



wwPDB EM Validation Summary Report ⓘ

Sep 16, 2026 – 03:35 PM EDT

PDB ID : 7N2C / pdb_00007n2c
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

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:

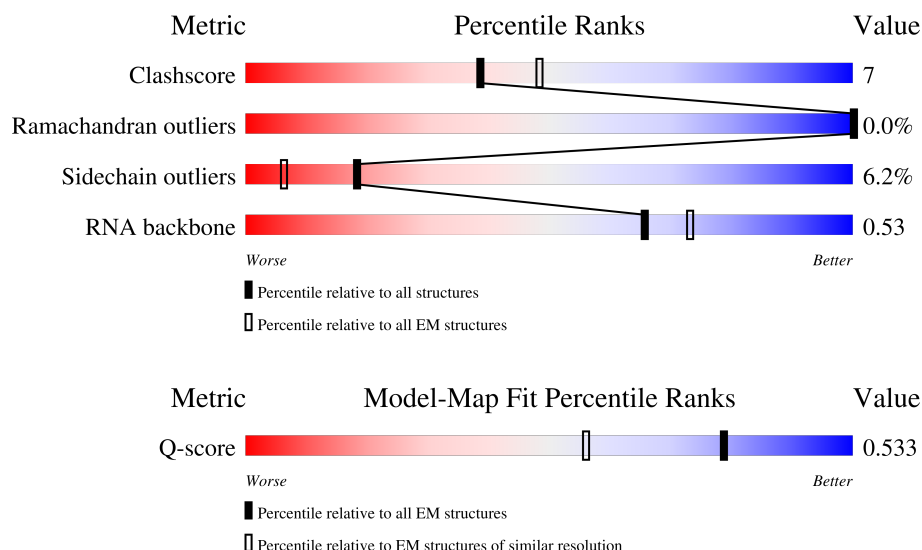
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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)	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	10355 (2.22 - 3.22)

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	

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Mol	Chain	Length	Quality of chain
4	SD	206	
5	SE	167	
6	SF	135	
7	SG	179	
8	SH	130	
9	SI	130	
10	SJ	103	
11	SK	129	
12	SL	124	
13	SM	118	
14	SN	101	
15	SO	89	
16	SP	82	
17	SQ	84	
18	SR	75	
19	SS	92	
20	ST	87	
21	SU	71	
22	mR	60	
23	23	2904	
24	5	120	
25	LA	234	
26	LB	273	
27	LC	209	
28	LD	201	

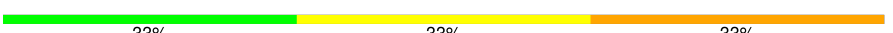
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Mol	Chain	Length	Quality of chain
29	LE	179	
30	LF	177	
31	LG	121	
32	LI	149	
33	LJ	165	
34	LK	142	
35	LM	142	
36	LN	123	
37	LO	144	
38	LP	136	
39	LQ	127	
40	LR	117	
41	LS	115	
42	LT	118	
43	LU	103	
44	LV	110	
45	LW	100	
46	LX	104	
47	LY	94	
48	La	85	
49	Lb	78	
50	Lc	63	
51	Ld	59	
52	Le	70	
53	Lf	57	

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Mol	Chain	Length	Quality of chain
54	Lg	55	
55	Lh	46	
56	Li	65	
57	Lj	38	
58	EF	704	
59	Pp	3	
60	Pt	76	
61	Dt	76	

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		

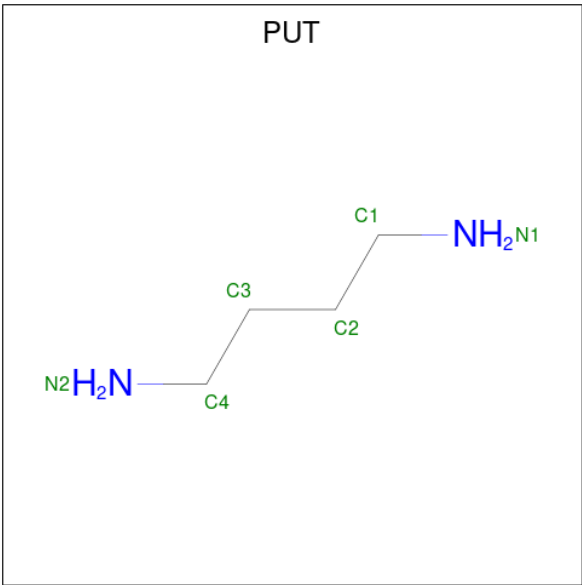
- Molecule 60 is a RNA chain called Chains: Pt.

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-DIAMINOBTANE (CCD ID: PUT) (formula: C₄H₁₂N₂) (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 (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

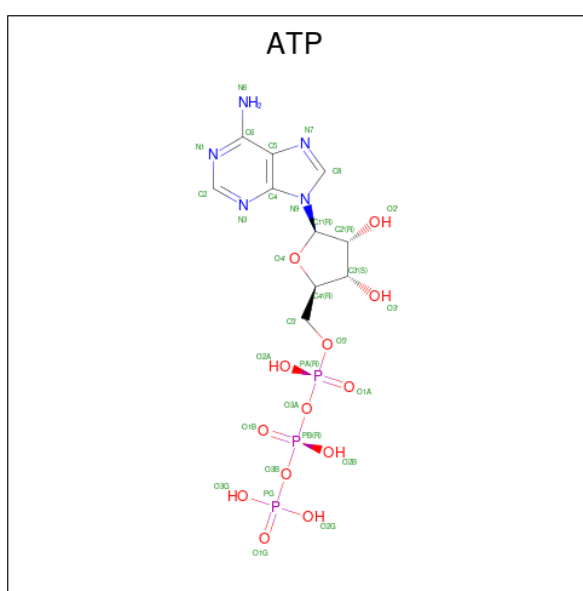
Mol	Chain	Residues	Atoms		AltConf
63	16	40	Total	Mg	0
			40	40	
63	SN	2	Total	Mg	0
			2	2	
63	23	144	Total	Mg	0
			144	144	
63	5	4	Total	Mg	0
			4	4	
63	LB	1	Total	Mg	0
			1	1	
63	LC	1	Total	Mg	0
			1	1	
63	LD	1	Total	Mg	0
			1	1	
63	LQ	1	Total	Mg	0
			1	1	
63	LW	1	Total	Mg	0
			1	1	
63	Lf	1	Total	Mg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

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by

depositor).

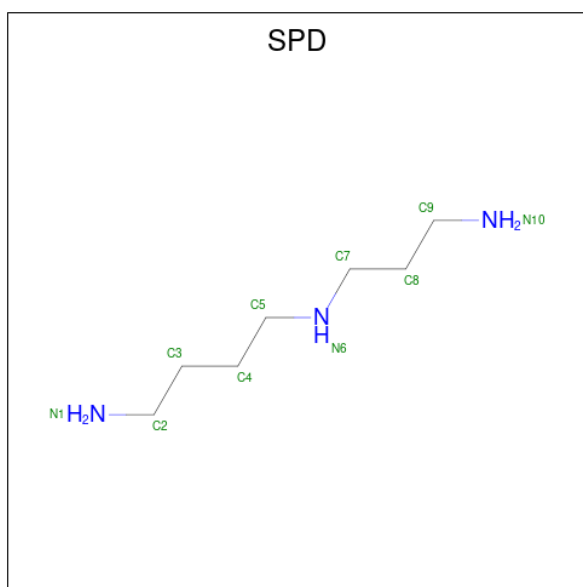
Mol	Chain	Residues	Atoms		AltConf
64	SB	1	Total	Zn	0
			1	1	
64	Le	1	Total	Zn	0
			1	1	
64	Lj	1	Total	Zn	0
			1	1	

- Molecule 65 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



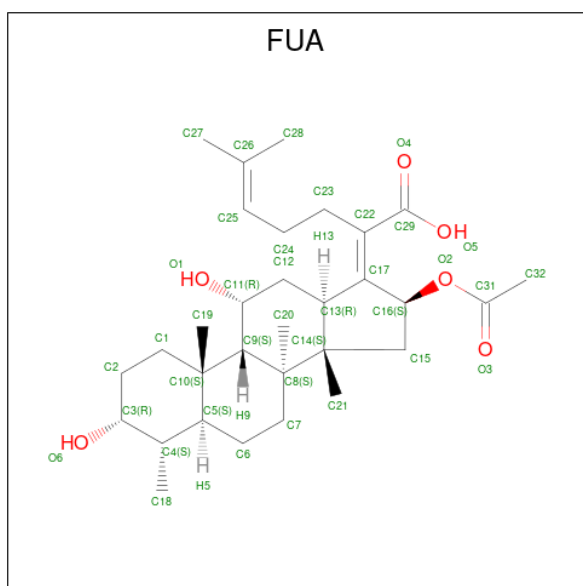
Mol	Chain	Residues	Atoms					AltConf
65	23	1	Total	C	N	O	P	0
			31	10	5	13	3	
65	23	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 66 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



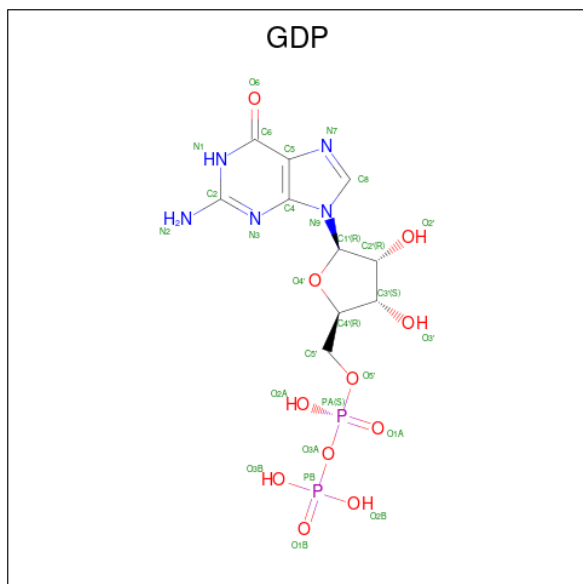
Mol	Chain	Residues	Atoms			AltConf
66	23	1	Total	C	N	0
			10	7	3	
66	23	1	Total	C	N	0
			10	7	3	
66	23	1	Total	C	N	0
			10	7	3	

- Molecule 67 is FUSIDIC ACID (CCD ID: 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	

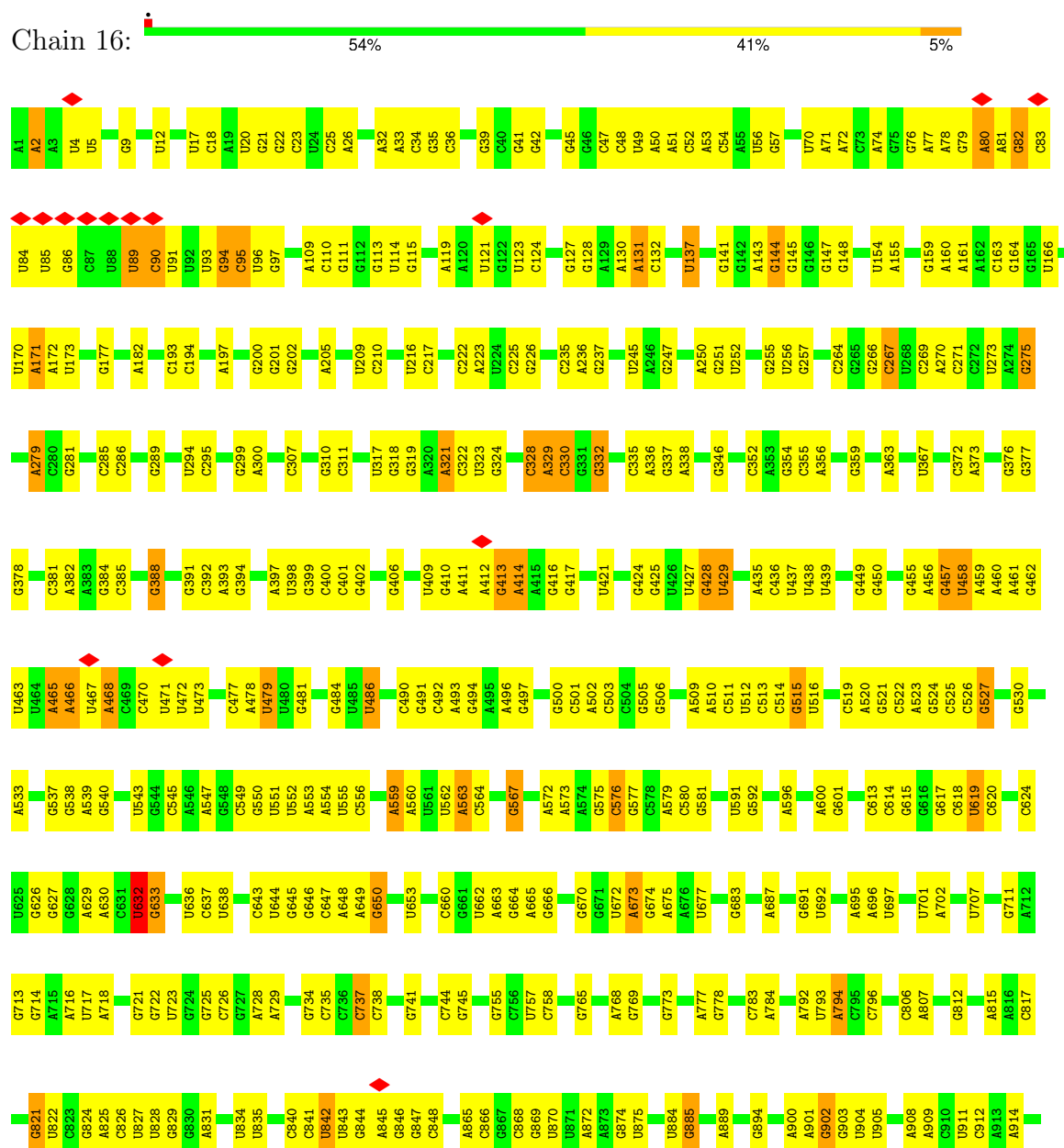
- Molecule 68 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



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

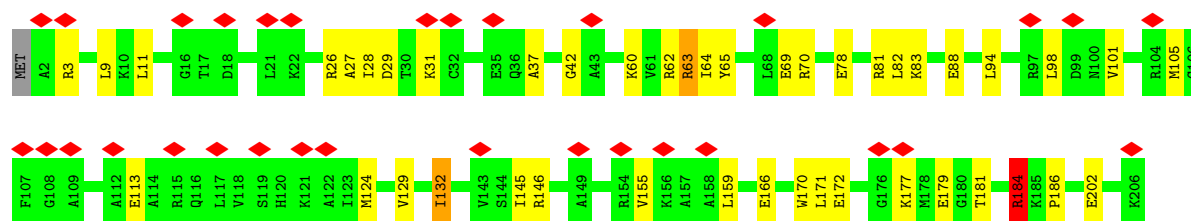




VAL
GLU
GLN
PRO
GLU
LYS
PRO
ALA
ALA
GLN
PRO
LYS
LYS
GLN
GLN
ARG
LYS
GLY
ARG
LYS

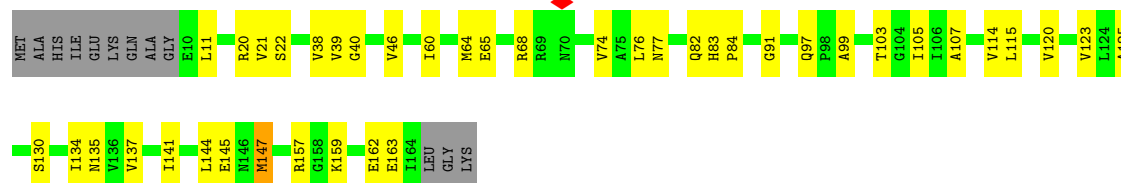
• Molecule 4: 30S ribosomal protein S4

Chain SD: 15% 78% 20%



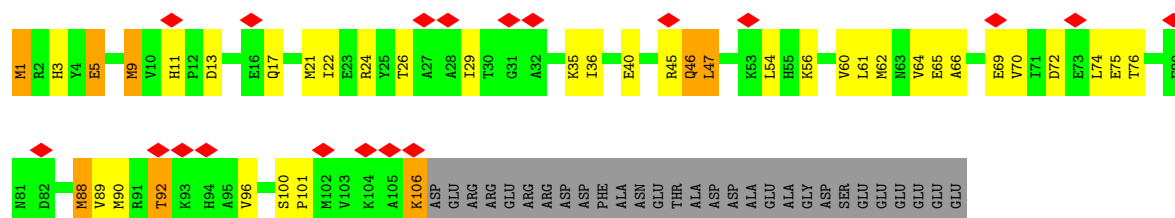
• Molecule 5: 30S ribosomal protein S5

Chain SE: 68% 24% 7%



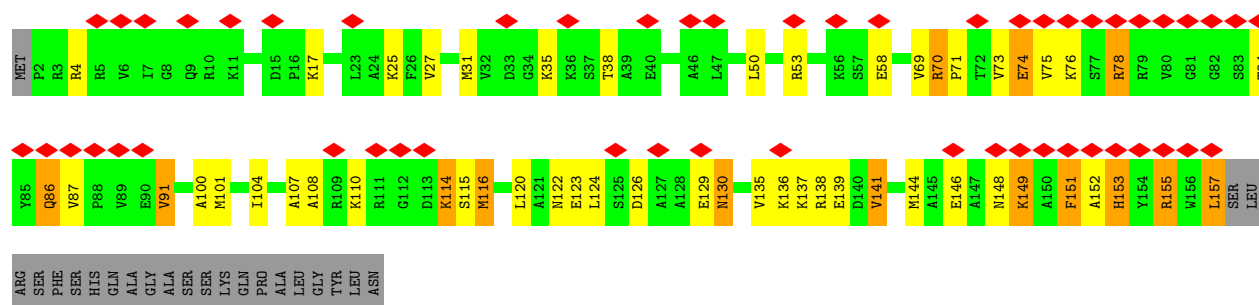
• Molecule 6: 30S ribosomal protein S6

Chain SF: 14% 49% 24% 6% 21%



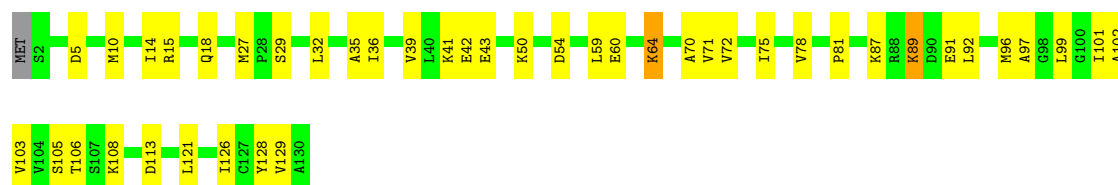
• Molecule 7: 30S ribosomal protein S7

Chain SG: 29% 58% 22% 8% 13%



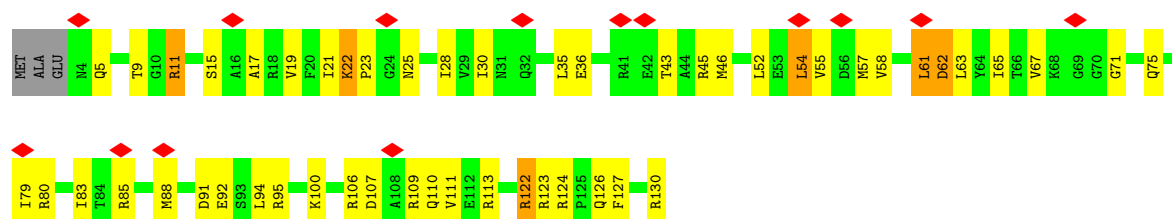
• Molecule 8: 30S ribosomal protein S8

Chain SH:  66% 32% ..



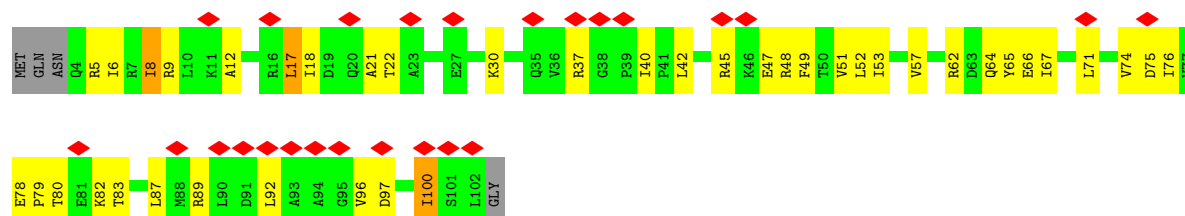
• Molecule 9: 30S ribosomal protein S9

Chain SI:  11% 58% 35% 5% .



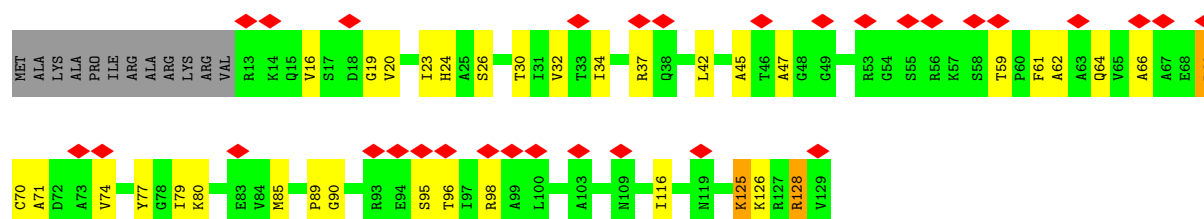
• Molecule 10: 30S ribosomal protein S10

Chain SJ:  24% 56% 37% . .



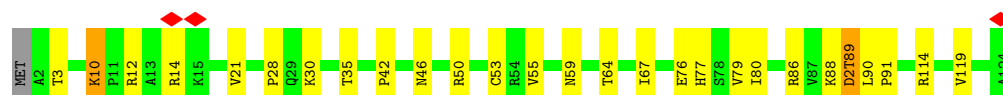
• Molecule 11: 30S ribosomal protein S11

Chain SK:  24% 64% 25% 9% .

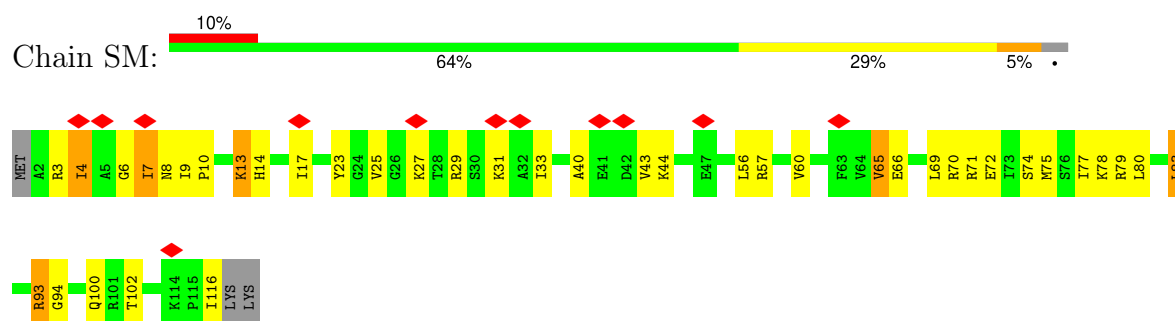


• Molecule 12: 30S ribosomal protein S12

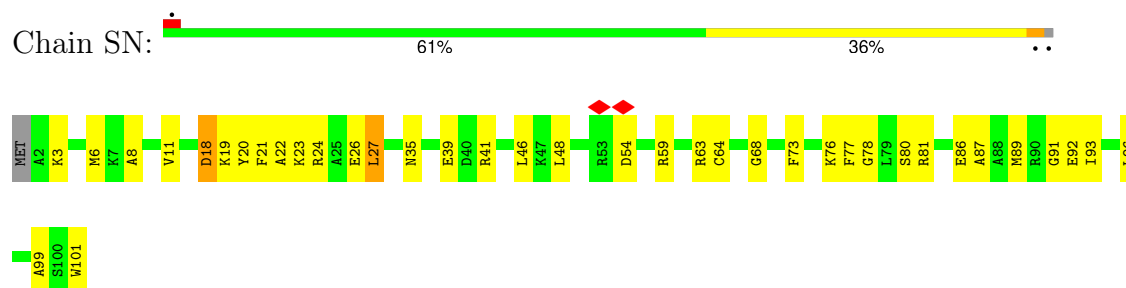
Chain SL:  77% 20% ..



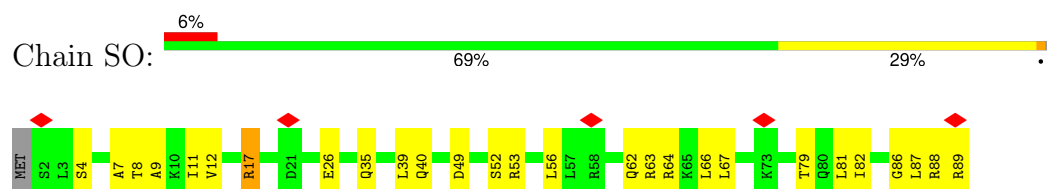
• Molecule 13: 30S ribosomal protein S13



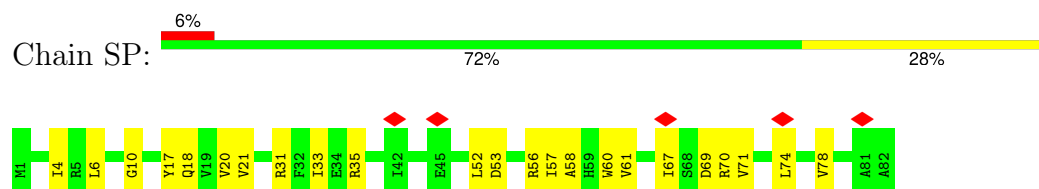
• Molecule 14: 30S ribosomal protein S14



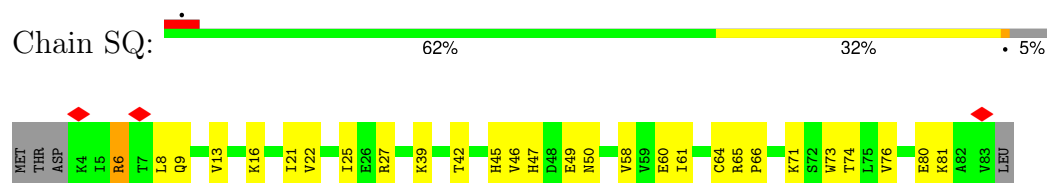
• Molecule 15: 30S ribosomal protein S15



• Molecule 16: 30S ribosomal protein S16

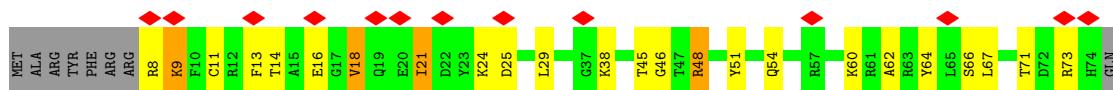


• Molecule 17: 30S ribosomal protein S17

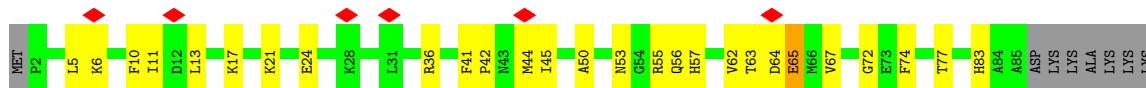


• Molecule 18: 30S ribosomal protein S18

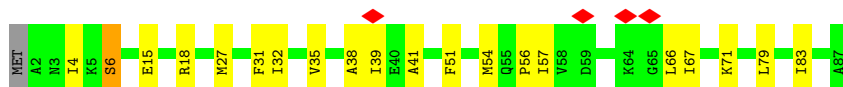
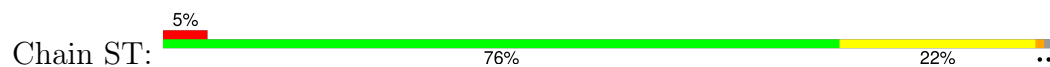




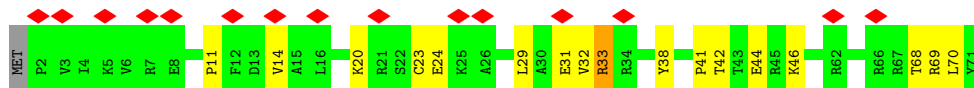
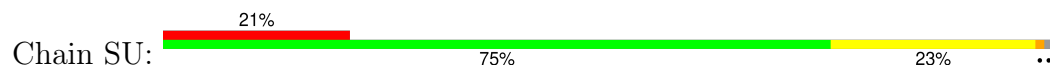
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



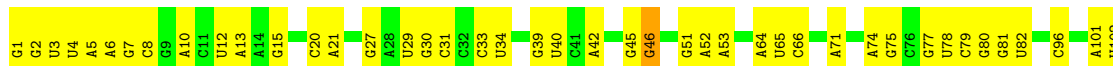
- Molecule 21: 30S ribosomal protein S21



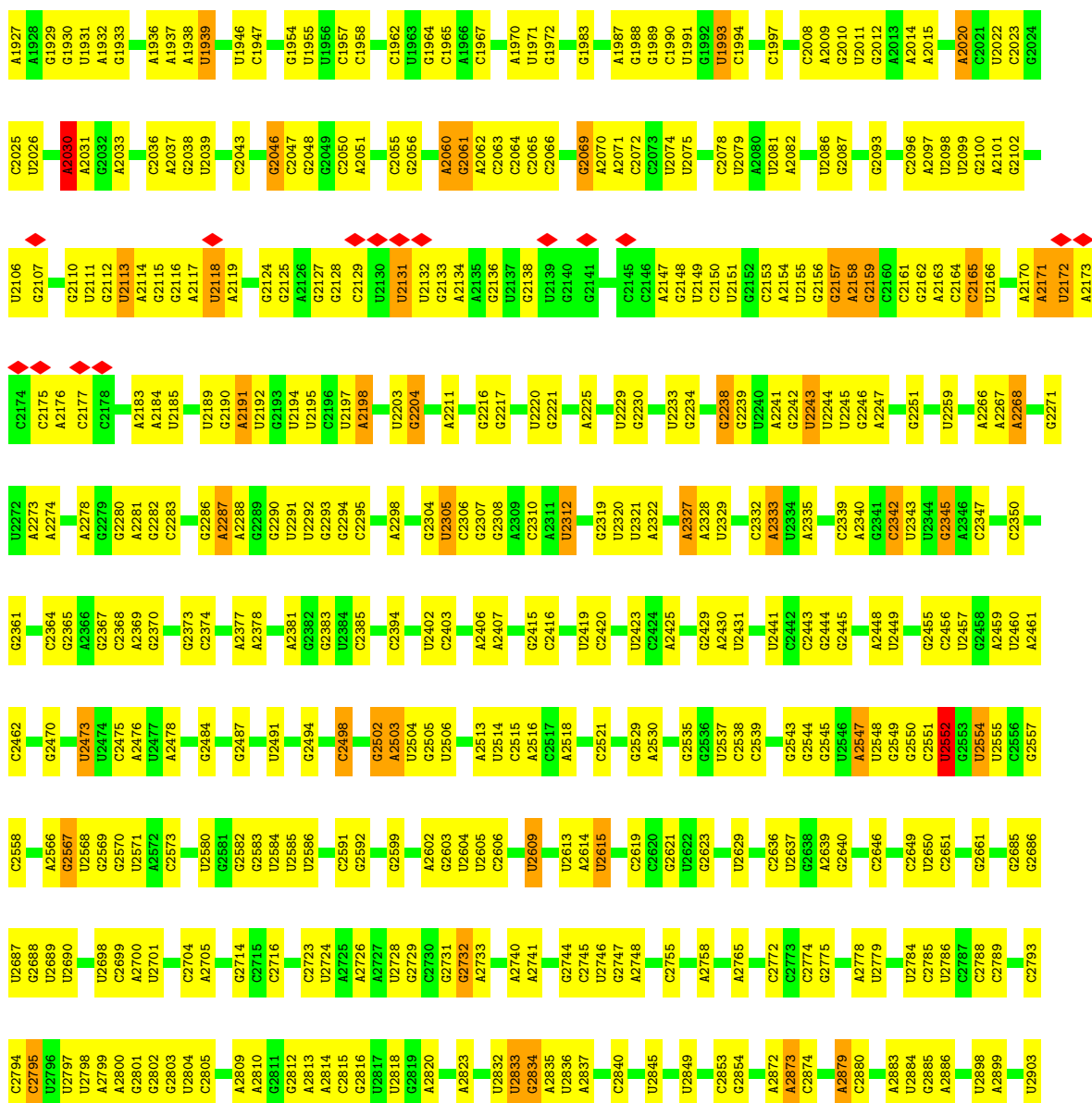
- Molecule 22: Chains: mR



- Molecule 23: 23S rRNA



C1838	A1739	U1405	U1282	A1174	G1087	A1000	A892	C814	G597	G494
G1842	C1740	U1406	A1286	A1175	A1088	A1001	C893	C817	U598	U499
C1843	C1741	G1410	A1287	U1176	A1089	A1009	U894	G600	A599	A504
C1844	G1742	U1411	G1288	U1177	A1090	A1010	U895	A819	A505	A505
G1845	A1743	U1412	G1289	C1178	G1091	A1011	A896	A603	A608	C509
G1846	A1744	A1413	G1290	U1179	U1094	G1011	C897	G822	A609	C510
A1847	U1745	G1416	C1291	U1180	U1097	U1012	C903	C823	U615	A513
A1848	U1747	U1647	C1292	U1181	U1097	C1013	G904	U827	U615	A513
G1849	C1748	U1183	G1295	U1182	U1101	A1014	U906	A829	A627	U521
A1853	G1756	U1184	C1297	U1184	C1102	G1017	G907	G830	A631	A522
A1854	U1649	U1298	C1298	G1195	U1105	U1018	C908	A833	A632	A528
G1857	A1665	G1428	G1299	C1196	G1106	U1019	A909	G834	A633	A529
A1858	U1666	G1429	G1300	U1197	G1107	A1020	A910	G834	A634	G530
A1858	G1667	A1430	A1301	U1198	G1107	G1021	A911	G843	C635	C531
G1862	G1667	A1535	A1302	U1199	G1110	G1022	C912	A844	C636	A532
A1866	A1672	C1432	C1306	U1200	G1111	U1023	A917	A845	A637	A538
G1867	G1673	A1433	A1307	C1201	G1112	G1026	G926	U846	G638	G539
C1868	G1674	G1435	A1308	G1212	G1113	A1027	A927	U847	U639	A547
C1868	C1675	G1436	C1315	U1219	G1114	G1028	U928	C851	U641	G548
G1869	A1676	C1437	U1316	U1220	G1115	A1029	G930	C852	A644	G549
C1870	A1677	A1438	G1317	U1221	G1116	G1033	U931	G856	U654	U554
A1871	A1678	U1439	U1318	G1222	G1117	U1034	U932	G857	G645	G555
A1872	G1679	U1440	U1319	U1223	G1118	G1035	U933	G858	G647	U558
A1873	G1680	U1441	A1321	A1226	G1119	G1036	U934	G859	A654	G559
C1874	G1681	U1442	A1322	G1227	G1120	A1045	U935	G860	A655	A563
G1875	U1682	U1443	C1323	U1228	G1121	G1047	U936	G861	G656	G567
A1876	U1683	G1444	G1324	U1229	G1122	A1050	U937	G862	U658	U566
C1881	U1684	C1445	U1325	U1230	G1123	G1051	A939	G863	A668	U567
U1882	C1685	U1446	U1326	G1231	G1124	A1054	A940	G864	G669	U568
A1885	U1686	G1447	U1327	U1232	G1125	G1055	A941	G869	A670	U569
A1889	A1689	G1448	A1328	G1233	G1126	G1056	C946	U870	C671	U573
A1900	A1690	U1449	U1329	U1234	G1127	U1059	C947	U871	G674	A574
A1901	G1691	G1450	U1330	U1235	G1128	U1060	C948	U872	A675	A575
G1906	U1692	U1451	A1331	G1236	G1129	A1067	G949	G875	C680	G579
G1907	A1693	G1452	C1332	U1237	G1130	A1068	G950	G876	G681	U580
U1910	U1694	U1453	U1333	G1238	G1131	G1069	U951	G877	G682	C581
U1911	A1695	U1454	A1334	U1239	G1132	A1070	U952	C796	A685	A586
A1912	U1696	U1455	U1335	G1240	G1133	C1076	A953	G797	U686	C587
A1913	C1704	U1456	G1336	U1241	G1134	A1077	A954	G801	U588	U588
3TD1915	C1705	A1457	U1337	U1242	G1135	U1078	A955	U884	A689	U589
A1916	C1706	U1458	A1338	U1243	G1136	C1079	A956	G805	G690	A590
U1917	G1707	U1459	U1339	U1244	G1137	A1080	G957	G806	A699	U591
A1918	C1708	U1460	A1340	U1245	G1138	U1083	U970	G809	G700	U593
C1830	U1709	U1461	U1341	G1250	G1139	A1084	A980	U810	G703	U594
C1831	G1710	U1462	A1342	U1251	G1140	U1085	A981	C812	U703	C595
C1832	A1711	U1463	U1343	U1252	G1141	A1086	A982	C813	G704	U596
U1919	G1715	U1464	A1344	U1253	G1142	C1076	A983	C814		
C1920	U1716	U1465	U1345	U1254	G1143	A1077	A984	U811		
G1921	G1717	U1466	U1346	U1255	G1144	U1078	A985	C812		
	U1720	U1467	A1347	U1256	G1145	C1079	A986	C813		
	G1721	U1468	U1348	U1257	G1146	A1080	A987	C814		
	U1721	U1469	A1349	U1258	G1147	U1083	A988	C815		
	C1727	U1470	U1350	U1259	G1148	U1084	A989	C816		
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	U1730	U1472	U1352	U1261	G1150	U1086	A991	C818		
	G1731	U1473	A1353	U1262	G1151	U1087	A992	C819		
	U1736	U1474	U1354	U1263	G1152	U1088	A993	C820		
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	G1738	U1476	U1356	U1265	G1154	U1090	A995	C822		
		U1477	U1357	U1266	G1155	U1091	A996	C823		
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		U1479	U1359	U1268	G1157	U1093	A998	C825		
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		U1483	U1363	U1272	G1161	U1097	A1002	C829		
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		U1487	U1367	U1276	G1165	U1101	A1006	C833		
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		U1497	U1377	U1286	G1175	U1111	A1016	C843		
		U1498	U1378	U1287	G1176	U1112	A1017	C844		
		U1499	U1379	U1288	G1177	U1113	A1018	C845		
		U1500	U1380	U1289	G1178	U1114	A1019	C846		
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		U1505	U1385	U1294	G1183	U1119	A1024	C851		
		U1506	U1386	U1295	G1184	U1120	A1025	C852		
		U1507	U1387	U1296	G1185	U1121	A1026	C853		
		U1508	U1388	U1297	G1186	U1122	A1027	C854		
		U1509	U1389	U1298	G1187	U1123	A1028	C855		
		U1510	U1390	U1299	G1188	U1124	A1029	C856		
		U1511	U1391	U1300	G1189	U1125	A1030	C857		
		U1512	U1392	U1301	G1190	U1126	A1031	C858		
		U1513	U1393	U1302	G1191	U1127	A1032	C859		
		U1514	U1394	U1303	G1192	U1128	A1033	C860		
		U1515	U1395	U1304	G1193	U1129	A1034	C861		
		U1516	U1396	U1305	G1194	U1130	A1035	C862		
		U1517	U1397	U1306	G1195	U1131	A1036	C863		
		U1518	U1398	U1307	G1196	U1132	A1037	C864		
		U1519	U1399	U1308	G1197	U1133	A1038	C865		
		U1520	U1400	U1309	G1198	U1134	A1039	C866		
		U1521	U1401	U1310	G1199	U1135	A1040	C867		
		U1522	U1402	U1311	G1200	U1136	A1041	C868		
		U1523	U1403	U1312	G1201	U1137	A1042	C869		
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		U1525	U1405	U1314	G1203	U1139	A1044	C871		
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		U1531	U1411	U1320	G1209	U1145	A1050	C877		
		U1532	U1412	U1321	G1210	U1146	A1051	C878		
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		U1534	U1414	U1323	G1212	U1148	A1053	C880		
		U1535	U1415	U1324	G1213	U1149	A1054	C881		
		U1536	U1416	U1325	G1214	U1150	A1055	C882		
		U1537	U1417	U1326	G1215	U1151	A1056	C883		
		U1538	U1418	U1327	G1216	U1152	A1057	C884		
		U1539	U1419	U1328	G1217	U1153	A1058	C885		
		U1540	U1420	U1329	G1218	U1154	A1059	C886		
		U1541	U1421	U1330	G1219	U1155	A1060	C887		
		U1542	U1422	U1331	G1220	U1156	A1061	C888		
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		U1544	U1424	U1333	G1222	U1158	A1063	C890		
		U1545	U1425	U1334	G1223	U1159	A1064	C891		
		U1546	U1426	U1335	G1224	U1160	A1065	C892		
		U1547	U1427	U1336	G1225	U1161	A1066	C893		
		U1548	U1428	U1337	G1226	U1162	A1067	C894		
		U1549	U1429	U1338	G1227	U1163	A1068	C895		
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• Molecule 24: 5S rRNA

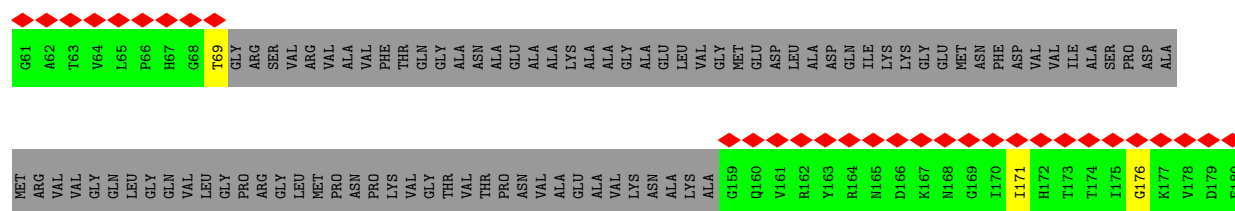
Chain 5: 72% 27%



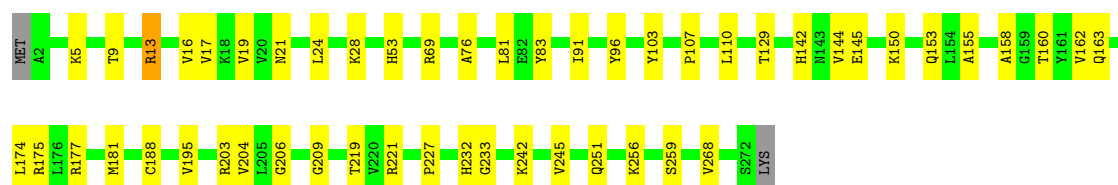
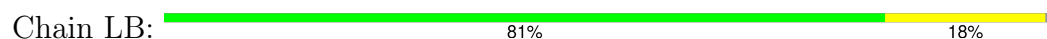
• Molecule 25: 50S ribosomal protein L1

Chain LA: 51% 38% 18% 43%

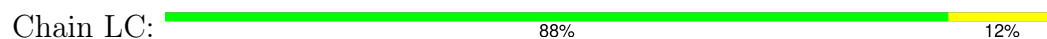




• Molecule 26: 50S ribosomal protein L2



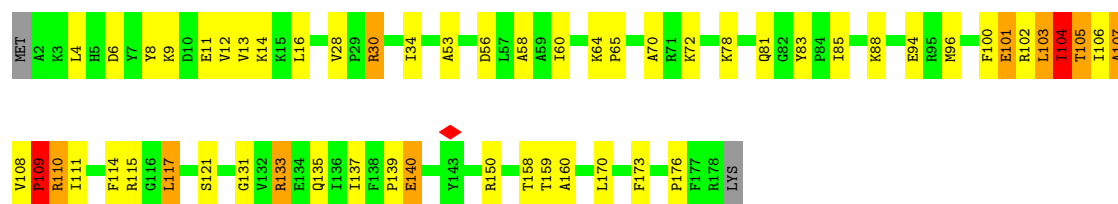
• Molecule 27: 50S ribosomal protein L3



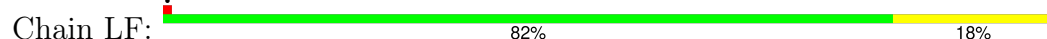
• Molecule 28: 50S ribosomal protein L4

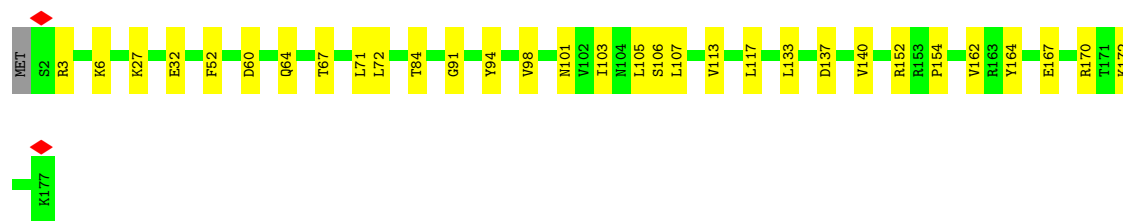


• Molecule 29: 50S ribosomal protein L5

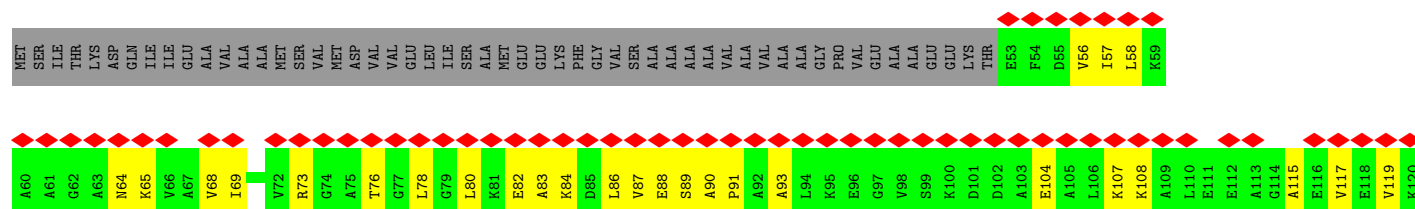
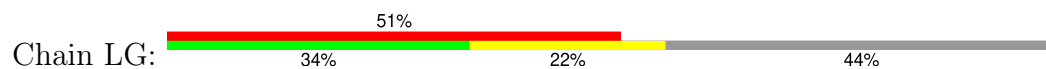


• Molecule 30: 50S ribosomal protein L6

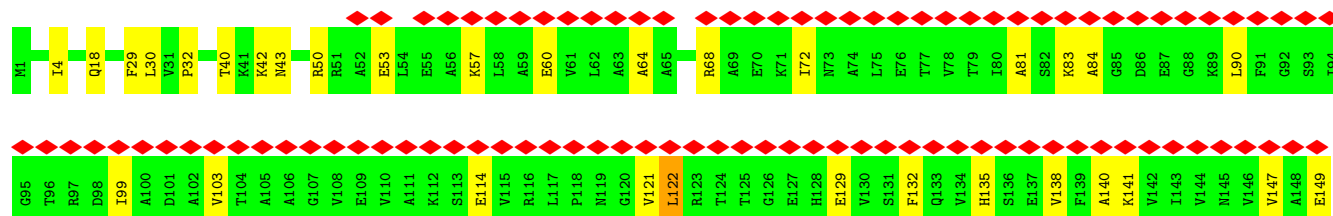
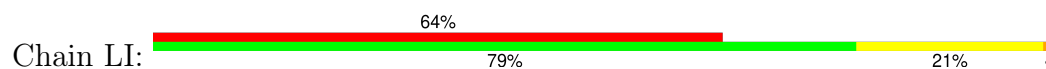




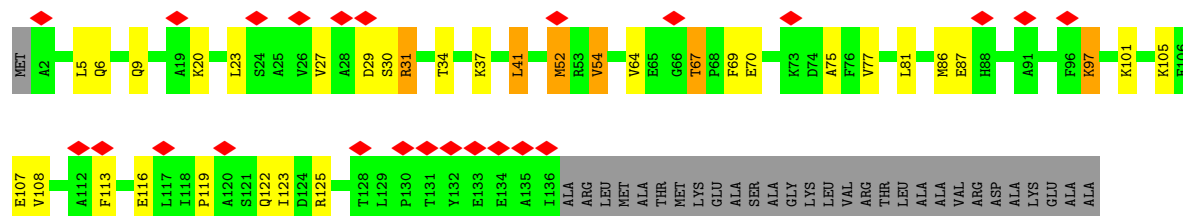
- Molecule 31: 50S ribosomal protein L7/L12

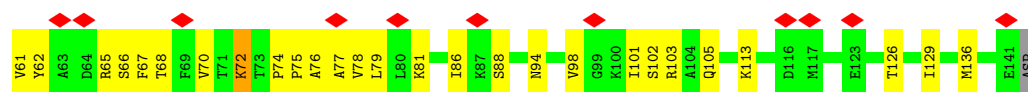


- Molecule 32: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L10





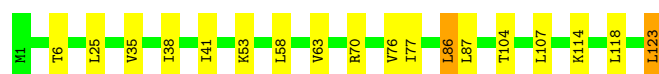
- Molecule 35: 50S ribosomal protein L13

Chain LM: 83% 17%



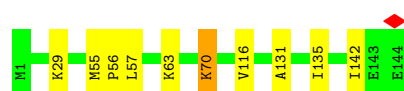
- Molecule 36: 50S ribosomal protein L14

Chain LN: 85% 13%



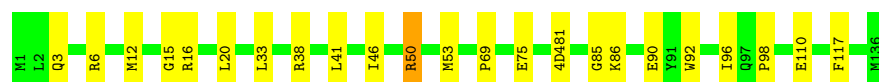
- Molecule 37: 50S ribosomal protein L15

Chain LO: 93% 6%



- Molecule 38: 50S ribosomal protein L16

Chain LP: 83% 16%



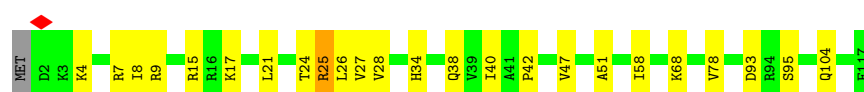
- Molecule 39: 50S ribosomal protein L17

Chain LQ: 84% 10% 6%



- Molecule 40: 50S ribosomal protein L18

Chain LR: 79% 20%



- Molecule 41: 50S ribosomal protein L19

Chain LS:  78% 21%



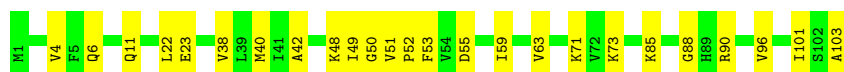
- Molecule 42: 50S ribosomal protein L20

Chain LT:  85% 13%



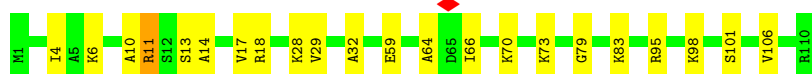
- Molecule 43: 50S ribosomal protein L21

Chain LU:  76% 24%



- Molecule 44: 50S ribosomal protein L22

Chain LV:  80% 19%



- Molecule 45: 50S ribosomal protein L23

Chain LW:  71% 22% 7%



- Molecule 46: 50S ribosomal protein L24

Chain LX:  88% 10%

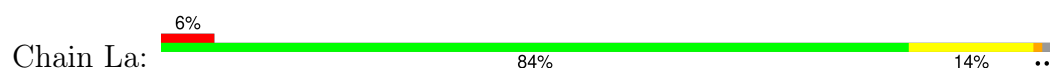


- Molecule 47: 50S ribosomal protein L25

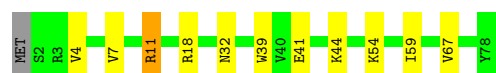
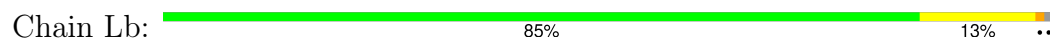
Chain LY:  83% 15%



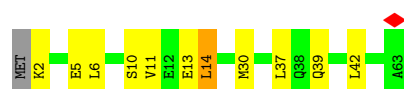
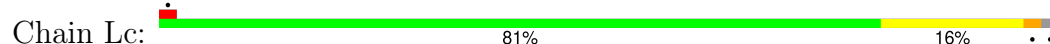
- Molecule 48: 50S ribosomal protein L27



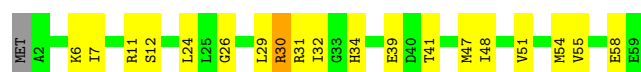
- Molecule 49: 50S ribosomal protein L28



- Molecule 50: 50S ribosomal protein L29



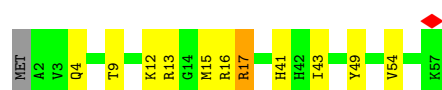
- Molecule 51: 50S ribosomal protein L30



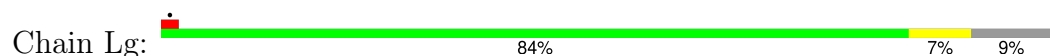
- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



- Molecule 54: 50S ribosomal protein L33



- Molecule 55: 50S ribosomal protein L34

Chain Lh:  74% 26%



- Molecule 56: 50S ribosomal protein L35

Chain Li:  88% 11%



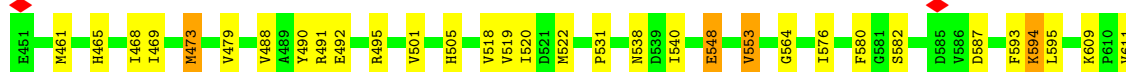
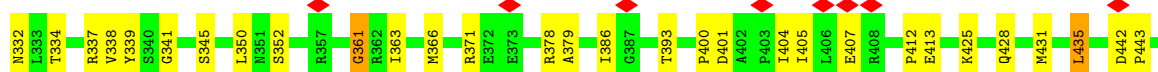
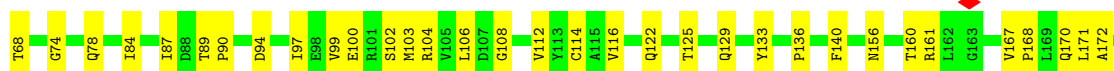
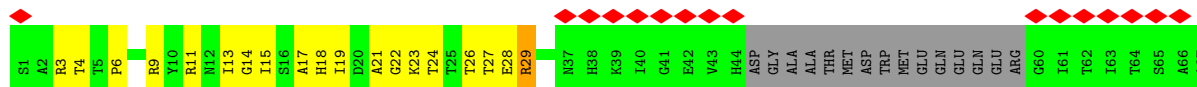
- Molecule 57: 50S ribosomal protein L36

Chain Lj:  87% 11%

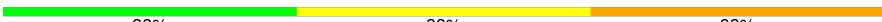


- Molecule 58: Elongation factor G

Chain EF:  6% 75% 21%

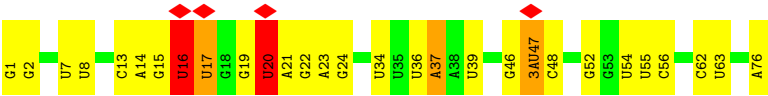


- Molecule 59: Polypeptide

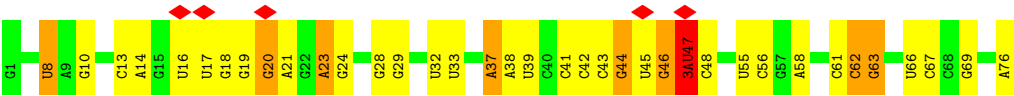
Chain Pp:  33% 33% 33%



• 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: OMG, OMC, T6A, MG, 2MG, 3TD, MIA, 4OC, 4D4, 2MA, U8U, SPD, UR3, D2T, PUT, FUA, ZN, 6MZ, H2U, ATP, 3AU, 4SU, PSU, 1MG, G7M, MA6, 5MU, GDP, OMU, 5MC

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	0.28	0/36619	0.41	1/57122 (0.0%)
2	SB	0.62	0/1800	0.90	3/2425 (0.1%)
3	SC	0.35	0/1651	0.56	0/2225
4	SD	0.39	0/1665	0.65	0/2227
5	SE	0.47	0/1157	0.68	0/1557
6	SF	0.69	0/881	0.90	0/1189
7	SG	0.82	0/1253	1.11	5/1681 (0.3%)
8	SH	0.39	0/989	0.66	0/1326
9	SI	0.59	0/1034	0.87	1/1375 (0.1%)
10	SJ	0.82	0/805	1.16	2/1089 (0.2%)
11	SK	0.32	0/893	0.52	0/1205
12	SL	0.64	0/960	0.88	0/1286
13	SM	0.72	1/900 (0.1%)	1.22	5/1204 (0.4%)
14	SN	0.73	0/817	1.02	2/1088 (0.2%)
15	SO	0.38	0/722	0.63	1/964 (0.1%)
16	SP	0.45	0/659	0.75	0/884
17	SQ	0.43	0/657	0.61	0/881
18	SR	0.67	0/564	0.98	0/756
19	SS	0.45	0/685	0.66	0/922
20	ST	0.40	0/676	0.73	0/895
21	SU	0.34	0/597	0.56	0/792
22	mR	0.34	0/280	0.49	0/433
23	23	0.25	1/69239 (0.0%)	0.34	5/108014 (0.0%)
24	5	0.29	0/2873	0.41	1/4478 (0.0%)
25	LA	0.50	0/1033	0.74	0/1387
26	LB	0.34	1/2121 (0.0%)	0.52	1/2852 (0.0%)
27	LC	0.30	0/1586	0.44	0/2134
28	LD	0.22	0/1571	0.37	0/2113
29	LE	0.56	3/1434 (0.2%)	0.90	8/1926 (0.4%)
30	LF	0.24	0/1343	0.45	0/1816
31	LG	0.37	0/488	0.75	1/652 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LI	0.30	0/1122	0.50	0/1515
33	LJ	0.66	0/1037	0.97	1/1400 (0.1%)
34	LK	0.79	0/987	0.99	0/1334
35	LM	0.22	0/1152	0.34	0/1551
36	LN	0.38	0/956	0.59	0/1279
37	LO	0.36	0/1062	0.55	1/1413 (0.1%)
38	LP	0.37	0/1081	0.57	0/1443
39	LQ	0.27	0/973	0.43	0/1301
40	LR	0.36	0/902	0.64	0/1209
41	LS	0.36	0/929	0.51	0/1242
42	LT	0.33	0/960	0.48	0/1278
43	LU	0.42	0/829	0.64	0/1107
44	LV	0.36	0/864	0.55	0/1156
45	LW	0.28	0/744	0.44	0/994
46	LX	0.24	0/787	0.43	0/1051
47	LY	0.33	0/766	0.54	0/1025
48	La	0.30	0/642	0.46	0/848
49	Lb	0.35	0/635	0.55	0/848
50	Lc	0.37	0/502	0.60	0/667
51	Ld	0.33	0/453	0.54	0/605
52	Le	0.42	0/539	0.63	0/721
53	Lf	0.45	0/450	0.62	0/599
54	Lg	0.20	0/416	0.32	0/554
55	Lh	0.32	0/380	0.52	0/498
56	Li	0.32	0/513	0.50	0/676
57	Lj	0.30	0/303	0.47	0/397
58	EF	0.63	0/5097	0.88	4/6933 (0.1%)
59	Pp	0.31	0/28	1.17	0/34
60	Pt	0.29	0/1600	0.40	0/2486
61	Dt	0.34	1/1654 (0.1%)	0.51	1/2572 (0.0%)
All	All	0.35	7/166315 (0.0%)	0.50	43/247634 (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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	2069	G7M	O3'-P	7.64	1.63	1.56
26	LB	81	LEU	C-N	6.23	1.42	1.33
29	LE	101	GLU	C-O	5.92	1.30	1.24
13	SM	93	ARG	NE-CZ	5.50	1.39	1.33
29	LE	103	LEU	C-O	-5.10	1.18	1.24

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	SM	93	ARG	CB-CG-CD	18.65	154.19	111.30
13	SM	93	ARG	CG-CD-NE	17.59	150.71	112.00
10	SJ	37	ARG	N-CA-C	-13.36	89.09	110.20
29	LE	109	PRO	CA-N-CD	-10.64	97.10	112.00
2	SB	47	VAL	O-C-N	-7.57	114.69	120.07

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	408	0
2	SB	1769	0	1795	38	0
3	SC	1624	0	1696	38	0
4	SD	1643	0	1707	25	0
5	SE	1144	0	1185	21	0
6	SF	862	0	864	21	0
7	SG	1235	0	1286	28	0
8	SH	979	0	1031	28	0
9	SI	1022	0	1070	24	0
10	SJ	795	0	836	22	0
11	SK	877	0	887	23	0
12	SL	957	0	1017	16	0
13	SM	891	0	952	25	0
14	SN	805	0	844	23	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	14	0
19	SS	668	0	693	22	0
20	ST	670	0	719	12	0
21	SU	589	0	629	9	0
22	mR	252	0	128	4	0
23	23	62334	0	31374	614	0
24	5	2570	0	1301	11	0
25	LA	1026	0	1092	30	0
26	LB	2082	0	2154	33	0
27	LC	1565	0	1616	15	0
28	LD	1552	0	1618	17	0
29	LE	1410	0	1444	44	0
30	LF	1323	0	1371	17	0
31	LG	487	0	515	16	0
32	LI	1111	0	1148	20	0
33	LJ	1023	0	1050	16	0
34	LK	973	0	1017	25	0
35	LM	1129	0	1162	14	0
36	LN	947	0	1023	11	0
37	LO	1053	0	1129	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	LP	1075	0	1155	13	0
39	LQ	960	0	1000	8	0
40	LR	892	0	923	12	0
41	LS	917	0	960	13	0
42	LT	947	0	1019	13	0
43	LU	816	0	839	16	0
44	LV	857	0	922	13	0
45	LW	738	0	807	11	0
46	LX	779	0	831	5	0
47	LY	753	0	780	7	0
48	La	634	0	653	11	0
49	Lb	625	0	652	7	0
50	Lc	501	0	531	6	0
51	Ld	449	0	488	13	0
52	Le	529	0	527	12	0
53	Lf	444	0	458	7	0
54	Lg	409	0	440	2	0
55	Lh	377	0	418	9	0
56	Li	504	0	572	4	0
57	Lj	302	0	340	3	0
58	EF	4999	0	4781	89	0
59	Pp	28	0	33	2	0
60	Pt	1636	0	840	10	0
61	Dt	1641	0	843	11	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	1911	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 1911 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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SB	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	35
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%)	158 (84%)	30 (16%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	SC	170/190 (90%)	166 (98%)	4 (2%)	43	70
4	SD	172/173 (99%)	162 (94%)	10 (6%)	18	41
5	SE	118/126 (94%)	110 (93%)	8 (7%)	14	33
6	SF	92/116 (79%)	71 (77%)	21 (23%)	1	2
7	SG	129/147 (88%)	102 (79%)	27 (21%)	1	3
8	SH	104/105 (99%)	99 (95%)	5 (5%)	23	48
9	SI	105/107 (98%)	86 (82%)	19 (18%)	2	4
10	SJ	87/90 (97%)	74 (85%)	13 (15%)	3	7
11	SK	90/99 (91%)	87 (97%)	3 (3%)	33	61
12	SL	102/103 (99%)	91 (89%)	11 (11%)	6	15
13	SM	93/96 (97%)	82 (88%)	11 (12%)	5	12
14	SN	83/84 (99%)	72 (87%)	11 (13%)	4	9
15	SO	76/77 (99%)	72 (95%)	4 (5%)	20	44
16	SP	65/65 (100%)	65 (100%)	0	100	100
17	SQ	74/78 (95%)	69 (93%)	5 (7%)	14	33
18	SR	58/65 (89%)	48 (83%)	10 (17%)	2	5
19	SS	72/79 (91%)	69 (96%)	3 (4%)	26	53
20	ST	65/66 (98%)	62 (95%)	3 (5%)	24	50
21	SU	60/61 (98%)	56 (93%)	4 (7%)	15	34
25	LA	110/181 (61%)	104 (94%)	6 (6%)	19	43
26	LB	216/218 (99%)	211 (98%)	5 (2%)	44	71
27	LC	164/164 (100%)	162 (99%)	2 (1%)	63	82
28	LD	165/165 (100%)	165 (100%)	0	100	100
29	LE	148/150 (99%)	140 (95%)	8 (5%)	20	43
30	LF	137/138 (99%)	137 (100%)	0	100	100
31	LG	47/85 (55%)	45 (96%)	2 (4%)	26	52
32	LI	114/114 (100%)	109 (96%)	5 (4%)	25	51
33	LJ	103/123 (84%)	89 (86%)	14 (14%)	3	8
34	LK	103/110 (94%)	80 (78%)	23 (22%)	1	2
35	LM	116/116 (100%)	115 (99%)	1 (1%)	70	86
36	LN	104/104 (100%)	101 (97%)	3 (3%)	37	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	LO	103/103 (100%)	102 (99%)	1 (1%)	68	85
38	LP	108/108 (100%)	105 (97%)	3 (3%)	38	67
39	LQ	100/103 (97%)	100 (100%)	0	100	100
40	LR	86/87 (99%)	83 (96%)	3 (4%)	32	59
41	LS	99/100 (99%)	96 (97%)	3 (3%)	36	64
42	LT	89/90 (99%)	85 (96%)	4 (4%)	24	50
43	LU	84/84 (100%)	83 (99%)	1 (1%)	63	82
44	LV	93/93 (100%)	90 (97%)	3 (3%)	34	62
45	LW	80/84 (95%)	76 (95%)	4 (5%)	22	46
46	LX	83/85 (98%)	81 (98%)	2 (2%)	43	70
47	LY	78/78 (100%)	74 (95%)	4 (5%)	21	46
48	La	62/63 (98%)	61 (98%)	1 (2%)	55	78
49	Lb	67/68 (98%)	66 (98%)	1 (2%)	57	79
50	Lc	54/55 (98%)	50 (93%)	4 (7%)	13	30
51	Ld	48/49 (98%)	48 (100%)	0	100	100
52	Le	60/62 (97%)	57 (95%)	3 (5%)	22	46
53	Lf	47/48 (98%)	46 (98%)	1 (2%)	47	73
54	Lg	45/49 (92%)	44 (98%)	1 (2%)	45	72
55	Lh	38/38 (100%)	38 (100%)	0	100	100
56	Li	51/52 (98%)	48 (94%)	3 (6%)	18	40
57	Lj	34/34 (100%)	32 (94%)	2 (6%)	18	40
58	EF	480/578 (83%)	451 (94%)	29 (6%)	17	39
59	Pp	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	5522/5908 (94%)	5177 (94%)	345 (6%)	18	38

5 of 345 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	LJ	30	SER
44	LV	11	ARG
33	LJ	67	THR
34	LK	59	ILE
49	Lb	54	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
38	LP	13	HIS
58	EF	465	HIS
47	LY	80	HIS
58	EF	37	ASN
12	SL	73	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1533/1534 (99%)	283 (18%)	14 (0%)
22	mR	11/60 (18%)	3 (27%)	0
23	23	2902/2904 (99%)	485 (16%)	12 (0%)
24	5	119/120 (99%)	19 (15%)	2 (1%)
60	Pt	75/76 (98%)	15 (20%)	0
61	Dt	75/76 (98%)	23 (30%)	0
All	All	4715/4770 (98%)	828 (17%)	28 (0%)

5 of 828 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$
61	PSU	Dt	39	61	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
23	PSU	23	2457	23	18,21,22	1.41	2 (11%)	21,30,33	2.12	5 (23%)
1	2MG	16	1516	1	23,26,27	1.25	3 (13%)	33,38,41	2.20	7 (21%)
23	PSU	23	2580	23	18,21,22	1.41	3 (16%)	21,30,33	2.08	4 (19%)
61	4SU	Dt	8	61	18,21,22	1.96	4 (22%)	25,30,33	2.25	6 (24%)
1	4OC	16	1402	1	20,23,24	0.76	0	25,32,35	0.94	1 (4%)
23	PSU	23	1917	23	18,21,22	6.15	12 (66%)	21,30,33	2.04	5 (23%)
23	5MU	23	747	23	19,22,23	1.40	5 (26%)	27,32,35	2.12	6 (22%)
61	PSU	Dt	32	61	18,21,22	1.37	2 (11%)	21,30,33	2.02	3 (14%)
23	6MZ	23	1618	23	22,25,26	1.45	5 (22%)	29,36,39	2.18	9 (31%)
1	UR3	16	1498	1	19,22,23	0.96	0	26,32,35	1.72	2 (7%)
23	PSU	23	955	23	18,21,22	1.40	3 (16%)	21,30,33	2.12	4 (19%)
23	PSU	23	2604	23	18,21,22	1.50	4 (22%)	21,30,33	2.20	4 (19%)
60	U8U	Pt	34	22,60	20,24,25	1.50	3 (15%)	22,34,37	1.25	3 (13%)
12	D2T	SL	89	12	8,9,10	2.44	1 (12%)	6,11,13	2.91	4 (66%)
23	OMC	23	2498	23,63	19,22,23	0.81	0	25,31,34	0.91	1 (4%)
60	PSU	Pt	55	60	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)
1	MA6	16	1518	1	23,26,27	1.67	5 (21%)	33,38,41	2.22	9 (27%)
60	5MU	Pt	54	60	19,22,23	1.39	6 (31%)	27,32,35	2.08	6 (22%)
1	G7M	16	527	1	23,26,27	2.34	5 (21%)	34,39,42	3.09	12 (35%)
1	PSU	16	516	1	18,21,22	1.42	3 (16%)	21,30,33	2.09	4 (19%)
23	H2U	23	2449	23	18,21,22	1.09	3 (16%)	19,30,33	1.02	1 (5%)
23	1MG	23	745	23	23,26,27	1.21	3 (13%)	33,39,42	1.87	7 (21%)
61	3AU	Dt	47	61	24,28,29	1.02	0	30,40,43	1.60	4 (13%)
23	PSU	23	1911	23	18,21,22	6.15	13 (72%)	21,30,33	1.98	5 (23%)
23	OMG	23	2251	23,60	23,26,27	0.51	0	32,38,41	0.45	0
60	H2U	Pt	17	60	18,21,22	0.97	2 (11%)	19,30,33	0.99	2 (10%)
60	T6A	Pt	37	60	31,34,35	1.42	4 (12%)	43,49,52	1.85	9 (20%)
1	5MC	16	967	1	19,22,23	1.58	3 (15%)	26,32,35	1.21	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	6MZ	23	2030	23	22,25,26	1.44	5 (22%)	29,36,39	2.31	10 (34%)
38	4D4	LP	81	38	9,11,12	2.19	2 (22%)	7,13,15	2.07	3 (42%)
61	G7M	Dt	46	61	23,26,27	2.37	6 (26%)	34,39,42	3.03	10 (29%)
60	H2U	Pt	20	60	18,21,22	1.07	2 (11%)	19,30,33	1.33	4 (21%)
23	2MG	23	2445	23	23,26,27	1.27	4 (17%)	33,38,41	2.23	7 (21%)
23	OMU	23	2552	23	19,22,23	1.24	3 (15%)	25,31,34	1.86	5 (20%)
23	PSU	23	2605	23	18,21,22	1.40	4 (22%)	21,30,33	2.02	4 (19%)
23	2MG	23	1835	23	23,26,27	1.26	4 (17%)	33,38,41	2.22	8 (24%)
23	G7M	23	2069	23	23,26,27	2.42	5 (21%)	34,39,42	3.37	14 (41%)
23	PSU	23	746	23,63	18,21,22	1.40	3 (16%)	21,30,33	1.99	4 (19%)
23	5MU	23	1939	23	19,22,23	1.43	5 (26%)	27,32,35	2.35	6 (22%)
23	2MA	23	2503	23,63	22,25,26	1.48	5 (22%)	32,37,40	2.31	9 (28%)
23	3TD	23	1915	23	19,22,23	1.38	2 (10%)	23,32,35	2.31	4 (17%)
23	PSU	23	2504	23	18,21,22	1.39	3 (16%)	21,30,33	2.09	3 (14%)
60	3AU	Pt	47	60	24,28,29	1.03	0	30,40,43	1.57	5 (16%)
61	MIA	Dt	37	61	28,31,32	2.39	7 (25%)	38,44,47	2.88	15 (39%)
1	MA6	16	1519	1	23,26,27	1.52	3 (13%)	33,38,41	2.22	9 (27%)
60	H2U	Pt	16	60	18,21,22	1.03	2 (11%)	19,30,33	1.09	2 (10%)
61	PSU	Dt	55	61	18,21,22	1.43	2 (11%)	21,30,33	2.20	4 (19%)
60	PSU	Pt	39	60	18,21,22	1.40	2 (11%)	21,30,33	2.01	4 (19%)
1	5MC	16	1407	1	19,22,23	1.59	3 (15%)	26,32,35	1.12	3 (11%)
1	2MG	16	966	1	23,26,27	1.29	4 (17%)	33,38,41	2.21	6 (18%)
23	5MC	23	1962	23	19,22,23	1.54	3 (15%)	26,32,35	1.12	2 (7%)

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	PSU	Dt	39	61	-	2/7/25/26	0/2/2/2
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
1	2MG	16	1516	1	-	0/9/27/28	0/3/3/3
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
61	4SU	Dt	8	61	-	3/7/25/26	0/2/2/2
1	4OC	16	1402	1	-	0/9/29/30	0/2/2/2
23	PSU	23	1917	23	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	5MU	23	747	23	-	0/7/25/26	0/2/2/2
61	PSU	Dt	32	61	-	0/7/25/26	0/2/2/2
23	6MZ	23	1618	23	-	0/9/27/28	0/3/3/3
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
60	U8U	Pt	34	22,60	-	4/10/28/29	0/2/2/2
12	D2T	SL	89	12	-	3/7/12/14	-
23	OMC	23	2498	23,63	-	2/9/27/28	0/2/2/2
60	PSU	Pt	55	60	-	0/7/25/26	0/2/2/2
1	MA6	16	1518	1	-	3/11/29/30	0/3/3/3
60	5MU	Pt	54	60	-	0/7/25/26	0/2/2/2
1	G7M	16	527	1	-	2/7/25/26	0/3/3/3
1	PSU	16	516	1	-	0/7/25/26	0/2/2/2
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2
23	1MG	23	745	23	-	0/7/25/26	0/3/3/3
61	3AU	Dt	47	61	-	9/16/34/35	0/2/2/2
23	PSU	23	1911	23	-	0/7/25/26	0/2/2/2
23	OMG	23	2251	23,60	-	1/9/27/28	0/3/3/3
60	H2U	Pt	17	60	-	3/7/38/39	0/2/2/2
60	T6A	Pt	37	60	-	10/23/41/42	0/3/3/3
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
23	6MZ	23	2030	23	-	2/9/27/28	0/3/3/3
38	4D4	LP	81	38	-	4/11/12/14	-
61	G7M	Dt	46	61	-	1/7/25/26	0/3/3/3
60	H2U	Pt	20	60	-	5/7/38/39	0/2/2/2
23	2MG	23	2445	23	-	1/9/27/28	0/3/3/3
23	OMU	23	2552	23	-	2/9/27/28	0/2/2/2
23	PSU	23	2605	23	-	2/7/25/26	0/2/2/2
23	2MG	23	1835	23	-	0/9/27/28	0/3/3/3
23	G7M	23	2069	23	-	0/7/25/26	0/3/3/3
23	PSU	23	746	23,63	-	4/7/25/26	0/2/2/2
23	5MU	23	1939	23	-	2/7/25/26	0/2/2/2
23	2MA	23	2503	23,63	-	0/7/25/26	0/3/3/3
23	3TD	23	1915	23	-	0/7/25/26	0/2/2/2
23	PSU	23	2504	23	-	2/7/25/26	0/2/2/2
60	3AU	Pt	47	60	-	2/16/34/35	0/2/2/2
61	MIA	Dt	37	61	-	5/15/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	16	1519	1	-	6/11/29/30	0/3/3/3
60	H2U	Pt	16	60	-	3/7/38/39	0/2/2/2
61	PSU	Dt	55	61	-	0/7/25/26	0/2/2/2
60	PSU	Pt	39	60	-	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	-	0/9/27/28	0/3/3/3
23	5MC	23	1962	23	-	4/7/25/26	0/2/2/2

The worst 5 of 177 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 275 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	2069	G7M	CN7-N7-C8	-8.87	111.36	124.79
1	16	527	G7M	CN7-N7-C8	-8.69	111.63	124.79
61	Dt	46	G7M	CN7-N7-C8	-8.45	111.99	124.79
23	23	2503	2MA	C5-C4-N3	-8.25	118.48	127.18

There are no chirality outliers.

5 of 87 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	1519	MA6	O4'-C4'-C5'-O5'
1	16	1519	MA6	C5-C6-N6-C10
12	SL	89	D2T	CG-CB-SB-CB1
23	23	746	PSU	C2'-C1'-C5-C4
23	23	746	PSU	C2'-C1'-C5-C6

There are no ring outliers.

19 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	16	1516	2MG	1	0
1	16	1402	4OC	1	0
23	23	955	PSU	1	0
12	SL	89	D2T	5	0
1	16	1518	MA6	1	0
61	Dt	47	3AU	1	0
23	23	1911	PSU	1	0
23	23	2251	OMG	1	0
60	Pt	37	T6A	2	0
1	16	967	5MC	2	0
23	23	2030	6MZ	2	0
60	Pt	20	H2U	1	0
23	23	2552	OMU	1	0
23	23	2503	2MA	1	0
23	23	1915	3TD	1	0
61	Dt	37	MIA	2	0
1	16	1519	MA6	1	0
60	Pt	16	H2U	1	0
1	16	966	2MG	1	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	LC	301	-	5,5,5	0.10	0	4,4,4	0.13	0
66	SPD	23	3021	-	9,9,9	0.32	0	8,8,8	0.91	0
62	PUT	16	1601	-	5,5,5	0.12	0	4,4,4	0.12	0
62	PUT	23	3014	-	5,5,5	0.10	0	4,4,4	0.12	0
67	FUA	EF	802	63	39,40,40	2.06	13 (33%)	50,64,64	2.79	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	GDP	EF	803	63	29,30,30	1.15	3 (10%)	45,47,47	1.78	7 (15%)
62	PUT	23	3009	-	5,5,5	0.09	0	4,4,4	0.13	0
62	PUT	23	3006	-	5,5,5	0.09	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	3007	-	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
66	SPD	23	3023	-	9,9,9	0.16	0	8,8,8	0.23	0
62	PUT	23	3020	-	5,5,5	0.16	0	4,4,4	0.20	0
62	PUT	23	3010	-	5,5,5	0.10	0	4,4,4	0.13	0
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
62	PUT	23	3005	-	5,5,5	0.11	0	4,4,4	0.13	0
62	PUT	23	3015	-	5,5,5	0.14	0	4,4,4	0.19	0
62	PUT	23	3017	-	5,5,5	0.12	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	3008	-	5,5,5	0.10	0	4,4,4	0.14	0
62	PUT	23	3013	-	5,5,5	0.10	0	4,4,4	0.13	0
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
65	ATP	23	3002	-	32,33,33	0.26	0	48,52,52	0.27	0
65	ATP	23	3001	-	32,33,33	0.26	0	48,52,52	0.28	0
62	PUT	23	3012	-	5,5,5	0.11	0	4,4,4	0.13	0
62	PUT	23	3016	-	5,5,5	0.09	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	LC	301	-	-	1/3/3/3	-
66	SPD	23	3021	-	-	2/7/7/7	-
62	PUT	16	1601	-	-	0/3/3/3	-
62	PUT	23	3014	-	-	1/3/3/3	-
67	FUA	EF	802	63	-	5/16/92/92	0/4/4/4
68	GDP	EF	803	63	-	4/16/32/32	0/3/3/3
62	PUT	23	3009	-	-	0/3/3/3	-
62	PUT	23	3006	-	-	0/3/3/3	-
62	PUT	23	3018	-	-	1/3/3/3	-
62	PUT	23	3007	-	-	1/3/3/3	-
62	PUT	23	3011	-	-	1/3/3/3	-
66	SPD	23	3023	-	-	2/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PUT	23	3020	-	-	0/3/3/3	-
62	PUT	23	3010	-	-	1/3/3/3	-
62	PUT	16	1602	-	-	2/3/3/3	-
62	PUT	23	3019	-	-	0/3/3/3	-
62	PUT	23	3005	-	-	0/3/3/3	-
62	PUT	23	3015	-	-	1/3/3/3	-
62	PUT	23	3017	-	-	1/3/3/3	-
62	PUT	23	3003	-	-	0/3/3/3	-
62	PUT	23	3008	-	-	0/3/3/3	-
62	PUT	23	3013	-	-	0/3/3/3	-
62	PUT	23	3004	-	-	0/3/3/3	-
66	SPD	23	3022	-	-	0/7/7/7	-
65	ATP	23	3002	-	-	5/22/38/38	0/3/3/3
65	ATP	23	3001	-	-	5/22/38/38	0/3/3/3
62	PUT	23	3012	-	-	0/3/3/3	-
62	PUT	23	3016	-	-	1/3/3/3	-

The worst 5 of 16 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
68	EF	803	GDP	C5-C4	3.00	1.47	1.38

The worst 5 of 26 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
68	EF	803	GDP	C5-C4-N3	-6.14	118.62	128.39
67	EF	802	FUA	C27-C26-C25	5.56	139.33	122.66

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

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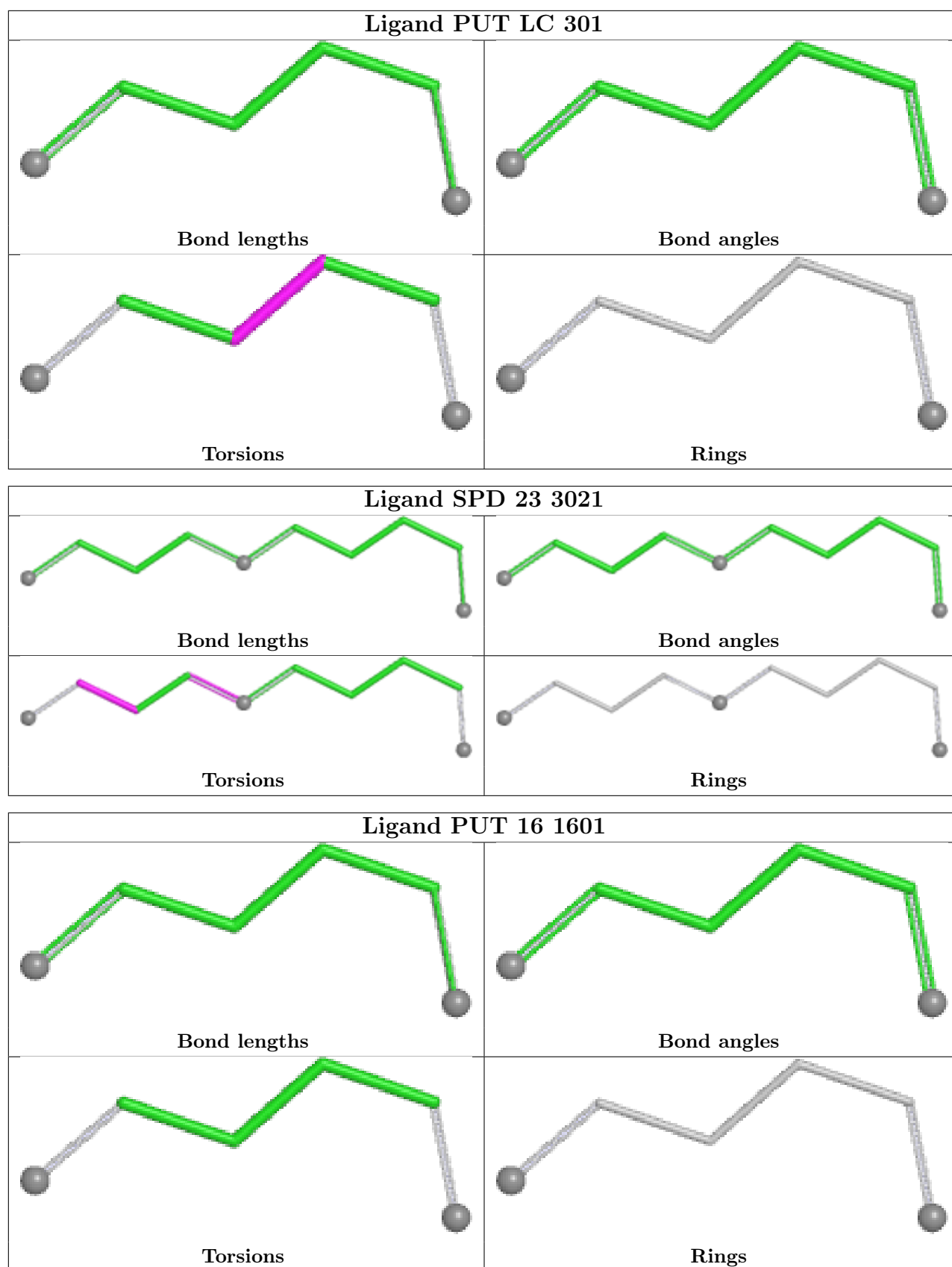
Mol	Chain	Res	Type	Atoms
65	23	3002	ATP	O4'-C4'-C5'-O5'
67	EF	802	FUA	C23-C22-C29-O5
67	EF	802	FUA	O3-C31-O2-C16

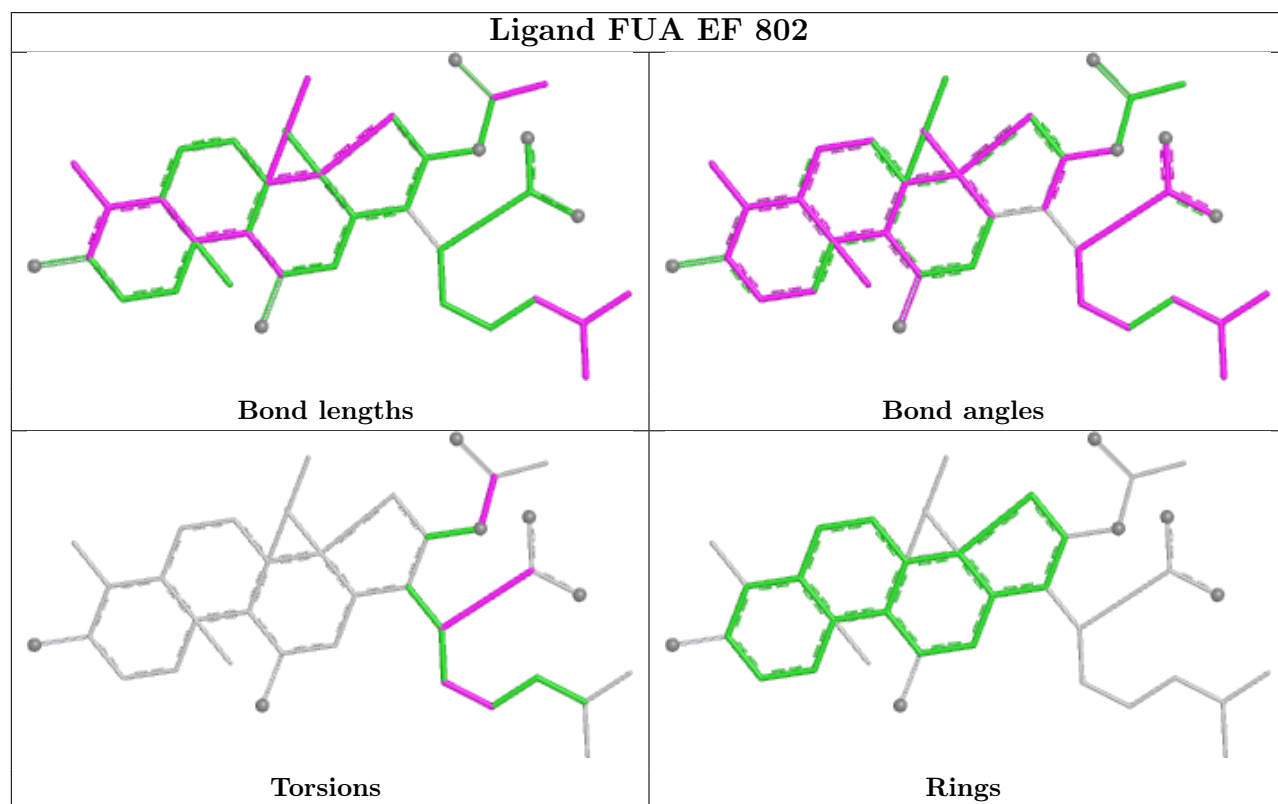
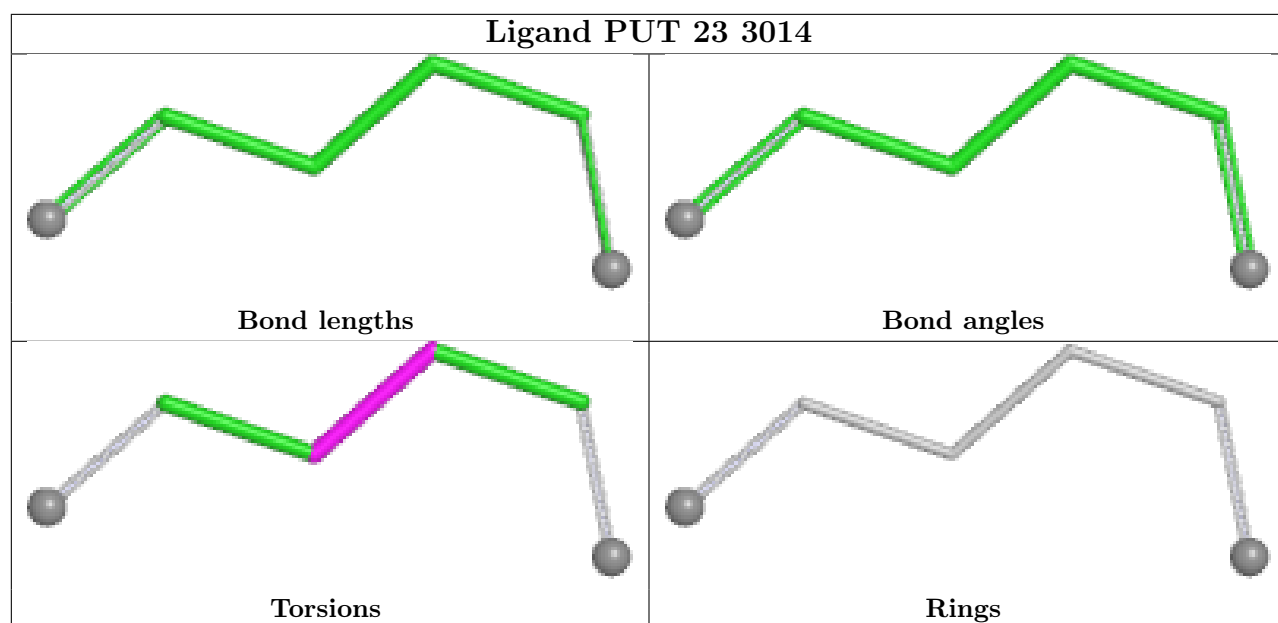
There are no ring outliers.

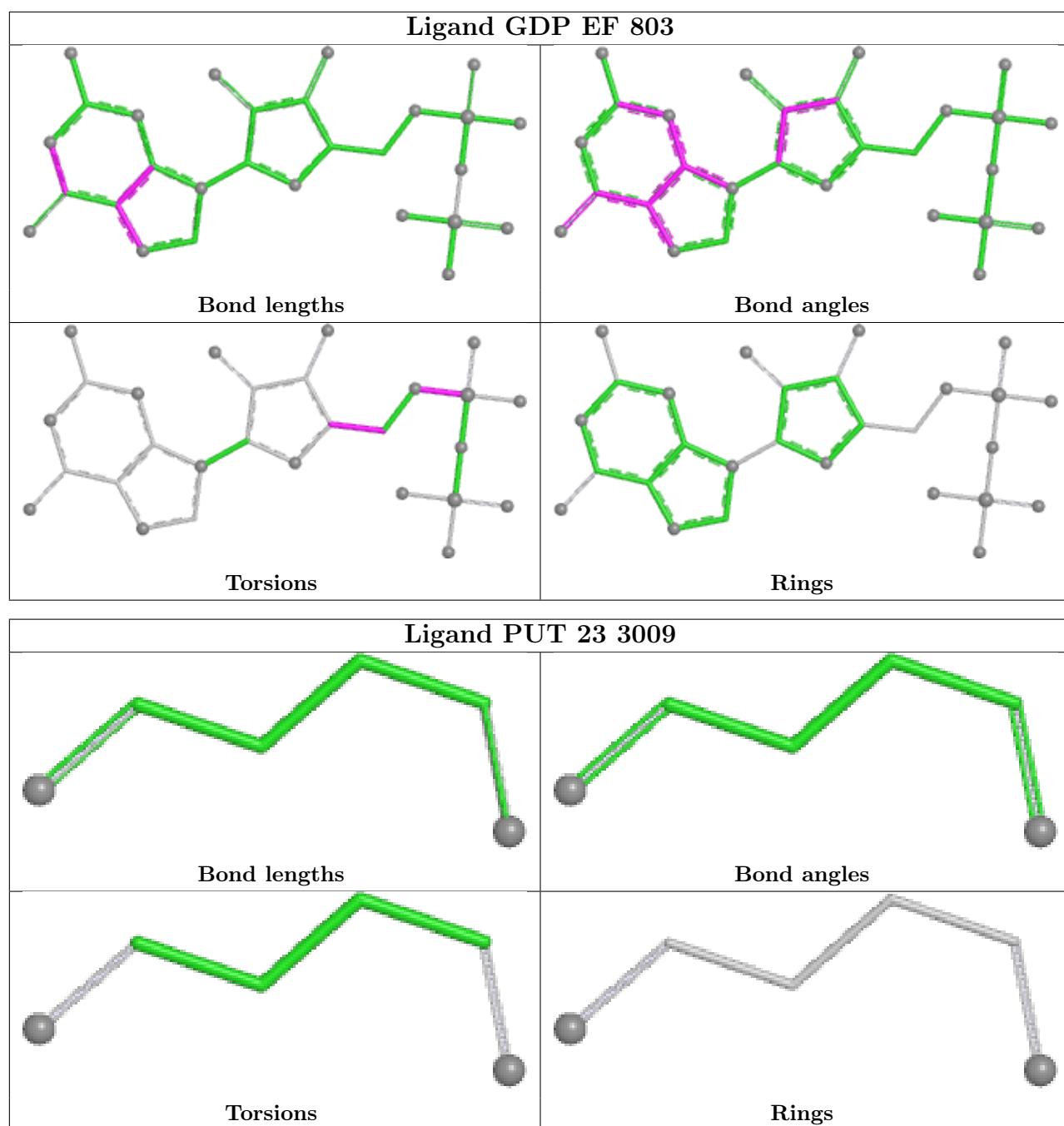
6 monomers are involved in 21 short contacts:

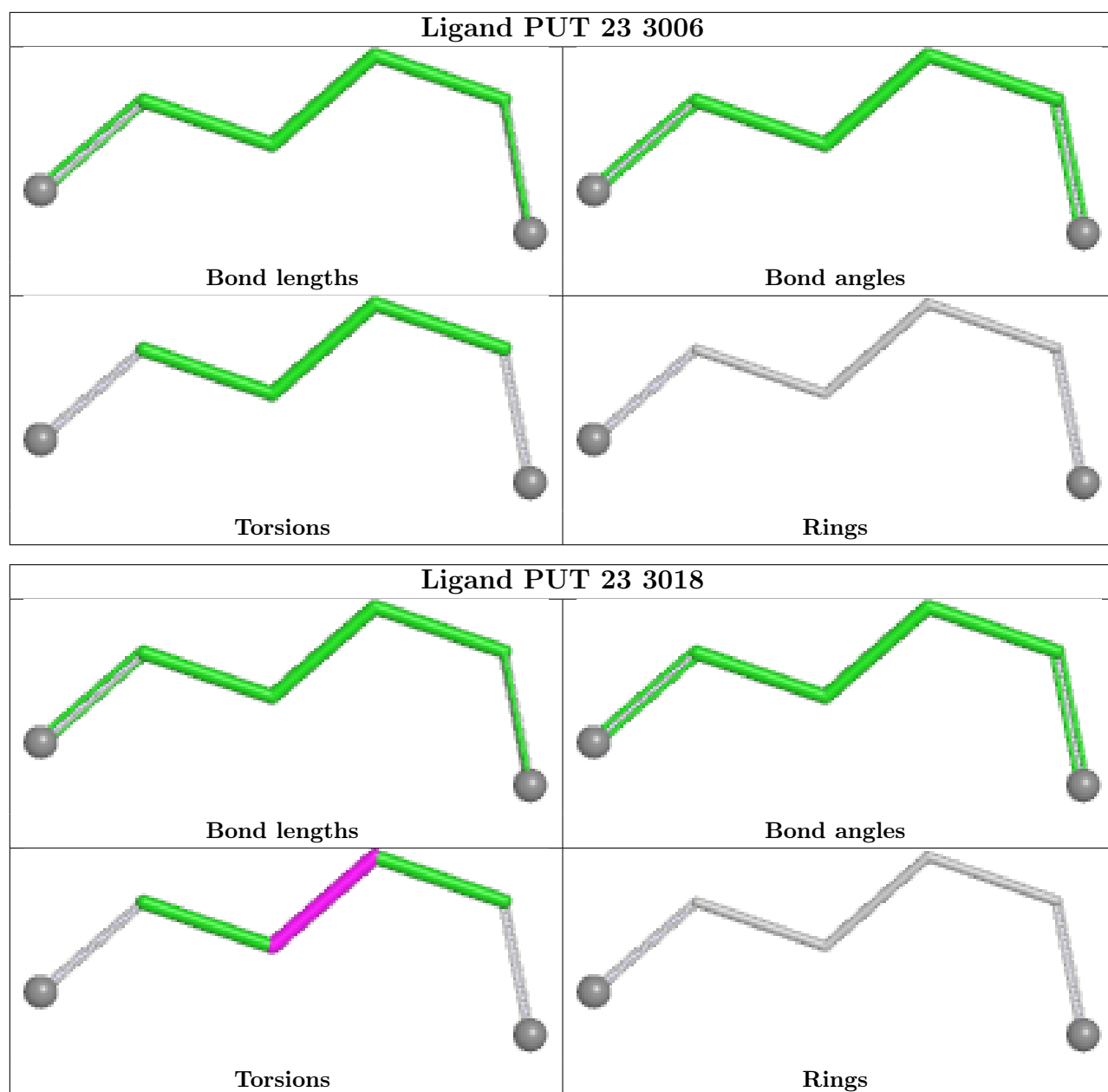
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	LC	301	PUT	1	0
67	EF	802	FUA	15	0
62	23	3020	PUT	2	0
62	23	3010	PUT	1	0
62	16	1602	PUT	1	0
62	23	3013	PUT	1	0

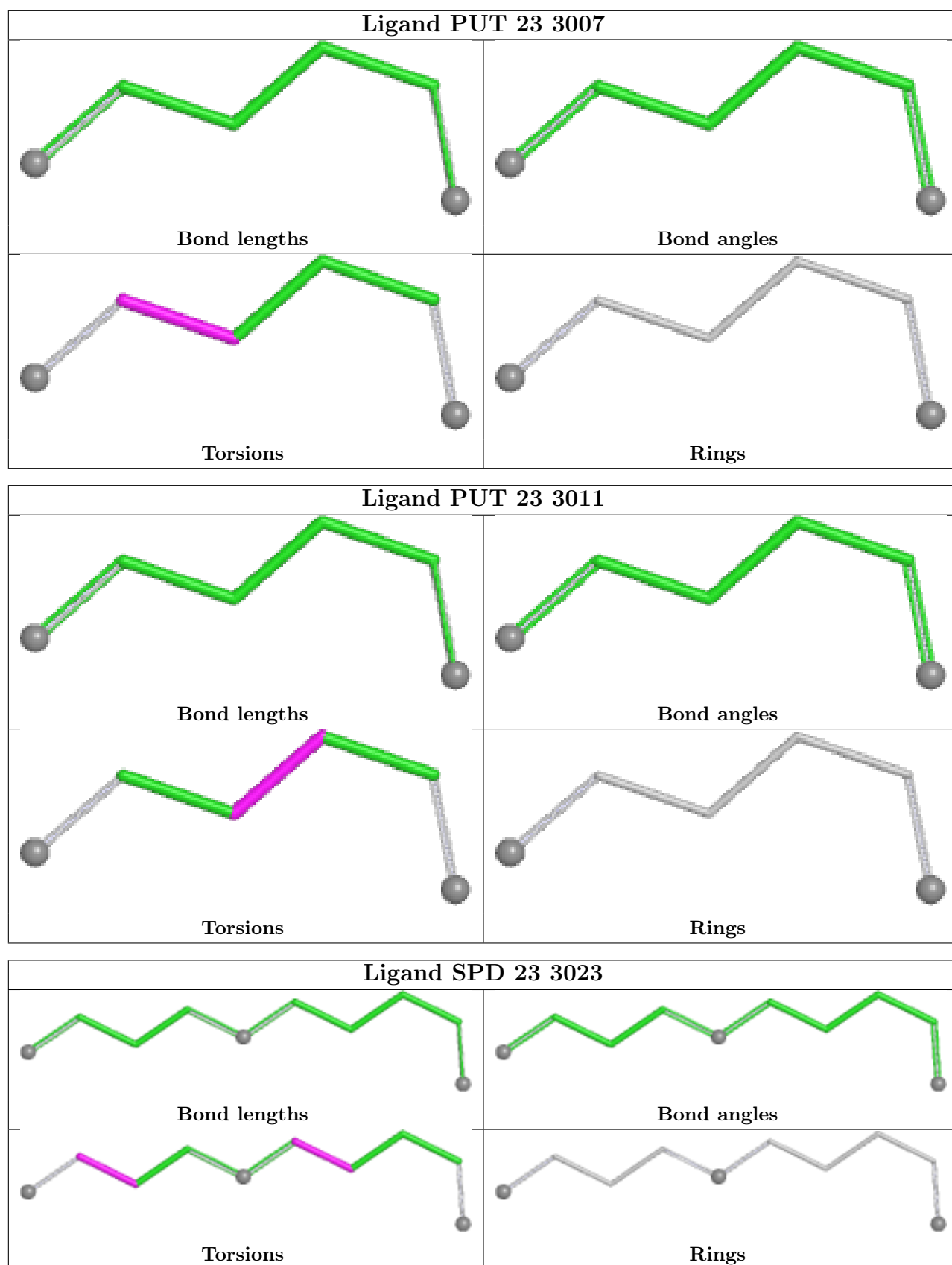
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

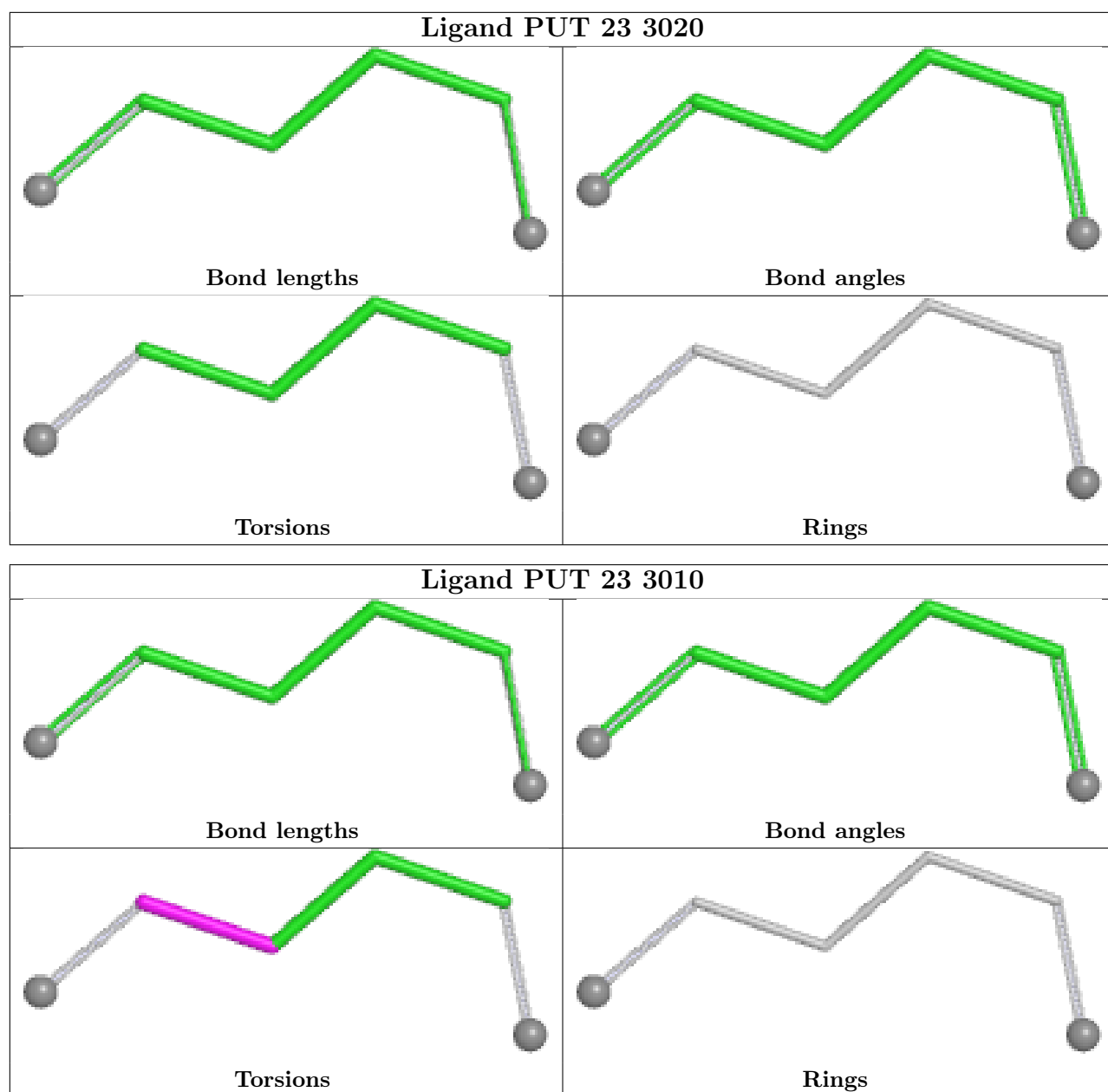


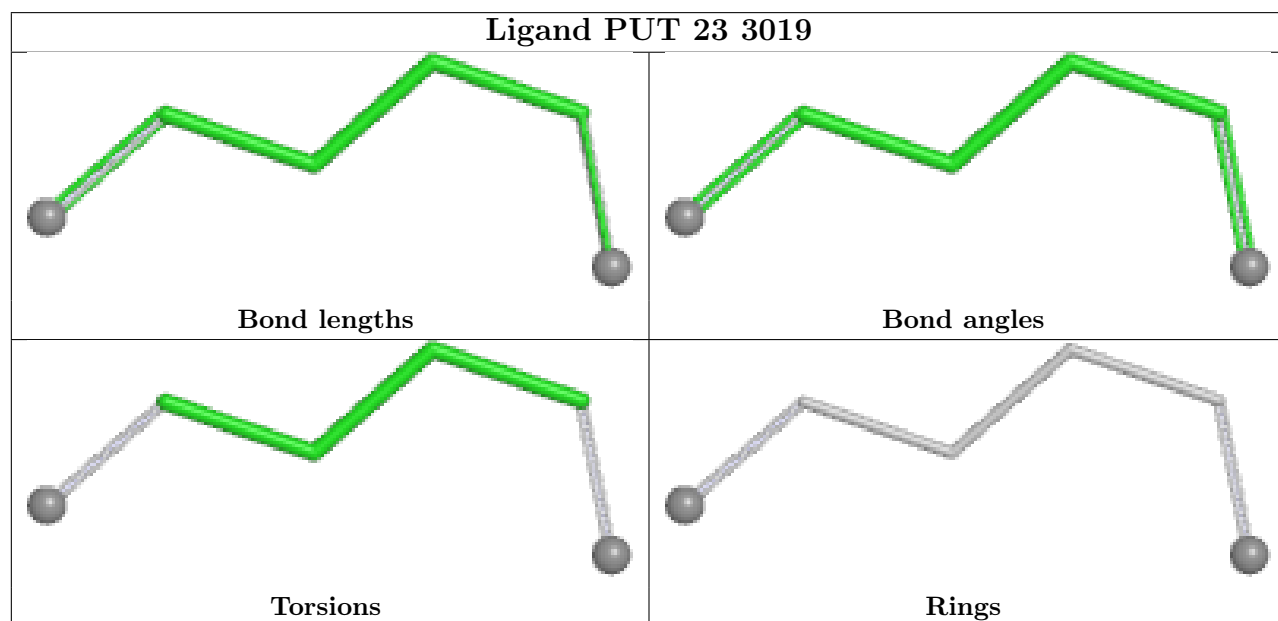
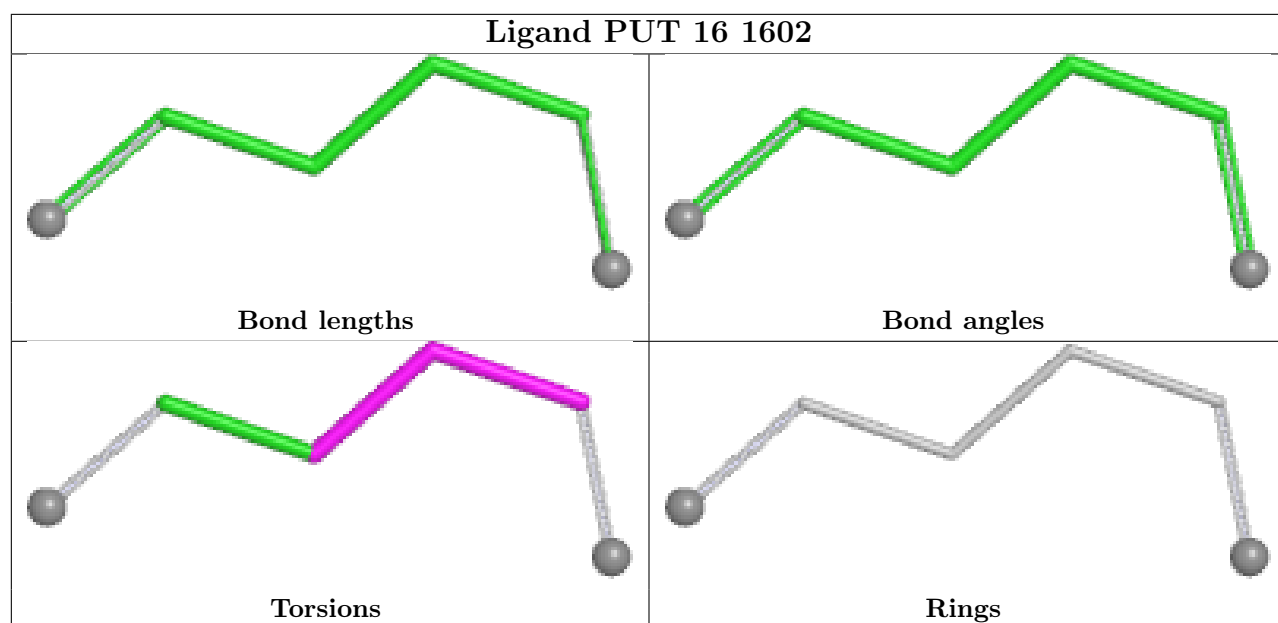


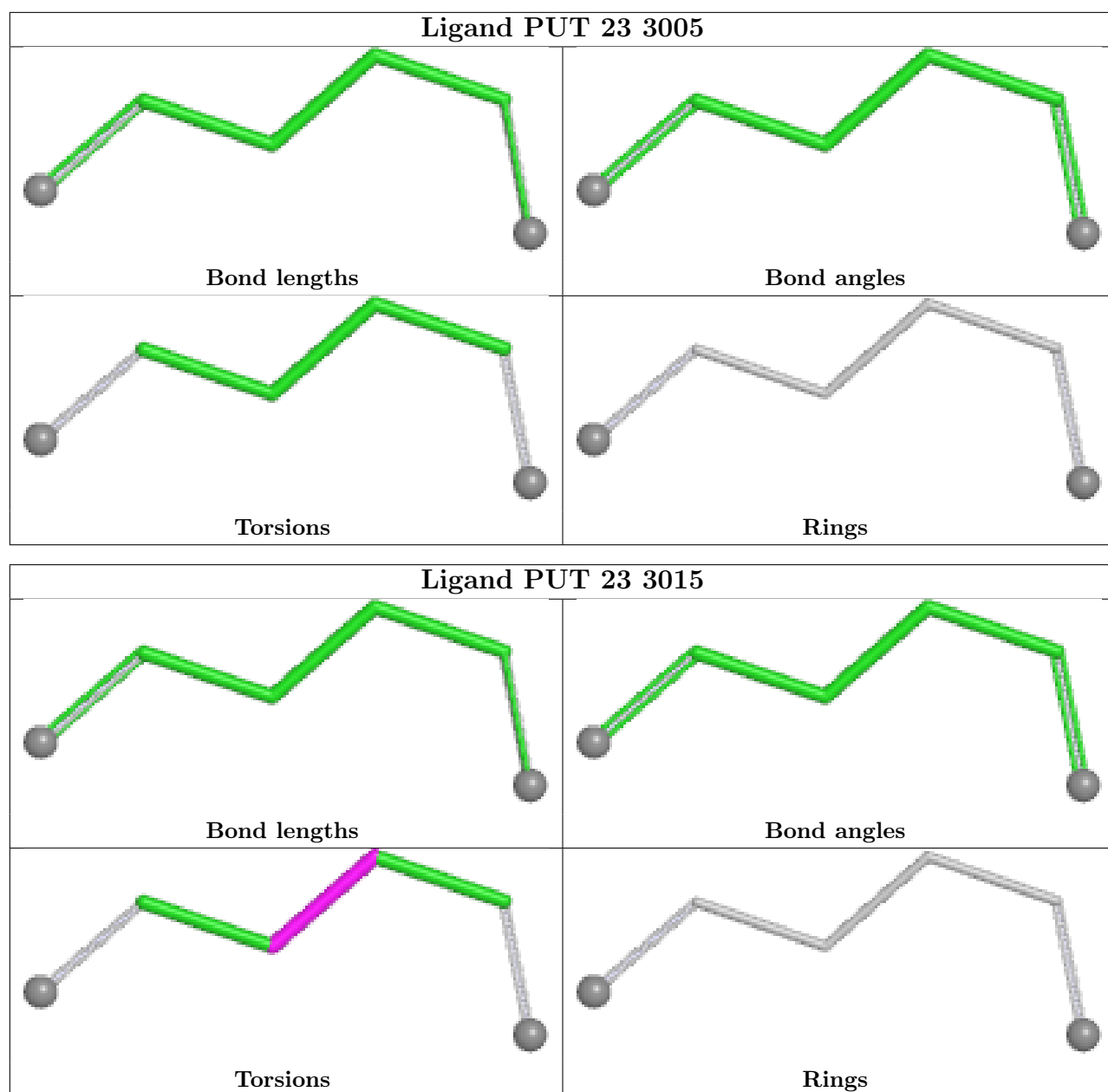


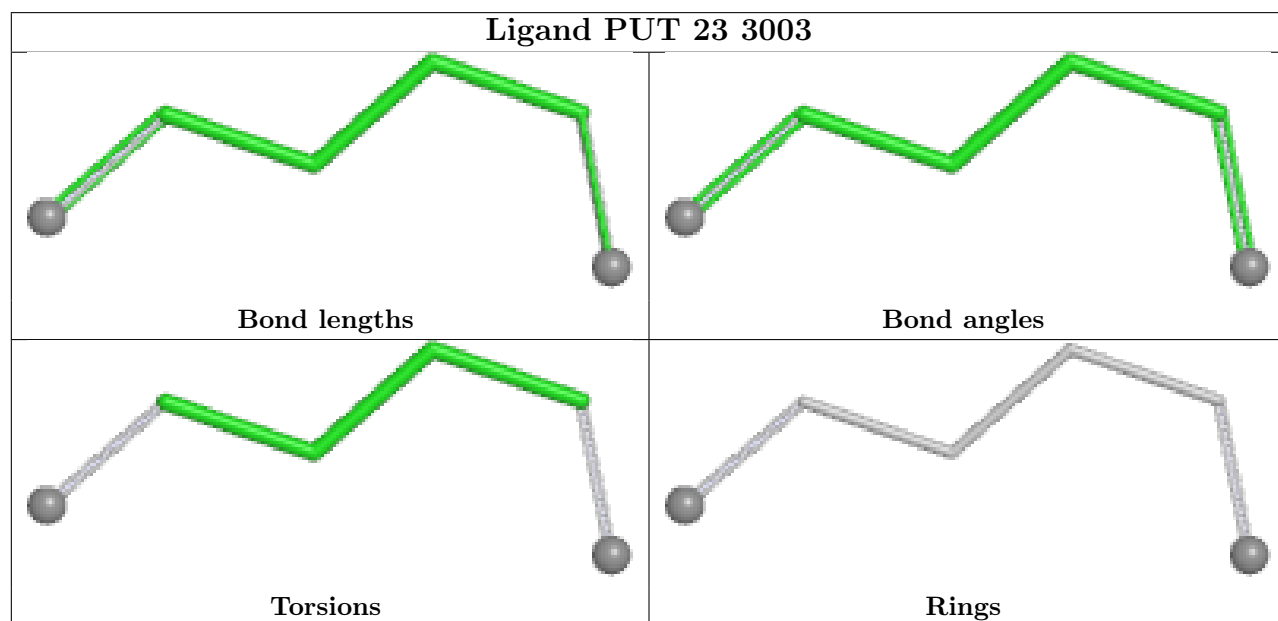
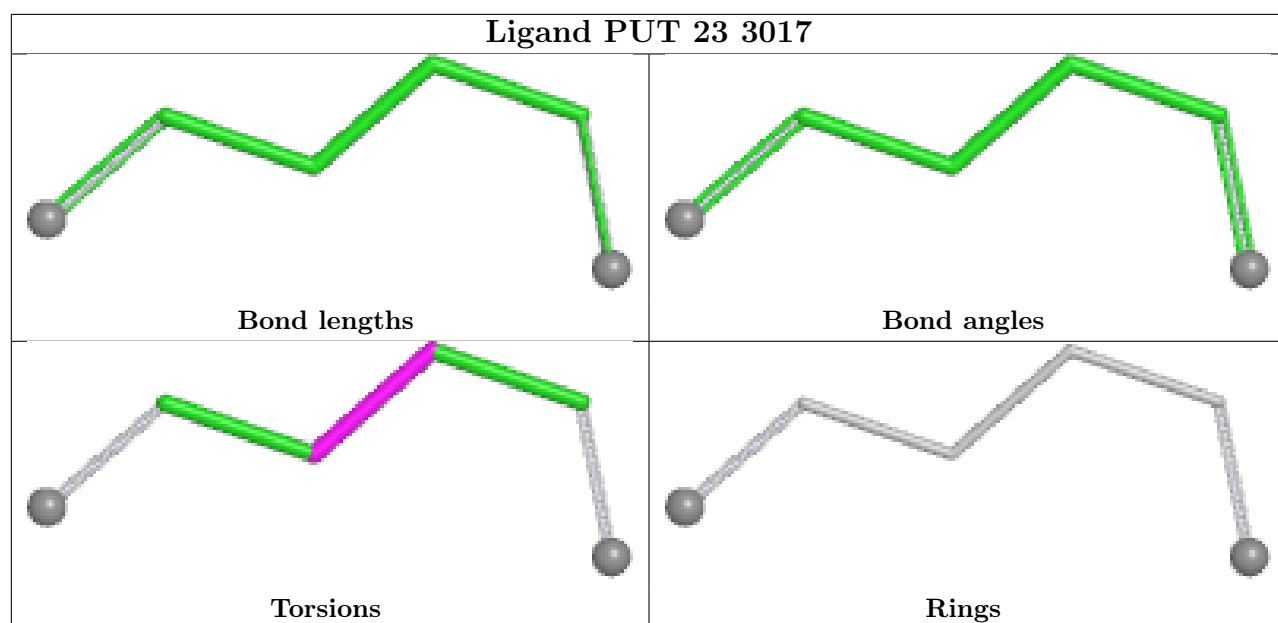


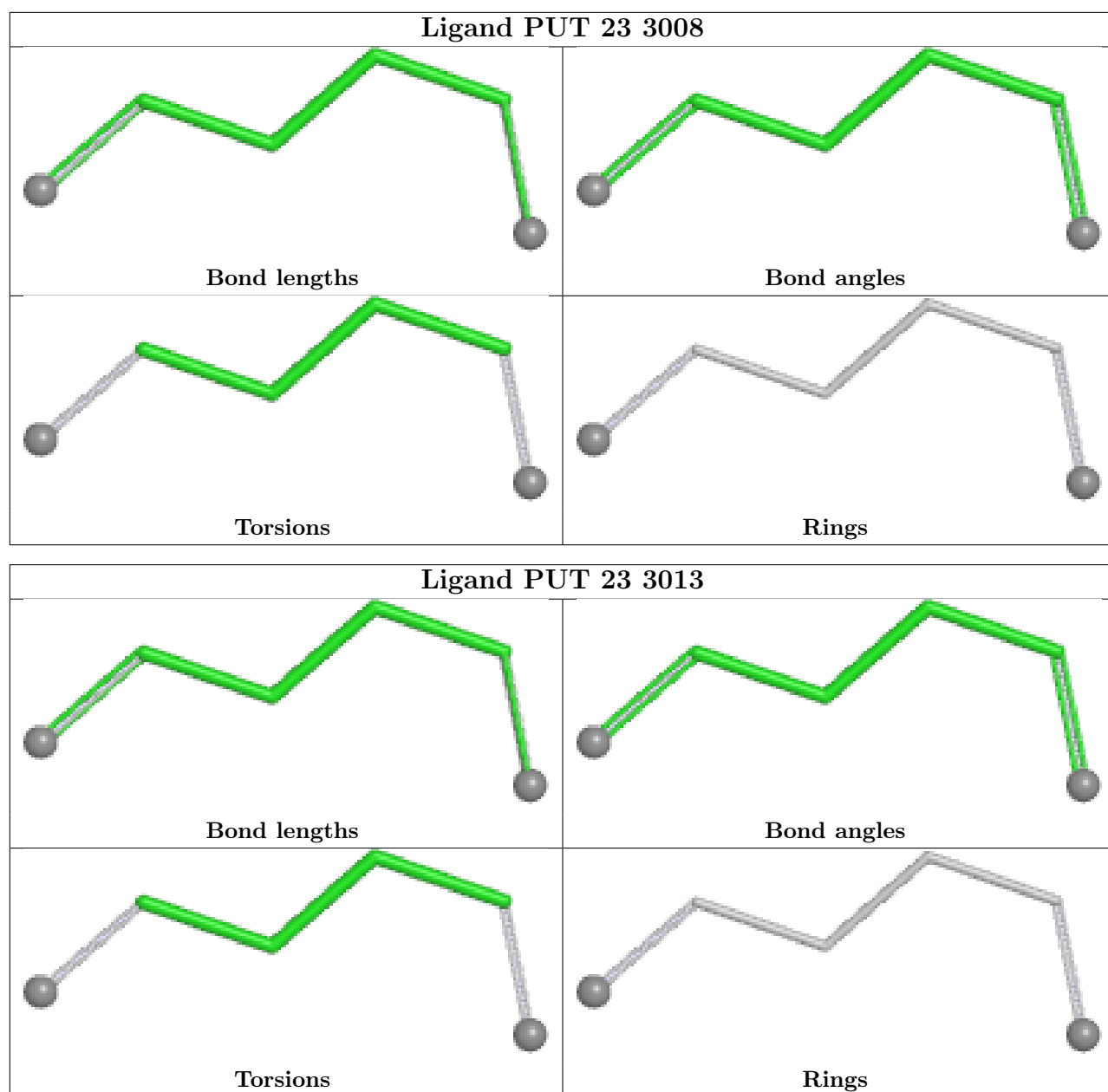


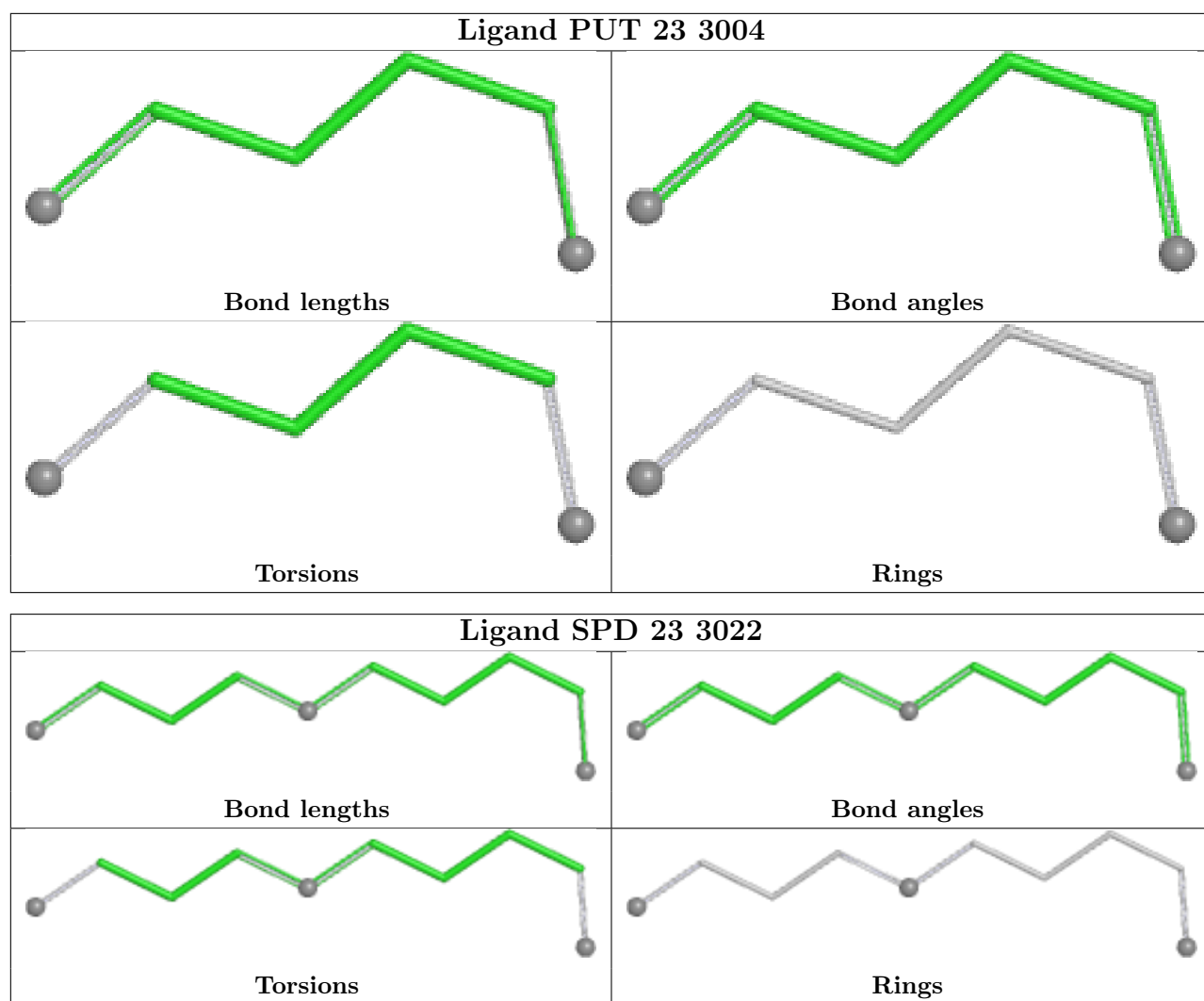


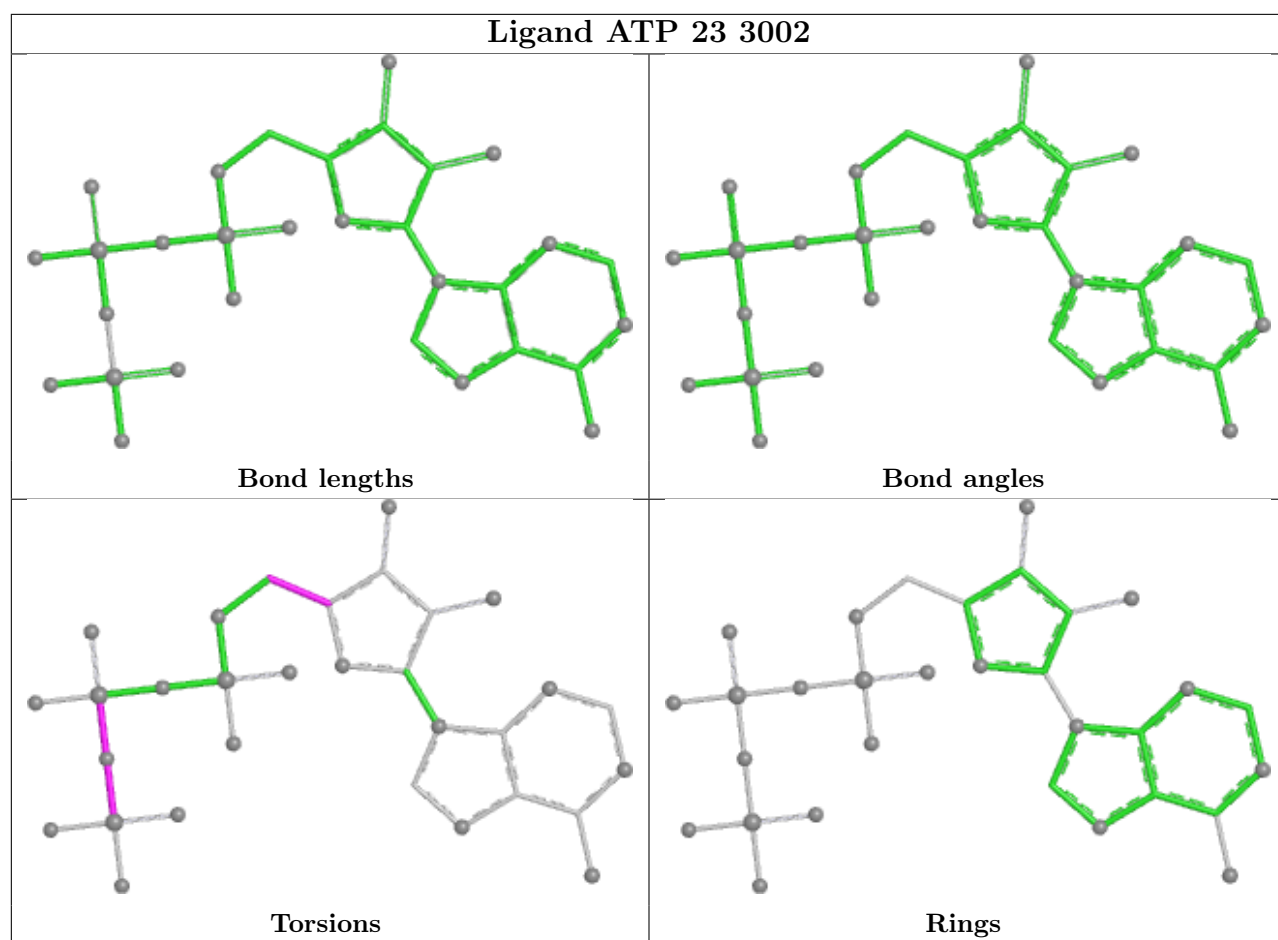




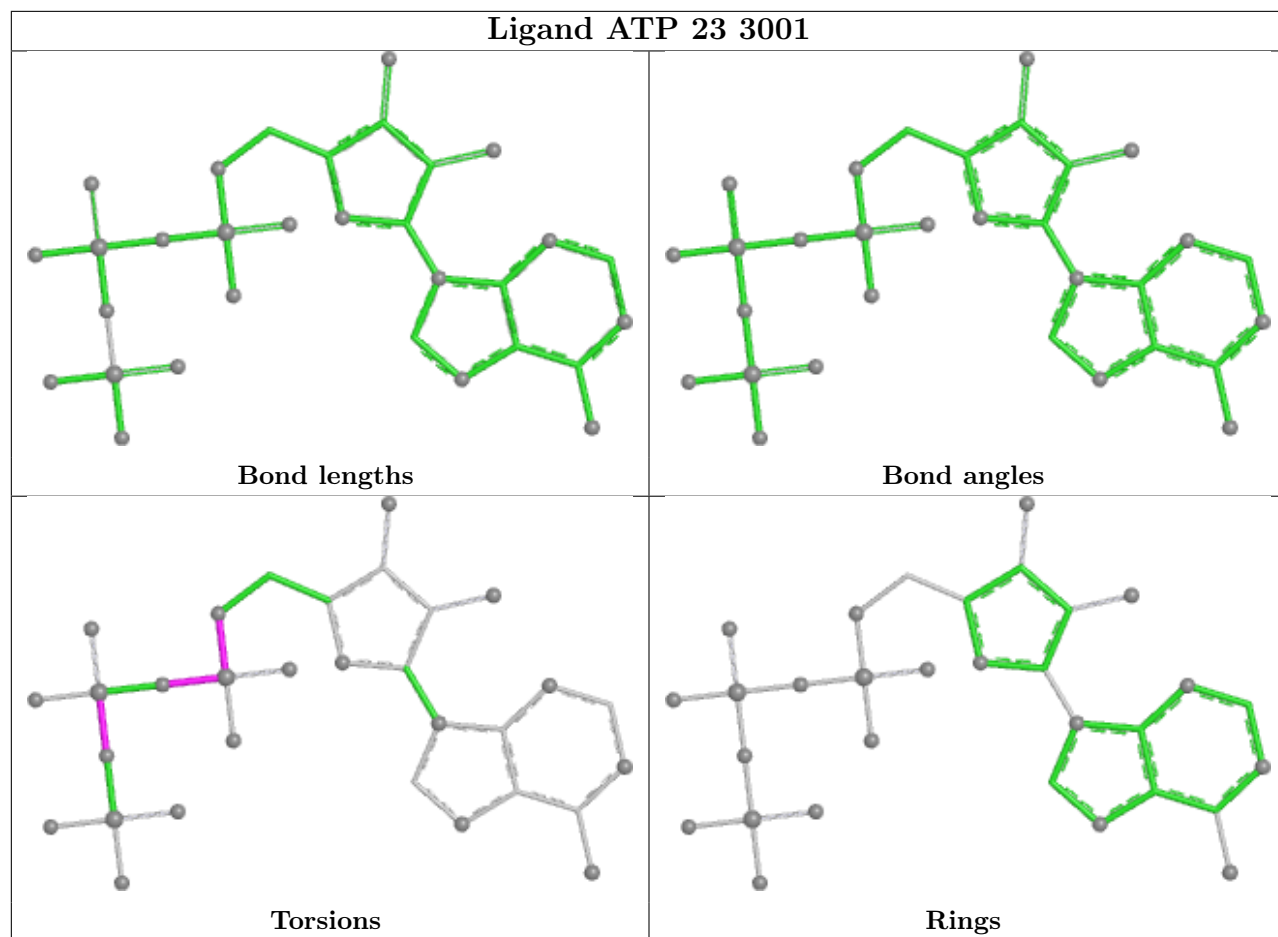




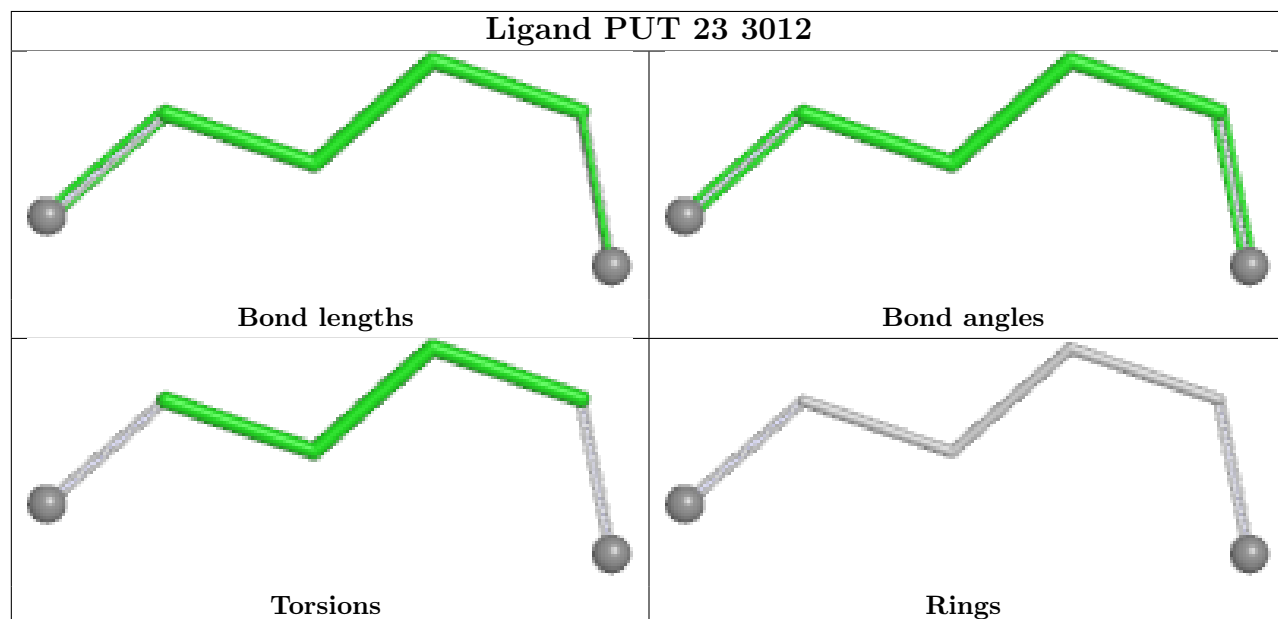


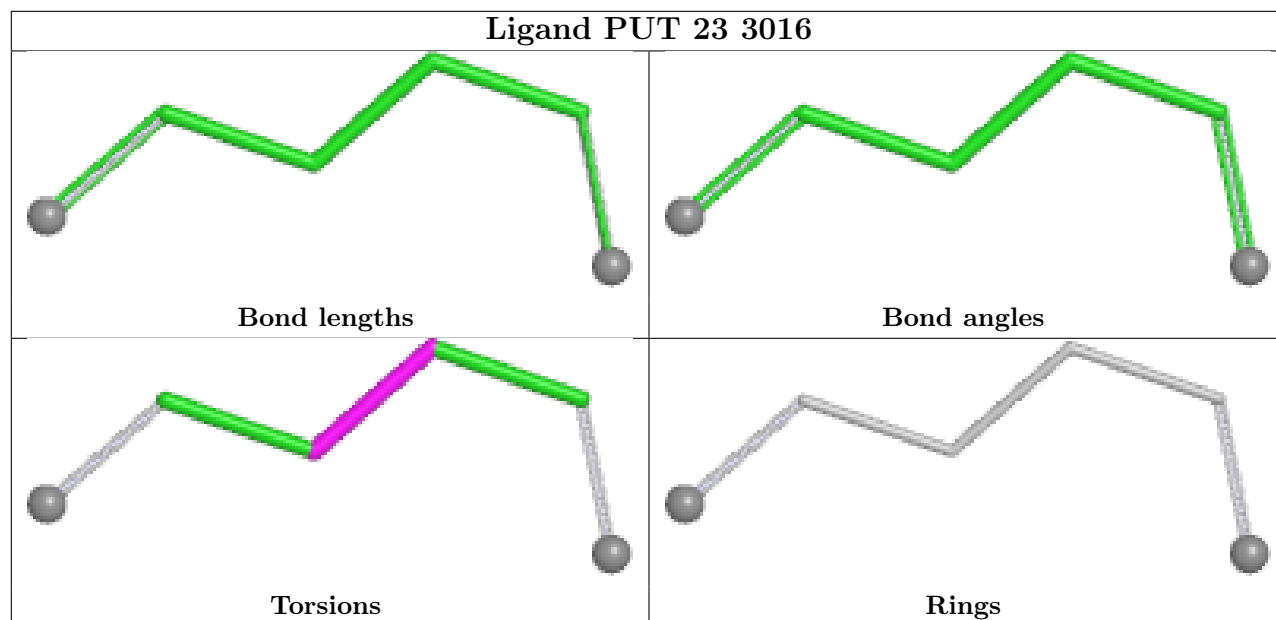


Ligand ATP 23 3001



Ligand PUT 23 3012





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

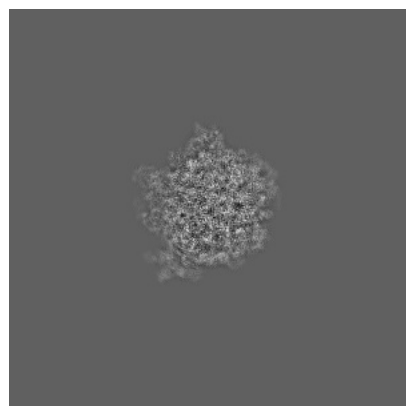
6 Map visualisation [i](#)

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

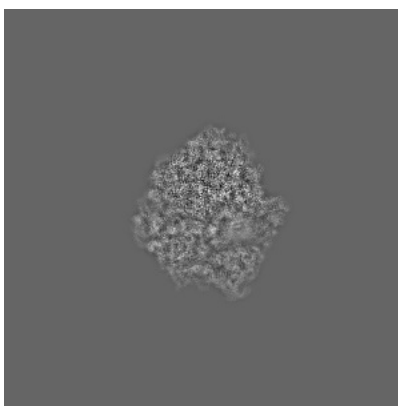
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

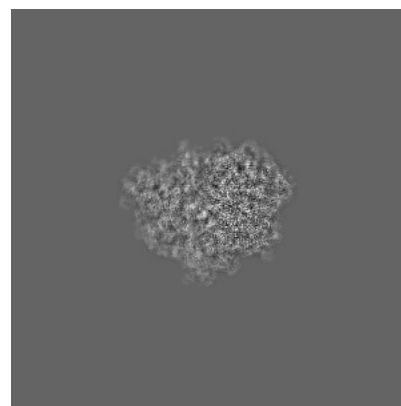
6.1.1 Primary map



X

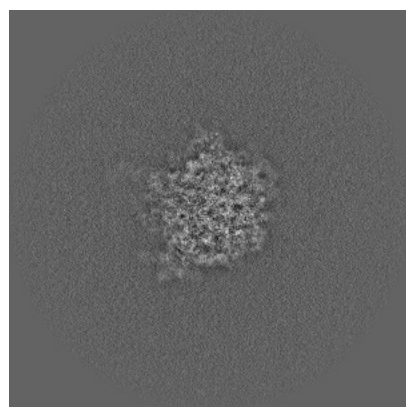


Y

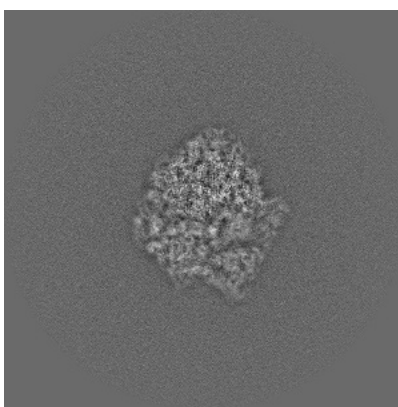


Z

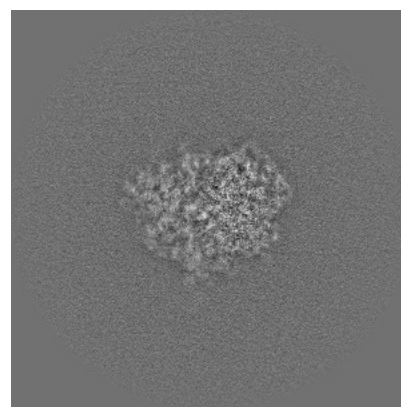
6.1.2 Raw map



X



Y

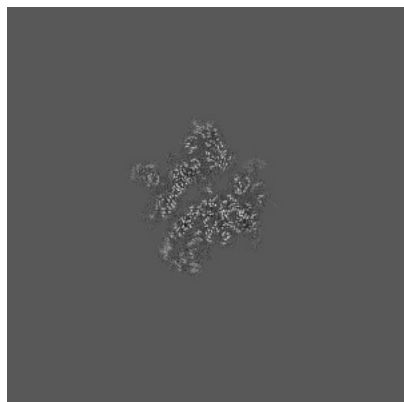


Z

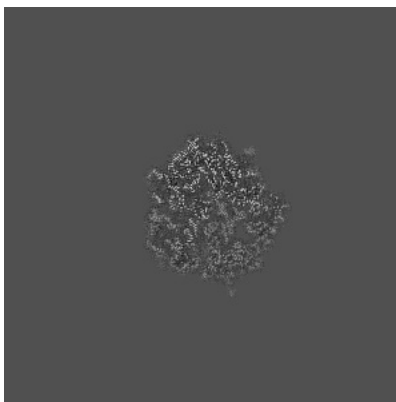
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

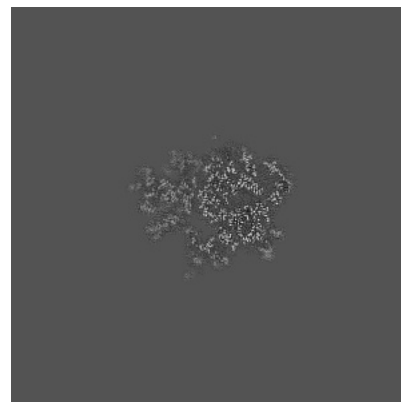
6.2.1 Primary map



X Index: 288

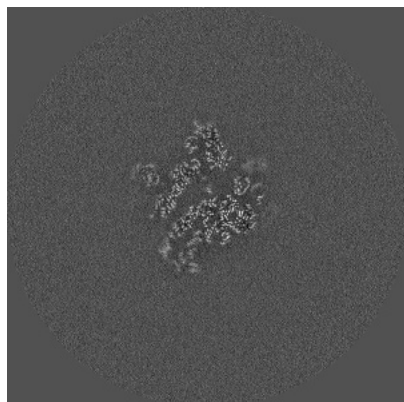


Y Index: 288

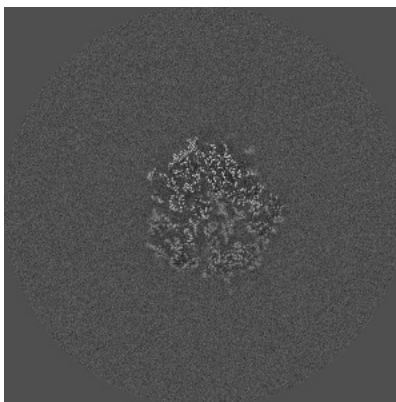


Z Index: 288

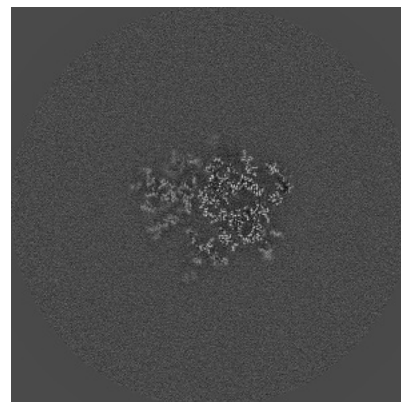
6.2.2 Raw map



X Index: 288



Y Index: 288

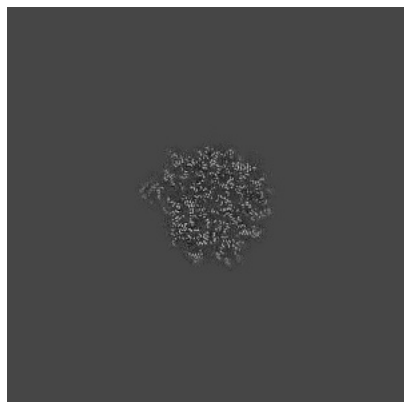


Z Index: 288

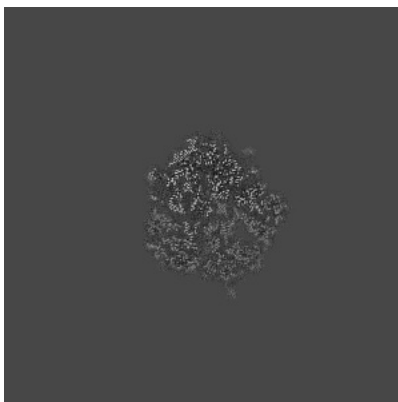
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

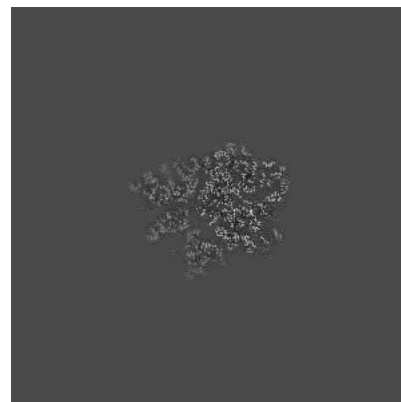
6.3.1 Primary map



X Index: 315

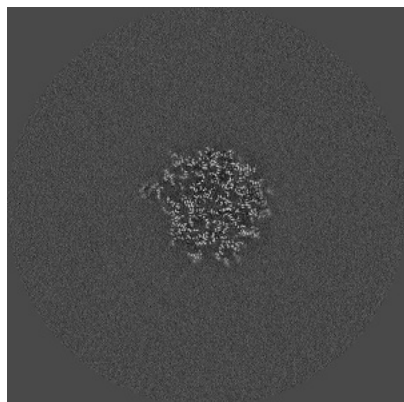


Y Index: 290

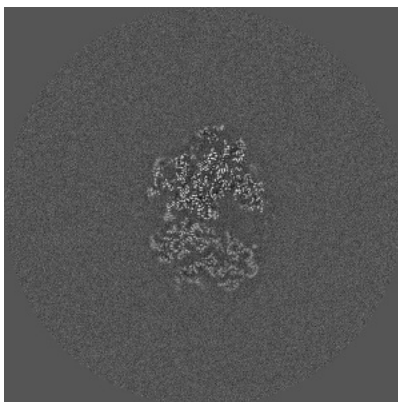


Z Index: 282

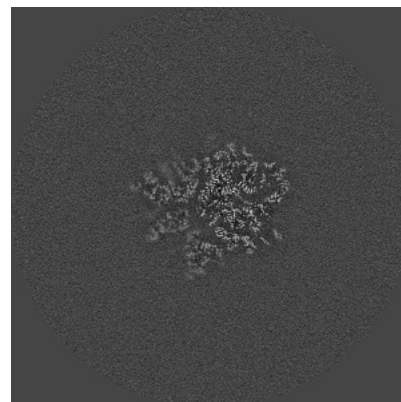
6.3.2 Raw map



X Index: 315



Y Index: 312

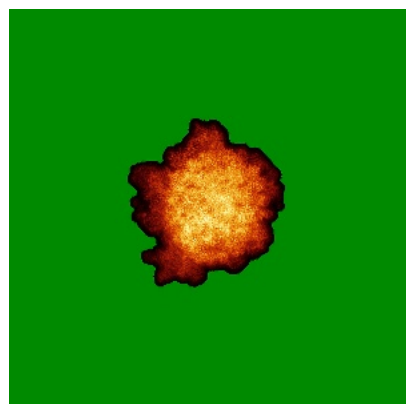


Z Index: 282

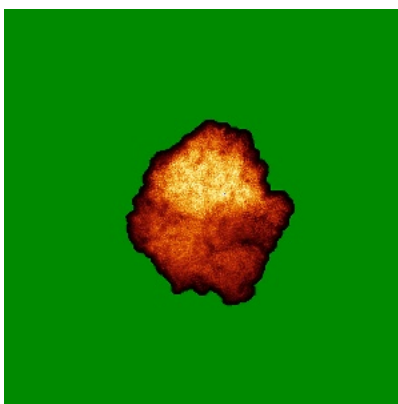
The images above show the largest variance slices of the map in three orthogonal directions.

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

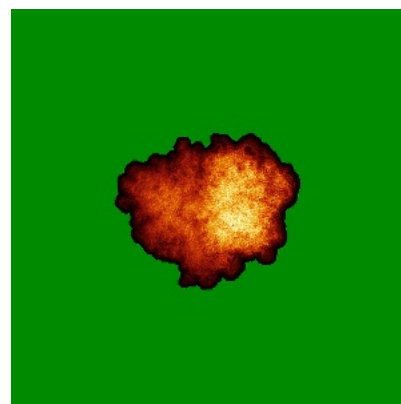
6.4.1 Primary map



X

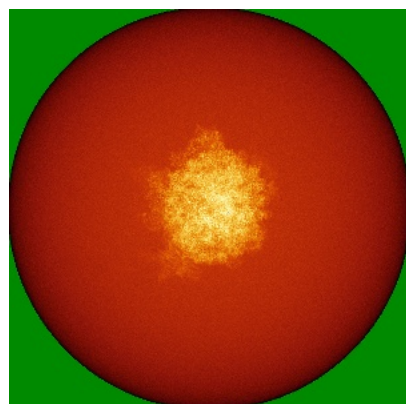


Y

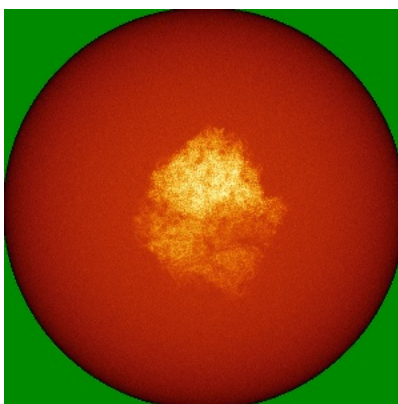


Z

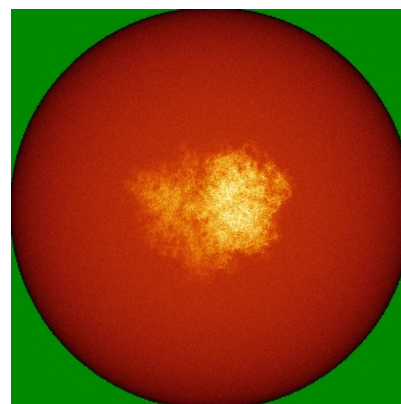
6.4.2 Raw map



X



Y

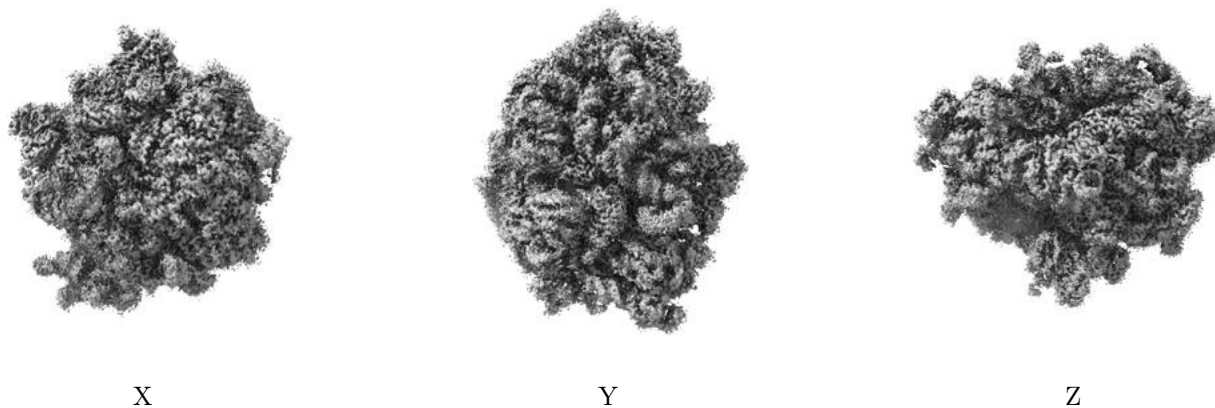


Z

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.

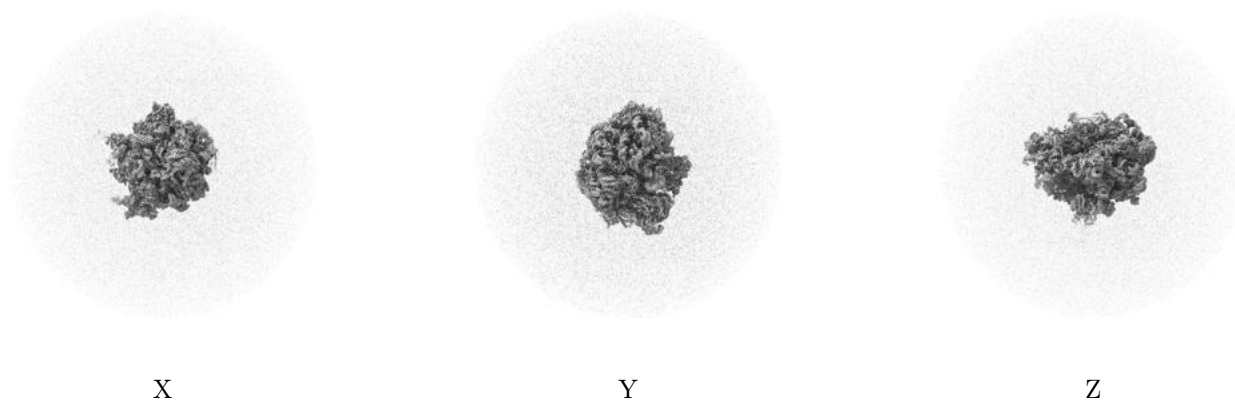
6.5 Orthogonal surface views [i](#)

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.

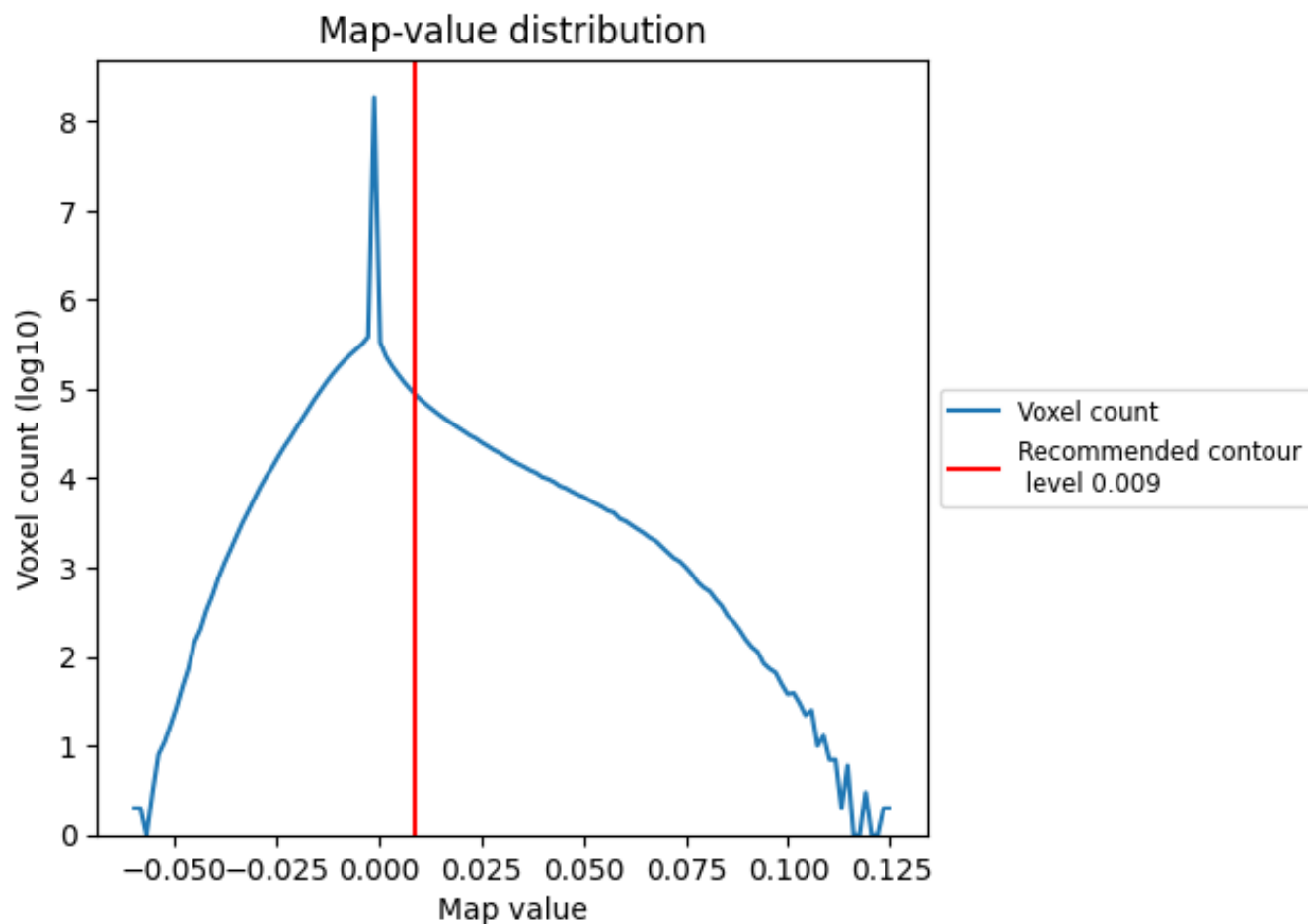
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

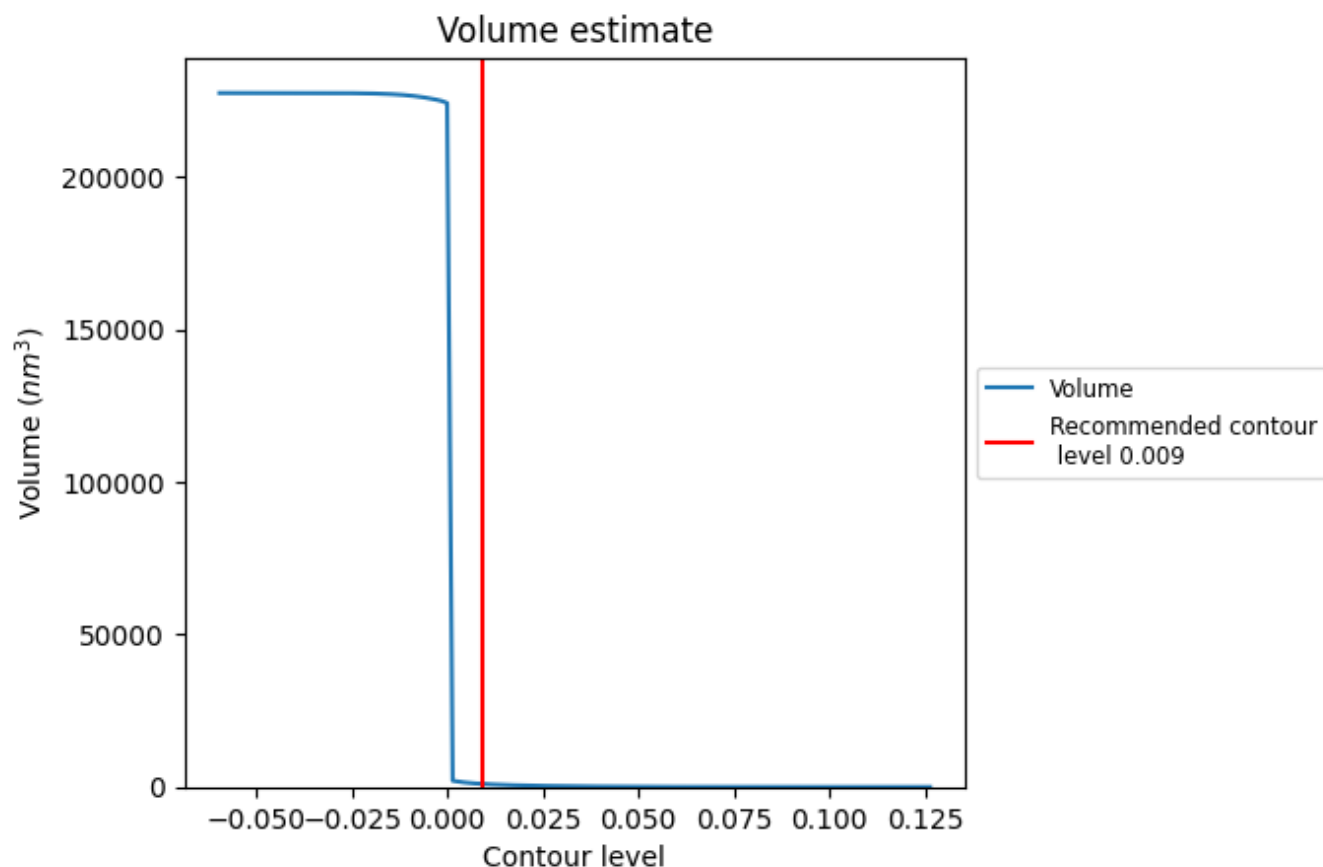
This section contains the results of statistical analysis of the map.

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.

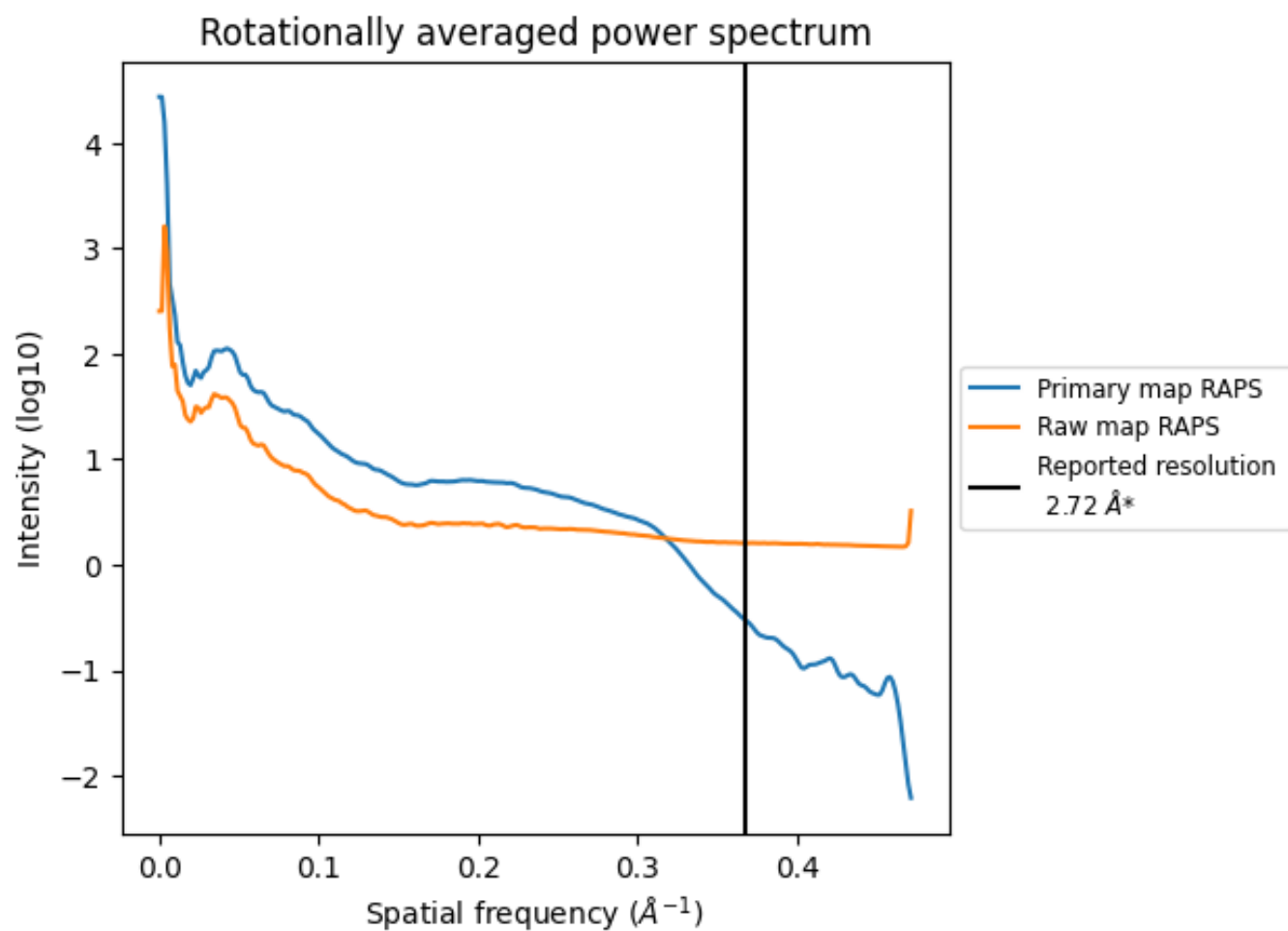
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1017 nm³; 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 ⓘ

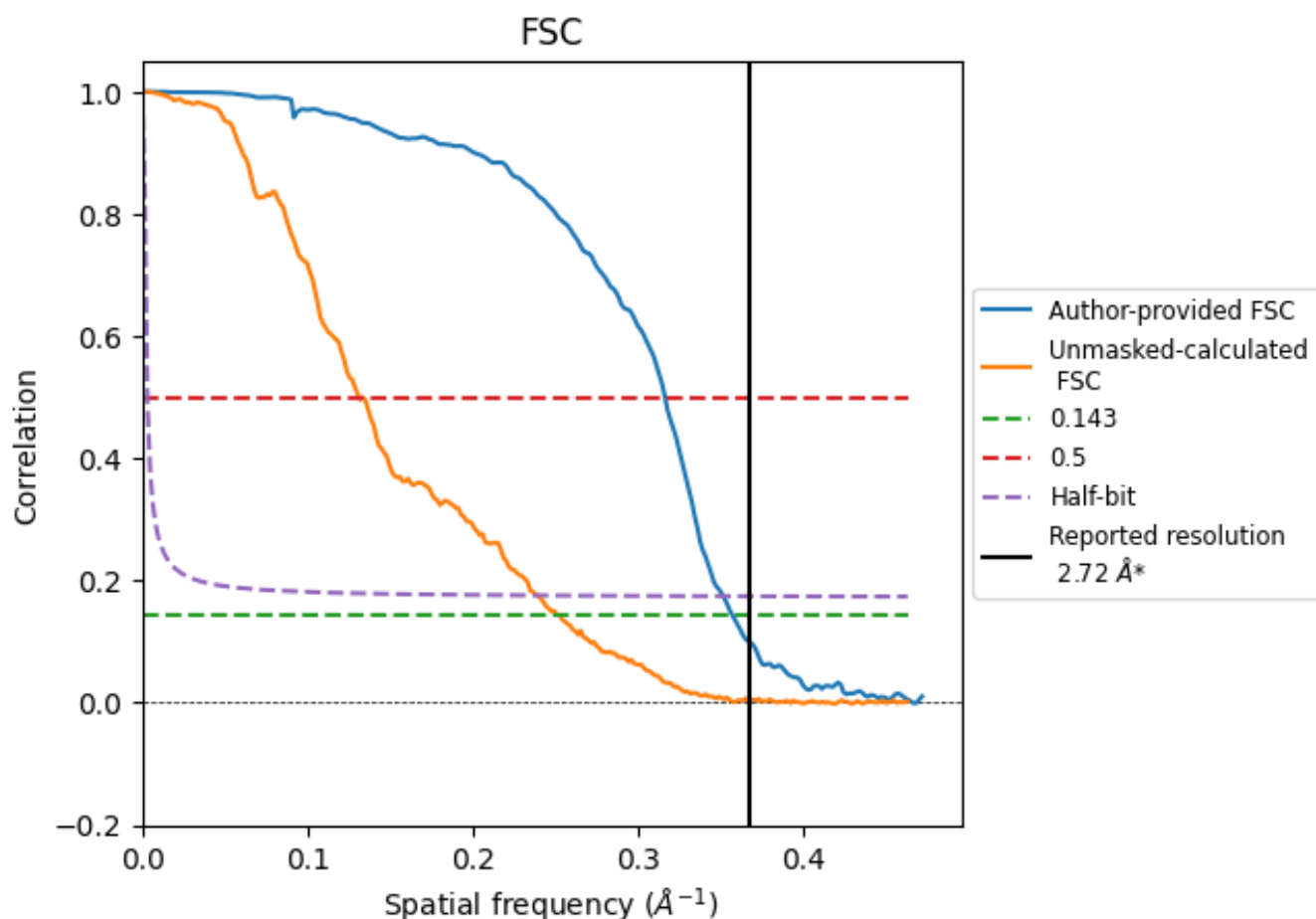


*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

8.2 Resolution estimates [i](#)

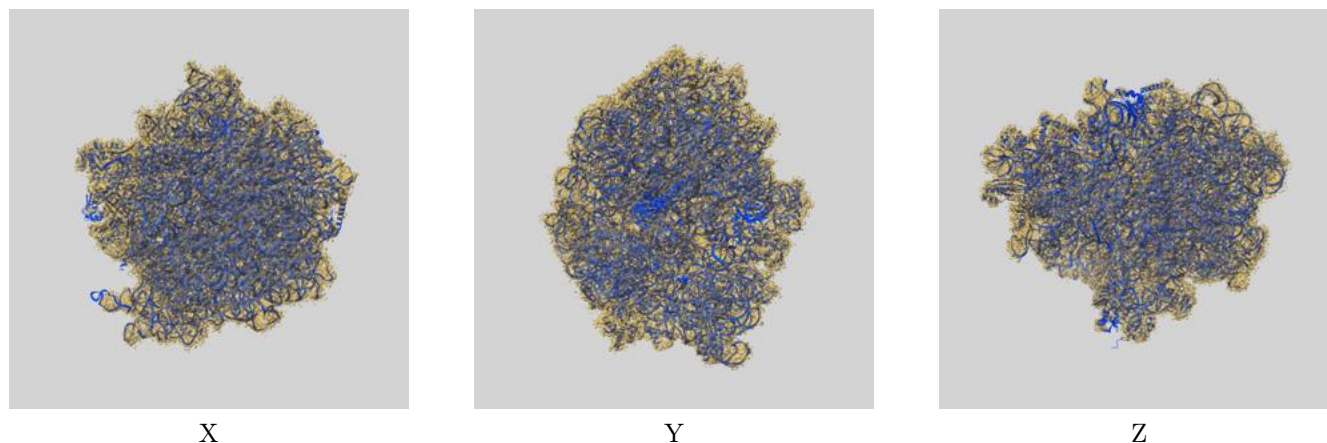
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.80	3.16	2.85
Unmasked-calculated*	3.96	7.63	4.18

*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](#)

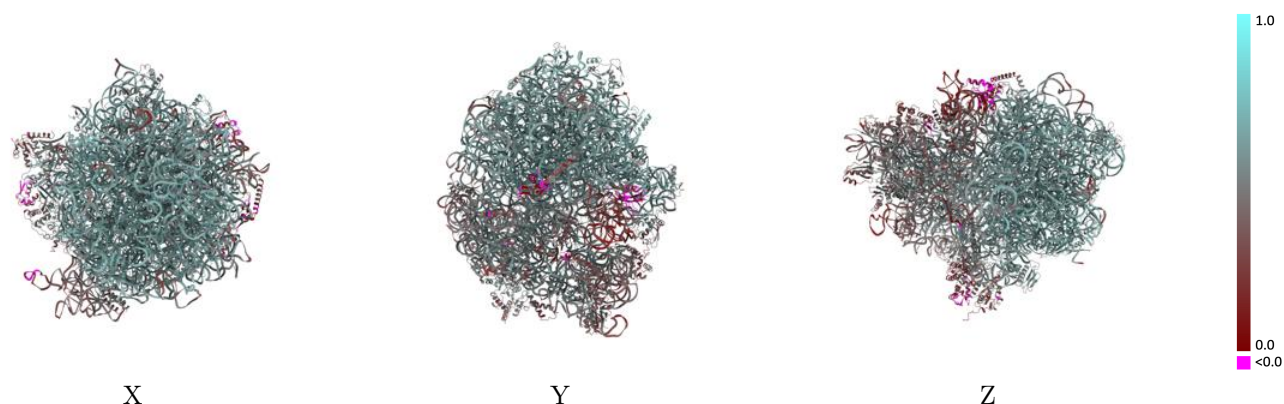
This section contains information regarding the fit between EMDB map EMD-24132 and PDB model 7N2C. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



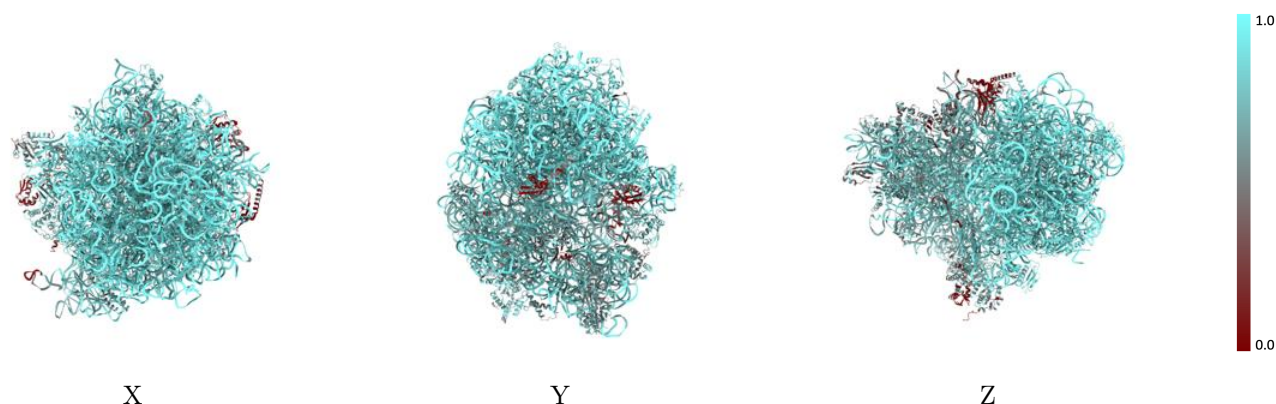
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



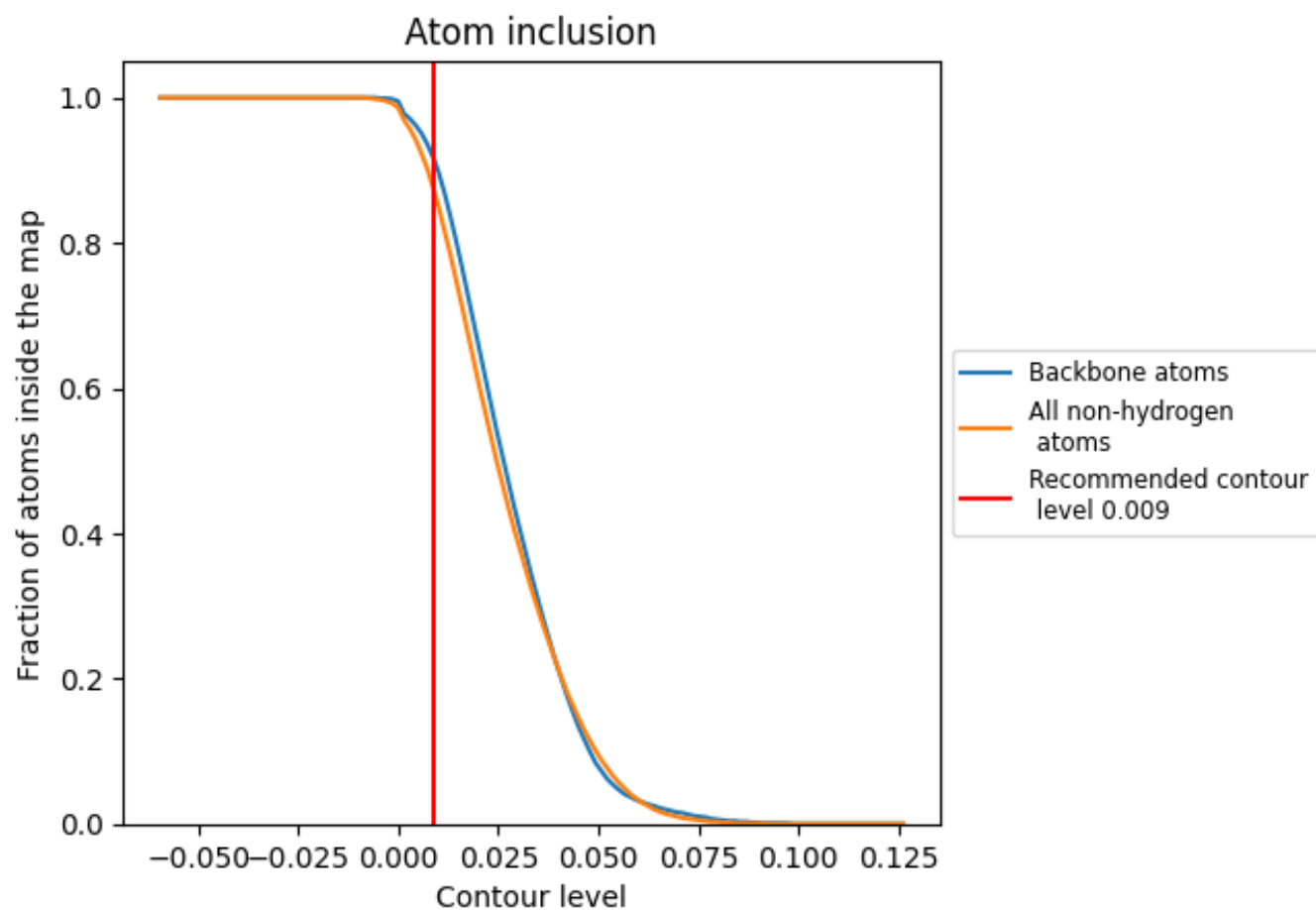
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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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