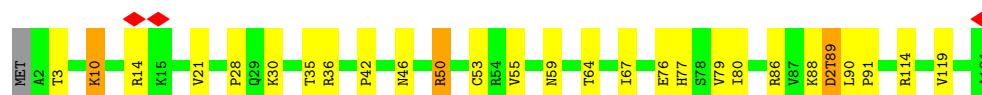
• Molecule 11: 30S ribosomal protein S11

Chain SK:  24% 66% 22% 9% ..

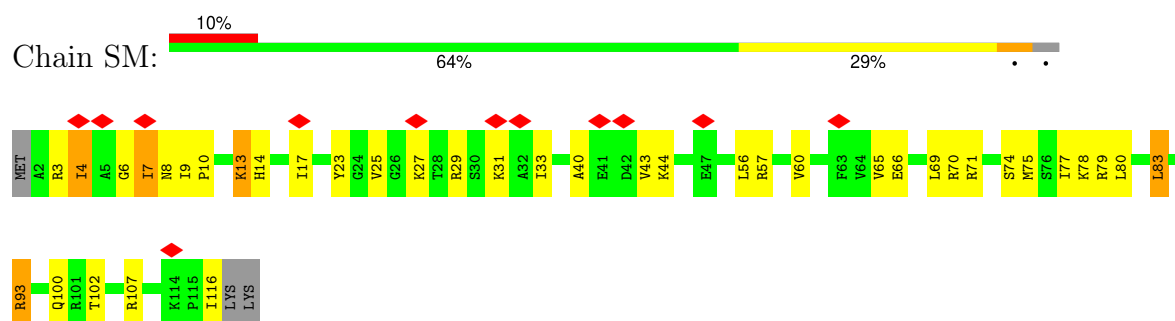


• Molecule 12: 30S ribosomal protein S12

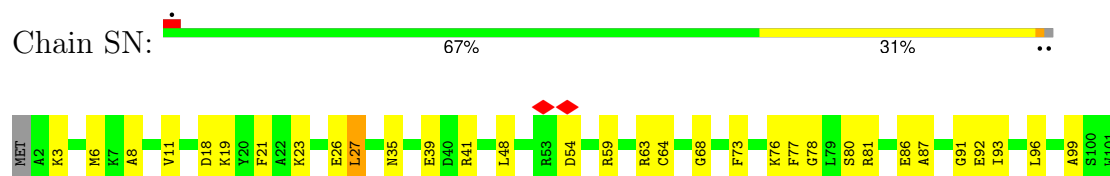
Chain SL:  77% 19% ..



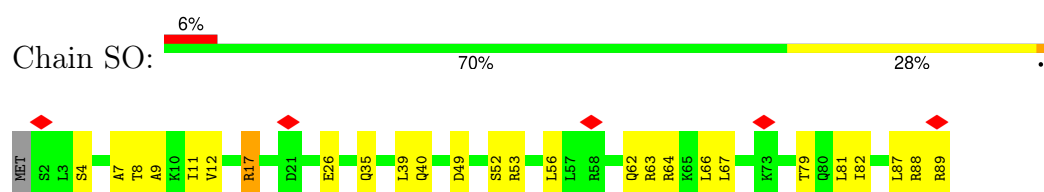
- Molecule 13: 30S ribosomal protein S13



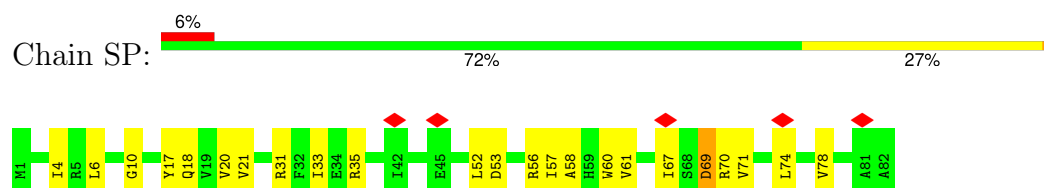
- Molecule 14: 30S ribosomal protein S14



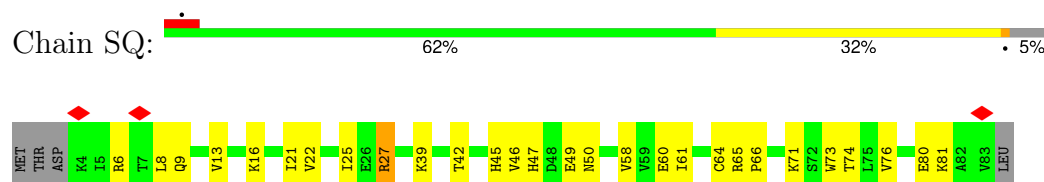
- Molecule 15: 30S ribosomal protein S15



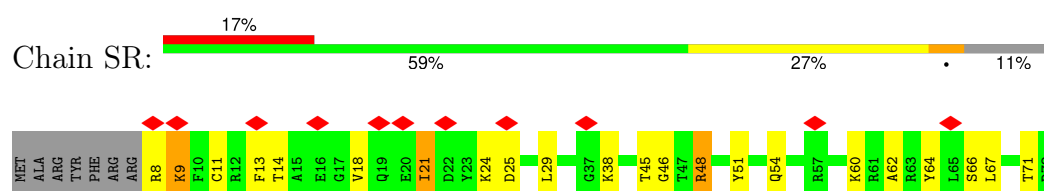
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

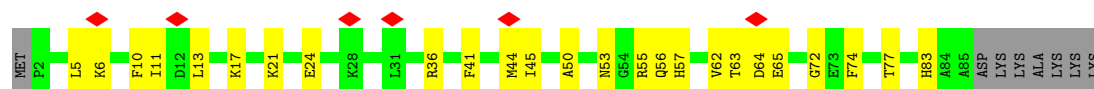


- Molecule 18: 30S ribosomal protein S18

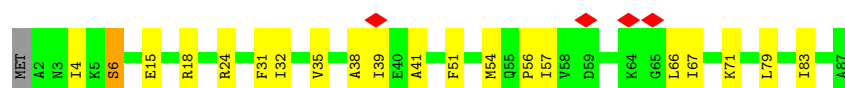
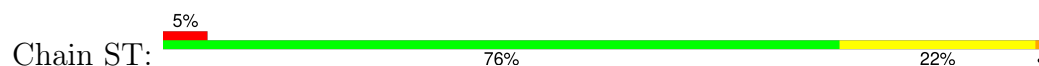


- Molecule 19: 30S ribosomal protein S19

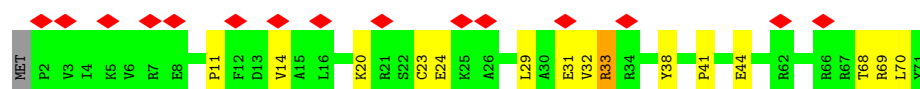
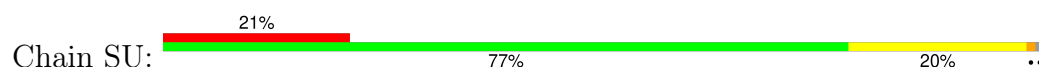




- Molecule 20: 30S ribosomal protein S20



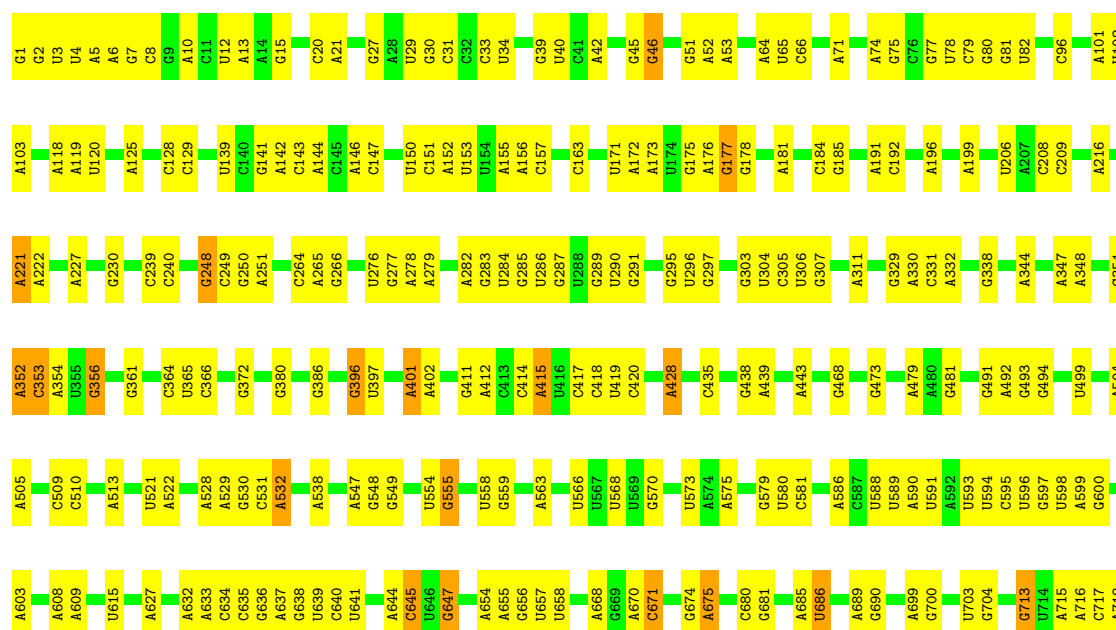
- Molecule 21: 30S ribosomal protein S21



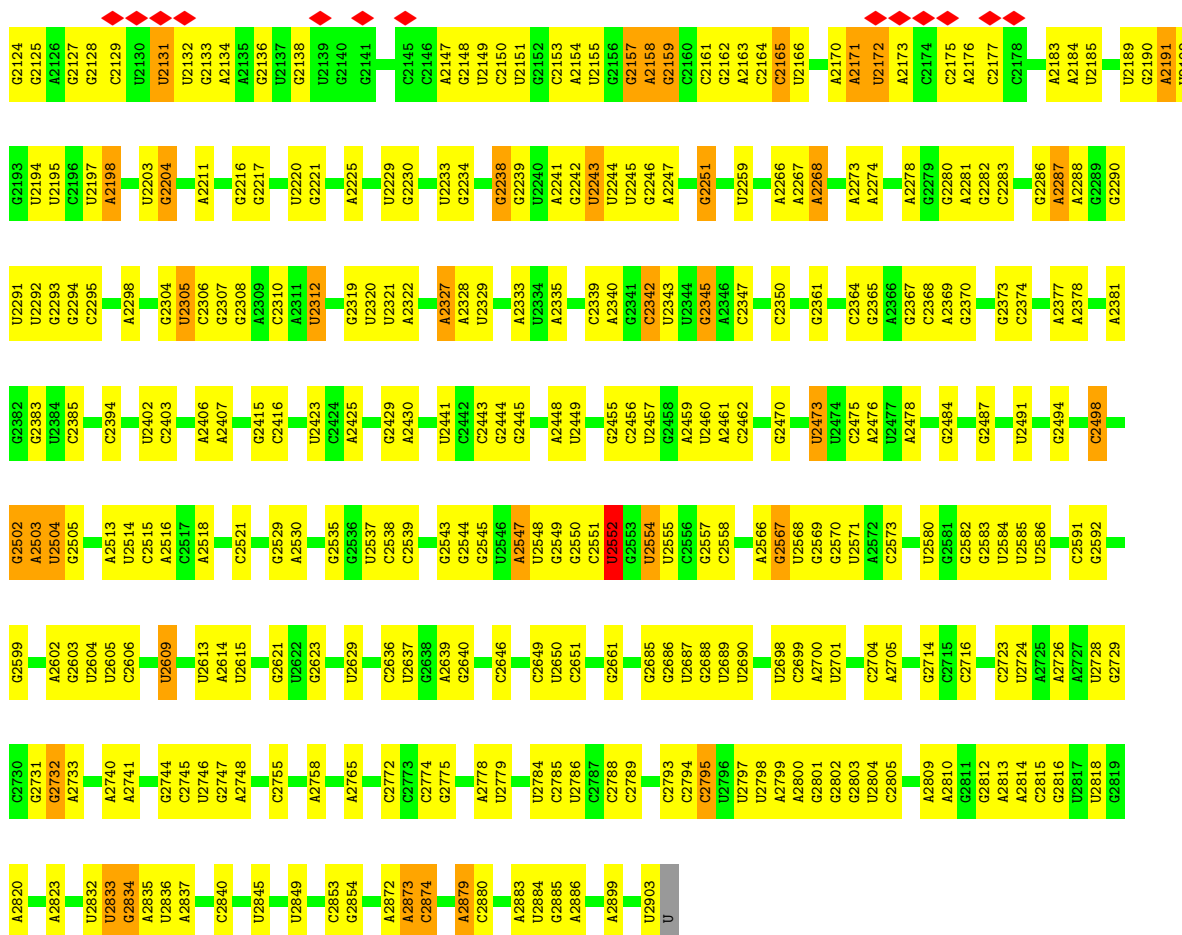
- Molecule 22: Chains: mR



- Molecule 23: 23S rRNA



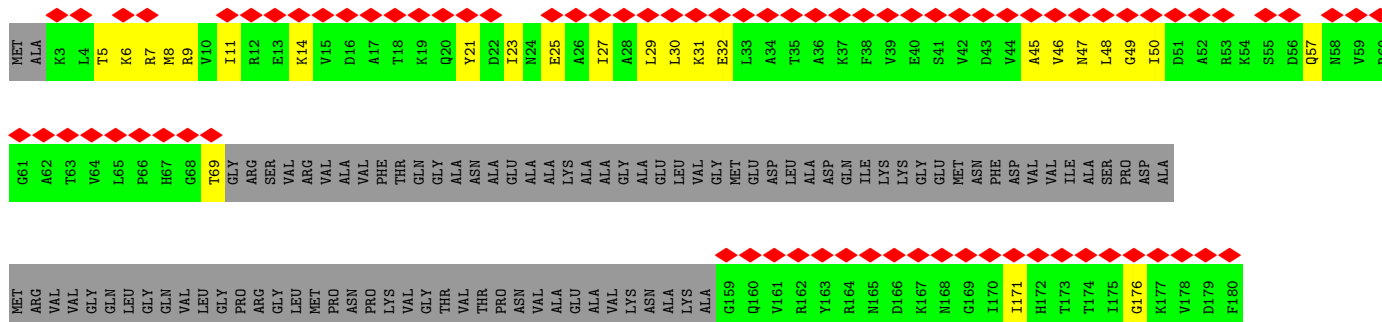
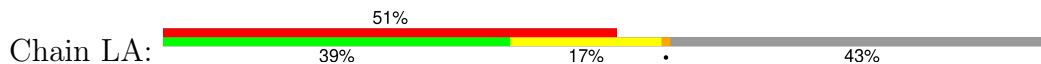
G2046	C1947	A1854	C1764	G1649	A1532	C1428	G1299	C1196	G1107	G1022	A905	U827	A721
C2047	G1954	G1857	G1770	A1665	C1533	G1429	G1300	G1197	G1110	U1023	U906	U828	A722
G2048	U1955	A1858	C1771	G1666	U1534	G1430	A1301	U1198	A1111	C908	C907	A829	C723
C2049	U1956	G1862	A1772	G1667	C1535	G1431	C1306	C1200	G1112	G1026	A909	G830	U724
A2051	C1958		A1773	A1672	C1536	A1432	A1307	G1212	G1115	A1028	A910	A833	G729
		A1866	C1774	G1673	G1540	A1433	U1313		G1116	A1029	C912	G834	A730
C2055	C1962	G1867	U1782	G1674	C1541	A1434	C1314	U1219	C1117	U1033	A917	G843	C740
G2056	U1963	C1868	A1783	C1675	U1542	G1435	C1315	G1223	C1118	G1034	A926	A845	U741
A2060	G1964	G1869	A1784	A1576	C1543	G1436	U1316	U1224	G1125	U1035	G926	U846	A742
G2061	C1965	C1870	A1785	A1677	G1543	U1438	G1317	G1225			A927	U847	A743
A2062	A1966	A1871	A1786	A1678	G1543	A1439	U1318	A1226		G1038	A928	C848	U744
	C1967	A1872	A1786	A1679	A1548	U1440		G1227	U1132	A1039	U931	U850	G745
C2063	G1970	G1873	A1794	U1680	A1549	G1441	A1321		A1133		U931	U851	U747
G2064	U1971	C1876	C1795	G1681	G1560	U1442	A1322	U1231	A1134	C1045	U931		
C2065	G1972	A1876	U1796	G1682	U1561	U1443	C1323	G1232	C1135	A1046	U941	U852	
G2066		G1881	G1797	G1684	U1563	G1444	A1327	U1233	G1136	G1047			U754
	G1983	U1882	C1800	G1685	C1564	G1447	A1328	G1234	G1138	A1050	C946	G856	U755
A2070		A1885	A1801		C1565	G1448	G1339	U1235	G1139	G1051	A947	G857	A756
G2071	G1987		A1802	A1689	A1566	G1449	G1340	G1236	U1140		C948	G858	G757
C2072	U1988	A1889	A1803	A1690	U1569	G1452	A1353	G1237	U1141	A1054	U955	U860	G760
G2073	C1989			U1693	A1570	A1453	A1354	U1238	A1142	G1055		A861	A761
U2074	G1990	G1896	A1808		A1571	G1459	C1357	A1247	G1149	G1056		G862	U762
U2075	U1991		A1809	C1704	A1572		G1358	G1248	C1150		A959	A863	G763
	U1992		A1810	A1705	U1578	A1469	G1359	U1249	A1151	G1059	A960	G864	A764
C2078	C1994		U1811	G1706		A1470	A1365	G1250	C1152	U1060	C961		
U2079		G1906	U1812	G1707	U1583	G1478	G1368	G1251	G1153		G962	G869	G775
A2080	C1997	G1907	G1813	G1708	U1584		G1368	G1252	G1154	G1067	C963	U870	G776
U2081			C1816	G1709	C1585	G1482	A1378	U1253	A1155	G1068	C964	U871	
A2082			U1819	G1710	U1586	G1483	U1379	G1254	A1156	A1069	C966	U872	A782
	C2008	G1910	C1822	A1711	G1587	U1485	A1384	U1255	C1161	A1070	U967	G875	A783
U2086	U2011	U1911	U1820	G1715	A1590	U1486	A1385	G1266	G1163	C1076	U967	G876	G784
G2087		A1912	C1822	U1720	A1591		C1386	U1267	C1164	A1077	C968	G877	G785
	G2010	C1914	U1827	G1721		A1490	A1387	G1271	A1169	U1078	U970	A878	C786
G2093		A1915	U1829	C1727	A1597	C1493	A1387	U1272	C1170	A1080	G974	G879	C787
C2096	A2020	U1917	G1830	G1730	A1598	A1494	U1394	U1273	G1171	U1083	A980	G881	A788
U2098	C2021	A1918	C1831	G1731	C1604	A1495	A1395	G1278	C1172	A1084	U981	G882	A789
G2100	U2022	C1920	C1832	G1736	C1605	U1496	C1398	G1279	U1173	A1085	C982	U883	C796
C2102	C2023	G1921		G1737	A1608	C1498	C1399	U1280	U1174	A1086	A983	C884	G797
	G2024		G1835	U1738	A1609	C1498	U1405	G1281	A1175	G1087	A996	C885	G801
U2106	C2025	A1927	C1838	G1739	A1610	A1504	U1406	U1282	U1176	A1088		U886	G805
G2107	U2026	G1928	G1842	G1740	A1616	C1507	U1406	A1286	U1177	A1089	A996	C888	
	A2030	G1930	C1843	G1741	C1617	A1508	G1410	A1287	G1178	A1090	A1000	C889	U811
U2110	U2031	U1931	U1844	U1742	A1618	A1509	U1411	G1288	C1179	G1091	A1001	C890	U812
G2112	G2032	G1933	G1845	G1743	A1618	G1510	U1412		U1180	U1097	A1009	C891	U813
A2113	A2033		G1846	A1744	U1636	G1511	U1413	G1292	U1181	U1097	A1010	G892	C814
C2036	C2037	A1936	G1847	A1745	A1637	C1512	A1413	G1293	U1182	G1097	A1011	C893	C817
U2115	G2038	A1938	A1848	U1747	G1645	G1513	G1416	G1294	U1183	U1101	G1012	U894	G818
G2116		U1939	G1849	C1748	U1646	A1515	A1419	G1295	U1184	C1102	A1014	U895	A819
A2117				G1756	U1647	A1515	A1420	G1296	G1187	U1105		A896	G822
U2118			A1853		U1648	G1524		G1297	G1195	G1106		C903	
A2119		U1946						G1298				G904	



- Molecule 24: 5S rRNA



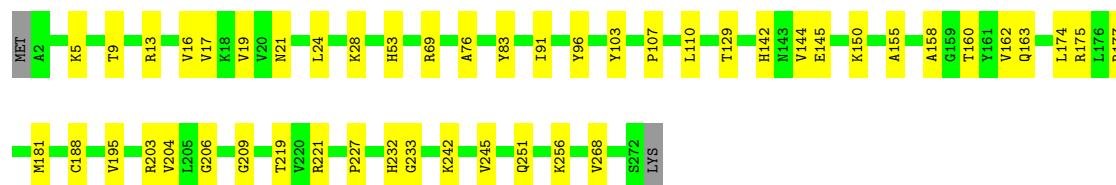
- Molecule 25: 50S ribosomal protein L1





- Molecule 26: 50S ribosomal protein L2

Chain LB: 82% 18%



- Molecule 27: 50S ribosomal protein L3

Chain LC: 89% 11%



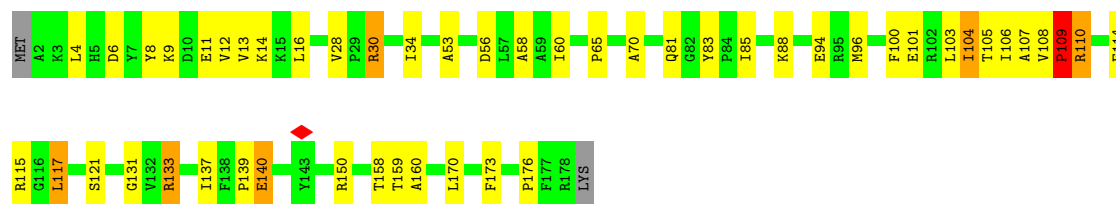
- Molecule 28: 50S ribosomal protein L4

Chain LD: 90% 10%



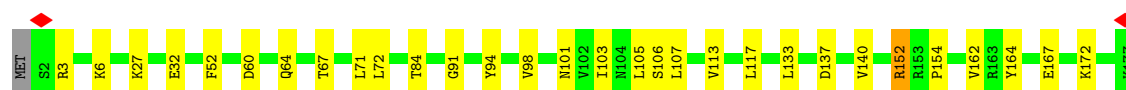
- Molecule 29: 50S ribosomal protein L5

Chain LE: 71% 24%



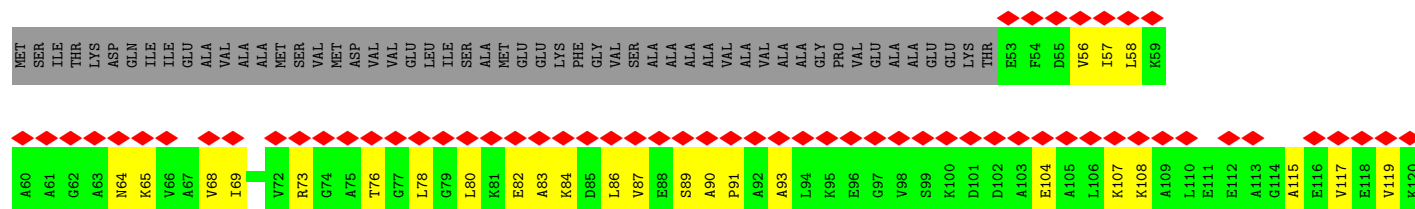
- Molecule 30: 50S ribosomal protein L6

Chain LF: 82% 16%

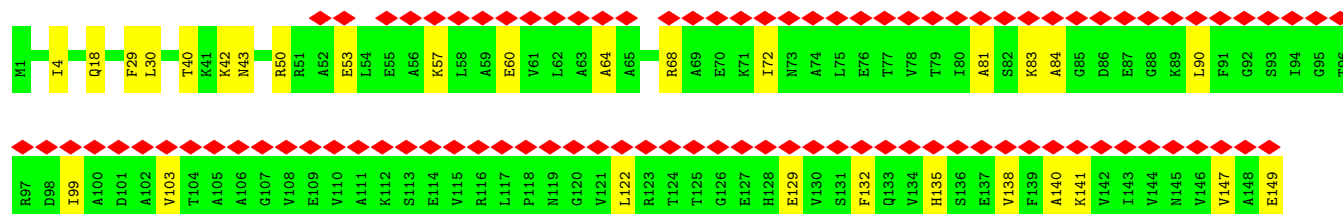
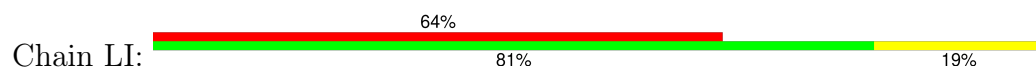


- Molecule 31: 50S ribosomal protein L7/L12

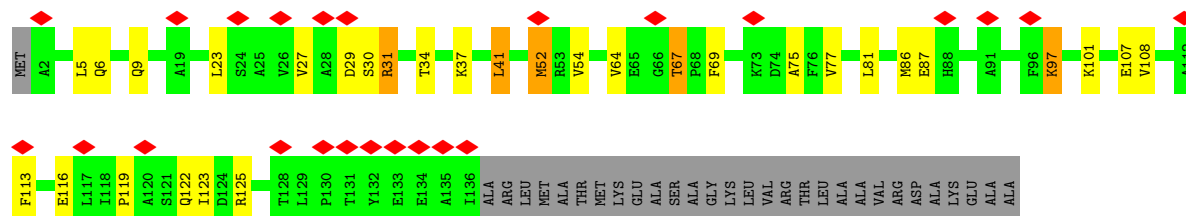
Chain LG: 35% 21% 44%



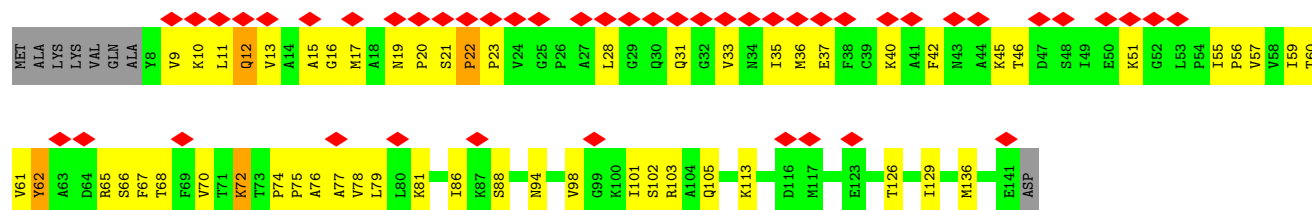
• Molecule 32: 50S ribosomal protein L9



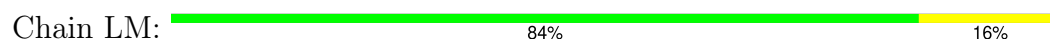
• Molecule 33: 50S ribosomal protein L10




• Molecule 34: 50S ribosomal protein L11

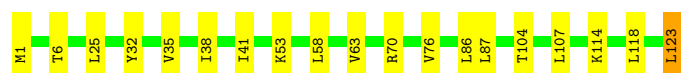


• Molecule 35: 50S ribosomal protein L13



• Molecule 36: 50S ribosomal protein L14

Chain LN:  85% 15%




- Molecule 37: 50S ribosomal protein L15

Chain LO:  94% 6%




- Molecule 38: 50S ribosomal protein L16

Chain LP:  85% 15%




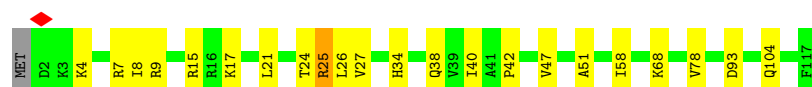
- Molecule 39: 50S ribosomal protein L17

Chain LQ:  84% 10% 6%




- Molecule 40: 50S ribosomal protein L18

Chain LR:  80% 18% ..




- Molecule 41: 50S ribosomal protein L19

Chain LS:  78% 21% .




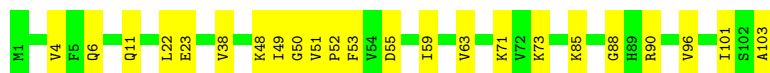
- Molecule 42: 50S ribosomal protein L20

Chain LT:  85% 14% ..




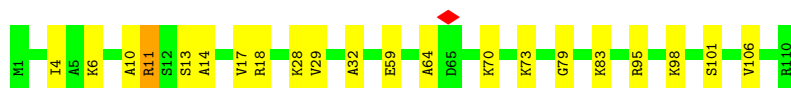
- Molecule 43: 50S ribosomal protein L21

Chain LU:  78% 22%



- Molecule 44: 50S ribosomal protein L22

Chain LV:  81% 18%



- Molecule 45: 50S ribosomal protein L23

Chain LW:  73% 20% 7%




- Molecule 46: 50S ribosomal protein L24

Chain LX:  90% 8%



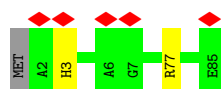
- Molecule 47: 50S ribosomal protein L25

Chain LY:  84% 14%



- Molecule 48: 50S ribosomal protein L27

Chain La:  6% 96%

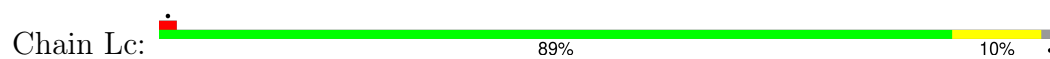


- Molecule 49: 50S ribosomal protein L28

Chain Lb:  96%



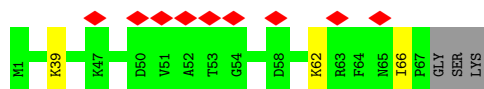
- Molecule 50: 50S ribosomal protein L29



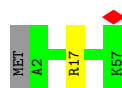
- Molecule 51: 50S ribosomal protein L30



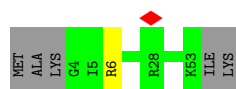
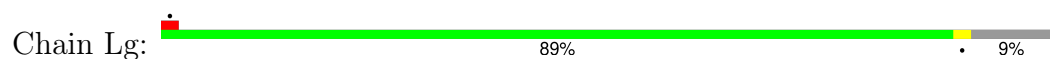
- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



- Molecule 54: 50S ribosomal protein L33



- Molecule 55: 50S ribosomal protein L34



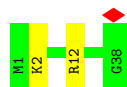
There are no outlier residues recorded for this chain.

- Molecule 56: 50S ribosomal protein L35

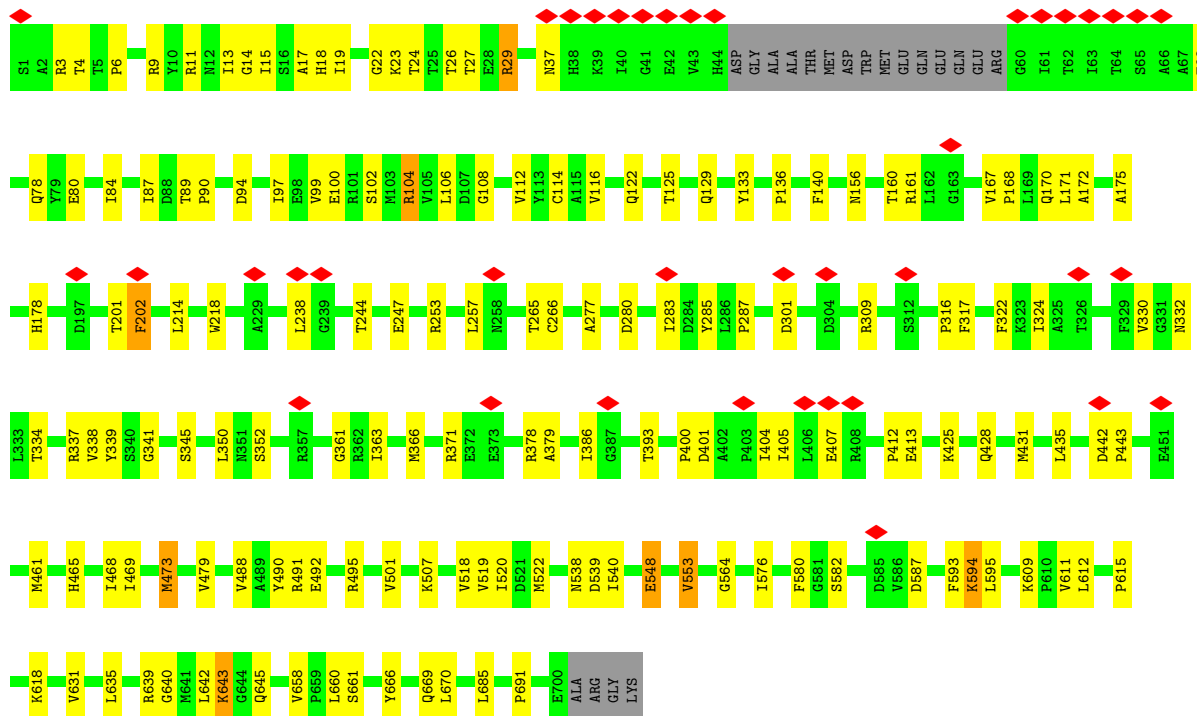
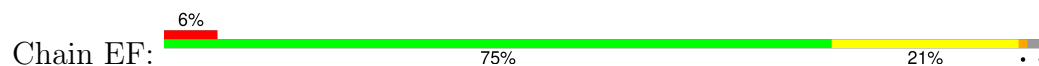


- Molecule 57: 50S ribosomal protein L36





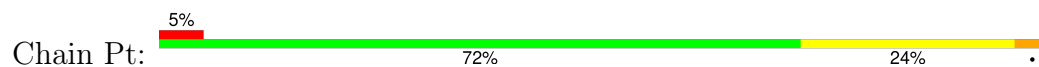
- Molecule 58: Elongation factor G



- Molecule 59: Polypeptide

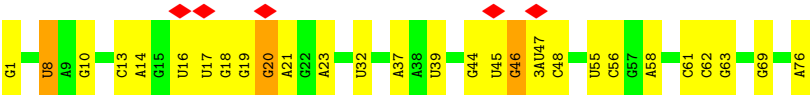


- Molecule 60: Chains: Pt



- Molecule 61: tRNA





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	113540	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	0.126	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	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: U8U, 2MA, G7M, OMG, ZN, PUT, GDP, MIA, ATP, MG, MA6, 3TD, OMC, 4OC, PSU, 4SU, H2U, OMU, T6A, FUA, 2MG, 5MC, 6MZ, SPD, D2T, 1MG, 3AU, UR3, 4D4, 5MU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	16	0.32	0/36619	0.73	4/57122 (0.0%)
2	SB	0.45	0/1800	0.59	0/2425
3	SC	0.32	0/1651	0.55	0/2225
4	SD	0.34	0/1665	0.56	0/2227
5	SE	0.39	0/1157	0.57	0/1557
6	SF	0.47	0/881	0.63	0/1189
7	SG	0.56	0/1253	0.66	0/1681
8	SH	0.35	0/989	0.59	0/1326
9	SI	0.43	0/1034	0.65	0/1375
10	SJ	0.53	0/805	0.74	1/1089 (0.1%)
11	SK	0.32	0/893	0.59	0/1205
12	SL	0.46	0/960	0.62	0/1286
13	SM	0.54	0/900	1.02	3/1204 (0.2%)
14	SN	0.51	0/817	0.61	0/1088
15	SO	0.33	0/722	0.53	0/964
16	SP	0.37	0/659	0.63	0/884
17	SQ	0.36	0/657	0.59	0/881
18	SR	0.47	0/564	0.67	0/756
19	SS	0.37	0/685	0.58	0/922
20	ST	0.35	0/676	0.54	0/895
21	SU	0.33	0/597	0.59	0/792
22	mR	0.24	0/280	0.64	0/433
23	23	0.41	0/69239	0.76	8/108014 (0.0%)
24	5	0.44	1/2873 (0.0%)	0.75	0/4478
25	LA	0.38	0/1033	0.61	0/1387
26	LB	0.34	0/2121	0.59	0/2852
27	LC	0.32	0/1586	0.55	0/2134
28	LD	0.29	0/1571	0.52	0/2113
29	LE	0.42	0/1434	0.67	2/1926 (0.1%)
30	LF	0.31	0/1343	0.53	0/1816
31	LG	0.33	0/488	0.62	0/652

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	LI	0.30	0/1122	0.51	0/1515
33	LJ	0.47	0/1037	0.63	0/1400
34	LK	0.52	0/987	0.64	0/1334
35	LM	0.31	0/1152	0.51	0/1551
36	LN	0.35	0/956	0.59	0/1279
37	LO	0.34	0/1062	0.59	0/1413
38	LP	0.33	0/1081	0.58	0/1443
39	LQ	0.31	0/973	0.61	0/1301
40	LR	0.33	0/902	0.58	0/1209
41	LS	0.34	0/929	0.58	0/1242
42	LT	0.35	0/960	0.53	0/1278
43	LU	0.35	0/829	0.61	0/1107
44	LV	0.34	0/864	0.57	0/1156
45	LW	0.30	0/744	0.53	0/994
46	LX	0.31	0/787	0.53	0/1051
47	LY	0.33	0/766	0.55	0/1025
48	La	0.33	0/642	0.53	0/848
49	Lb	0.33	0/635	0.57	0/848
50	Lc	0.33	0/502	0.59	1/667 (0.1%)
51	Ld	0.31	0/453	0.56	0/605
52	Le	0.37	0/539	0.62	0/721
53	Lf	0.36	0/450	0.59	0/599
54	Lg	0.28	0/416	0.49	0/554
55	Lh	0.32	0/380	0.68	0/498
56	Li	0.31	0/513	0.57	0/676
57	Lj	0.32	0/303	0.55	0/397
58	EF	0.45	0/5097	0.61	0/6933
59	Pp	0.41	0/28	0.97	0/34
60	Pt	0.41	1/1600 (0.1%)	0.73	0/2486
61	Dt	0.45	2/1654 (0.1%)	0.73	1/2572 (0.0%)
All	All	0.39	4/166315 (0.0%)	0.71	20/247634 (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
4	SD	0	1
6	SF	0	1
7	SG	0	1
9	SI	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	SJ	0	1
15	SO	0	2
21	SU	0	1
27	LC	0	1
29	LE	0	1
40	LR	0	1
46	LX	0	1
47	LY	0	2
48	La	0	1
49	Lb	0	1
51	Ld	0	1
53	Lf	0	1
All	All	0	18

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	Pt	1	G	OP3-P	-10.66	1.48	1.61
61	Dt	1	G	OP3-P	-10.65	1.48	1.61
24	5	1	U	OP3-P	-10.55	1.48	1.61
61	Dt	20	G	O3'-P	6.27	1.68	1.61

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	SM	93	ARG	CG-CD-NE	18.53	150.71	111.80
13	SM	93	ARG	CB-CG-CD	16.38	154.19	111.60
29	LE	109	PRO	CA-N-CD	-10.29	97.10	111.50
10	SJ	37	ARG	N-CA-C	-8.11	89.09	111.00
13	SM	93	ARG	CD-NE-CZ	7.94	134.72	123.60

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	SD	184	ARG	Sidechain
6	SF	45	ARG	Sidechain
7	SG	141	VAL	Mainchain
9	SI	113	ARG	Sidechain
10	SJ	89	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	16	32929	0	16589	404	0
2	SB	1769	0	1795	35	0
3	SC	1624	0	1696	37	0
4	SD	1643	0	1707	24	0
5	SE	1144	0	1185	20	0
6	SF	862	0	864	17	0
7	SG	1235	0	1286	25	0
8	SH	979	0	1031	25	0
9	SI	1022	0	1070	21	0
10	SJ	795	0	836	21	0
11	SK	877	0	887	20	0
12	SL	957	0	1017	15	0
13	SM	891	0	952	23	0
14	SN	805	0	844	19	0
15	SO	714	0	734	12	0
16	SP	649	0	666	20	0
17	SQ	648	0	691	17	0
18	SR	555	0	578	13	0
19	SS	668	0	693	18	0
20	ST	670	0	719	11	0
21	SU	589	0	629	7	0
22	mR	252	0	128	0	0
23	23	62334	0	31374	584	0
24	5	2570	0	1301	10	0
25	LA	1026	0	1092	26	0
26	LB	2082	0	2154	30	0
27	LC	1565	0	1616	13	0
28	LD	1552	0	1618	15	0
29	LE	1410	0	1444	37	0
30	LF	1323	0	1371	16	0
31	LG	487	0	515	16	0
32	LI	1111	0	1148	18	0
33	LJ	1023	0	1050	15	0
34	LK	973	0	1017	25	0
35	LM	1129	0	1162	13	0
36	LN	947	0	1023	12	0
37	LO	1053	0	1129	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	LP	1075	0	1155	9	0
39	LQ	960	0	1000	8	0
40	LR	892	0	923	11	0
41	LS	917	0	960	13	0
42	LT	947	0	1019	13	0
43	LU	816	0	839	15	0
44	LV	857	0	922	13	0
45	LW	738	0	807	10	0
46	LX	779	0	831	4	0
47	LY	753	0	780	7	0
48	La	634	0	653	0	0
49	Lb	625	0	652	0	0
50	Lc	501	0	531	0	0
51	Ld	449	0	488	0	0
52	Le	529	0	527	0	0
53	Lf	444	0	458	0	0
54	Lg	409	0	440	0	0
55	Lh	377	0	418	0	0
56	Li	504	0	572	0	0
57	Lj	302	0	340	0	0
58	EF	4999	0	4781	84	0
59	Pp	28	0	33	0	0
60	Pt	1636	0	840	0	0
61	Dt	1641	0	843	0	0
62	16	12	0	24	1	0
62	23	108	0	216	4	0
62	LC	6	0	12	1	0
63	16	40	0	0	0	0
63	23	144	0	0	0	0
63	5	4	0	0	0	0
63	EF	1	0	0	0	0
63	LB	1	0	0	0	0
63	LC	1	0	0	0	0
63	LD	1	0	0	0	0
63	LQ	1	0	0	0	0
63	LW	1	0	0	0	0
63	Lf	1	0	0	0	0
63	SN	2	0	0	0	0
64	Le	1	0	0	0	0
64	Lj	1	0	0	0	0
64	SB	1	0	0	0	0
65	23	62	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
66	23	30	0	57	0	0
67	EF	37	0	47	15	0
68	EF	28	0	12	0	0
All	All	155157	0	106815	1742	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 7.

The worst 5 of 1742 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)
23:23:713:G:N2	23:23:718:A:N1	1.92	1.17
6:SF:46:GLN:HA	6:SF:56:LYS:HG2	1.41	1.00
32:LI:147:VAL:HG12	32:LI:149:GLU:HG3	1.43	0.98
29:LE:106:ILE:HG21	29:LE:139:PRO:HD3	1.45	0.97
36:LN:123:LEU:HG	36:LN:123:LEU:O	1.66	0.94

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	224/241 (93%)	209 (93%)	15 (7%)	0	100	100
3	SC	204/233 (88%)	198 (97%)	6 (3%)	0	100	100
4	SD	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
5	SE	153/167 (92%)	147 (96%)	6 (4%)	0	100	100
6	SF	104/135 (77%)	96 (92%)	8 (8%)	0	100	100
7	SG	154/179 (86%)	145 (94%)	9 (6%)	0	100	100
8	SH	127/130 (98%)	123 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	SI	125/130 (96%)	112 (90%)	13 (10%)	0	100	100
10	SJ	97/103 (94%)	92 (95%)	5 (5%)	0	100	100
11	SK	115/129 (89%)	106 (92%)	9 (8%)	0	100	100
12	SL	120/124 (97%)	112 (93%)	8 (7%)	0	100	100
13	SM	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
14	SN	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
15	SO	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
16	SP	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
17	SQ	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
18	SR	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
19	SS	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
20	ST	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	SU	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
25	LA	130/234 (56%)	127 (98%)	3 (2%)	0	100	100
26	LB	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
27	LC	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
28	LD	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
29	LE	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
30	LF	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
31	LG	66/121 (54%)	61 (92%)	5 (8%)	0	100	100
32	LI	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
33	LJ	133/165 (81%)	122 (92%)	11 (8%)	0	100	100
34	LK	132/142 (93%)	110 (83%)	21 (16%)	1 (1%)	16	36
35	LM	140/142 (99%)	140 (100%)	0	0	100	100
36	LN	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
37	LO	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
38	LP	133/136 (98%)	133 (100%)	0	0	100	100
39	LQ	118/127 (93%)	115 (98%)	3 (2%)	0	100	100
40	LR	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
41	LS	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
42	LT	115/118 (98%)	113 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	LU	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
44	LV	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
45	LW	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
46	LX	100/104 (96%)	91 (91%)	9 (9%)	0	100	100
47	LY	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
48	La	82/85 (96%)	81 (99%)	1 (1%)	0	100	100
49	Lb	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
50	Lc	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
51	Ld	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
52	Le	65/70 (93%)	54 (83%)	11 (17%)	0	100	100
53	Lf	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
54	Lg	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
55	Lh	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
56	Li	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
57	Lj	36/38 (95%)	36 (100%)	0	0	100	100
58	EF	681/704 (97%)	646 (95%)	35 (5%)	0	100	100
59	Pp	1/3 (33%)	1 (100%)	0	0	100	100
All	All	6763/7282 (93%)	6447 (95%)	315 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	LK	22	PRO

### 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	188/199 (94%)	162 (86%)	26 (14%)	3	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	SC	170/190 (90%)	164 (96%)	6 (4%)	31	58
4	SD	172/173 (99%)	162 (94%)	10 (6%)	17	37
5	SE	118/126 (94%)	111 (94%)	7 (6%)	16	37
6	SF	92/116 (79%)	75 (82%)	17 (18%)	1	3
7	SG	129/147 (88%)	106 (82%)	23 (18%)	1	3
8	SH	104/105 (99%)	100 (96%)	4 (4%)	28	55
9	SI	105/107 (98%)	86 (82%)	19 (18%)	1	3
10	SJ	87/90 (97%)	77 (88%)	10 (12%)	4	10
11	SK	90/99 (91%)	87 (97%)	3 (3%)	33	61
12	SL	102/103 (99%)	90 (88%)	12 (12%)	4	10
13	SM	93/96 (97%)	81 (87%)	12 (13%)	3	8
14	SN	83/84 (99%)	74 (89%)	9 (11%)	5	12
15	SO	76/77 (99%)	72 (95%)	4 (5%)	19	42
16	SP	65/65 (100%)	64 (98%)	1 (2%)	60	82
17	SQ	74/78 (95%)	69 (93%)	5 (7%)	13	31
18	SR	58/65 (89%)	49 (84%)	9 (16%)	2	5
19	SS	72/79 (91%)	70 (97%)	2 (3%)	38	66
20	ST	65/66 (98%)	61 (94%)	4 (6%)	15	34
21	SU	60/61 (98%)	56 (93%)	4 (7%)	13	31
25	LA	110/181 (61%)	102 (93%)	8 (7%)	11	27
26	LB	216/218 (99%)	211 (98%)	5 (2%)	45	73
27	LC	164/164 (100%)	162 (99%)	2 (1%)	67	85
28	LD	165/165 (100%)	165 (100%)	0	100	100
29	LE	148/150 (99%)	141 (95%)	7 (5%)	22	47
30	LF	137/138 (99%)	136 (99%)	1 (1%)	81	92
31	LG	47/85 (55%)	45 (96%)	2 (4%)	25	50
32	LI	114/114 (100%)	110 (96%)	4 (4%)	31	58
33	LJ	103/123 (84%)	91 (88%)	12 (12%)	4	10
34	LK	103/110 (94%)	80 (78%)	23 (22%)	1	2
35	LM	116/116 (100%)	115 (99%)	1 (1%)	75	89
36	LN	104/104 (100%)	103 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	LO	103/103 (100%)	102 (99%)	1 (1%)	73	88
38	LP	108/108 (100%)	105 (97%)	3 (3%)	38	66
39	LQ	100/103 (97%)	100 (100%)	0	100	100
40	LR	86/87 (99%)	83 (96%)	3 (4%)	31	58
41	LS	99/100 (99%)	96 (97%)	3 (3%)	36	64
42	LT	89/90 (99%)	86 (97%)	3 (3%)	32	59
43	LU	84/84 (100%)	83 (99%)	1 (1%)	67	85
44	LV	93/93 (100%)	91 (98%)	2 (2%)	47	74
45	LW	80/84 (95%)	77 (96%)	3 (4%)	28	55
46	LX	83/85 (98%)	82 (99%)	1 (1%)	67	85
47	LY	78/78 (100%)	75 (96%)	3 (4%)	28	55
48	La	62/63 (98%)	61 (98%)	1 (2%)	58	81
49	Lb	67/68 (98%)	65 (97%)	2 (3%)	36	64
50	Lc	54/55 (98%)	49 (91%)	5 (9%)	7	17
51	Ld	48/49 (98%)	48 (100%)	0	100	100
52	Le	60/62 (97%)	57 (95%)	3 (5%)	20	44
53	Lf	47/48 (98%)	47 (100%)	0	100	100
54	Lg	45/49 (92%)	44 (98%)	1 (2%)	47	74
55	Lh	38/38 (100%)	38 (100%)	0	100	100
56	Li	51/52 (98%)	49 (96%)	2 (4%)	27	54
57	Lj	34/34 (100%)	32 (94%)	2 (6%)	16	37
58	EF	480/578 (83%)	446 (93%)	34 (7%)	12	29
59	Pp	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	5522/5908 (94%)	5195 (94%)	327 (6%)	19	37

5 of 327 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	LK	12	GLN
52	Le	66	ILE
34	LK	37	GLU
41	LS	34	GLU
58	EF	202	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
52	Le	6	HIS
58	EF	37	ASN
58	EF	428	GLN
12	SL	73	ASN
11	SK	64	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1530/1534 (99%)	281 (18%)	14 (0%)
22	mR	11/60 (18%)	3 (27%)	0
23	23	2898/2904 (99%)	484 (16%)	12 (0%)
24	5	119/120 (99%)	19 (15%)	2 (1%)
60	Pt	73/76 (96%)	14 (19%)	0
61	Dt	73/76 (96%)	22 (30%)	0
All	All	4704/4770 (98%)	823 (17%)	28 (0%)

5 of 823 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	2	A
1	16	4	U
1	16	5	U
1	16	9	G
1	16	32	A

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	23	12	U
24	5	108	A
23	23	889	C
23	23	2430	A
23	23	784	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
23	2MA	23	2503	63,23	18,25,26	0.68	0	20,37,40	1.99	4 (20%)
60	H2U	Pt	20	60	18,21,22	1.07	2 (11%)	19,30,33	1.33	4 (21%)
61	PSU	Dt	39	61	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
23	PSU	23	2605	23	18,21,22	1.40	4 (22%)	21,30,33	2.02	4 (19%)
60	3AU	Pt	47	60	24,28,29	1.03	0	30,40,43	1.57	5 (16%)
23	2MG	23	1835	23	18,26,27	0.90	1 (5%)	16,38,41	1.32	3 (18%)
23	PSU	23	2504	23	18,21,22	1.39	3 (16%)	21,30,33	2.09	3 (14%)
1	MA6	16	1518	1	19,26,27	1.30	3 (15%)	18,38,41	2.25	6 (33%)
23	PSU	23	955	23	18,21,22	1.40	3 (16%)	21,30,33	2.12	4 (19%)
61	PSU	Dt	32	61	18,21,22	1.37	2 (11%)	21,30,33	2.02	3 (14%)
60	H2U	Pt	17	60	18,21,22	0.97	2 (11%)	19,30,33	0.99	2 (10%)
61	MIA	Dt	37	61	24,31,32	2.30	3 (12%)	22,44,47	2.78	7 (31%)
60	5MU	Pt	54	60	19,22,23	1.39	6 (31%)	27,32,35	2.08	6 (22%)
61	G7M	Dt	46	61	20,26,27	2.60	4 (20%)	16,39,42	1.27	2 (12%)
23	OMC	23	2498	63,23	19,22,23	0.81	0	25,31,34	0.91	1 (4%)
23	PSU	23	746	63,23	18,21,22	1.40	3 (16%)	21,30,33	1.99	4 (19%)
23	6MZ	23	1618	23	17,25,26	0.93	1 (5%)	15,36,39	2.20	4 (26%)
23	G7M	23	2069	23	20,26,27	2.79	5 (25%)	16,39,42	2.11	4 (25%)
60	U8U	Pt	34	60,22	20,24,25	1.50	3 (15%)	22,34,37	1.25	3 (13%)
38	4D4	LP	81	38	9,11,12	2.19	2 (22%)	7,13,15	2.07	3 (42%)
61	PSU	Dt	55	61	18,21,22	1.43	2 (11%)	21,30,33	2.20	4 (19%)
1	2MG	16	1516	1	18,26,27	0.90	1 (5%)	16,38,41	1.36	3 (18%)
1	PSU	16	516	1	18,21,22	1.42	3 (16%)	21,30,33	2.09	4 (19%)
61	3AU	Dt	47	61	24,28,29	1.02	0	30,40,43	1.60	4 (13%)
23	OMG	23	2251	60,23	19,26,27	1.18	2 (10%)	21,38,41	0.83	1 (4%)
60	T6A	Pt	37	60	26,34,35	0.97	1 (3%)	28,49,52	1.71	5 (17%)
61	4SU	Dt	8	61	18,21,22	1.96	4 (22%)	25,30,33	2.25	6 (24%)
12	D2T	SL	89	12	8,9,10	2.44	1 (12%)	6,11,13	2.91	4 (66%)
23	PSU	23	1911	23	18,21,22	6.15	13 (72%)	21,30,33	1.98	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4OC	16	1402	1	20,23,24	0.76	0	25,32,35	0.94	1 (4%)
23	H2U	23	2449	23	18,21,22	1.09	3 (16%)	19,30,33	1.02	1 (5%)
23	5MU	23	747	23	19,22,23	1.40	5 (26%)	27,32,35	2.12	6 (22%)
23	6MZ	23	2030	23	17,25,26	0.88	1 (5%)	15,36,39	2.41	4 (26%)
23	OMU	23	2552	23	19,22,23	1.24	3 (15%)	25,31,34	1.86	5 (20%)
23	PSU	23	2580	23	18,21,22	1.41	3 (16%)	21,30,33	2.08	4 (19%)
60	PSU	Pt	39	60	18,21,22	1.40	2 (11%)	21,30,33	2.01	4 (19%)
23	PSU	23	1917	23	18,21,22	6.15	12 (66%)	21,30,33	2.04	5 (23%)
1	5MC	16	1407	1	19,22,23	1.59	3 (15%)	26,32,35	1.12	3 (11%)
1	2MG	16	966	1	18,26,27	1.01	1 (5%)	16,38,41	1.33	2 (12%)
1	UR3	16	1498	1	19,22,23	0.96	0	26,32,35	1.72	2 (7%)
1	MA6	16	1519	1	19,26,27	1.14	2 (10%)	18,38,41	2.03	4 (22%)
23	5MU	23	1939	23	19,22,23	1.43	5 (26%)	27,32,35	2.35	6 (22%)
23	1MG	23	745	23	19,26,27	0.99	1 (5%)	18,39,42	1.57	3 (16%)
23	PSU	23	2604	23	18,21,22	1.50	4 (22%)	21,30,33	2.20	4 (19%)
23	3TD	23	1915	23	19,22,23	1.38	2 (10%)	23,32,35	2.31	4 (17%)
23	2MG	23	2445	23	18,26,27	0.91	1 (5%)	16,38,41	1.27	2 (12%)
1	G7M	16	527	1	20,26,27	2.60	4 (20%)	16,39,42	1.27	2 (12%)
60	H2U	Pt	16	60	18,21,22	1.03	2 (11%)	19,30,33	1.09	2 (10%)
60	PSU	Pt	55	60	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)
23	5MC	23	1962	23	19,22,23	1.54	3 (15%)	26,32,35	1.12	2 (7%)
1	5MC	16	967	1	19,22,23	1.58	3 (15%)	26,32,35	1.21	3 (11%)
23	PSU	23	2457	23	18,21,22	1.41	2 (11%)	21,30,33	2.12	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	2MA	23	2503	63,23	-	0/3/25/26	0/3/3/3
60	H2U	Pt	20	60	-	5/7/38/39	0/2/2/2
61	PSU	Dt	39	61	-	2/7/25/26	0/2/2/2
23	PSU	23	2605	23	-	2/7/25/26	0/2/2/2
60	3AU	Pt	47	60	-	2/16/34/35	0/2/2/2
23	2MG	23	1835	23	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	23	2504	23	-	2/7/25/26	0/2/2/2
1	MA6	16	1518	1	-	1/7/29/30	0/3/3/3
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
61	PSU	Dt	32	61	-	0/7/25/26	0/2/2/2
60	H2U	Pt	17	60	-	3/7/38/39	0/2/2/2
61	MIA	Dt	37	61	-	5/11/33/34	0/3/3/3
60	5MU	Pt	54	60	-	0/7/25/26	0/2/2/2
61	G7M	Dt	46	61	-	1/3/25/26	0/3/3/3
23	OMC	23	2498	63,23	-	2/9/27/28	0/2/2/2
23	PSU	23	746	63,23	-	4/7/25/26	0/2/2/2
23	6MZ	23	1618	23	-	0/5/27/28	0/3/3/3
23	G7M	23	2069	23	-	0/3/25/26	0/3/3/3
60	U8U	Pt	34	60,22	-	4/10/28/29	0/2/2/2
38	4D4	LP	81	38	-	4/11/12/14	-
61	PSU	Dt	55	61	-	0/7/25/26	0/2/2/2
1	2MG	16	1516	1	-	0/5/27/28	0/3/3/3
1	PSU	16	516	1	-	0/7/25/26	0/2/2/2
61	3AU	Dt	47	61	-	9/16/34/35	0/2/2/2
23	OMG	23	2251	60,23	-	1/5/27/28	0/3/3/3
60	T6A	Pt	37	60	-	10/19/41/42	0/3/3/3
61	4SU	Dt	8	61	-	3/7/25/26	0/2/2/2
12	D2T	SL	89	12	-	3/7/12/14	-
23	PSU	23	1911	23	-	0/7/25/26	0/2/2/2
1	4OC	16	1402	1	-	0/9/29/30	0/2/2/2
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2
23	5MU	23	747	23	-	0/7/25/26	0/2/2/2
23	6MZ	23	2030	23	-	2/5/27/28	0/3/3/3
23	OMU	23	2552	23	-	2/9/27/28	0/2/2/2
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
60	PSU	Pt	39	60	-	0/7/25/26	0/2/2/2
23	PSU	23	1917	23	-	0/7/25/26	0/2/2/2
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	16	966	1	-	0/5/27/28	0/3/3/3
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	16	1519	1	-	4/7/29/30	0/3/3/3
23	5MU	23	1939	23	-	2/7/25/26	0/2/2/2
23	1MG	23	745	23	-	0/3/25/26	0/3/3/3
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
23	3TD	23	1915	23	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	2MG	23	2445	23	-	1/5/27/28	0/3/3/3
1	G7M	16	527	1	-	2/3/25/26	0/3/3/3
60	H2U	Pt	16	60	-	3/7/38/39	0/2/2/2
60	PSU	Pt	55	60	-	0/7/25/26	0/2/2/2
23	5MC	23	1962	23	-	4/7/25/26	0/2/2/2
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2

The worst 5 of 140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	1911	PSU	C6-C5	12.36	1.49	1.35
23	23	1917	PSU	C6-C5	12.25	1.48	1.35
23	23	1911	PSU	C2-N1	12.18	1.52	1.36
23	23	1917	PSU	C2-N1	12.18	1.52	1.36
23	23	1917	PSU	O4'-C1'	10.45	1.58	1.43

The worst 5 of 190 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	Dt	37	MIA	C12-C13-C14	-9.04	110.78	127.01
23	23	1915	3TD	N1-C2-N3	8.10	122.02	116.13
23	23	2503	2MA	C2-N3-C4	7.06	121.16	115.46
1	16	1498	UR3	C4-N3-C2	-6.80	119.11	124.58
23	23	2604	PSU	N1-C2-N3	6.73	122.27	115.17

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'
12	SL	89	D2T	CG-CB-SB-CB1
23	23	746	PSU	C2'-C1'-C5-C4
23	23	746	PSU	C2'-C1'-C5-C6
23	23	2251	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

13 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	23	2503	2MA	1	0
1	16	1518	MA6	1	0
1	16	1516	2MG	1	0
23	23	2251	OMG	1	0
12	SL	89	D2T	4	0
23	23	1911	PSU	1	0
1	16	1402	4OC	1	0
23	23	2030	6MZ	2	0
23	23	2552	OMU	1	0
1	16	966	2MG	1	0
1	16	1519	MA6	1	0
23	23	1915	3TD	1	0
1	16	967	5MC	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 228 ligands modelled in this entry, 200 are monoatomic - leaving 28 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	$\# Z  > 2$
62	PUT	23	3010	-	5,5,5	0.10	0	4,4,4	0.13	0
62	PUT	23	3018	-	5,5,5	0.11	0	4,4,4	0.13	0
62	PUT	23	3013	-	5,5,5	0.10	0	4,4,4	0.13	0
62	PUT	23	3003	-	5,5,5	0.15	0	4,4,4	0.22	0
62	PUT	23	3009	-	5,5,5	0.09	0	4,4,4	0.13	0
65	ATP	23	3002	-	28,33,33	0.64	0	34,52,52	0.58	1 (2%)
62	PUT	23	3016	-	5,5,5	0.09	0	4,4,4	0.13	0
62	PUT	16	1601	-	5,5,5	0.12	0	4,4,4	0.12	0
62	PUT	23	3008	-	5,5,5	0.10	0	4,4,4	0.14	0
66	SPD	23	3023	-	9,9,9	0.16	0	8,8,8	0.23	0
62	PUT	23	3006	-	5,5,5	0.09	0	4,4,4	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
66	SPD	23	3021	-	9,9,9	0.32	0	8,8,8	0.91	0
62	PUT	23	3007	-	5,5,5	0.10	0	4,4,4	0.12	0
62	PUT	LC	301	-	5,5,5	0.10	0	4,4,4	0.13	0
62	PUT	23	3014	-	5,5,5	0.10	0	4,4,4	0.12	0
62	PUT	23	3011	-	5,5,5	0.09	0	4,4,4	0.13	0
62	PUT	23	3020	-	5,5,5	0.16	0	4,4,4	0.20	0
62	PUT	23	3005	-	5,5,5	0.11	0	4,4,4	0.13	0
65	ATP	23	3001	-	28,33,33	0.64	0	34,52,52	0.58	1 (2%)
62	PUT	23	3017	-	5,5,5	0.12	0	4,4,4	0.13	0
62	PUT	23	3015	-	5,5,5	0.14	0	4,4,4	0.19	0
68	GDP	EF	803	63	25,30,30	0.97	1 (4%)	30,47,47	1.16	3 (10%)
62	PUT	16	1602	-	5,5,5	0.15	0	4,4,4	0.22	0
62	PUT	23	3019	-	5,5,5	0.12	0	4,4,4	0.13	0
67	FUA	EF	802	63	39,40,40	2.06	13 (33%)	50,64,64	2.79	19 (38%)
62	PUT	23	3004	-	5,5,5	0.10	0	4,4,4	0.12	0
66	SPD	23	3022	-	9,9,9	0.32	0	8,8,8	0.89	0
62	PUT	23	3012	-	5,5,5	0.11	0	4,4,4	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PUT	23	3010	-	-	1/3/3/3	-
62	PUT	23	3018	-	-	1/3/3/3	-
62	PUT	23	3013	-	-	0/3/3/3	-
62	PUT	23	3003	-	-	0/3/3/3	-
62	PUT	23	3009	-	-	0/3/3/3	-
65	ATP	23	3002	-	-	5/18/38/38	0/3/3/3
62	PUT	23	3016	-	-	1/3/3/3	-
62	PUT	16	1601	-	-	0/3/3/3	-
62	PUT	23	3008	-	-	0/3/3/3	-
66	SPD	23	3023	-	-	2/7/7/7	-
62	PUT	23	3006	-	-	0/3/3/3	-
66	SPD	23	3021	-	-	2/7/7/7	-
62	PUT	23	3007	-	-	1/3/3/3	-
62	PUT	LC	301	-	-	1/3/3/3	-
62	PUT	23	3014	-	-	1/3/3/3	-
62	PUT	23	3011	-	-	1/3/3/3	-
62	PUT	23	3020	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PUT	23	3005	-	-	0/3/3/3	-
65	ATP	23	3001	-	-	5/18/38/38	0/3/3/3
62	PUT	23	3017	-	-	1/3/3/3	-
62	PUT	23	3015	-	-	1/3/3/3	-
68	GDP	EF	803	63	-	4/12/32/32	0/3/3/3
62	PUT	16	1602	-	-	2/3/3/3	-
62	PUT	23	3019	-	-	0/3/3/3	-
67	FUA	EF	802	63	-	5/16/92/92	0/4/4/4
62	PUT	23	3004	-	-	0/3/3/3	-
66	SPD	23	3022	-	-	0/7/7/7	-
62	PUT	23	3012	-	-	0/3/3/3	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	EF	802	FUA	C9-C11	5.22	1.61	1.54
67	EF	802	FUA	C10-C5	-4.17	1.48	1.56
67	EF	802	FUA	C28-C26	4.06	1.61	1.50
67	EF	802	FUA	C20-C8	-3.80	1.47	1.54
67	EF	802	FUA	C27-C26	2.83	1.58	1.50

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	EF	802	FUA	C18-C4-C3	-7.63	102.42	111.35
67	EF	802	FUA	C28-C26-C27	-6.86	98.79	114.59
67	EF	802	FUA	C21-C14-C8	6.34	117.49	112.23
67	EF	802	FUA	C27-C26-C25	5.56	139.33	122.66
67	EF	802	FUA	C10-C5-C4	4.91	119.16	113.20

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

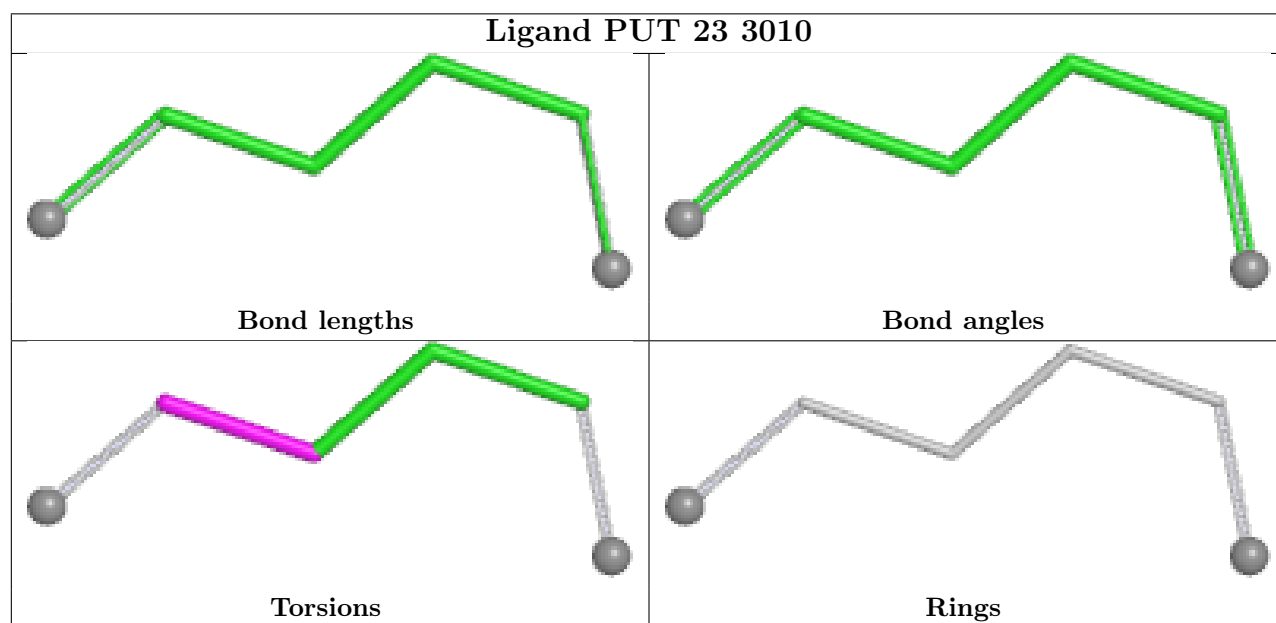
Mol	Chain	Res	Type	Atoms
65	23	3001	ATP	C5'-O5'-PA-O3A
65	23	3002	ATP	PB-O3B-PG-O3G
65	23	3002	ATP	O4'-C4'-C5'-O5'
67	EF	802	FUA	C23-C22-C29-O5
67	EF	802	FUA	O3-C31-O2-C16

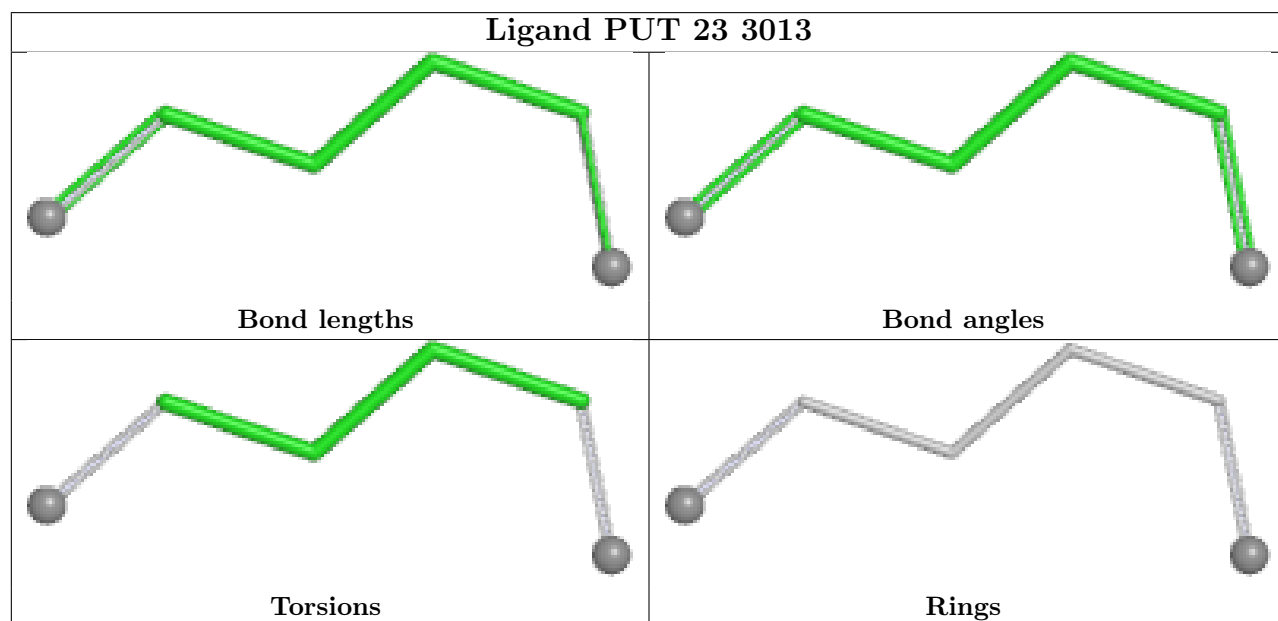
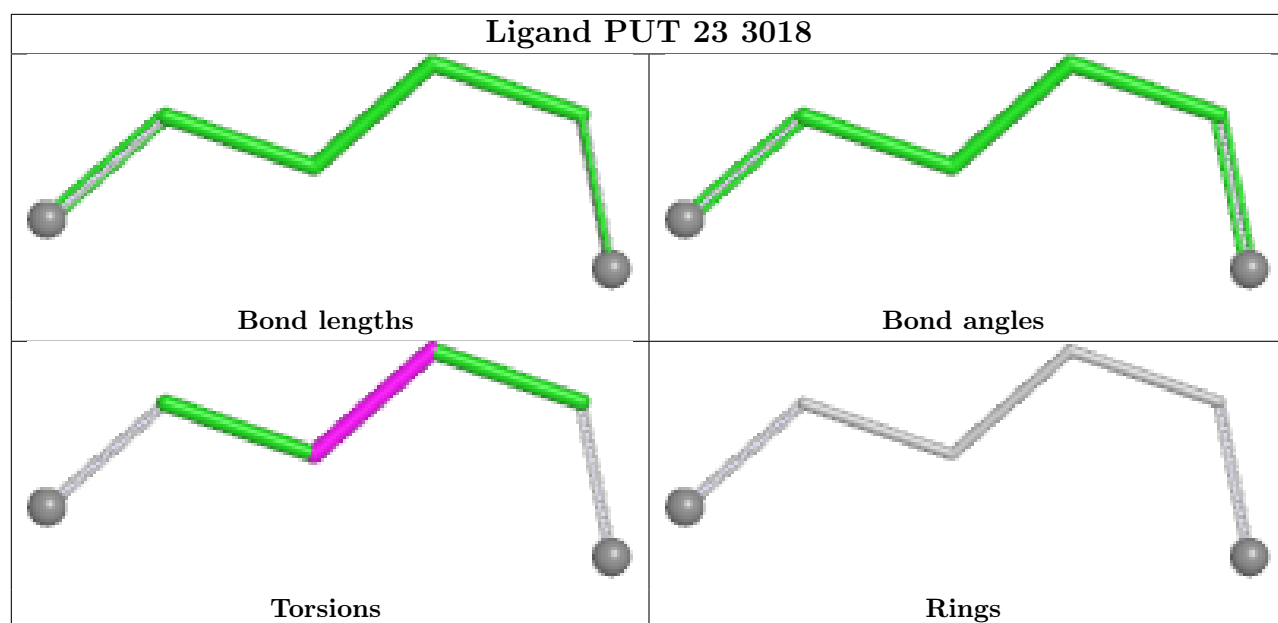
There are no ring outliers.

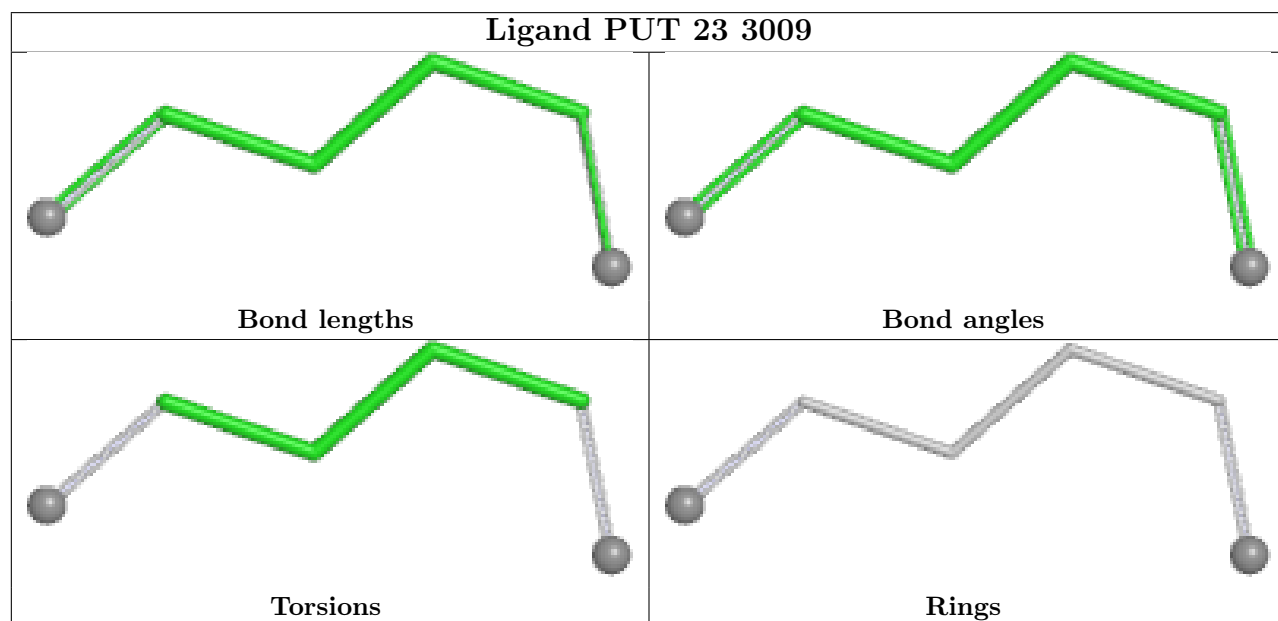
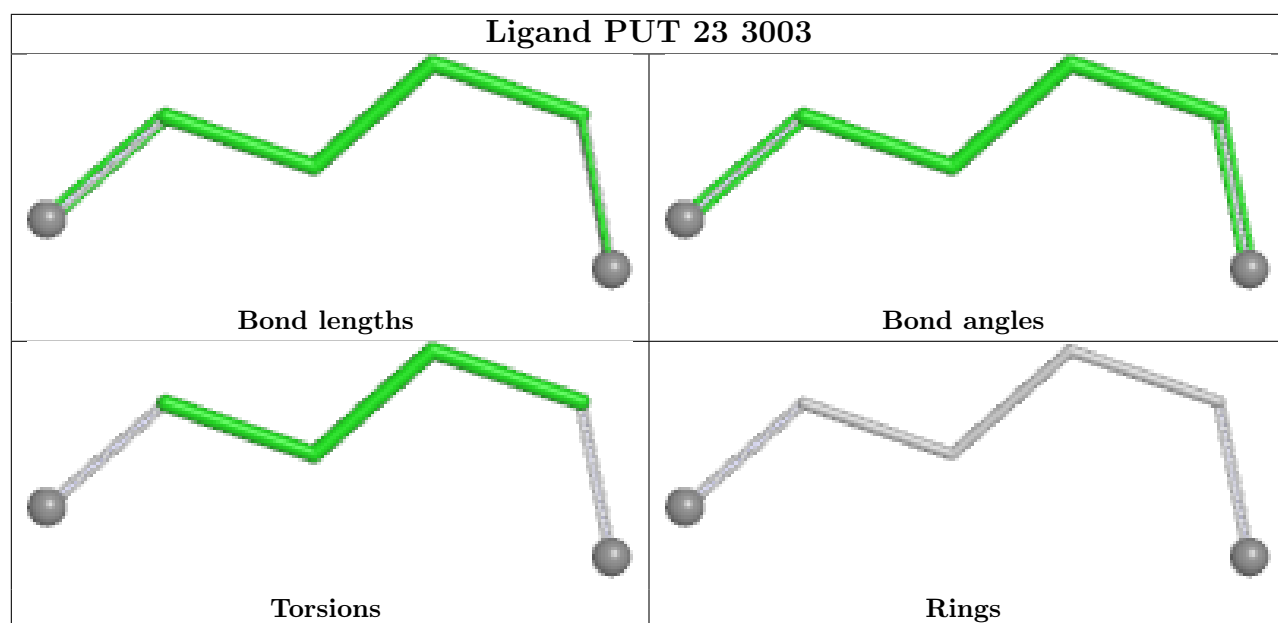
6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	23	3010	PUT	1	0
62	23	3013	PUT	1	0
62	LC	301	PUT	1	0
62	23	3020	PUT	2	0
62	16	1602	PUT	1	0
67	EF	802	FUA	15	0

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

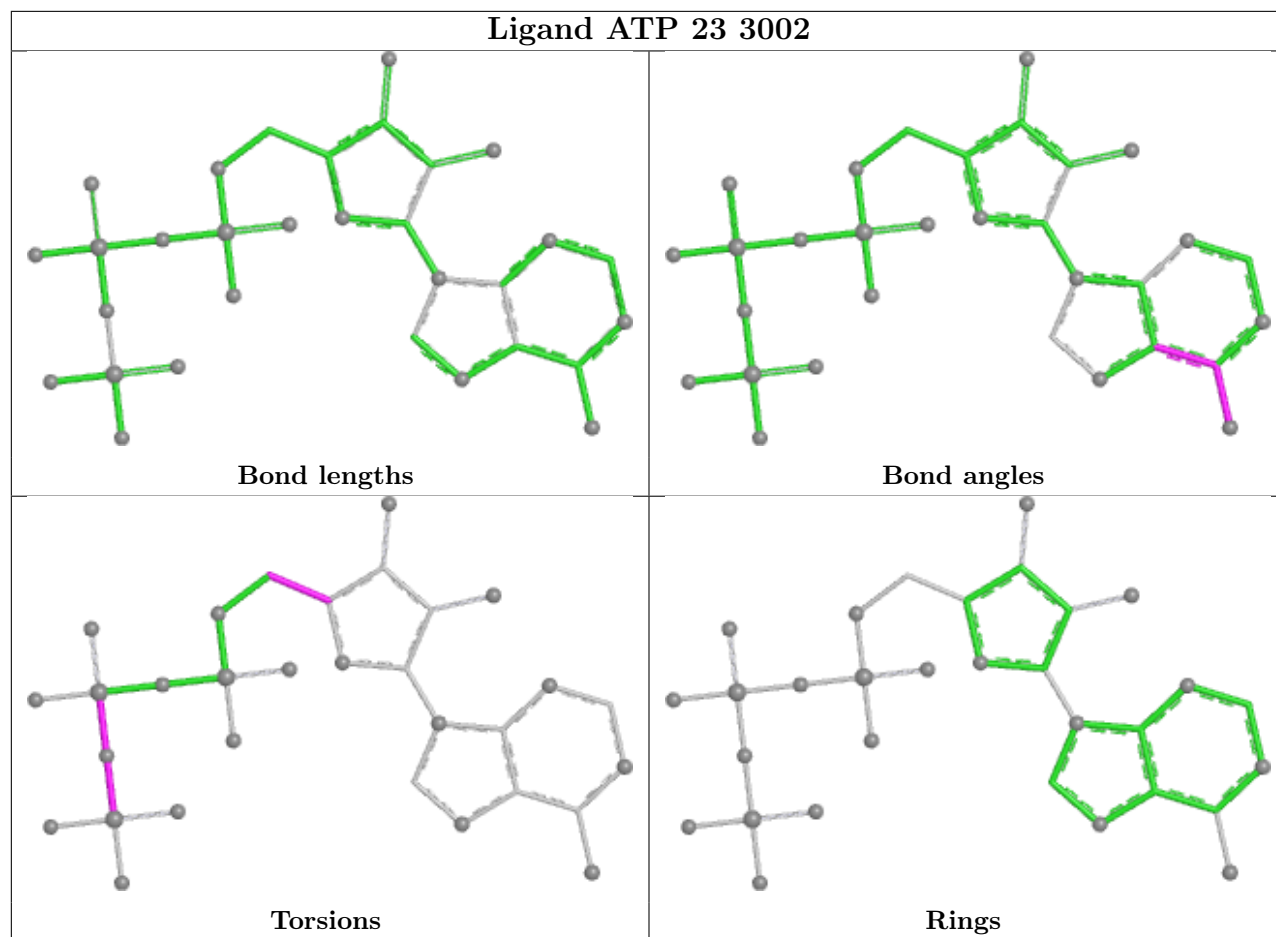




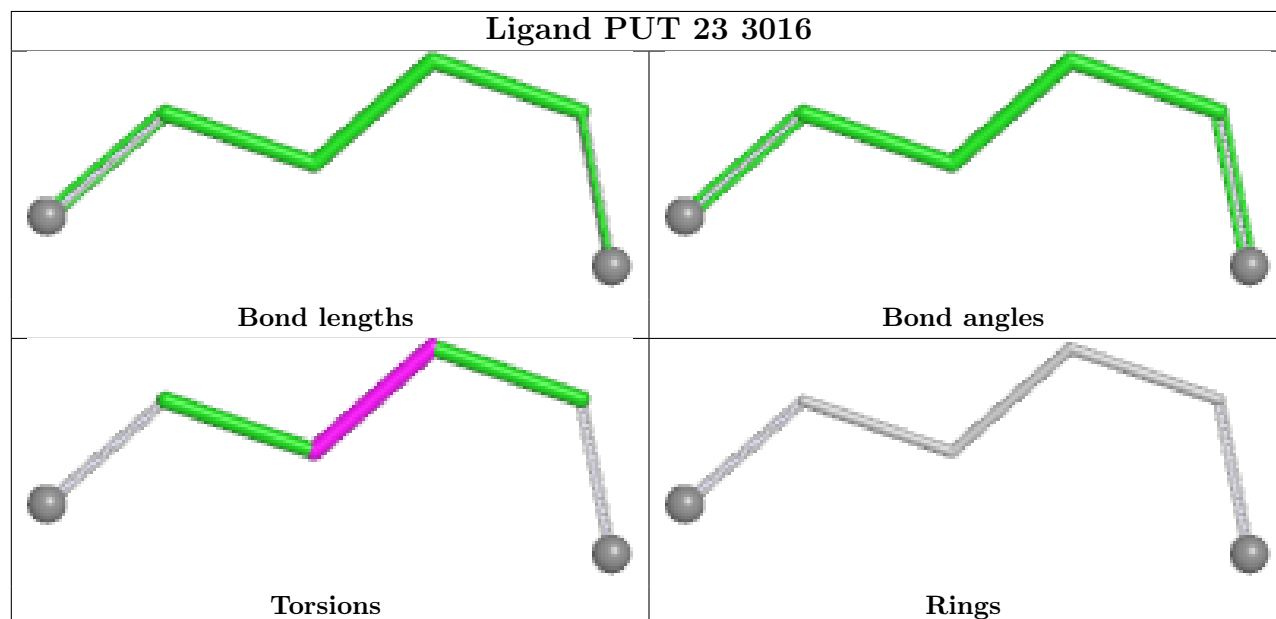


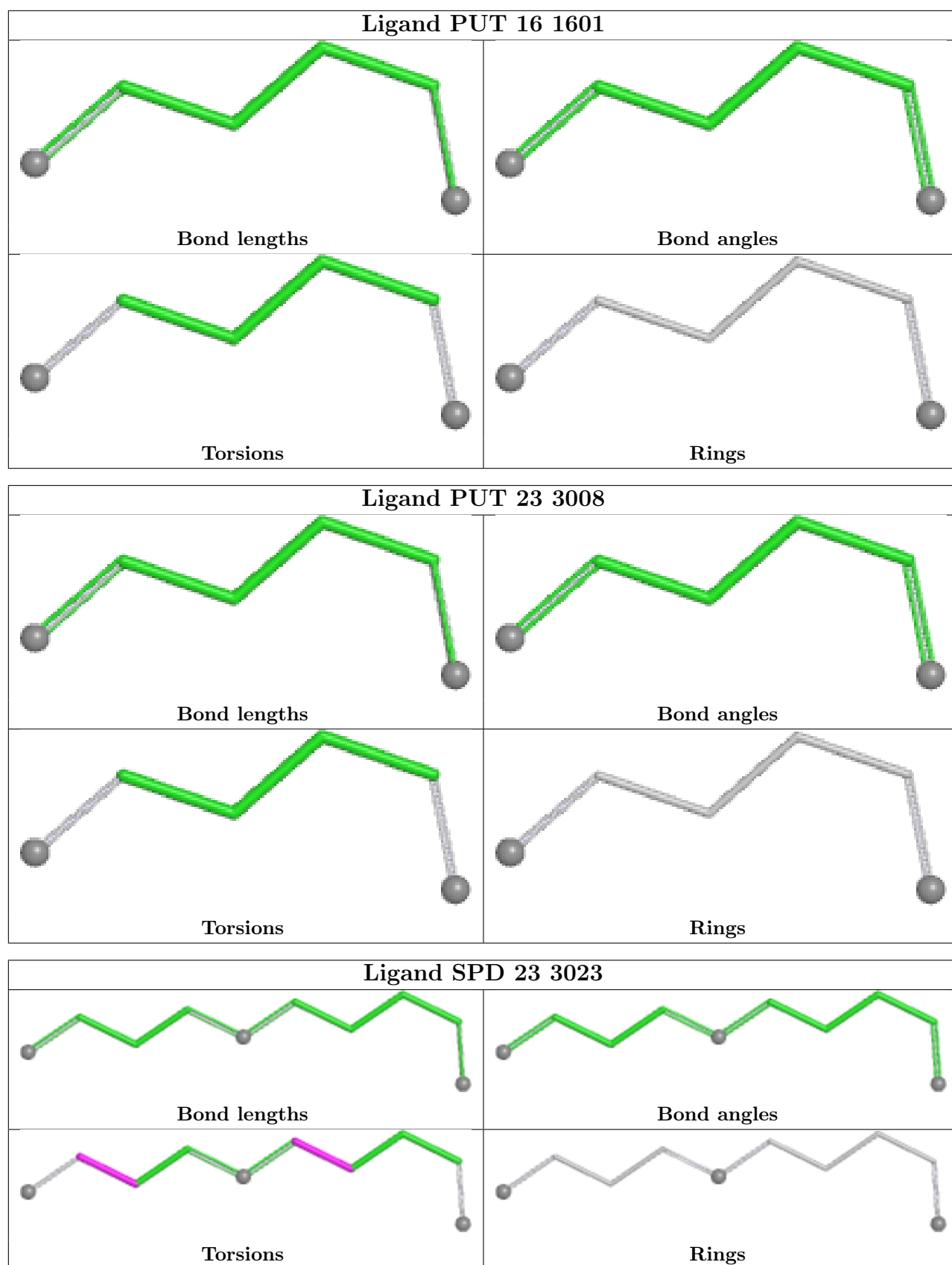


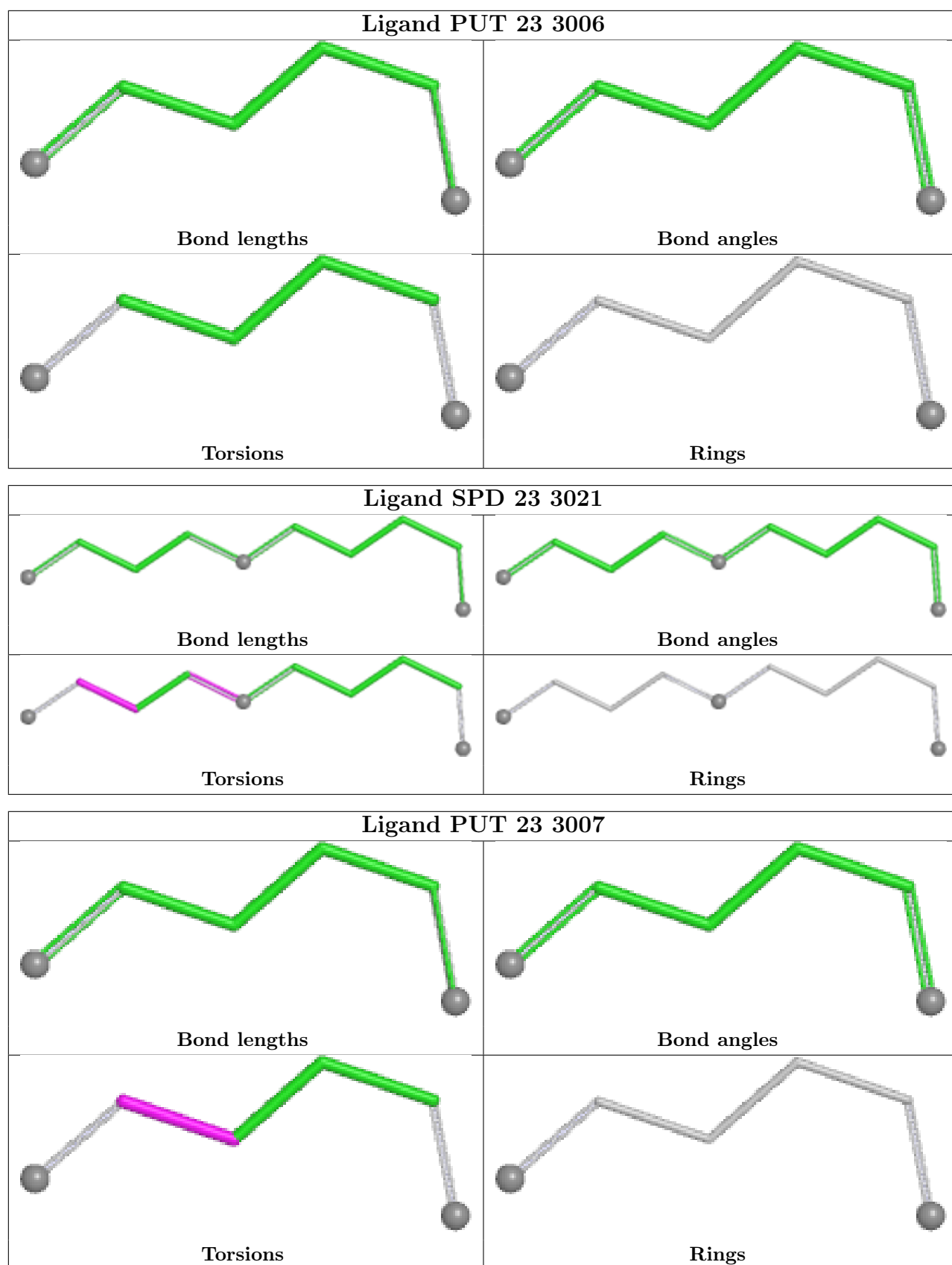
## Ligand ATP 23 3002

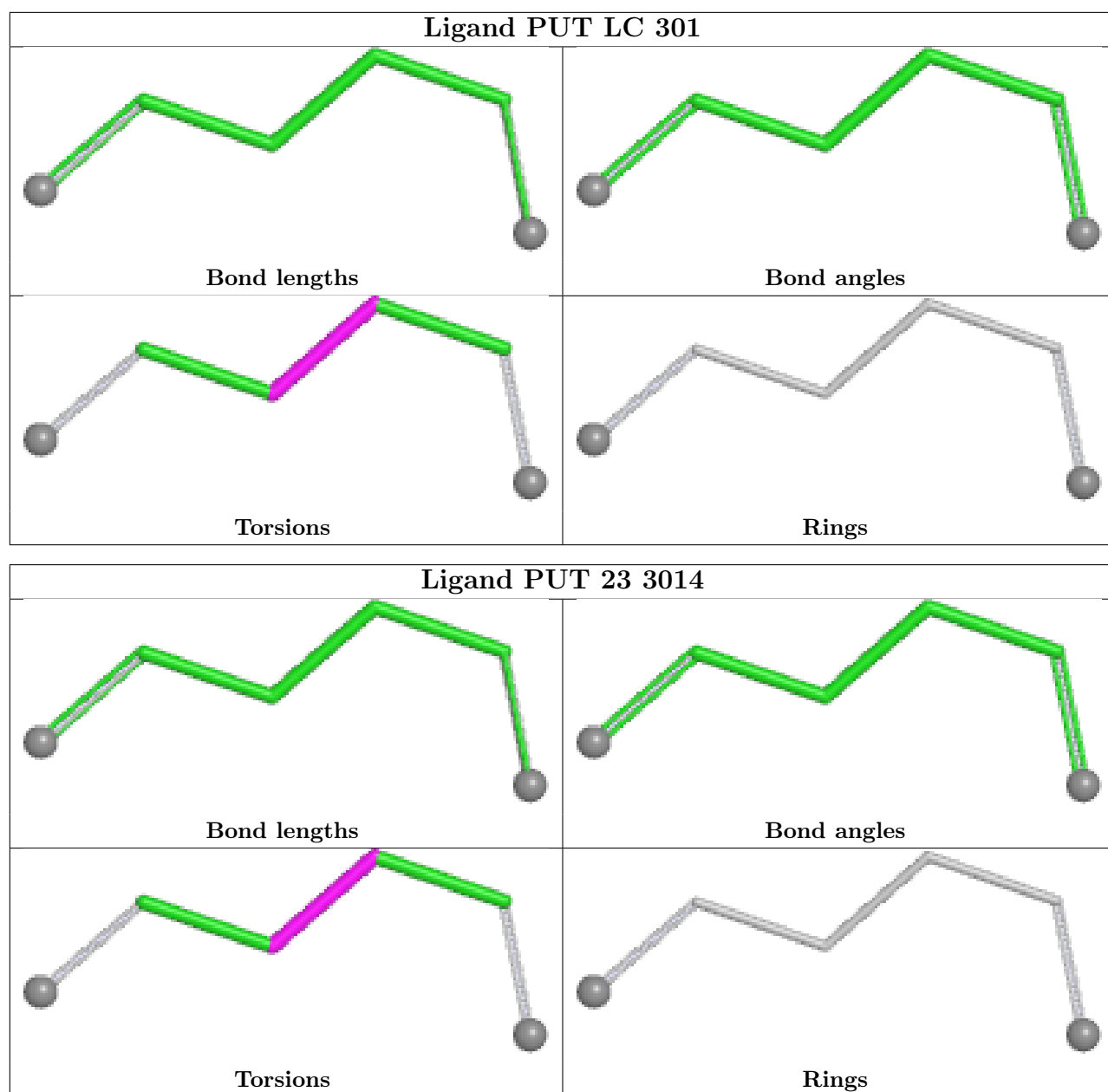


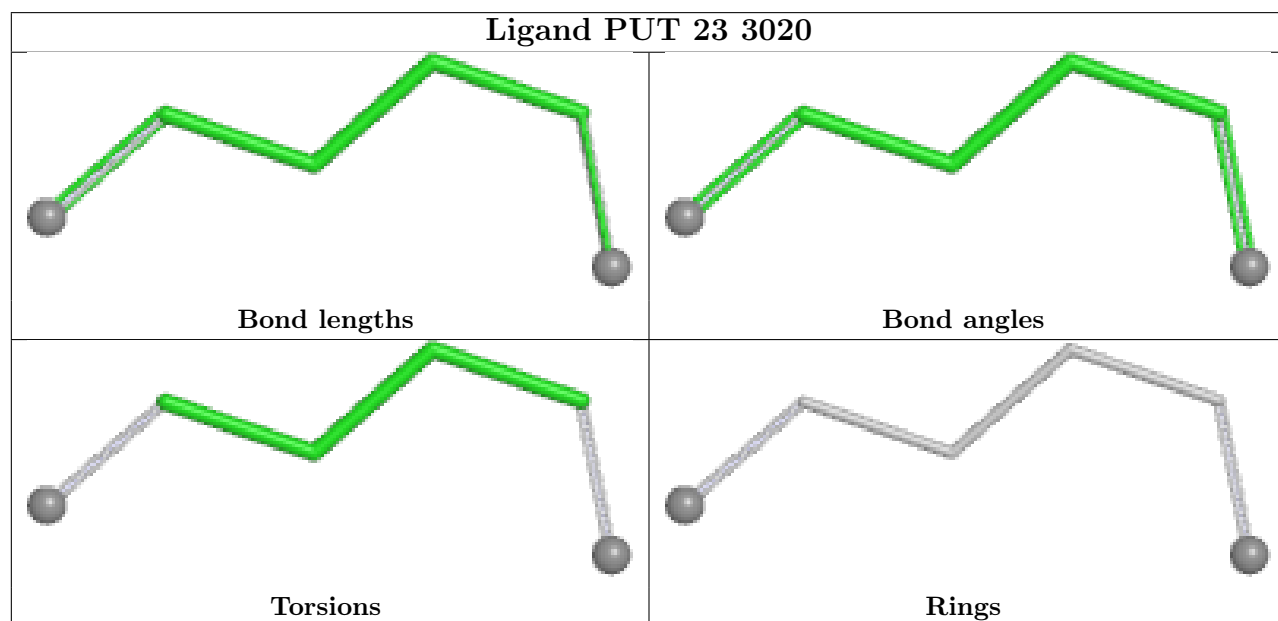
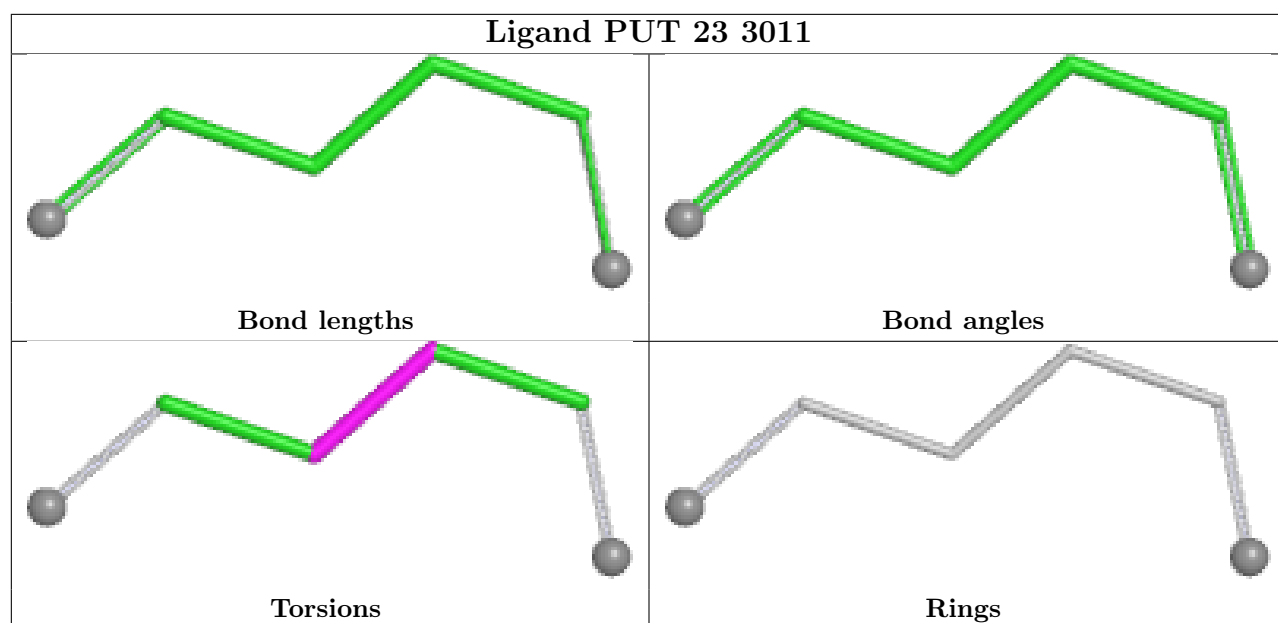
## Ligand PUT 23 3016

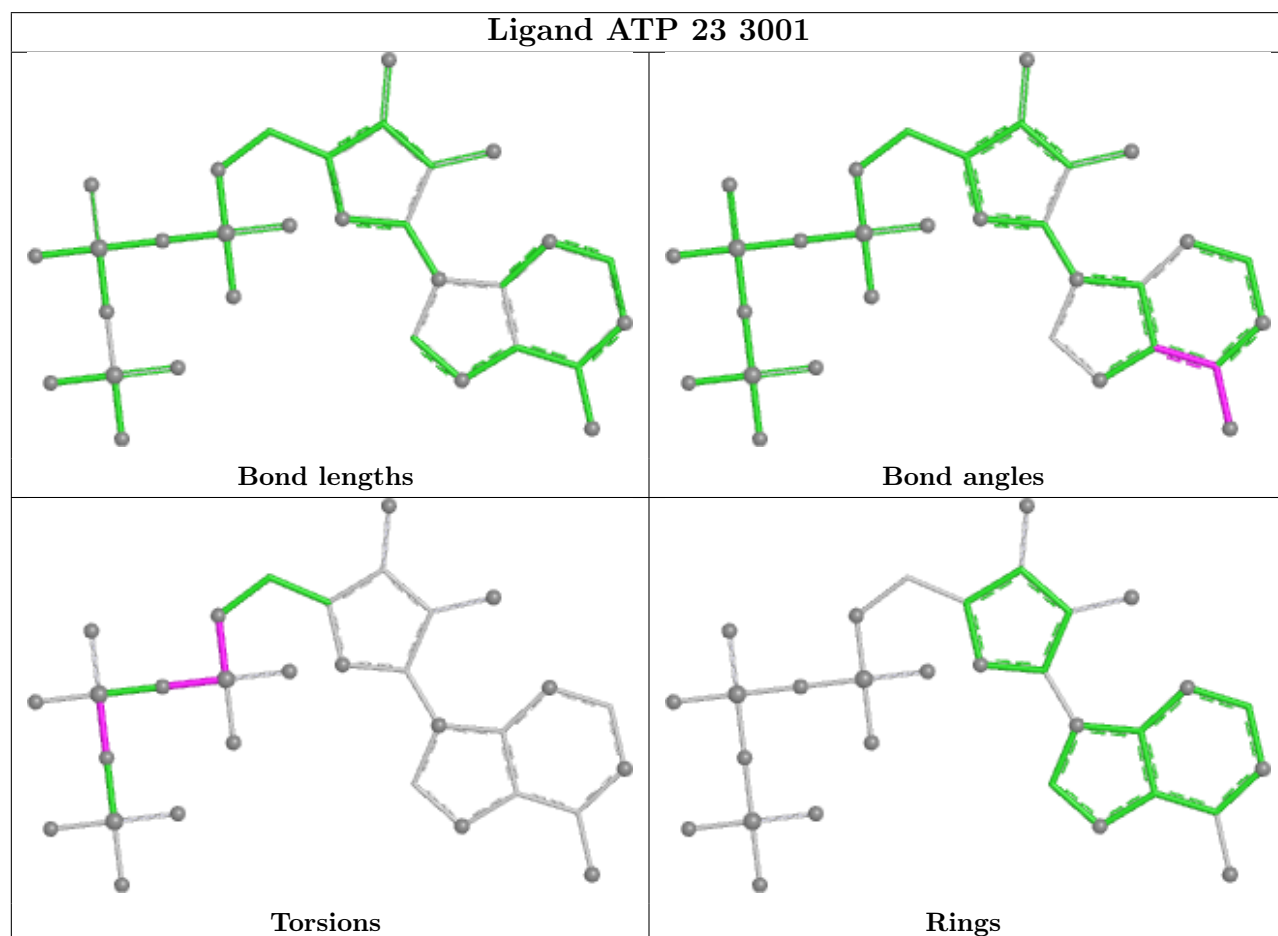
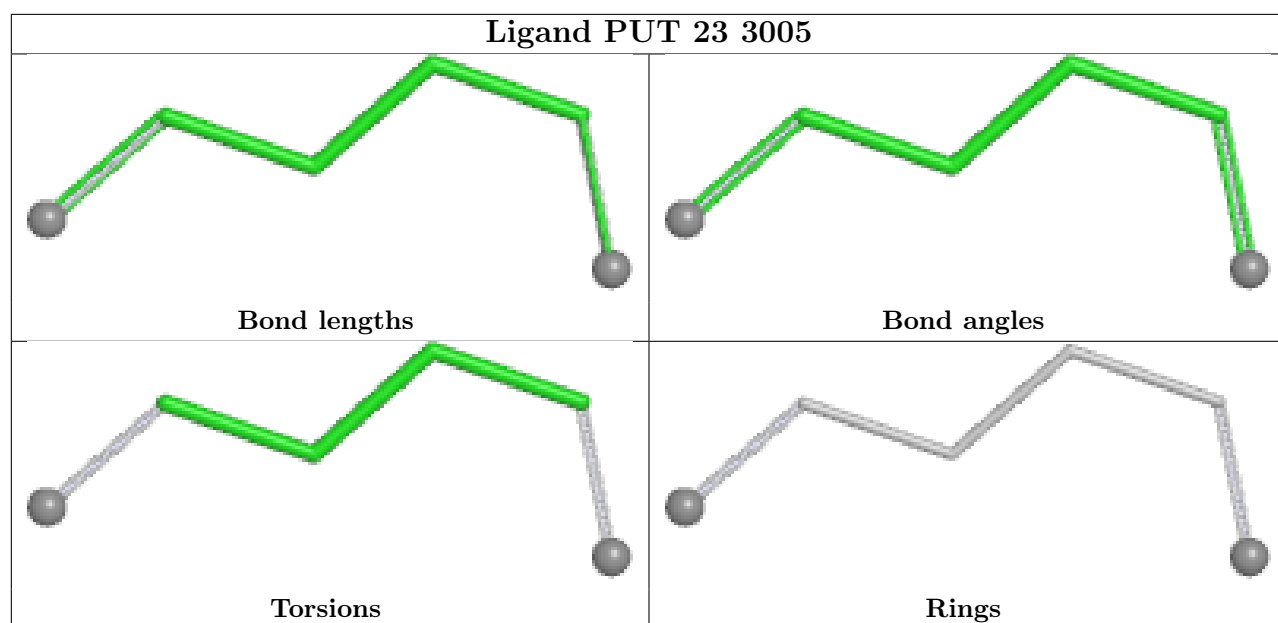


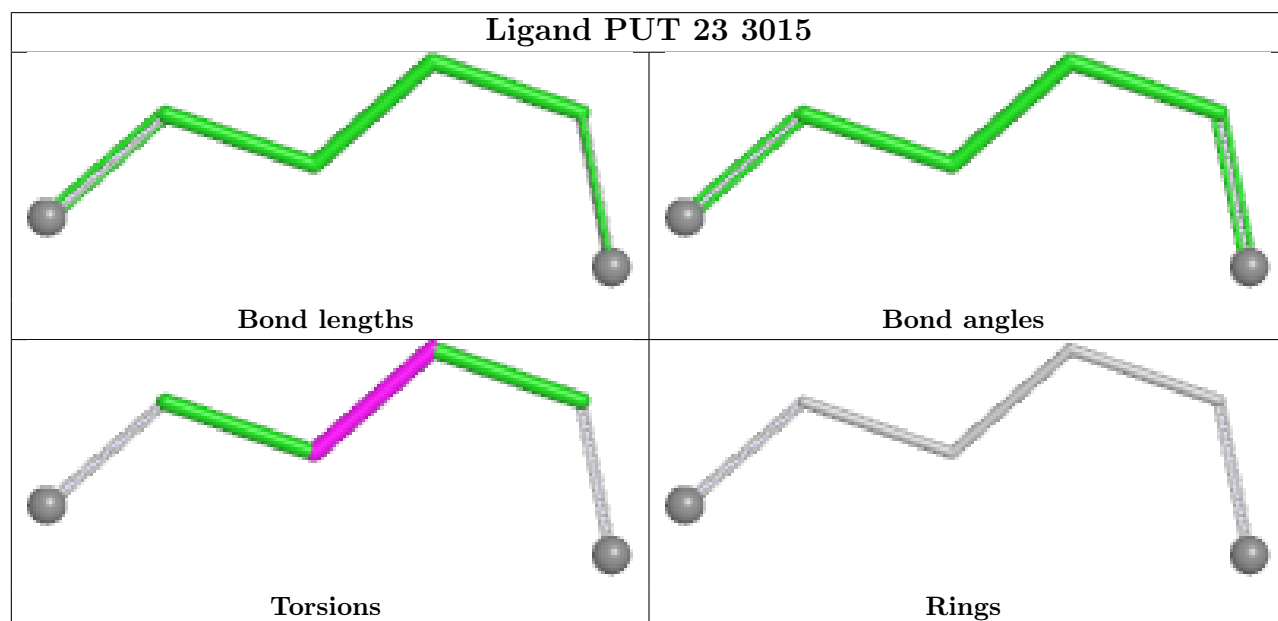
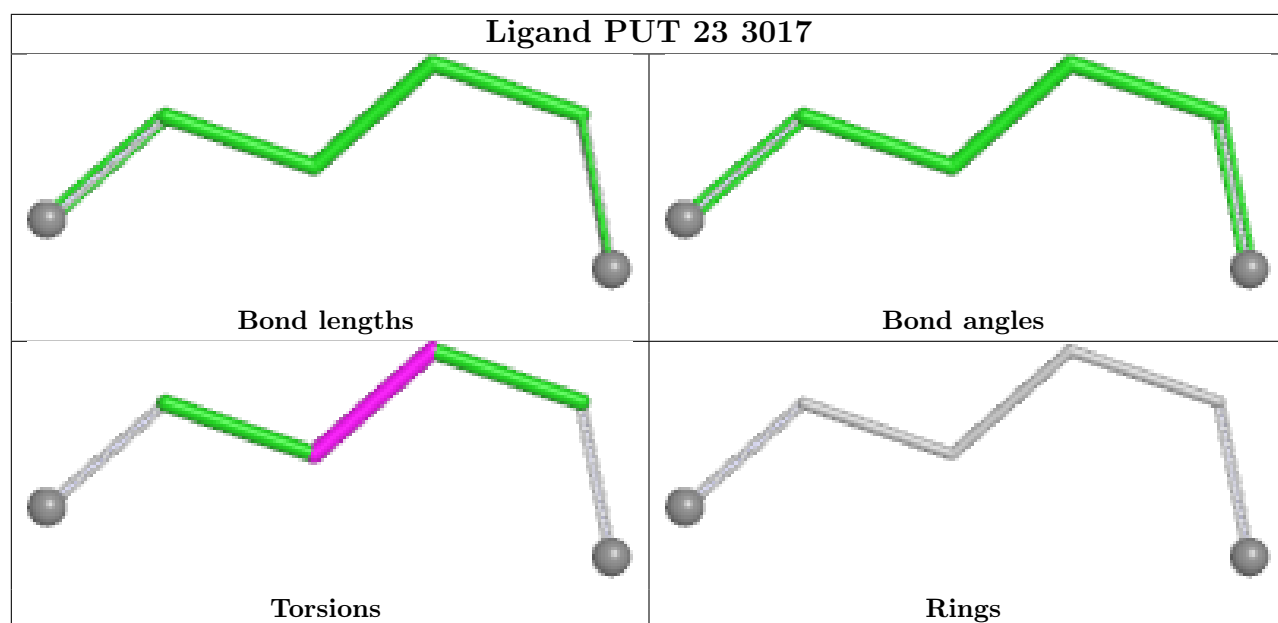


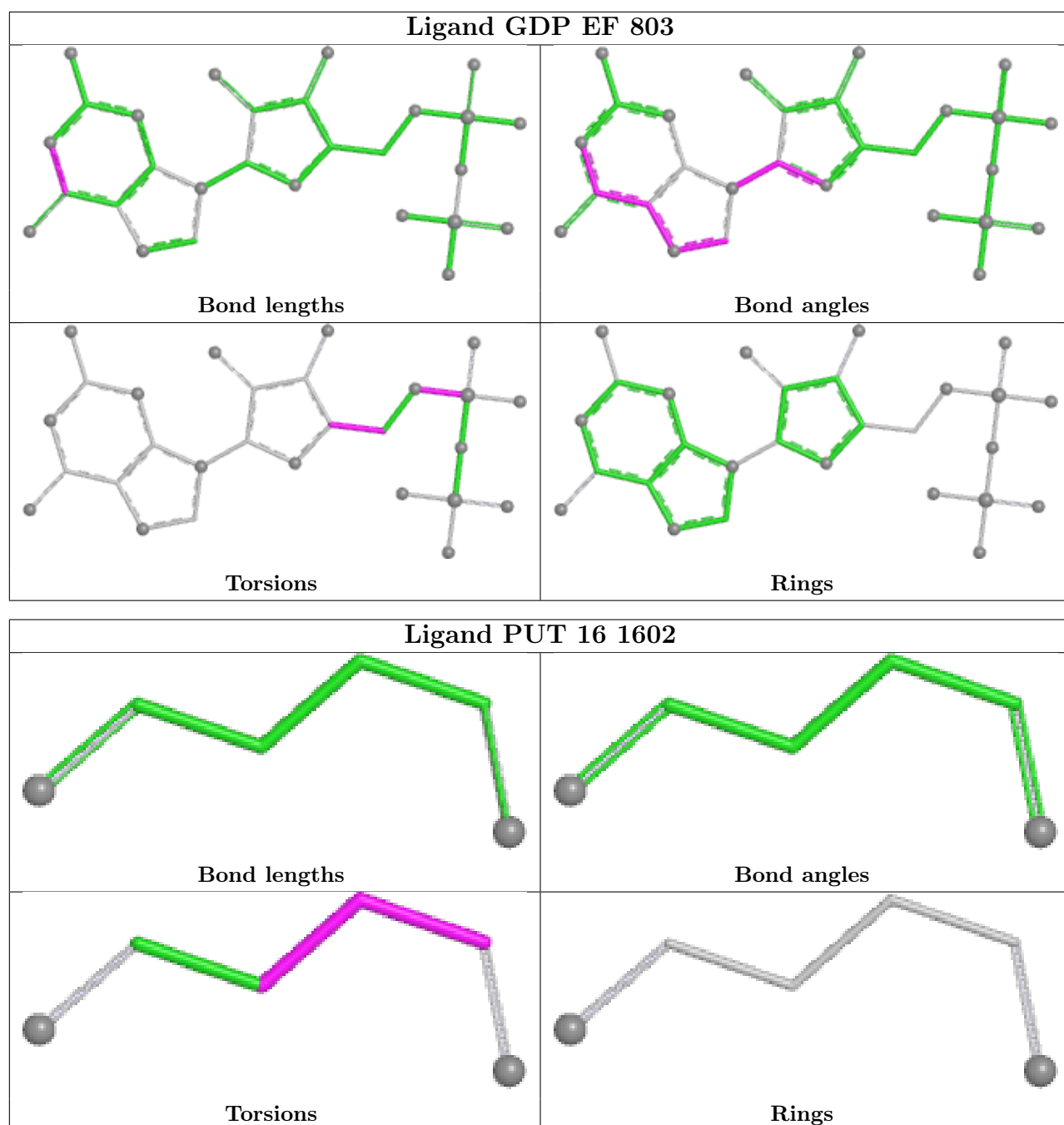




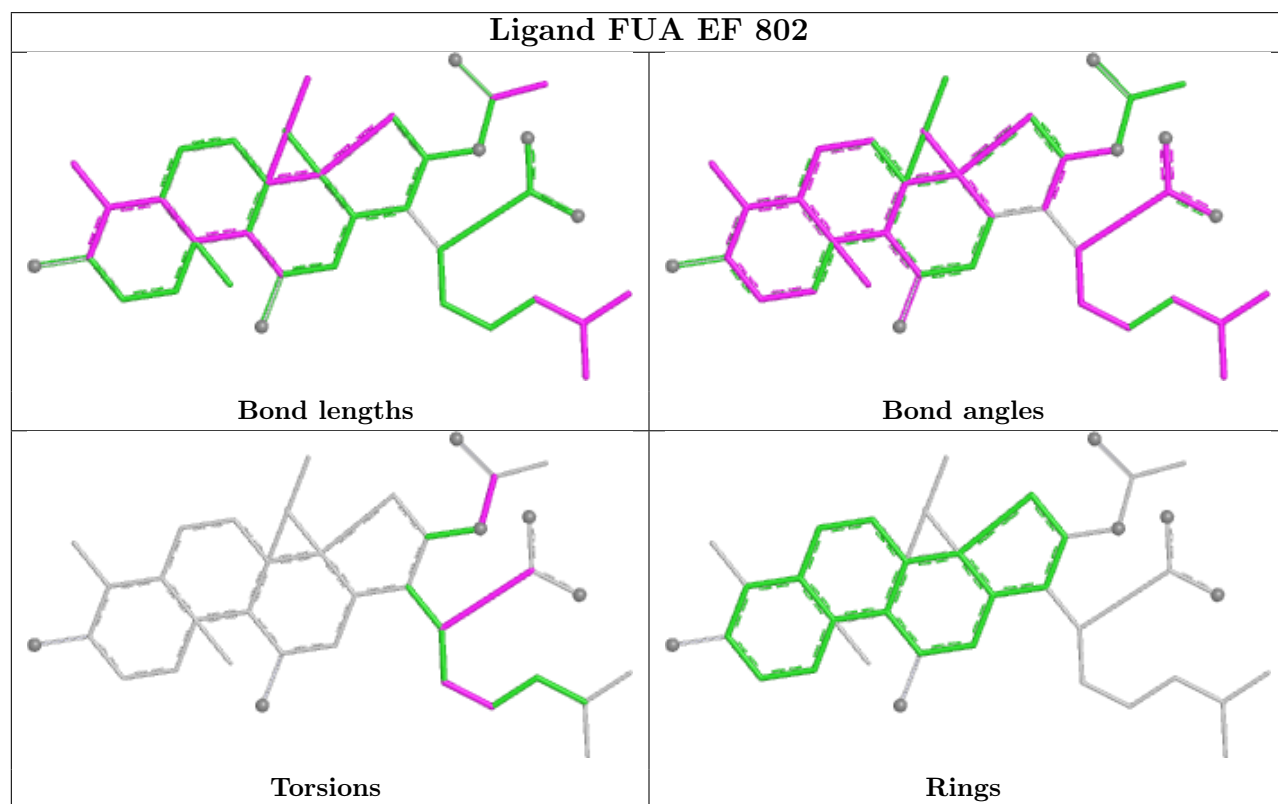
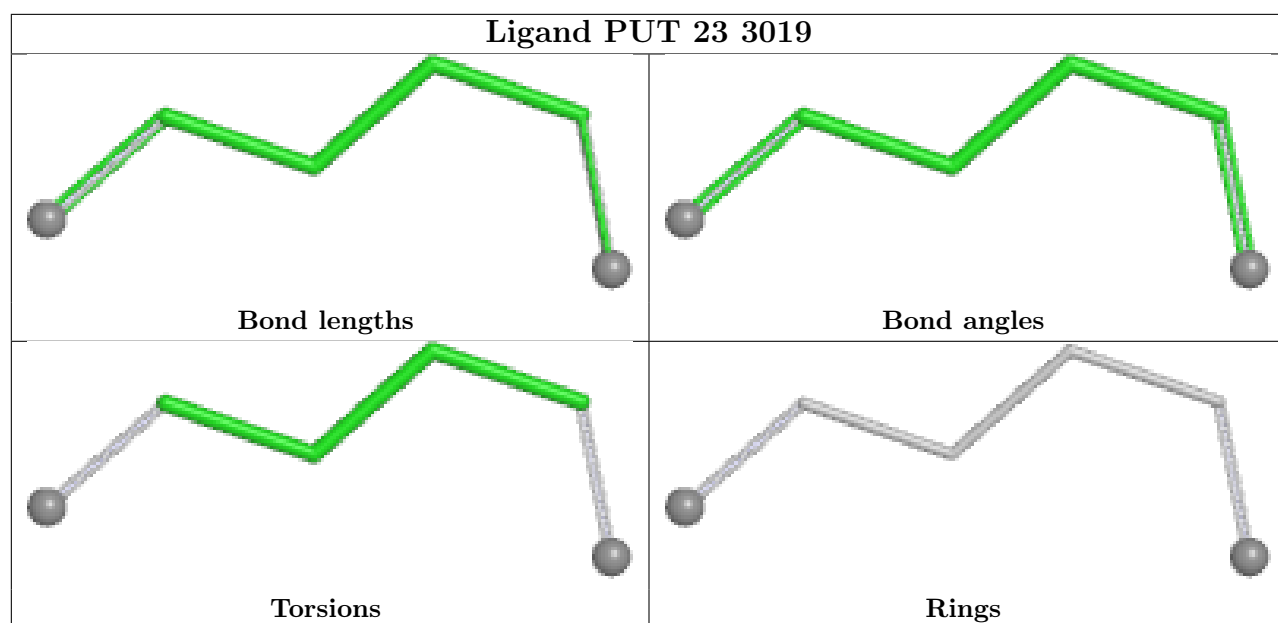


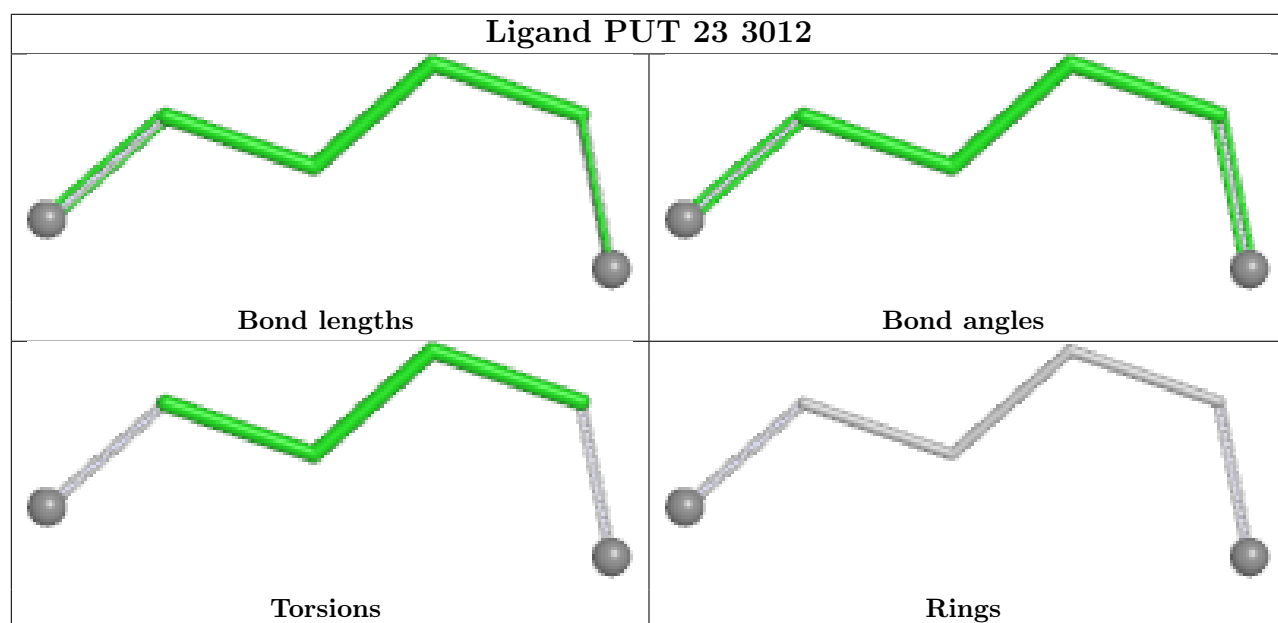
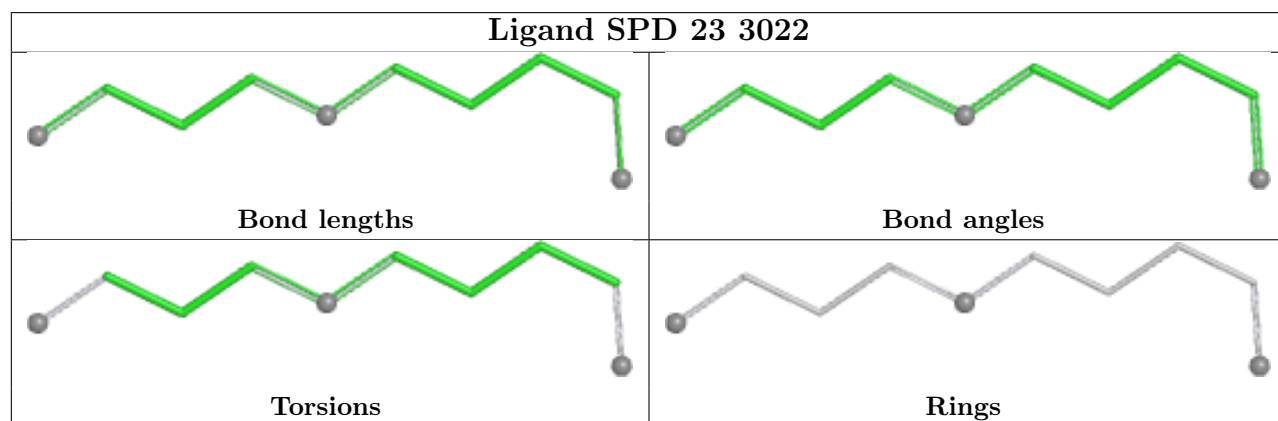
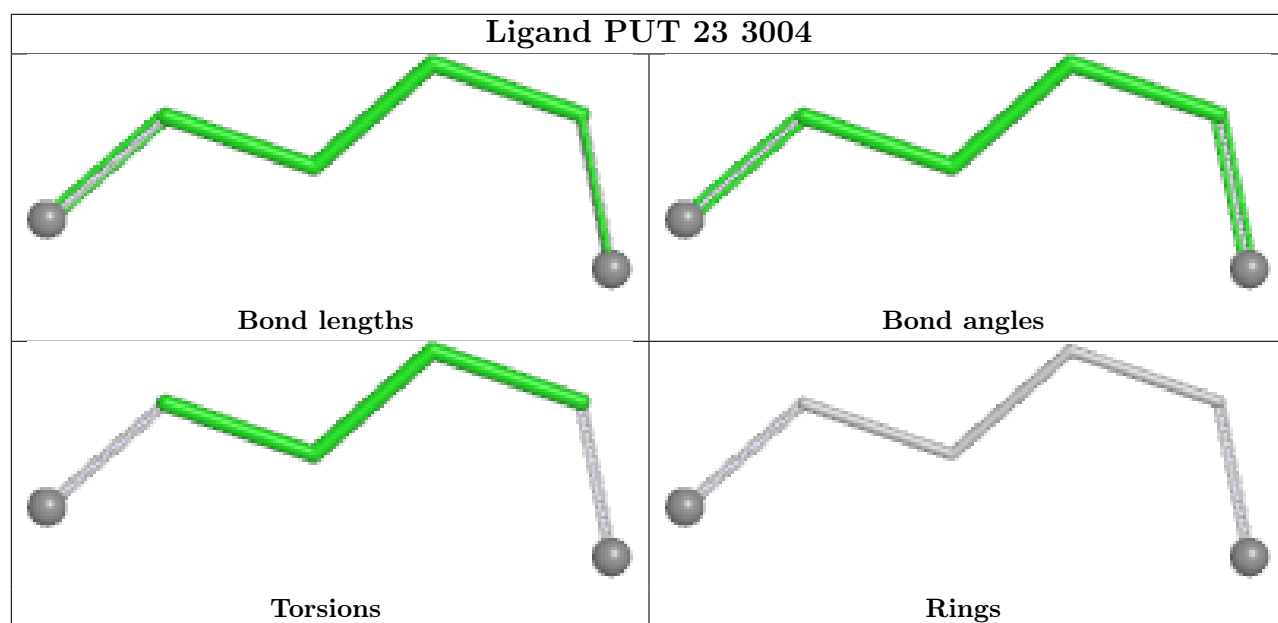












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

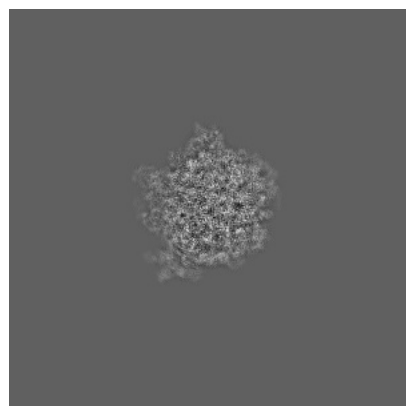
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24132. These allow visual inspection of the internal detail of the map and identification of artifacts.

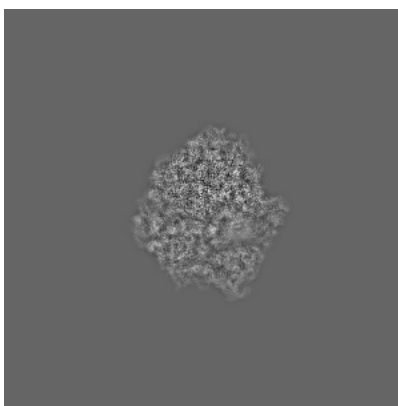
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

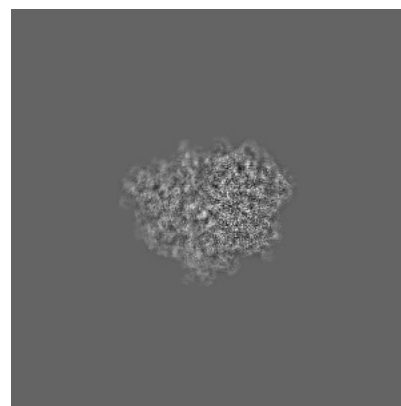
#### 6.1.1 Primary map



X

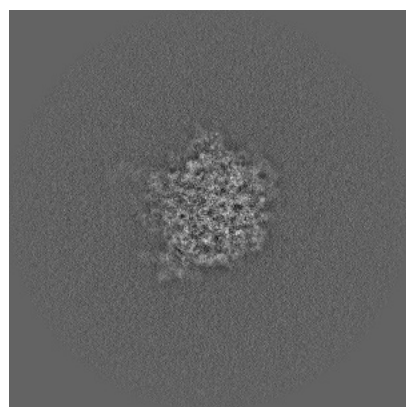


Y

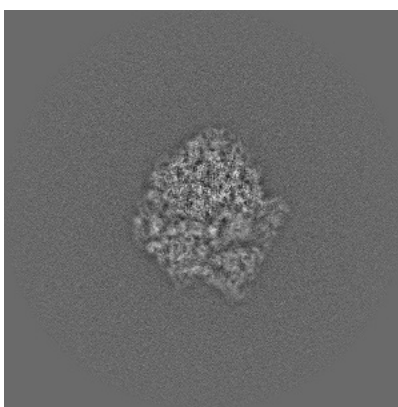


Z

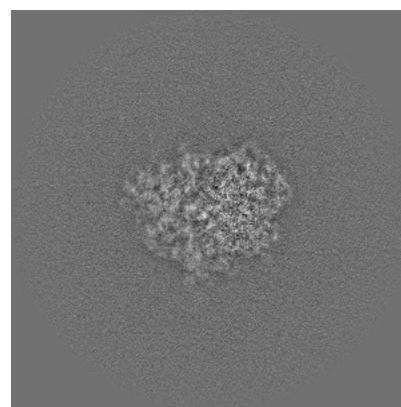
#### 6.1.2 Raw map



X



Y

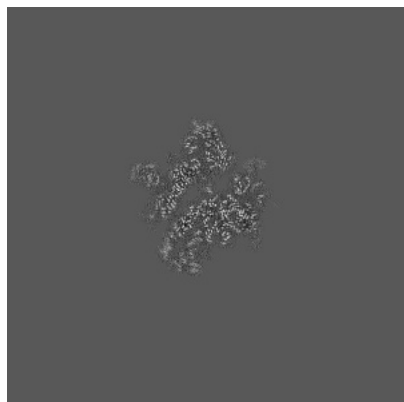


Z

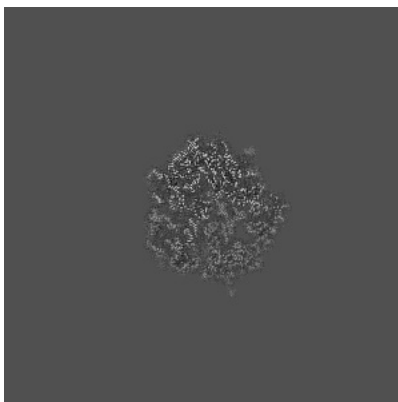
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

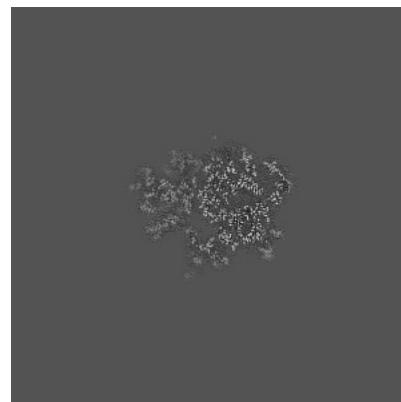
### 6.2.1 Primary map



X Index: 288

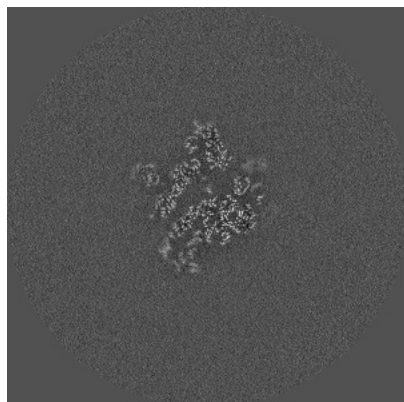


Y Index: 288

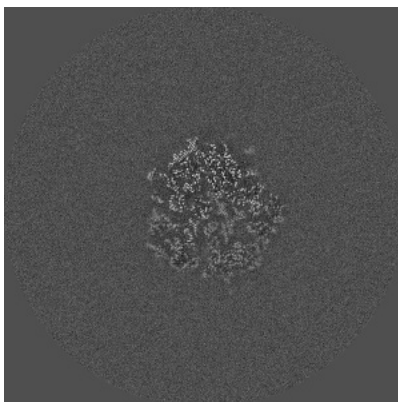


Z Index: 288

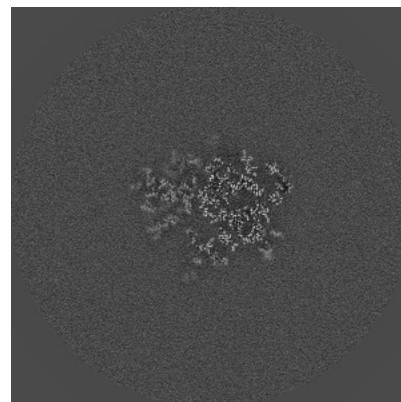
### 6.2.2 Raw map



X Index: 288



Y Index: 288

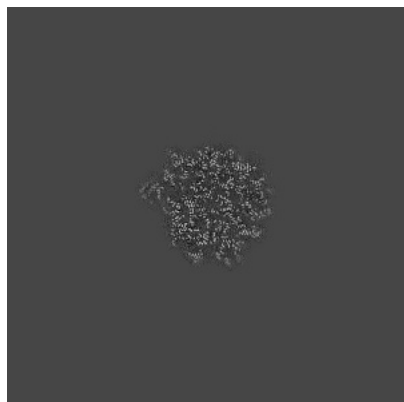


Z Index: 288

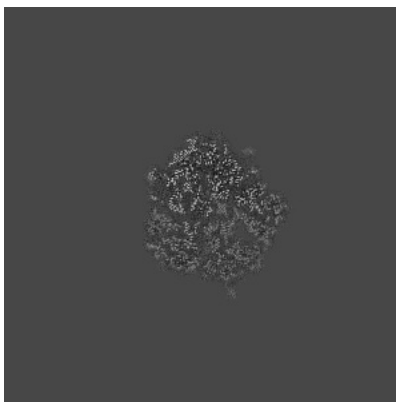
The images above show central slices of the map in three orthogonal directions.

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

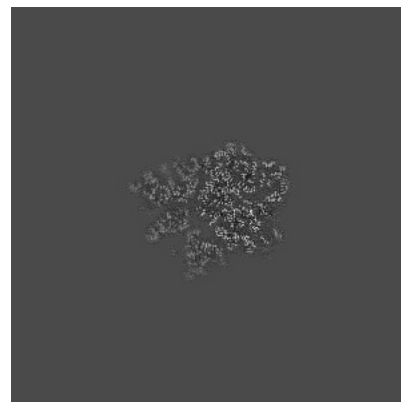
### 6.3.1 Primary map



X Index: 315

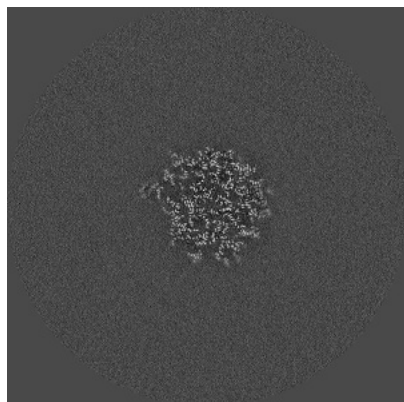


Y Index: 290

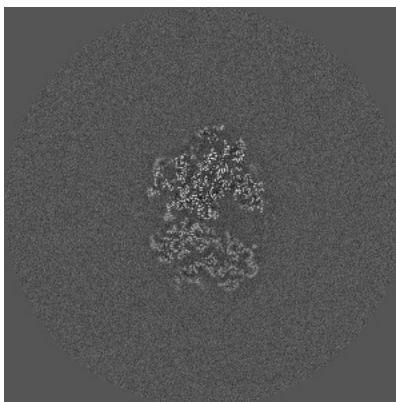


Z Index: 282

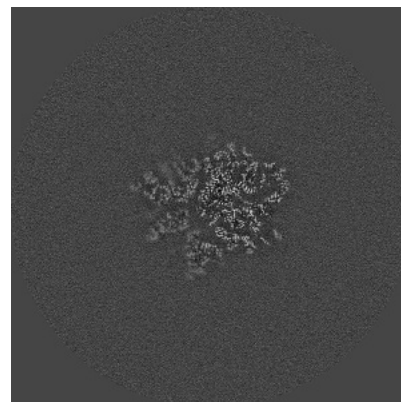
### 6.3.2 Raw map



X Index: 315



Y Index: 312

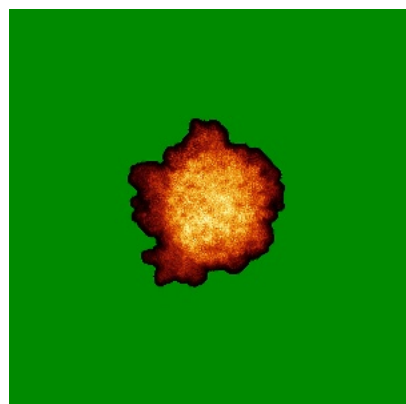


Z Index: 282

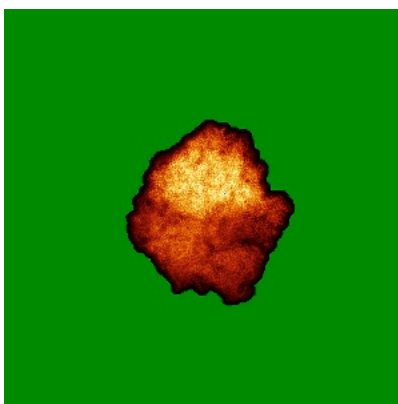
The images above show the largest variance slices of the map in three orthogonal directions.

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

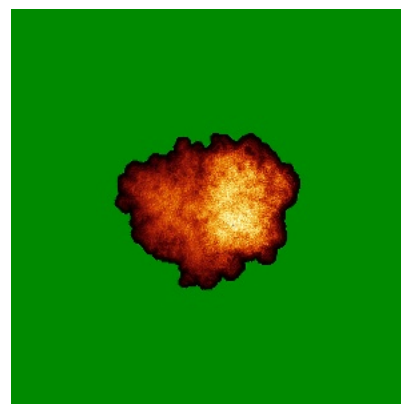
### 6.4.1 Primary map



X

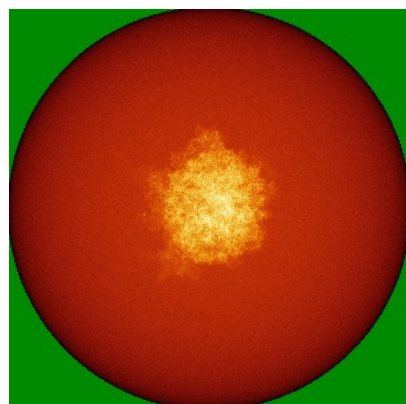


Y

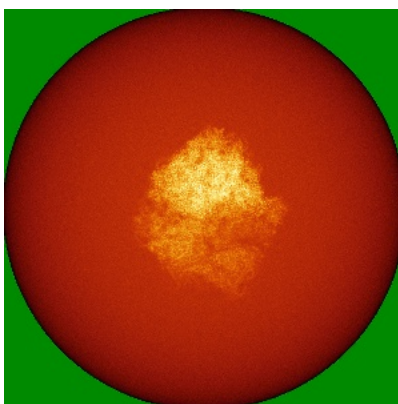


Z

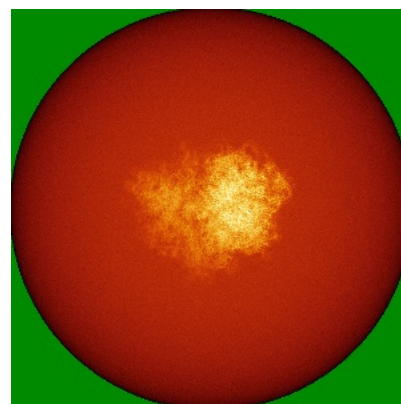
### 6.4.2 Raw map



X



Y



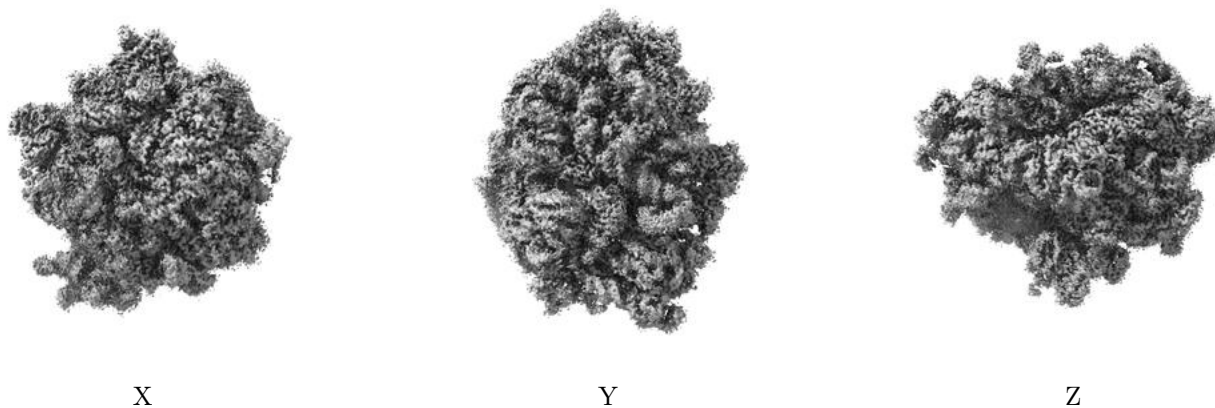
Z

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.



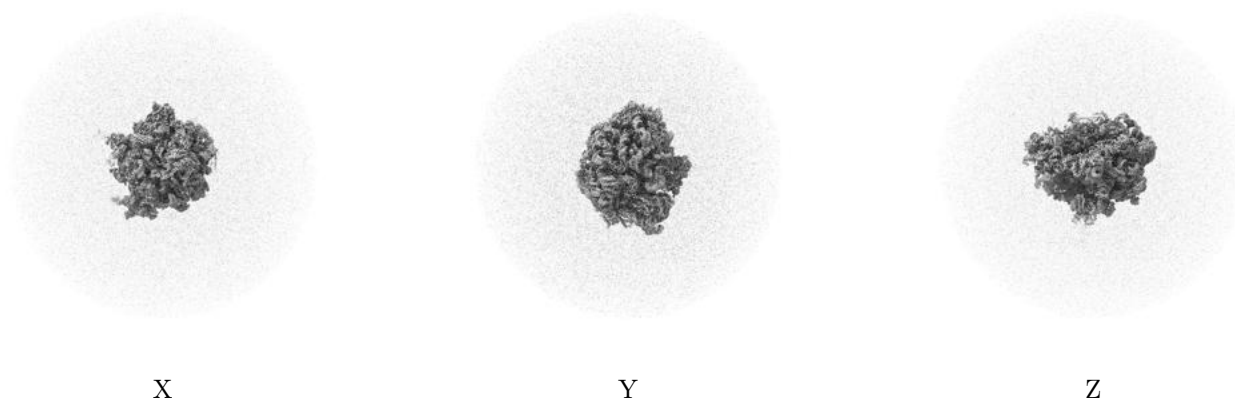
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. 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](#)

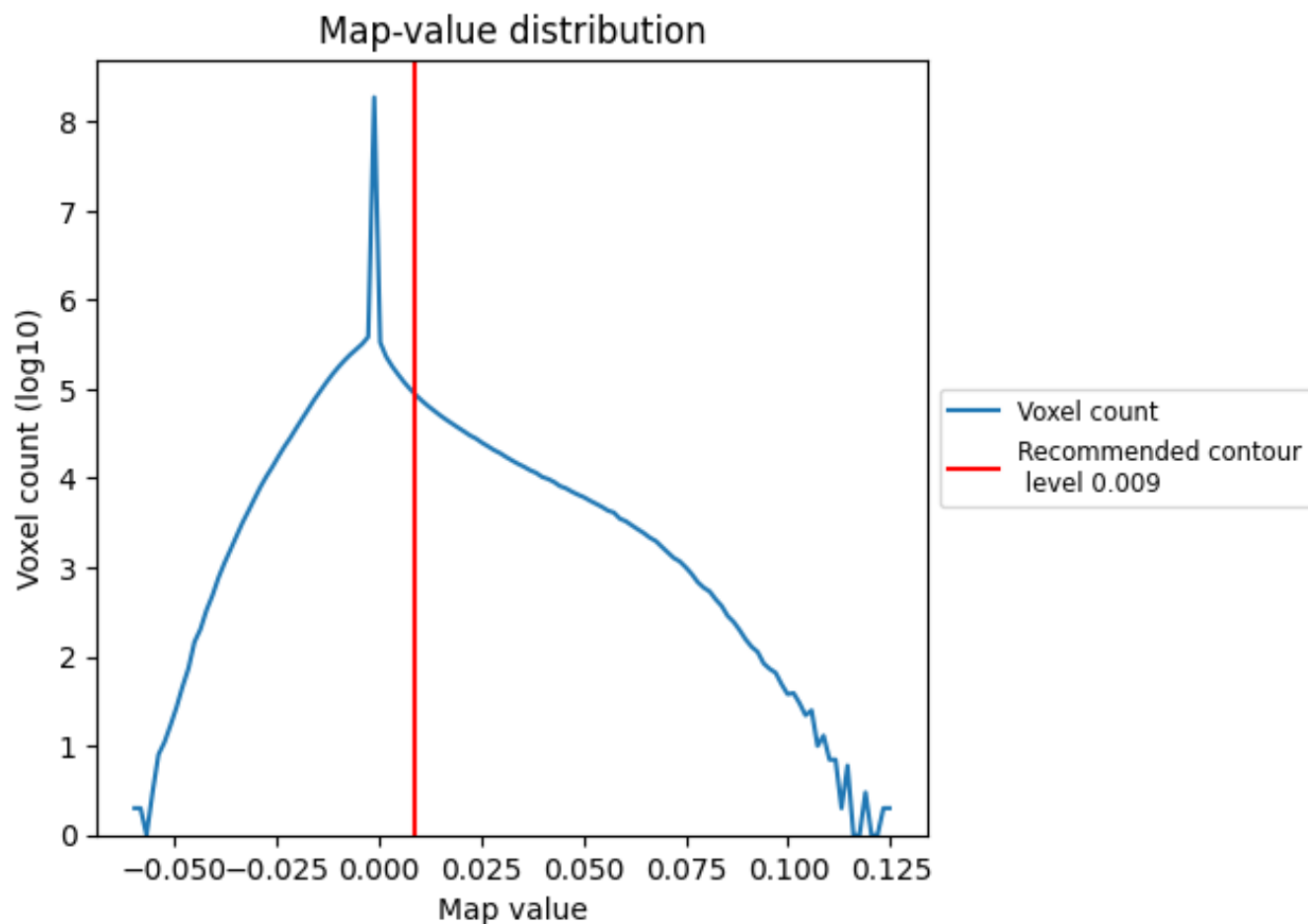
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

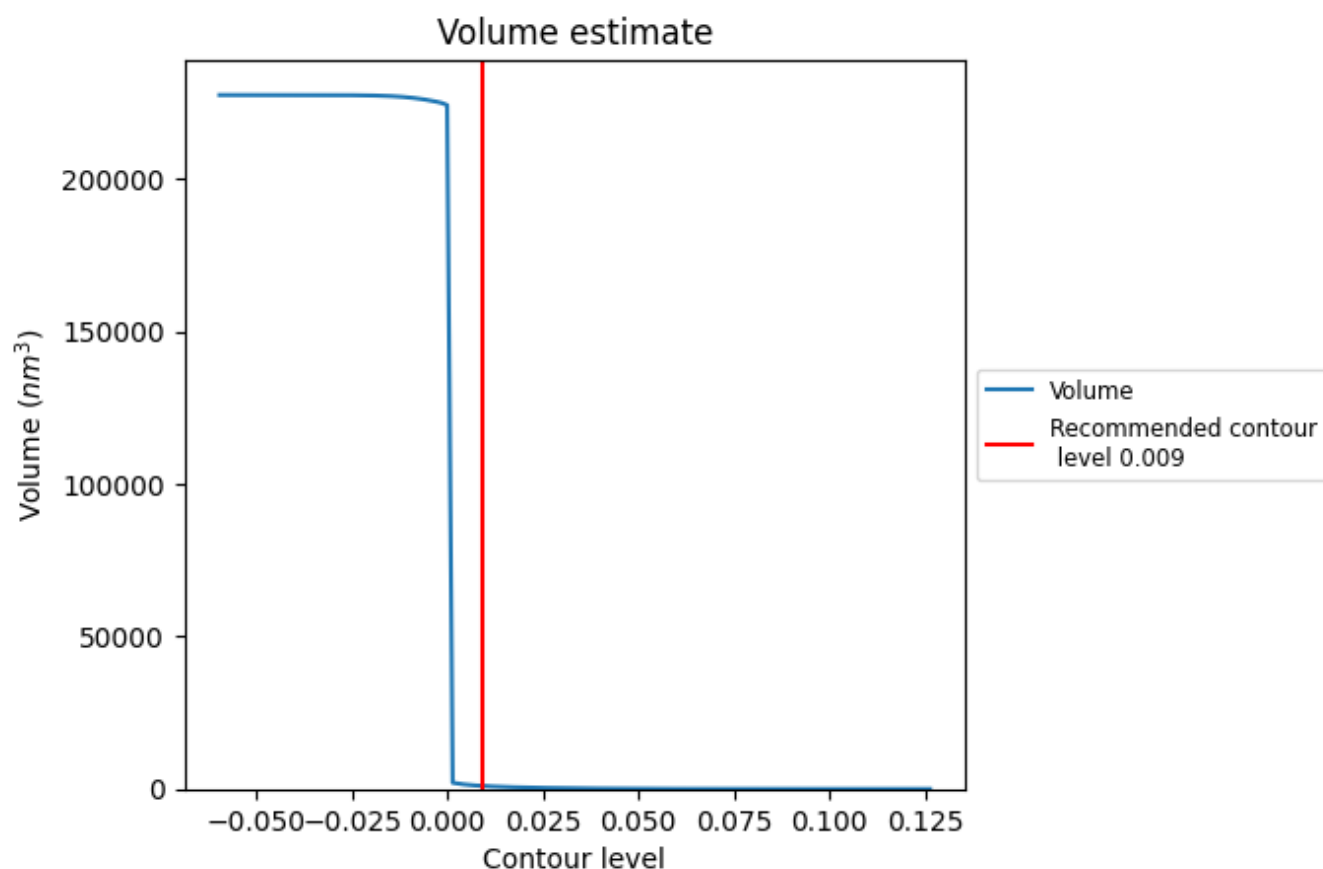
This section contains the results of statistical analysis of the map.

### 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.

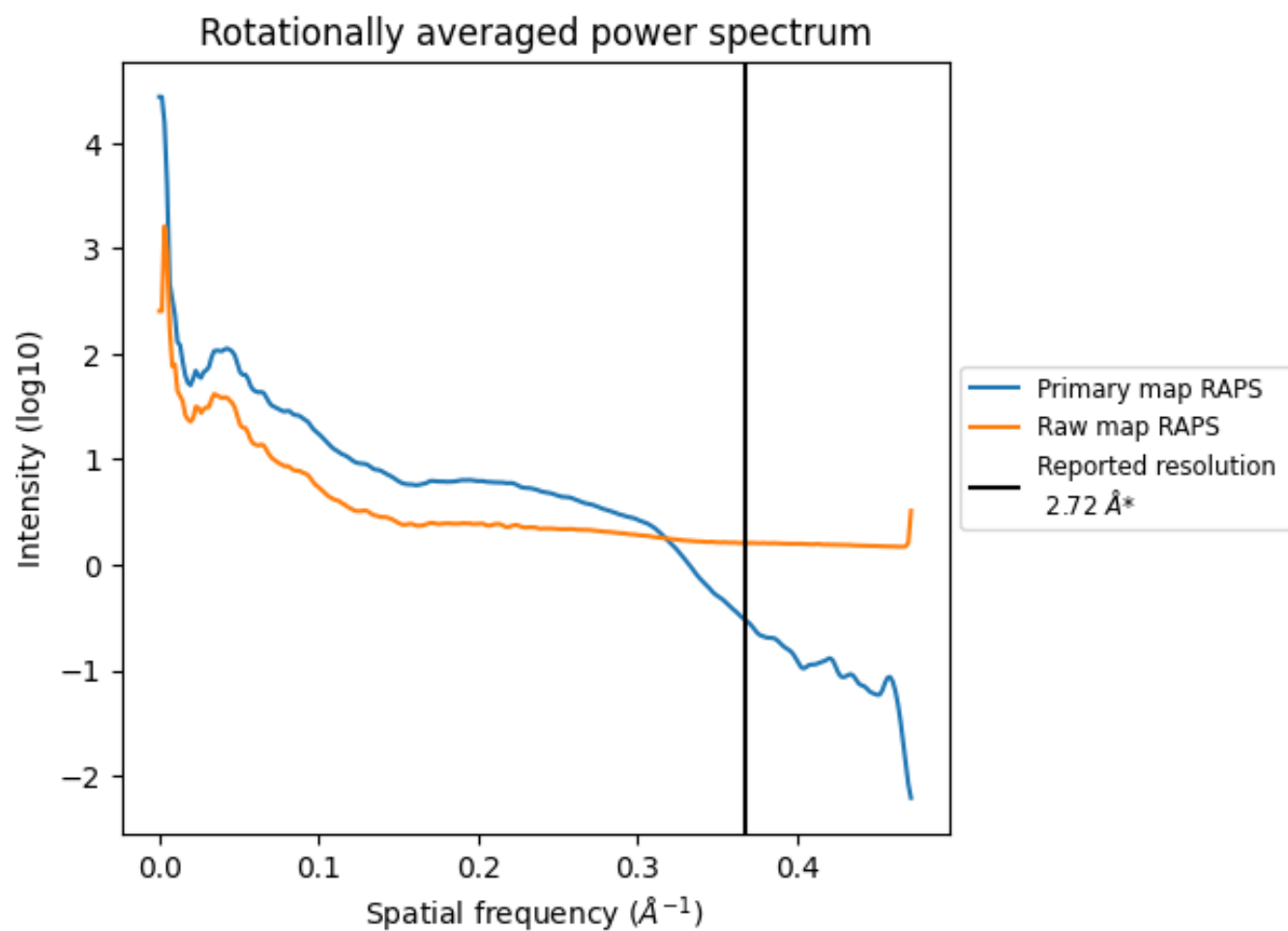
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1017 nm<sup>3</sup>; this corresponds to an approximate mass of 919 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 ⓘ

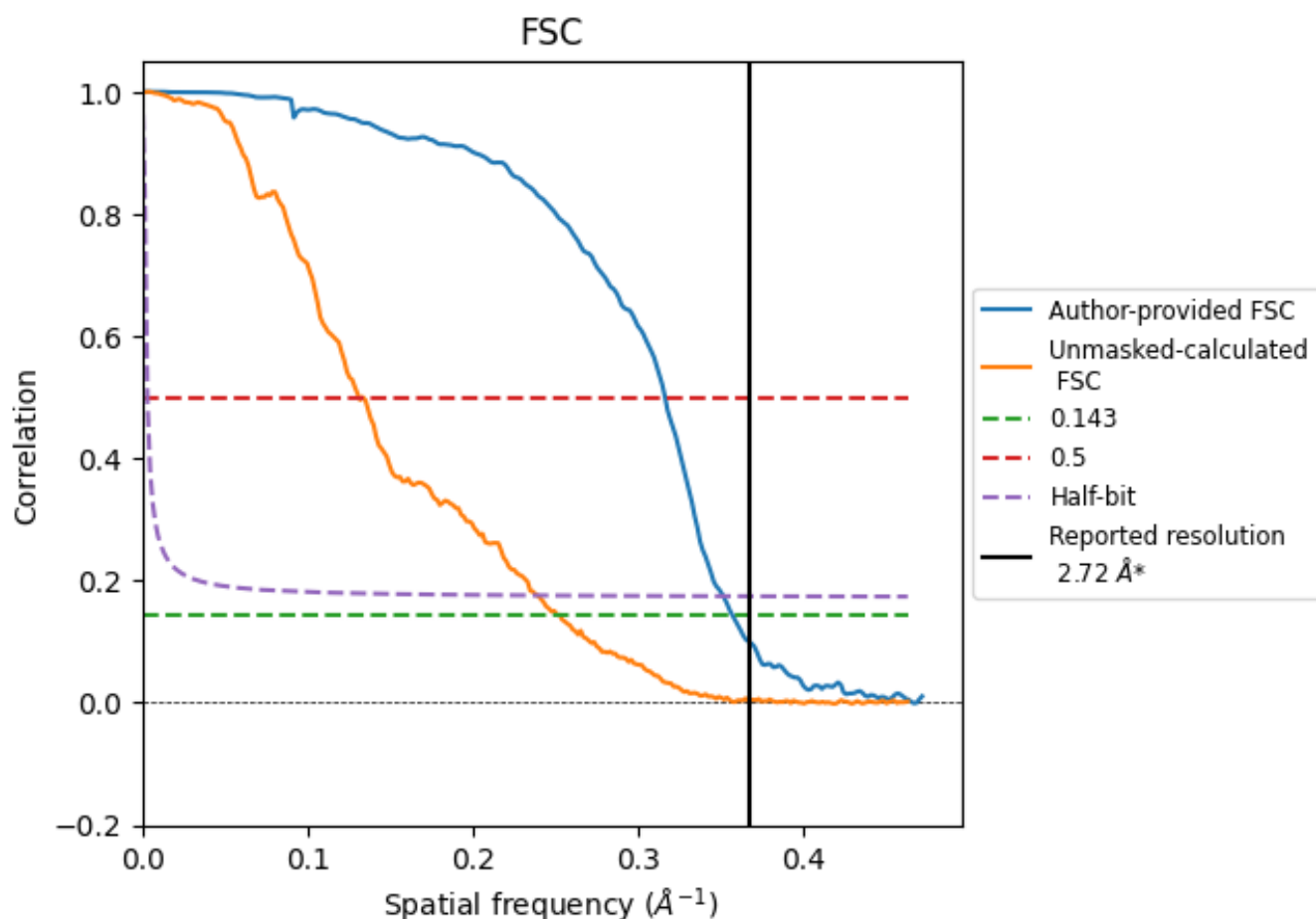


\*Reported resolution corresponds to spatial frequency of 0.368  $\text{\AA}^{-1}$

## 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  $0.368 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

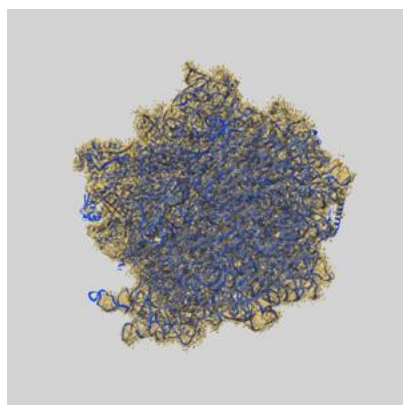
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.80	3.16	2.85
Unmasked-calculated*	3.96	7.63	4.18

\*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 3.96 differs from the reported value 2.72 by more than 10 %

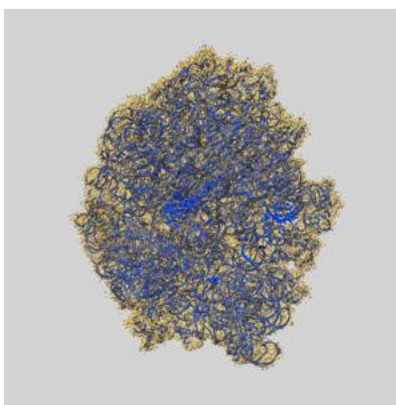
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24132 and PDB model 7N2C. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

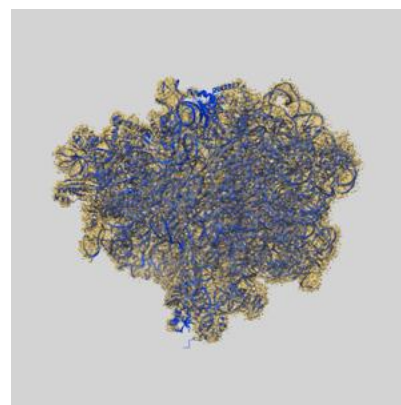
### 9.1 Map-model overlay [i](#)



X



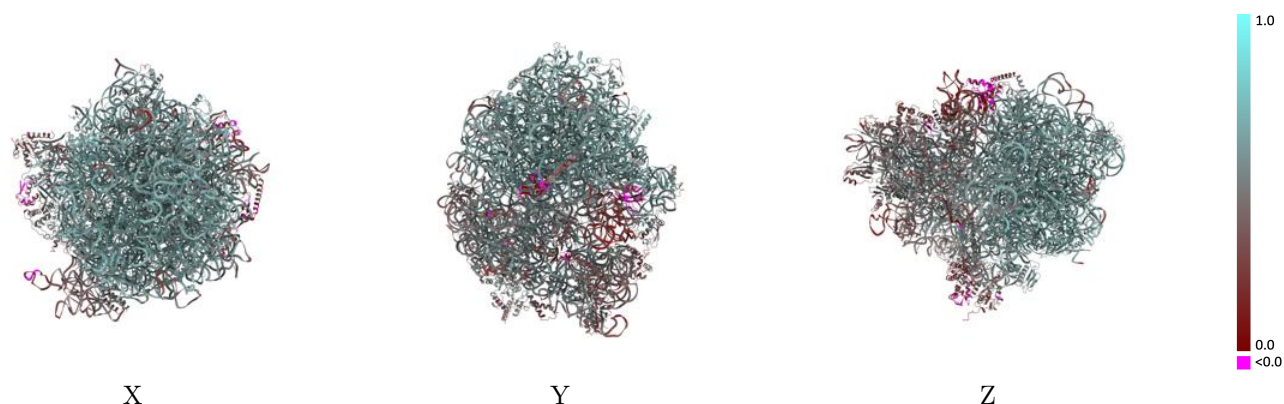
Y



Z

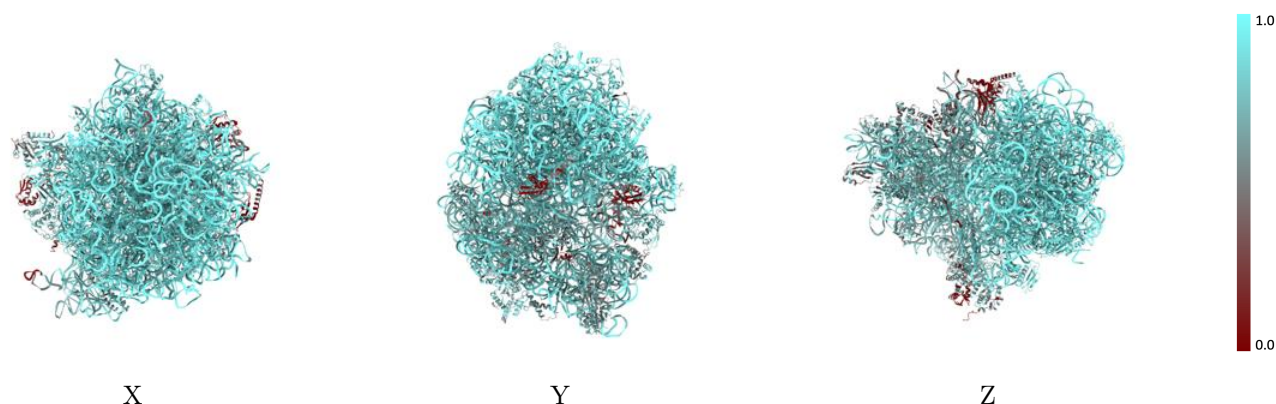
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



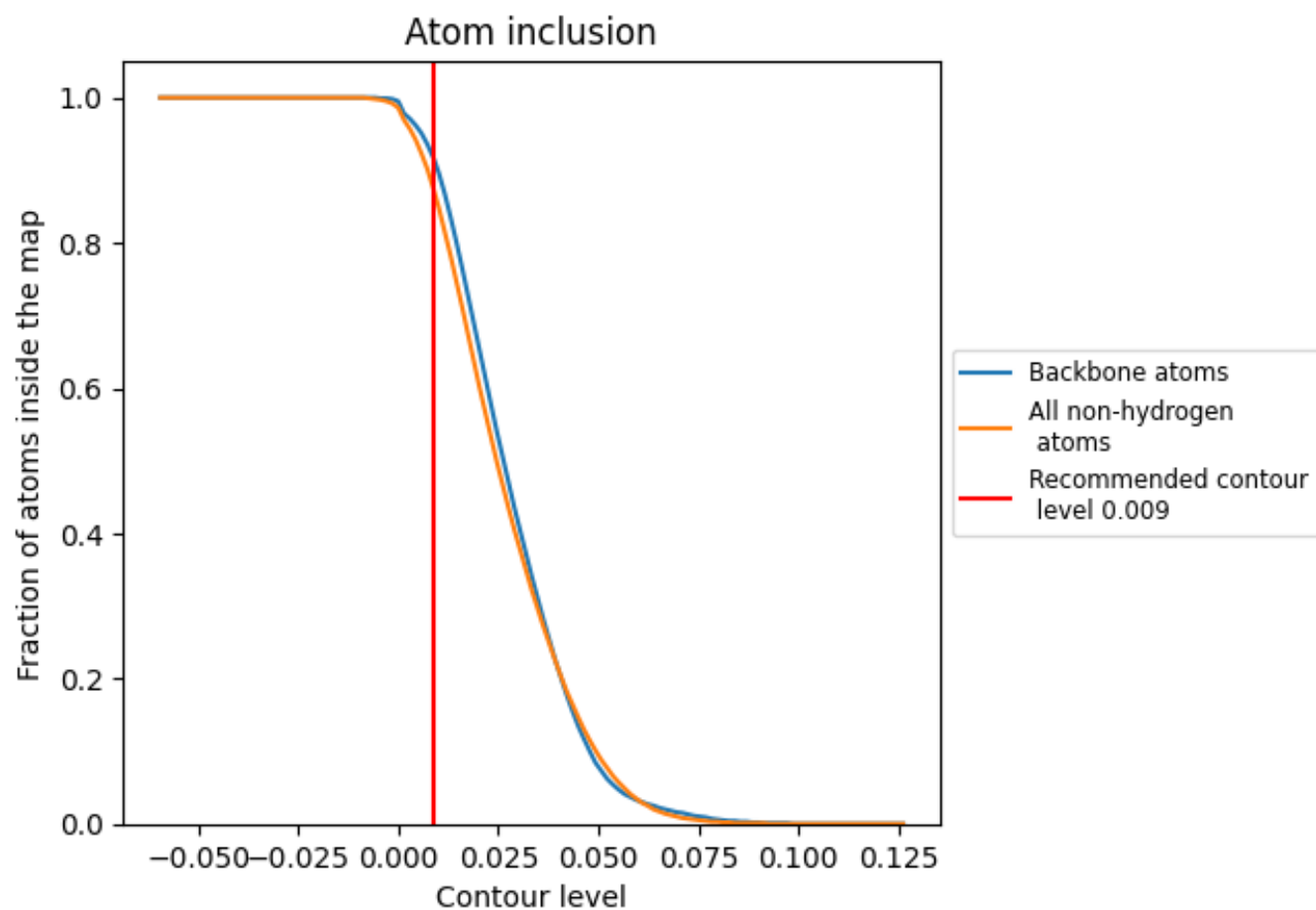
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 91% of all backbone atoms, 87% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8700	 0.5330
16	 0.8780	 0.4890
23	 0.9590	 0.5920
5	 0.9630	 0.5780
Dt	 0.8430	 0.4490
EF	 0.7550	 0.4750
LA	 0.1540	 0.1230
LB	 0.9220	 0.6190
LC	 0.9350	 0.6220
LD	 0.8990	 0.5890
LE	 0.7650	 0.4910
LF	 0.8420	 0.5400
LG	 0.0910	 0.0660
LI	 0.3390	 0.2440
LJ	 0.5900	 0.3430
LK	 0.4850	 0.2890
LM	 0.9370	 0.6240
LN	 0.9150	 0.6140
LO	 0.9070	 0.6040
LP	 0.9270	 0.6130
LQ	 0.9580	 0.6330
LR	 0.8520	 0.5540
LS	 0.9090	 0.5930
LT	 0.9330	 0.6270
LU	 0.9130	 0.6020
LV	 0.9160	 0.6150
LW	 0.8820	 0.5900
LX	 0.9060	 0.5750
LY	 0.8960	 0.5750
La	 0.8720	 0.6080
Lb	 0.9320	 0.6070
Lc	 0.8610	 0.5440
Ld	 0.9450	 0.6140
Le	 0.6760	 0.3740
Lf	 0.9280	 0.6290



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
Lg	 0.8480	 0.5720
Lh	 0.9320	 0.6330
Li	 0.9370	 0.6280
Lj	 0.8800	 0.6010
Pp	 0.6790	 0.4830
Pt	 0.8470	 0.4840
SB	 0.6980	 0.4340
SC	 0.7520	 0.4810
SD	 0.6430	 0.3970
SE	 0.7880	 0.5010
SF	 0.5830	 0.3690
SG	 0.4650	 0.2960
SH	 0.7810	 0.5200
SI	 0.6330	 0.4330
SJ	 0.5710	 0.3950
SK	 0.5850	 0.4270
SL	 0.8040	 0.5380
SM	 0.6660	 0.3980
SN	 0.7130	 0.4730
SO	 0.7360	 0.4690
SP	 0.7180	 0.4760
SQ	 0.7180	 0.4660
SR	 0.5920	 0.4250
SS	 0.7120	 0.4760
ST	 0.7190	 0.4460
SU	 0.5800	 0.3660
mR	 0.6270	 0.3910