



## Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 01:29 AM EDT

PDB ID : 7N30  
EMDB ID : EMD-24135  
Title : Elongating 70S ribosome complex in a hybrid-H2\* pre-translocation (PRE-H2\*) conformation  
Authors : Rundlet, E.J.; Holm, M.; Schacherl, M.; Natchiar, K.S.; Altman, R.B.; Spahn, C.M.T.; Myasnikov, A.G.; Blanchard, S.C.  
Deposited on : 2021-05-30  
Resolution : 2.66 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

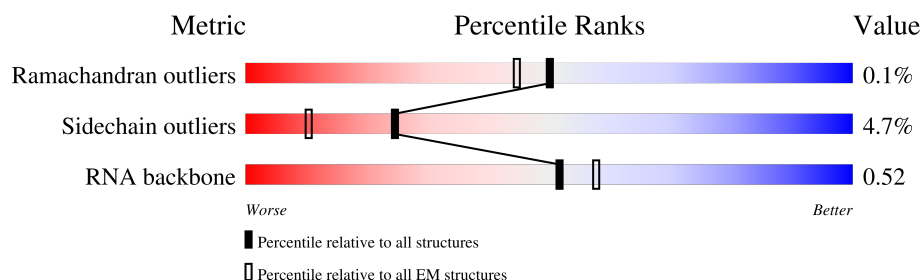
EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41.4

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.66 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>17%</div> <div>82%</div> <div>17%</div> <div>•</div> </div>
2	SB	241	<div> <div>60%</div> <div>89%</div> <div>7%</div> <div>•</div> </div>
3	SC	233	<div> <div>44%</div> <div>88%</div> <div>9%</div> <div>•</div> </div>
4	SD	206	<div> <div>71%</div> <div>96%</div> <div>•</div> <div>•</div> </div>
5	SE	167	<div> <div>17%</div> <div>89%</div> <div>7%</div> <div>•</div> </div>
6	SF	135	<div> <div>58%</div> <div>73%</div> <div>5%</div> <div>21%</div> </div>
7	SG	179	<div> <div>78%</div> <div>78%</div> <div>6%</div> <div>16%</div> </div>
8	SH	130	<div> <div>18%</div> <div>95%</div> <div>•</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
9	SI	130	<div>81%</div> <div>92%</div> <div>6%</div>
10	SJ	103	<div>75%</div> <div>90%</div> <div>6%</div>
11	SK	129	<div>48%</div> <div>88%</div> <div>9%</div>
12	SL	124	<div>14%</div> <div>94%</div> <div>• •</div>
13	SM	118	<div>89%</div> <div>89%</div> <div>8%</div>
14	SN	101	<div>64%</div> <div>96%</div> <div>• •</div>
15	SO	89	<div>38%</div> <div>97%</div> <div>• •</div>
16	SP	82	<div>35%</div> <div>98%</div> <div>•</div>
17	SQ	84	<div>40%</div> <div>92%</div> <div>• 5%</div>
18	SR	75	<div>36%</div> <div>85%</div> <div>• 12%</div>
19	SS	92	<div>87%</div> <div>84%</div> <div>5% 11%</div>
20	ST	87	<div>59%</div> <div>95%</div> <div>• •</div>
21	SU	71	<div>73%</div> <div>80%</div> <div>18%</div>
22	mR	60	<div>•</div> <div>18%</div> <div>82%</div>
23	23	2904	<div>12%</div> <div>81%</div> <div>18%</div>
24	5	120	<div>12%</div> <div>87%</div> <div>13%</div>
25	LB	273	<div>5%</div> <div>98%</div> <div>• •</div>
26	LC	209	<div>7%</div> <div>96%</div> <div>•</div>
27	LD	201	<div>18%</div> <div>98%</div> <div>•</div>
28	LE	179	<div>97%</div> <div>90%</div> <div>8% • •</div>
29	LF	177	<div>59%</div> <div>95%</div> <div>• • •</div>
30	LI	149	<div>93%</div> <div>93%</div> <div>7%</div>
31	LM	142	<div>8%</div> <div>100%</div> <div></div>
32	LN	123	<div>8%</div> <div>96%</div> <div>• •</div>
33	LO	144	<div>8%</div> <div>94%</div> <div>6%</div>

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

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 146268 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	1526	Total	C	N	O	P	0	0
			32762	14619	6014	10603	1526		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SC	212	Total	C	N	O	S	0	0
			1658	1049	311	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SD	204	Total	C	N	O	S	0	0
			1633	1020	313	296	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
			1143	712	216	209	6		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SH	128	Total	C	N	O	S	0	0
			973	613	172	182	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	122	Total	C	N	O	S	0	0
			951	588	195	163	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SO	88	Total	C	N	O	S	0	0
			713	439	144	129	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SP	82	Total	C	N	O	S	0	0
			648	406	128	113	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	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SS	82	Total	C	N	O	S	0	0
			656	419	125	110	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
			590	366	125	98	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	mR	11	Total	C	N	O	P	0	0
			234	105	41	77	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	23	2901	Total	C	N	O	P	0	0
			62293	27796	11460	20136	2901		

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

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

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

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

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

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

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

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

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



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

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

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

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

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

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LS	114	Total	C	N	O	S	1	0
			928	580	183	164	1		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LW	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
43	LY	94	Total	C	N	O	S	
			752	479	137	133	3	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
44	La	75	Total	C	N	O	S	
			575	356	116	102	1	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lf	56	Total	C	N	O	S	0	0
			443	269	94	79	1		

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

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

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

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

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

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

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

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

- Molecule 54 is a protein called Nascent peptide.

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

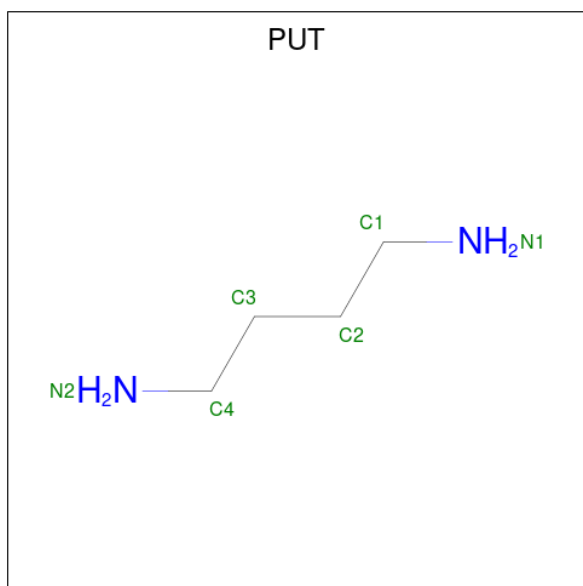
- Molecule 55 is a RNA chain called tRNA.

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

- Molecule 56 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	Dt	76	Total	C	N	O	P	S	0	0
			1637	735	294	531	75	2		

- Molecule 57 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula:  $C_4H_{12}N_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
57	16	1	Total	C	N	0
			6	4	2	
57	23	1	Total	C	N	0
			6	4	2	
57	23	1	Total	C	N	0
			6	4	2	
57	23	1	Total	C	N	0
			6	4	2	
57	23	1	Total	C	N	0
			6	4	2	
57	23	1	Total	C	N	0
			6	4	2	
57	23	1	Total	C	N	0
			6	4	2	
57	23	1	Total	C	N	0
			6	4	2	

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Mol	Chain	Residues	Atoms			AltConf
57	23	1	Total	C	N	0
			6	4	2	

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
58	16	76	Total	Mg	0
			76	76	
58	SD	1	Total	Mg	0
			1	1	
58	SS	1	Total	Mg	0
			1	1	
58	23	210	Total	Mg	0
			210	210	
58	5	4	Total	Mg	0
			4	4	
58	LC	1	Total	Mg	0
			1	1	
58	LD	1	Total	Mg	0
			1	1	
58	LX	1	Total	Mg	0
			1	1	
58	Lf	1	Total	Mg	0
			1	1	

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

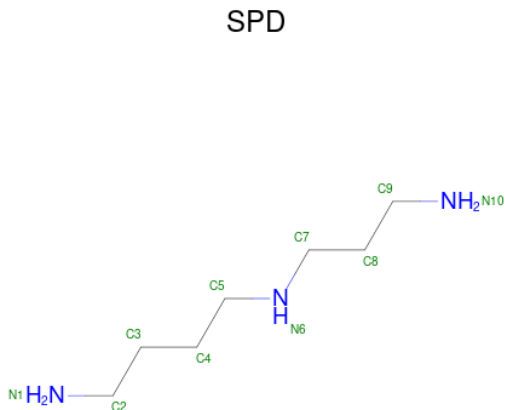
Mol	Chain	Residues	Atoms		AltConf
59	SB	1	Total	Zn	0
			1	1	

- Molecule 60 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
60	23	1	Total 31	C 10	N 5	O 13	P 3	0
60	23	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 61 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ) (labeled as "Lig- and of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
61	23	1	Total	C	N	0
			10	7	3	

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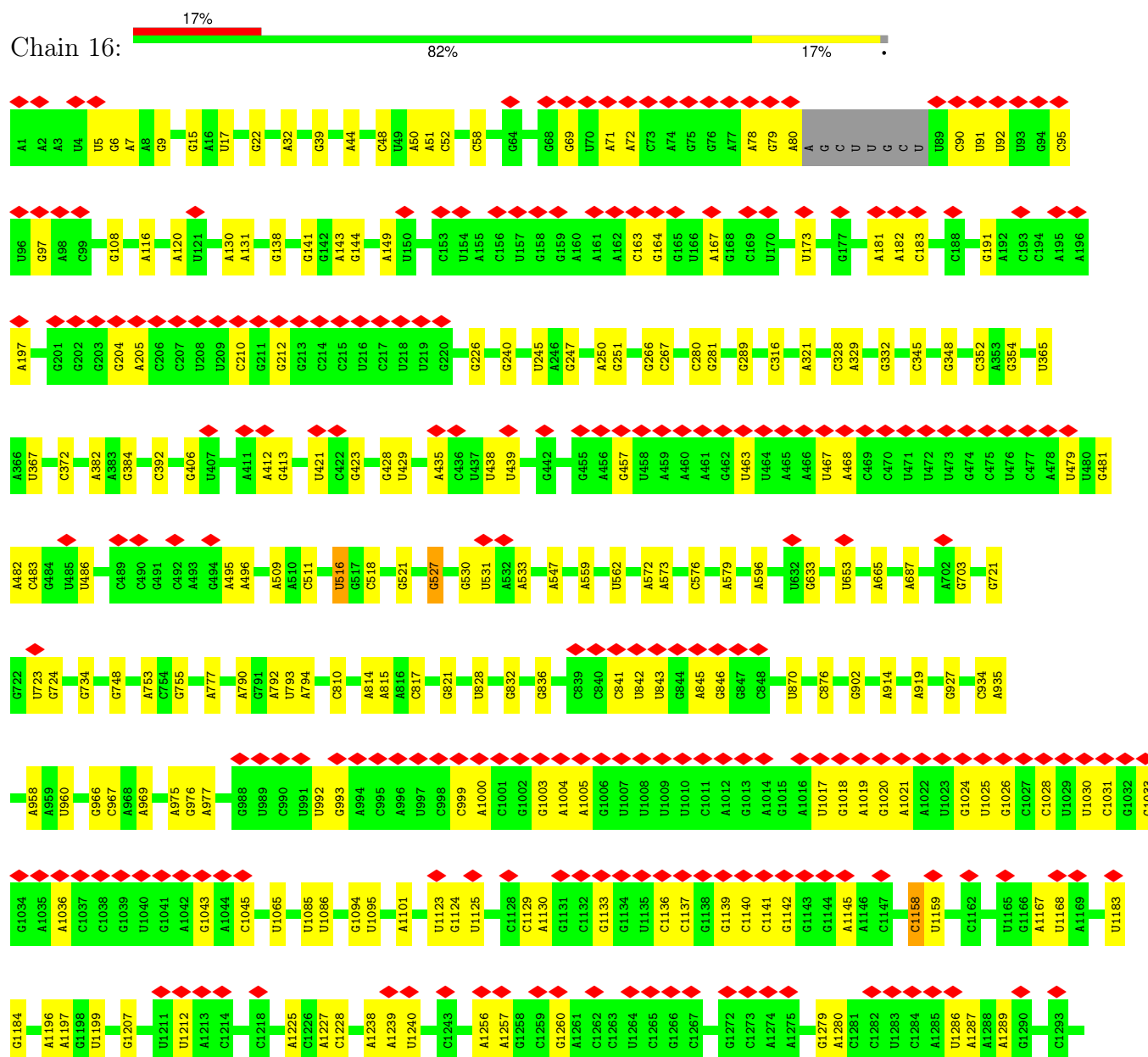
Mol	Chain	Residues	Atoms			AltConf
61	23	1	Total	C	N	0
			10	7	3	
61	23	1	Total	C	N	0
			10	7	3	
61	23	1	Total	C	N	0
			10	7	3	

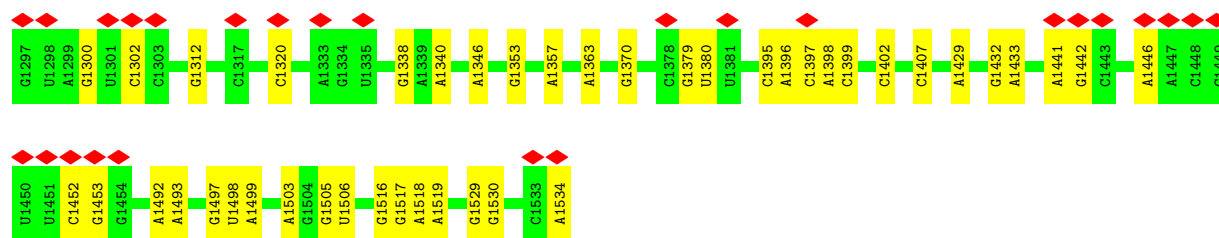


### 3 Residue-property plots

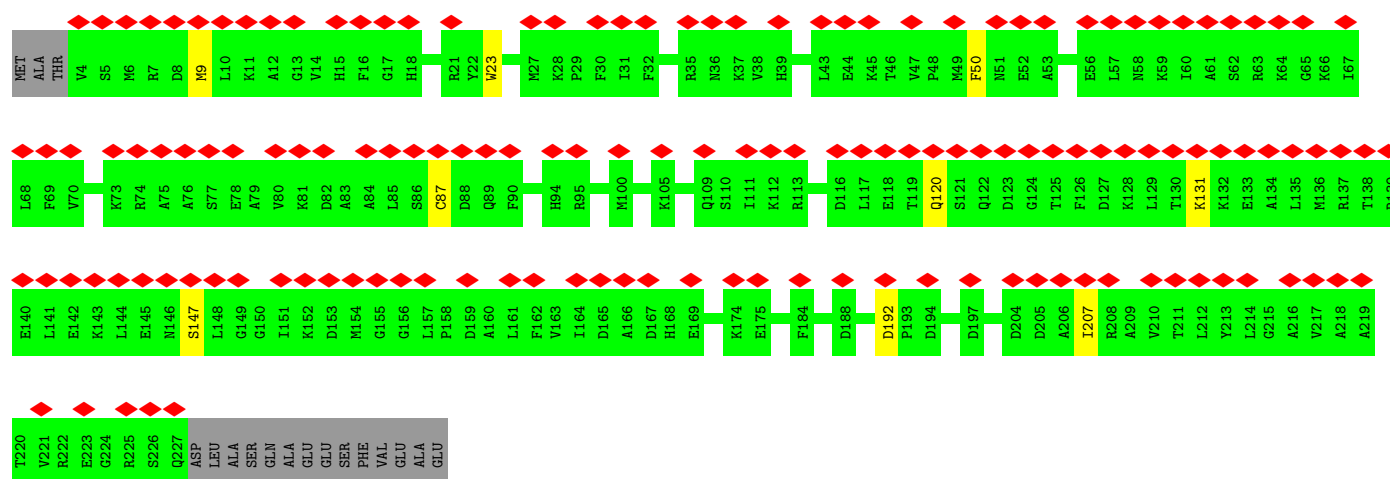
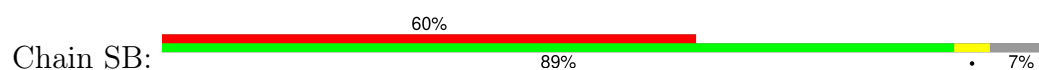
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 16S rRNA

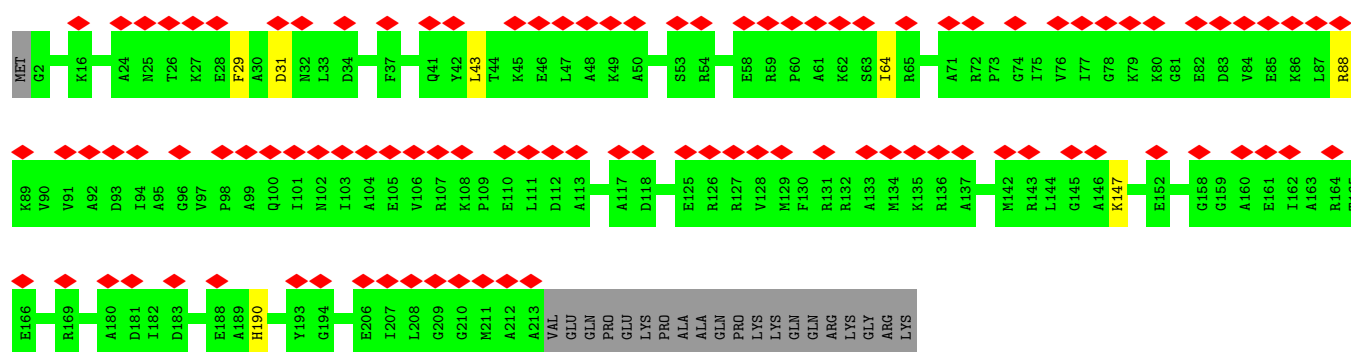




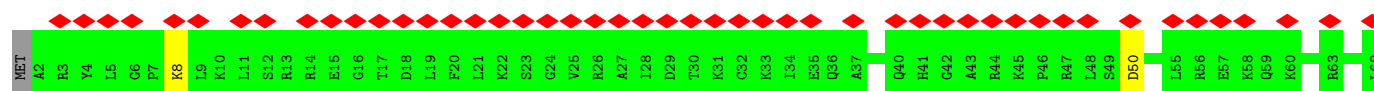
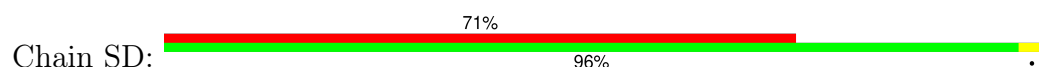
• Molecule 2: 30S ribosomal protein S2

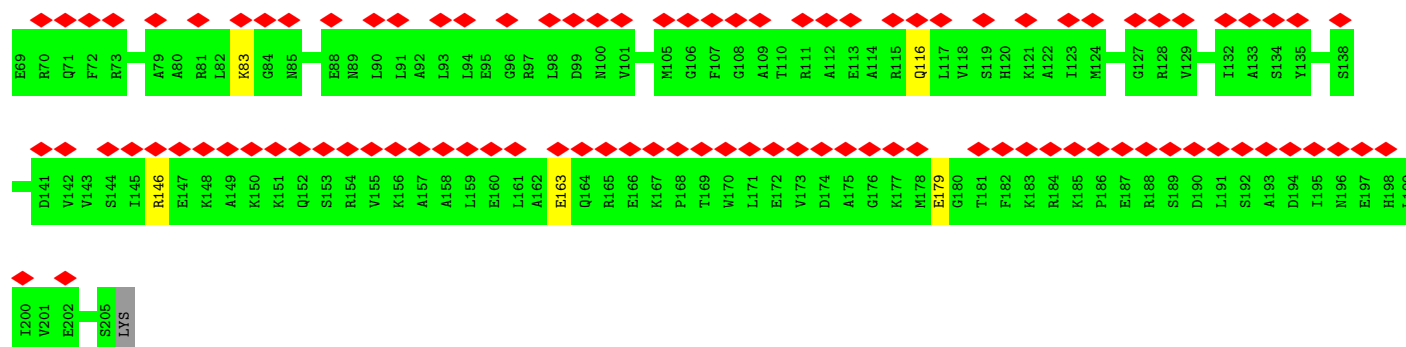


• Molecule 3: 30S ribosomal protein S3

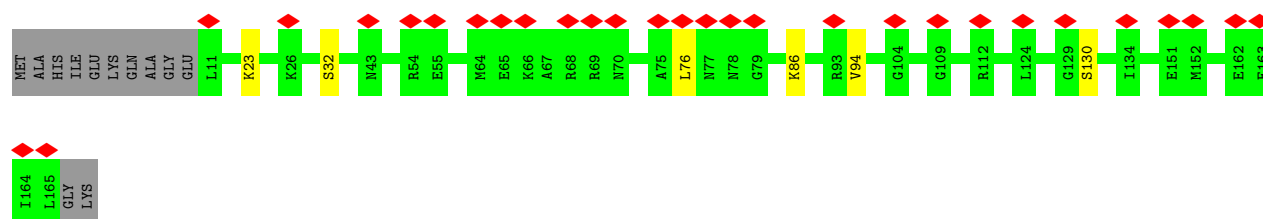
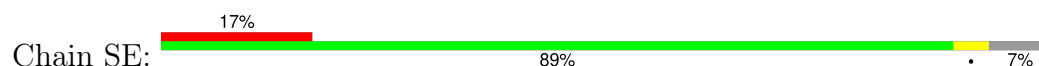


• Molecule 4: 30S ribosomal protein S4

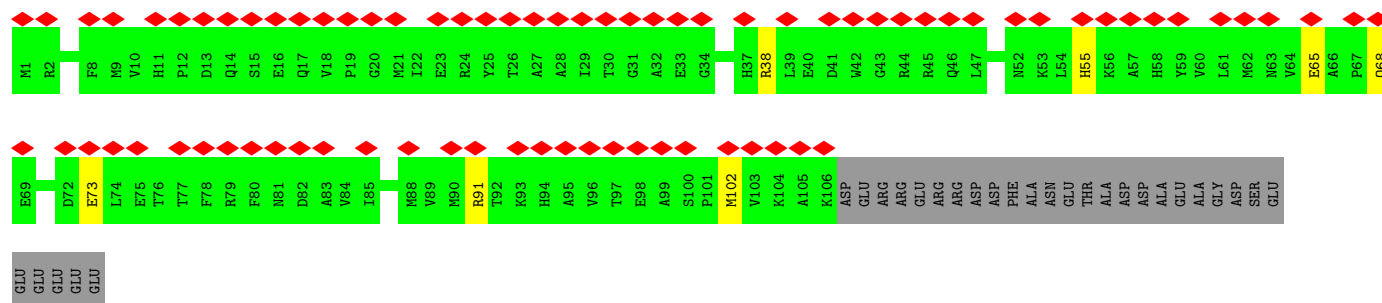
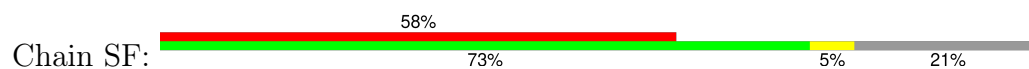




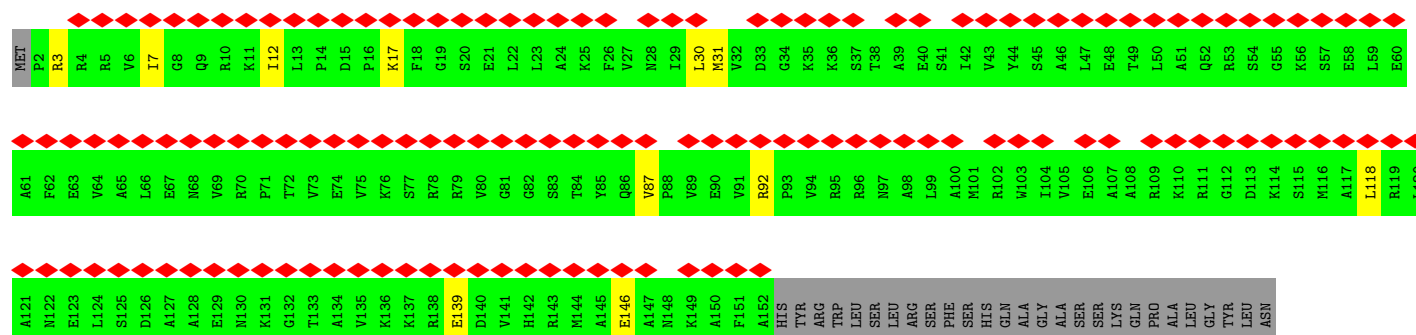
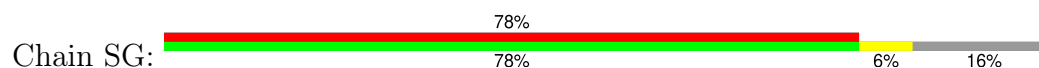
• Molecule 5: 30S ribosomal protein S5



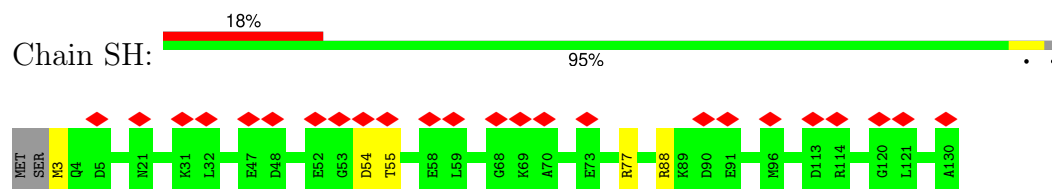
• Molecule 6: 30S ribosomal protein S6



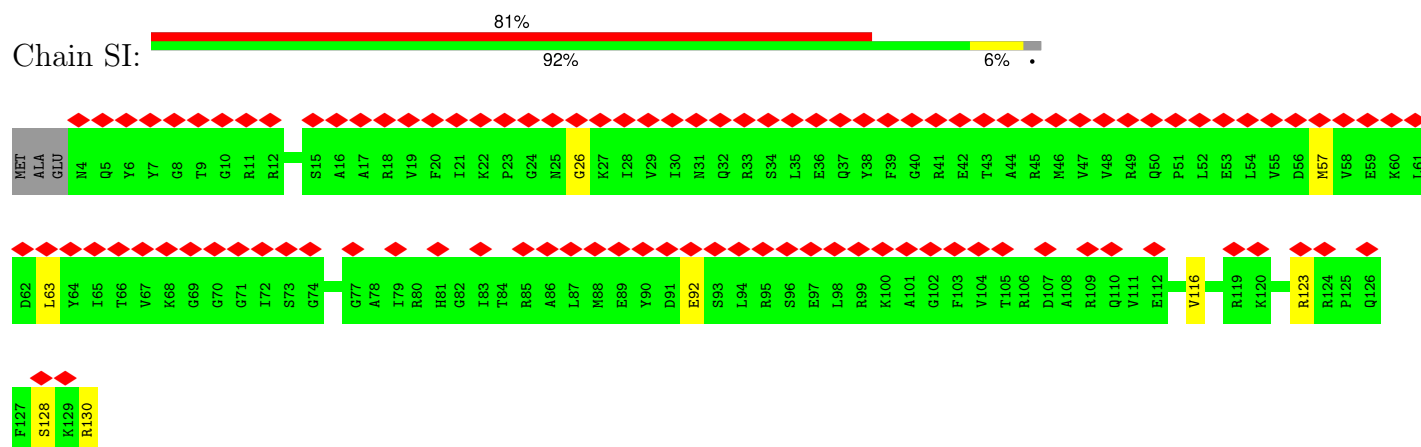
• Molecule 7: 30S ribosomal protein S7



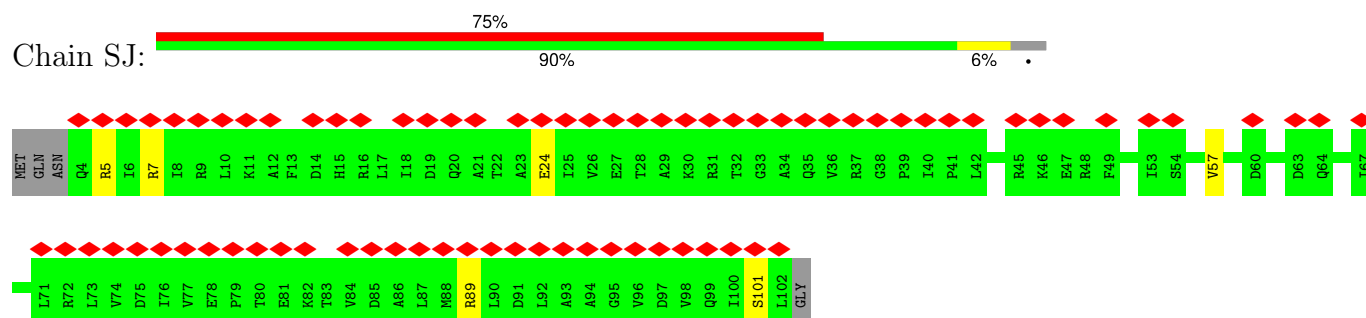
- Molecule 8: 30S ribosomal protein S8



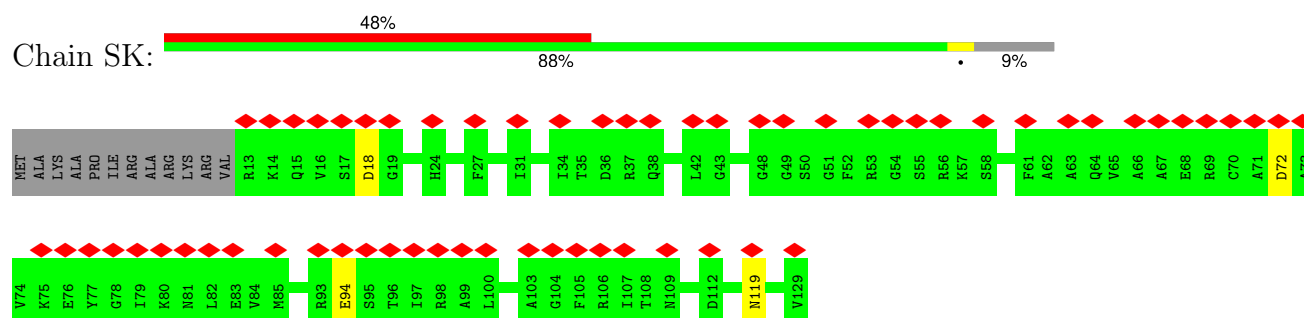
- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10

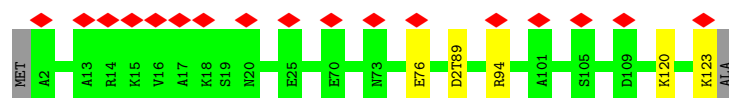


- Molecule 11: 30S ribosomal protein S11

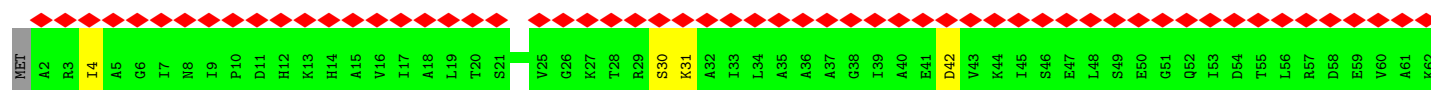


- Molecule 12: 30S ribosomal protein S12

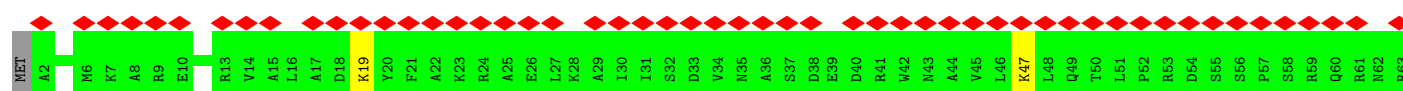




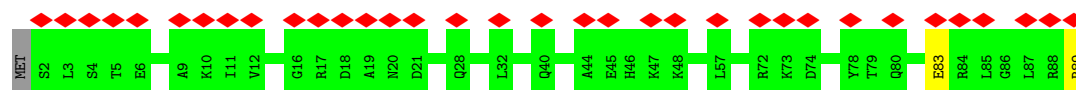
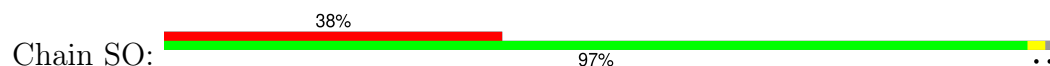
- Molecule 13: 30S ribosomal protein S13



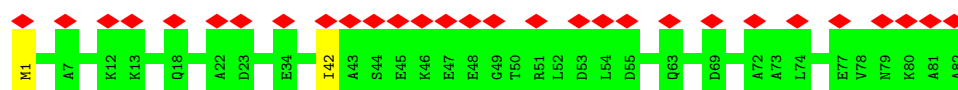
- Molecule 14: 30S ribosomal protein S14



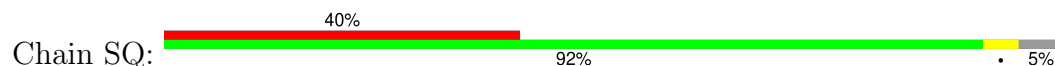
- Molecule 15: 30S ribosomal protein S15



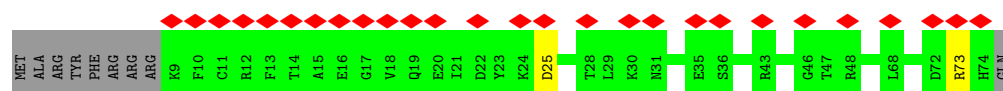
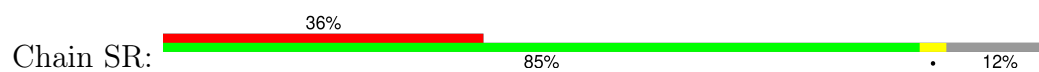
- Molecule 16: 30S ribosomal protein S16



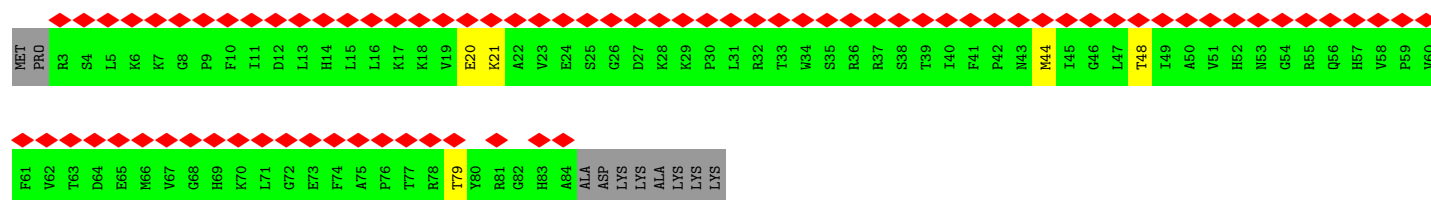
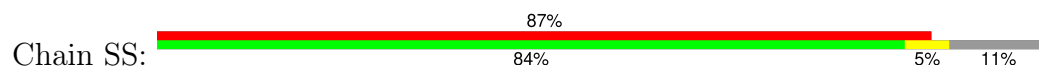
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



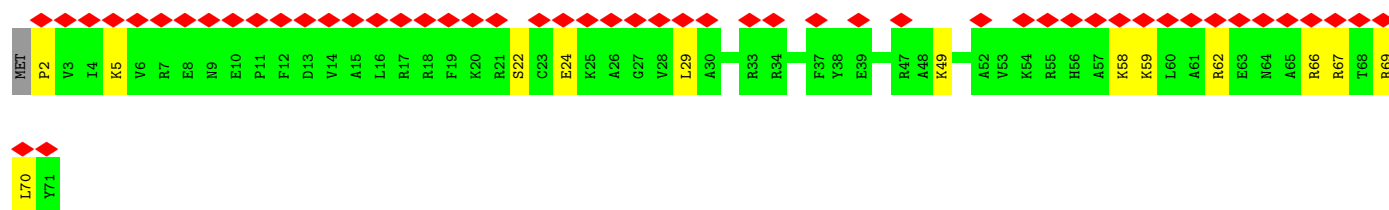
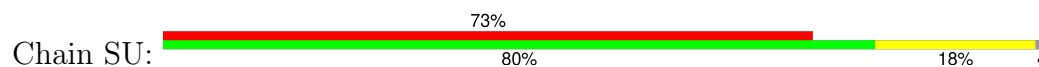
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



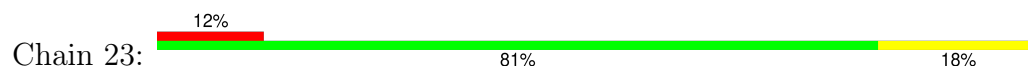
- Molecule 21: 30S ribosomal protein S21

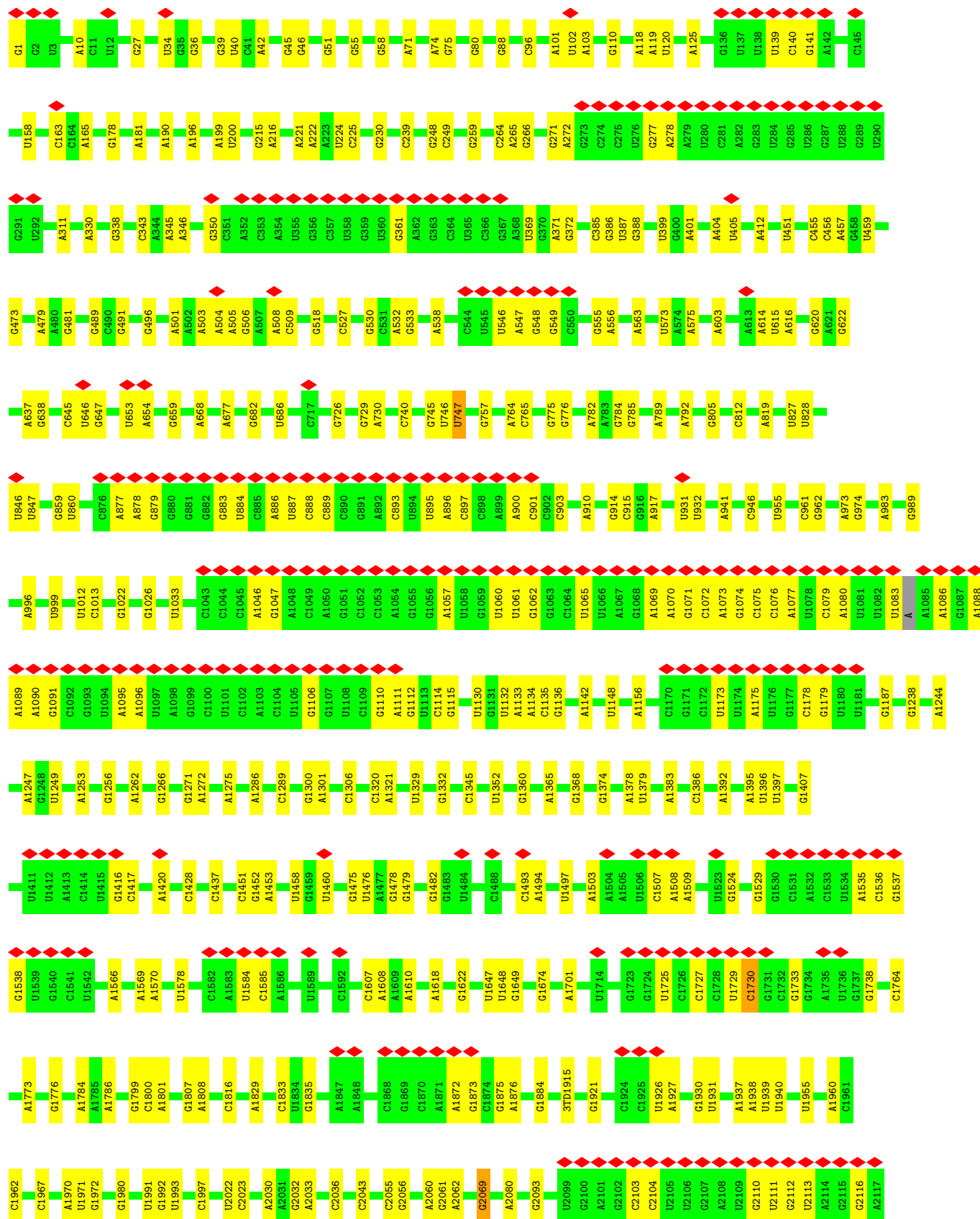


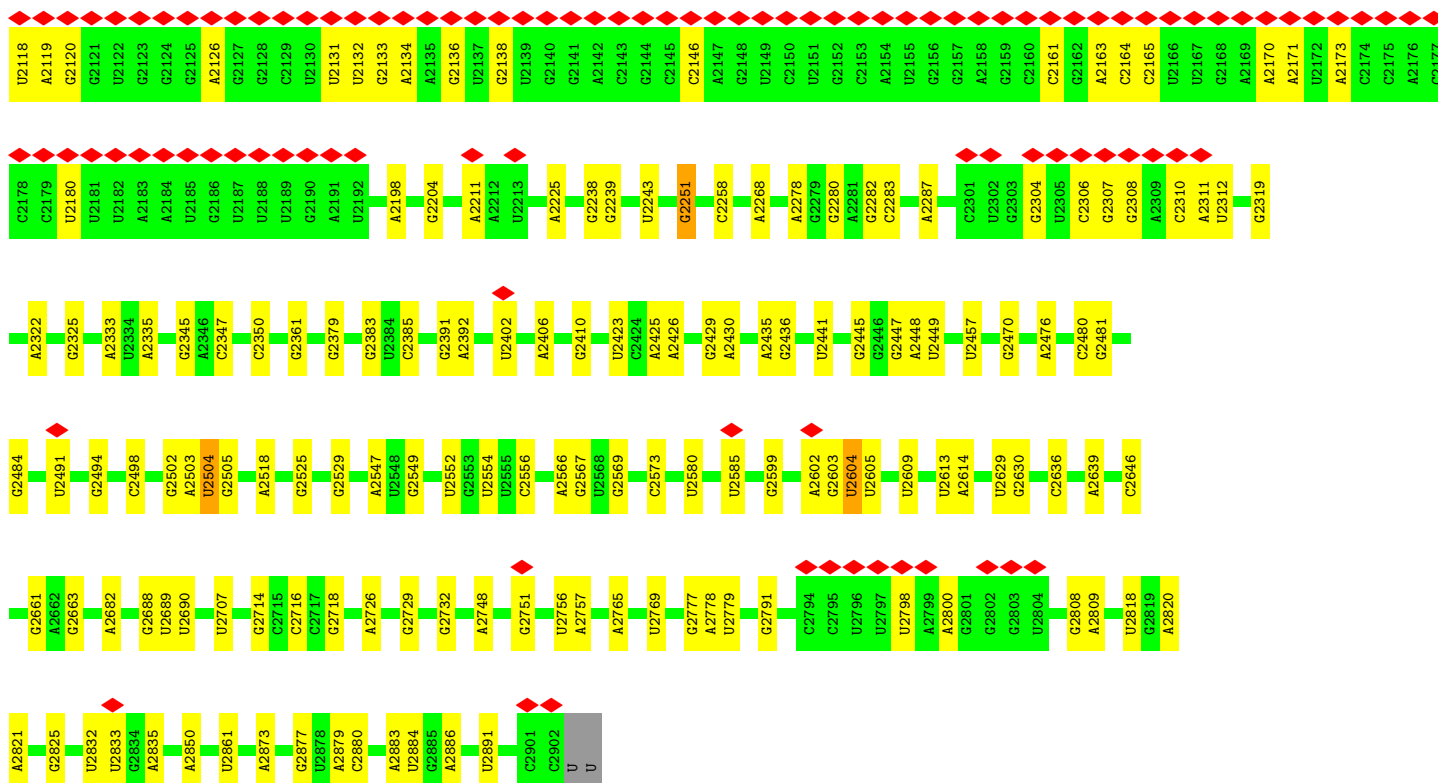
- Molecule 22: mRNA



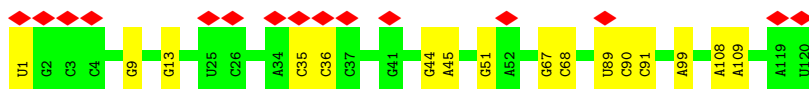
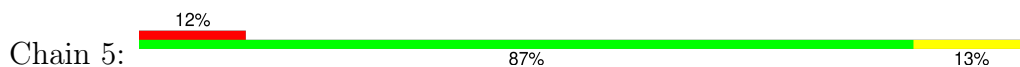
- Molecule 23: 23S rRNA







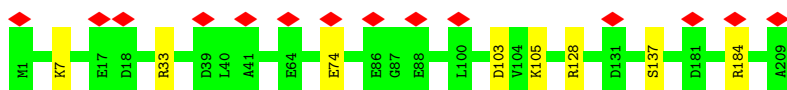
• Molecule 24: 5S rRNA



• Molecule 25: 50S ribosomal protein L2



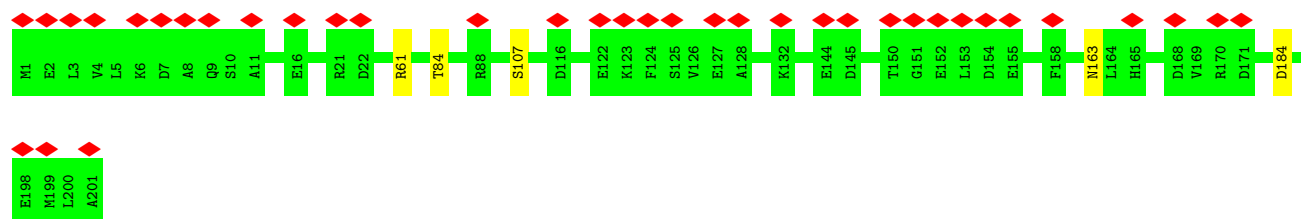
• Molecule 26: 50S ribosomal protein L3



• Molecule 27: 50S ribosomal protein L4

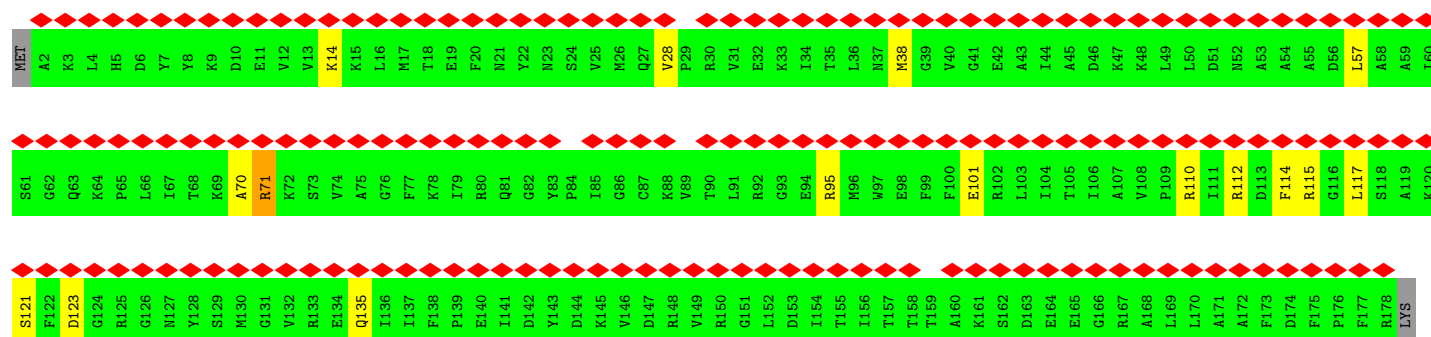






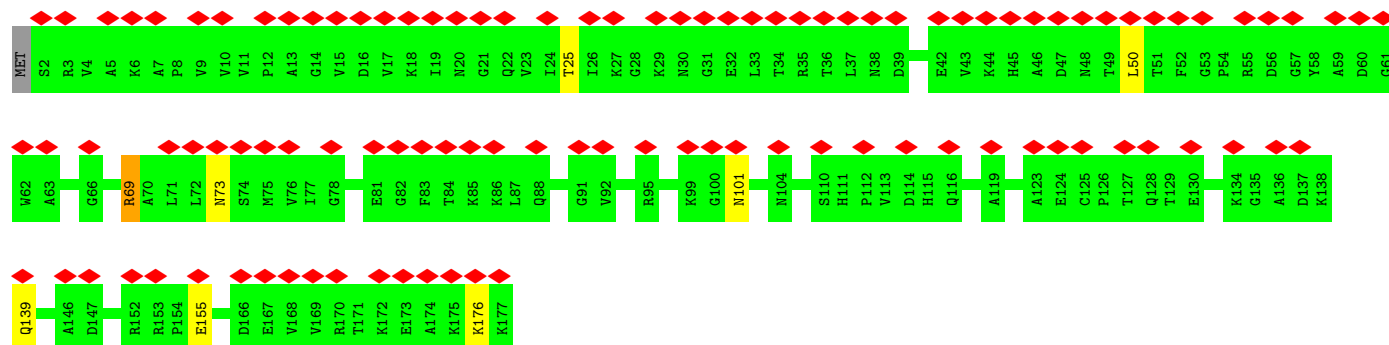
• Molecule 28: 50S ribosomal protein L5

Chain LE: 97%  
90% 8% ..



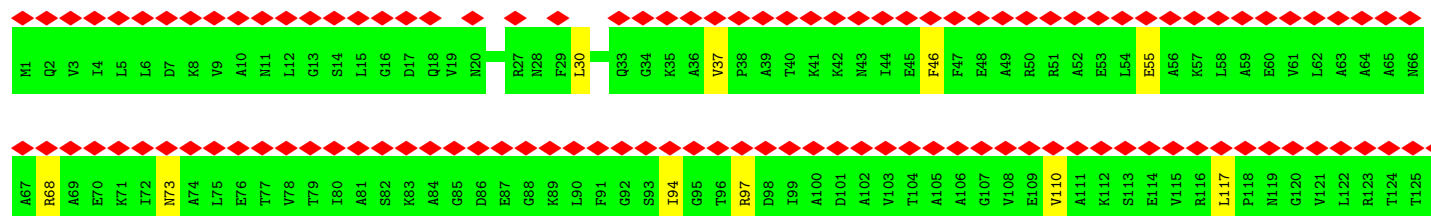
• Molecule 29: 50S ribosomal protein L6

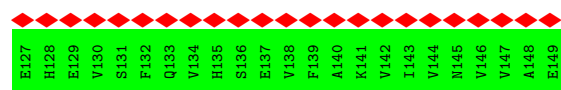
Chain LF: 59%  
95% 7% ..



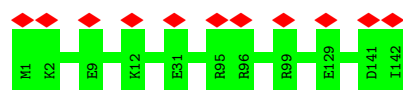
• Molecule 30: 50S ribosomal protein L9

Chain LI: 93%  
93% 7%

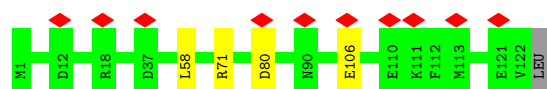




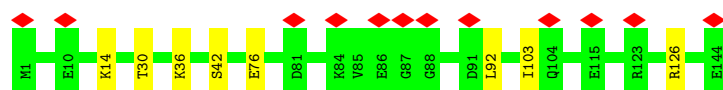
- Molecule 31: 50S ribosomal protein L13



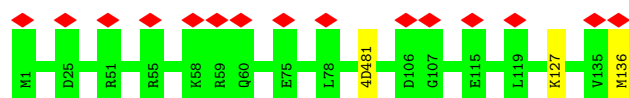
- Molecule 32: 50S ribosomal protein L14



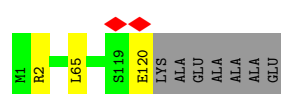
- Molecule 33: 50S ribosomal protein L15



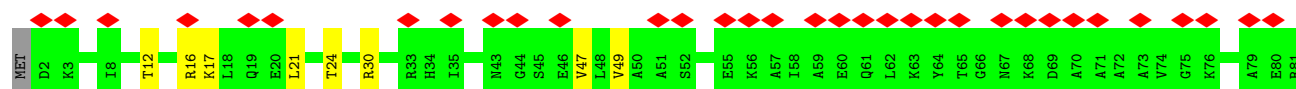
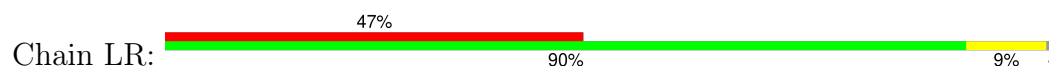
- Molecule 34: 50S ribosomal protein L16

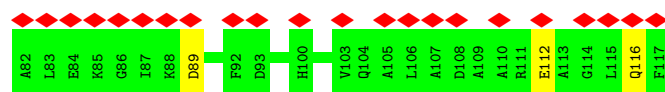


- Molecule 35: 50S ribosomal protein L17



- Molecule 36: 50S ribosomal protein L18

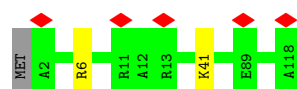




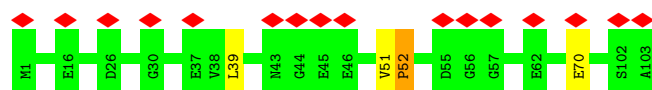
- Molecule 37: 50S ribosomal protein L19



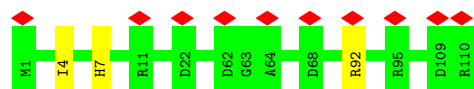
- Molecule 38: 50S ribosomal protein L20



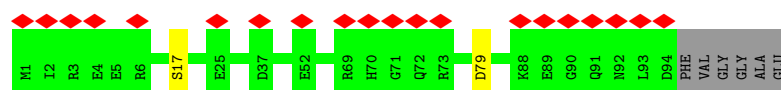
- Molecule 39: 50S ribosomal protein L21



- Molecule 40: 50S ribosomal protein L22



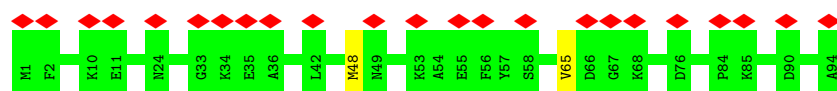
- Molecule 41: 50S ribosomal protein L23



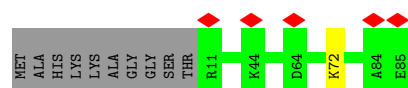
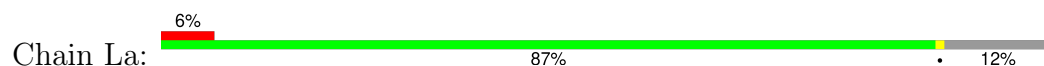
- Molecule 42: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L25



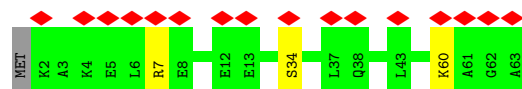
- Molecule 44: 50S ribosomal protein L27



- Molecule 45: 50S ribosomal protein L28



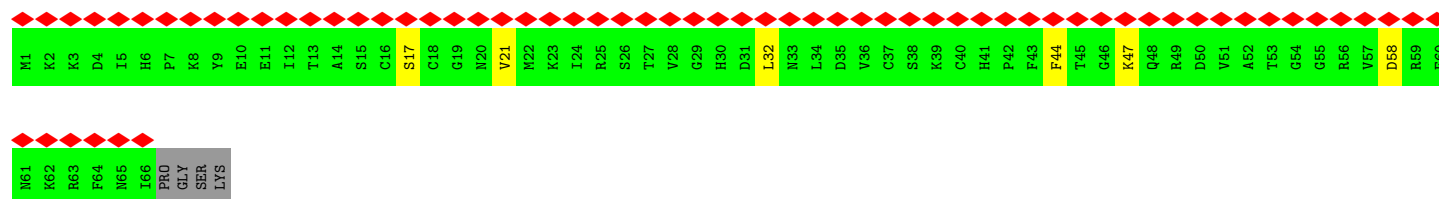
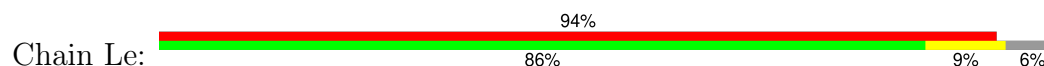
- Molecule 46: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L30

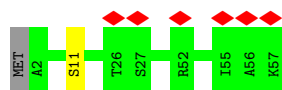


- Molecule 48: 50S ribosomal protein L31

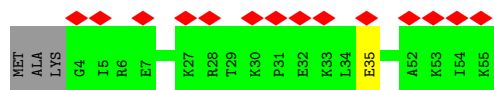


- Molecule 49: 50S ribosomal protein L32

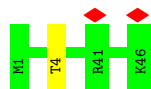




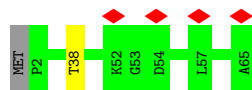
- Molecule 50: 50S ribosomal protein L33



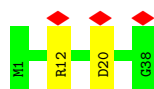
- Molecule 51: 50S ribosomal protein L34



- Molecule 52: 50S ribosomal protein L35



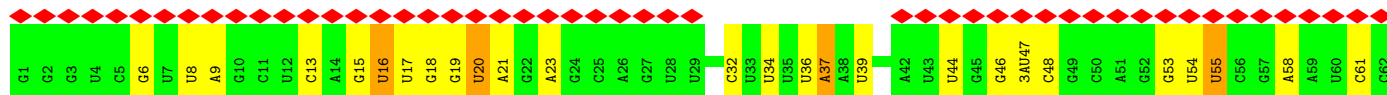
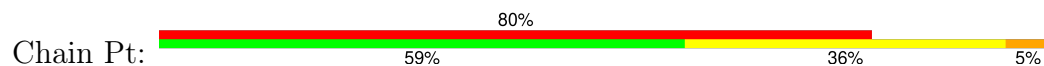
- Molecule 53: 50S ribosomal protein L36

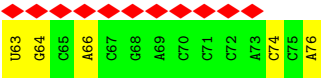


- Molecule 54: Nascent peptide

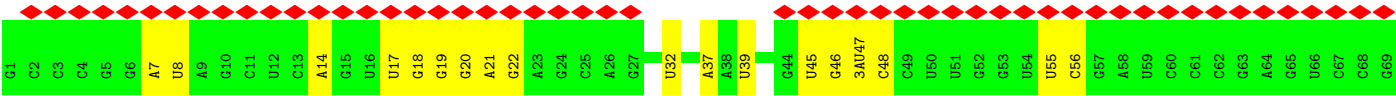
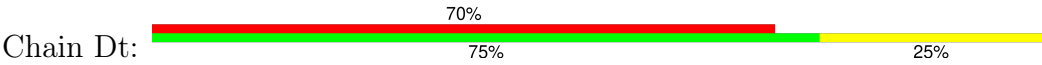


- Molecule 55: tRNA





● Molecule 56: tRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87818	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	0.133	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0193	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: 5MU, PUT, D2T, ZN, MIA, UR3, H2U, 6MZ, OMG, 4D4, T6A, ATP, 5MC, 4SU, 1MG, G7M, MA6, 3AU, PSU, 3TD, OMC, MG, 2MA, OMU, 4OC, SPD, 2MG, U8U

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	0.52	0/36405	0.69	1/56786 (0.0%)
2	SB	0.43	0/1784	0.62	0/2403
3	SC	0.45	0/1685	0.62	0/2270
4	SD	0.45	0/1655	0.63	1/2216 (0.0%)
5	SE	0.48	0/1156	0.64	0/1556
6	SF	0.43	0/881	0.62	0/1189
7	SG	0.49	0/1195	0.64	0/1602
8	SH	0.45	0/983	0.63	0/1318
9	SI	0.42	0/1034	0.70	0/1375
10	SJ	0.48	0/805	0.70	0/1089
11	SK	0.47	0/893	0.65	0/1205
12	SL	0.44	0/954	0.67	0/1279
13	SM	0.48	0/892	0.71	0/1193
14	SN	0.43	0/817	0.58	0/1088
15	SO	0.45	0/721	0.61	0/964
16	SP	0.49	0/658	0.73	0/884
17	SQ	0.45	0/657	0.65	0/881
18	SR	0.45	0/553	0.63	1/742 (0.1%)
19	SS	0.45	0/672	0.65	0/904
20	ST	0.37	0/676	0.56	0/895
21	SU	0.46	0/598	0.68	0/792
22	mR	0.45	0/261	0.61	0/404
23	23	0.56	1/69236 (0.0%)	0.70	1/108005 (0.0%)
24	5	0.59	1/2873 (0.0%)	0.71	0/4478
25	LB	0.45	0/2121	0.69	1/2852 (0.0%)
26	LC	0.45	0/1586	0.65	0/2134
27	LD	0.40	0/1571	0.61	0/2113
28	LE	0.54	0/1434	0.69	0/1926
29	LF	0.45	0/1343	0.63	0/1816
30	LI	0.49	0/1122	0.63	0/1515
31	LM	0.44	0/1152	0.58	0/1551



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	LN	0.45	0/947	0.67	0/1268
33	LO	0.43	0/1062	0.70	1/1413 (0.1%)
34	LP	0.43	0/1081	0.64	0/1443
35	LQ	0.43	0/973	0.62	0/1301
36	LR	0.43	0/901	0.68	0/1209
37	LS	0.44	0/940	0.64	0/1256
38	LT	0.47	0/960	0.69	0/1278
39	LU	0.52	1/829 (0.1%)	0.98	3/1107 (0.3%)
40	LV	0.46	0/864	0.65	0/1156
41	LW	0.41	0/752	0.62	0/1005
42	LX	0.47	0/787	0.65	0/1051
43	LY	0.45	0/765	0.63	0/1025
44	La	0.39	0/582	0.63	0/769
45	Lb	0.49	0/634	0.73	0/848
46	Lc	0.39	0/502	0.59	0/667
47	Ld	0.41	0/453	0.61	0/605
48	Le	0.58	0/531	0.66	0/709
49	Lf	0.51	0/449	0.72	0/599
50	Lg	0.45	0/434	0.63	0/576
51	Lh	0.47	0/380	0.79	0/498
52	Li	0.44	0/513	0.66	0/676
53	Lj	0.43	0/303	0.65	0/397
54	Pp	0.56	0/28	1.13	0/34
55	Pt	0.34	0/1573	0.68	0/2445
56	Dt	0.40	0/1650	0.65	0/2568
All	All	0.52	3/157266 (0.0%)	0.69	9/235328 (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
8	SH	0	1
12	SL	0	1
13	SM	0	1
26	LC	0	1
28	LE	0	1
29	LF	0	1
46	Lc	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	1	U	OP3-P	-10.72	1.48	1.61
23	23	1	G	OP3-P	-10.30	1.48	1.61
39	LU	52	PRO	N-CD	-7.29	1.37	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	LU	51	VAL	C-N-CD	-23.12	69.73	120.60
23	23	1730	C	N1-C1'-C2'	6.15	122.00	114.00
33	LO	36	LYS	N-CA-C	5.80	126.66	111.00
39	LU	52	PRO	CA-N-CD	5.54	119.46	111.70
18	SR	25	ASP	CB-CG-OD1	5.24	123.02	118.30
1	16	1158	C	N1-C2-O2	5.08	121.95	118.90
25	LB	232	HIS	CB-CA-C	5.04	120.48	110.40
4	SD	50	ASP	CB-CG-OD1	5.04	122.83	118.30
39	LU	51	VAL	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	LC	128	ARG	Sidechain
28	LE	112	ARG	Sidechain
29	LF	69	ARG	Sidechain
46	Lc	7	ARG	Sidechain
8	SH	77	ARG	Sidechain
12	SL	94	ARG	Sidechain
13	SM	70	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SB	222/241 (92%)	208 (94%)	13 (6%)	1 (0%)	25	40
3	SC	210/233 (90%)	203 (97%)	7 (3%)	0	100	100
4	SD	202/206 (98%)	200 (99%)	2 (1%)	0	100	100
5	SE	153/167 (92%)	146 (95%)	7 (5%)	0	100	100
6	SF	104/135 (77%)	100 (96%)	4 (4%)	0	100	100
7	SG	149/179 (83%)	144 (97%)	5 (3%)	0	100	100
8	SH	126/130 (97%)	119 (94%)	7 (6%)	0	100	100
9	SI	125/130 (96%)	114 (91%)	10 (8%)	1 (1%)	16	28
10	SJ	97/103 (94%)	91 (94%)	5 (5%)	1 (1%)	13	21
11	SK	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
12	SL	119/124 (96%)	117 (98%)	2 (2%)	0	100	100
13	SM	112/118 (95%)	107 (96%)	4 (4%)	1 (1%)	14	25
14	SN	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
15	SO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	SP	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	SQ	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
18	SR	64/75 (85%)	64 (100%)	0	0	100	100
19	SS	80/92 (87%)	78 (98%)	2 (2%)	0	100	100
20	ST	84/87 (97%)	84 (100%)	0	0	100	100
21	SU	68/71 (96%)	68 (100%)	0	0	100	100
25	LB	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
26	LC	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
27	LD	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
28	LE	175/179 (98%)	167 (95%)	6 (3%)	2 (1%)	12	19
29	LF	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
30	LI	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
31	LM	140/142 (99%)	140 (100%)	0	0	100	100
32	LN	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
33	LO	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
34	LP	133/136 (98%)	131 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	LQ	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
36	LR	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
37	LS	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
38	LT	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
39	LU	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	13	21
40	LV	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	LW	92/100 (92%)	91 (99%)	1 (1%)	0	100	100
42	LX	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
43	LY	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
44	La	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
45	Lb	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
46	Lc	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
47	Ld	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	Le	64/70 (91%)	57 (89%)	6 (9%)	1 (2%)	8	13
49	Lf	54/57 (95%)	54 (100%)	0	0	100	100
50	Lg	50/55 (91%)	47 (94%)	3 (6%)	0	100	100
51	Lh	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
52	Li	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
53	Lj	36/38 (95%)	36 (100%)	0	0	100	100
54	Pp	1/3 (33%)	1 (100%)	0	0	100	100
All	All	5606/5916 (95%)	5404 (96%)	194 (4%)	8 (0%)	50	67

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	SB	131	LYS
10	SJ	57	VAL
39	LU	52	PRO
28	LE	70	ALA
48	Le	47	LYS
28	LE	71	ARG
9	SI	26	GLY
13	SM	4	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SB	186/199 (94%)	178 (96%)	8 (4%)	25	41
3	SC	172/190 (90%)	165 (96%)	7 (4%)	26	43
4	SD	171/173 (99%)	165 (96%)	6 (4%)	31	50
5	SE	118/126 (94%)	112 (95%)	6 (5%)	20	34
6	SF	92/116 (79%)	85 (92%)	7 (8%)	11	18
7	SG	124/147 (84%)	113 (91%)	11 (9%)	8	12
8	SH	103/105 (98%)	99 (96%)	4 (4%)	27	45
9	SI	105/107 (98%)	98 (93%)	7 (7%)	13	22
10	SJ	87/90 (97%)	82 (94%)	5 (6%)	17	29
11	SK	90/99 (91%)	86 (96%)	4 (4%)	24	40
12	SL	102/103 (99%)	99 (97%)	3 (3%)	37	58
13	SM	92/96 (96%)	85 (92%)	7 (8%)	11	18
14	SN	83/84 (99%)	80 (96%)	3 (4%)	30	48
15	SO	76/77 (99%)	74 (97%)	2 (3%)	41	63
16	SP	65/65 (100%)	63 (97%)	2 (3%)	35	55
17	SQ	74/78 (95%)	71 (96%)	3 (4%)	26	43
18	SR	57/65 (88%)	56 (98%)	1 (2%)	54	73
19	SS	71/79 (90%)	66 (93%)	5 (7%)	12	21
20	ST	65/66 (98%)	62 (95%)	3 (5%)	23	38
21	SU	60/61 (98%)	47 (78%)	13 (22%)	1	0
25	LB	216/218 (99%)	214 (99%)	2 (1%)	75	87
26	LC	164/164 (100%)	157 (96%)	7 (4%)	25	41
27	LD	165/165 (100%)	160 (97%)	5 (3%)	36	56
28	LE	148/150 (99%)	134 (90%)	14 (10%)	7	11
29	LF	137/138 (99%)	129 (94%)	8 (6%)	17	29
30	LI	114/114 (100%)	104 (91%)	10 (9%)	8	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	LM	116/116 (100%)	116 (100%)	0	100	100
32	LN	103/104 (99%)	99 (96%)	4 (4%)	27	45
33	LO	103/103 (100%)	96 (93%)	7 (7%)	13	22
34	LP	108/108 (100%)	106 (98%)	2 (2%)	52	72
35	LQ	100/103 (97%)	97 (97%)	3 (3%)	36	56
36	LR	86/87 (99%)	75 (87%)	11 (13%)	3	5
37	LS	100/100 (100%)	92 (92%)	8 (8%)	10	16
38	LT	89/90 (99%)	87 (98%)	2 (2%)	47	68
39	LU	84/84 (100%)	82 (98%)	2 (2%)	44	65
40	LV	93/93 (100%)	90 (97%)	3 (3%)	34	54
41	LW	81/84 (96%)	79 (98%)	2 (2%)	42	64
42	LX	83/85 (98%)	80 (96%)	3 (4%)	30	48
43	LY	78/78 (100%)	76 (97%)	2 (3%)	41	63
44	La	57/63 (90%)	56 (98%)	1 (2%)	54	73
45	Lb	67/68 (98%)	65 (97%)	2 (3%)	36	56
46	Lc	54/55 (98%)	52 (96%)	2 (4%)	29	48
47	Ld	48/49 (98%)	46 (96%)	2 (4%)	25	42
48	Le	59/62 (95%)	54 (92%)	5 (8%)	8	13
49	Lf	47/48 (98%)	46 (98%)	1 (2%)	48	70
50	Lg	47/49 (96%)	46 (98%)	1 (2%)	48	70
51	Lh	38/38 (100%)	37 (97%)	1 (3%)	41	63
52	Li	51/52 (98%)	50 (98%)	1 (2%)	50	71
53	Lj	34/34 (100%)	32 (94%)	2 (6%)	16	28
54	Pp	3/3 (100%)	3 (100%)	0	100	100
All	All	4666/4831 (97%)	4446 (95%)	220 (5%)	24	37

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	9	MET
2	SB	23	TRP
2	SB	50	PHE
2	SB	87	CYS
2	SB	120	GLN

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Mol	Chain	Res	Type
2	SB	147	SER
2	SB	192	ASP
2	SB	207	ILE
3	SC	29	PHE
3	SC	31	ASP
3	SC	43	LEU
3	SC	64	ILE
3	SC	88	ARG
3	SC	147	LYS
3	SC	190	HIS
4	SD	8	LYS
4	SD	83	LYS
4	SD	116	GLN
4	SD	146	ARG
4	SD	163	GLU
4	SD	179	GLU
5	SE	23	LYS
5	SE	32	SER
5	SE	76	LEU
5	SE	86	LYS
5	SE	94	VAL
5	SE	130	SER
6	SF	38	ARG
6	SF	55	HIS
6	SF	65	GLU
6	SF	68	GLN
6	SF	73	GLU
6	SF	91	ARG
6	SF	102	MET
7	SG	3	ARG
7	SG	7	ILE
7	SG	12	ILE
7	SG	17	LYS
7	SG	30	LEU
7	SG	31	MET
7	SG	87	VAL
7	SG	92	ARG
7	SG	118	LEU
7	SG	139	GLU
7	SG	146	GLU
8	SH	3	MET
8	SH	54	ASP

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Mol	Chain	Res	Type
8	SH	55	THR
8	SH	88	ARG
9	SI	57	MET
9	SI	63	LEU
9	SI	92	GLU
9	SI	116	VAL
9	SI	123	ARG
9	SI	128	SER
9	SI	130	ARG
10	SJ	5	ARG
10	SJ	7	ARG
10	SJ	24	GLU
10	SJ	89	ARG
10	SJ	101	SER
11	SK	18	ASP
11	SK	72	ASP
11	SK	94	GLU
11	SK	119	ASN
12	SL	76	GLU
12	SL	120	LYS
12	SL	123	LYS
13	SM	30	SER
13	SM	31	LYS
13	SM	42	ASP
13	SM	79	ARG
13	SM	97	VAL
13	SM	107	ARG
13	SM	113	ARG
14	SN	19	LYS
14	SN	47	LYS
14	SN	76	LYS
15	SO	83	GLU
15	SO	89	ARG
16	SP	1	MET
16	SP	42	ILE
17	SQ	28	PHE
17	SQ	62	ARG
17	SQ	65	ARG
18	SR	73	ARG
19	SS	20	GLU
19	SS	21	LYS
19	SS	44	MET

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Mol	Chain	Res	Type
19	SS	48	THR
19	SS	79	THR
20	ST	52	ASN
20	ST	55	GLN
20	ST	69	LYS
21	SU	2	PRO
21	SU	5	LYS
21	SU	22	SER
21	SU	24	GLU
21	SU	29	LEU
21	SU	49	LYS
21	SU	58	LYS
21	SU	59	LYS
21	SU	62	ARG
21	SU	66	ARG
21	SU	67	ARG
21	SU	69	ARG
21	SU	70	LEU
25	LB	130	LEU
25	LB	157	SER
26	LC	7	LYS
26	LC	33	ARG
26	LC	74	GLU
26	LC	103	ASP
26	LC	105	LYS
26	LC	137	SER
26	LC	184	ARG
27	LD	61	ARG
27	LD	84	THR
27	LD	107	SER
27	LD	163	ASN
27	LD	184	ASP
28	LE	14	LYS
28	LE	28	VAL
28	LE	38	MET
28	LE	57	LEU
28	LE	71	ARG
28	LE	95	ARG
28	LE	101	GLU
28	LE	110	ARG
28	LE	114	PHE
28	LE	115	ARG

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Mol	Chain	Res	Type
28	LE	117	LEU
28	LE	121	SER
28	LE	123	ASP
28	LE	135	GLN
29	LF	25	THR
29	LF	50	LEU
29	LF	69	ARG
29	LF	73	ASN
29	LF	101	ASN
29	LF	139	GLN
29	LF	155	GLU
29	LF	176	LYS
30	LI	30	LEU
30	LI	37	VAL
30	LI	46	PHE
30	LI	55	GLU
30	LI	68	ARG
30	LI	73	ASN
30	LI	94	ILE
30	LI	97	ARG
30	LI	110	VAL
30	LI	117	LEU
32	LN	58	LEU
32	LN	71	ARG
32	LN	80	ASP
32	LN	106	GLU
33	LO	14	LYS
33	LO	30	THR
33	LO	42	SER
33	LO	76	GLU
33	LO	92	LEU
33	LO	103	ILE
33	LO	126	ARG
34	LP	127	LYS
34	LP	136	MET
35	LQ	2	ARG
35	LQ	65	LEU
35	LQ	120	GLU
36	LR	12	THR
36	LR	16	ARG
36	LR	17	LYS
36	LR	21	LEU

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Mol	Chain	Res	Type
36	LR	24	THR
36	LR	30	ARG
36	LR	47	VAL
36	LR	49	VAL
36	LR	89	ASP
36	LR	112	GLU
36	LR	116	GLN
37	LS	13	MET
37	LS	16	ASP
37	LS	19	SER
37	LS	21	ARG
37	LS	39[A]	ARG
37	LS	39[B]	ARG
37	LS	78	SER
37	LS	87	LYS
38	LT	6	ARG
38	LT	41	LYS
39	LU	39	LEU
39	LU	70	GLU
40	LV	4	ILE
40	LV	7	HIS
40	LV	92	ARG
41	LW	17	SER
41	LW	79	ASP
42	LX	53	ASN
42	LX	81	ASP
42	LX	99	ASN
43	LY	48	MET
43	LY	65	VAL
44	La	72	LYS
45	Lb	35	SER
45	Lb	54	LYS
46	Lc	34	SER
46	Lc	60	LYS
47	Ld	16	ARG
47	Ld	54	MET
48	Le	17	SER
48	Le	21	VAL
48	Le	32	LEU
48	Le	44	PHE
48	Le	58	ASP
49	Lf	11	SER

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Mol	Chain	Res	Type
50	Lg	35	GLU
51	Lh	4	THR
52	Li	38	THR
53	Lj	12	ARG
53	Lj	20	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	SB	177	ASN
3	SC	176	HIS
5	SE	78	ASN
5	SE	82	GLN
6	SF	14	GLN
6	SF	46	GLN
6	SF	68	GLN
10	SJ	58	ASN
11	SK	119	ASN
14	SN	66	GLN
16	SP	63	GLN
16	SP	79	ASN
19	SS	57	HIS
20	ST	55	GLN
26	LC	49	GLN
26	LC	150	GLN
27	LD	163	ASN
28	LE	37	ASN
29	LF	30	ASN
29	LF	101	ASN
29	LF	116	GLN
30	LI	11	ASN
30	LI	66	ASN
30	LI	133	GLN
36	LR	38	GLN
36	LR	116	GLN
38	LT	52	GLN
39	LU	86	GLN
41	LW	91	GLN
43	LY	24	ASN
48	Le	33	ASN
50	Lg	45	GLN
52	Li	31	HIS

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1521/1534 (99%)	252 (16%)	20 (1%)
22	mR	10/60 (16%)	0	0
23	23	2895/2904 (99%)	511 (17%)	41 (1%)
24	5	119/120 (99%)	15 (12%)	1 (0%)
55	Pt	73/76 (96%)	25 (34%)	0
56	Dt	73/76 (96%)	12 (16%)	0
All	All	4691/4770 (98%)	815 (17%)	62 (1%)

All (815) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	5	U
1	16	6	G
1	16	7	A
1	16	9	G
1	16	15	G
1	16	17	U
1	16	22	G
1	16	32	A
1	16	39	G
1	16	44	A
1	16	48	C
1	16	50	A
1	16	51	A
1	16	52	C
1	16	58	C
1	16	69	G
1	16	71	A
1	16	72	A
1	16	78	A
1	16	79	G
1	16	80	A
1	16	90	C
1	16	91	U
1	16	92	U
1	16	95	C
1	16	97	G
1	16	108	G
1	16	116	A
1	16	120	A
1	16	130	A

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Mol	Chain	Res	Type
1	16	131	A
1	16	138	G
1	16	141	G
1	16	143	A
1	16	144	G
1	16	149	A
1	16	163	C
1	16	164	G
1	16	167	A
1	16	173	U
1	16	182	A
1	16	183	C
1	16	191	G
1	16	197	A
1	16	204	G
1	16	205	A
1	16	210	C
1	16	212	G
1	16	226	G
1	16	240	G
1	16	245	U
1	16	247	G
1	16	250	A
1	16	251	G
1	16	266	G
1	16	267	C
1	16	280	C
1	16	281	G
1	16	289	G
1	16	316	C
1	16	321	A
1	16	328	C
1	16	329	A
1	16	332	G
1	16	345	C
1	16	348	G
1	16	352	C
1	16	354	G
1	16	365	U
1	16	367	U
1	16	372	C
1	16	382	A

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Mol	Chain	Res	Type
1	16	384	G
1	16	392	C
1	16	406	G
1	16	412	A
1	16	413	G
1	16	421	U
1	16	423	G
1	16	429	U
1	16	435	A
1	16	439	U
1	16	457	G
1	16	463	U
1	16	467	U
1	16	468	A
1	16	479	U
1	16	481	G
1	16	482	A
1	16	483	C
1	16	486	U
1	16	495	A
1	16	496	A
1	16	509	A
1	16	511	C
1	16	516	PSU
1	16	518	C
1	16	521	G
1	16	527	G7M
1	16	531	U
1	16	533	A
1	16	547	A
1	16	559	A
1	16	562	U
1	16	572	A
1	16	573	A
1	16	576	C
1	16	579	A
1	16	596	A
1	16	633	G
1	16	653	U
1	16	665	A
1	16	687	A
1	16	703	G

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Mol	Chain	Res	Type
1	16	721	G
1	16	723	U
1	16	724	G
1	16	734	G
1	16	748	G
1	16	753	A
1	16	755	G
1	16	777	A
1	16	790	A
1	16	792	A
1	16	793	U
1	16	794	A
1	16	810	C
1	16	814	A
1	16	815	A
1	16	817	C
1	16	821	G
1	16	828	U
1	16	832	G
1	16	836	G
1	16	841	C
1	16	842	U
1	16	843	U
1	16	845	A
1	16	846	G
1	16	870	U
1	16	876	C
1	16	902	G
1	16	914	A
1	16	919	A
1	16	927	G
1	16	934	C
1	16	935	A
1	16	958	A
1	16	960	U
1	16	969	A
1	16	975	A
1	16	976	G
1	16	977	A
1	16	992	U
1	16	993	G
1	16	999	C

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Mol	Chain	Res	Type
1	16	1000	A
1	16	1003	G
1	16	1004	A
1	16	1005	A
1	16	1017	U
1	16	1018	G
1	16	1019	A
1	16	1020	G
1	16	1021	A
1	16	1025	U
1	16	1026	G
1	16	1028	C
1	16	1030	U
1	16	1031	C
1	16	1033	G
1	16	1036	A
1	16	1043	G
1	16	1045	C
1	16	1065	U
1	16	1085	U
1	16	1086	U
1	16	1094	G
1	16	1095	U
1	16	1101	A
1	16	1123	U
1	16	1124	G
1	16	1125	U
1	16	1129	C
1	16	1130	A
1	16	1133	G
1	16	1136	C
1	16	1137	C
1	16	1139	G
1	16	1140	C
1	16	1141	C
1	16	1142	G
1	16	1145	A
1	16	1158	C
1	16	1159	U
1	16	1167	A
1	16	1168	U
1	16	1184	G

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Mol	Chain	Res	Type
1	16	1196	A
1	16	1197	A
1	16	1199	U
1	16	1212	U
1	16	1227	A
1	16	1228	C
1	16	1238	A
1	16	1239	A
1	16	1240	U
1	16	1256	A
1	16	1257	A
1	16	1260	G
1	16	1279	G
1	16	1280	A
1	16	1286	U
1	16	1287	A
1	16	1289	A
1	16	1300	G
1	16	1302	C
1	16	1312	G
1	16	1320	C
1	16	1338	G
1	16	1340	A
1	16	1346	A
1	16	1353	G
1	16	1357	A
1	16	1363	A
1	16	1370	G
1	16	1379	G
1	16	1380	U
1	16	1395	C
1	16	1396	A
1	16	1397	C
1	16	1398	A
1	16	1399	C
1	16	1429	A
1	16	1432	G
1	16	1433	A
1	16	1441	A
1	16	1442	G
1	16	1446	A
1	16	1452	C

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Mol	Chain	Res	Type
1	16	1453	G
1	16	1492	A
1	16	1493	A
1	16	1497	G
1	16	1499	A
1	16	1503	A
1	16	1505	G
1	16	1506	U
1	16	1517	G
1	16	1529	G
1	16	1530	G
1	16	1534	A
23	23	10	A
23	23	27	G
23	23	34	U
23	23	36	G
23	23	39	G
23	23	40	U
23	23	42	A
23	23	45	G
23	23	46	G
23	23	51	G
23	23	55	G
23	23	58	G
23	23	71	A
23	23	74	A
23	23	75	G
23	23	80	G
23	23	88	G
23	23	96	C
23	23	101	A
23	23	102	U
23	23	103	A
23	23	110	G
23	23	118	A
23	23	119	A
23	23	120	U
23	23	125	A
23	23	139	U
23	23	140	C
23	23	141	G
23	23	158	U

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Mol	Chain	Res	Type
23	23	163	C
23	23	165	A
23	23	178	G
23	23	181	A
23	23	190	A
23	23	196	A
23	23	199	A
23	23	200	U
23	23	215	G
23	23	216	A
23	23	221	A
23	23	222	A
23	23	224	U
23	23	225	C
23	23	230	G
23	23	239	C
23	23	248	G
23	23	259	G
23	23	264	C
23	23	265	A
23	23	266	G
23	23	271	G
23	23	272	A
23	23	278	A
23	23	311	A
23	23	330	A
23	23	338	G
23	23	343	C
23	23	345	A
23	23	346	A
23	23	350	G
23	23	361	G
23	23	371	A
23	23	372	G
23	23	385	C
23	23	386	G
23	23	387	U
23	23	388	G
23	23	399	U
23	23	401	A
23	23	405	U
23	23	412	A

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Mol	Chain	Res	Type
23	23	451	U
23	23	455	C
23	23	456	C
23	23	457	A
23	23	459	U
23	23	473	G
23	23	481	G
23	23	489	G
23	23	491	G
23	23	496	G
23	23	501	A
23	23	503	A
23	23	504	A
23	23	505	A
23	23	506	G
23	23	508	A
23	23	509	C
23	23	518	G
23	23	527	C
23	23	530	G
23	23	532	A
23	23	533	G
23	23	538	A
23	23	546	U
23	23	547	A
23	23	548	G
23	23	549	G
23	23	556	A
23	23	563	A
23	23	573	U
23	23	575	A
23	23	603	A
23	23	614	A
23	23	615	U
23	23	616	A
23	23	622	G
23	23	637	A
23	23	638	G
23	23	645	C
23	23	646	U
23	23	647	G
23	23	653	U

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Mol	Chain	Res	Type
23	23	654	A
23	23	659	G
23	23	668	A
23	23	677	A
23	23	682	G
23	23	686	U
23	23	726	G
23	23	729	G
23	23	730	A
23	23	740	C
23	23	747	5MU
23	23	757	G
23	23	764	A
23	23	765	C
23	23	775	G
23	23	776	G
23	23	782	A
23	23	784	G
23	23	785	G
23	23	789	A
23	23	792	A
23	23	805	G
23	23	812	C
23	23	819	A
23	23	827	U
23	23	828	U
23	23	846	U
23	23	847	U
23	23	859	G
23	23	860	U
23	23	877	A
23	23	878	A
23	23	879	G
23	23	883	G
23	23	884	U
23	23	886	A
23	23	887	U
23	23	888	C
23	23	889	C
23	23	893	C
23	23	895	U
23	23	896	A

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Mol	Chain	Res	Type
23	23	897	C
23	23	900	A
23	23	901	C
23	23	903	C
23	23	910	A
23	23	914	G
23	23	915	C
23	23	917	A
23	23	931	U
23	23	932	U
23	23	941	A
23	23	946	C
23	23	961	C
23	23	962	G
23	23	973	A
23	23	974	G
23	23	983	A
23	23	989	G
23	23	996	A
23	23	999	U
23	23	1012	U
23	23	1013	C
23	23	1022	G
23	23	1026	G
23	23	1033	U
23	23	1046	A
23	23	1047	G
23	23	1057	A
23	23	1060	U
23	23	1061	U
23	23	1062	G
23	23	1065	U
23	23	1069	A
23	23	1070	A
23	23	1071	G
23	23	1072	C
23	23	1073	A
23	23	1074	G
23	23	1075	C
23	23	1076	C
23	23	1077	A
23	23	1079	C

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Mol	Chain	Res	Type
23	23	1080	A
23	23	1083	U
23	23	1086	A
23	23	1088	A
23	23	1089	A
23	23	1090	A
23	23	1091	G
23	23	1095	A
23	23	1096	A
23	23	1106	G
23	23	1110	G
23	23	1111	A
23	23	1112	G
23	23	1114	C
23	23	1115	G
23	23	1130	U
23	23	1132	U
23	23	1133	A
23	23	1134	A
23	23	1135	C
23	23	1136	G
23	23	1142	A
23	23	1148	U
23	23	1156	A
23	23	1173	U
23	23	1175	A
23	23	1178	C
23	23	1179	G
23	23	1187	G
23	23	1238	G
23	23	1244	A
23	23	1247	A
23	23	1249	U
23	23	1253	A
23	23	1256	G
23	23	1262	A
23	23	1266	G
23	23	1271	G
23	23	1272	A
23	23	1275	A
23	23	1289	C
23	23	1300	G

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Mol	Chain	Res	Type
23	23	1301	A
23	23	1306	C
23	23	1320	C
23	23	1321	A
23	23	1329	U
23	23	1332	G
23	23	1345	C
23	23	1352	U
23	23	1360	G
23	23	1365	A
23	23	1368	G
23	23	1374	G
23	23	1378	A
23	23	1379	U
23	23	1383	A
23	23	1386	C
23	23	1392	A
23	23	1395	A
23	23	1396	U
23	23	1397	U
23	23	1407	G
23	23	1416	G
23	23	1417	C
23	23	1420	A
23	23	1428	C
23	23	1437	C
23	23	1451	C
23	23	1452	G
23	23	1453	A
23	23	1458	U
23	23	1460	U
23	23	1475	G
23	23	1476	U
23	23	1478	G
23	23	1479	G
23	23	1482	G
23	23	1493	C
23	23	1494	A
23	23	1497	U
23	23	1503	A
23	23	1507	C
23	23	1508	A

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Mol	Chain	Res	Type
23	23	1509	A
23	23	1524	G
23	23	1529	G
23	23	1535	A
23	23	1536	C
23	23	1537	G
23	23	1538	G
23	23	1566	A
23	23	1569	A
23	23	1570	A
23	23	1578	U
23	23	1584	U
23	23	1585	C
23	23	1607	C
23	23	1608	A
23	23	1610	A
23	23	1622	G
23	23	1647	U
23	23	1648	U
23	23	1649	G
23	23	1674	G
23	23	1701	A
23	23	1725	U
23	23	1727	C
23	23	1729	U
23	23	1730	C
23	23	1733	G
23	23	1738	G
23	23	1764	C
23	23	1773	A
23	23	1776	G
23	23	1784	A
23	23	1786	A
23	23	1799	G
23	23	1800	C
23	23	1801	A
23	23	1807	G
23	23	1808	A
23	23	1816	C
23	23	1829	A
23	23	1833	C
23	23	1872	A

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Mol	Chain	Res	Type
23	23	1873	G
23	23	1875	G
23	23	1876	A
23	23	1884	G
23	23	1921	G
23	23	1926	U
23	23	1927	A
23	23	1930	G
23	23	1931	U
23	23	1937	A
23	23	1938	A
23	23	1940	U
23	23	1955	U
23	23	1960	A
23	23	1967	C
23	23	1970	A
23	23	1971	U
23	23	1972	G
23	23	1980	G
23	23	1991	U
23	23	1992	G
23	23	1993	U
23	23	1997	C
23	23	2022	U
23	23	2023	C
23	23	2032	G
23	23	2033	A
23	23	2036	C
23	23	2043	C
23	23	2055	C
23	23	2056	G
23	23	2060	A
23	23	2061	G
23	23	2062	A
23	23	2069	G7M
23	23	2080	A
23	23	2093	G
23	23	2103	C
23	23	2104	C
23	23	2110	G
23	23	2111	U
23	23	2112	G

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Mol	Chain	Res	Type
23	23	2113	U
23	23	2116	G
23	23	2118	U
23	23	2119	A
23	23	2120	G
23	23	2126	A
23	23	2131	U
23	23	2132	U
23	23	2133	G
23	23	2134	A
23	23	2136	G
23	23	2138	G
23	23	2146	C
23	23	2161	C
23	23	2163	A
23	23	2164	C
23	23	2165	C
23	23	2170	A
23	23	2171	A
23	23	2173	A
23	23	2180	U
23	23	2198	A
23	23	2204	G
23	23	2211	A
23	23	2225	A
23	23	2238	G
23	23	2239	G
23	23	2243	U
23	23	2251	OMG
23	23	2258	C
23	23	2268	A
23	23	2278	A
23	23	2280	G
23	23	2283	C
23	23	2287	A
23	23	2304	G
23	23	2306	C
23	23	2307	G
23	23	2308	G
23	23	2310	C
23	23	2311	A
23	23	2312	U

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Mol	Chain	Res	Type
23	23	2319	G
23	23	2322	A
23	23	2325	G
23	23	2333	A
23	23	2335	A
23	23	2345	G
23	23	2347	C
23	23	2350	C
23	23	2361	G
23	23	2379	G
23	23	2383	G
23	23	2385	C
23	23	2391	G
23	23	2392	A
23	23	2402	U
23	23	2406	A
23	23	2410	G
23	23	2423	U
23	23	2425	A
23	23	2426	A
23	23	2429	G
23	23	2430	A
23	23	2435	A
23	23	2436	G
23	23	2441	U
23	23	2448	A
23	23	2470	G
23	23	2476	A
23	23	2480	C
23	23	2481	G
23	23	2484	G
23	23	2491	U
23	23	2494	G
23	23	2502	G
23	23	2504	PSU
23	23	2505	G
23	23	2518	A
23	23	2525	G
23	23	2529	G
23	23	2547	A
23	23	2549	G
23	23	2554	U

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Mol	Chain	Res	Type
23	23	2556	C
23	23	2566	A
23	23	2567	G
23	23	2569	G
23	23	2573	C
23	23	2585	U
23	23	2599	G
23	23	2602	A
23	23	2603	G
23	23	2604	PSU
23	23	2609	U
23	23	2613	U
23	23	2614	A
23	23	2629	U
23	23	2630	G
23	23	2636	C
23	23	2639	A
23	23	2646	C
23	23	2661	G
23	23	2663	G
23	23	2682	A
23	23	2688	G
23	23	2689	U
23	23	2690	U
23	23	2707	U
23	23	2714	G
23	23	2716	C
23	23	2718	G
23	23	2726	A
23	23	2729	G
23	23	2732	G
23	23	2748	A
23	23	2751	G
23	23	2757	A
23	23	2765	A
23	23	2769	U
23	23	2777	G
23	23	2778	A
23	23	2779	U
23	23	2791	G
23	23	2798	U
23	23	2800	A

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Mol	Chain	Res	Type
23	23	2808	G
23	23	2809	A
23	23	2818	U
23	23	2820	A
23	23	2821	A
23	23	2825	G
23	23	2832	U
23	23	2833	U
23	23	2835	A
23	23	2850	A
23	23	2861	U
23	23	2873	A
23	23	2877	G
23	23	2879	A
23	23	2880	C
23	23	2883	A
23	23	2884	U
23	23	2886	A
23	23	2891	U
24	5	9	G
24	5	13	G
24	5	35	C
24	5	36	C
24	5	44	G
24	5	45	A
24	5	51	G
24	5	67	G
24	5	68	C
24	5	89	U
24	5	90	C
24	5	91	C
24	5	99	A
24	5	108	A
24	5	109	A
55	Pt	6	G
55	Pt	8	U
55	Pt	9	A
55	Pt	13	C
55	Pt	15	G
55	Pt	16	H2U
55	Pt	18	G
55	Pt	19	G

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Mol	Chain	Res	Type
55	Pt	20	H2U
55	Pt	21	A
55	Pt	23	A
55	Pt	32	C
55	Pt	36	U
55	Pt	37	T6A
55	Pt	44	U
55	Pt	48	C
55	Pt	53	G
55	Pt	55	PSU
55	Pt	58	A
55	Pt	61	C
55	Pt	63	U
55	Pt	64	G
55	Pt	66	A
55	Pt	74	C
55	Pt	76	A
56	Dt	7	A
56	Dt	14	A
56	Dt	17	U
56	Dt	18	G
56	Dt	19	G
56	Dt	20	G
56	Dt	21	A
56	Dt	22	G
56	Dt	45	U
56	Dt	48	C
56	Dt	56	C
56	Dt	76	A

All (62) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	16	181	A
1	16	251	G
1	16	329	A
1	16	413	G
1	16	428	G
1	16	438	U
1	16	530	G
1	16	1024	G
1	16	1124	G

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Mol	Chain	Res	Type
1	16	1129	C
1	16	1137	C
1	16	1145	A
1	16	1183	U
1	16	1225	A
1	16	1239	A
1	16	1346	A
1	16	1432	G
1	16	1452	C
1	16	1492	A
1	16	1505	G
23	23	140	C
23	23	196	A
23	23	199	A
23	23	221	A
23	23	249	C
23	23	277	G
23	23	278	A
23	23	345	A
23	23	369	U
23	23	387	U
23	23	404	A
23	23	479	A
23	23	503	A
23	23	504	A
23	23	555	G
23	23	620	G
23	23	784	G
23	23	895	U
23	23	1060	U
23	23	1069	A
23	23	1070	A
23	23	1079	C
23	23	1110	G
23	23	1178	C
23	23	1286	A
23	23	1416	G
23	23	1451	C
23	23	1535	A
23	23	1584	U
23	23	1647	U
23	23	2111	U

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Mol	Chain	Res	Type
23	23	2119	A
23	23	2282	G
23	23	2308	G
23	23	2311	A
23	23	2430	A
23	23	2447	G
23	23	2481	G
23	23	2756	U
23	23	2779	U
23	23	2820	A
24	5	108	A

## 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	$\# Z  > 2$
55	H2U	Pt	17	55	18,21,22	1.08	2 (11%)	19,30,33	1.02	1 (5%)
23	5MC	23	1962	23	19,22,23	1.44	3 (15%)	26,32,35	1.21	2 (7%)
23	G7M	23	2069	23	20,26,27	2.42	4 (20%)	16,39,42	1.19	1 (6%)
23	2MA	23	2503	23,58	18,25,26	0.77	0	20,37,40	2.11	4 (20%)
55	U8U	Pt	34	22,55	20,24,25	1.72	3 (15%)	22,34,37	1.30	4 (18%)
23	6MZ	23	1618	23	17,25,26	0.92	1 (5%)	15,36,39	2.57	5 (33%)
55	3AU	Pt	47	55	24,28,29	1.03	1 (4%)	30,40,43	1.44	3 (10%)
23	OMG	23	2251	23,55	19,26,27	1.07	1 (5%)	21,38,41	1.46	4 (19%)
56	G7M	Dt	46	56	20,26,27	2.63	4 (20%)	16,39,42	1.72	3 (18%)
23	6MZ	23	2030	23	17,25,26	0.89	0	15,36,39	2.62	4 (26%)
1	MA6	16	1519	1	19,26,27	1.00	1 (5%)	18,38,41	1.97	4 (22%)
23	2MG	23	1835	23	18,26,27	1.00	1 (5%)	16,38,41	1.75	6 (37%)
23	PSU	23	2580	23	18,21,22	1.73	6 (33%)	21,30,33	2.30	6 (28%)
23	PSU	23	955	23	18,21,22	1.55	5 (27%)	21,30,33	2.26	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	OMC	23	2498	23,58	19,22,23	0.87	0	25,31,34	0.96	1 (4%)
34	4D4	LP	81	34	9,11,12	2.16	2 (22%)	7,13,15	2.04	3 (42%)
23	3TD	23	1915	23	19,22,23	1.28	2 (10%)	23,32,35	2.03	3 (13%)
23	5MU	23	1939	23,58	19,22,23	1.48	4 (21%)	27,32,35	2.33	6 (22%)
1	2MG	16	1516	1	18,26,27	1.09	1 (5%)	16,38,41	1.66	4 (25%)
55	PSU	Pt	39	55	18,21,22	1.55	4 (22%)	21,30,33	2.04	3 (14%)
23	PSU	23	746	23,58	18,21,22	1.45	3 (16%)	21,30,33	2.20	4 (19%)
56	MIA	Dt	37	56	24,31,32	2.33	2 (8%)	22,44,47	2.58	7 (31%)
56	PSU	Dt	39	56	18,21,22	1.56	4 (22%)	21,30,33	1.99	3 (14%)
1	5MC	16	1407	1	19,22,23	1.40	3 (15%)	26,32,35	1.34	3 (11%)
1	PSU	16	516	58,1	18,21,22	1.56	4 (22%)	21,30,33	2.28	4 (19%)
1	2MG	16	966	1	18,26,27	1.11	1 (5%)	16,38,41	1.42	3 (18%)
23	PSU	23	2605	23	18,21,22	1.62	5 (27%)	21,30,33	2.08	4 (19%)
23	5MU	23	747	23	19,22,23	1.54	6 (31%)	27,32,35	2.21	8 (29%)
55	T6A	Pt	37	55	26,34,35	0.99	0	28,49,52	2.35	6 (21%)
56	4SU	Dt	8	56	18,21,22	1.94	5 (27%)	25,30,33	2.21	6 (24%)
56	3AU	Dt	47	56	24,28,29	1.07	1 (4%)	30,40,43	1.56	5 (16%)
23	H2U	23	2449	23	18,21,22	1.29	3 (16%)	19,30,33	1.30	2 (10%)
23	OMU	23	2552	23	19,22,23	1.44	4 (21%)	25,31,34	2.16	7 (28%)
55	G7M	Pt	46	55	20,26,27	2.61	4 (20%)	16,39,42	1.09	1 (6%)
55	5MU	Pt	54	55	19,22,23	1.43	5 (26%)	27,32,35	1.98	5 (18%)
23	PSU	23	2457	23	18,21,22	1.65	4 (22%)	21,30,33	2.30	6 (28%)
1	4OC	16	1402	1	20,23,24	0.82	1 (5%)	25,32,35	1.20	2 (8%)
55	H2U	Pt	16	55	18,21,22	1.00	2 (11%)	19,30,33	1.25	3 (15%)
1	UR3	16	1498	1	19,22,23	0.93	0	26,32,35	1.96	3 (11%)
1	5MC	16	967	1	19,22,23	1.45	3 (15%)	26,32,35	1.13	2 (7%)
55	PSU	Pt	55	55	18,21,22	1.41	3 (16%)	21,30,33	2.07	5 (23%)
56	PSU	Dt	55	56	18,21,22	1.42	3 (16%)	21,30,33	2.11	4 (19%)
12	D2T	SL	89	12	8,9,10	2.05	2 (25%)	6,11,13	1.66	3 (50%)
23	PSU	23	2504	23,58	18,21,22	1.51	3 (16%)	21,30,33	2.26	6 (28%)
1	2MG	16	1207	1	18,26,27	1.10	1 (5%)	16,38,41	1.67	5 (31%)
23	PSU	23	2604	23	18,21,22	1.68	5 (27%)	21,30,33	2.32	6 (28%)
1	G7M	16	527	1	20,26,27	2.55	4 (20%)	16,39,42	1.46	3 (18%)
55	H2U	Pt	20	55	18,21,22	1.12	2 (11%)	19,30,33	0.89	1 (5%)
23	1MG	23	745	23	19,26,27	0.78	0	18,39,42	1.63	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	PSU	Dt	32	56	18,21,22	1.49	4 (22%)	21,30,33	2.19	3 (14%)
1	MA6	16	1518	1	19,26,27	0.99	1 (5%)	18,38,41	2.19	3 (16%)
23	2MG	23	2445	23	18,26,27	1.11	2 (11%)	16,38,41	1.30	2 (12%)

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
55	H2U	Pt	17	55	-	5/7/38/39	0/2/2/2
23	5MC	23	1962	23	-	0/7/25/26	0/2/2/2
23	G7M	23	2069	23	-	1/3/25/26	0/3/3/3
23	2MA	23	2503	23,58	-	0/3/25/26	0/3/3/3
55	U8U	Pt	34	22,55	-	0/10/28/29	0/2/2/2
23	6MZ	23	1618	23	-	0/5/27/28	0/3/3/3
55	3AU	Pt	47	55	-	9/16/34/35	0/2/2/2
23	OMG	23	2251	23,55	-	3/5/27/28	0/3/3/3
56	G7M	Dt	46	56	-	0/3/25/26	0/3/3/3
23	6MZ	23	2030	23	-	2/5/27/28	0/3/3/3
1	MA6	16	1519	1	-	0/7/29/30	0/3/3/3
23	2MG	23	1835	23	-	0/5/27/28	0/3/3/3
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
23	OMC	23	2498	23,58	-	0/9/27/28	0/2/2/2
34	4D4	LP	81	34	-	3/11/12/14	-
23	3TD	23	1915	23	-	0/7/25/26	0/2/2/2
23	5MU	23	1939	23,58	-	0/7/25/26	0/2/2/2
1	2MG	16	1516	1	-	0/5/27/28	0/3/3/3
55	PSU	Pt	39	55	-	0/7/25/26	0/2/2/2
23	PSU	23	746	23,58	-	2/7/25/26	0/2/2/2
56	MIA	Dt	37	56	-	3/11/33/34	0/3/3/3
56	PSU	Dt	39	56	-	0/7/25/26	0/2/2/2
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
1	PSU	16	516	58,1	-	2/7/25/26	0/2/2/2
1	2MG	16	966	1	-	0/5/27/28	0/3/3/3
23	PSU	23	2605	23	-	0/7/25/26	0/2/2/2
23	5MU	23	747	23	-	0/7/25/26	0/2/2/2
55	T6A	Pt	37	55	-	4/19/41/42	0/3/3/3
56	4SU	Dt	8	56	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	3AU	Dt	47	56	-	6/16/34/35	0/2/2/2
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2
23	OMU	23	2552	23	-	0/9/27/28	0/2/2/2
55	G7M	Pt	46	55	-	0/3/25/26	0/3/3/3
55	5MU	Pt	54	55	-	0/7/25/26	0/2/2/2
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
1	4OC	16	1402	1	-	1/9/29/30	0/2/2/2
55	H2U	Pt	16	55	-	4/7/38/39	0/2/2/2
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
55	PSU	Pt	55	55	-	1/7/25/26	0/2/2/2
56	PSU	Dt	55	56	-	0/7/25/26	0/2/2/2
12	D2T	SL	89	12	-	1/7/12/14	-
23	PSU	23	2504	23,58	-	0/7/25/26	0/2/2/2
1	2MG	16	1207	1	-	0/5/27/28	0/3/3/3
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
1	G7M	16	527	1	-	2/3/25/26	0/3/3/3
55	H2U	Pt	20	55	-	5/7/38/39	0/2/2/2
23	1MG	23	745	23	-	0/3/25/26	0/3/3/3
56	PSU	Dt	32	56	-	0/7/25/26	0/2/2/2
1	MA6	16	1518	1	-	0/7/29/30	0/3/3/3
23	2MG	23	2445	23	-	1/5/27/28	0/3/3/3

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Dt	37	MIA	C2-S10	-8.17	1.69	1.75
56	Dt	46	G7M	C8-N9	7.45	1.46	1.33
1	16	527	G7M	C8-N9	7.33	1.46	1.33
55	Pt	46	G7M	C8-N9	7.21	1.46	1.33
55	Pt	46	G7M	C8-N7	7.11	1.46	1.33
56	Dt	46	G7M	C8-N7	7.09	1.46	1.33
23	23	2069	G7M	C8-N9	6.82	1.45	1.33
56	Dt	37	MIA	C13-C14	6.69	1.52	1.32
1	16	527	G7M	C8-N7	6.63	1.45	1.33
23	23	2069	G7M	C8-N7	6.54	1.45	1.33
55	Pt	34	U8U	C2-S2	-5.42	1.59	1.67
56	Dt	8	4SU	C4-S4	-5.12	1.59	1.68
34	LP	81	4D4	CZ-NE	5.00	1.42	1.33
1	16	967	5MC	C5-C4	4.91	1.47	1.44
23	23	1962	5MC	C5-C4	4.73	1.47	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	1407	5MC	C5-C4	4.61	1.47	1.44
12	SL	89	D2T	CB-CA	-4.46	1.53	1.54
56	Dt	46	G7M	C5-C4	4.33	1.47	1.39
55	Pt	46	G7M	C5-C4	4.18	1.47	1.39
1	16	527	G7M	C5-C4	4.04	1.47	1.39
23	23	2580	PSU	C4-N3	-3.84	1.31	1.38
23	23	2552	OMU	C4-N3	-3.75	1.32	1.38
23	23	2457	PSU	C4-N3	-3.62	1.32	1.38
56	Dt	8	4SU	C4-N3	-3.59	1.33	1.37
23	23	2604	PSU	C4-N3	-3.51	1.32	1.38
23	23	2605	PSU	C4-N3	-3.49	1.32	1.38
23	23	2069	G7M	C5-C4	3.46	1.46	1.39
34	LP	81	4D4	CZ-NH2	3.43	1.44	1.32
23	23	1915	3TD	C6-C5	3.39	1.39	1.35
56	Dt	55	PSU	C6-C5	3.37	1.39	1.35
23	23	2504	PSU	C6-C5	3.33	1.39	1.35
55	Pt	34	U8U	C6-N1	-3.33	1.32	1.38
23	23	2504	PSU	C4-N3	-3.31	1.32	1.38
23	23	955	PSU	C4-N3	-3.28	1.32	1.38
23	23	747	5MU	C4-N3	-3.25	1.32	1.38
23	23	1939	5MU	C4-N3	-3.23	1.32	1.38
55	Pt	39	PSU	C6-C5	3.20	1.38	1.35
1	16	516	PSU	C4-N3	-3.19	1.32	1.38
23	23	2457	PSU	C6-C5	3.19	1.38	1.35
55	Pt	55	PSU	C6-C5	3.17	1.38	1.35
56	Dt	39	PSU	C6-C5	3.16	1.38	1.35
55	Pt	39	PSU	C4-N3	-3.15	1.32	1.38
23	23	2604	PSU	C2-N3	-3.09	1.32	1.37
55	Pt	20	H2U	C2-N3	-3.06	1.32	1.38
56	Dt	39	PSU	C4-N3	-3.04	1.33	1.38
56	Dt	32	PSU	C6-C5	3.03	1.38	1.35
23	23	955	PSU	C2-N3	-3.03	1.32	1.37
23	23	2605	PSU	C2-N3	-3.02	1.32	1.37
23	23	2552	OMU	C2-N3	-2.99	1.32	1.38
23	23	746	PSU	C4-N3	-2.98	1.33	1.38
23	23	2449	H2U	C2-N3	-2.98	1.32	1.38
1	16	966	2MG	C6-N1	-2.96	1.33	1.37
56	Dt	8	4SU	C5-C4	-2.94	1.39	1.42
56	Dt	32	PSU	C4-N3	-2.93	1.33	1.38
1	16	1516	2MG	C6-N1	-2.90	1.33	1.37
23	23	2604	PSU	C6-C5	2.89	1.38	1.35
55	Pt	54	5MU	C4-N3	-2.88	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	Pt	34	U8U	C4-N3	-2.88	1.33	1.38
23	23	2605	PSU	C6-C5	2.85	1.38	1.35
23	23	2580	PSU	C2-N3	-2.85	1.32	1.37
23	23	2251	OMG	C6-N1	-2.84	1.33	1.37
55	Pt	55	PSU	C4-N3	-2.82	1.33	1.38
56	Dt	55	PSU	C4-N3	-2.81	1.33	1.38
23	23	2580	PSU	C6-C5	2.81	1.38	1.35
1	16	516	PSU	C6-C5	2.81	1.38	1.35
23	23	2445	2MG	C6-N1	-2.80	1.33	1.37
23	23	2449	H2U	C4-N3	-2.80	1.32	1.37
55	Pt	17	H2U	C2-N3	-2.79	1.33	1.38
23	23	1939	5MU	C2-N3	-2.78	1.33	1.38
55	Pt	20	H2U	C4-N3	-2.78	1.32	1.37
1	16	1207	2MG	C6-N1	-2.77	1.33	1.37
23	23	1915	3TD	C2-N1	-2.73	1.33	1.37
1	16	527	G7M	C6-N1	-2.73	1.33	1.37
23	23	747	5MU	C2-N3	-2.67	1.33	1.38
23	23	2457	PSU	C2-N3	-2.66	1.33	1.37
23	23	1835	2MG	C6-N1	-2.65	1.33	1.37
23	23	1939	5MU	C6-C5	2.63	1.38	1.34
23	23	1962	5MC	C6-N1	-2.63	1.33	1.38
23	23	747	5MU	C6-N1	-2.61	1.33	1.38
23	23	2552	OMU	C5-C4	-2.59	1.38	1.43
55	Pt	16	H2U	C2-N3	-2.59	1.33	1.38
1	16	967	5MC	C6-N1	-2.55	1.33	1.38
55	Pt	17	H2U	C4-N3	-2.50	1.33	1.37
55	Pt	54	5MU	C6-C5	2.47	1.38	1.34
23	23	746	PSU	C6-C5	2.47	1.38	1.35
1	16	516	PSU	C2-N1	-2.45	1.33	1.36
23	23	2604	PSU	C2-N1	-2.45	1.33	1.36
55	Pt	39	PSU	C2-N3	-2.44	1.33	1.37
23	23	955	PSU	C6-C5	2.44	1.38	1.35
1	16	1519	MA6	C6-C5	2.43	1.48	1.44
1	16	516	PSU	C2-N3	-2.43	1.33	1.37
23	23	2504	PSU	C2-N3	-2.43	1.33	1.37
56	Dt	8	4SU	C2-N1	2.42	1.42	1.38
55	Pt	46	G7M	C6-N1	-2.39	1.34	1.37
23	23	747	5MU	C4-C5	2.39	1.48	1.44
56	Dt	39	PSU	C2-N1	-2.39	1.33	1.36
56	Dt	39	PSU	C2-N3	-2.38	1.33	1.37
1	16	1407	5MC	C6-C5	2.38	1.38	1.34
23	23	1939	5MU	C6-N1	-2.37	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Dt	47	3AU	C2-N1	2.37	1.41	1.38
23	23	1962	5MC	C6-C5	2.37	1.38	1.34
23	23	2605	PSU	C2-N1	-2.35	1.33	1.36
23	23	746	PSU	C2-N3	-2.35	1.33	1.37
23	23	2069	G7M	C6-N1	-2.31	1.34	1.37
55	Pt	54	5MU	C2-N3	-2.29	1.34	1.38
55	Pt	39	PSU	C2-N1	-2.29	1.33	1.36
23	23	2449	H2U	C2-N1	-2.28	1.32	1.35
56	Dt	32	PSU	C2-N3	-2.27	1.33	1.37
55	Pt	54	5MU	C6-N1	-2.27	1.34	1.38
1	16	1407	5MC	C6-N1	-2.27	1.34	1.38
56	Dt	8	4SU	C2-N3	-2.26	1.34	1.38
55	Pt	16	H2U	C4-N3	-2.25	1.33	1.37
23	23	2445	2MG	C2-N1	-2.23	1.33	1.36
23	23	2580	PSU	C2'-C1'	-2.22	1.50	1.53
23	23	747	5MU	C6-C5	2.20	1.38	1.34
23	23	955	PSU	C2-N1	-2.19	1.33	1.36
23	23	2457	PSU	C2-N1	-2.19	1.33	1.36
12	SL	89	D2T	CB1-SB	-2.19	1.75	1.79
56	Dt	32	PSU	C2-N1	-2.16	1.33	1.36
55	Pt	54	5MU	C2-N1	2.15	1.41	1.38
23	23	747	5MU	C2-N1	2.14	1.41	1.38
23	23	955	PSU	C2'-C1'	-2.14	1.50	1.53
1	16	967	5MC	C6-C5	2.13	1.38	1.34
55	Pt	55	PSU	C2-N3	-2.12	1.34	1.37
23	23	2580	PSU	C6-N1	-2.11	1.32	1.36
1	16	1518	MA6	C6-C5	2.08	1.48	1.44
56	Dt	55	PSU	C2-N3	-2.08	1.34	1.37
23	23	2580	PSU	C2-N1	-2.07	1.34	1.36
56	Dt	46	G7M	C6-N1	-2.04	1.34	1.37
23	23	2604	PSU	C2'-C1'	-2.02	1.51	1.53
23	23	2605	PSU	C2'-C1'	-2.01	1.51	1.53
1	16	1402	4OC	C6-N1	-2.01	1.33	1.38
23	23	1618	6MZ	C6-C5	2.00	1.47	1.44
55	Pt	47	3AU	C2-N1	2.00	1.41	1.38
23	23	2552	OMU	C6-N1	-2.00	1.33	1.38

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Dt	37	MIA	C12-C13-C14	-9.08	110.72	127.01
55	Pt	37	T6A	C2-N1-C6	7.69	122.57	116.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16	1498	UR3	C4-N3-C2	-7.62	118.45	124.58
23	23	2503	2MA	C2-N3-C4	7.50	121.51	115.46
23	23	2457	PSU	N1-C2-N3	7.24	122.80	115.17
23	23	955	PSU	N1-C2-N3	7.19	122.75	115.17
23	23	1618	6MZ	C2-N1-C6	7.16	122.16	116.60
23	23	2580	PSU	N1-C2-N3	7.10	122.66	115.17
1	16	516	PSU	N1-C2-N3	7.09	122.64	115.17
23	23	2504	PSU	N1-C2-N3	7.01	122.56	115.17
1	16	1518	MA6	C2-N1-C6	6.91	123.62	116.84
23	23	1915	3TD	N1-C2-N3	6.84	121.10	116.13
23	23	2604	PSU	N1-C2-N3	6.84	122.38	115.17
23	23	2030	6MZ	C2-N1-C6	6.81	121.89	116.60
56	Dt	32	PSU	N1-C2-N3	6.77	122.31	115.17
55	Pt	39	PSU	N1-C2-N3	6.64	122.17	115.17
23	23	2605	PSU	N1-C2-N3	6.59	122.12	115.17
23	23	746	PSU	N1-C2-N3	6.48	122.00	115.17
56	Dt	39	PSU	N1-C2-N3	6.36	121.88	115.17
55	Pt	55	PSU	N1-C2-N3	6.35	121.87	115.17
56	Dt	55	PSU	N1-C2-N3	6.25	121.76	115.17
56	Dt	8	4SU	C4-N3-C2	-5.91	121.65	127.31
23	23	1939	5MU	C4-N3-C2	-5.67	119.91	127.34
56	Dt	8	4SU	C5-C4-N3	5.63	119.99	114.75
23	23	1939	5MU	N3-C2-N1	5.62	122.21	114.89
1	16	1519	MA6	C2-N1-C6	5.49	122.23	116.84
23	23	747	5MU	N3-C2-N1	5.37	121.89	114.89
55	Pt	37	T6A	N6-C10-N11	5.23	120.96	113.77
23	23	1915	3TD	C4-N3-C2	-5.19	119.12	124.61
23	23	747	5MU	C4-N3-C2	-5.10	120.65	127.34
23	23	1939	5MU	C5-C4-N3	5.07	119.73	115.32
23	23	2552	OMU	C2'-C1'-N1	-5.01	104.73	114.24
23	23	746	PSU	C4-N3-C2	-4.93	119.58	126.37
55	Pt	47	3AU	C4-N3-C2	-4.93	118.87	124.66
56	Dt	47	3AU	C4-N3-C2	-4.90	118.90	124.66
23	23	2552	OMU	C4-N3-C2	-4.84	120.61	126.61
23	23	955	PSU	C4-N3-C2	-4.82	119.74	126.37
23	23	2504	PSU	C4-N3-C2	-4.71	119.88	126.37
55	Pt	54	5MU	N3-C2-N1	4.70	121.01	114.89
23	23	2552	OMU	N3-C2-N1	4.67	120.97	114.89
55	Pt	54	5MU	C4-N3-C2	-4.53	121.40	127.34
23	23	2030	6MZ	C9-N6-C6	-4.51	118.66	122.85
23	23	1618	6MZ	N3-C2-N1	-4.51	122.55	128.67
55	Pt	37	T6A	N6-C6-N1	4.49	123.76	118.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Dt	46	G7M	O4'-C1'-N9	4.42	114.60	108.75
55	Pt	37	T6A	N3-C2-N1	-4.28	122.86	128.67
56	Dt	32	PSU	C4-N3-C2	-4.26	120.51	126.37
23	23	1939	5MU	C5-C6-N1	-4.23	118.72	123.31
1	16	516	PSU	C4-N3-C2	-4.22	120.56	126.37
23	23	2457	PSU	C4-N3-C2	-4.20	120.58	126.37
1	16	516	PSU	O2-C2-N1	-4.16	118.49	122.79
23	23	747	5MU	C5-C4-N3	4.16	118.94	115.32
23	23	1939	5MU	O4-C4-C5	-4.13	120.19	124.92
1	16	1518	MA6	N3-C2-N1	-4.13	123.06	128.67
56	Dt	55	PSU	C4-N3-C2	-4.11	120.70	126.37
23	23	2604	PSU	C4-N3-C2	-4.10	120.73	126.37
55	Pt	54	5MU	O4-C4-C5	-4.06	120.27	124.92
55	Pt	54	5MU	C5-C4-N3	4.05	118.84	115.32
23	23	2552	OMU	C5-C4-N3	4.03	120.45	114.80
23	23	2580	PSU	C4-N3-C2	-4.03	120.82	126.37
56	Dt	32	PSU	O2-C2-N1	-4.02	118.64	122.79
23	23	2605	PSU	C4-N3-C2	-3.98	120.89	126.37
55	Pt	55	PSU	C4-N3-C2	-3.97	120.91	126.37
56	Dt	37	MIA	C15-C14-C13	-3.94	110.83	122.66
55	Pt	39	PSU	C4-N3-C2	-3.92	120.97	126.37
56	Dt	37	MIA	C16-C14-C13	-3.92	110.89	122.66
56	Dt	8	4SU	C5-C4-S4	-3.86	119.90	124.31
56	Dt	8	4SU	N3-C2-N1	3.85	119.90	114.89
23	23	2030	6MZ	N3-C2-N1	-3.85	123.45	128.67
23	23	2604	PSU	C3'-C2'-C1'	3.84	106.22	101.69
23	23	746	PSU	O2-C2-N1	-3.77	118.90	122.79
23	23	1835	2MG	N1-C2-N2	3.69	120.32	116.56
55	Pt	55	PSU	O2-C2-N1	-3.67	119.00	122.79
23	23	1962	5MC	C5-C6-N1	-3.65	119.35	123.31
1	16	1519	MA6	N3-C2-N1	-3.65	123.72	128.67
56	Dt	39	PSU	C4-N3-C2	-3.65	121.35	126.37
34	LP	81	4D4	NE-CZ-NH2	-3.57	114.54	120.67
1	16	1498	UR3	C5-C4-N3	3.56	119.73	115.04
23	23	2030	6MZ	C4-C5-N7	-3.51	105.63	109.34
23	23	747	5MU	C5-C6-N1	-3.46	119.56	123.31
23	23	1618	6MZ	C9-N6-C6	-3.45	119.65	122.85
23	23	2580	PSU	C3'-C2'-C1'	3.45	105.75	101.69
56	Dt	55	PSU	O2-C2-N1	-3.41	119.27	122.79
55	Pt	39	PSU	O2-C2-N1	-3.39	119.29	122.79
23	23	2457	PSU	O2-C2-N1	-3.29	119.40	122.79
34	LP	81	4D4	NH1-CZ-NE	3.28	126.72	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	Dt	39	PSU	O2-C2-N1	-3.27	119.41	122.79
1	16	1519	MA6	C4-C5-N7	-3.22	105.93	109.34
1	16	1516	2MG	N1-C2-N2	3.22	119.84	116.56
23	23	2251	OMG	O6-C6-C5	-3.19	117.99	124.32
55	Pt	34	U8U	C1'-N1-C6	-3.12	116.02	121.15
23	23	2504	PSU	O2-C2-N1	-3.11	119.58	122.79
23	23	745	1MG	C5-C6-N1	3.08	118.41	113.96
23	23	2580	PSU	O2-C2-N1	-3.07	119.62	122.79
23	23	2445	2MG	C8-N7-C5	3.06	107.75	102.55
1	16	1207	2MG	C8-N7-C5	3.05	107.74	102.55
23	23	747	5MU	O4-C4-C5	-3.04	121.44	124.92
56	Dt	47	3AU	C5-C4-N3	3.01	119.80	115.64
56	Dt	8	4SU	C1'-N1-C2	3.00	122.98	117.59
55	Pt	54	5MU	C5-C6-N1	-2.99	120.06	123.31
23	23	746	PSU	C5-C6-N1	-2.99	117.99	122.14
23	23	745	1MG	C8-N7-C5	2.95	107.57	102.55
56	Dt	46	G7M	C4'-O4'-C1'	-2.94	107.23	109.92
1	16	527	G7M	CN7-N7-C8	-2.92	111.36	125.43
23	23	745	1MG	CM1-N1-C6	2.91	121.49	117.54
1	16	1518	MA6	C4-C5-N7	-2.88	106.30	109.34
55	Pt	47	3AU	C5-C4-N3	2.88	119.62	115.64
1	16	967	5MC	C5-C6-N1	-2.86	120.20	123.31
23	23	2604	PSU	O2-C2-N1	-2.86	119.84	122.79
23	23	2251	OMG	C2'-C1'-N9	-2.84	106.25	112.56
23	23	2251	OMG	C5-C6-N1	2.83	119.47	114.07
23	23	2503	2MA	C4-C5-N7	-2.79	106.39	109.34
56	Dt	46	G7M	CN7-N7-C8	-2.78	112.03	125.43
23	23	2069	G7M	CN7-N7-C8	-2.78	112.03	125.43
23	23	2457	PSU	C3'-C2'-C1'	2.76	104.95	101.69
55	Pt	46	G7M	CN7-N7-C8	-2.76	112.13	125.43
1	16	1402	4OC	O2-C2-N3	-2.76	117.98	122.33
23	23	1835	2MG	N2-C2-N3	-2.75	117.00	120.51
23	23	2605	PSU	O2-C2-N3	-2.73	117.00	121.86
1	16	1516	2MG	C8-N7-C5	2.73	107.19	102.55
23	23	955	PSU	O2-C2-N1	-2.71	120.00	122.79
1	16	1407	5MC	O2-C2-N3	-2.69	118.08	122.33
1	16	967	5MC	C5-C4-N3	-2.69	119.00	121.75
1	16	966	2MG	C8-N7-C5	2.68	107.11	102.55
1	16	1516	2MG	O4'-C1'-N9	2.67	112.28	108.75
55	Pt	55	PSU	C3'-C2'-C1'	2.66	104.83	101.69
23	23	2503	2MA	C2-N1-C6	2.66	122.19	118.10
23	23	2449	H2U	C5-C4-N3	2.64	119.49	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	Pt	16	H2U	O4'-C1'-N1	2.63	112.88	109.30
1	16	1407	5MC	C5-C6-N1	-2.62	120.46	123.31
56	Dt	47	3AU	C10-N3-C2	2.60	121.48	117.64
1	16	1402	4OC	C6-C5-C4	2.60	120.13	117.00
23	23	955	PSU	O2-C2-N3	-2.59	117.25	121.86
23	23	747	5MU	C3'-C2'-C1'	2.59	106.36	101.46
56	Dt	37	MIA	C4-C5-N7	-2.58	106.61	109.34
1	16	1407	5MC	C5-C4-N3	-2.55	119.14	121.75
23	23	1939	5MU	O2-C2-N1	-2.55	119.47	122.80
23	23	2449	H2U	O4'-C1'-N1	2.54	112.75	109.30
23	23	1835	2MG	C8-N7-C5	2.52	106.84	102.55
23	23	1835	2MG	O6-C6-C5	-2.50	119.36	124.32
23	23	1835	2MG	C5-C6-N1	2.48	118.79	114.07
55	Pt	16	H2U	C5-C6-N1	-2.47	104.06	111.52
23	23	747	5MU	C5M-C5-C4	2.46	121.41	118.78
1	16	1516	2MG	C5-C6-N1	2.45	118.75	114.07
56	Dt	37	MIA	C2-N1-C6	2.44	121.77	117.42
1	16	1207	2MG	N1-C2-N2	2.44	119.05	116.56
23	23	1962	5MC	C5-C4-N3	-2.44	119.25	121.75
56	Dt	55	PSU	C6-C5-C4	-2.42	116.54	118.17
1	16	527	G7M	O4'-C1'-N9	2.42	111.95	108.75
56	Dt	47	3AU	C3'-C2'-C1'	2.41	106.03	101.46
56	Dt	37	MIA	C11-S10-C2	-2.41	100.44	102.25
23	23	1835	2MG	CM2-N2-C2	-2.40	118.50	123.65
55	Pt	47	3AU	C10-N3-C2	2.38	121.15	117.64
23	23	2580	PSU	C5-C6-N1	-2.38	118.84	122.14
23	23	2504	PSU	C5-C6-N1	-2.37	118.85	122.14
55	Pt	34	U8U	O4-C4-C5	-2.37	120.72	124.71
23	23	955	PSU	C5-C6-N1	-2.36	118.86	122.14
55	Pt	16	H2U	C5-C4-N3	2.36	119.20	116.69
56	Dt	47	3AU	C1'-N1-C2	2.35	120.88	117.04
23	23	2580	PSU	O2-C2-N3	-2.33	117.72	121.86
1	16	966	2MG	O4'-C1'-N9	2.32	111.83	108.75
23	23	2605	PSU	C5-C6-N1	-2.32	118.92	122.14
23	23	2251	OMG	C8-N7-C5	2.32	106.50	102.55
23	23	1915	3TD	C3'-C2'-C1'	2.32	104.42	101.69
56	Dt	37	MIA	N3-C2-N1	-2.32	122.79	127.03
1	16	1207	2MG	CM2-N2-C2	-2.32	118.67	123.65
23	23	2604	PSU	O2-C2-N3	-2.30	117.77	121.86
23	23	2552	OMU	O4-C4-C5	-2.30	121.20	125.16
1	16	1519	MA6	C1'-N9-C4	-2.30	122.61	126.64
23	23	2457	PSU	O2-C2-N3	-2.29	117.80	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16	1207	2MG	C5-C6-N1	2.27	118.41	114.07
23	23	2504	PSU	O2-C2-N3	-2.27	117.83	121.86
1	16	1498	UR3	C3U-N3-C4	2.26	121.00	117.87
23	23	2498	OMC	O2-C2-N3	-2.25	118.78	122.33
55	Pt	37	T6A	O10-C10-N6	-2.24	119.66	123.64
1	16	966	2MG	C5-C6-N1	2.24	118.34	114.07
23	23	2445	2MG	C5-C6-N1	2.23	118.33	114.07
23	23	2552	OMU	O4'-C1'-N1	2.22	113.39	108.36
23	23	747	5MU	C5M-C5-C6	-2.22	119.85	122.85
55	Pt	37	T6A	C4-C5-N7	-2.19	107.03	109.34
23	23	2604	PSU	C5-C6-N1	-2.18	119.11	122.14
12	SL	89	D2T	OD2-CG-CB	2.16	117.83	113.15
1	16	1207	2MG	N2-C2-N3	-2.15	117.77	120.51
1	16	516	PSU	C3'-C2'-C1'	2.14	104.21	101.69
23	23	1618	6MZ	C4-C5-N7	-2.13	107.08	109.34
12	SL	89	D2T	CB-CA-N	2.13	113.41	109.10
34	LP	81	4D4	O-C-CA	-2.11	119.34	124.77
55	Pt	17	H2U	C3'-C2'-C1'	2.11	105.46	101.46
23	23	2457	PSU	C5-C6-N1	-2.10	119.22	122.14
55	Pt	34	U8U	C-C5-C6	-2.09	118.07	121.21
23	23	1618	6MZ	O3'-C3'-C2'	-2.08	105.15	111.82
23	23	2504	PSU	C3'-C2'-C1'	2.06	104.12	101.69
23	23	2552	OMU	O2-C2-N1	-2.06	120.12	122.80
55	Pt	55	PSU	C5-C6-N1	-2.04	119.30	122.14
12	SL	89	D2T	O-C-CA	-2.04	119.52	124.77
55	Pt	20	H2U	C3'-C2'-C1'	2.02	105.29	101.46
55	Pt	34	U8U	C5-C4-N3	2.02	118.29	115.21
1	16	527	G7M	C2'-C3'-C4'	-2.02	98.71	102.61
56	Dt	8	4SU	C6-N1-C2	-2.01	118.55	121.00
23	23	2503	2MA	C5-C6-N1	-2.00	118.47	120.84
23	23	745	1MG	O4'-C1'-N9	2.00	111.40	108.75

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	516	PSU	O4'-C4'-C5'-O5'
1	16	527	G7M	O4'-C4'-C5'-O5'
1	16	527	G7M	C3'-C4'-C5'-O5'
23	23	2251	OMG	O4'-C4'-C5'-O5'
23	23	2251	OMG	C1'-C2'-O2'-CM2
55	Pt	16	H2U	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
55	Pt	16	H2U	C3'-C4'-C5'-O5'
55	Pt	16	H2U	O4'-C1'-N1-C2
55	Pt	16	H2U	O4'-C1'-N1-C6
55	Pt	37	T6A	O4'-C4'-C5'-O5'
55	Pt	47	3AU	C2'-C1'-N1-C2
55	Pt	47	3AU	C2'-C1'-N1-C6
55	Pt	55	PSU	C4'-C5'-O5'-P
56	Dt	37	MIA	O4'-C4'-C5'-O5'
56	Dt	37	MIA	C12-C13-C14-C16
56	Dt	47	3AU	C2'-C1'-N1-C2
56	Dt	47	3AU	C2'-C1'-N1-C6
56	Dt	47	3AU	C10-C11-C12-N40
55	Pt	47	3AU	C11-C12-C13-O31
23	23	2251	OMG	C3'-C4'-C5'-O5'
55	Pt	37	T6A	C3'-C4'-C5'-O5'
56	Dt	37	MIA	C3'-C4'-C5'-O5'
23	23	2030	6MZ	O4'-C4'-C5'-O5'
55	Pt	47	3AU	N40-C12-C13-O31
55	Pt	17	H2U	C2'-C1'-N1-C6
55	Pt	20	H2U	C2'-C1'-N1-C6
1	16	516	PSU	C3'-C4'-C5'-O5'
23	23	2030	6MZ	C3'-C4'-C5'-O5'
55	Pt	47	3AU	C11-C12-C13-O30
56	Dt	47	3AU	O4'-C1'-N1-C6
55	Pt	47	3AU	N40-C12-C13-O30
56	Dt	47	3AU	O4'-C1'-N1-C2
55	Pt	47	3AU	C10-C11-C12-C13
34	LP	81	4D4	OB-CB-CG-CD
55	Pt	20	H2U	C2'-C1'-N1-C2
55	Pt	17	H2U	C2'-C1'-N1-C2
55	Pt	20	H2U	O4'-C1'-N1-C6
34	LP	81	4D4	CA-CB-CG-CD
55	Pt	20	H2U	O4'-C1'-N1-C2
1	16	1402	4OC	O4'-C4'-C5'-O5'
56	Dt	47	3AU	C4'-C5'-O5'-P
55	Pt	37	T6A	N11-C12-C13-ODA
55	Pt	37	T6A	N11-C12-C13-ODB
23	23	2445	2MG	C3'-C4'-C5'-O5'
23	23	2069	G7M	C4'-C5'-O5'-P
55	Pt	47	3AU	O4'-C1'-N1-C6
55	Pt	17	H2U	C4'-C5'-O5'-P
55	Pt	17	H2U	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
55	Pt	20	H2U	C4'-C5'-O5'-P
55	Pt	47	3AU	O4'-C1'-N1-C2
23	23	746	PSU	O4'-C1'-C5-C6
12	SL	89	D2T	CG-CB-SB-CB1
23	23	746	PSU	C2'-C1'-C5-C6
55	Pt	17	H2U	O4'-C1'-N1-C6
34	LP	81	4D4	CG-CD-NE-CZ

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 314 ligands modelled in this entry, 297 are monoatomic - leaving 17 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	$\# Z  > 2$
57	PUT	23	3003	-	5,5,5	0.13	0	4,4,4	0.18	0
57	PUT	23	3004	-	5,5,5	0.12	0	4,4,4	0.23	0
61	SPD	23	3015	-	9,9,9	0.14	0	8,8,8	0.24	0
60	ATP	23	3001	-	28,33,33	0.77	0	34,52,52	0.81	1 (2%)
61	SPD	23	3013	-	9,9,9	0.16	0	8,8,8	0.28	0
57	PUT	23	3008	-	5,5,5	0.12	0	4,4,4	0.14	0
61	SPD	23	3016	-	9,9,9	0.32	0	8,8,8	0.90	0
57	PUT	23	3009	-	5,5,5	0.12	0	4,4,4	0.16	0
57	PUT	23	3010	-	5,5,5	0.13	0	4,4,4	0.23	0
61	SPD	23	3014	-	9,9,9	0.17	0	8,8,8	0.32	0
57	PUT	16	1601	-	5,5,5	0.13	0	4,4,4	0.24	0
60	ATP	23	3002	-	28,33,33	0.80	0	34,52,52	0.83	1 (2%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	PUT	23	3007	-	5,5,5	0.14	0	4,4,4	0.21	0
57	PUT	23	3006	-	5,5,5	0.12	0	4,4,4	0.21	0
57	PUT	23	3012	-	5,5,5	0.12	0	4,4,4	0.20	0
57	PUT	23	3011	-	5,5,5	0.14	0	4,4,4	0.22	0
57	PUT	23	3005	-	5,5,5	0.12	0	4,4,4	0.24	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
57	PUT	23	3003	-	-	0/3/3/3	-
57	PUT	23	3004	-	-	0/3/3/3	-
61	SPD	23	3015	-	-	4/7/7/7	-
60	ATP	23	3001	-	-	6/18/38/38	0/3/3/3
61	SPD	23	3013	-	-	3/7/7/7	-
57	PUT	23	3008	-	-	0/3/3/3	-
61	SPD	23	3016	-	-	1/7/7/7	-
57	PUT	23	3009	-	-	1/3/3/3	-
57	PUT	23	3010	-	-	0/3/3/3	-
61	SPD	23	3014	-	-	2/7/7/7	-
57	PUT	16	1601	-	-	0/3/3/3	-
60	ATP	23	3002	-	-	6/18/38/38	0/3/3/3
57	PUT	23	3007	-	-	0/3/3/3	-
57	PUT	23	3006	-	-	2/3/3/3	-
57	PUT	23	3012	-	-	1/3/3/3	-
57	PUT	23	3011	-	-	2/3/3/3	-
57	PUT	23	3005	-	-	0/3/3/3	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	23	3002	ATP	C5-C6-N6	2.46	124.06	120.31
60	23	3001	ATP	C5-C6-N6	2.35	123.88	120.31

There are no chirality outliers.

All (28) torsion outliers are listed below:

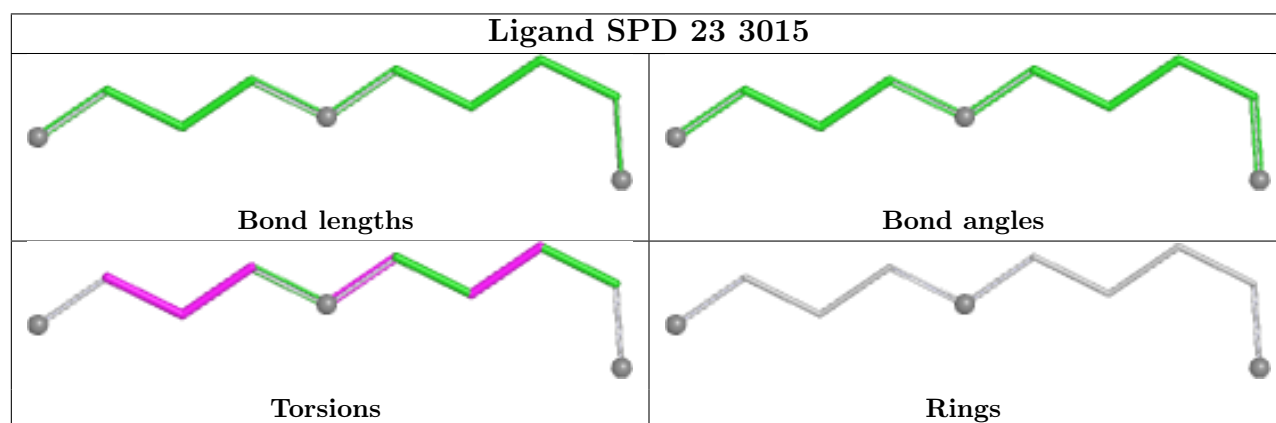
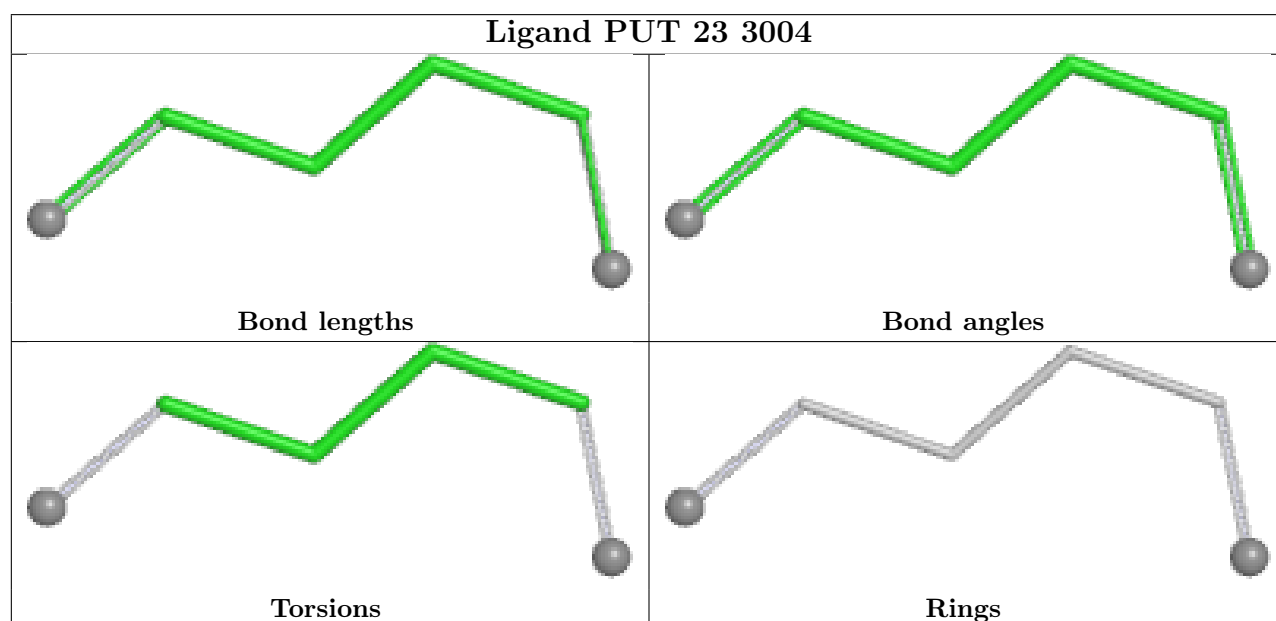
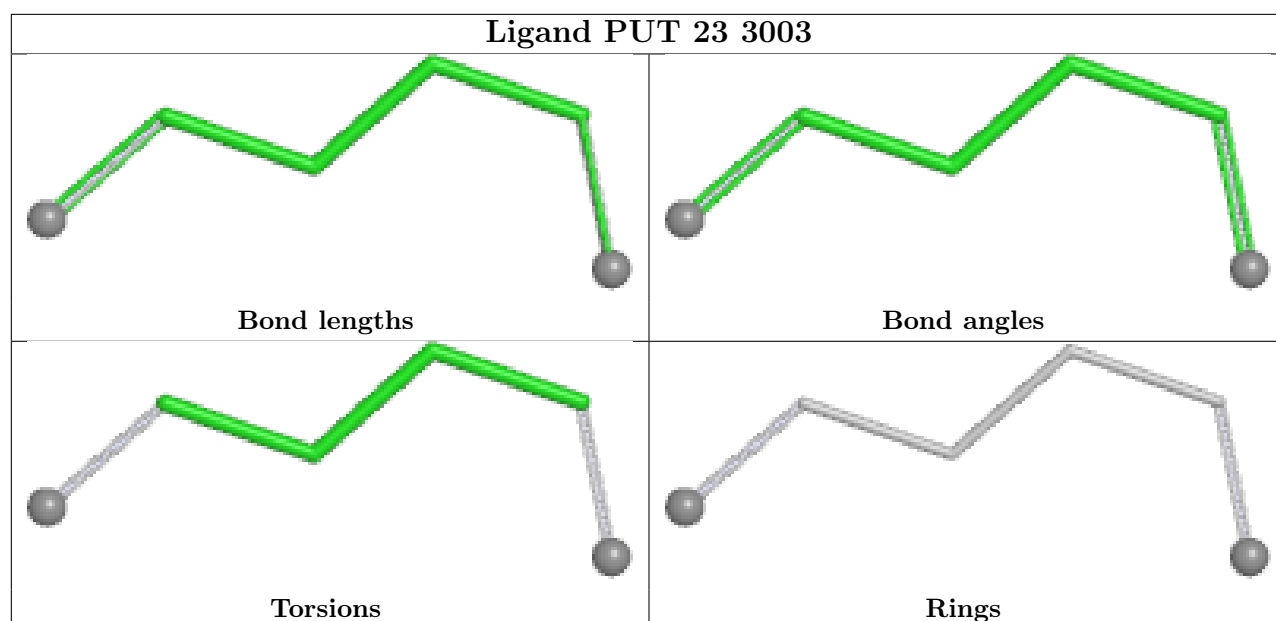


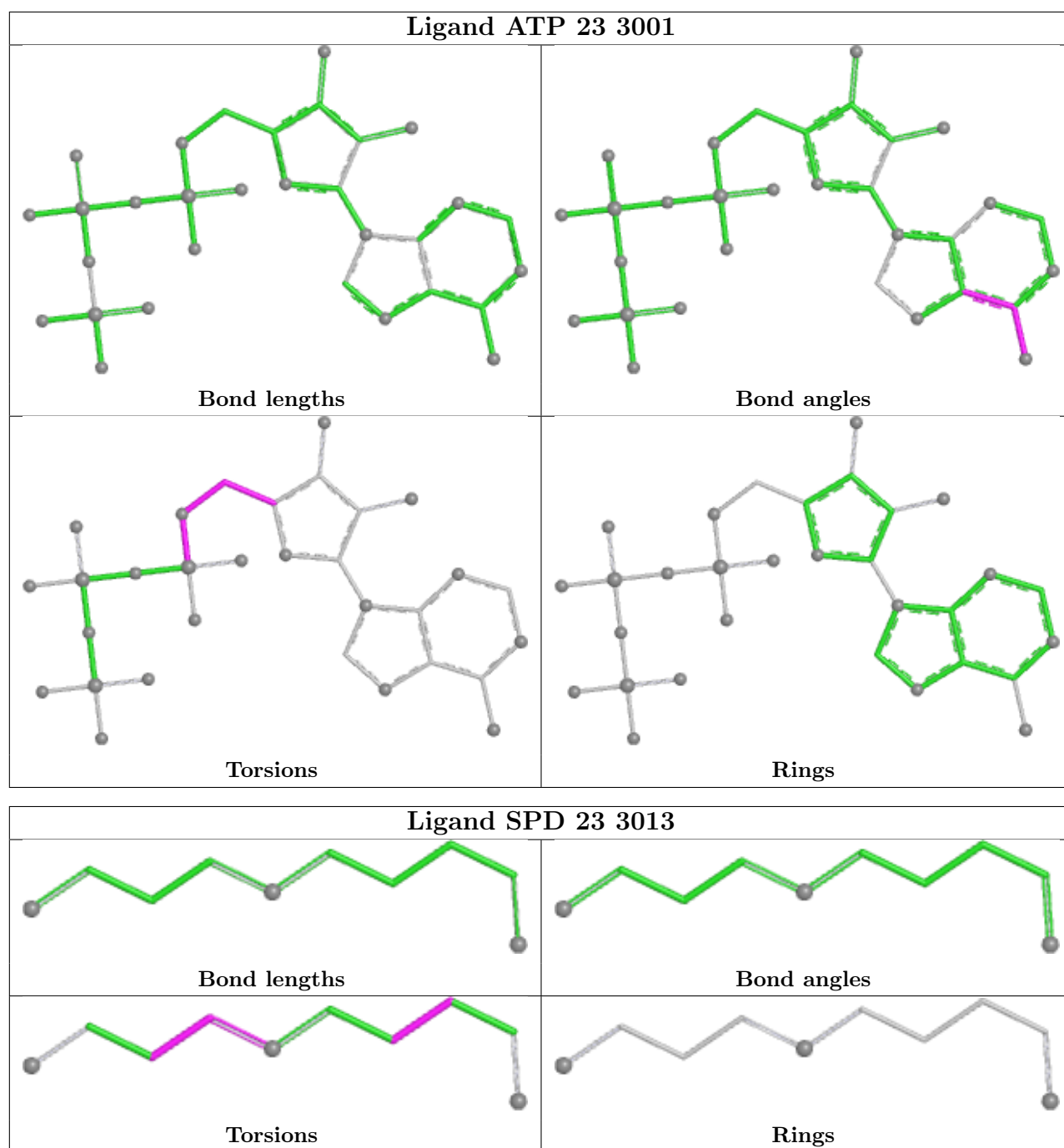
Mol	Chain	Res	Type	Atoms
60	23	3001	ATP	C5'-O5'-PA-O2A
60	23	3001	ATP	C5'-O5'-PA-O3A
60	23	3002	ATP	PB-O3B-PG-O2G
61	23	3013	SPD	N6-C7-C8-C9
57	23	3012	PUT	C2-C3-C4-N2
61	23	3014	SPD	C3-C4-C5-N6
61	23	3015	SPD	C2-C3-C4-C5
61	23	3015	SPD	N6-C7-C8-C9
61	23	3015	SPD	C7-C8-C9-N10
60	23	3001	ATP	C3'-C4'-C5'-O5'
60	23	3002	ATP	PG-O3B-PB-O1B
61	23	3014	SPD	C8-C7-N6-C5
60	23	3001	ATP	C5'-O5'-PA-O1A
57	23	3011	PUT	C2-C3-C4-N2
60	23	3001	ATP	C4'-C5'-O5'-PA
60	23	3001	ATP	O4'-C4'-C5'-O5'
60	23	3002	ATP	PB-O3A-PA-O2A
57	23	3006	PUT	N1-C1-C2-C3
61	23	3013	SPD	C8-C7-N6-C5
61	23	3013	SPD	C2-C3-C4-C5
61	23	3015	SPD	C4-C5-N6-C7
57	23	3009	PUT	N1-C1-C2-C3
60	23	3002	ATP	PB-O3B-PG-O1G
57	23	3006	PUT	C2-C3-C4-N2
57	23	3011	PUT	N1-C1-C2-C3
60	23	3002	ATP	PG-O3B-PB-O2B
61	23	3016	SPD	C7-C8-C9-N10
60	23	3002	ATP	PA-O3A-PB-O1B

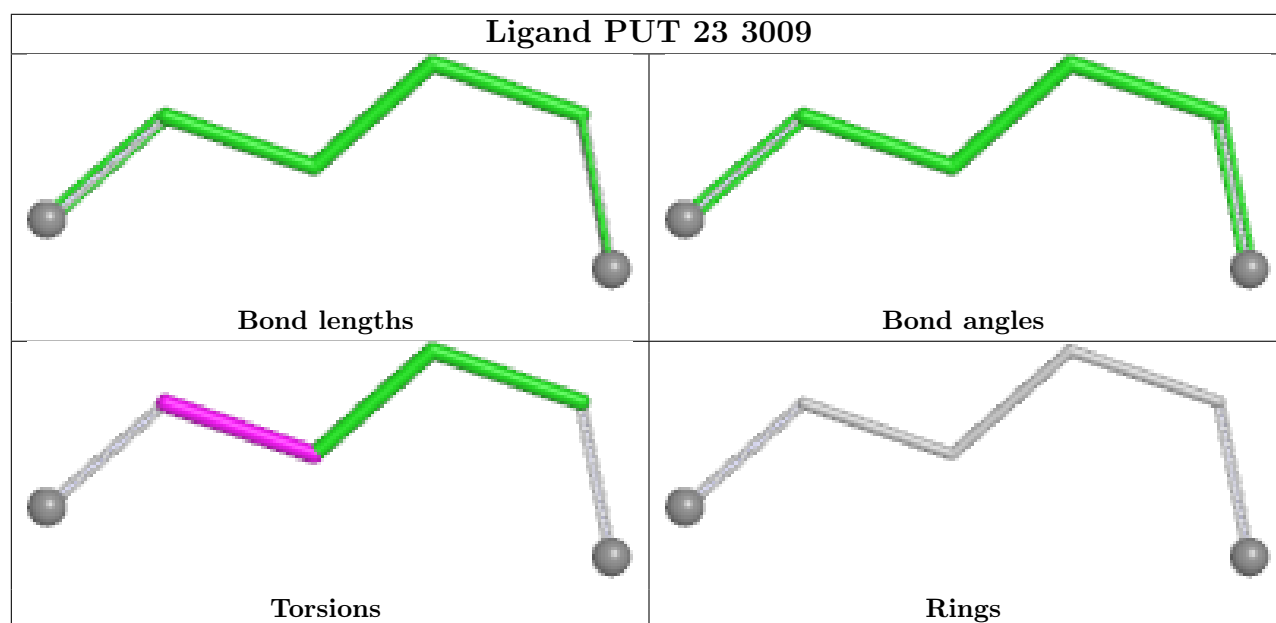
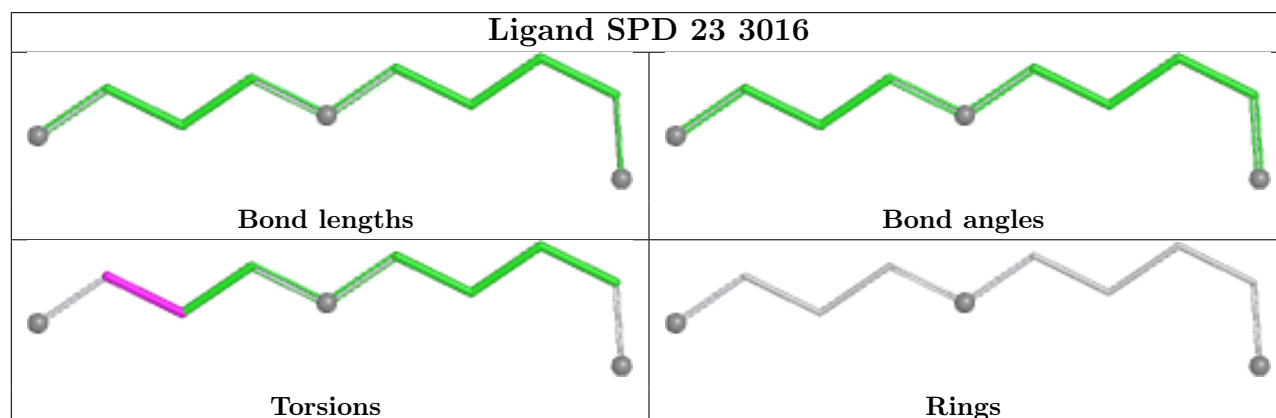
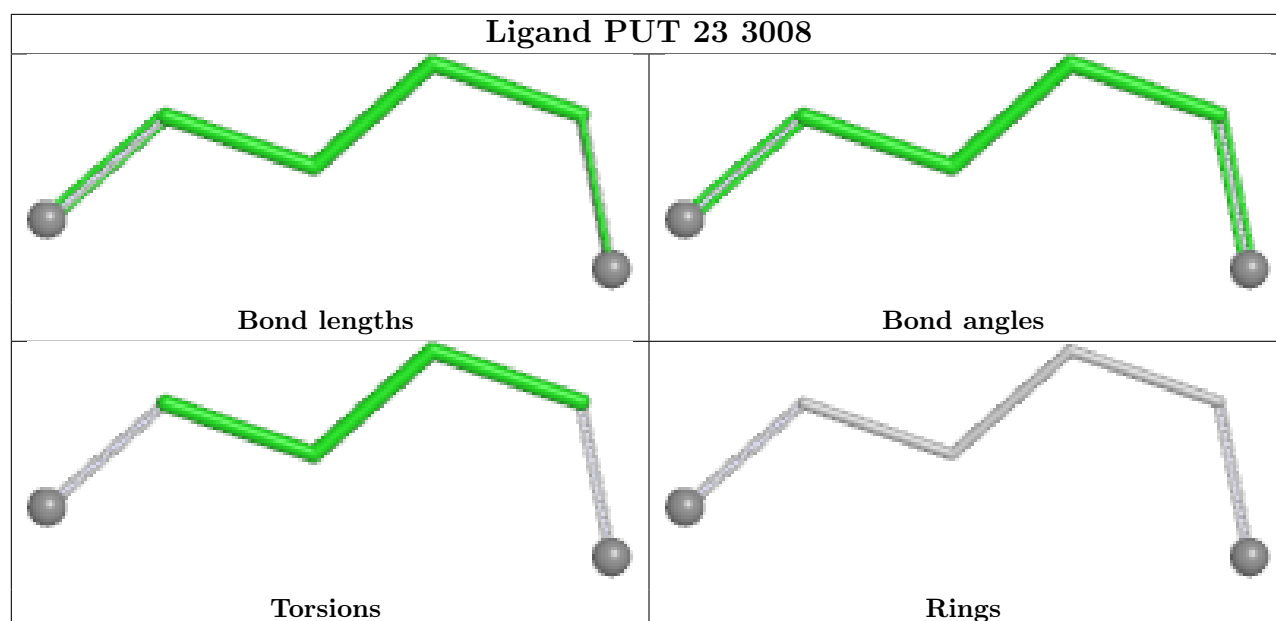
There are no ring outliers.

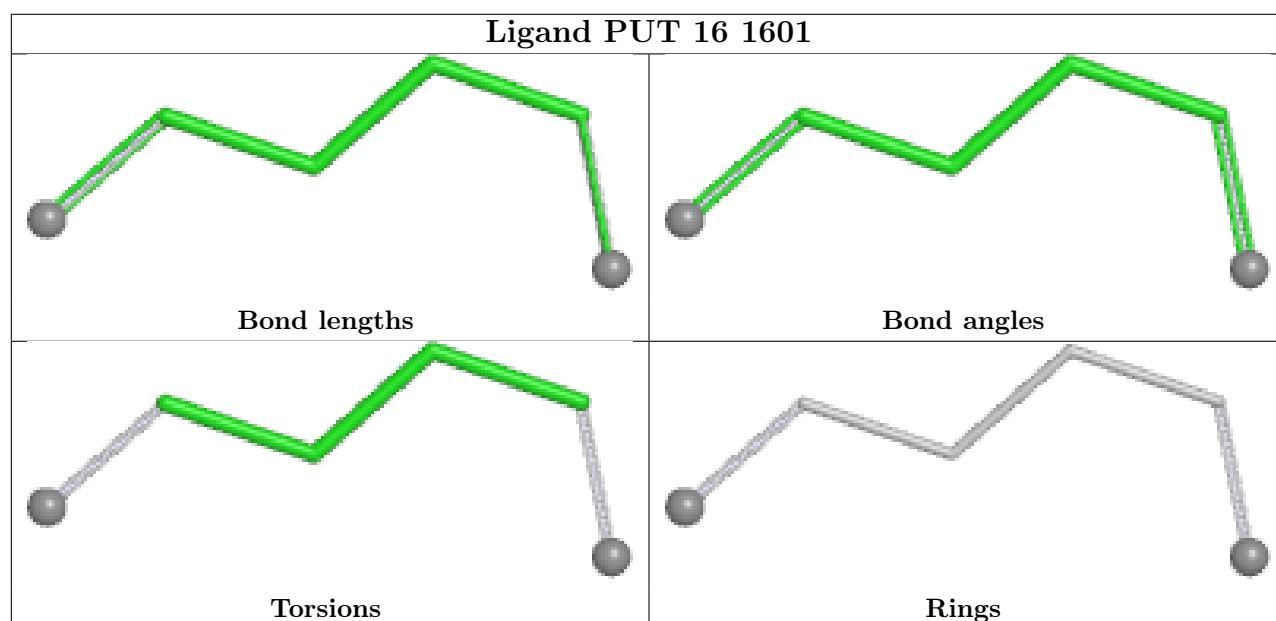
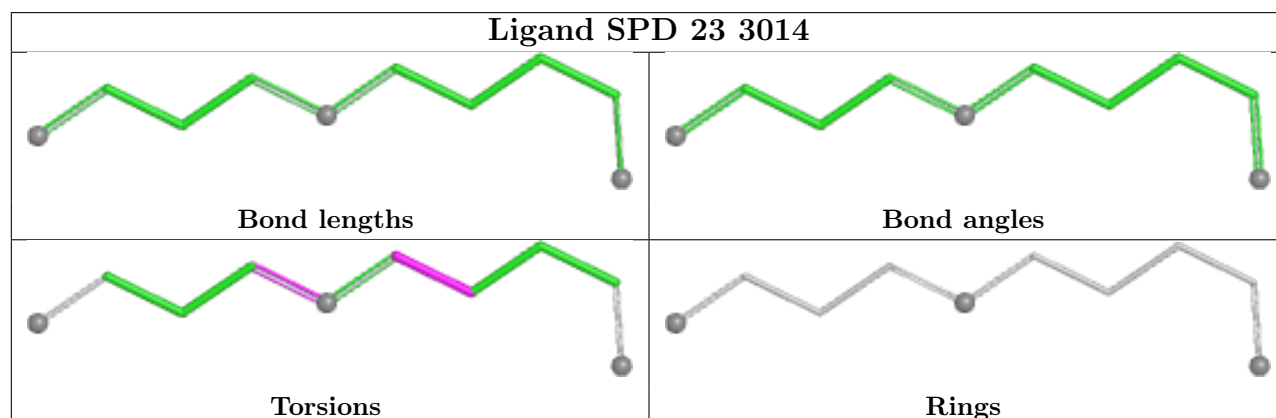
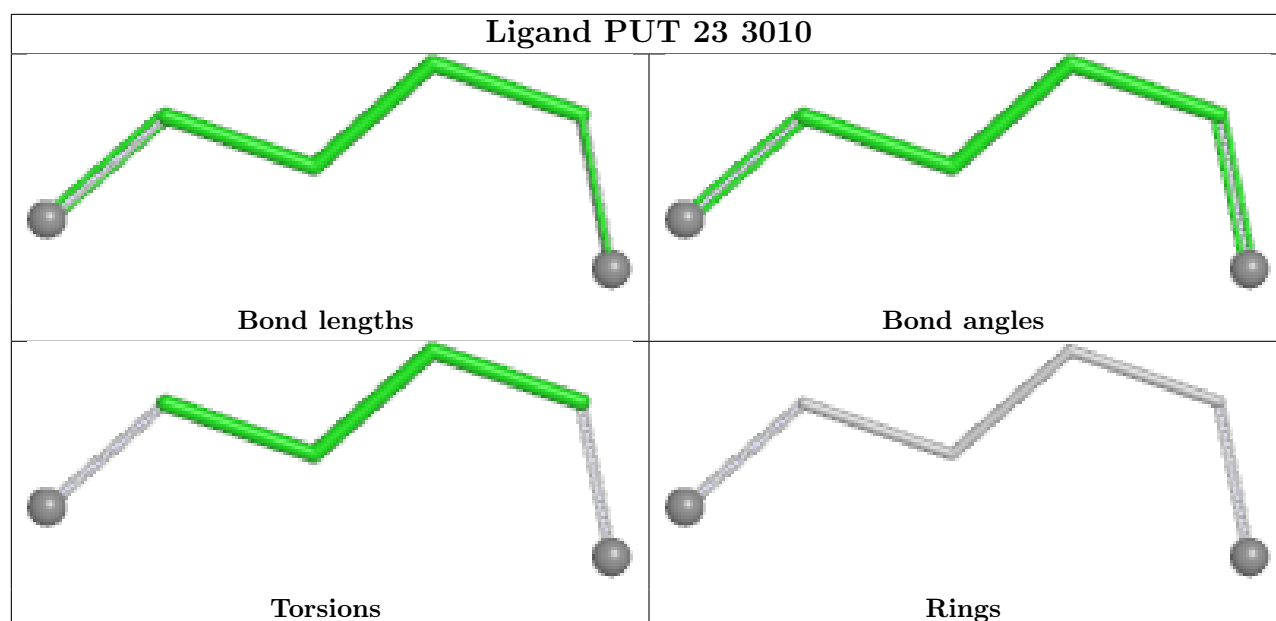
No monomer is involved in short contacts.

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

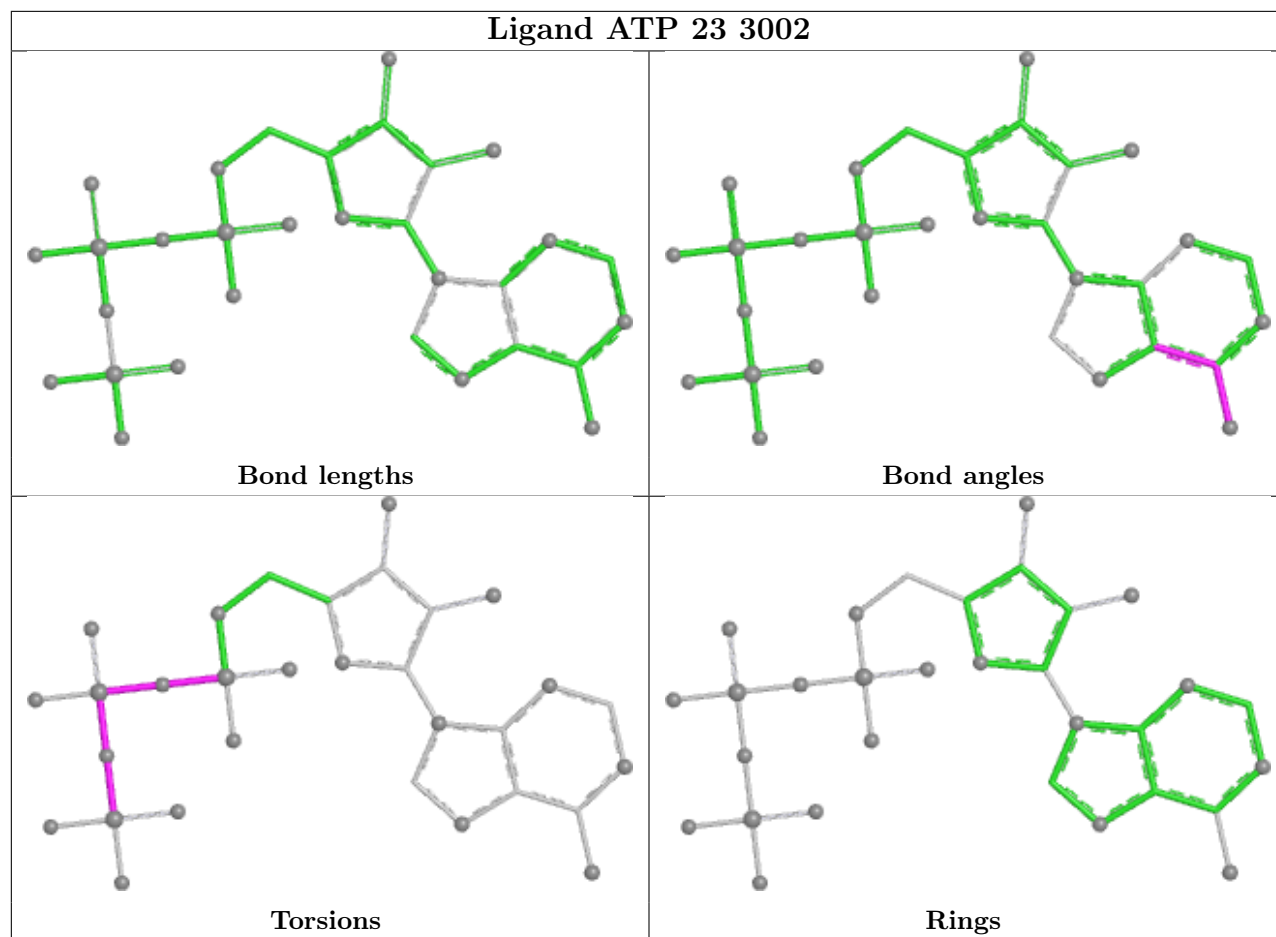




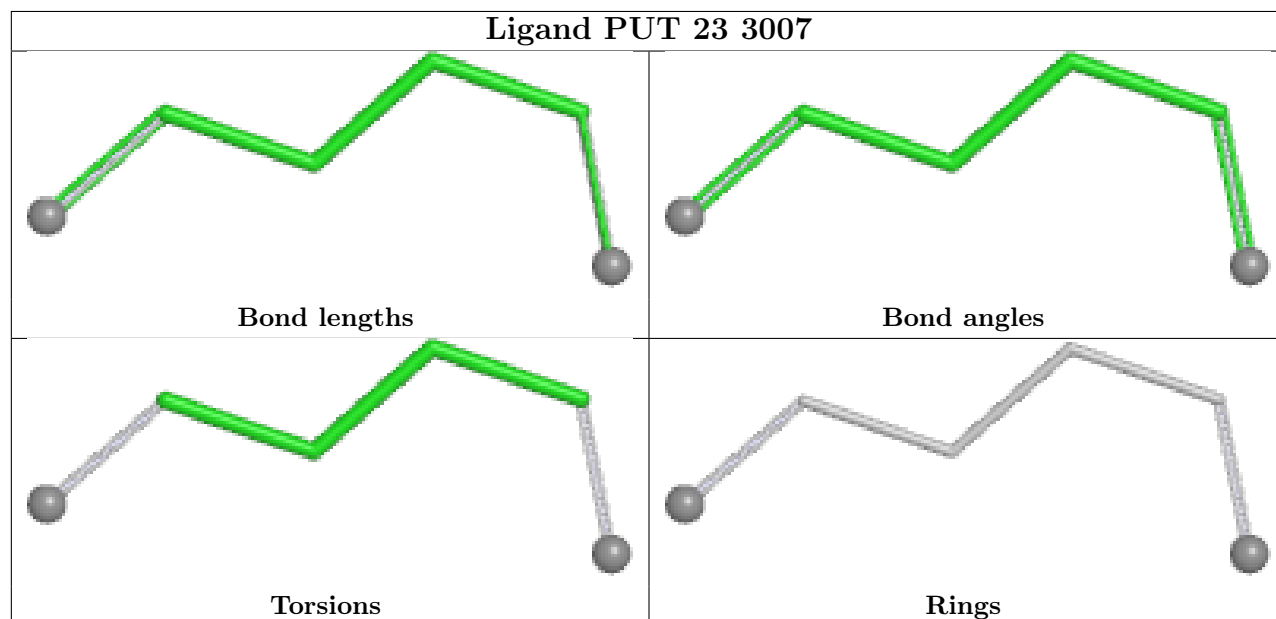


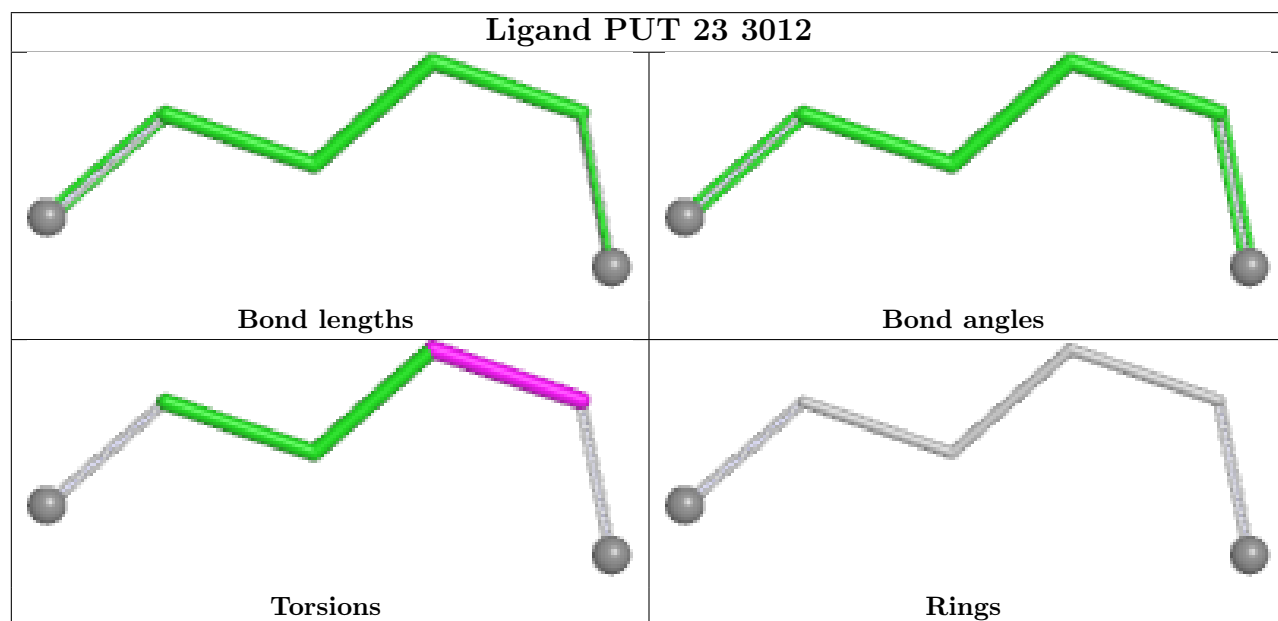
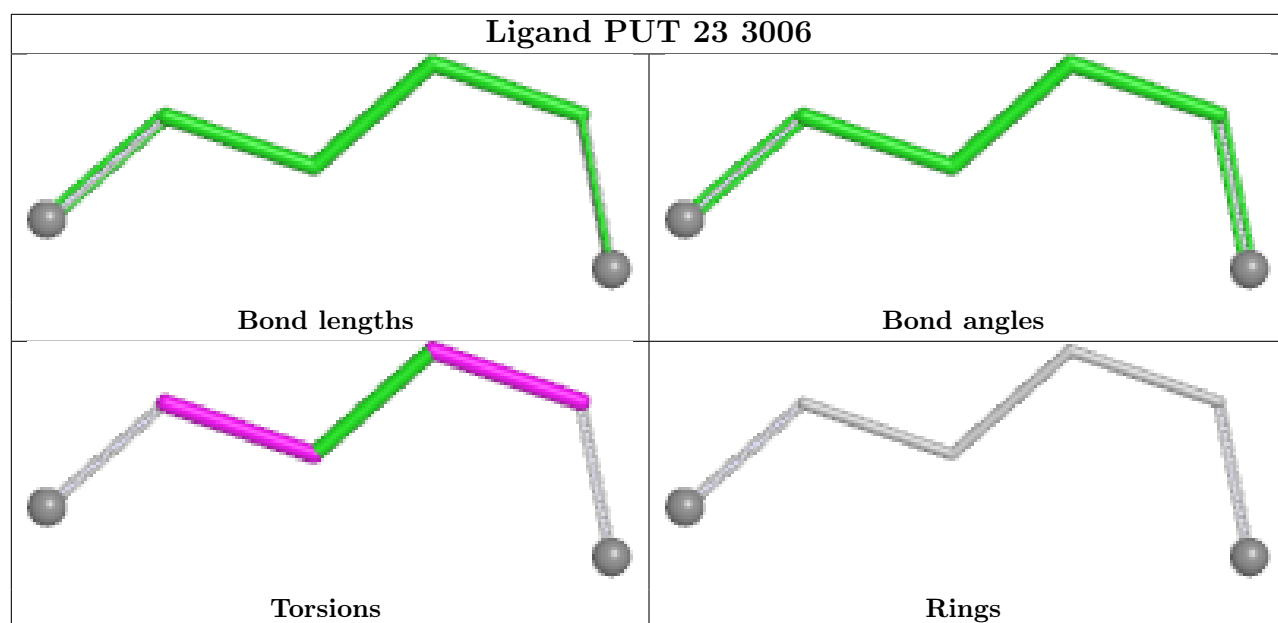


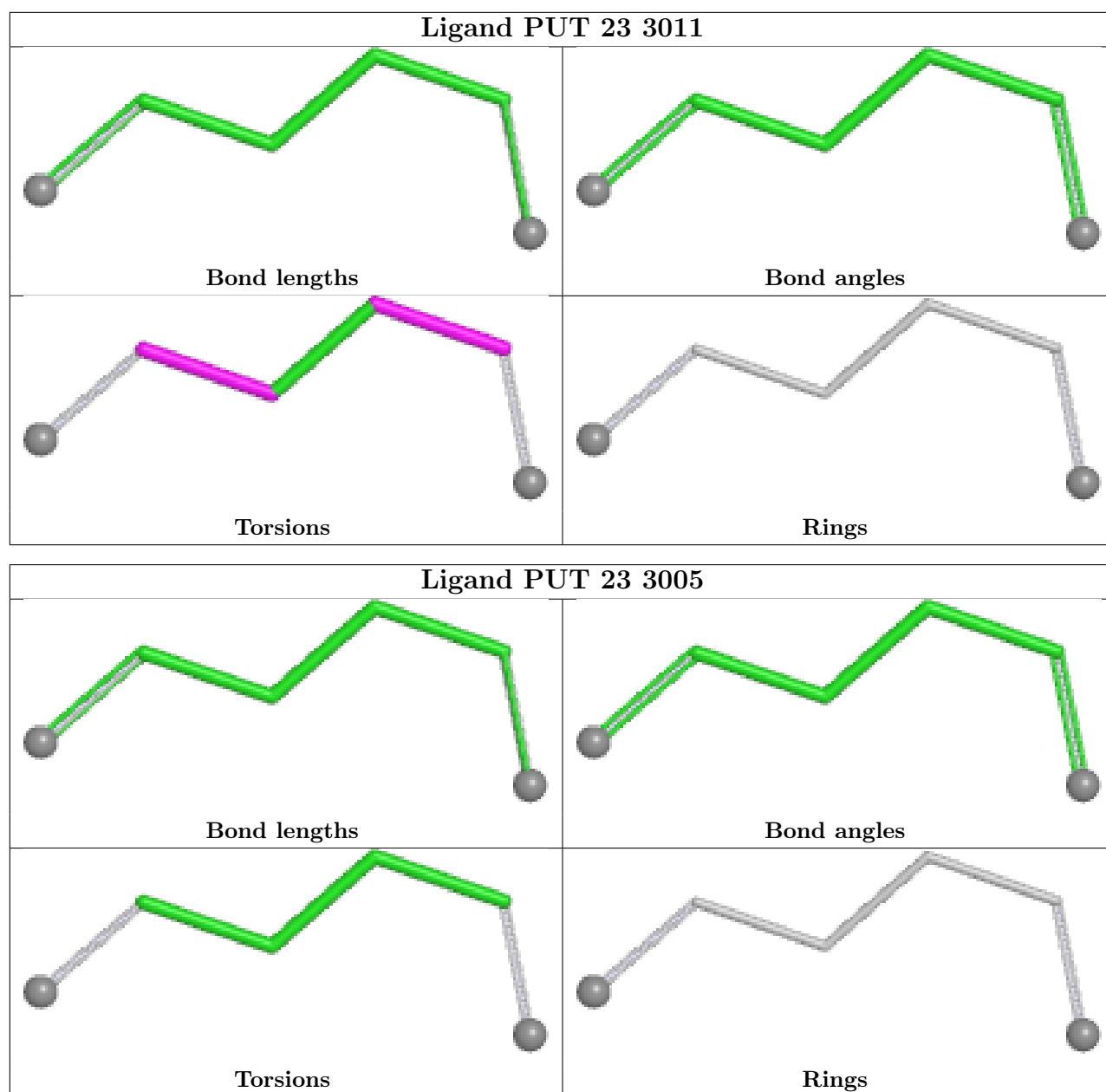
## Ligand ATP 23 3002



## Ligand PUT 23 3007







## 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.



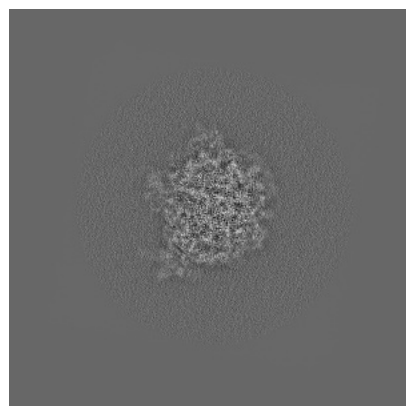
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24135. These allow visual inspection of the internal detail of the map and identification of artifacts.

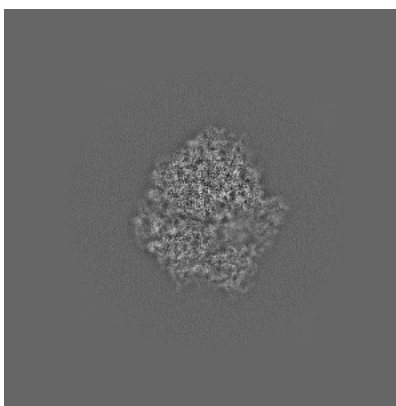
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

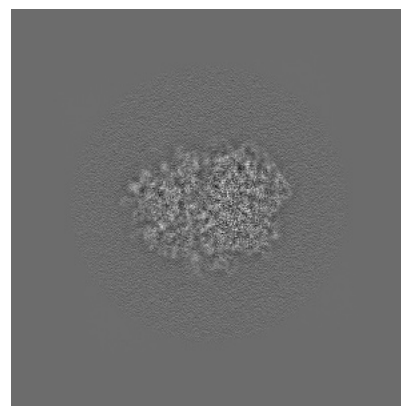
#### 6.1.1 Primary map



X

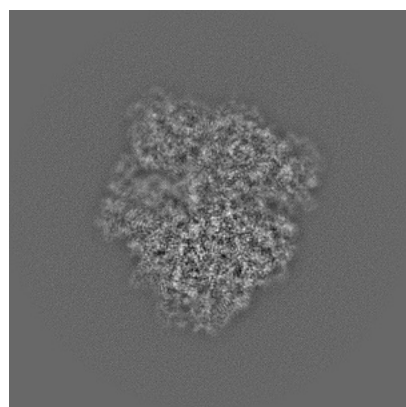


Y

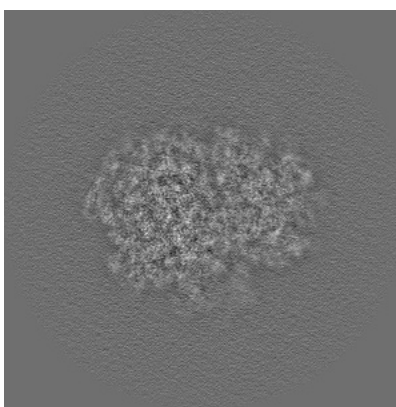


Z

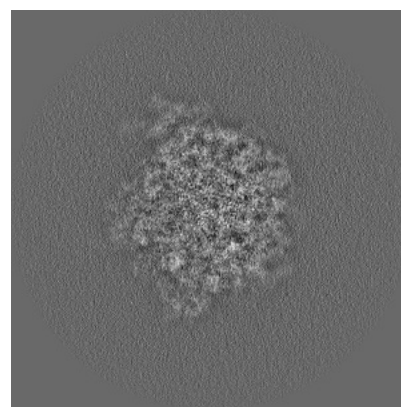
#### 6.1.2 Raw map



X



Y

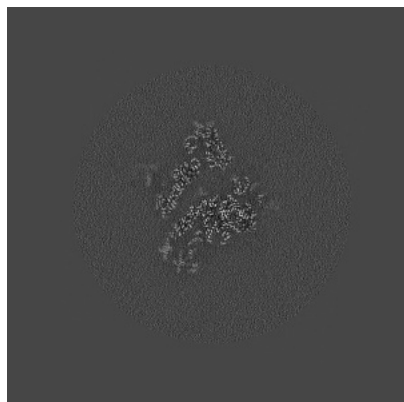


Z

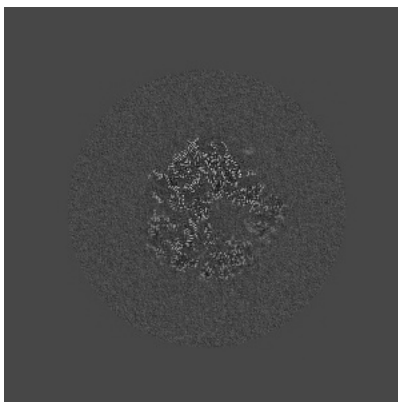
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

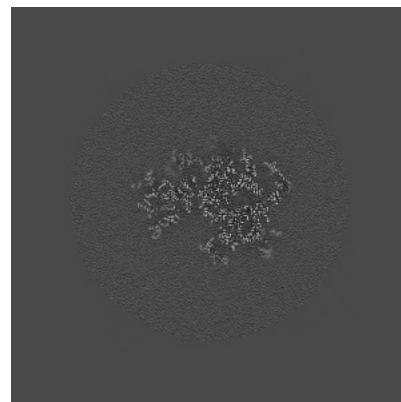
### 6.2.1 Primary map



X Index: 288

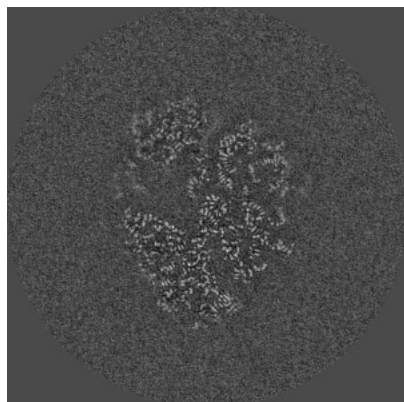


Y Index: 288

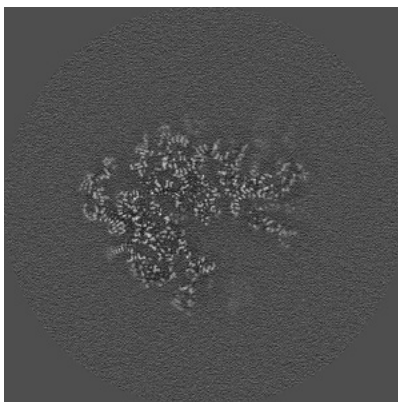


Z Index: 288

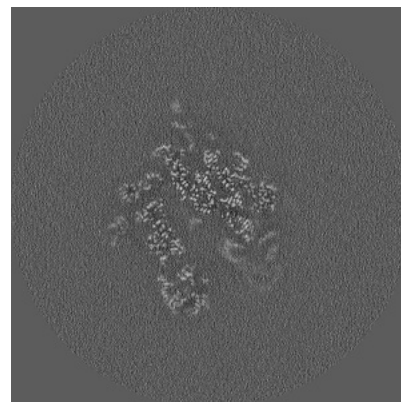
### 6.2.2 Raw map



X Index: 256



Y Index: 256

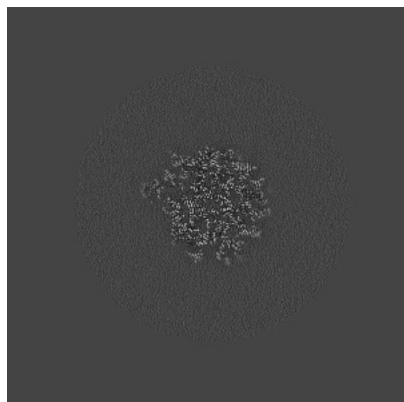


Z Index: 256

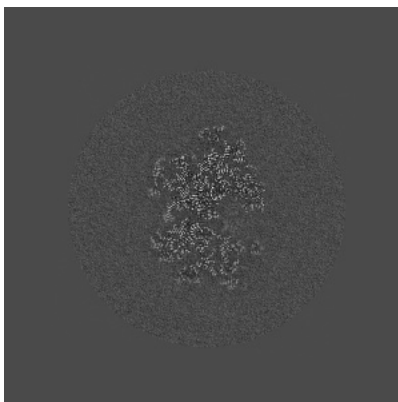
The images above show central slices of the map in three orthogonal directions.

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

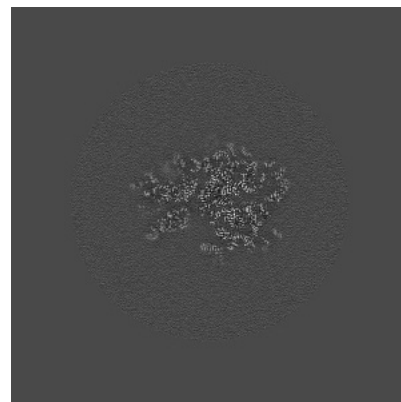
### 6.3.1 Primary map



X Index: 315

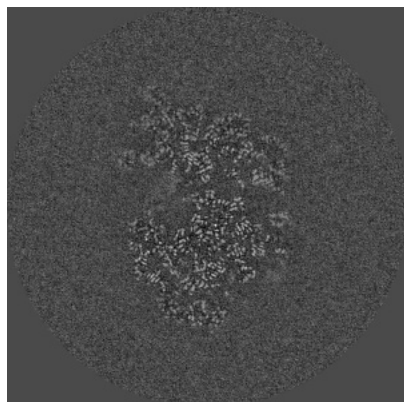


Y Index: 313

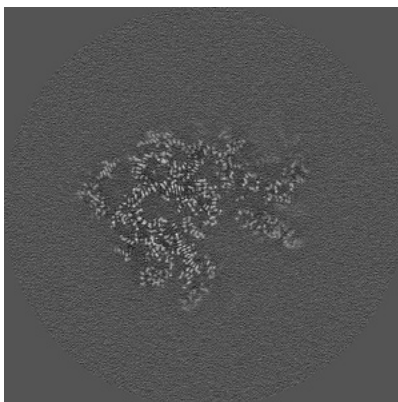


Z Index: 283

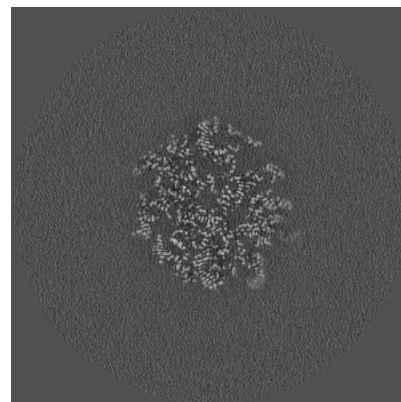
### 6.3.2 Raw map



X Index: 270



Y Index: 264

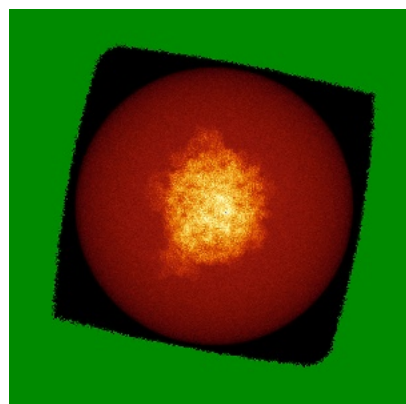


Z Index: 210

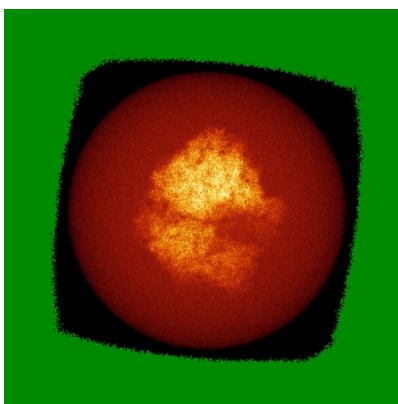
The images above show the largest variance slices of the map in three orthogonal directions.

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

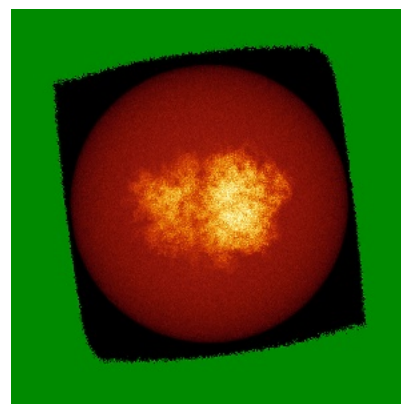
### 6.4.1 Primary map



X

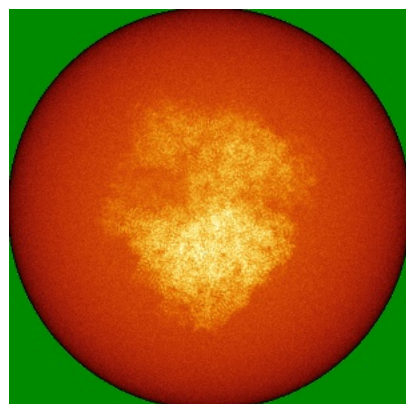


Y

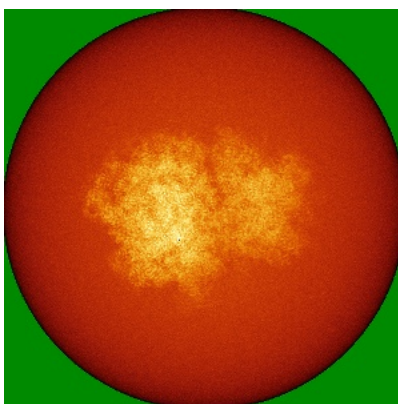


Z

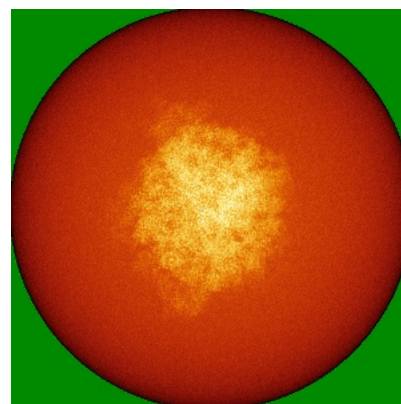
### 6.4.2 Raw map



X



Y



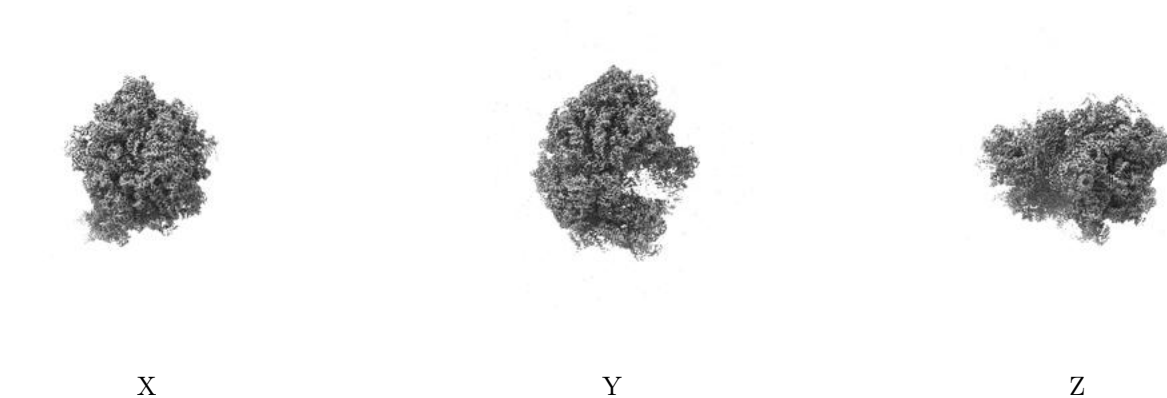
Z

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.



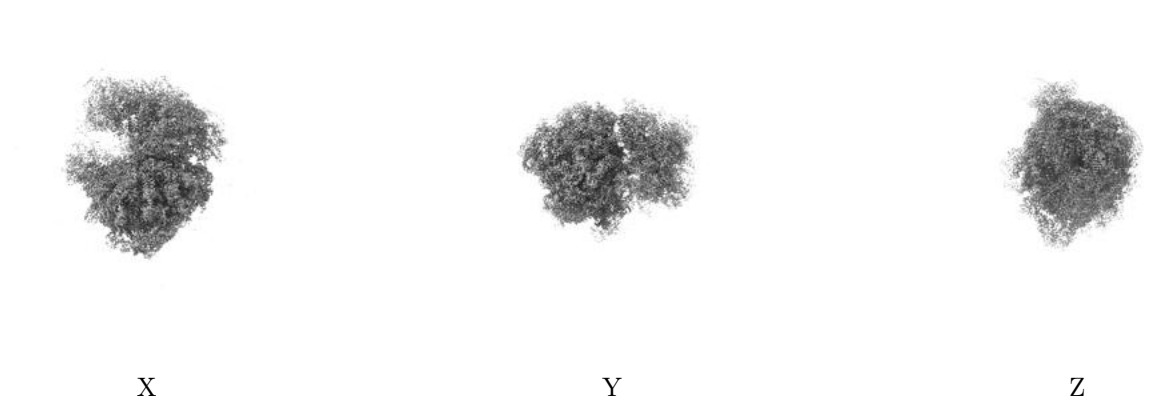
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0193. 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.

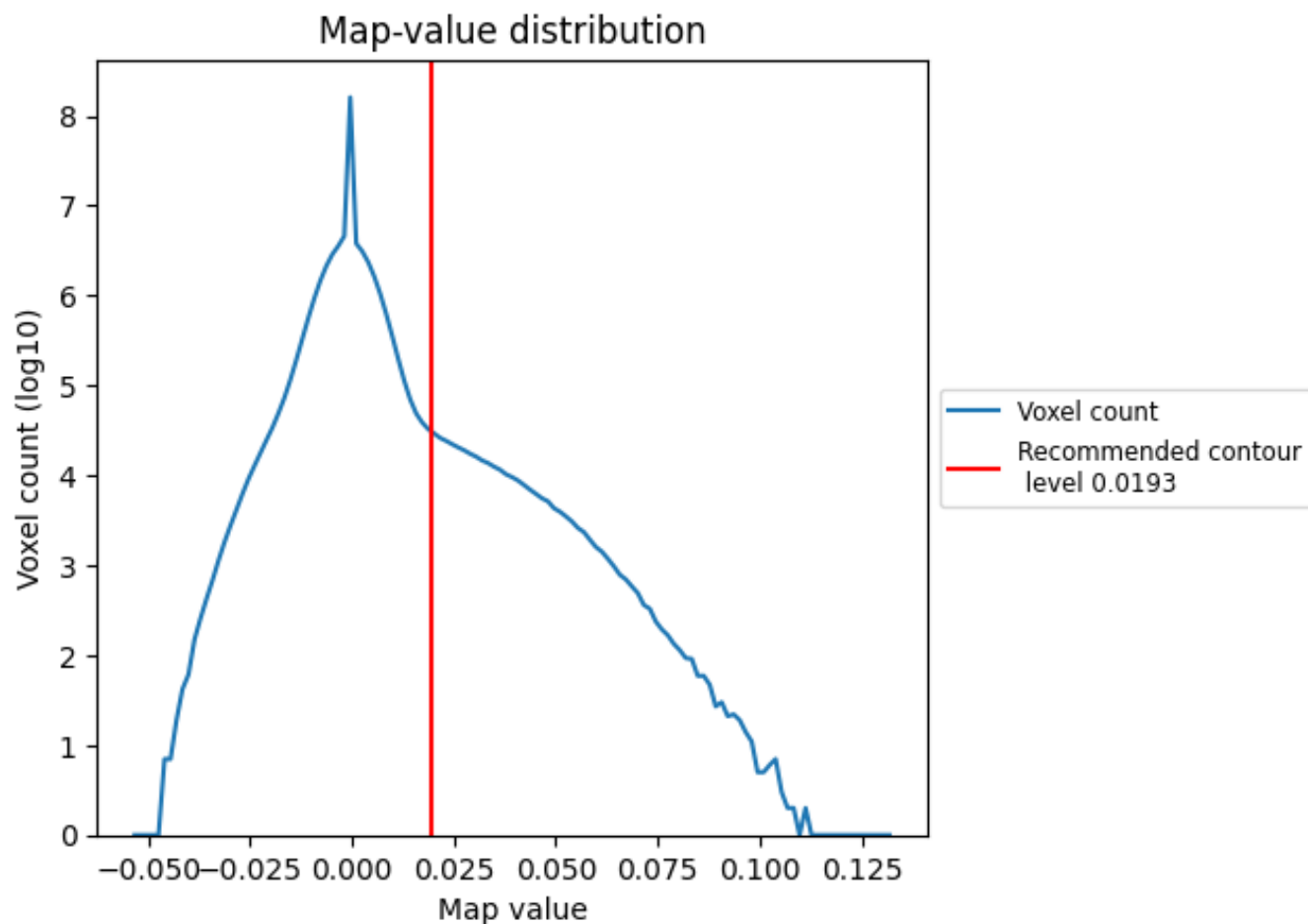
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

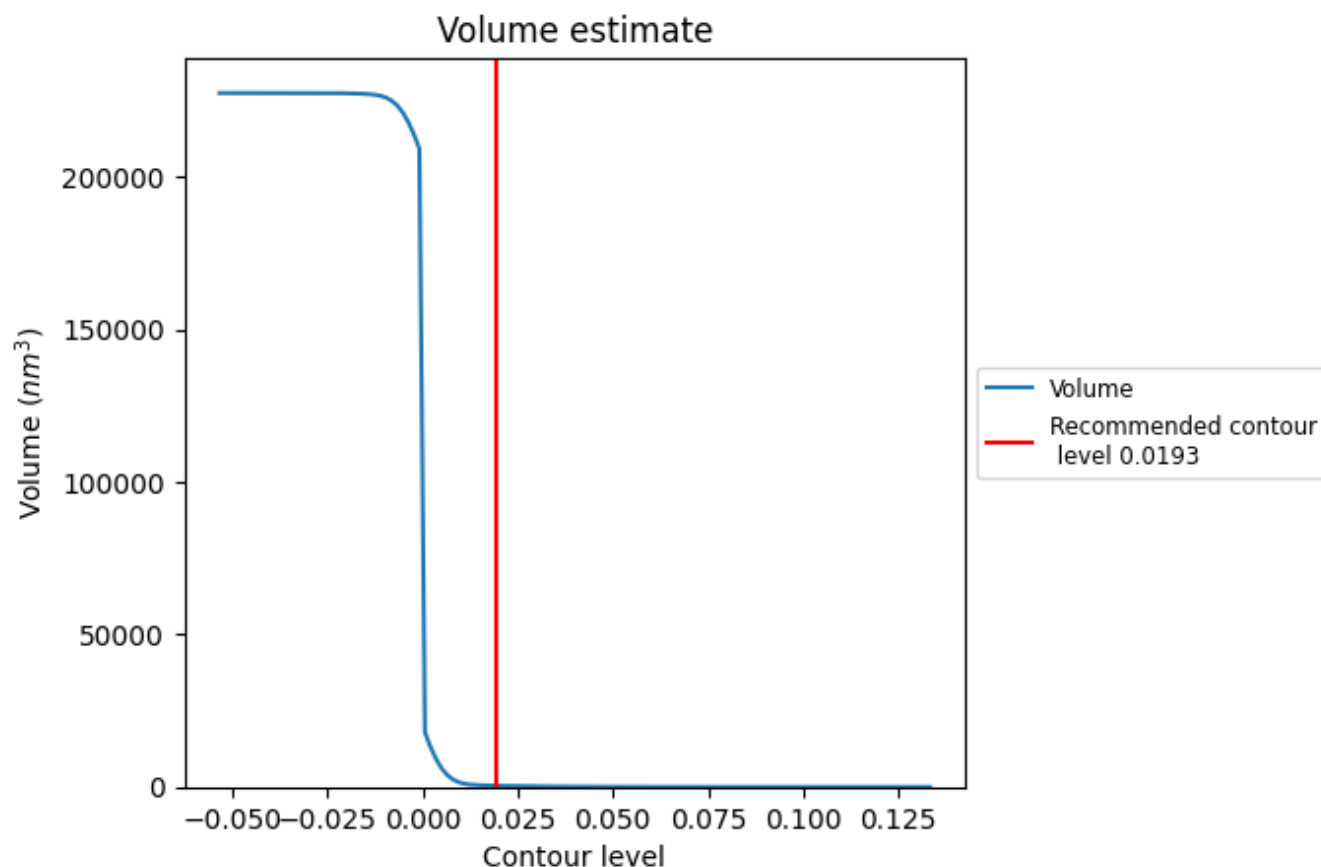
This section contains the results of statistical analysis of the map.

### 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.

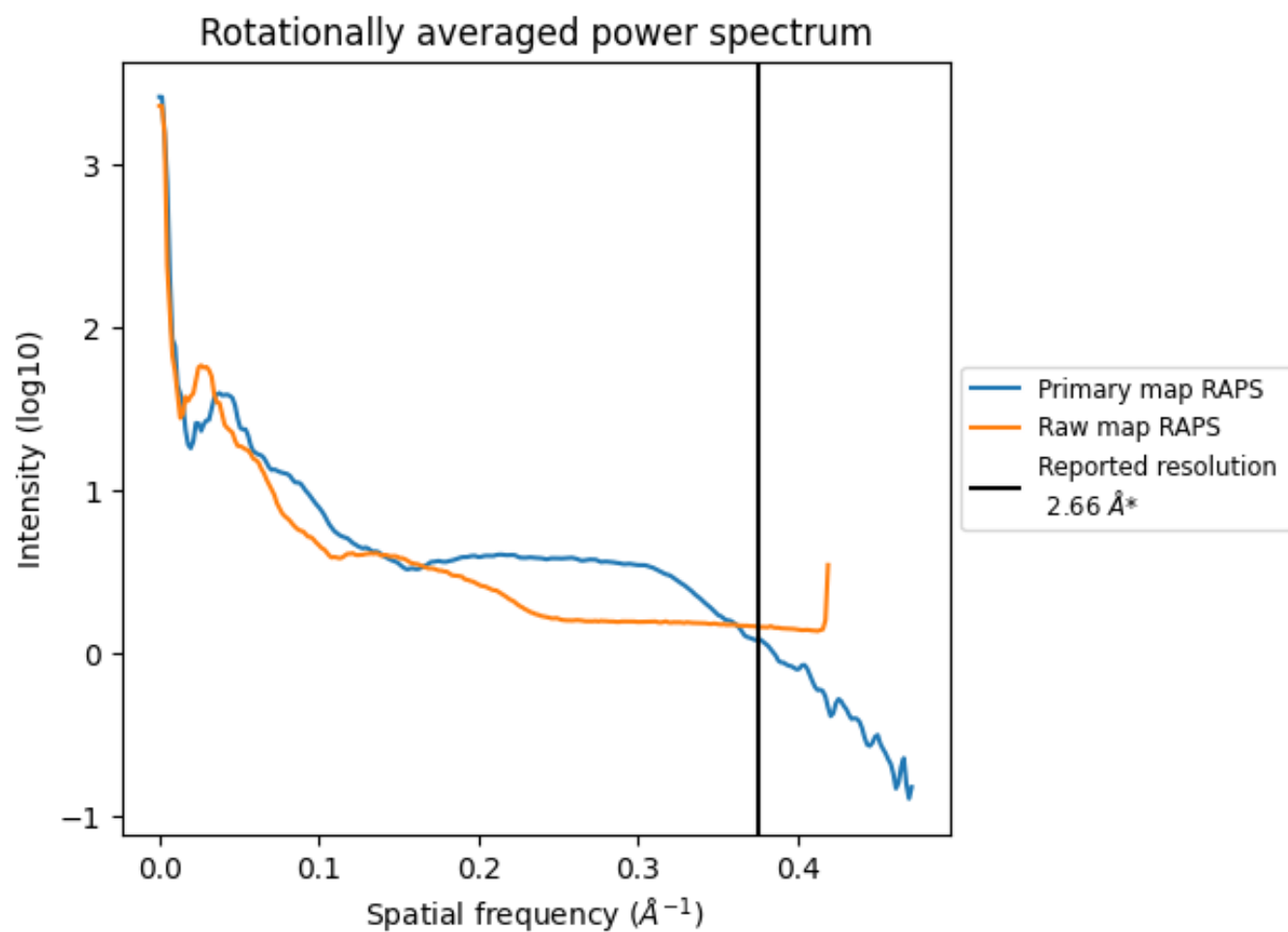
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 403  $\text{nm}^3$ ; this corresponds to an approximate mass of 364 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 ⓘ



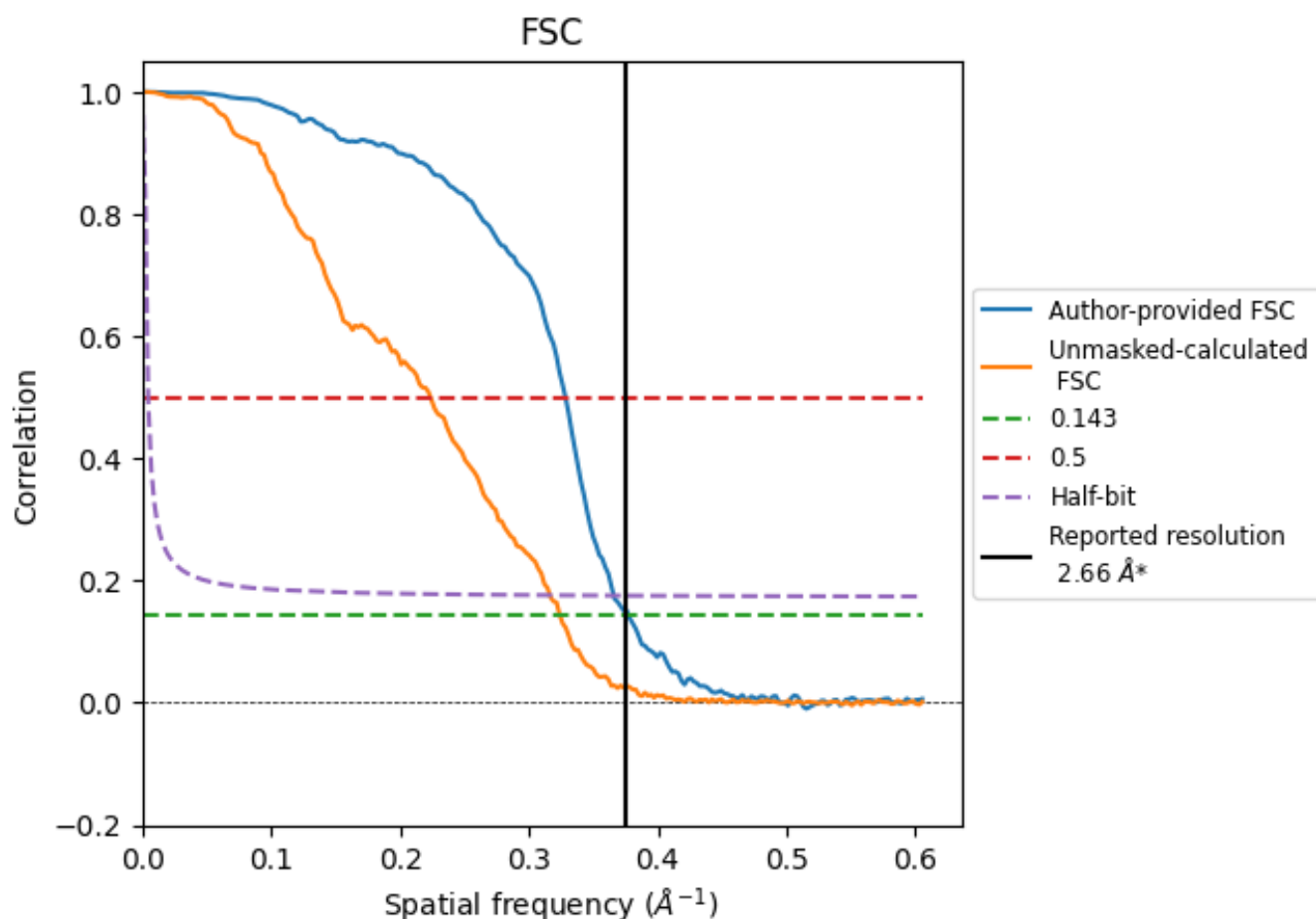
\*Reported resolution corresponds to spatial frequency of 0.376 Å<sup>-1</sup>



## 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 0.376 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

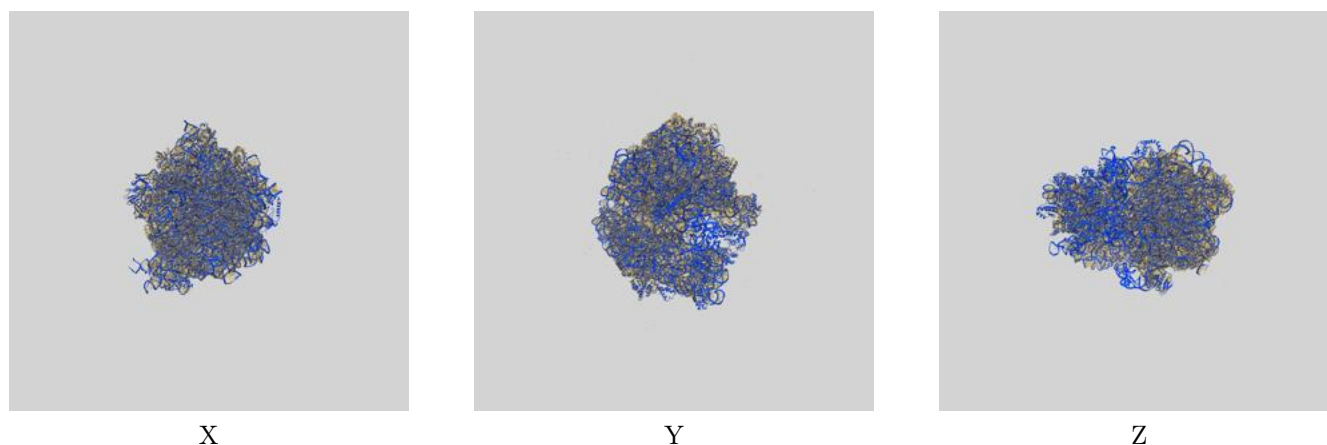
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	2.65	3.04	2.73
Unmasked-calculated*	3.08	4.47	3.16

\*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 3.08 differs from the reported value 2.66 by more than 10 %

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

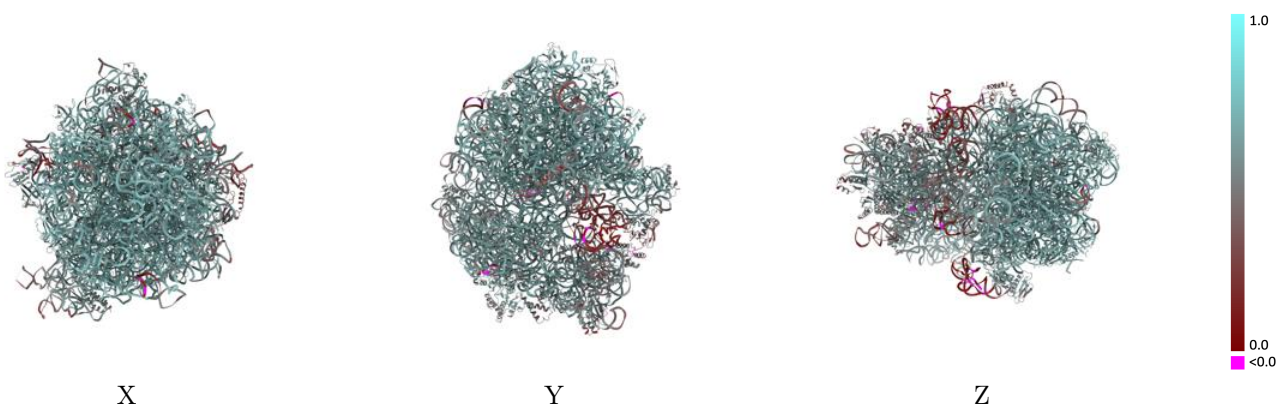
This section contains information regarding the fit between EMDB map EMD-24135 and PDB model 7N30. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

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



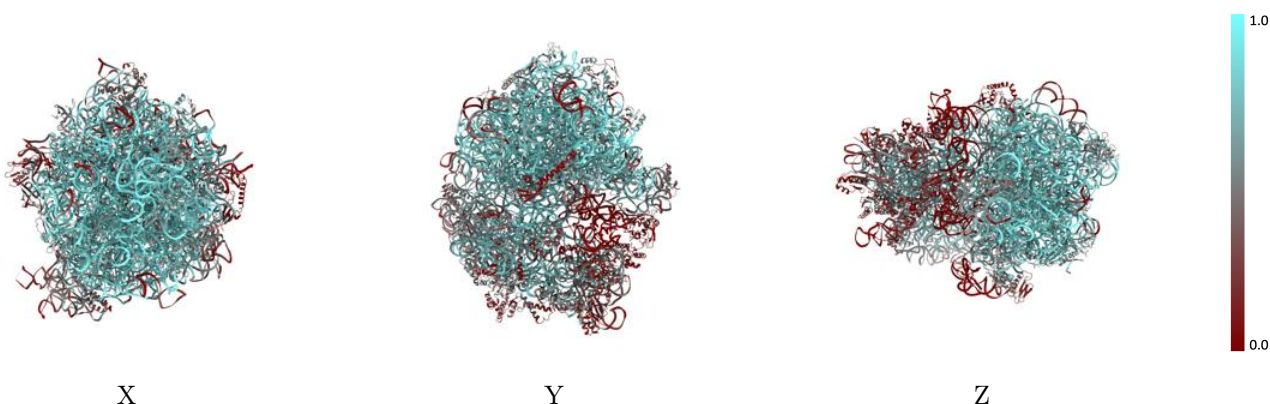
The images above show the 3D surface view of the map at the recommended contour level 0.0193 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



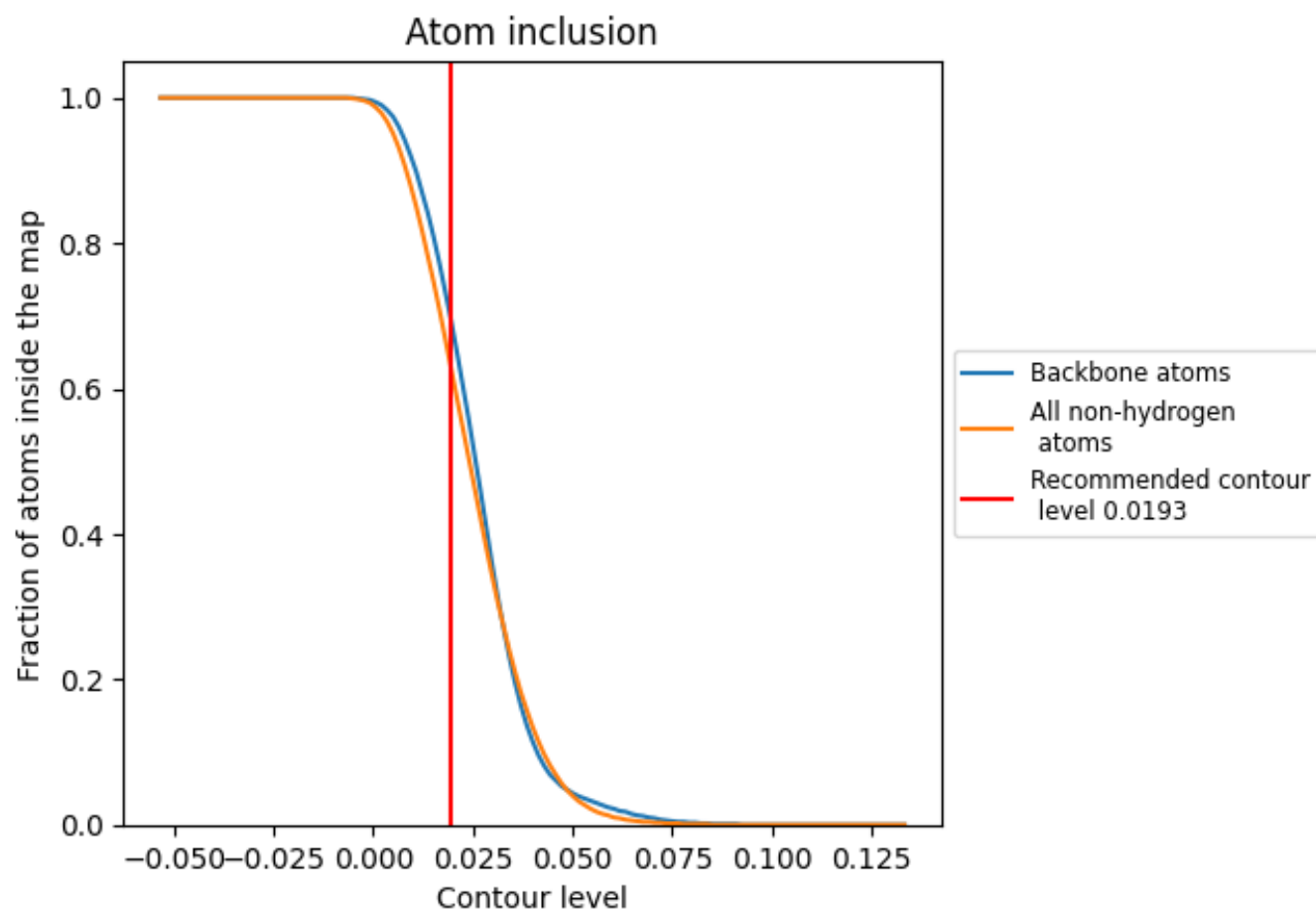
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0193).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 64% 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 (0.0193) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6360	 0.5920
16	 0.6320	 0.5900
23	 0.7640	 0.6100
5	 0.6420	 0.5960
Dt	 0.2680	 0.4110
LB	 0.7110	 0.6610
LC	 0.7020	 0.6500
LD	 0.6260	 0.6240
LE	 0.1170	 0.4470
LF	 0.3610	 0.5510
LI	 0.0760	 0.3770
LM	 0.7120	 0.6510
LN	 0.6750	 0.6540
LO	 0.6640	 0.6420
LP	 0.6690	 0.6460
LQ	 0.7500	 0.6640
LR	 0.4410	 0.5610
LS	 0.6220	 0.6310
LT	 0.7520	 0.6700
LU	 0.6390	 0.6250
LV	 0.6910	 0.6540
LW	 0.5590	 0.6010
LX	 0.5290	 0.6090
LY	 0.5490	 0.6070
La	 0.6730	 0.6480
Lb	 0.6380	 0.6410
Lc	 0.5090	 0.5710
Ld	 0.6750	 0.6260
Le	 0.0390	 0.2800
Lf	 0.6920	 0.6420
Lg	 0.5130	 0.6220
Lh	 0.7690	 0.6760
Li	 0.7480	 0.6670
Lj	 0.6370	 0.6390
Pp	 0.2860	 0.6300



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Chain	Atom inclusion	Q-score
Pt	 0.2270	 0.4610
SB	 0.3260	 0.5240
SC	 0.4260	 0.5700
SD	 0.3120	 0.5490
SE	 0.5640	 0.6080
SF	 0.3030	 0.5190
SG	 0.1490	 0.4500
SH	 0.5410	 0.6160
SI	 0.2530	 0.5180
SJ	 0.2420	 0.4980
SK	 0.4100	 0.5760
SL	 0.5830	 0.6260
SM	 0.1890	 0.4880
SN	 0.3370	 0.5490
SO	 0.4980	 0.5880
SP	 0.4700	 0.5760
SQ	 0.4450	 0.5800
SR	 0.4210	 0.5780
SS	 0.1760	 0.5000
ST	 0.3800	 0.5660
SU	 0.2730	 0.5110
mR	 0.6540	 0.6060