



## wwPDB EM Validation Summary Report ⓘ

Nov 21, 2022 – 07:43 PM EST

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:

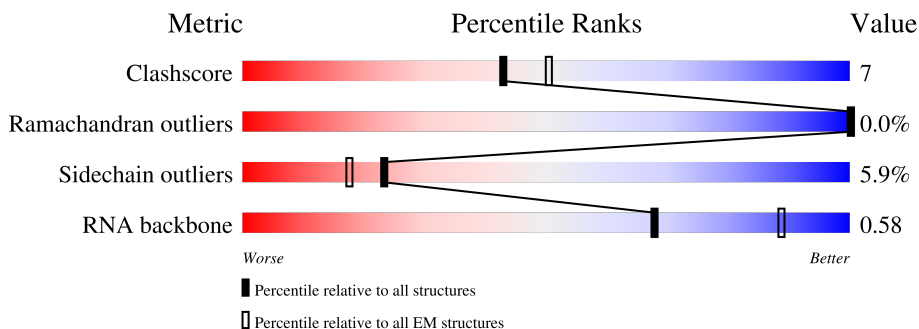
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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.



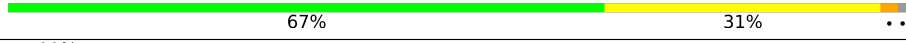



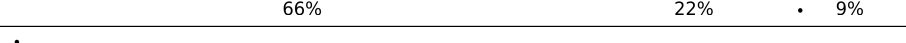
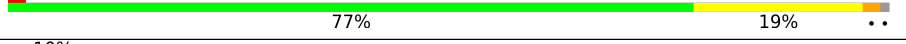



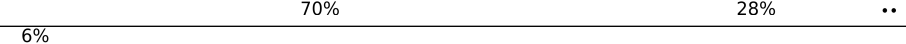



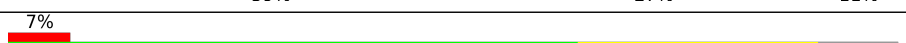
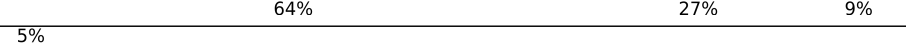




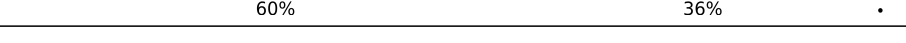

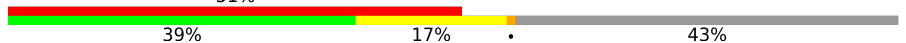



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	

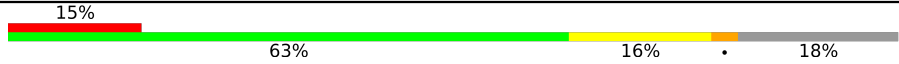
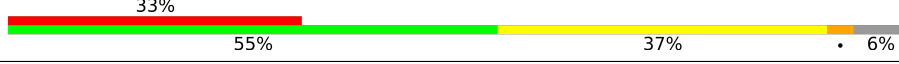



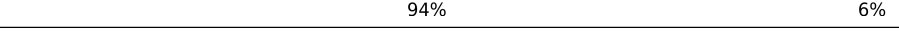



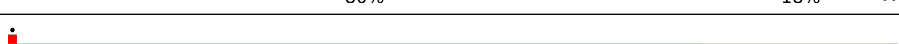
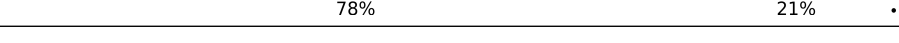




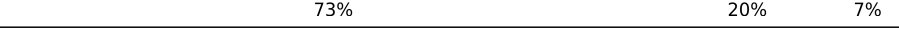



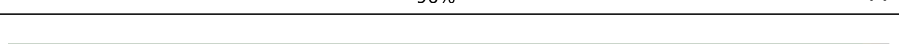
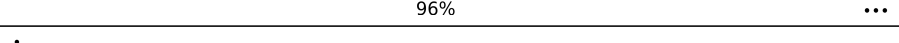

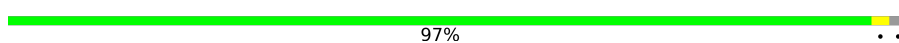

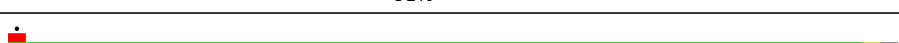
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Mol	Chain	Length	Quality of chain
8	SH	130	 67% 31% ..
9	SI	130	 11% 62% 33% ..
10	SJ	103	 24% 61% 32% ..
11	SK	129	 24% 66% 22% 9%
12	SL	124	 77% 19% ..
13	SM	118	 10% 64% 29% ..
14	SN	101	 67% 31% ..
15	SO	89	 6% 70% 28% ..
16	SP	82	 6% 72% 27% ..
17	SQ	84	 62% 32% 5%
18	SR	75	 17% 59% 27% 11%
19	SS	92	 7% 64% 27% 9%
20	ST	87	 5% 76% 22% ..
21	SU	71	 21% 77% 20% ..
22	mR	60	 7% 15% 5% 80%
23	23	2904	 60% 36% ..
24	5	120	 72% 26% ..
25	LA	234	 51% 39% 17% 43%
26	LB	273	 82% 18% ..
27	LC	209	 89% 11%
28	LD	201	 90% 10%
29	LE	179	 71% 24% ..
30	LF	177	 82% 16% ..
31	LG	121	 51% 35% 21% 44%
32	LI	149	 64% 81% 19%

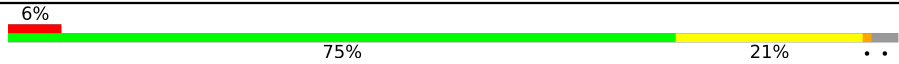



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Mol	Chain	Length	Quality of chain
33	LJ	165	
34	LK	142	
35	LM	142	
36	LN	123	
37	LO	144	
38	LP	136	
39	LQ	127	
40	LR	117	
41	LS	115	
42	LT	118	
43	LU	103	
44	LV	110	
45	LW	100	
46	LX	104	
47	LY	94	
48	La	85	
49	Lb	78	
50	Lc	63	
51	Ld	59	
52	Le	70	
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	
59	Pp	3	
60	Pt	76	
61	Dt	76	

## 2 Entry composition [i](#)

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
			Total	C	N	O	P		
1	16	1534	32929	14693	6041	10661	1534	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SB	226	1769	1119	317	325	8	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SG	156	1235	773	237	221	4	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SK	117	877	540	174	160	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SM	115	891	552	179	157	3	0	0

- 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
			Total	C	N	O	S		
35	LM	142	1129	714	212	199	4	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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		

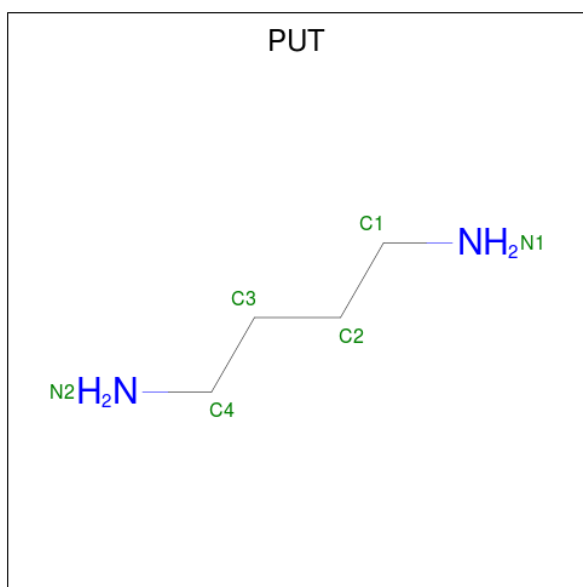
- Molecule 60 is a RNA chain called Chains: Pt.

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
			12	8	4	
62	16	1	Total	C	N	0
			12	8	4	
62	23	1	Total	C	N	0
			108	72	36	
62	23	1	Total	C	N	0
			108	72	36	
62	23	1	Total	C	N	0
			108	72	36	
62	23	1	Total	C	N	0
			108	72	36	
62	23	1	Total	C	N	0
			108	72	36	
62	23	1	Total	C	N	0
			108	72	36	
62	23	1	Total	C	N	0
			108	72	36	
62	23	1	Total	C	N	0
			108	72	36	
62	23	1	Total	C	N	0
			108	72	36	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
62	23	1	108	72	36	0
62	23	1	108	72	36	0
62	23	1	108	72	36	0
62	23	1	108	72	36	0
62	23	1	108	72	36	0
62	23	1	108	72	36	0
62	LC	1	6	4	2	0

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

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

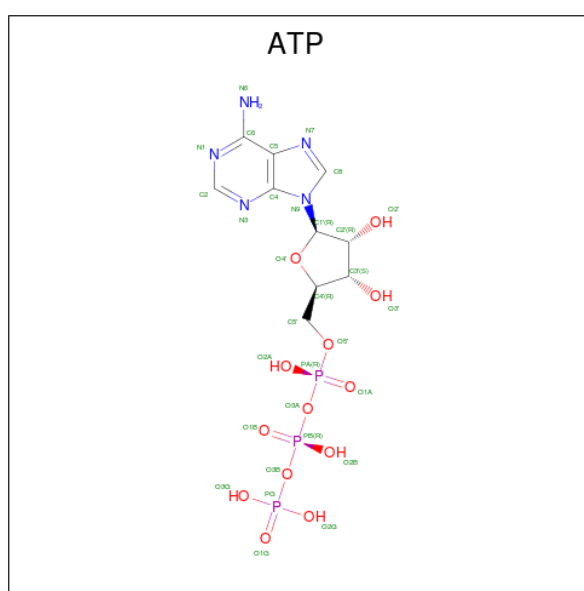
- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of

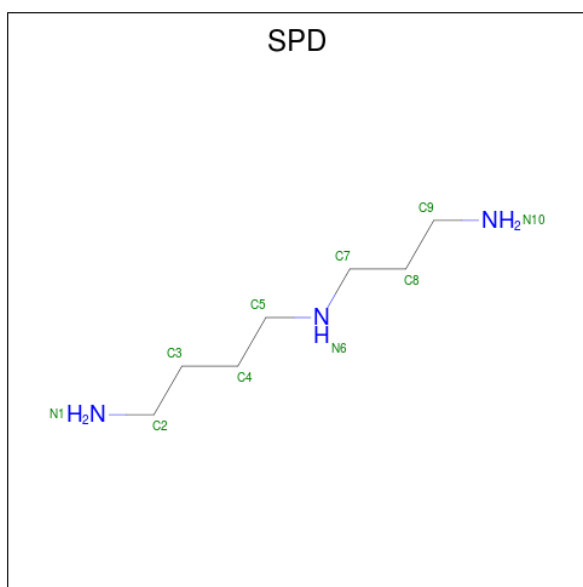


Interest" by depositor).

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	

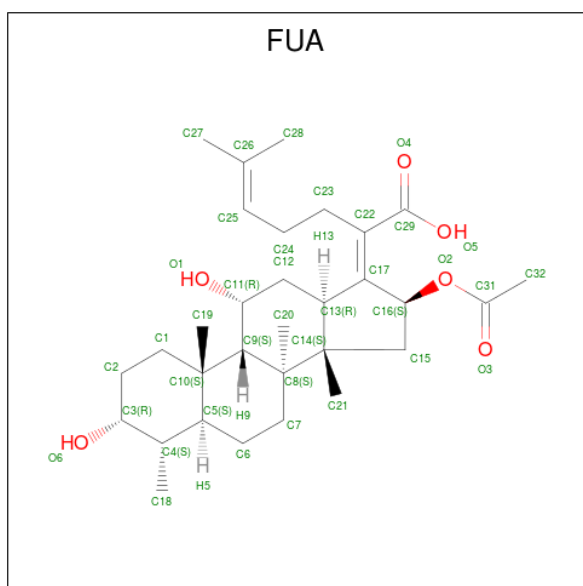
- Molecule 65 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			AltConf
66	23	1	Total	C	N	0
			30	21	9	
66	23	1	Total	C	N	0
			30	21	9	
66	23	1	Total	C	N	0
			30	21	9	

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

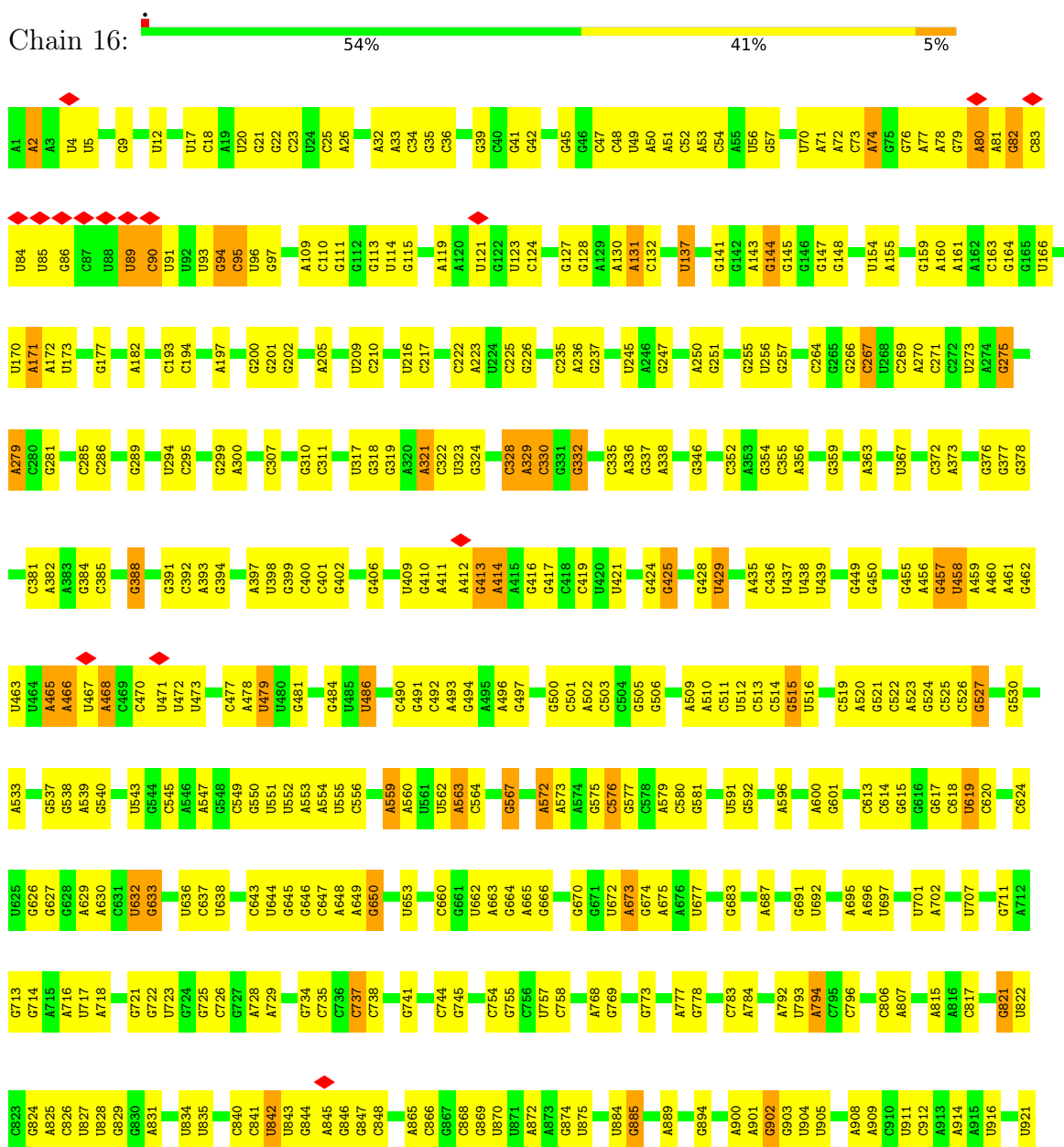


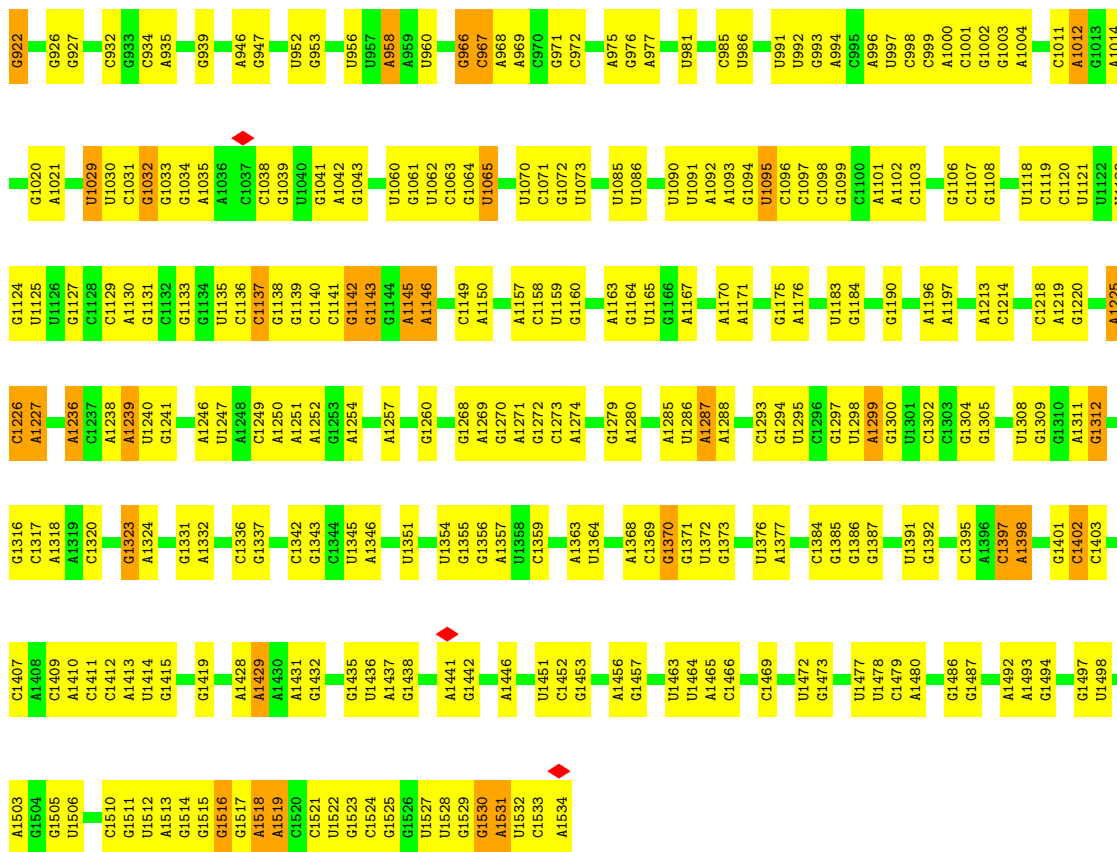


### 3 Residue-property plots

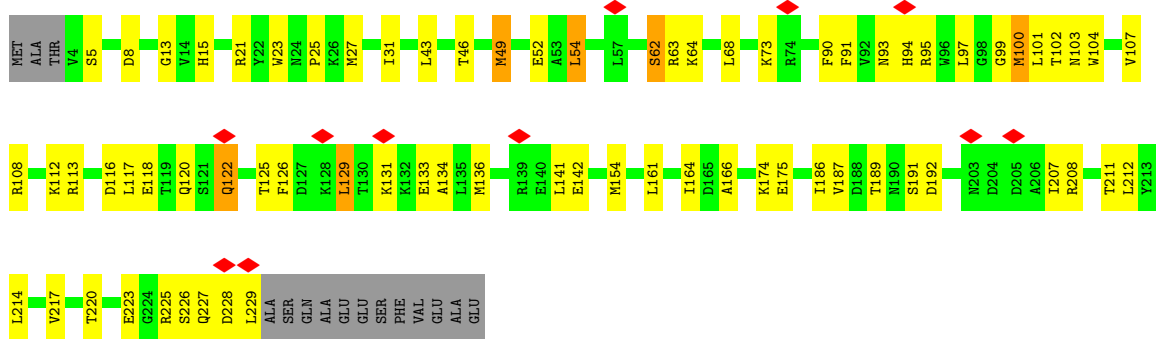
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

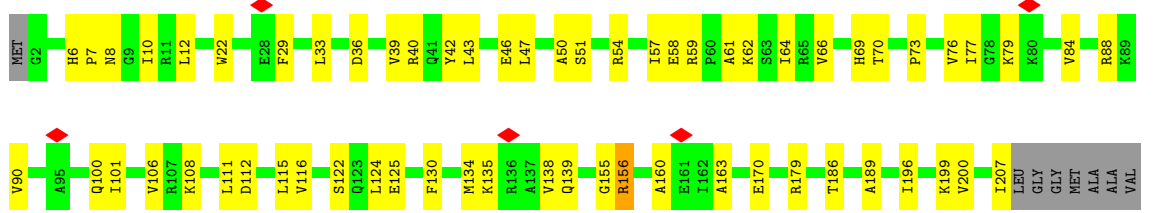




• Molecule 2: 30S ribosomal protein S2

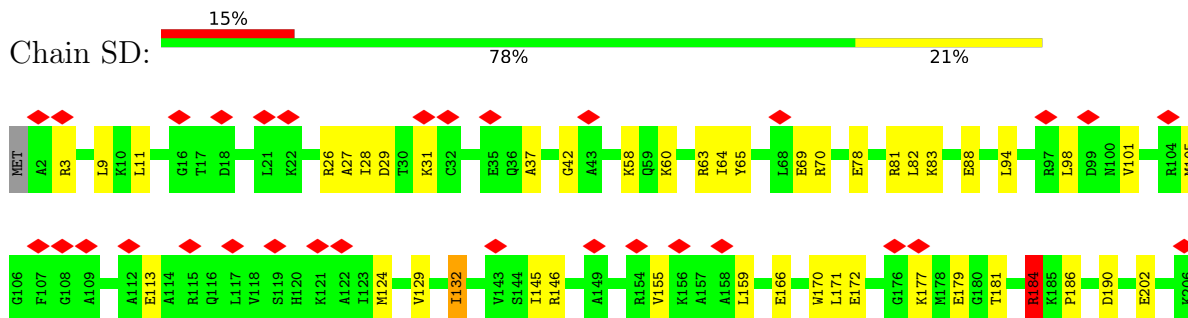


• Molecule 3: 30S ribosomal protein S3

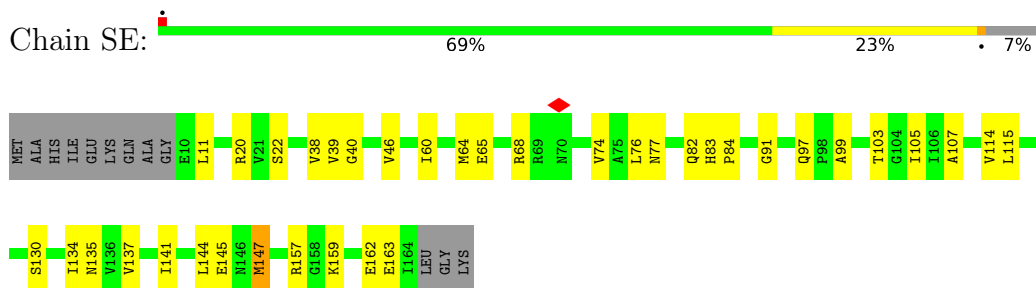


GLU  
GLN  
PRO  
GLU  
LYS  
PRO  
ALA  
GLN  
PRO  
LYS  
GLN  
GLN  
ARG  
LYS  
GLY  
ARG  
LYS

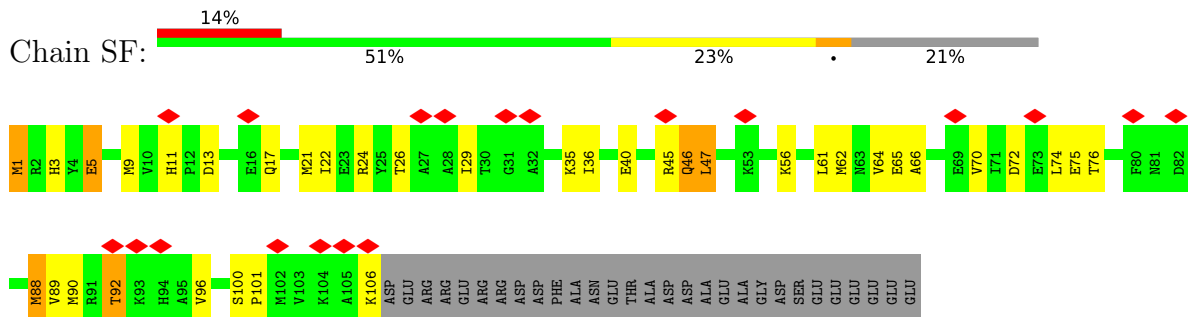
- Molecule 4: 30S ribosomal protein S4



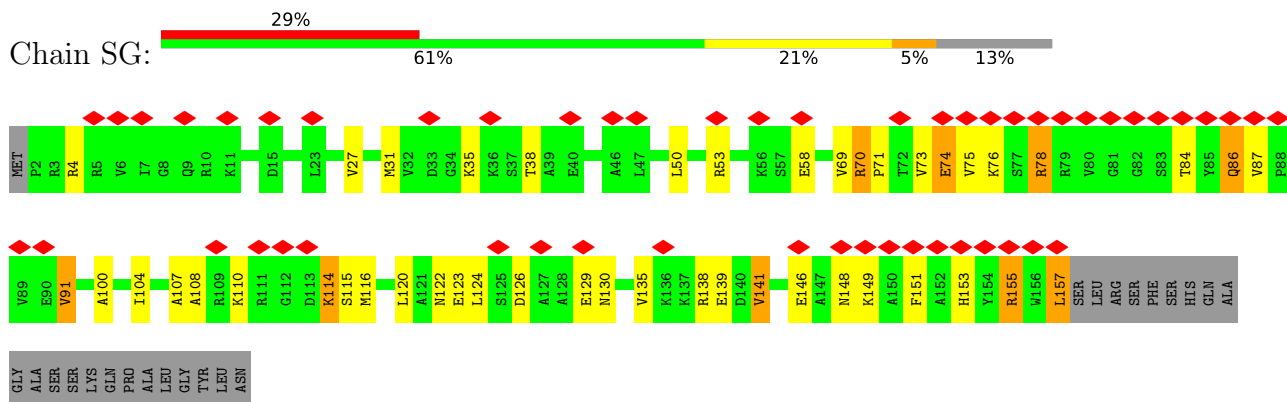
- Molecule 5: 30S ribosomal protein S5



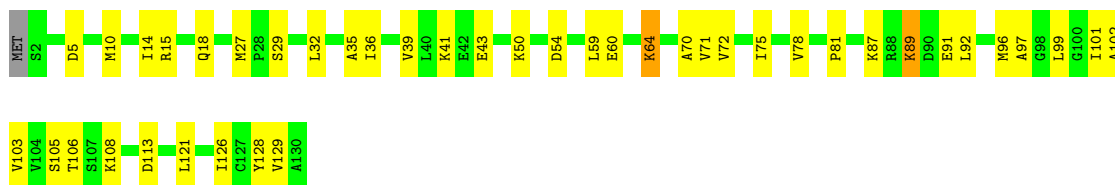
- Molecule 6: 30S ribosomal protein S6



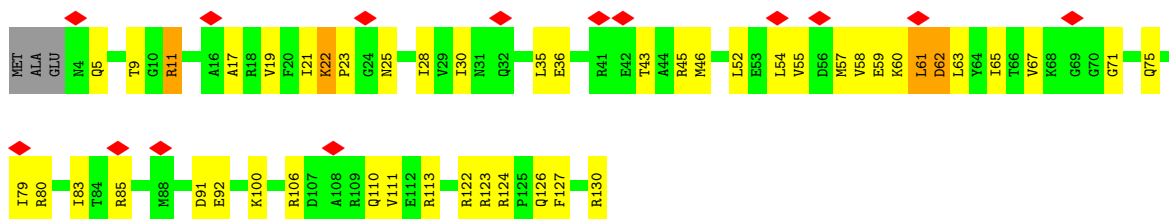
- Molecule 7: 30S ribosomal protein S7



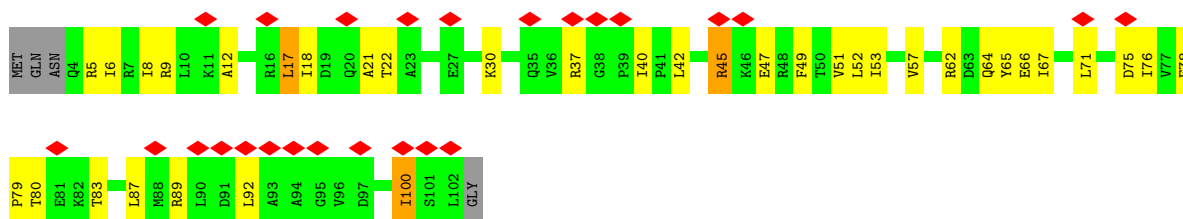
- Molecule 8: 30S ribosomal protein S8



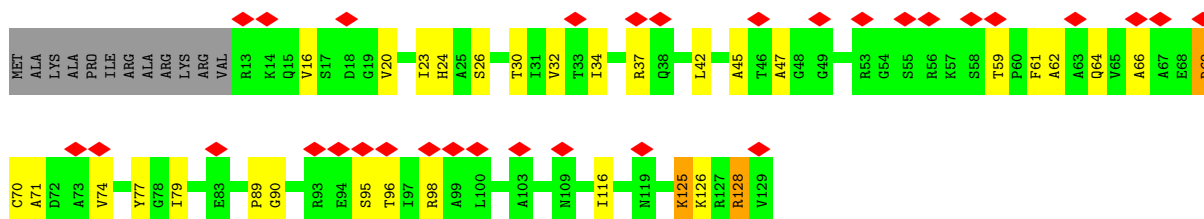
• Molecule 9: 30S ribosomal protein S9



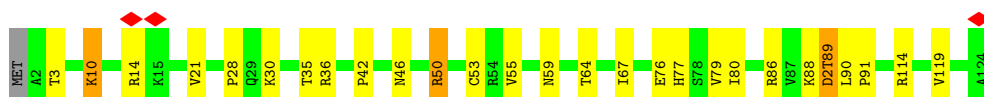
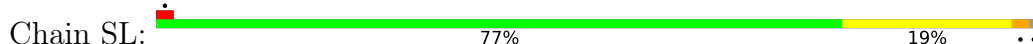
• Molecule 10: 30S ribosomal protein S10



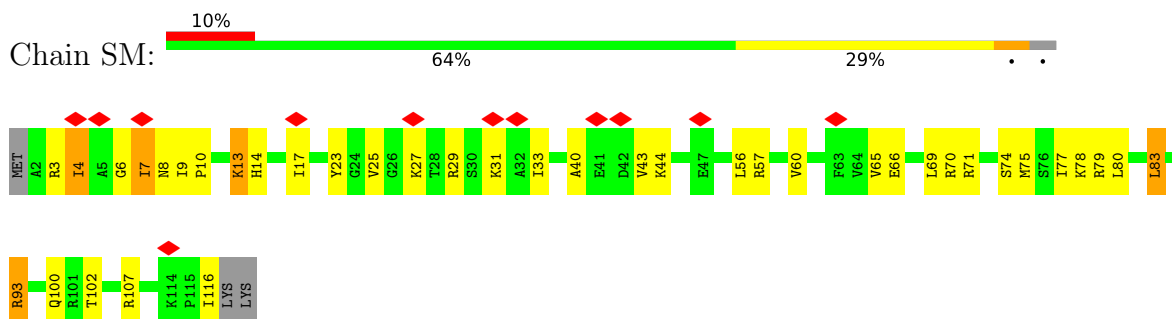
• Molecule 11: 30S ribosomal protein S11



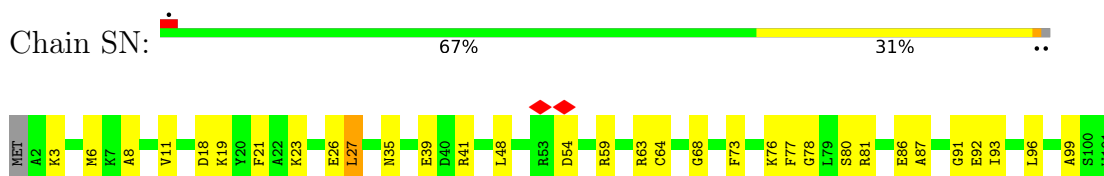
• Molecule 12: 30S ribosomal protein S12



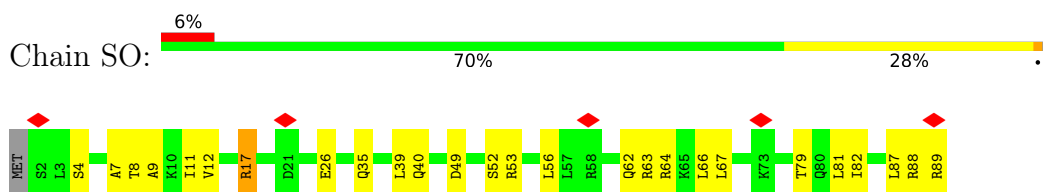
- Molecule 13: 30S ribosomal protein S13



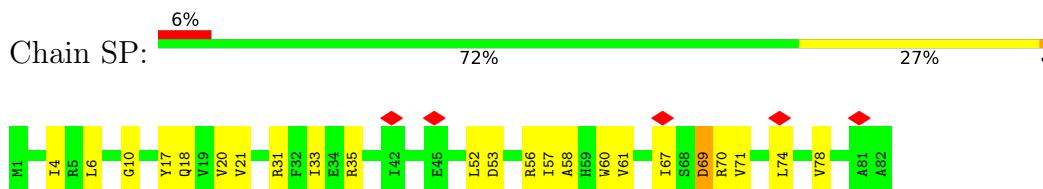
- Molecule 14: 30S ribosomal protein S14



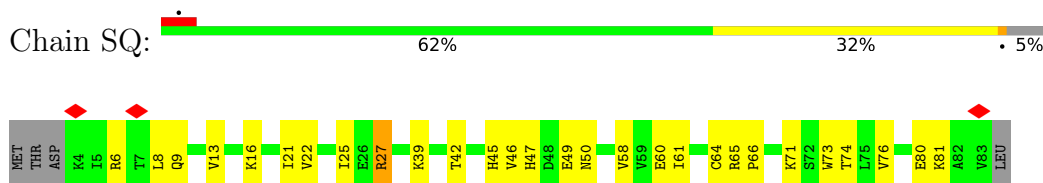
- Molecule 15: 30S ribosomal protein S15



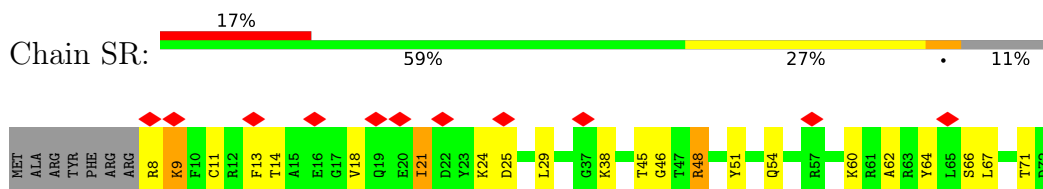
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

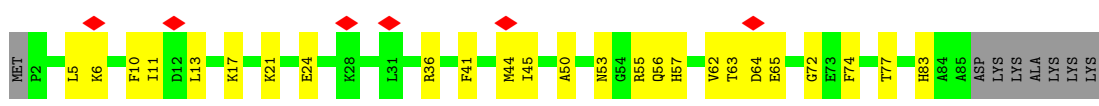


- Molecule 18: 30S ribosomal protein S18

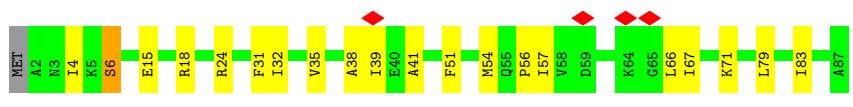
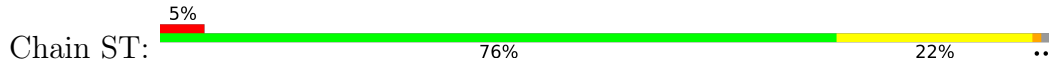


- Molecule 19: 30S ribosomal protein S19

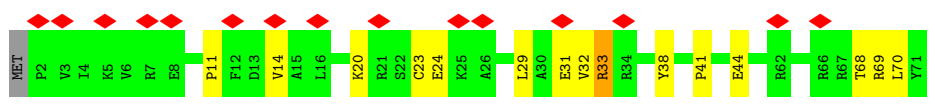
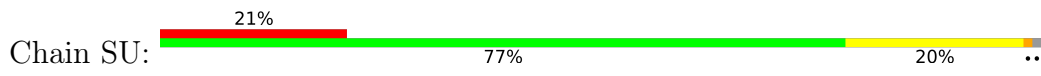




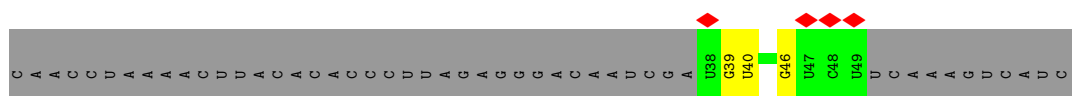
• Molecule 20: 30S ribosomal protein S20



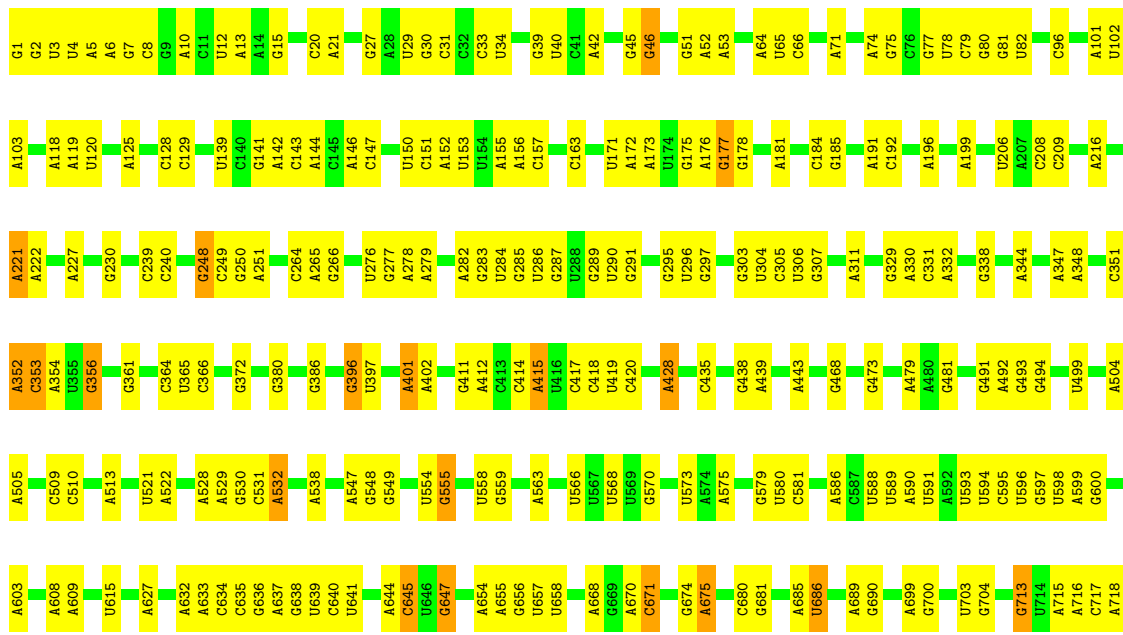
• Molecule 21: 30S ribosomal protein S21

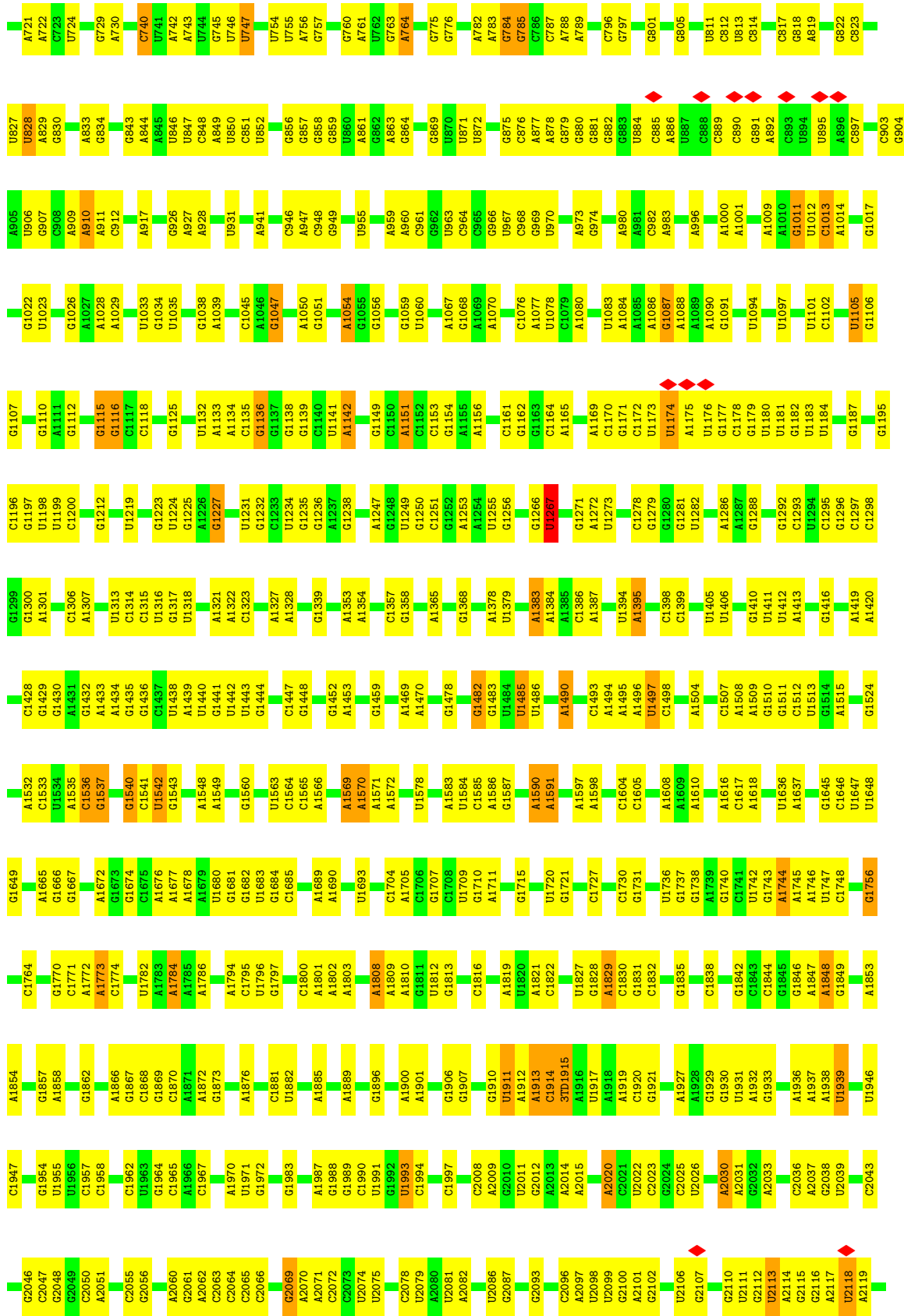


• Molecule 22: Chains: mR



• Molecule 23: 23S rRNA

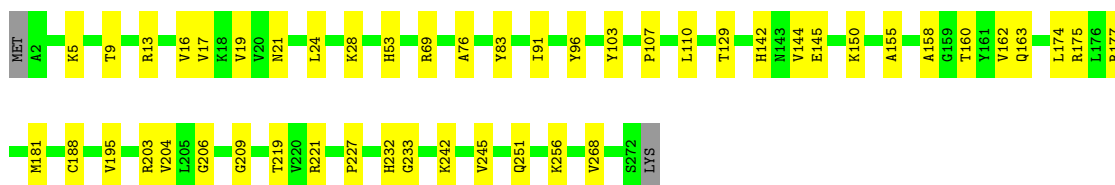
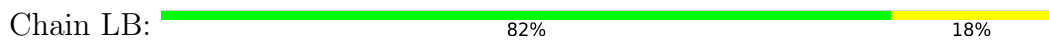




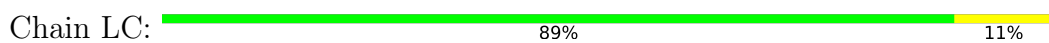




• Molecule 26: 50S ribosomal protein L2



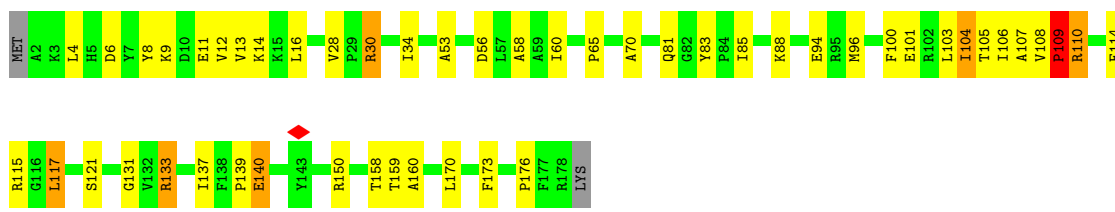
• Molecule 27: 50S ribosomal protein L3



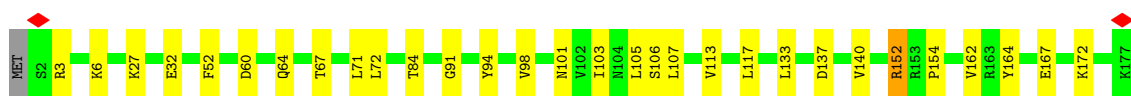
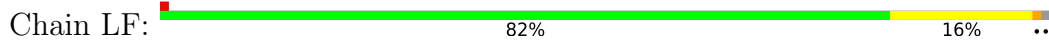
• Molecule 28: 50S ribosomal protein L4



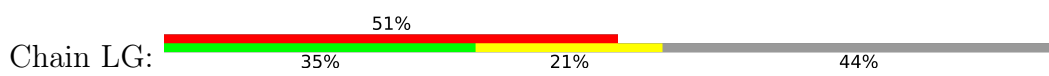
• Molecule 29: 50S ribosomal protein L5

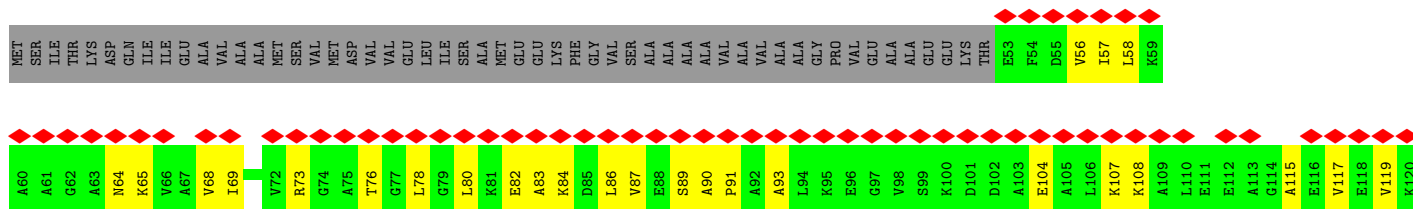


• Molecule 30: 50S ribosomal protein L6

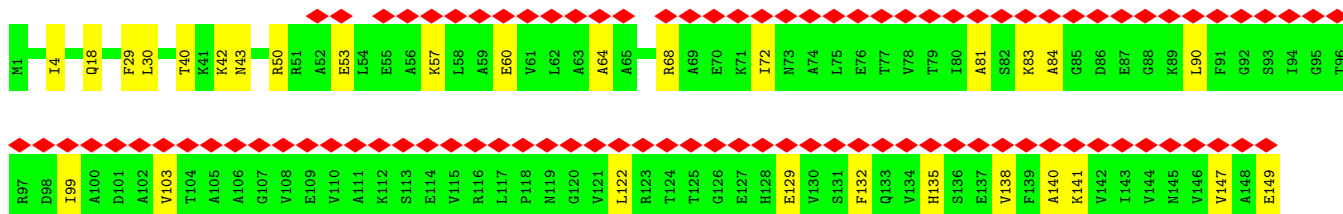
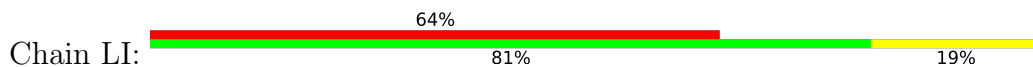


• Molecule 31: 50S ribosomal protein L7/L12

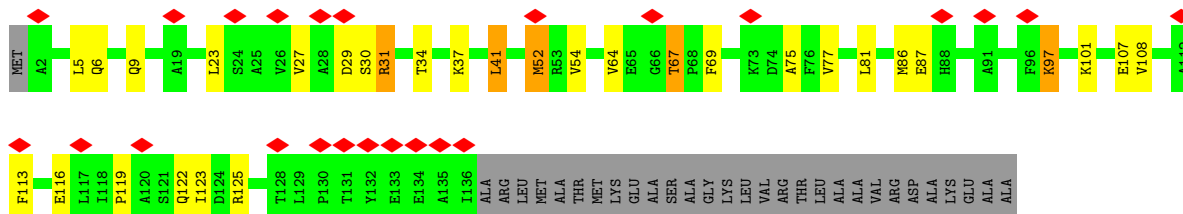




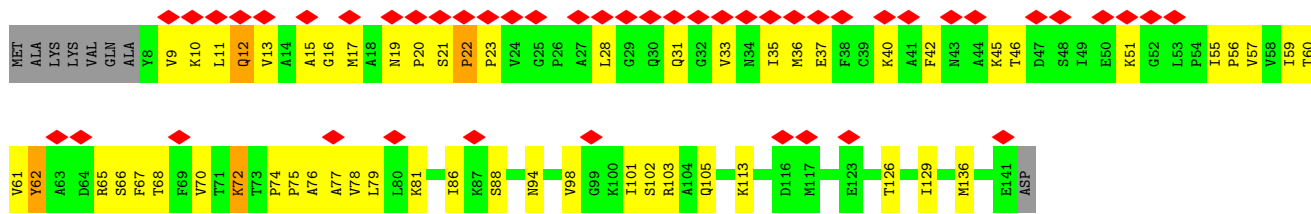
• Molecule 32: 50S ribosomal protein L9



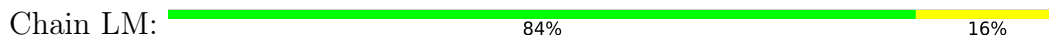
• Molecule 33: 50S ribosomal protein L10



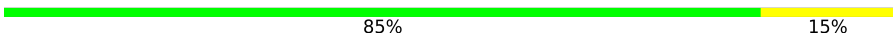
• Molecule 34: 50S ribosomal protein L11

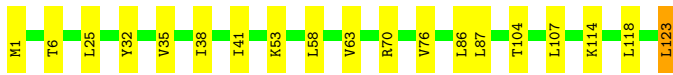


• Molecule 35: 50S ribosomal protein L13



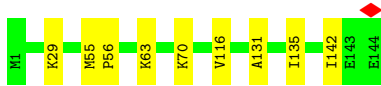
• Molecule 36: 50S ribosomal protein L14

Chain LN:  85% 15%




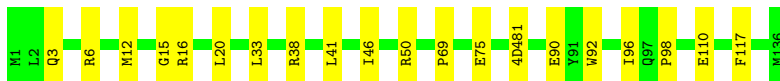
- Molecule 37: 50S ribosomal protein L15

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%




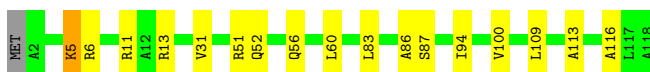
- Molecule 41: 50S ribosomal protein L19

Chain LS:  78% 21%

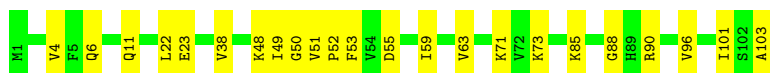
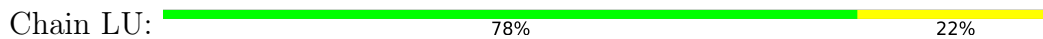


- Molecule 42: 50S ribosomal protein L20

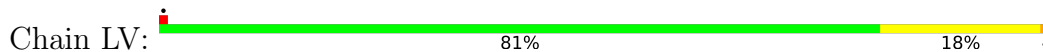
Chain LT:  85% 14%



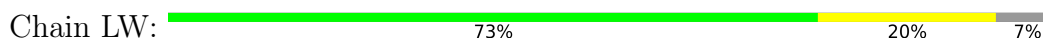
- Molecule 43: 50S ribosomal protein L21



• Molecule 44: 50S ribosomal protein L22



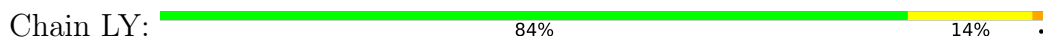
• Molecule 45: 50S ribosomal protein L23



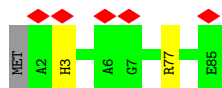
• Molecule 46: 50S ribosomal protein L24



• Molecule 47: 50S ribosomal protein L25



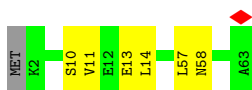
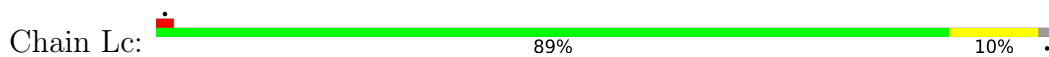
• Molecule 48: 50S ribosomal protein L27



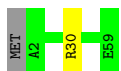
• Molecule 49: 50S ribosomal protein L28



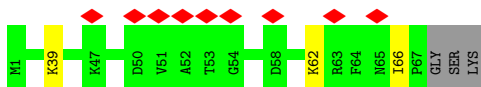
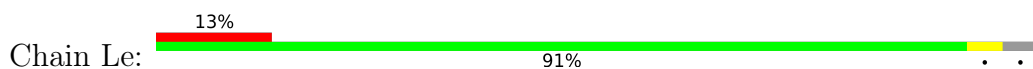
• Molecule 50: 50S ribosomal protein L29



- Molecule 51: 50S ribosomal protein L30



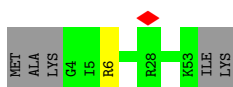
- Molecule 52: 50S ribosomal protein L31



- Molecule 53: 50S ribosomal protein L32



- Molecule 54: 50S ribosomal protein L33



- Molecule 55: 50S ribosomal protein L34



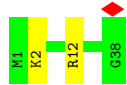
There are no outlier residues recorded for this chain.

- Molecule 56: 50S ribosomal protein L35

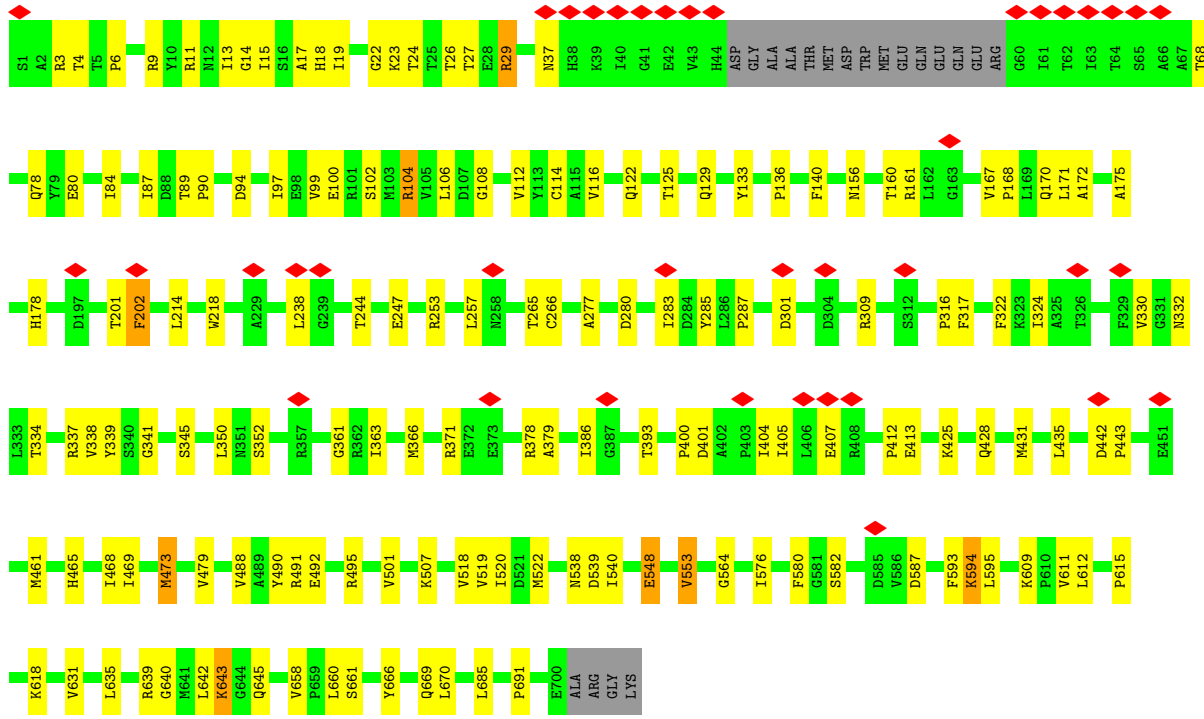
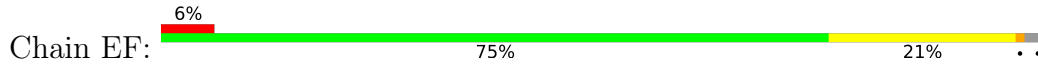


- Molecule 57: 50S ribosomal protein L36





• 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 i

### 5.1 Standard geometry i

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

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	16	32929	0	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 [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%)	19	41
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 [i](#)

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	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	SC	170/190 (90%)	164 (96%)	6 (4%)	36	63
4	SD	172/173 (99%)	162 (94%)	10 (6%)	20	42
5	SE	118/126 (94%)	111 (94%)	7 (6%)	19	41
6	SF	92/116 (79%)	75 (82%)	17 (18%)	1	3
7	SG	129/147 (88%)	106 (82%)	23 (18%)	2	4
8	SH	104/105 (99%)	100 (96%)	4 (4%)	33	60
9	SI	105/107 (98%)	86 (82%)	19 (18%)	1	4
10	SJ	87/90 (97%)	77 (88%)	10 (12%)	5	12
11	SK	90/99 (91%)	87 (97%)	3 (3%)	38	66
12	SL	102/103 (99%)	90 (88%)	12 (12%)	5	11
13	SM	93/96 (97%)	81 (87%)	12 (13%)	4	9
14	SN	83/84 (99%)	74 (89%)	9 (11%)	6	14
15	SO	76/77 (99%)	72 (95%)	4 (5%)	22	46
16	SP	65/65 (100%)	64 (98%)	1 (2%)	65	85
17	SQ	74/78 (95%)	69 (93%)	5 (7%)	16	35
18	SR	58/65 (89%)	49 (84%)	9 (16%)	2	6
19	SS	72/79 (91%)	70 (97%)	2 (3%)	43	71
20	ST	65/66 (98%)	61 (94%)	4 (6%)	18	39
21	SU	60/61 (98%)	56 (93%)	4 (7%)	16	35
25	LA	110/181 (61%)	102 (93%)	8 (7%)	14	31
26	LB	216/218 (99%)	211 (98%)	5 (2%)	50	77
27	LC	164/164 (100%)	162 (99%)	2 (1%)	71	88
28	LD	165/165 (100%)	165 (100%)	0	100	100
29	LE	148/150 (99%)	141 (95%)	7 (5%)	26	52
30	LF	137/138 (99%)	136 (99%)	1 (1%)	84	93
31	LG	47/85 (55%)	45 (96%)	2 (4%)	29	55
32	LI	114/114 (100%)	110 (96%)	4 (4%)	36	63
33	LJ	103/123 (84%)	91 (88%)	12 (12%)	5	12
34	LK	103/110 (94%)	80 (78%)	23 (22%)	1	2
35	LM	116/116 (100%)	115 (99%)	1 (1%)	78	91
36	LN	104/104 (100%)	103 (99%)	1 (1%)	76	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	LO	103/103 (100%)	102 (99%)	1 (1%)	76	90
38	LP	108/108 (100%)	105 (97%)	3 (3%)	43	71
39	LQ	100/103 (97%)	100 (100%)	0	100	100
40	LR	86/87 (99%)	83 (96%)	3 (4%)	36	63
41	LS	99/100 (99%)	96 (97%)	3 (3%)	41	69
42	LT	89/90 (99%)	86 (97%)	3 (3%)	37	65
43	LU	84/84 (100%)	83 (99%)	1 (1%)	71	88
44	LV	93/93 (100%)	91 (98%)	2 (2%)	52	78
45	LW	80/84 (95%)	77 (96%)	3 (4%)	33	60
46	LX	83/85 (98%)	82 (99%)	1 (1%)	71	88
47	LY	78/78 (100%)	75 (96%)	3 (4%)	33	60
48	La	62/63 (98%)	61 (98%)	1 (2%)	62	83
49	Lb	67/68 (98%)	65 (97%)	2 (3%)	41	69
50	Lc	54/55 (98%)	49 (91%)	5 (9%)	9	20
51	Ld	48/49 (98%)	48 (100%)	0	100	100
52	Le	60/62 (97%)	57 (95%)	3 (5%)	24	49
53	Lf	47/48 (98%)	47 (100%)	0	100	100
54	Lg	45/49 (92%)	44 (98%)	1 (2%)	52	78
55	Lh	38/38 (100%)	38 (100%)	0	100	100
56	Li	51/52 (98%)	49 (96%)	2 (4%)	32	59
57	Lj	34/34 (100%)	32 (94%)	2 (6%)	19	41
58	EF	480/578 (83%)	446 (93%)	34 (7%)	14	33
59	Pp	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	5522/5908 (94%)	5195 (94%)	327 (6%)	23	41

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 [i](#)

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 [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
23	PSU	23	2457	23	18,21,22	1.40	2 (11%)	22,30,33	1.95	5 (22%)
1	MA6	16	1518	1	19,26,27	1.20	2 (10%)	18,38,41	1.65	4 (22%)
1	UR3	16	1498	1	19,22,23	0.96	0	26,32,35	1.42	1 (3%)
61	4SU	Dt	8	61	18,21,22	1.85	4 (22%)	26,30,33	2.20	5 (19%)
23	PSU	23	2604	23	18,21,22	1.48	3 (16%)	22,30,33	2.05	4 (18%)
60	PSU	Pt	39	60	18,21,22	1.38	2 (11%)	22,30,33	1.85	4 (18%)
60	H2U	Pt	16	60	18,21,22	1.03	2 (11%)	21,30,33	1.32	3 (14%)
23	OMG	23	2251	60,23	18,26,27	1.17	2 (11%)	19,38,41	0.86	1 (5%)
23	PSU	23	2580	23	18,21,22	1.39	2 (11%)	22,30,33	1.92	4 (18%)
60	5MU	Pt	54	60	19,22,23	1.39	6 (31%)	28,32,35	2.06	6 (21%)
61	G7M	Dt	46	61	20,26,27	2.63	4 (20%)	17,39,42	0.98	1 (5%)
23	OMU	23	2552	23	19,22,23	1.22	3 (15%)	26,31,34	1.75	5 (19%)
23	PSU	23	955	23	18,21,22	1.38	3 (16%)	22,30,33	1.96	3 (13%)
23	G7M	23	2069	23	20,26,27	2.81	5 (25%)	17,39,42	2.05	4 (23%)
60	3AU	Pt	47	60	24,28,29	1.03	0	33,40,43	1.50	4 (12%)
1	MA6	16	1519	1	19,26,27	1.08	2 (10%)	18,38,41	1.43	2 (11%)
23	5MU	23	747	23	19,22,23	1.41	5 (26%)	28,32,35	2.10	6 (21%)
23	2MA	23	2503	63,23	17,25,26	0.99	1 (5%)	17,37,40	0.99	2 (11%)
1	4OC	16	1402	1	20,23,24	0.76	0	26,32,35	0.92	1 (3%)
23	PSU	23	746	63,23	18,21,22	1.39	3 (16%)	22,30,33	1.84	3 (13%)
23	PSU	23	2504	23	18,21,22	1.37	3 (16%)	22,30,33	1.93	3 (13%)
61	PSU	Dt	39	61	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
61	PSU	Dt	55	61	18,21,22	1.40	2 (11%)	22,30,33	2.05	4 (18%)
23	PSU	23	1917	23	18,21,22	6.01	12 (66%)	22,30,33	1.88	5 (22%)
60	H2U	Pt	17	60	18,21,22	0.96	2 (11%)	21,30,33	1.33	3 (14%)
23	2MG	23	2445	23	18,26,27	0.94	1 (5%)	16,38,41	1.15	2 (12%)
23	PSU	23	1911	23	18,21,22	6.01	13 (72%)	22,30,33	1.82	5 (22%)
1	G7M	16	527	1	20,26,27	2.63	4 (20%)	17,39,42	1.10	1 (5%)
60	PSU	Pt	55	60	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	2MG	23	1835	23	18,26,27	0.91	1 (5%)	16,38,41	1.15	3 (18%)
23	3TD	23	1915	23	18,22,23	1.36	2 (11%)	22,32,35	2.19	3 (13%)
12	D2T	SL	89	12	7,9,10	0.99	0	6,11,13	2.84	4 (66%)
23	PSU	23	2605	23	18,21,22	1.38	3 (16%)	22,30,33	1.87	4 (18%)
38	4D4	LP	81	38	9,11,12	2.09	2 (22%)	8,13,15	2.08	4 (50%)
23	5MU	23	1939	23	19,22,23	1.44	5 (26%)	28,32,35	2.32	6 (21%)
60	H2U	Pt	20	60	18,21,22	1.06	2 (11%)	21,30,33	2.73	4 (19%)
60	T6A	Pt	37	60	27,34,35	0.99	2 (7%)	29,49,52	1.55	5 (17%)
23	1MG	23	745	23	18,26,27	0.95	0	19,39,42	1.23	2 (10%)
1	2MG	16	1516	1	18,26,27	0.92	1 (5%)	16,38,41	1.15	2 (12%)
61	3AU	Dt	47	61	24,28,29	1.01	0	33,40,43	1.53	4 (12%)
23	OMC	23	2498	63,23	19,22,23	0.83	0	26,31,34	0.89	1 (3%)
1	5MC	16	967	1	18,22,23	0.98	2 (11%)	26,32,35	1.20	3 (11%)
23	6MZ	23	2030	23	18,25,26	0.85	1 (5%)	16,36,39	2.26	4 (25%)
61	MIA	Dt	37	61	24,31,32	2.31	3 (12%)	26,44,47	2.76	10 (38%)
23	6MZ	23	1618	23	18,25,26	0.86	1 (5%)	16,36,39	2.04	4 (25%)
1	2MG	16	966	1	18,26,27	1.05	1 (5%)	16,38,41	1.29	3 (18%)
23	5MC	23	1962	23	18,22,23	0.94	2 (11%)	26,32,35	1.14	2 (7%)
1	5MC	16	1407	1	18,22,23	0.93	2 (11%)	26,32,35	1.13	3 (11%)
61	PSU	Dt	32	61	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	16	516	1	18,21,22	1.41	3 (16%)	22,30,33	1.94	4 (18%)
60	U8U	Pt	34	60,22	19,24,25	1.57	3 (15%)	23,34,37	1.32	3 (13%)
23	H2U	23	2449	23	18,21,22	1.09	2 (11%)	21,30,33	1.44	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
1	MA6	16	1518	1	-	3/7/29/30	0/3/3/3
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
61	4SU	Dt	8	61	-	3/7/25/26	0/2/2/2
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
60	PSU	Pt	39	60	-	0/7/25/26	0/2/2/2
60	H2U	Pt	16	60	-	3/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	OMG	23	2251	60,23	-	1/5/27/28	0/3/3/3
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
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	OMU	23	2552	23	-	2/9/27/28	0/2/2/2
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
23	G7M	23	2069	23	-	1/3/25/26	0/3/3/3
60	3AU	Pt	47	60	-	3/16/34/35	0/2/2/2
1	MA6	16	1519	1	-	6/7/29/30	0/3/3/3
23	5MU	23	747	23	-	0/7/25/26	0/2/2/2
23	2MA	23	2503	63,23	-	1/3/25/26	0/3/3/3
1	4OC	16	1402	1	-	0/9/29/30	0/2/2/2
23	PSU	23	746	63,23	-	4/7/25/26	0/2/2/2
23	PSU	23	2504	23	-	2/7/25/26	0/2/2/2
61	PSU	Dt	39	61	-	2/7/25/26	0/2/2/2
61	PSU	Dt	55	61	-	0/7/25/26	0/2/2/2
23	PSU	23	1917	23	-	0/7/25/26	0/2/2/2
60	H2U	Pt	17	60	-	3/7/38/39	0/2/2/2
23	2MG	23	2445	23	-	1/5/27/28	0/3/3/3
23	PSU	23	1911	23	-	0/7/25/26	0/2/2/2
1	G7M	16	527	1	-	2/3/25/26	0/3/3/3
60	PSU	Pt	55	60	-	0/7/25/26	0/2/2/2
23	2MG	23	1835	23	-	0/5/27/28	0/3/3/3
23	3TD	23	1915	23	-	0/7/25/26	0/2/2/2
12	D2T	SL	89	12	-	3/7/12/14	-
23	PSU	23	2605	23	-	2/7/25/26	0/2/2/2
38	4D4	LP	81	38	-	4/11/12/14	-
23	5MU	23	1939	23	-	2/7/25/26	0/2/2/2
60	H2U	Pt	20	60	-	5/7/38/39	0/2/2/2
60	T6A	Pt	37	60	-	10/19/41/42	0/3/3/3
23	1MG	23	745	23	-	0/3/25/26	0/3/3/3
1	2MG	16	1516	1	-	0/5/27/28	0/3/3/3
61	3AU	Dt	47	61	-	9/16/34/35	0/2/2/2
23	OMC	23	2498	63,23	-	2/9/27/28	0/2/2/2
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
23	6MZ	23	2030	23	-	2/5/27/28	0/3/3/3
61	MIA	Dt	37	61	-	5/11/33/34	0/3/3/3
23	6MZ	23	1618	23	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	16	966	1	-	0/5/27/28	0/3/3/3
23	5MC	23	1962	23	-	4/7/25/26	0/2/2/2
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
61	PSU	Dt	32	61	-	0/7/25/26	0/2/2/2
1	PSU	16	516	1	-	0/7/25/26	0/2/2/2
60	U8U	Pt	34	60,22	-	4/9/28/29	0/2/2/2
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	1911	PSU	C6-C5	11.72	1.49	1.35
23	23	1911	PSU	C2-N1	11.69	1.52	1.36
23	23	1917	PSU	C2-N1	11.69	1.52	1.36
23	23	1917	PSU	C6-C5	11.62	1.48	1.35
23	23	1917	PSU	O4'-C1'	10.64	1.58	1.43

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	Pt	20	H2U	C4-N3-C2	-11.11	116.57	125.79
61	Dt	37	MIA	C12-C13-C14	-8.41	110.78	127.14
23	23	1915	3TD	N1-C2-N3	7.45	122.02	116.14
23	23	2604	PSU	N1-C2-N3	6.30	122.27	115.13
61	Dt	55	PSU	N1-C2-N3	6.28	122.25	115.13

There are no chirality outliers.

5 of 90 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	527	G7M	C3'-C4'-C5'-O5'
1	16	1518	MA6	C5-C6-N6-C9
1	16	1519	MA6	O4'-C4'-C5'-O5'
1	16	1519	MA6	C3'-C4'-C5'-O5'
1	16	1519	MA6	C5-C6-N6-C10

There are no ring outliers.

13 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	16	1518	MA6	1	0

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	3009	-	5,5,5	0.10	0	4,4,4	0.16	0
62	PUT	23	3015	-	5,5,5	0.15	0	4,4,4	0.18	0
62	PUT	23	3010	-	5,5,5	0.12	0	4,4,4	0.15	0
66	SPD	23	3021	-	9,9,9	0.32	0	8,8,8	0.92	0
62	PUT	23	3013	-	5,5,5	0.11	0	4,4,4	0.16	0
62	PUT	23	3004	-	5,5,5	0.11	0	4,4,4	0.15	0
62	PUT	23	3016	-	5,5,5	0.10	0	4,4,4	0.17	0
62	PUT	23	3020	-	5,5,5	0.18	0	4,4,4	0.18	0
62	PUT	LC	301	-	5,5,5	0.11	0	4,4,4	0.16	0
66	SPD	23	3023	-	9,9,9	0.16	0	8,8,8	0.24	0
62	PUT	16	1601	-	5,5,5	0.13	0	4,4,4	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
62	PUT	23	3017	-	5,5,5	0.13	0	4,4,4	0.16	0
68	GDP	EF	803	63	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
62	PUT	23	3019	-	5,5,5	0.13	0	4,4,4	0.16	0
62	PUT	23	3003	-	5,5,5	0.16	0	4,4,4	0.20	0
65	ATP	23	3002	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
62	PUT	16	1602	-	5,5,5	0.17	0	4,4,4	0.20	0
62	PUT	23	3006	-	5,5,5	0.10	0	4,4,4	0.16	0
62	PUT	23	3012	-	5,5,5	0.13	0	4,4,4	0.16	0
65	ATP	23	3001	-	26,33,33	0.60	0	31,52,52	0.73	2 (6%)
62	PUT	23	3007	-	5,5,5	0.11	0	4,4,4	0.15	0
62	PUT	23	3011	-	5,5,5	0.11	0	4,4,4	0.16	0
67	FUA	EF	802	63	39,40,40	2.10	14 (35%)	49,64,64	2.64	18 (36%)
62	PUT	23	3008	-	5,5,5	0.12	0	4,4,4	0.17	0
62	PUT	23	3018	-	5,5,5	0.12	0	4,4,4	0.16	0
62	PUT	23	3005	-	5,5,5	0.12	0	4,4,4	0.16	0
62	PUT	23	3014	-	5,5,5	0.11	0	4,4,4	0.16	0
66	SPD	23	3022	-	9,9,9	0.32	0	8,8,8	0.90	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	3009	-	-	0/3/3/3	-
62	PUT	23	3015	-	-	1/3/3/3	-
62	PUT	23	3010	-	-	1/3/3/3	-
66	SPD	23	3021	-	-	2/7/7/7	-
62	PUT	23	3013	-	-	0/3/3/3	-
62	PUT	23	3004	-	-	0/3/3/3	-
62	PUT	23	3016	-	-	1/3/3/3	-
62	PUT	23	3020	-	-	0/3/3/3	-
62	PUT	LC	301	-	-	1/3/3/3	-
66	SPD	23	3023	-	-	2/7/7/7	-
62	PUT	16	1601	-	-	0/3/3/3	-
62	PUT	23	3017	-	-	1/3/3/3	-
68	GDP	EF	803	63	-	4/12/32/32	0/3/3/3
62	PUT	23	3019	-	-	0/3/3/3	-
62	PUT	23	3003	-	-	0/3/3/3	-
65	ATP	23	3002	-	-	5/18/38/38	0/3/3/3
62	PUT	16	1602	-	-	3/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
62	PUT	23	3006	-	-	0/3/3/3	-
62	PUT	23	3012	-	-	0/3/3/3	-
65	ATP	23	3001	-	-	5/18/38/38	0/3/3/3
62	PUT	23	3007	-	-	1/3/3/3	-
62	PUT	23	3011	-	-	1/3/3/3	-
67	FUA	EF	802	63	-	5/15/92/92	0/4/4/4
62	PUT	23	3008	-	-	0/3/3/3	-
62	PUT	23	3018	-	-	1/3/3/3	-
62	PUT	23	3005	-	-	0/3/3/3	-
62	PUT	23	3014	-	-	1/3/3/3	-
66	SPD	23	3022	-	-	0/7/7/7	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	EF	802	FUA	C9-C11	5.08	1.61	1.54
67	EF	802	FUA	C13-C17	-4.19	1.46	1.52
67	EF	802	FUA	C28-C26	4.03	1.61	1.50
67	EF	802	FUA	C10-C5	-3.97	1.48	1.56
67	EF	802	FUA	C20-C8	-3.59	1.47	1.54

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	-7.29	102.42	111.36
67	EF	802	FUA	C28-C26-C27	-7.16	98.79	114.60
67	EF	802	FUA	C27-C26-C25	5.77	139.33	122.65
67	EF	802	FUA	C21-C14-C8	5.65	117.49	112.27
67	EF	802	FUA	C19-C10-C5	-4.51	104.97	111.18

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

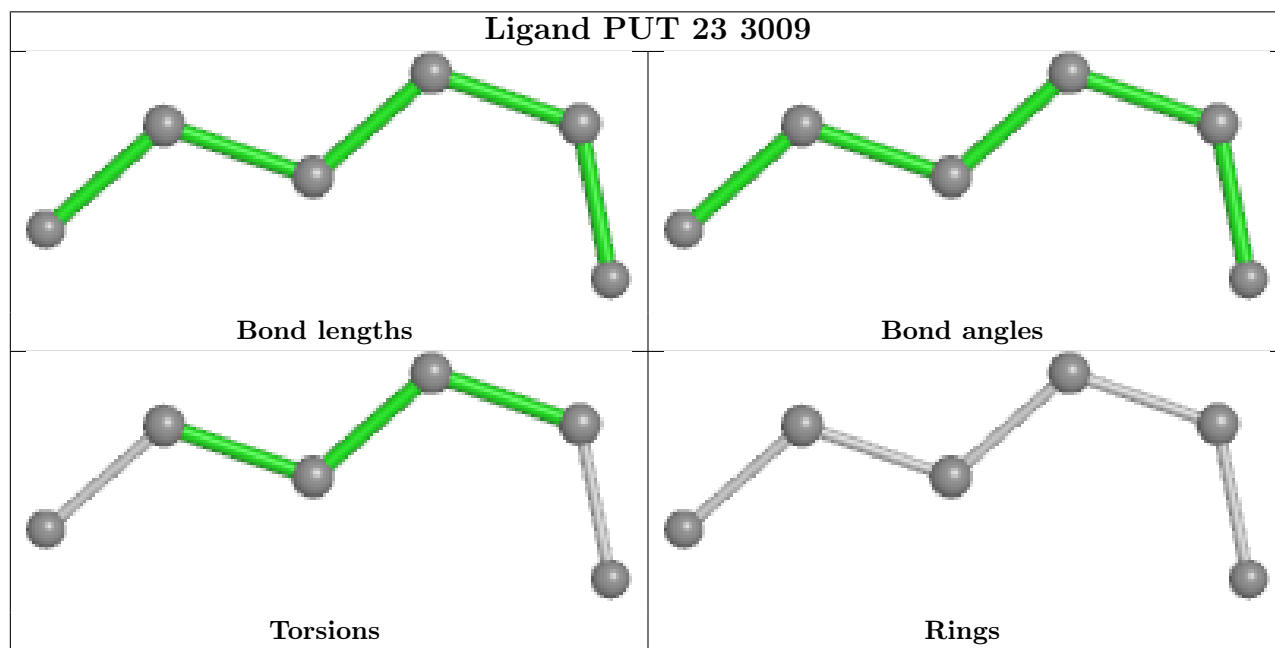
Mol	Chain	Res	Type	Atoms
65	23	3001	ATP	C5'-O5'-PA-O3A
65	23	3002	ATP	PB-O3B-PG-O3G
65	23	3002	ATP	O4'-C4'-C5'-O5'
65	23	3002	ATP	C3'-C4'-C5'-O5'
67	EF	802	FUA	C23-C22-C29-O5

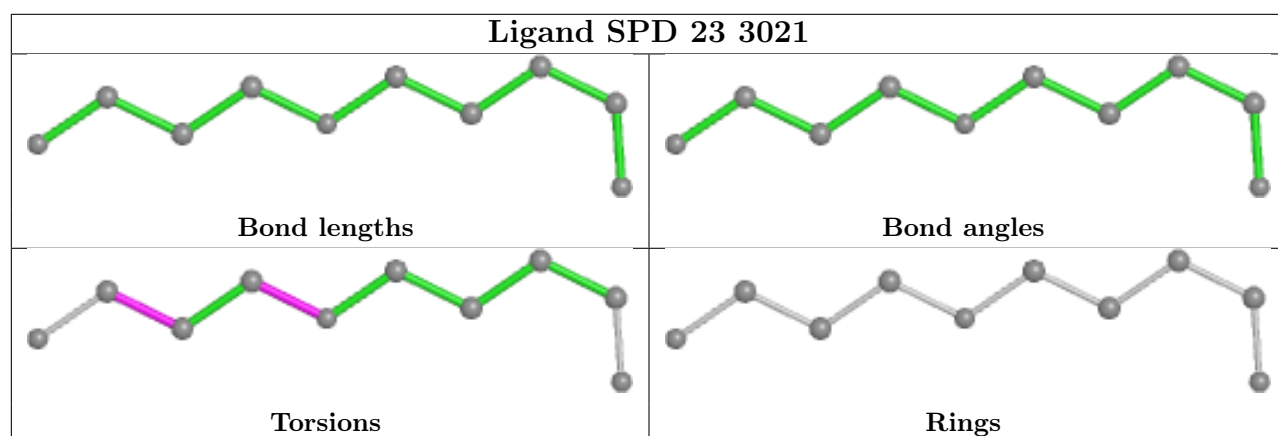
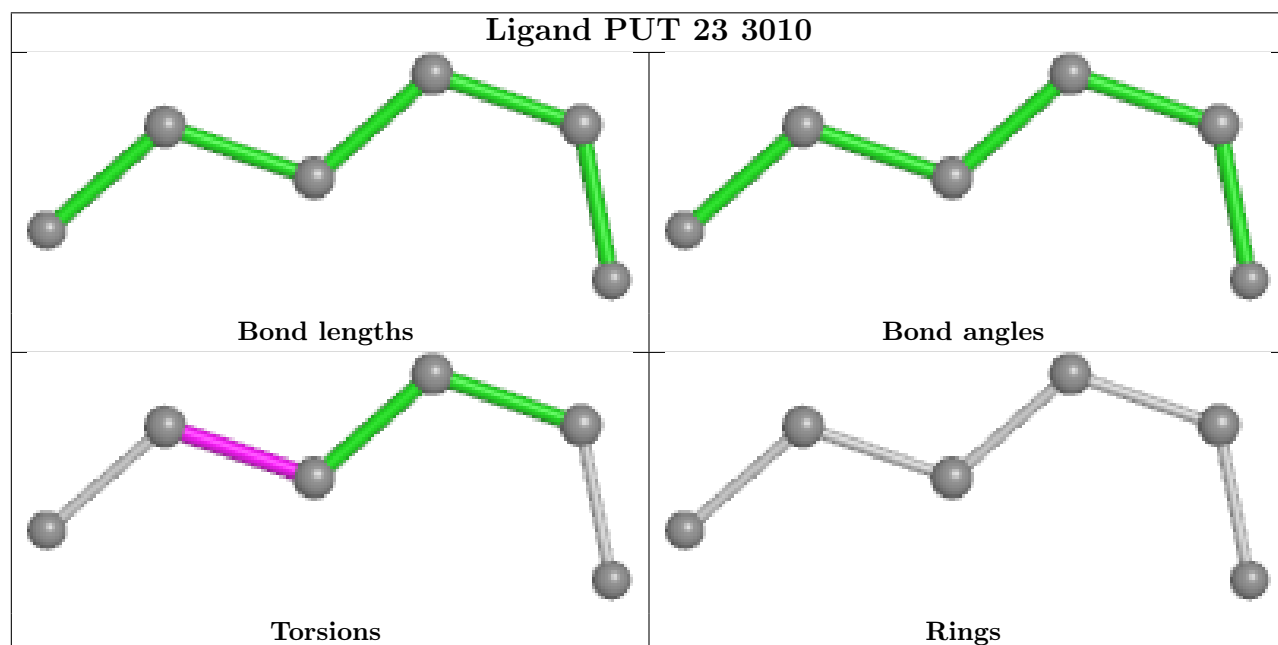
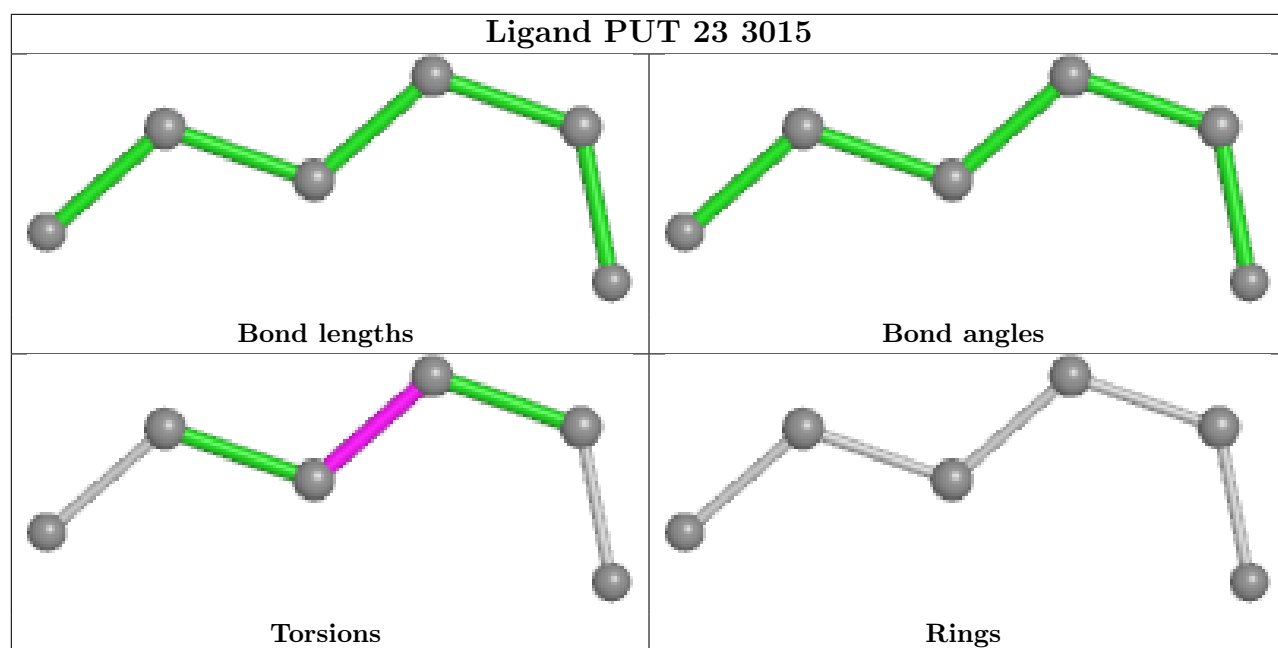
There are no ring outliers.

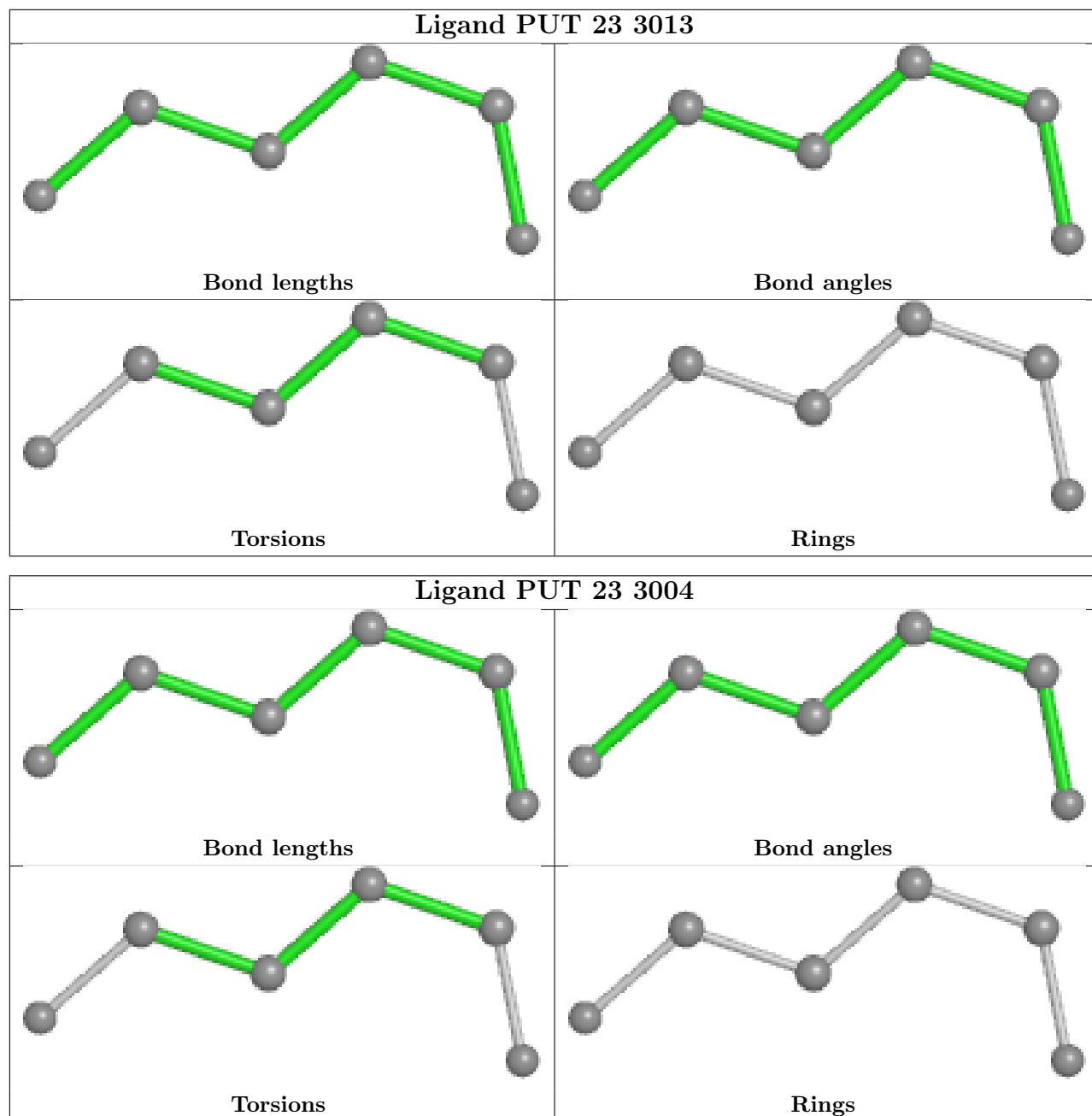
6 monomers are involved in 21 short contacts:

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

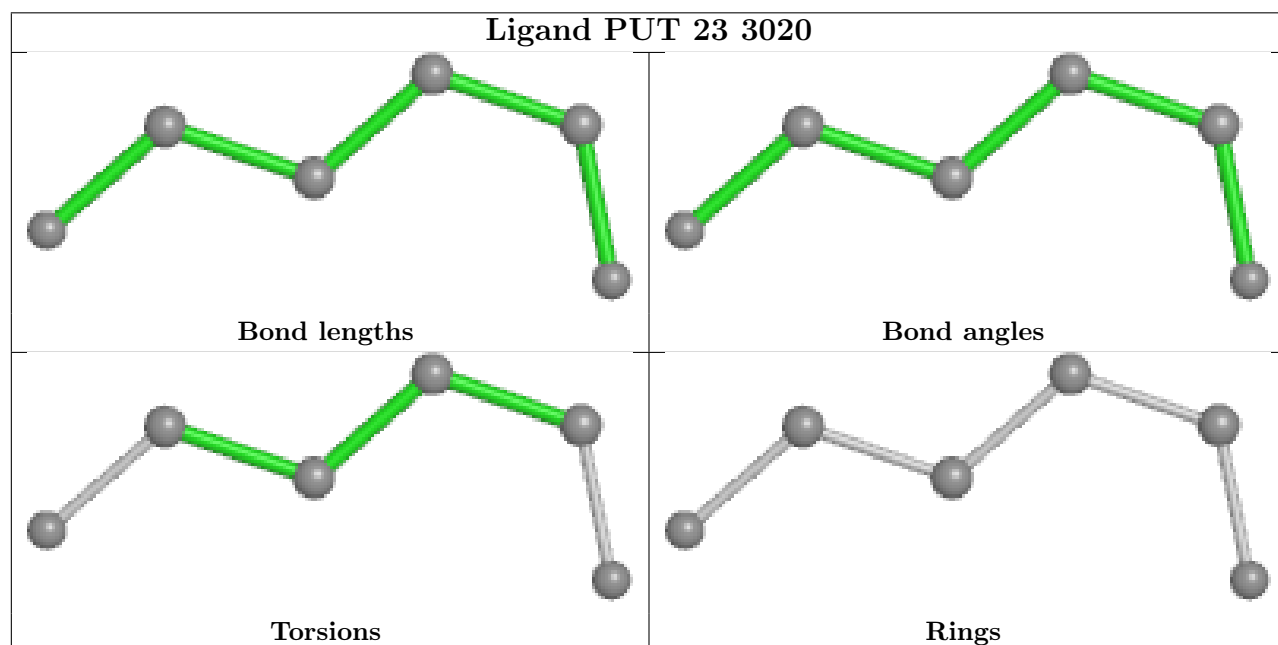
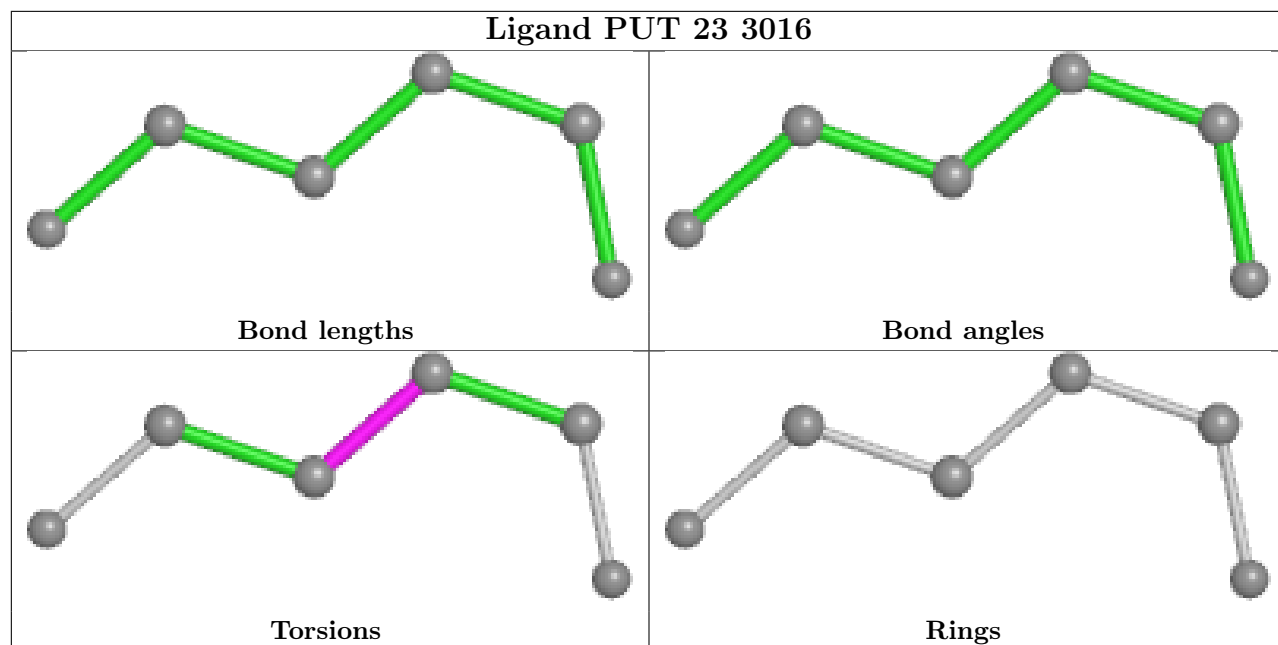
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

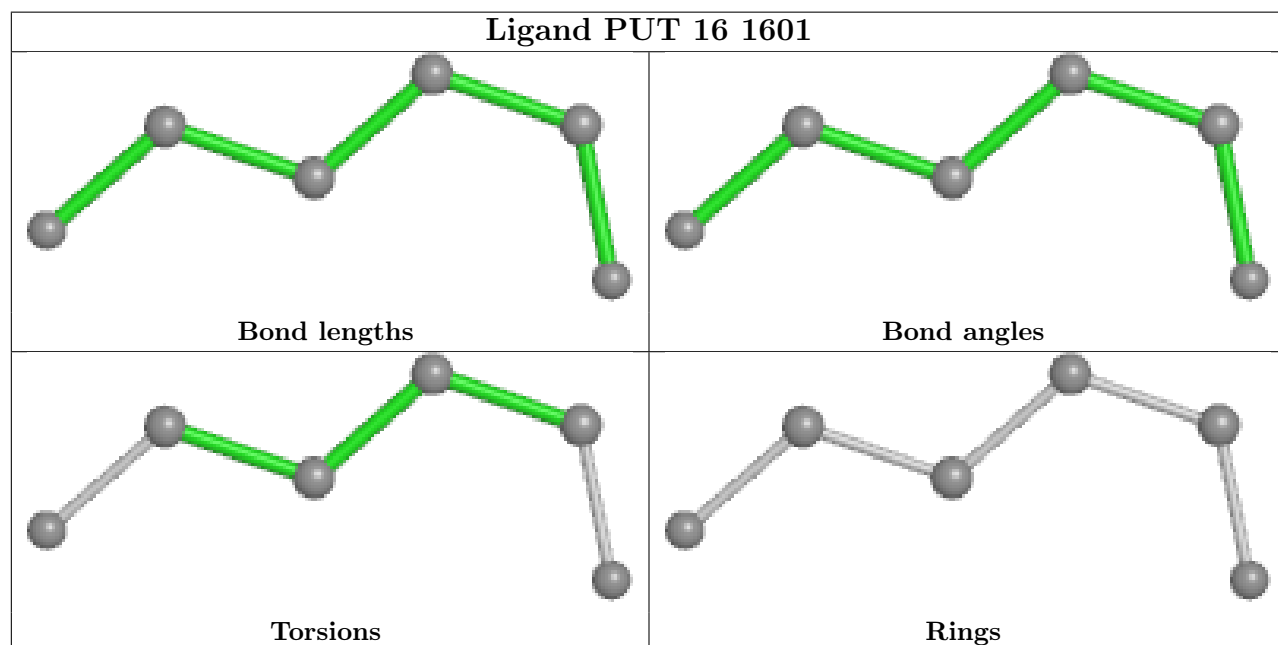
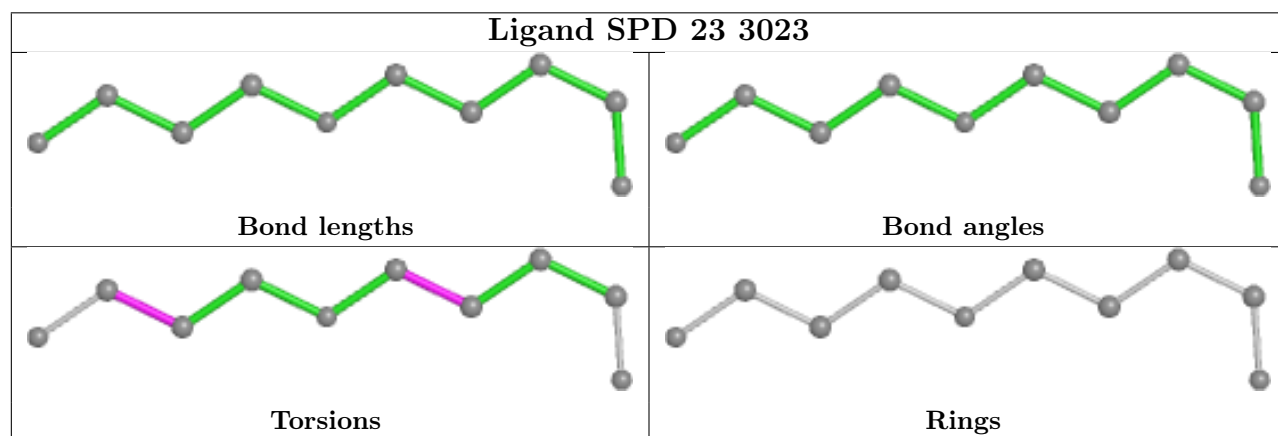
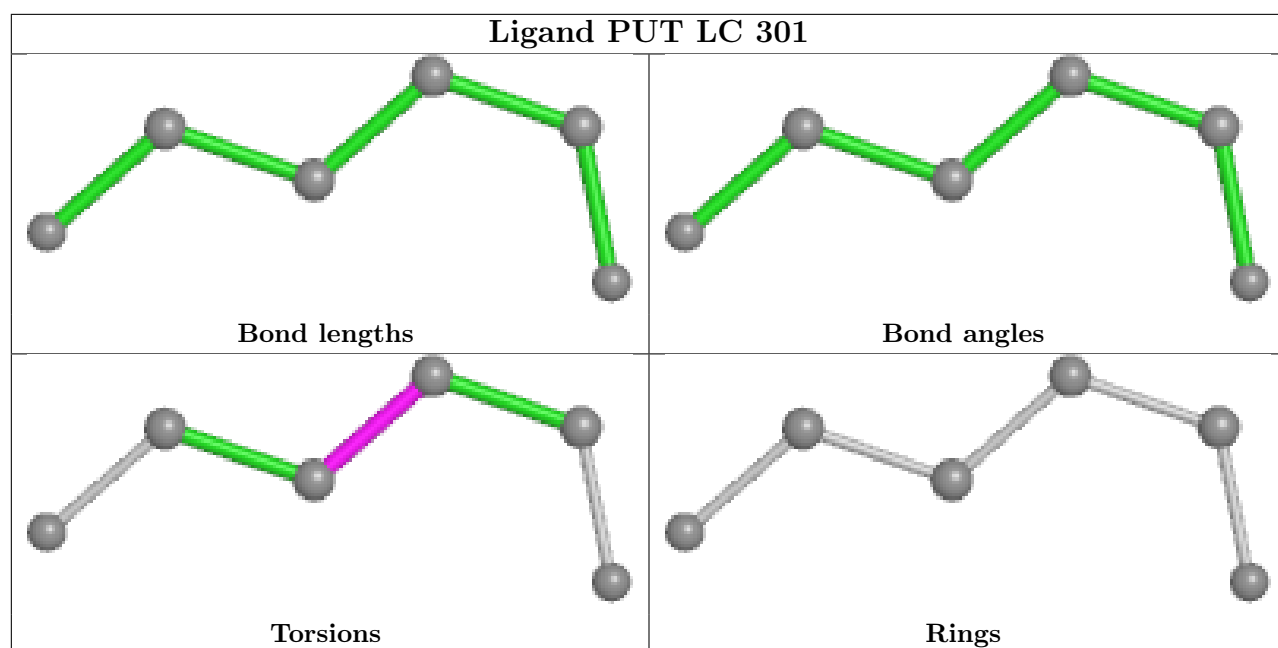


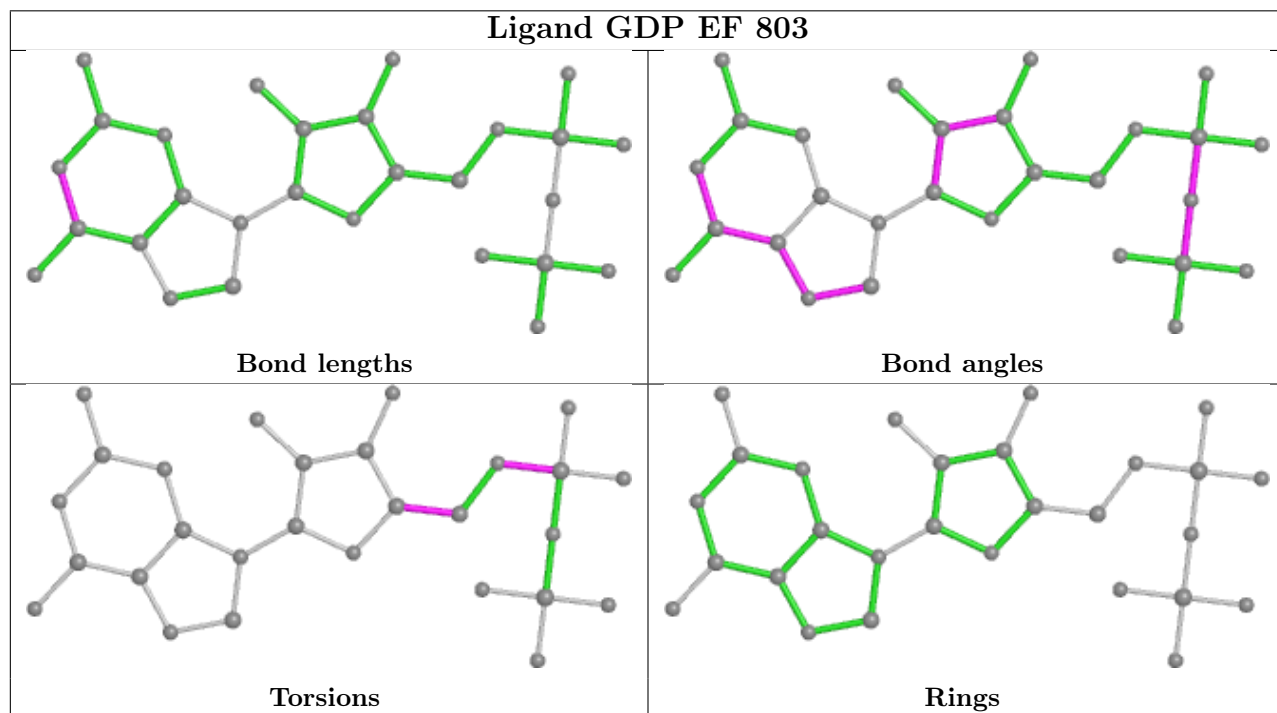
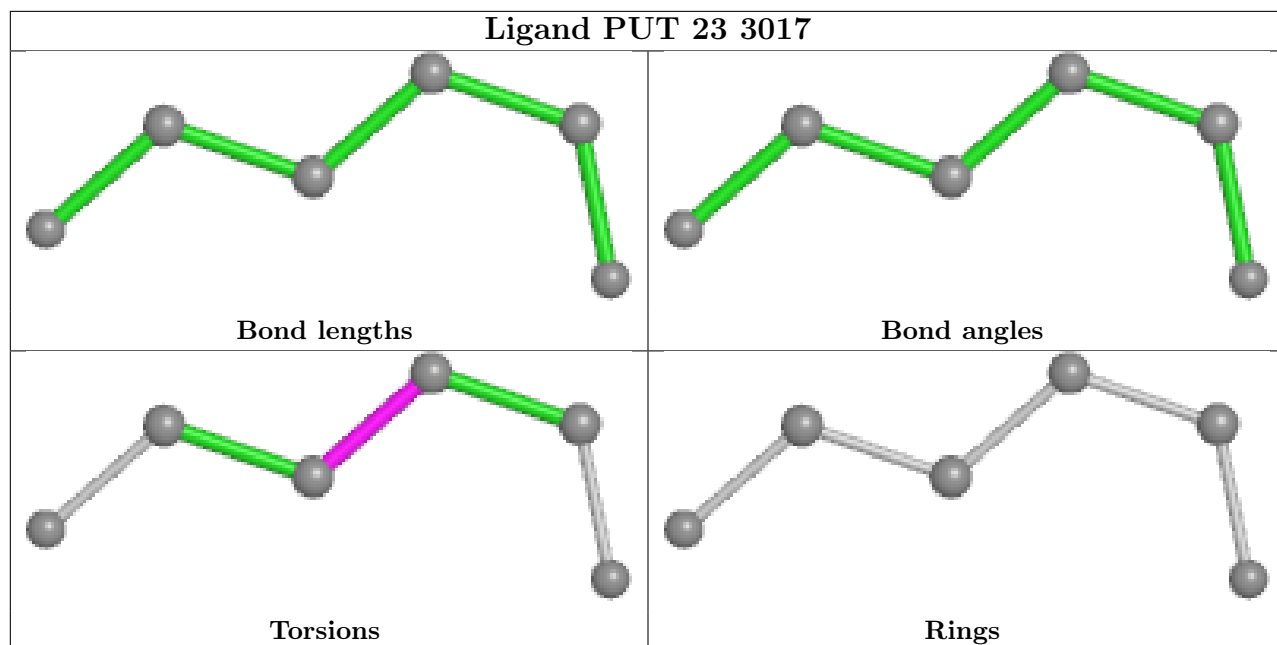


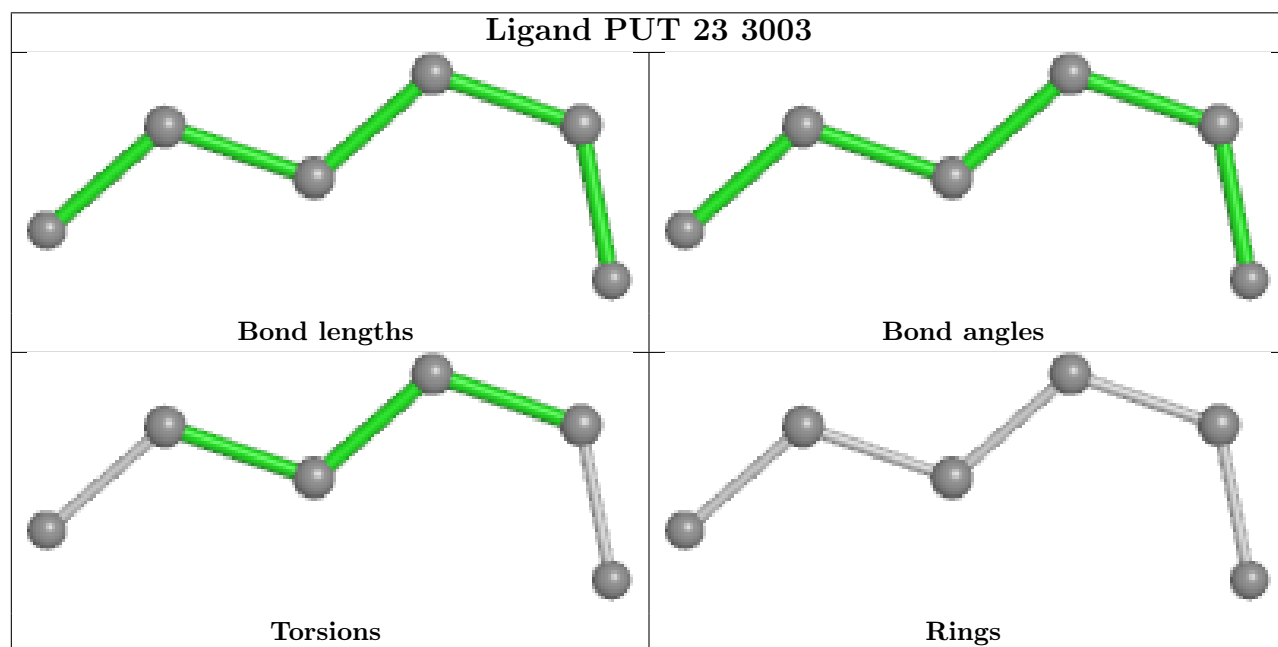
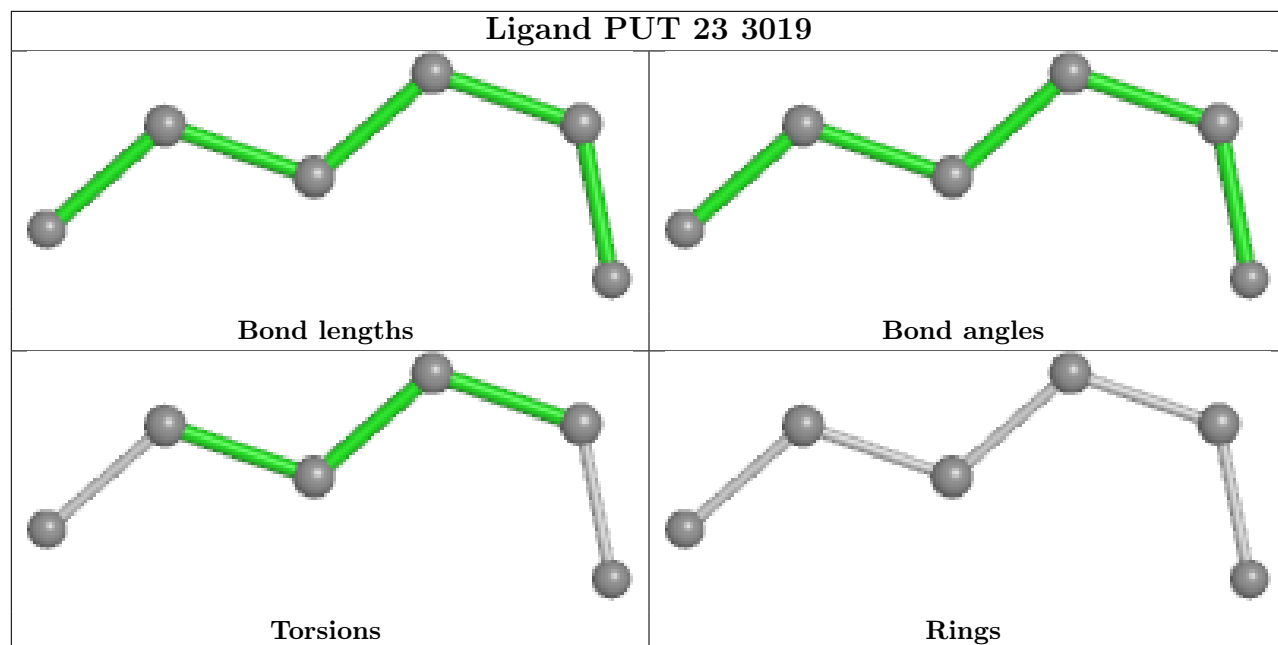


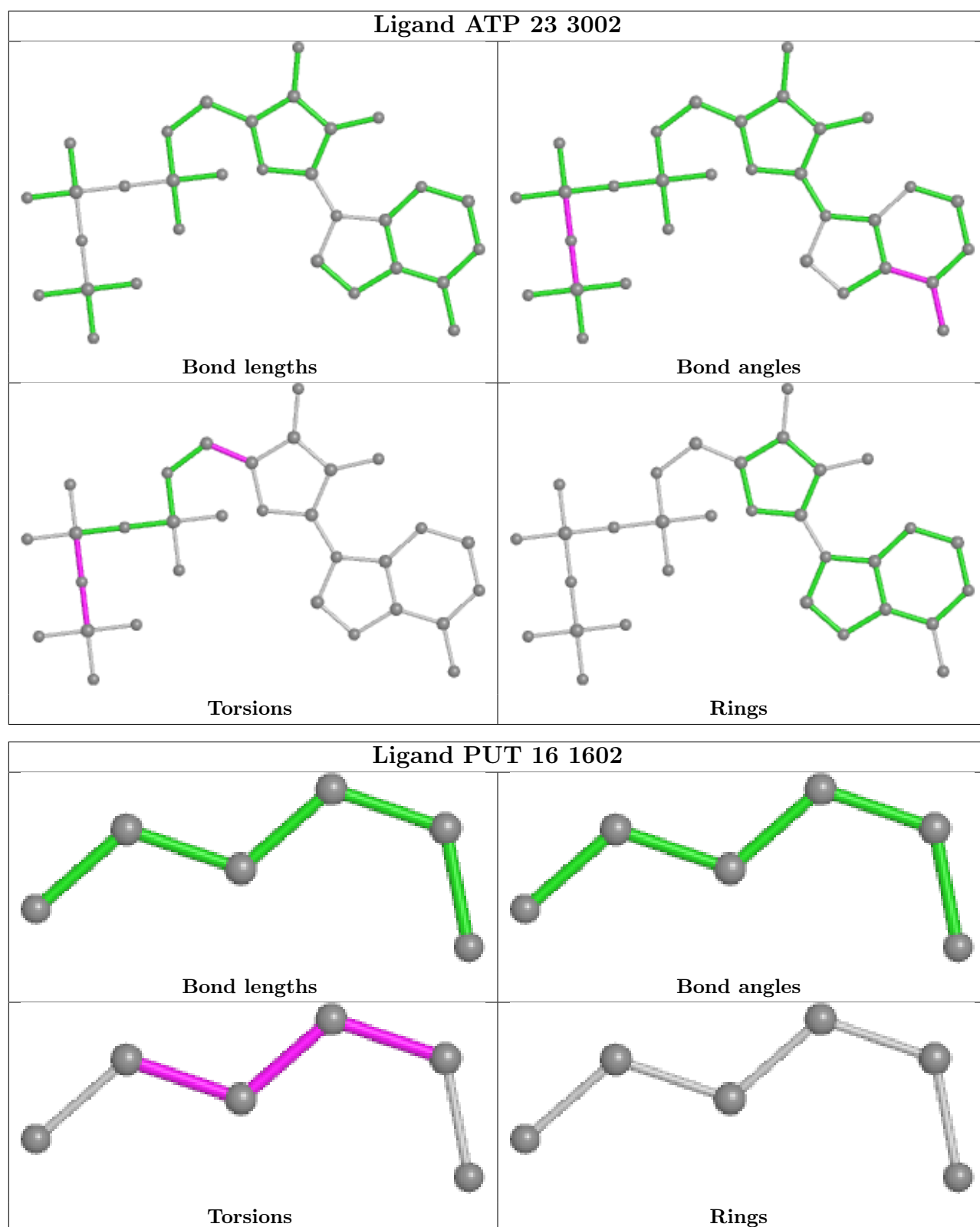


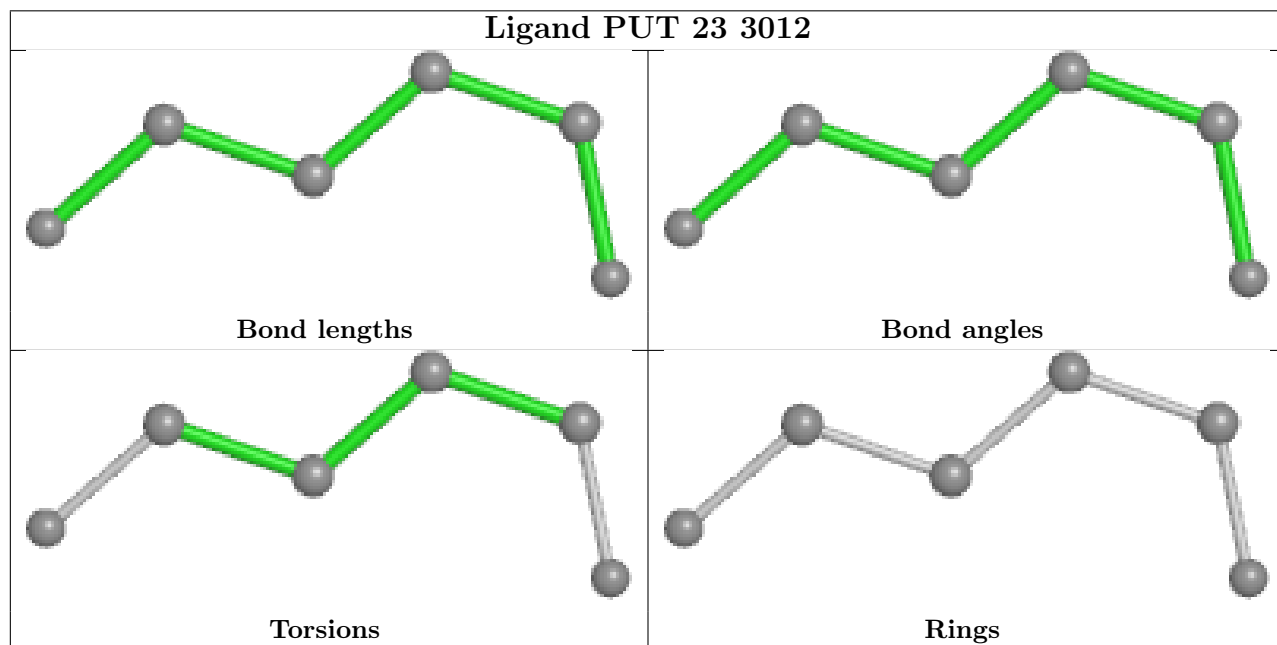
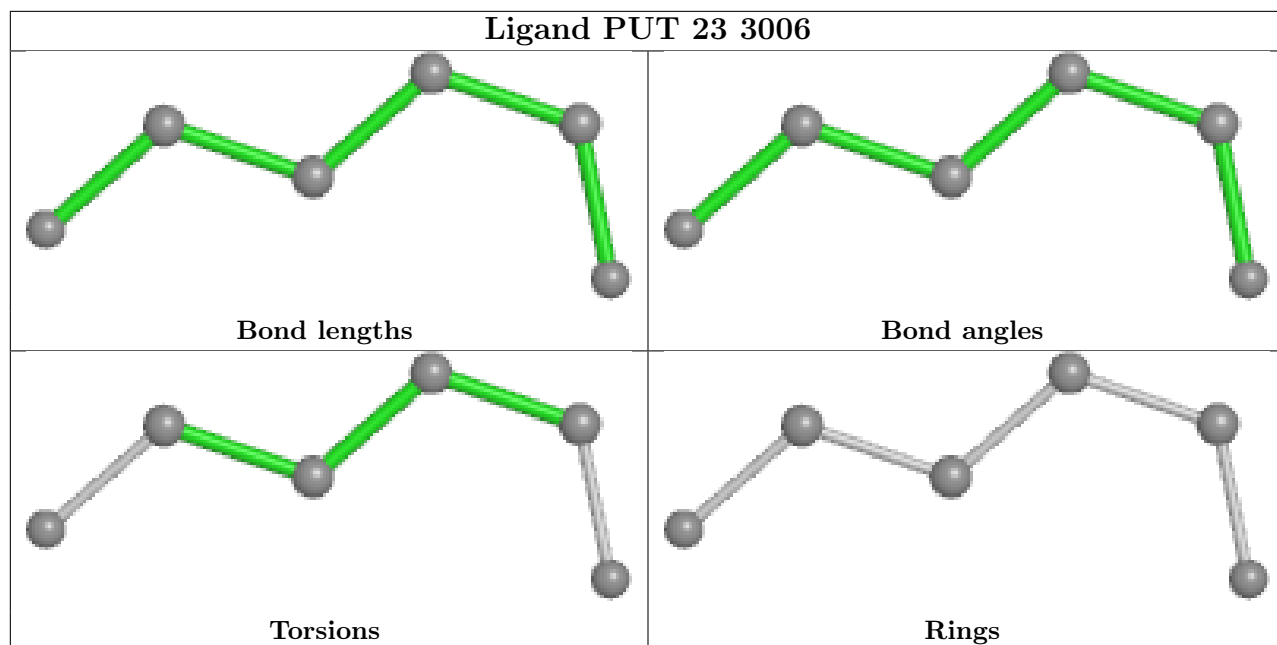


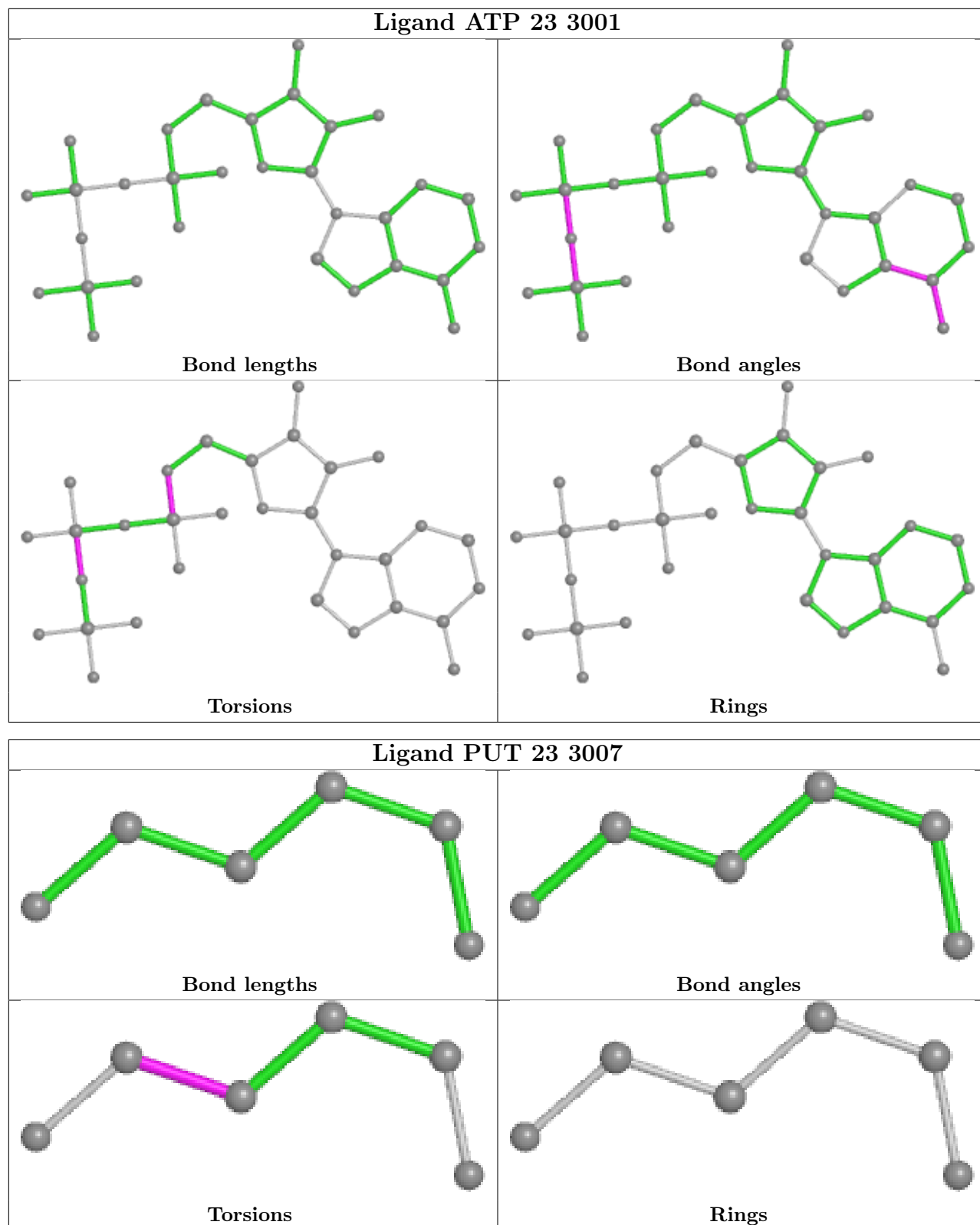


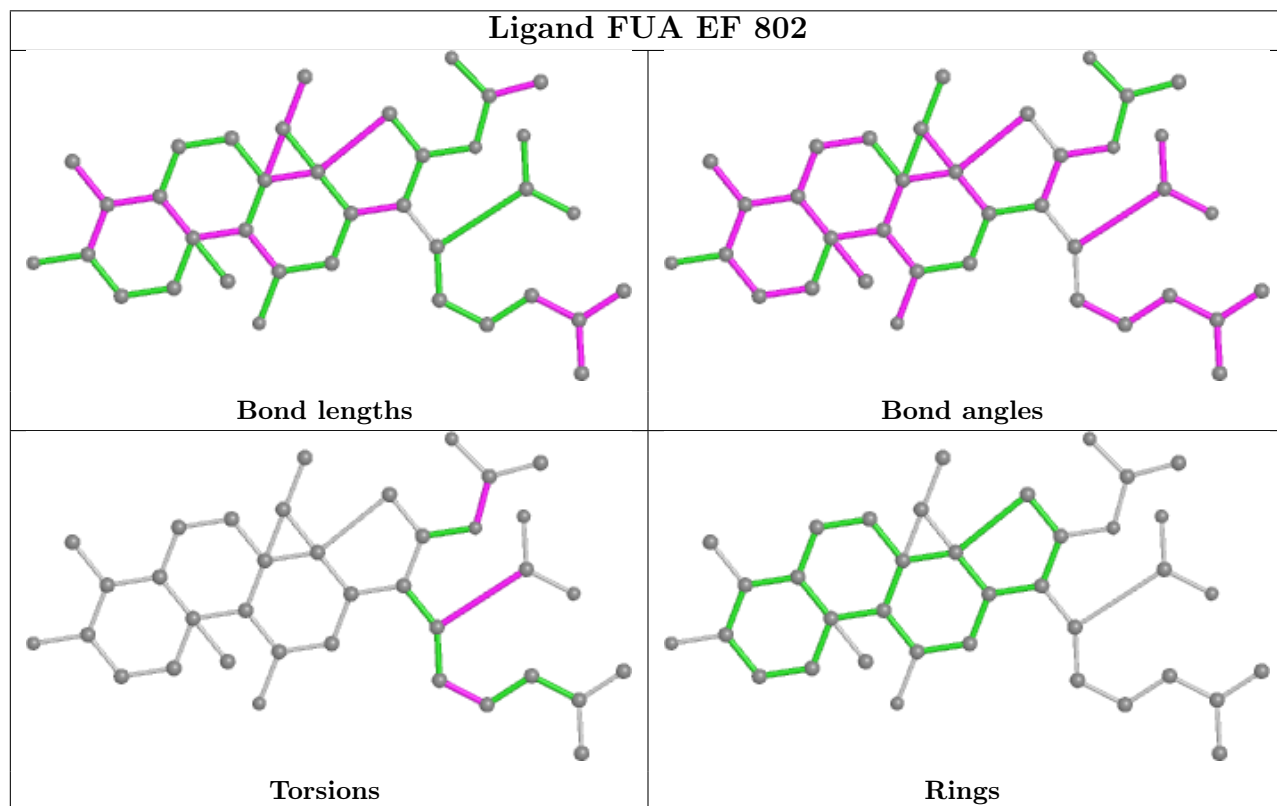
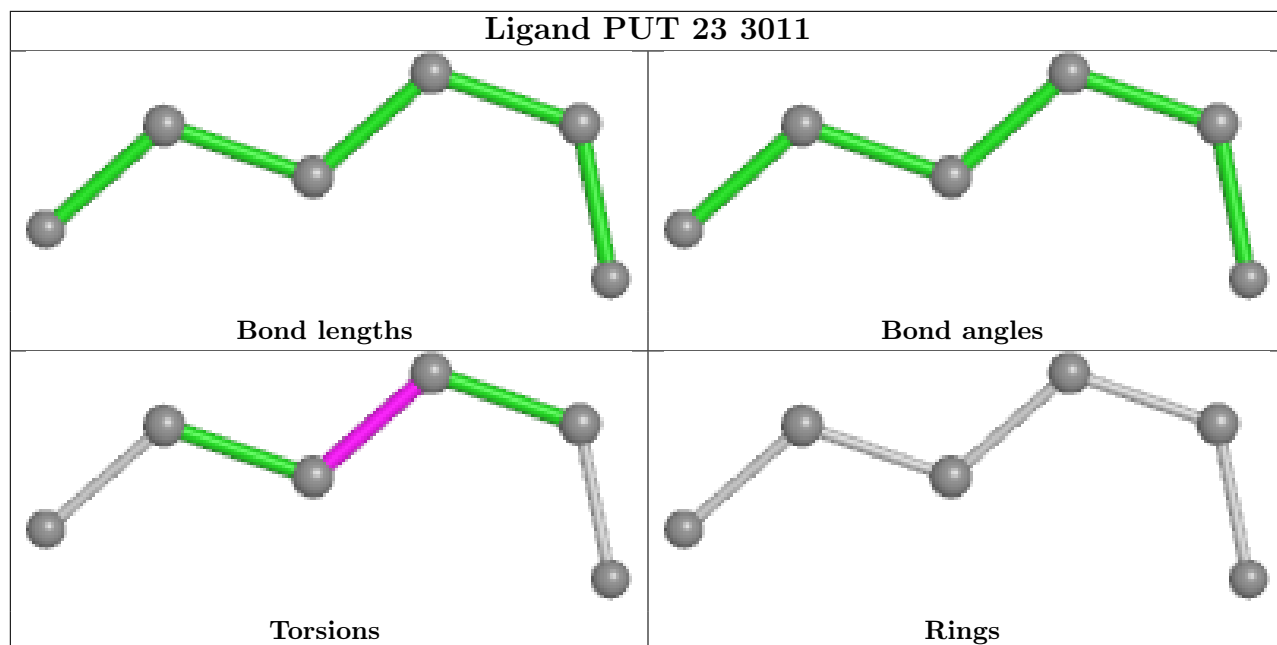




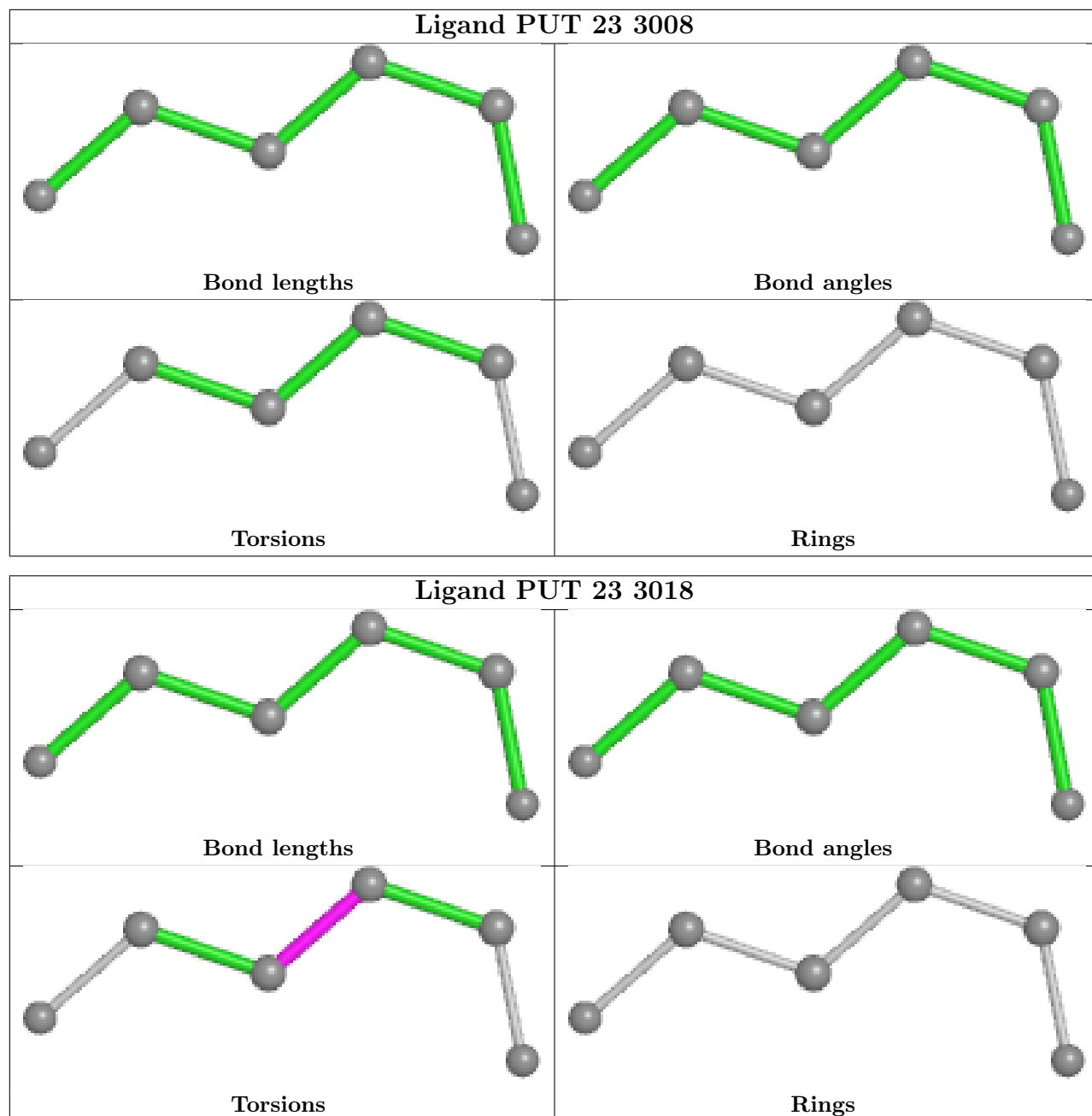


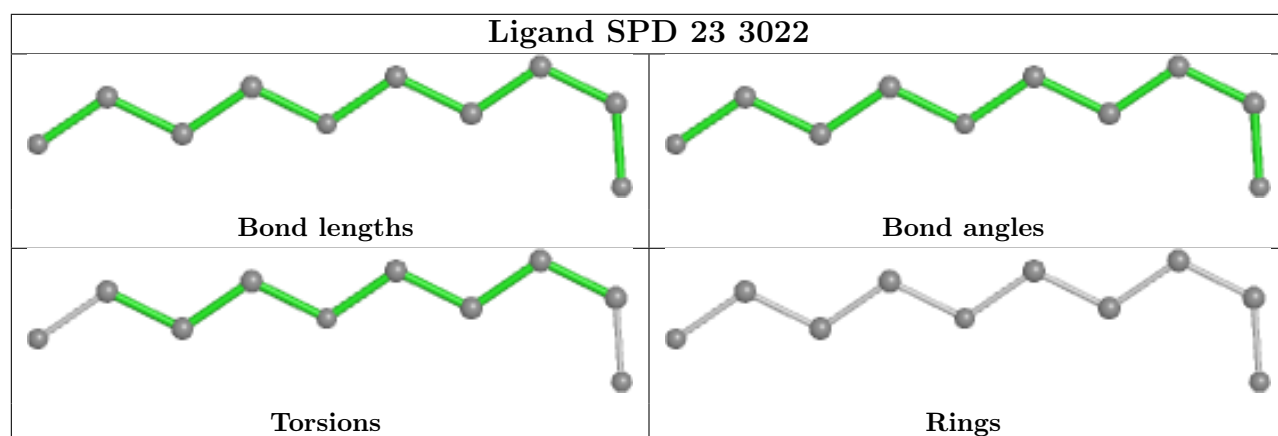
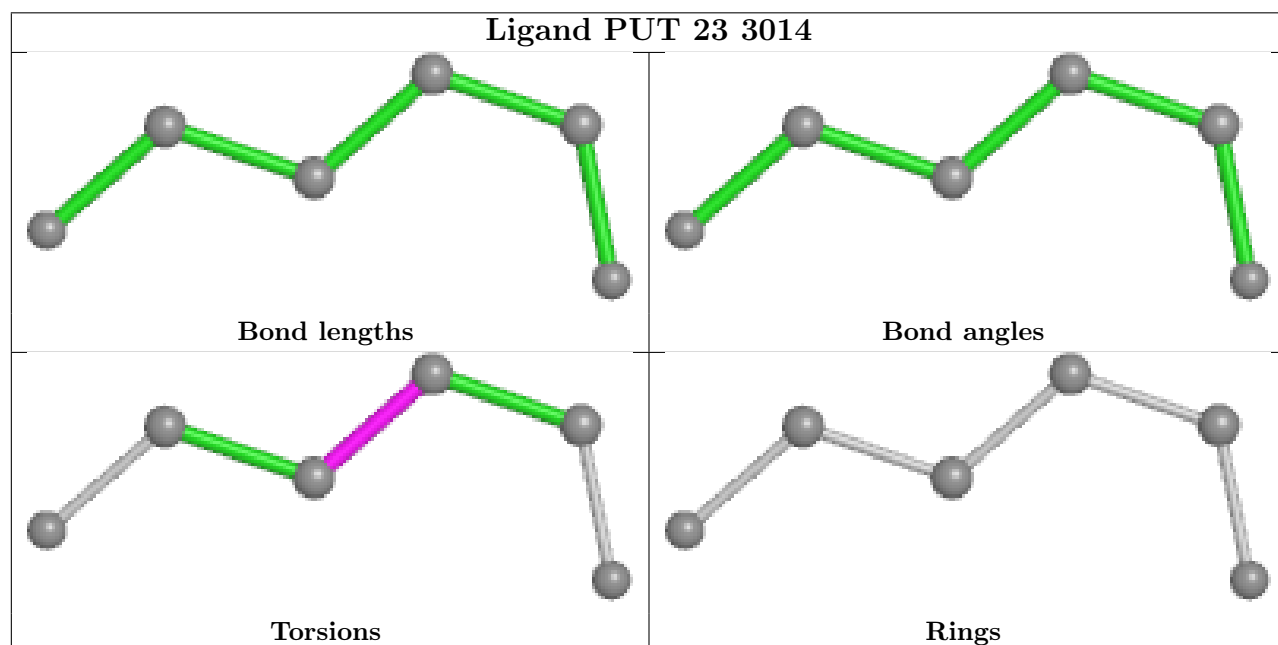
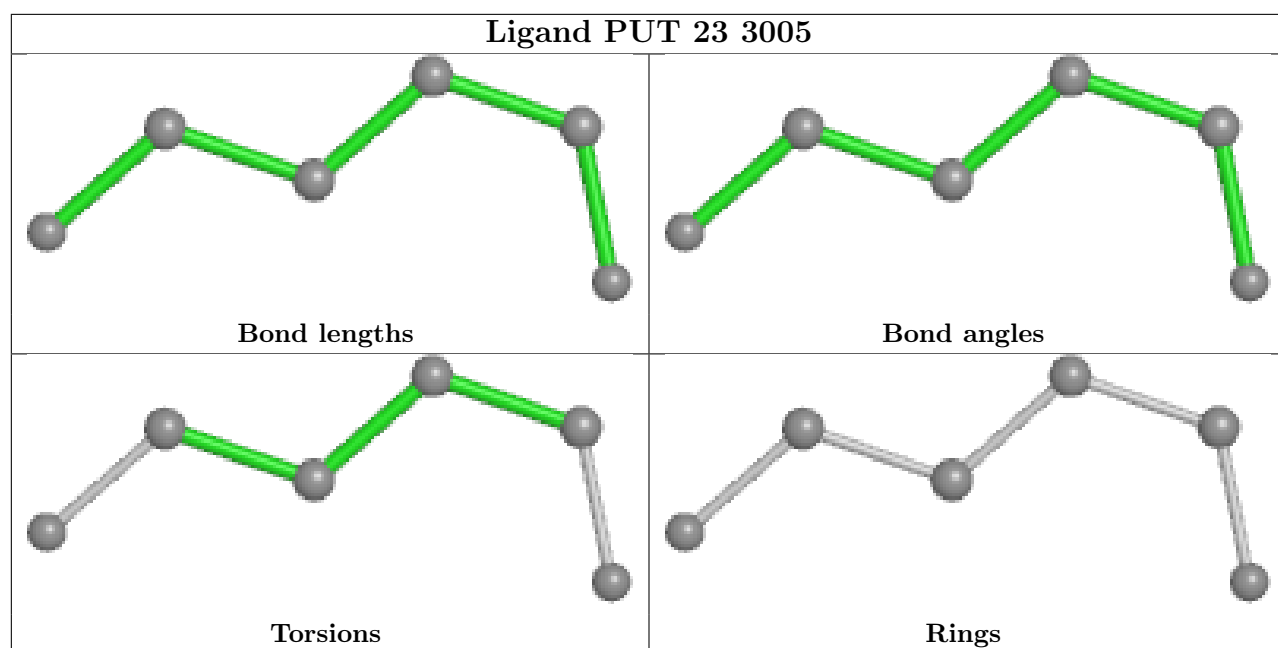












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

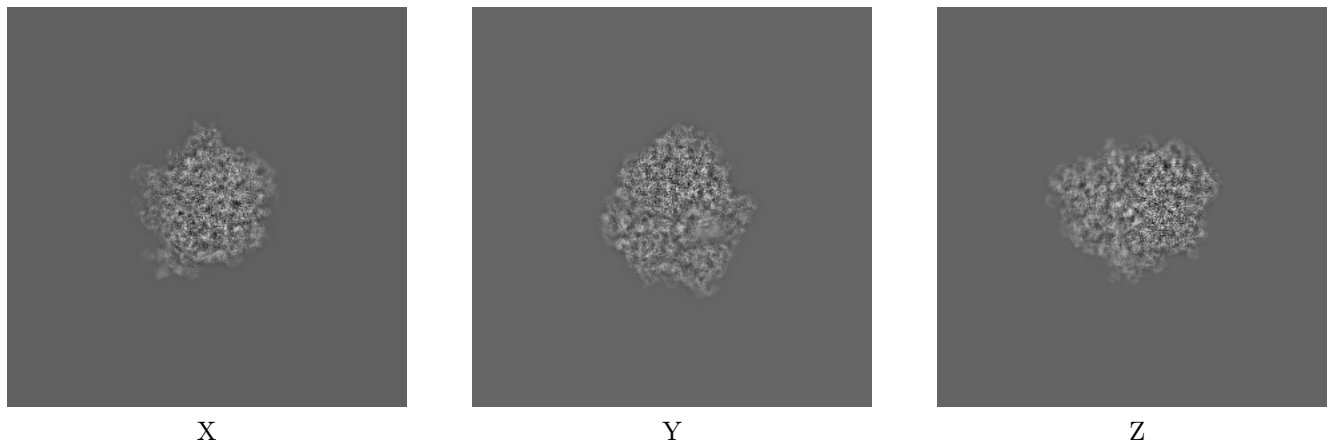
## 6 Map visualisation [i](#)

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.

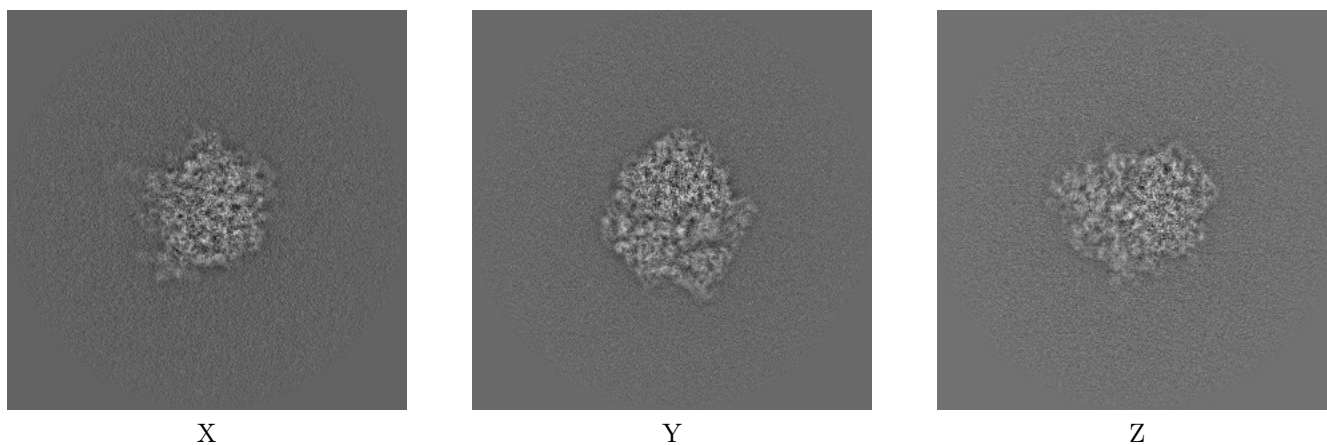
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



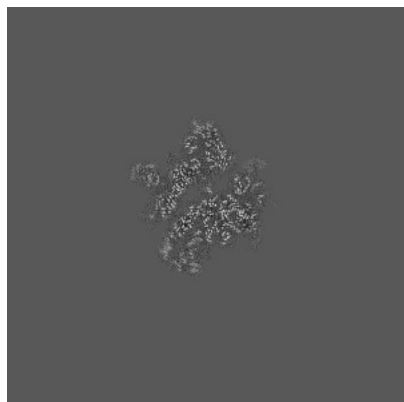
#### 6.1.2 Raw map



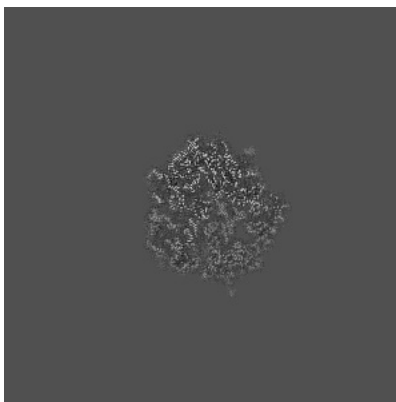
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

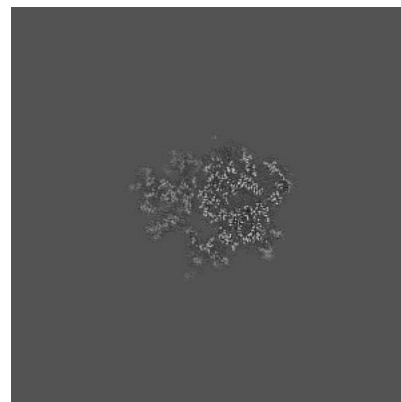
### 6.2.1 Primary map



X Index: 288

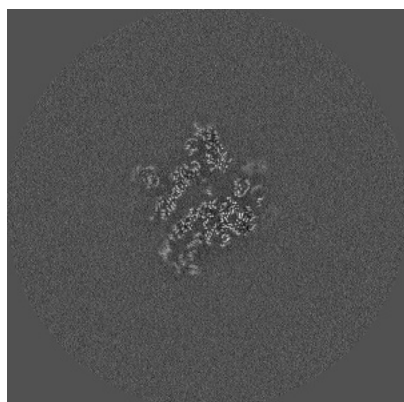


Y Index: 288

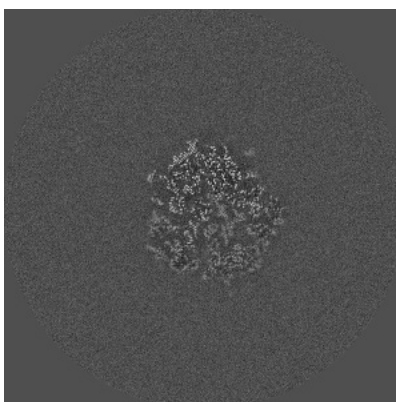


Z Index: 288

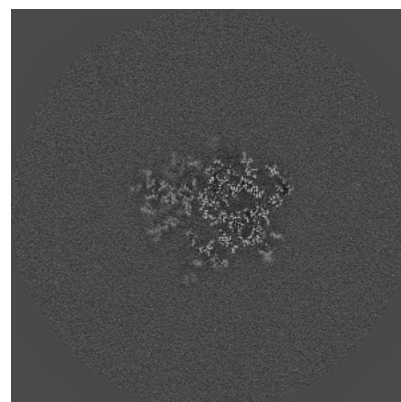
### 6.2.2 Raw map



X Index: 288



Y Index: 288

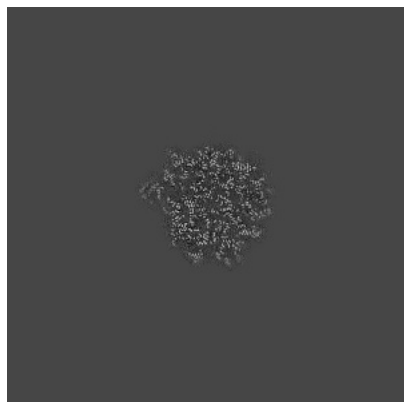


Z Index: 288

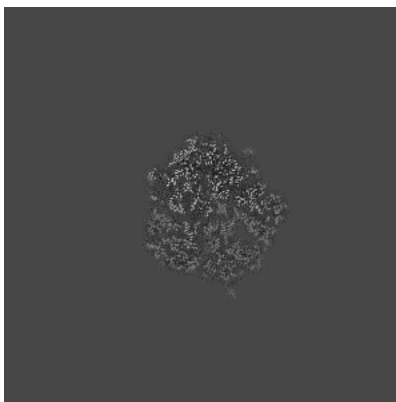
The images above show central slices of the map in three orthogonal directions.

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

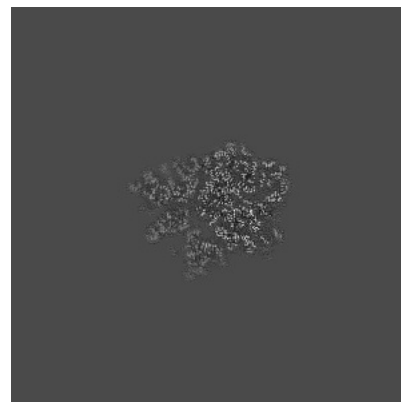
### 6.3.1 Primary map



X Index: 315

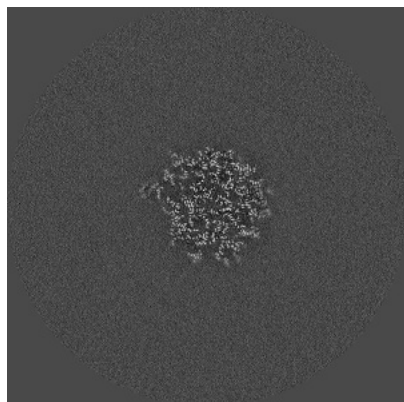


Y Index: 290

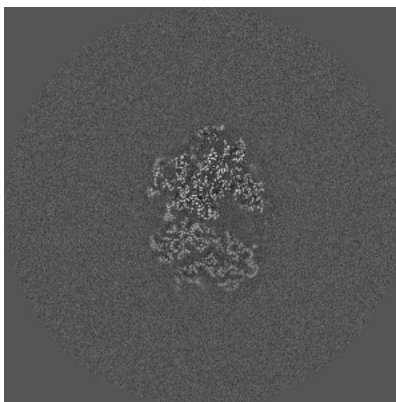


Z Index: 282

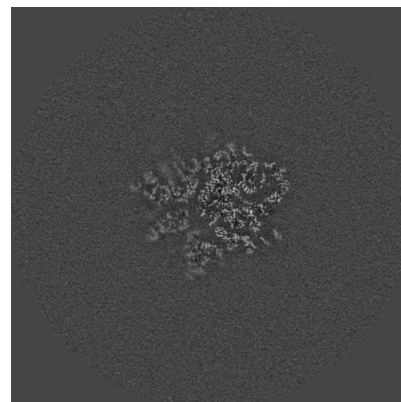
### 6.3.2 Raw map



X Index: 315



Y Index: 312

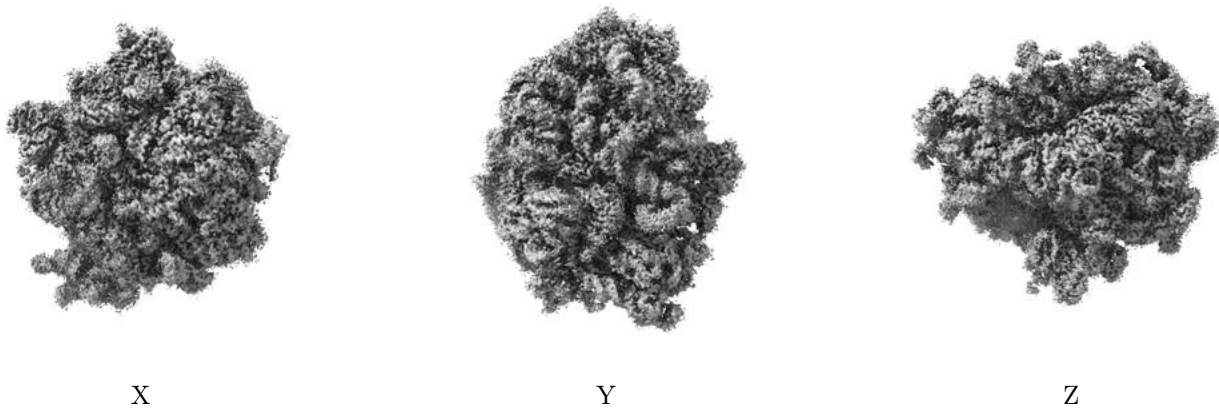


Z Index: 282

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

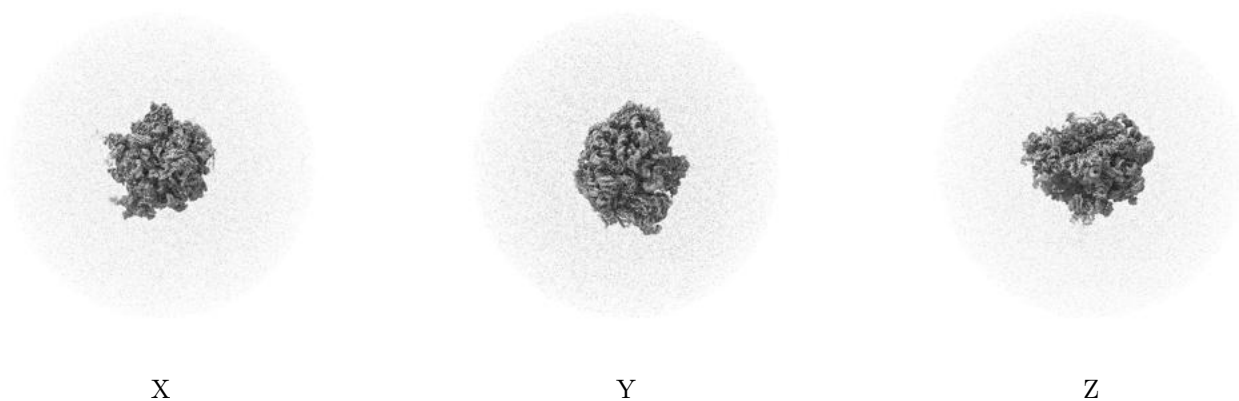
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 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.

### 6.4.2 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.

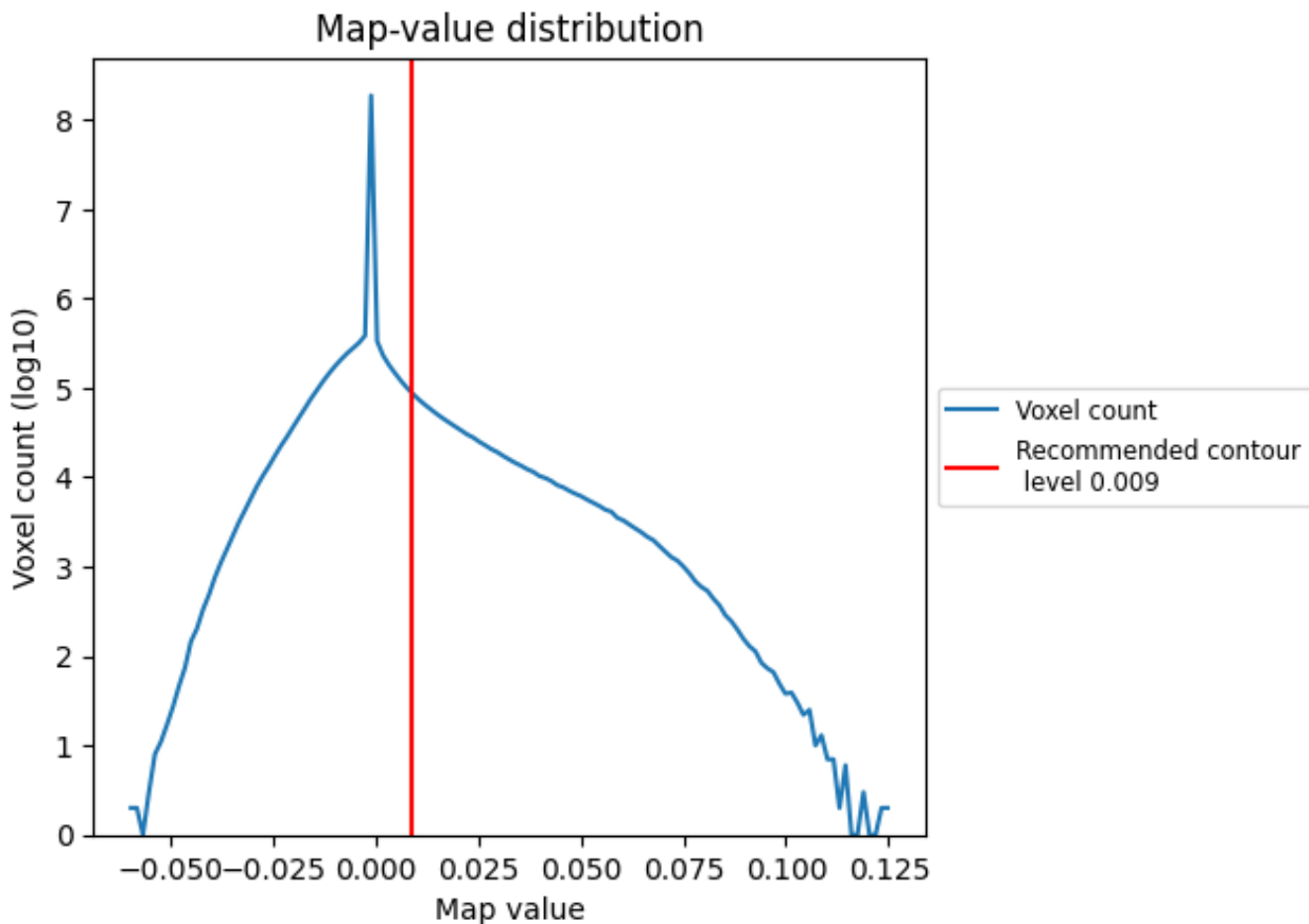
## 6.5 Mask visualisation [i](#)

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.

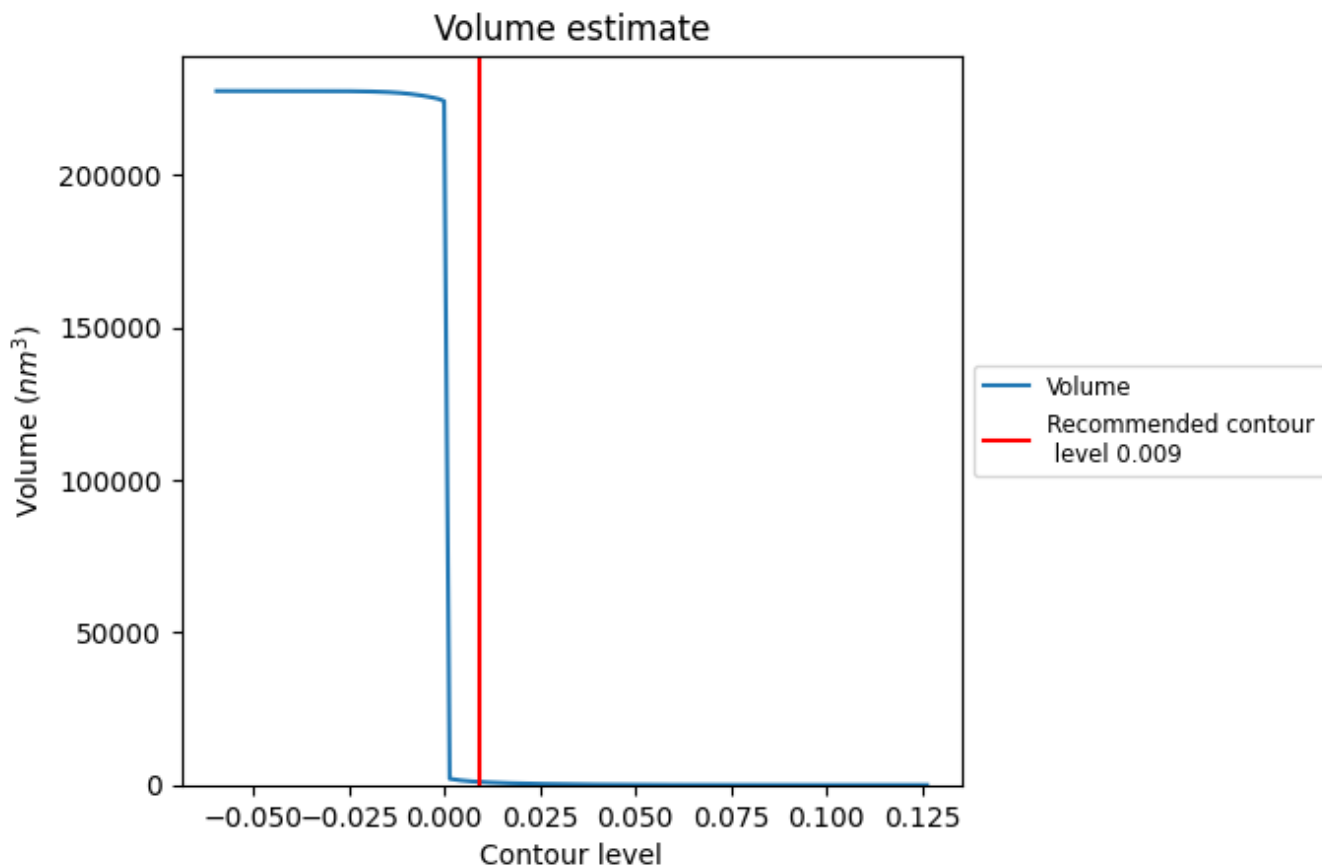
### 7.1 Map-value distribution [i](#)



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.



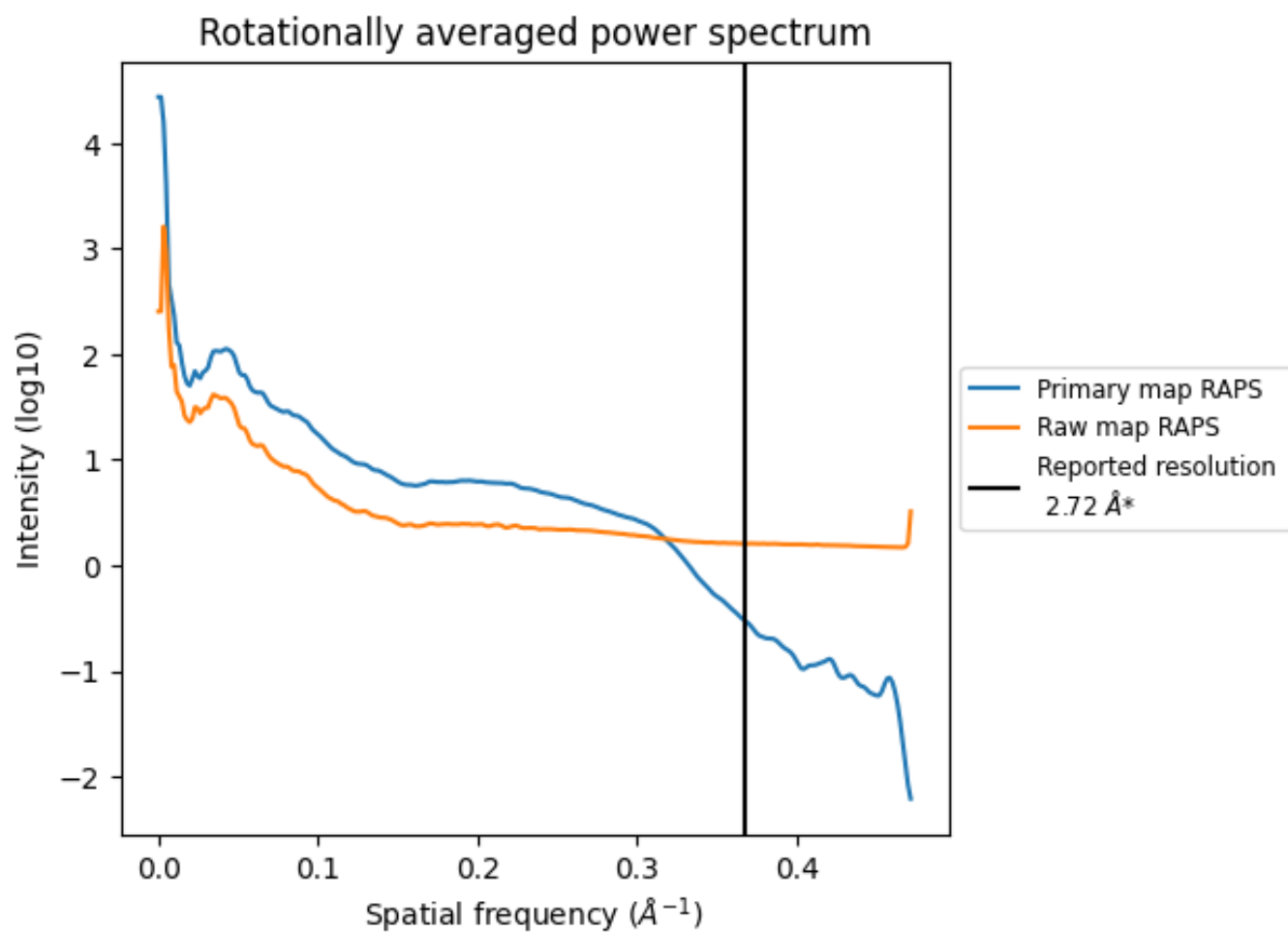
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is  $1017 \text{ nm}^3$ ; 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 i

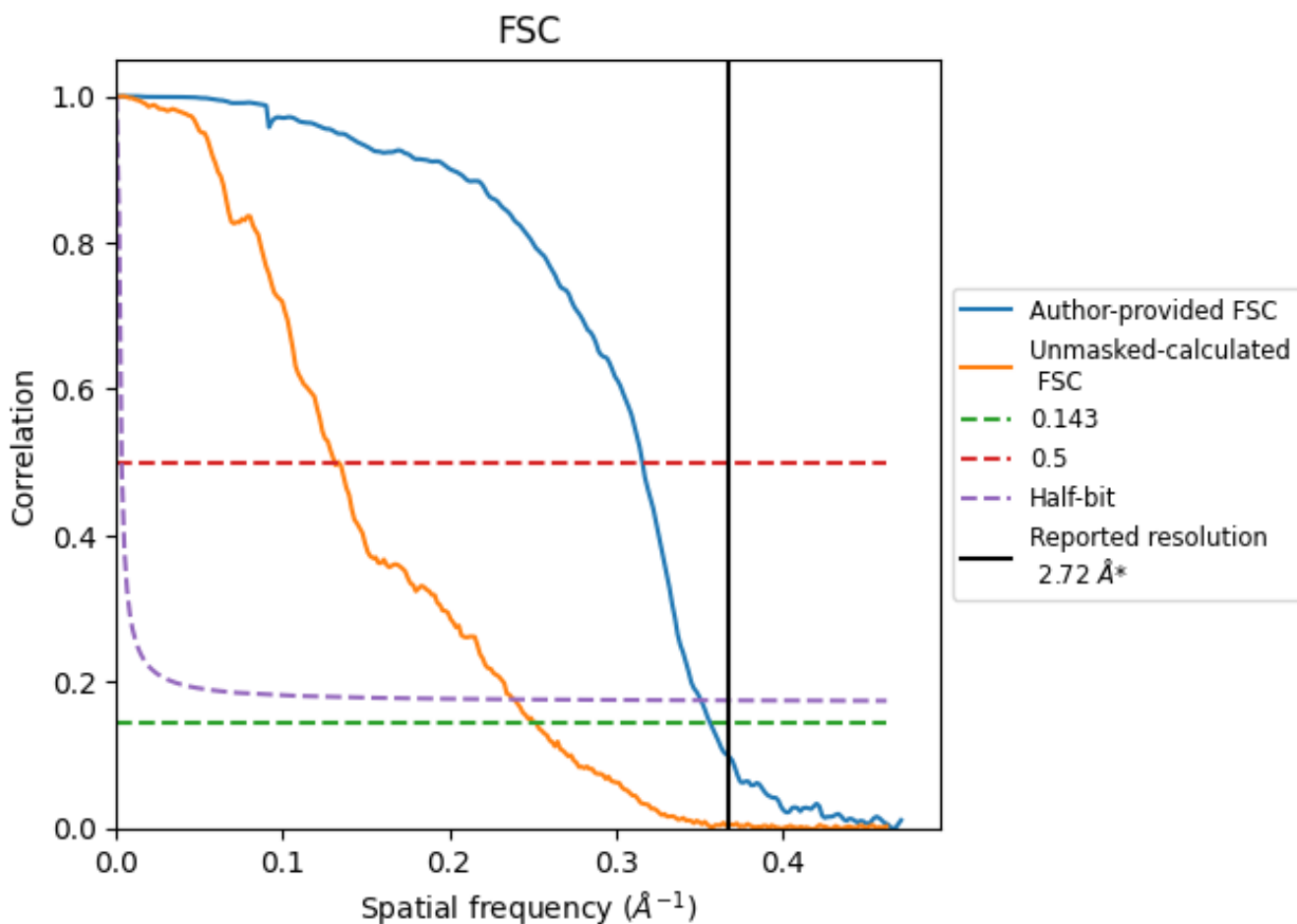


\*Reported resolution corresponds to spatial frequency of 0.368 Å<sup>-1</sup>

## 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<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

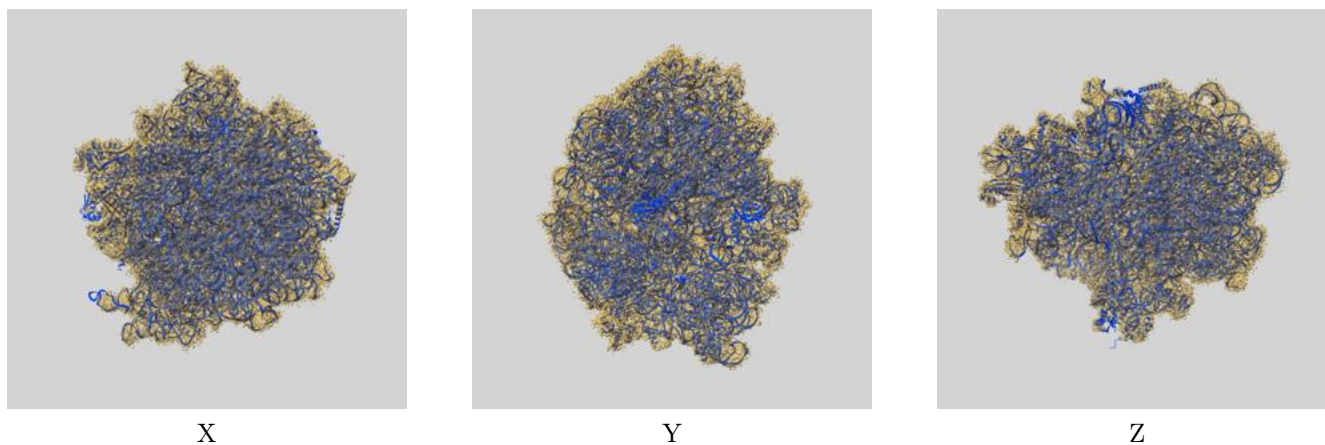
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.80	3.16	2.85
Unmasked-calculated*	3.96	7.63	4.18

\*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](#)

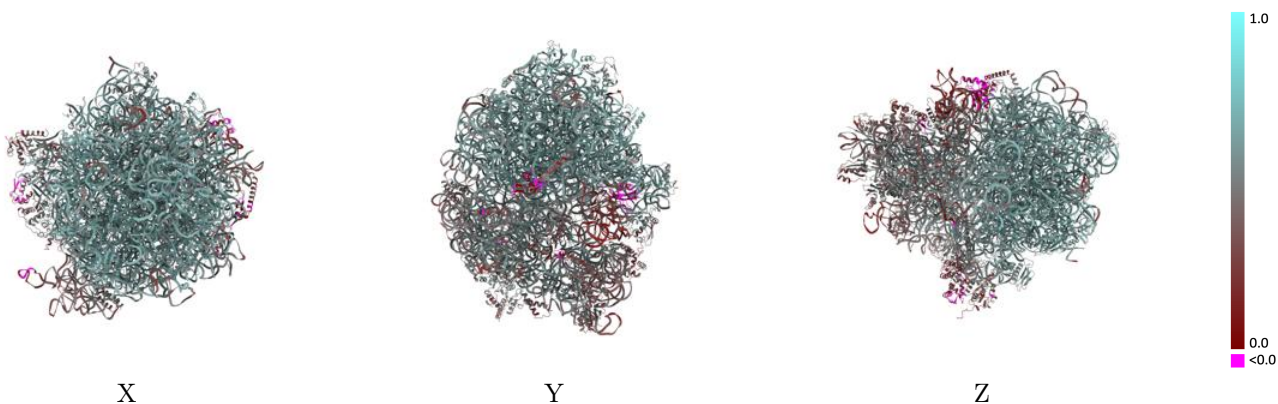
This section contains information regarding the fit between EMDB map EMD-24132 and PDB model 7N2C. Per-residue inclusion information can be found in section 3 on page 20.

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



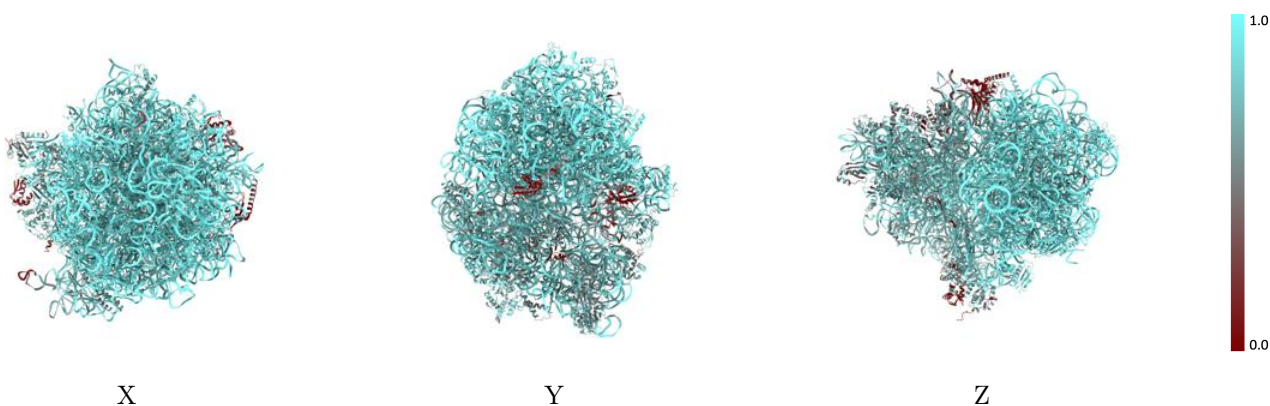
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



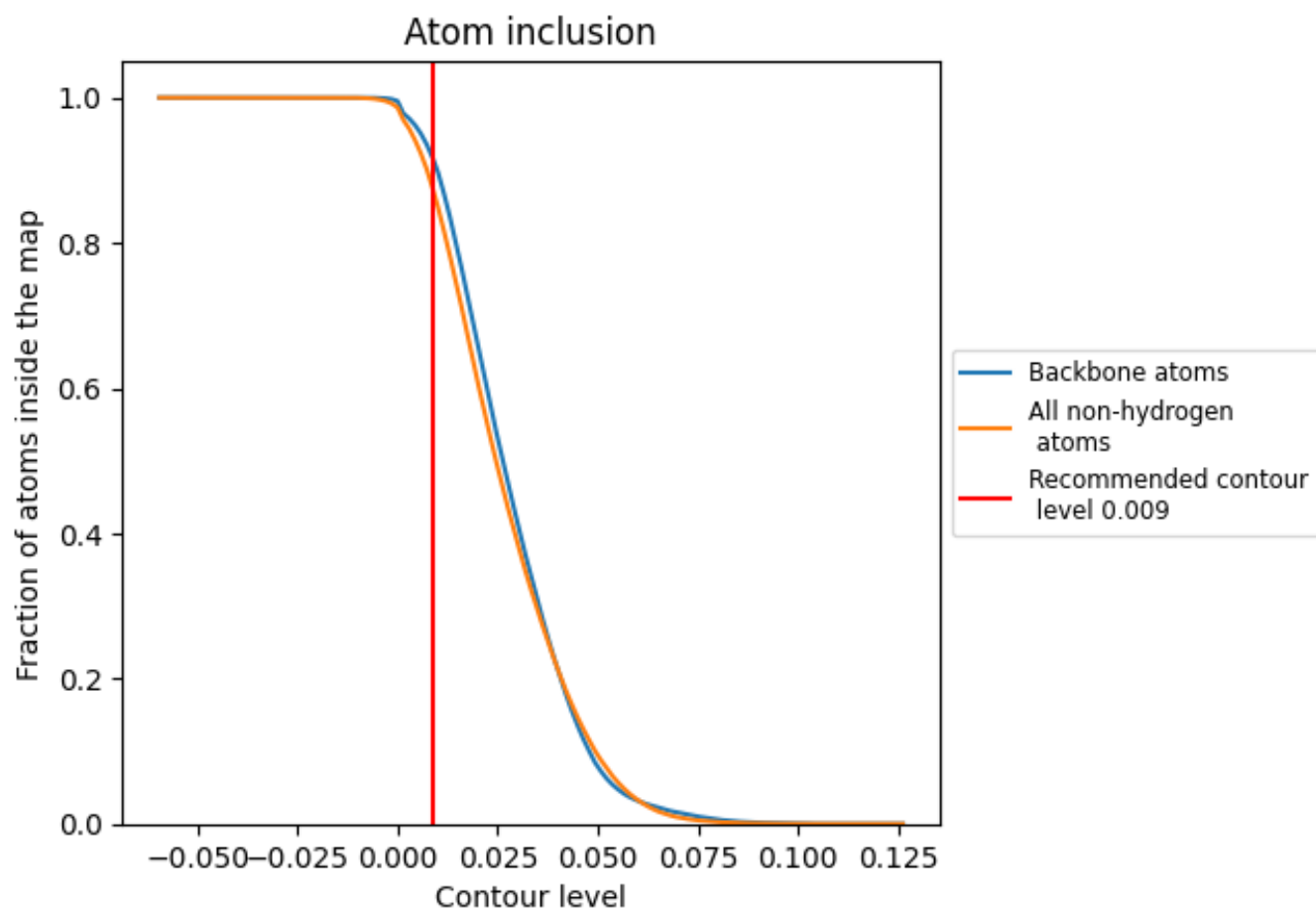
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.8702	 0.5330
16	 0.8776	 0.4890
23	 0.9592	 0.5920
5	 0.9631	 0.5780
Dt	 0.8428	 0.4490
EF	 0.7555	 0.4750
LA	 0.1536	 0.1230
LB	 0.9217	 0.6190
LC	 0.9346	 0.6220
LD	 0.8988	 0.5890
LE	 0.7647	 0.4910
LF	 0.8419	 0.5400
LG	 0.0907	 0.0660
LI	 0.3394	 0.2440
LJ	 0.5898	 0.3430
LK	 0.4850	 0.2890
LM	 0.9373	 0.6240
LN	 0.9154	 0.6140
LO	 0.9072	 0.6040
LP	 0.9271	 0.6130
LQ	 0.9577	 0.6330
LR	 0.8517	 0.5540
LS	 0.9088	 0.5930
LT	 0.9328	 0.6270
LU	 0.9134	 0.6020
LV	 0.9163	 0.6150
LW	 0.8824	 0.5900
LX	 0.9061	 0.5750
LY	 0.8957	 0.5750
La	 0.8722	 0.6080
Lb	 0.9318	 0.6070
Lc	 0.8609	 0.5440
Ld	 0.9451	 0.6140
Le	 0.6763	 0.3740
Lf	 0.9277	 0.6290



*Continued on next page...*



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Chain	Atom inclusion	Q-score
Lg	 0.8479	 0.5720
Lh	 0.9324	 0.6330
Li	 0.9369	 0.6280
Lj	 0.8805	 0.6010
Pp	 0.6786	 0.4830
Pt	 0.8472	 0.4840
SB	 0.6981	 0.4340
SC	 0.7522	 0.4810
SD	 0.6428	 0.3970
SE	 0.7879	 0.5010
SF	 0.5826	 0.3690
SG	 0.4653	 0.2960
SH	 0.7812	 0.5200
SI	 0.6333	 0.4330
SJ	 0.5714	 0.3950
SK	 0.5850	 0.4270
SL	 0.8039	 0.5380
SM	 0.6659	 0.3980
SN	 0.7126	 0.4730
SO	 0.7362	 0.4690
SP	 0.7177	 0.4760
SQ	 0.7184	 0.4660
SR	 0.5921	 0.4250
SS	 0.7117	 0.4760
ST	 0.7191	 0.4460
SU	 0.5796	 0.3660
mR	 0.6270	 0.3910