wwPDB EM Validation Summary Report (i)

Sep 16, 2026 – 08:05 PM EDT

PDB ID	:	7N1P / pdb_00007n1p
EMDB ID	:	EMD-24120
Title	:	Elongating 70S ribosome complex in a classical pre-translocation (PRE-C) conformation
Authors	:	Rundlet, E.J.; Holm, M.; Schacherl, M.; Natchiar, S.K.; Altman, R.B.; Spahn, C.M.T.; Myasnikov, A.G.; Blanchard, S.C.
Deposited on	:	2021-05-28
Resolution	:	2.33 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

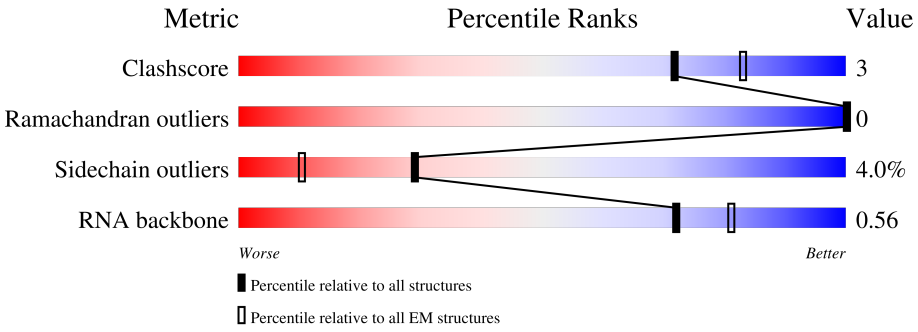
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

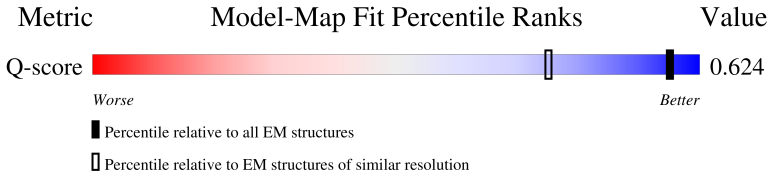
1 Overall quality at a glance

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

The reported resolution of this entry is 2.33 Å.

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





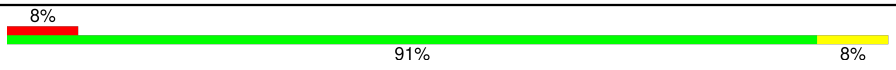
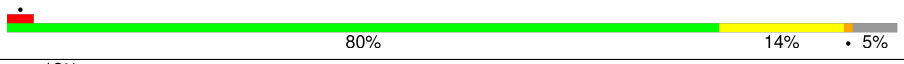
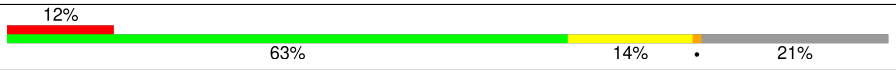
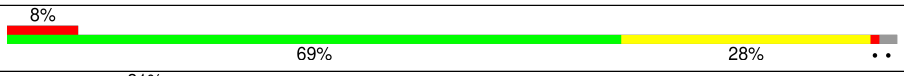
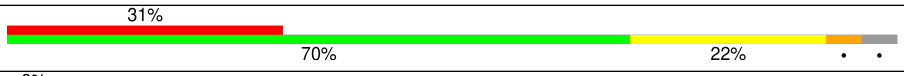
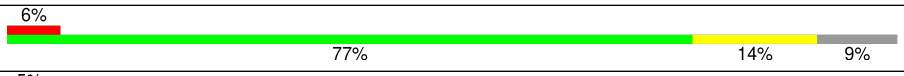
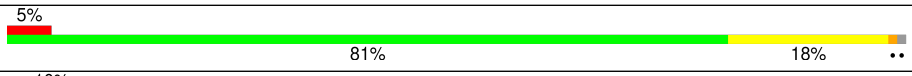
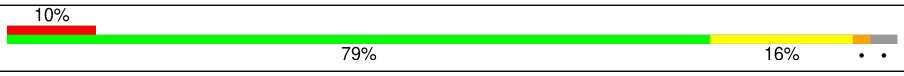
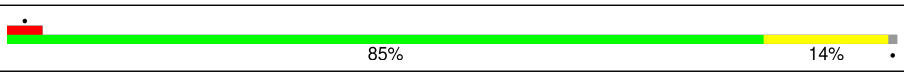
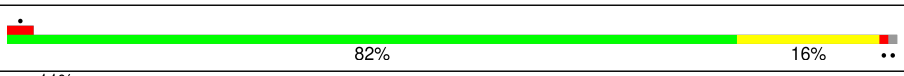
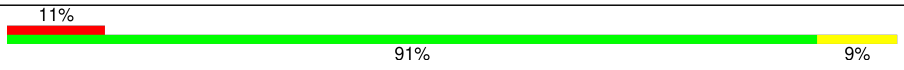
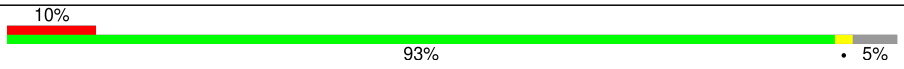
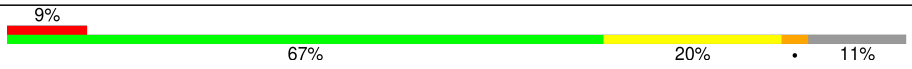
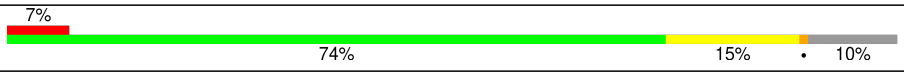
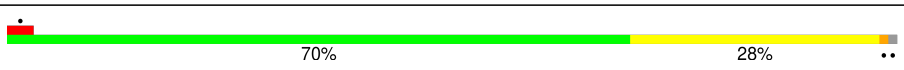
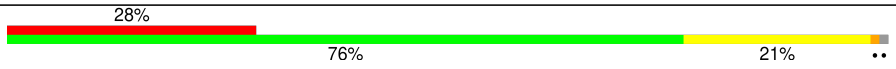
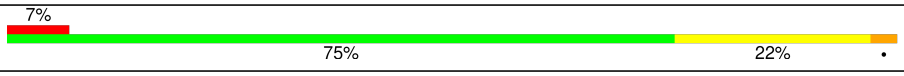
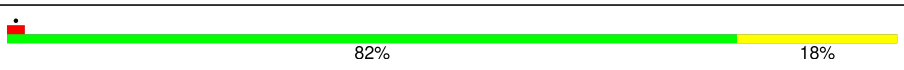
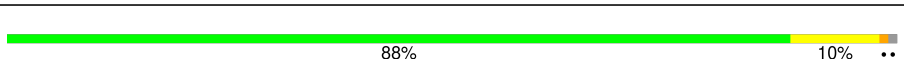
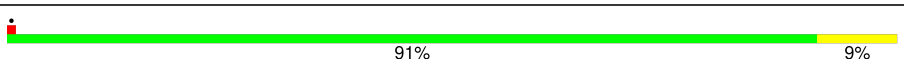
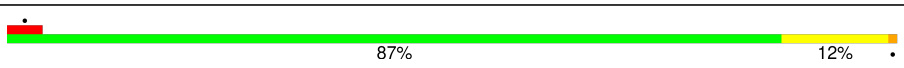
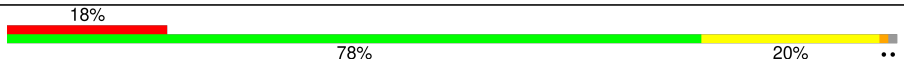
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	4434 (1.83 - 2.83)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1542	5% 75% 23% •
2	SB	241	20% 79% 15% • 5%
3	SC	233	7% 75% 15% • 9%

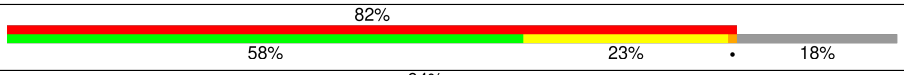
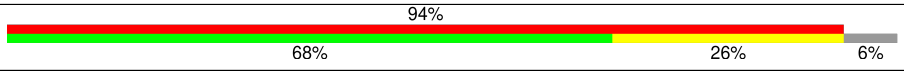
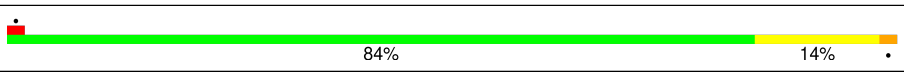
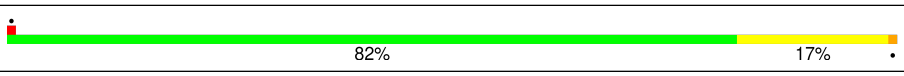
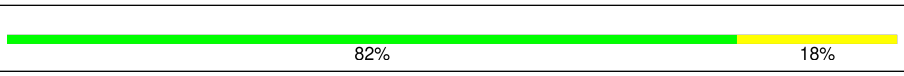
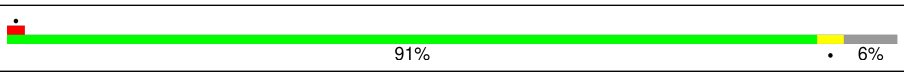
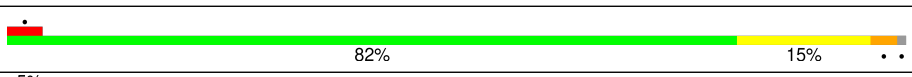
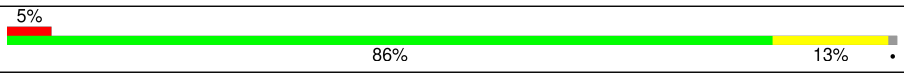
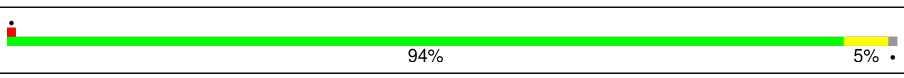
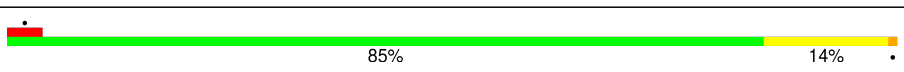
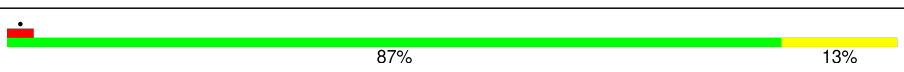
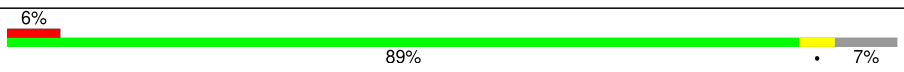
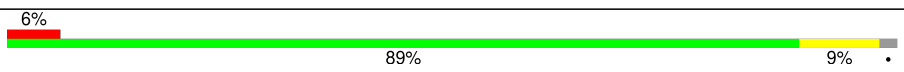
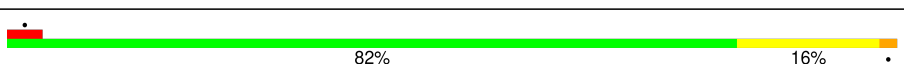
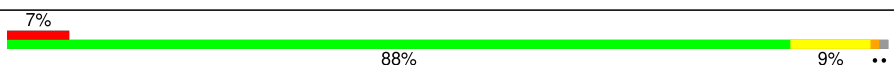
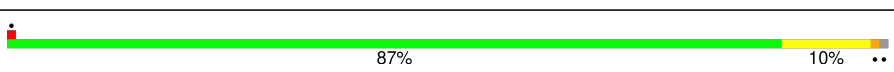
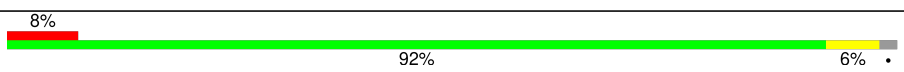
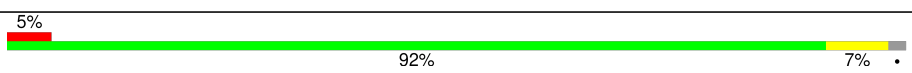
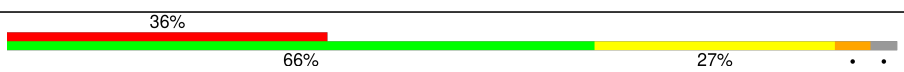
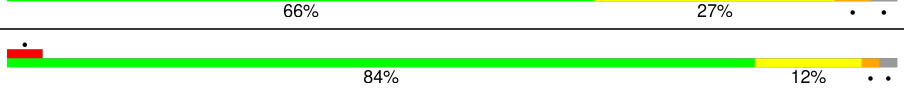
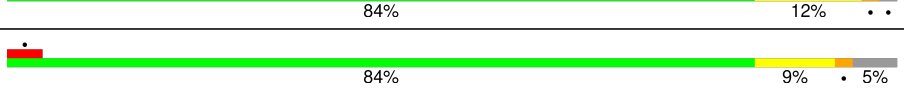
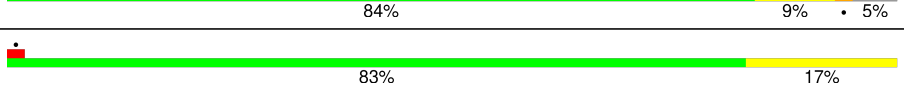
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Mol	Chain	Length	Quality of chain
4	SD	206	
5	SE	167	
6	SF	135	
7	SG	179	
8	SH	130	
9	SI	130	
10	SJ	103	
11	SK	129	
12	SL	124	
13	SM	118	
14	SN	101	
15	SO	89	
16	SP	82	
17	SQ	84	
18	SR	75	
19	SS	92	
20	ST	87	
21	SU	71	
22	mR	60	
23	23	2904	
24	5	120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

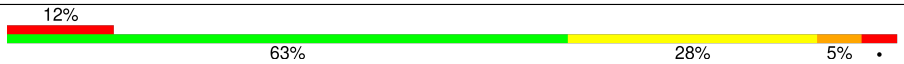
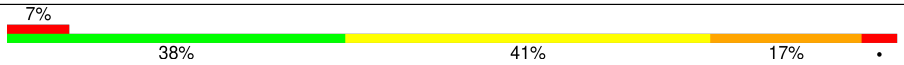
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Mol	Chain	Length	Quality of chain
29	LF	177	
30	LI	149	
31	LJ	165	
32	LK	142	
33	LM	142	
34	LN	123	
35	LO	144	
36	LP	136	
37	LQ	127	
38	LR	117	
39	LS	115	
40	LT	118	
41	LU	103	
42	LV	110	
43	LW	100	
44	LX	104	
45	LY	94	
46	La	85	
47	Lb	78	
48	Lc	63	
49	Ld	59	
50	Le	70	
51	Lf	57	
52	Lg	55	
53	Lh	46	

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Mol	Chain	Length	Quality of chain
54	Li	65	
55	Lj	38	
56	Pt	76	
57	Pp	3	
58	Dt	76	

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 149590 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	16	1542	33092	14767	6064	10719	1542	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SB	229	1787	1129	320	330	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SC	212	1666	1054	314	294	4	1	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SE	158	1166	725	220	215	6	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SG	155	Total	C	N	O	S	1	0
			1236	772	240	220	4		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SK	117	Total	C	N	O	S	1	0
			888	546	178	161	3		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SO	88	Total	C	N	O	S	2	0
			730	450	149	130	1		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SS	83	Total	C	N	O	S	0	0
			663	424	126	111	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	1	0
			598	374	125	98	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	mR	27	Total	C	N	O	P	3	0
			640	287	116	207	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	23	2904	Total	C	N	O	P	0	0
			62354	27824	11469	20157	2904		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LE	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LF	175	Total	C	N	O	S	0	0
			1313	826	241	244	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 L10.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LP	136	Total	C	N	O	S	1	0
			1086	692	209	179	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lb	77	Total	C	N	O	S	1	0
			632	393	131	106	2		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	Pt	76	Total	C	N	O	P	S	0	0
			1635	733	284	541	76	1		

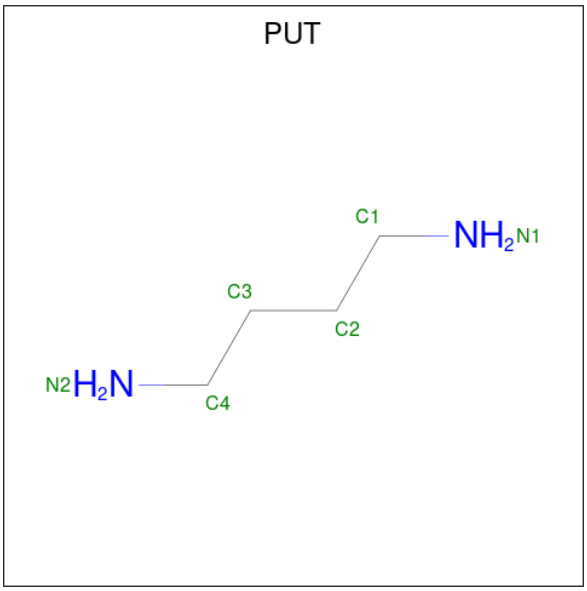
- Molecule 57 is a protein called Chains: Pp.

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

- Molecule 58 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	Dt	76	Total	C	N	O	P	S	0	0
			1638	734	291	535	76	2		

- Molecule 59 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
59	16	1	Total	C	N	0
			6	4	2	
59	16	1	Total	C	N	0
			6	4	2	
59	16	1	Total	C	N	0
			6	4	2	
59	23	1	Total	C	N	0
			6	4	2	

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Mol	Chain	Residues	Atoms	AltConf
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0
59	23	1	Total C N 6 4 2	0

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
60	16	113	Total Mg 113 113	0
60	SD	1	Total Mg 1 1	0
60	mR	1	Total Mg 1 1	0
60	23	275	Total Mg 275 275	0
60	5	5	Total Mg 5 5	0

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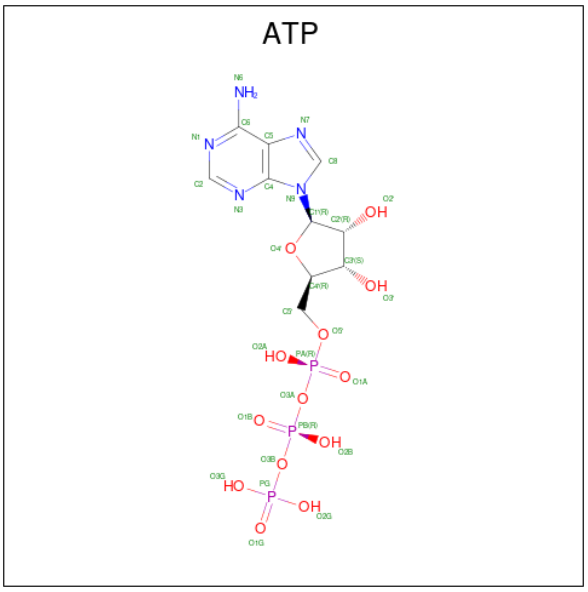
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Mol	Chain	Residues	Atoms	AltConf
60	LB	1	Total Mg 1 1	0
60	LC	1	Total Mg 1 1	0
60	LD	1	Total Mg 1 1	0
60	LE	1	Total Mg 1 1	0
60	Ld	1	Total Mg 1 1	0
60	Lf	1	Total Mg 1 1	0
60	Pt	1	Total Mg 1 1	0
60	Dt	3	Total Mg 3 3	0

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

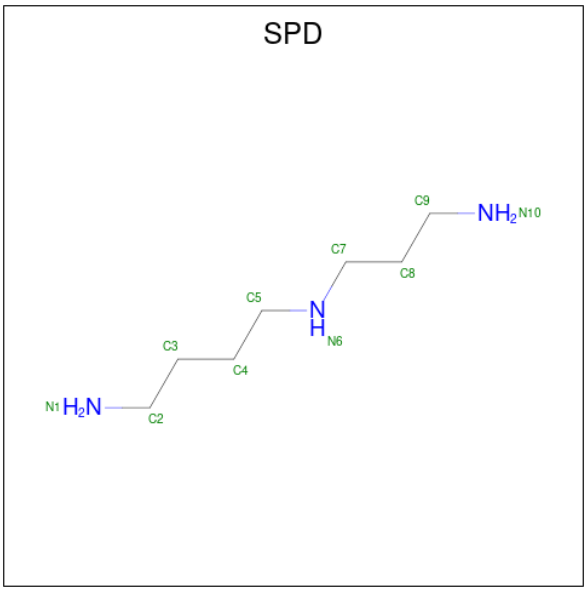
Mol	Chain	Residues	Atoms	AltConf
61	SB	1	Total Zn 1 1	0
61	Le	1	Total Zn 1 1	0
61	Lj	1	Total Zn 1 1	0

- Molecule 62 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
62	23	1	Total	C	N	O	P	0
			31	10	5	13	3	
62	23	1	Total	C	N	O	P	0
			31	10	5	13	3	
62	23	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 63 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
63	23	1	Total C N 10 7 3	0
63	23	1	Total C N 10 7 3	0
63	23	1	Total C N 10 7 3	0
63	23	1	Total C N 10 7 3	0
63	23	1	Total C N 10 7 3	0

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	AltConf
64	16	3	Total O 3 3	0
64	23	41	Total O 41 41	0
64	LB	3	Total O 3 3	0
64	LC	1	Total O 1 1	0
64	LT	1	Total O 1 1	0
64	LY	1	Total O 1 1	0

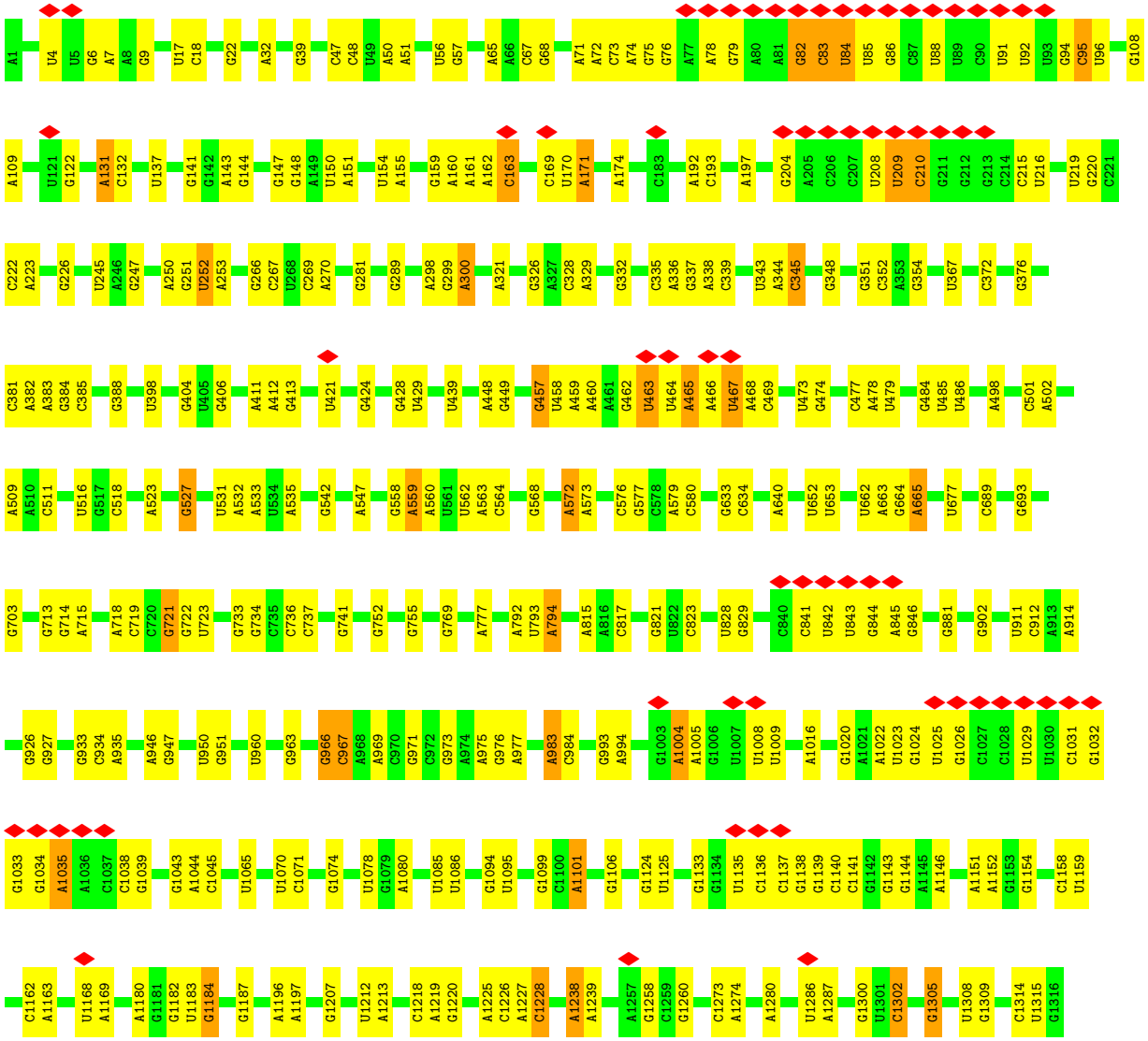
3 Residue-property plots (i)

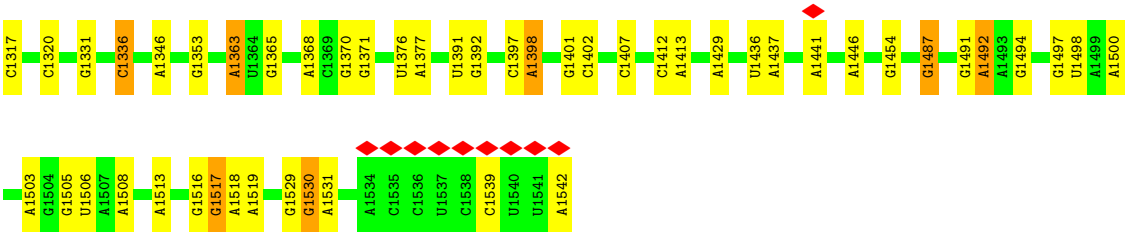
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

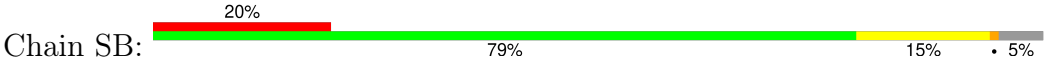
Chain 16:

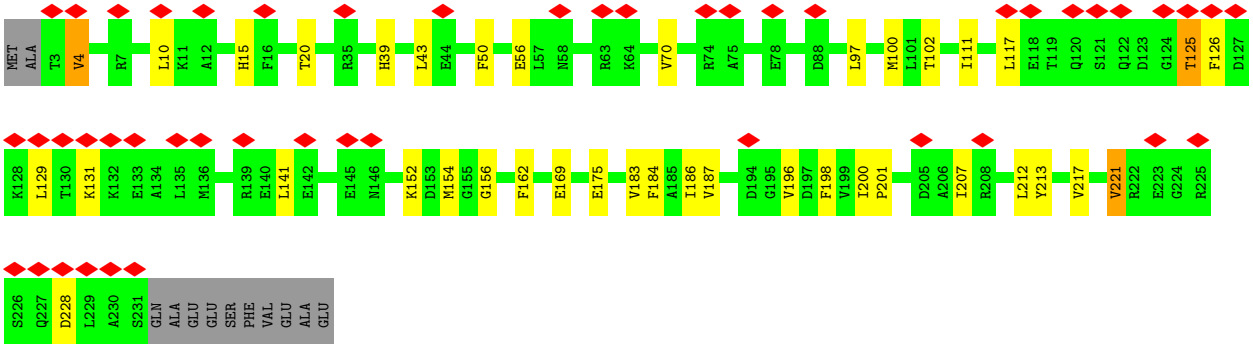




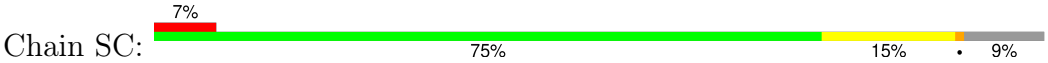


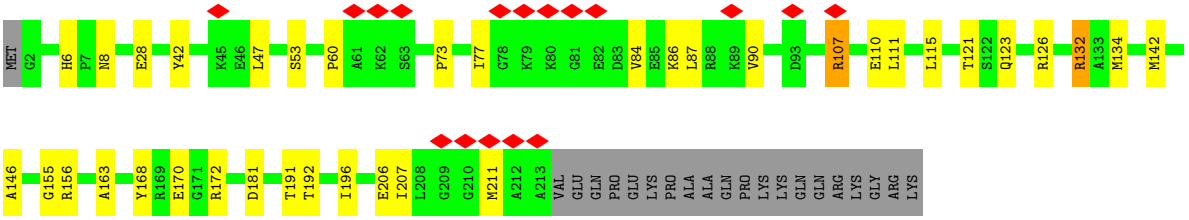
• Molecule 2: 30S ribosomal protein S2



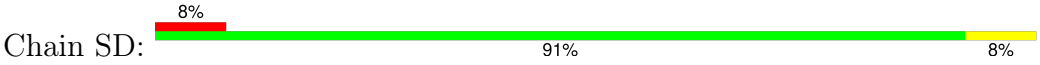


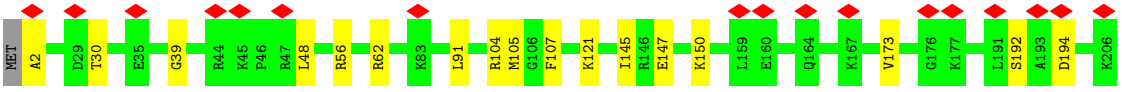
• Molecule 3: 30S ribosomal protein S3



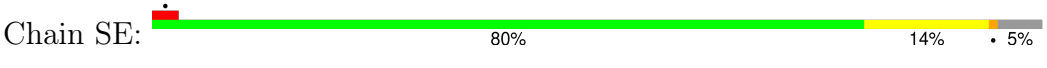


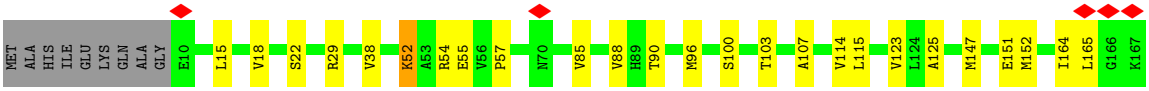
• Molecule 4: 30S ribosomal protein S4





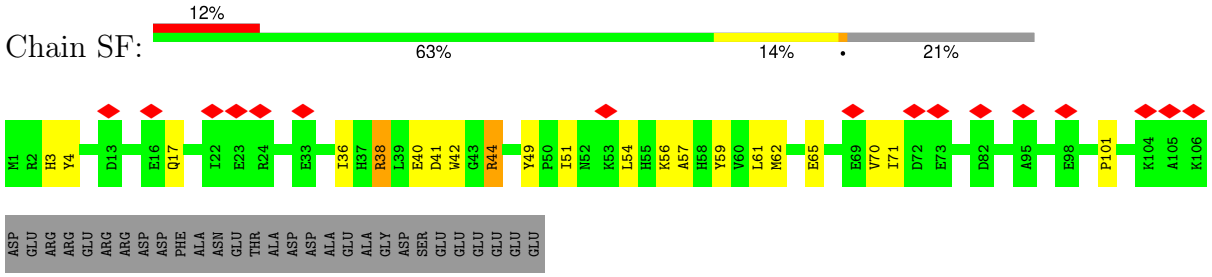
• Molecule 5: 30S ribosomal protein S5





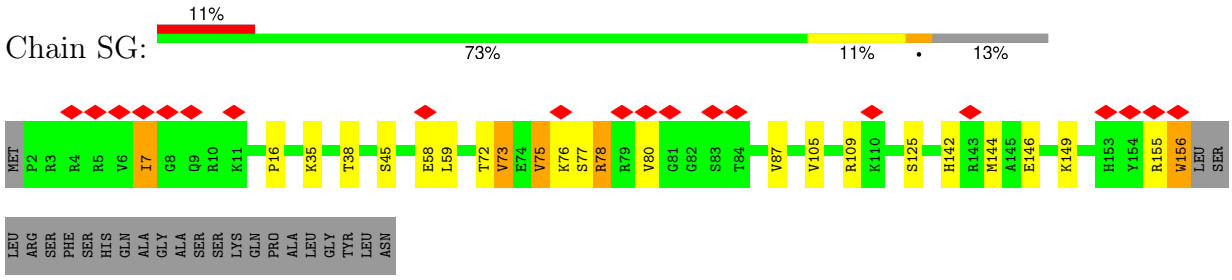
• Molecule 6: 30S ribosomal protein S6

Chain SF:



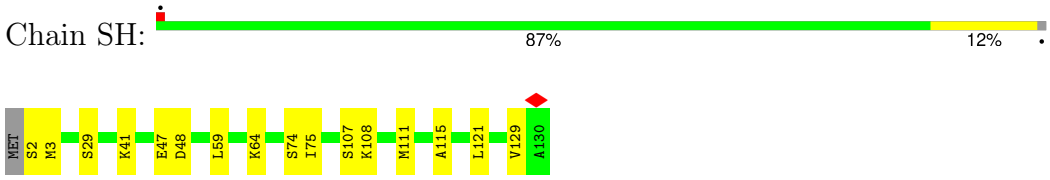
• Molecule 7: 30S ribosomal protein S7

Chain SG:



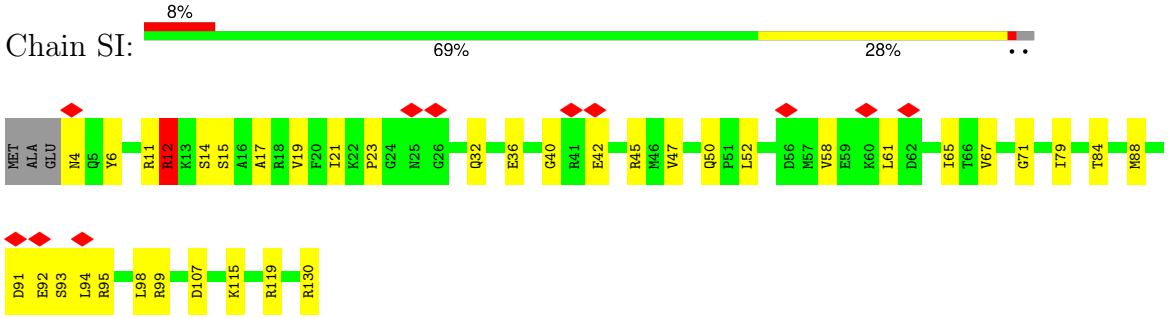
• Molecule 8: 30S ribosomal protein S8

Chain SH:



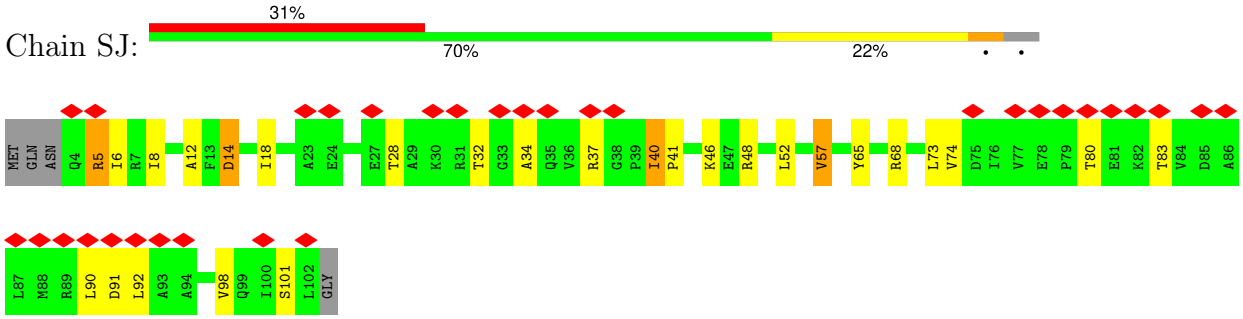
• Molecule 9: 30S ribosomal protein S9

Chain SI:



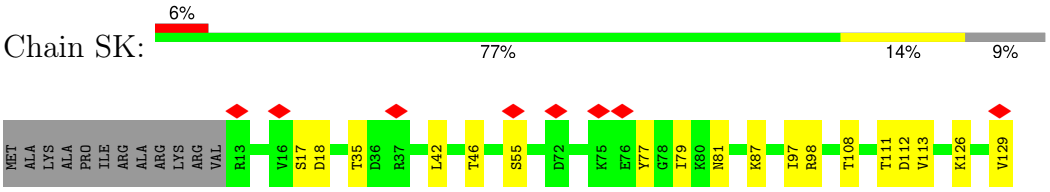
• Molecule 10: 30S ribosomal protein S10

Chain SJ:



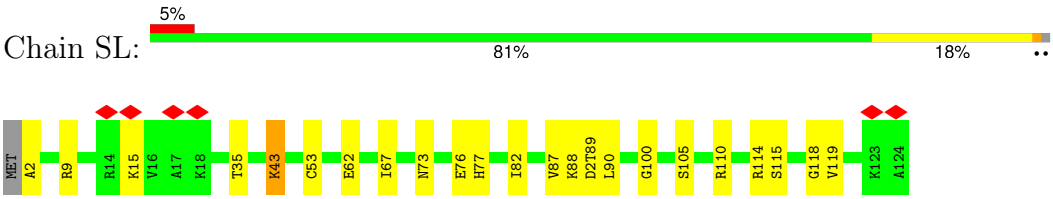
• Molecule 11: 30S ribosomal protein S11

Chain SK:



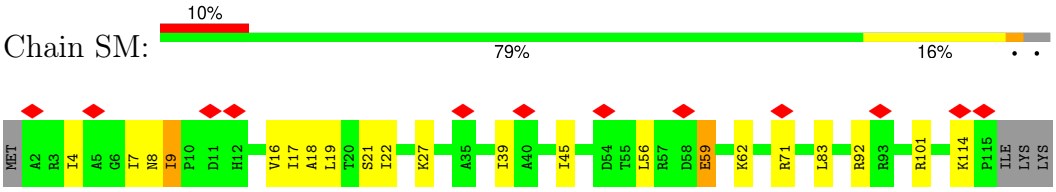
• Molecule 12: 30S ribosomal protein S12

Chain SL:



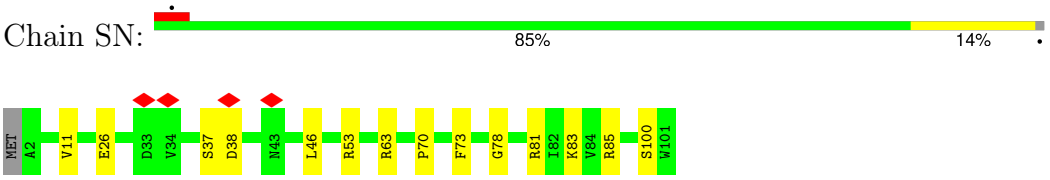
• Molecule 13: 30S ribosomal protein S13

Chain SM:



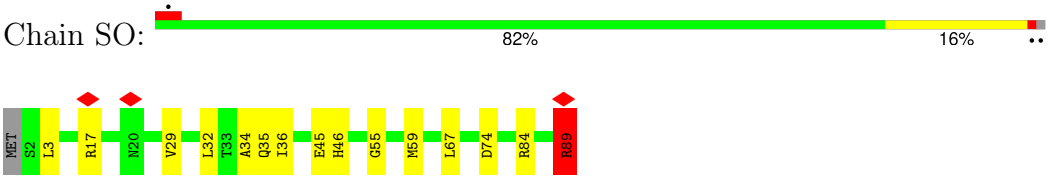
• Molecule 14: 30S ribosomal protein S14

Chain SN:



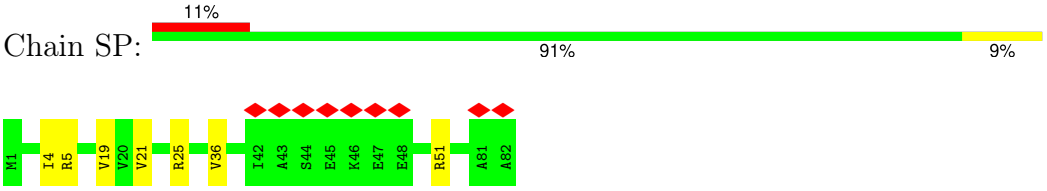
• Molecule 15: 30S ribosomal protein S15

Chain SO:



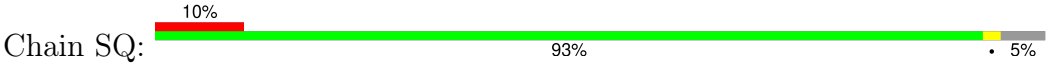
• Molecule 16: 30S ribosomal protein S16

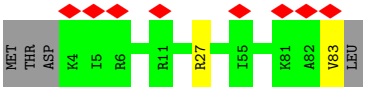
Chain SP:



• Molecule 17: 30S ribosomal protein S17

Chain SQ:

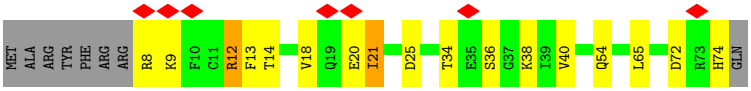




• Molecule 18: 30S ribosomal protein S18

Chain SR:

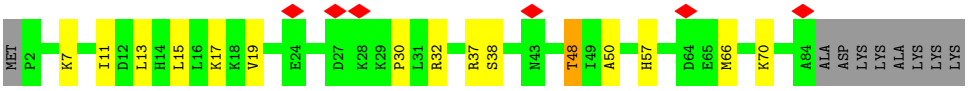




• Molecule 19: 30S ribosomal protein S19

Chain SS:

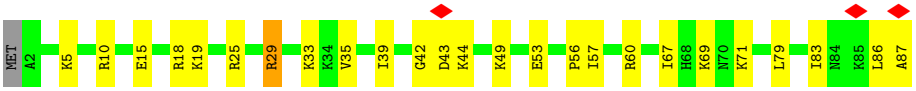




• Molecule 20: 30S ribosomal protein S20

Chain ST:

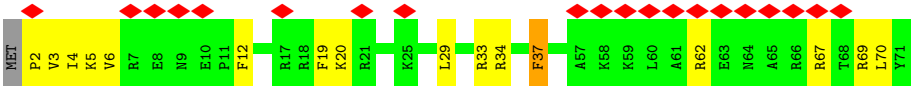




• Molecule 21: 30S ribosomal protein S21

Chain SU:

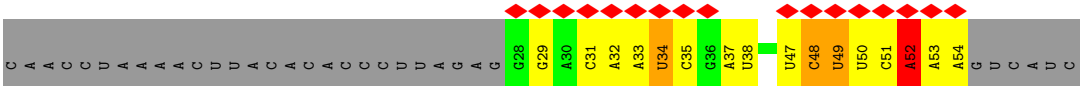




• Molecule 22: mRNA

Chain mR:

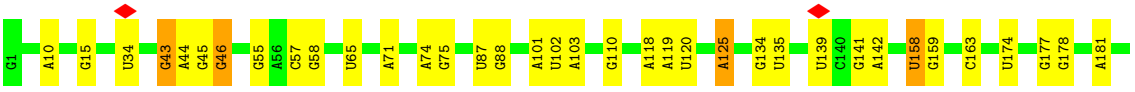


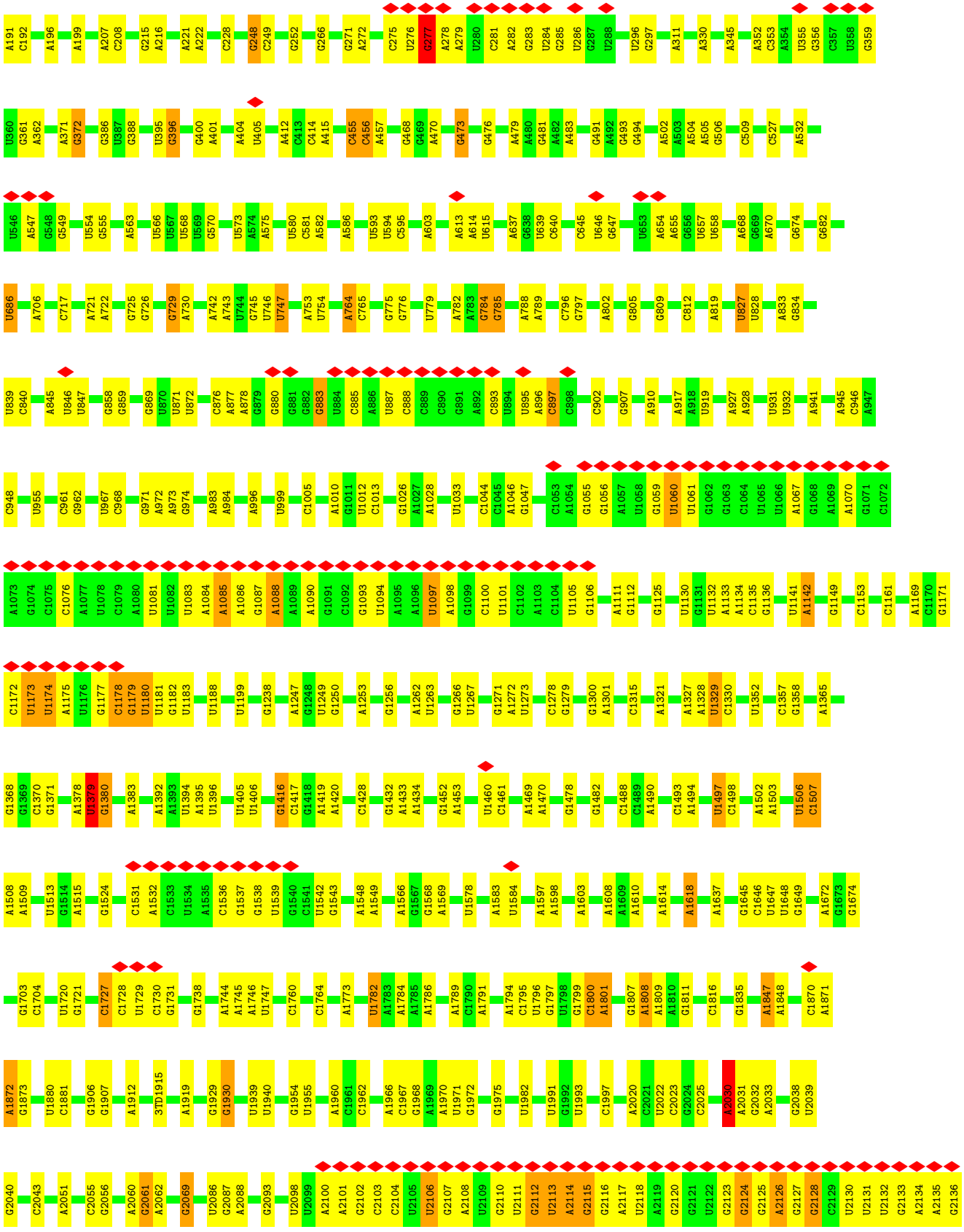


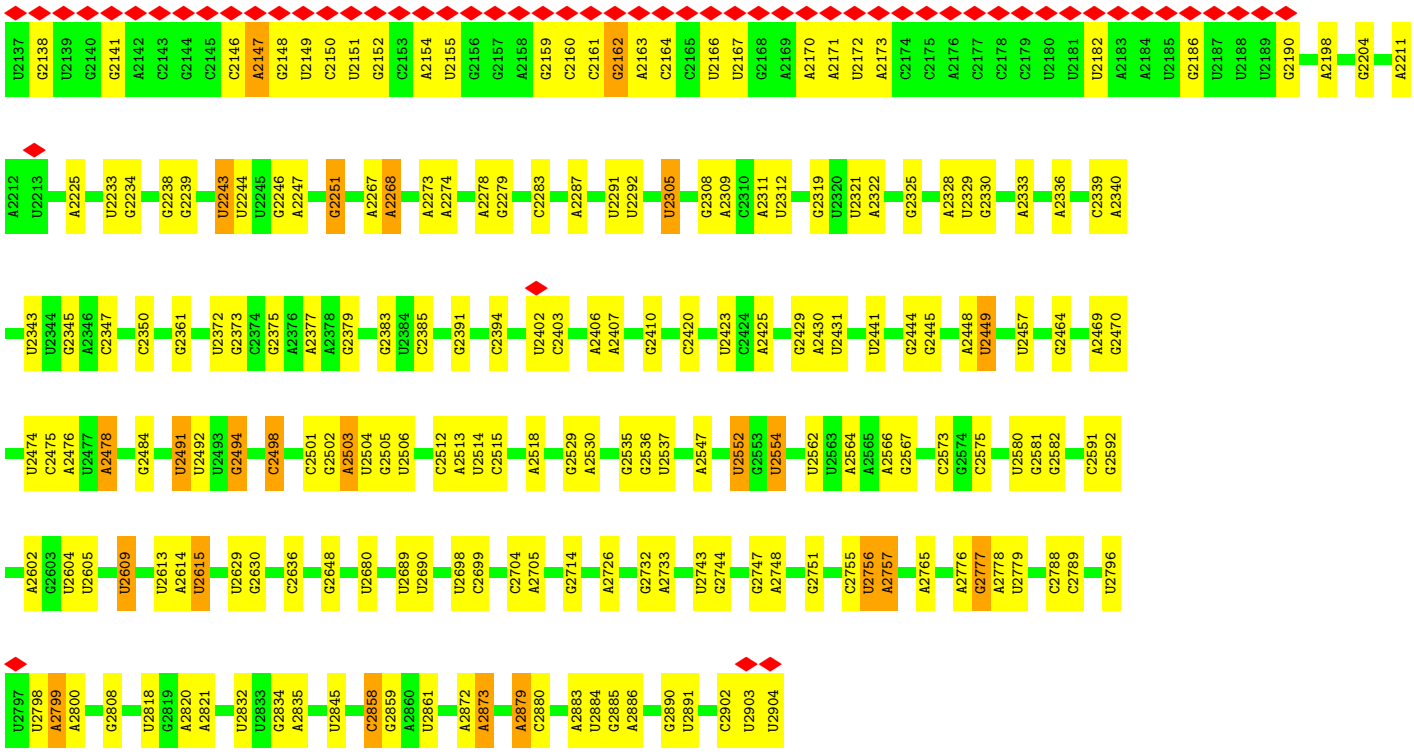
• Molecule 23: 23S rRNA

Chain 23:






A191 C192 A196 A199 A207 C208 G215 A216 A221 A222 C228 G248 C249 G252 G266 G271 A272 C275 U276 G277 A278 A279 U280 C281 A282 G283 U284 G285 U286 G287 U288 U296 G297 A311 A330 A345 A352 C353 A354 U355 G356 C357 U358 G359
U360 G361 A362 A371 G372 G386 U387 G388 U395 G396 G400 A401 A404 U405 A412 C413 C414 A415 C455 C456 A457 G468 G469 A470 G473 G476 A479 A480 G481 A482 A483 G491 A492 G493 G494 A502 A503 A504 A505 G506 C509 C527 A532
U546 A547 G548 G549 U554 G555 A563 U566 U567 U568 U569 G570 U573 A574 A575 U580 C581 A582 A586 U593 U594 C595 A603 A613 A614 U615 A637 G638 U639 C640 C645 U646 G647 U653 A654 A655 G656 U657 U658 A668 G669 A670 G674 G682
U686 A706 C717 A721 A722 G725 G726 G729 A730 A742 A743 U744 G745 U746 U747 A753 U754 A764 C765 G775 G776 U779 A782 A783 G784 G785 A788 A789 C796 G797 A802 G805 G809 C812 A819 U827 U828 A833 G834
U839 C840 A845 U846 U847 G858 G859 G869 U870 U871 U872 C876 A877 A878 G879 G880 G881 G882 G883 U884 C885 A886 U887 C888 C889 C890 G891 A892 C893 U894 U895 A896 C897 C898 C902 G907 A910 A917 A918 U919 A927 A928 U931 U932 A941 A945 C946 A947
C948 U955 C961 G962 U967 C968 G971 A972 A973 G974 A983 A984 A996 U999 C1005 A1010 G1011 U1012 C1013 G1026 A1027 A1028 U1033 C1044 C1045 A1046 G1047 C1053 A1054 G1055 G1056 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072
A1073 G1074 C1075 C1076 A1077 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 A1111 G1112 G1125 U1130 C1131 U1132 A1133 A1134 C1135 G1136 U1141 A1142 G1149 C1153 C1161 A1169 C1170 G1171
C1172 U1173 U1174 A1175 A1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1188 U1199 G1238 A1247 G1248 U1249 G1250 A1253 G1256 A1262 U1263 G1266 U1267 G1271 A1272 U1273 C1278 G1279 G1300 A1301 C1315 A1321 A1327 A1328 U1329 C1330 U1352 C1357 G1358 A1365
G1368 G1369 C1370 G1371 A1378 U1379 G1380 A1383 A1392 A1393 U1394 A1395 U1396 U1405 U1406 G1416 C1417 G1418 A1419 A1420 C1428 G1432 A1433 A1434 G1452 A1453 U1460 C1461 A1469 A1470 G1478 G1482 C1488 C1489 A1490 C1493 A1494 U1497 C1498 A1502 A1503 U1506 C1507
A1508 A1509 U1513 G1514 A1515 G1524 C1531 A1532 C1533 U1534 A1535 C1536 G1537 G1538 U1539 G1540 C1541 U1542 G1543 A1548 A1549 A1566 G1567 G1568 A1569 U1578 A1583 U1584 A1597 A1598 A1603 A1608 A1609 A1610 A1614 A1618 A1637 G1645 C1646 U1647 U1648 G1649 A1672 G1673 G1674
G1703 C1704 U1720 G1721 C1727 C1728 U1729 C1730 G1731 G1738 A1744 A1745 A1746 U1747 C1760 C1764 A1773 U1782 A1783 A1784 A1785 A1786 A1789 C1790 A1791 A1794 C1795 U1796 G1797 U1798 G1799 C1800 A1801 G1807 A1808 A1809 A1810 G1811 C1816 G1835 A1847 A1848 C1870 A1871
A1872 G1873 U1880 C1881 G1906 G1907 A1912 3TD1915 A1919 G1929 G1930 U1939 U1940 G1954 U1955 A1960 C1961 C1962 A1966 C1967 G1968 A1969 A1970 U1971 G1972 G1975 U1982 U1991 G1992 U1993 C1997 A2020 C2021 U2022 C2023 G2024 C2025 A2030 A2031 G2032 A2033 G2038 U2039
G2040 C2043 A2051 C2055 G2056 A2060 G2061 A2062 G2069 U2086 G2087 A2088 G2093 U2098 U2099 A2100 A2101 G2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 C2129 U2130 U2131 U2132 G2133 A2134 A2135 G2136



• Molecule 24: 5S rRNA

Chain 5:

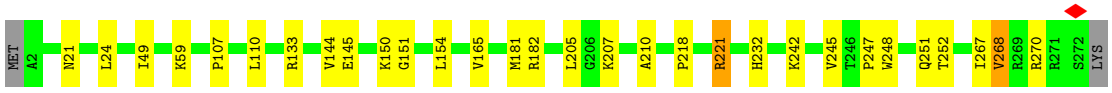




• Molecule 25: 50S ribosomal protein L2

Chain LB:





• Molecule 26: 50S ribosomal protein L3

Chain LC:

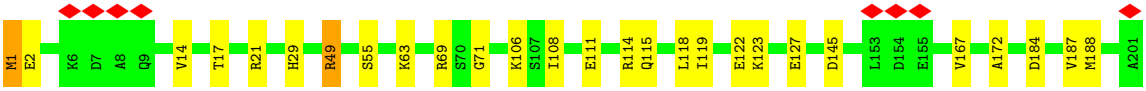




• Molecule 27: 50S ribosomal protein L4

Chain LD:

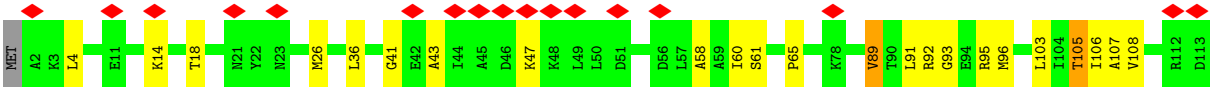


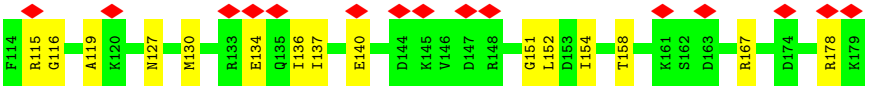


• Molecule 28: 50S ribosomal protein L5

Chain LE:



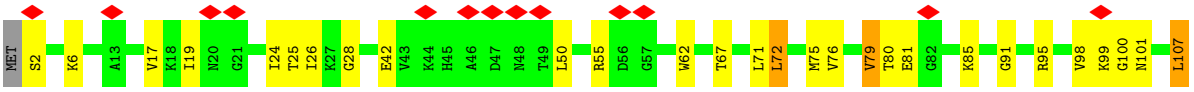


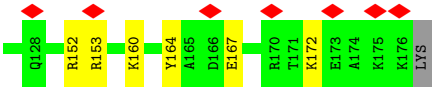


• Molecule 29: 50S ribosomal protein L6

Chain LF:



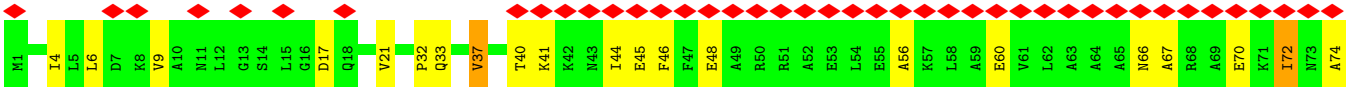


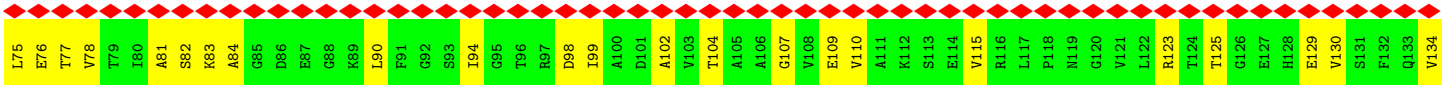


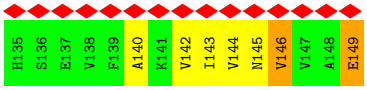
• Molecule 30: 50S ribosomal protein L9

Chain LI:





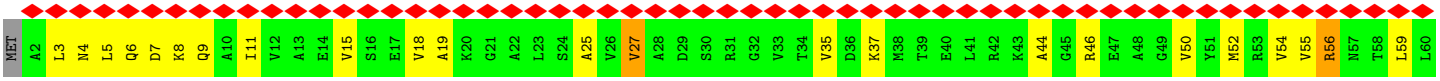


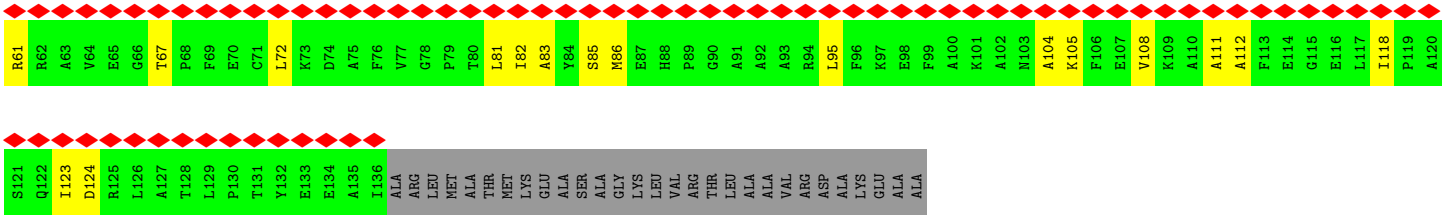


• Molecule 31: 50S ribosomal protein L10

Chain LJ:

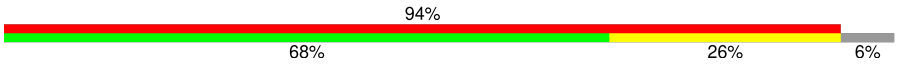


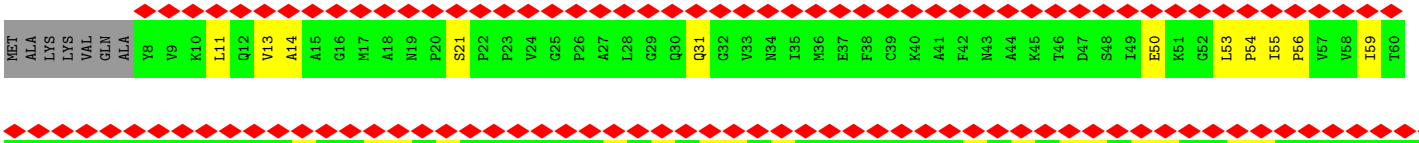




• Molecule 32: 50S ribosomal protein L11

Chain LK:

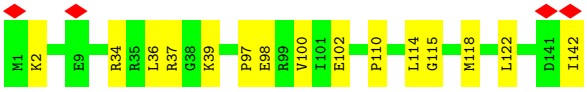




• Molecule 33: 50S ribosomal protein L13

Chain LM:





• Molecule 34: 50S ribosomal protein L14

Chain LN:

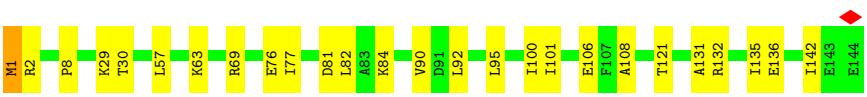




• Molecule 35: 50S ribosomal protein L15

Chain LO:

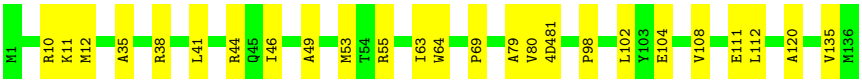




• Molecule 36: 50S ribosomal protein L16

Chain LP:

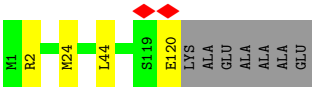




• Molecule 37: 50S ribosomal protein L17

Chain LQ:

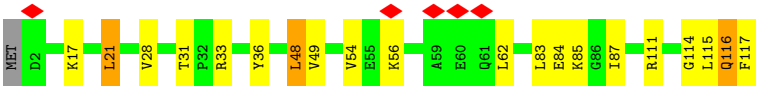




• Molecule 38: 50S ribosomal protein L18

Chain LR:

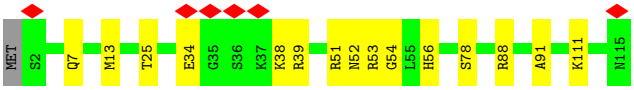




• Molecule 39: 50S ribosomal protein L19

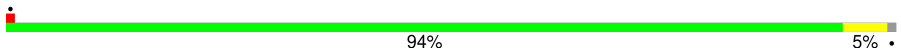
Chain LS:

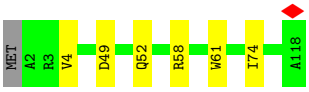




• Molecule 40: 50S ribosomal protein L20

Chain LT:

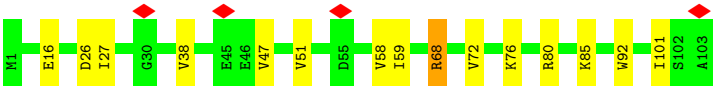




• Molecule 41: 50S ribosomal protein L21

Chain LU:

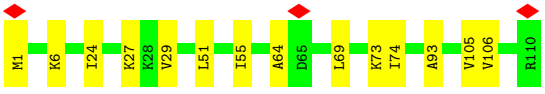




• Molecule 42: 50S ribosomal protein L22

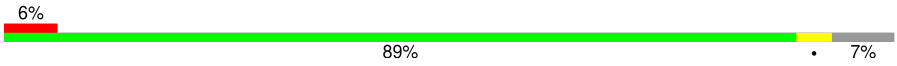
Chain LV:

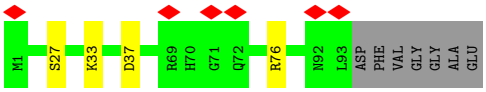




• Molecule 43: 50S ribosomal protein L23

Chain LW:

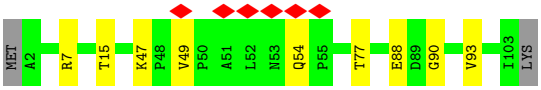




• Molecule 44: 50S ribosomal protein L24

Chain LX:

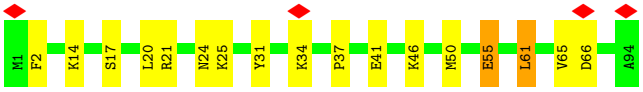




• Molecule 45: 50S ribosomal protein L25

Chain LY:





• Molecule 46: 50S ribosomal protein L27

Chain La:

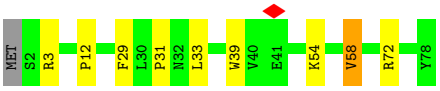




• Molecule 47: 50S ribosomal protein L28

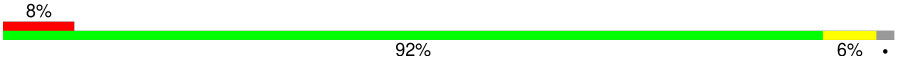
Chain Lb:

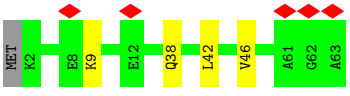




• Molecule 48: 50S ribosomal protein L29

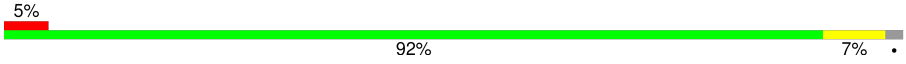
Chain Lc:

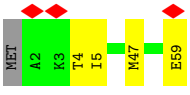




• Molecule 49: 50S ribosomal protein L30

Chain Ld:

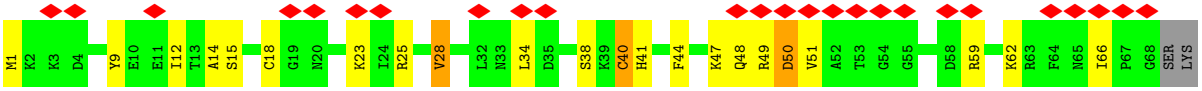




• Molecule 50: 50S ribosomal protein L31

Chain Le:

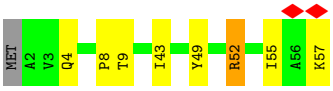




• Molecule 51: 50S ribosomal protein L32

Chain Lf:

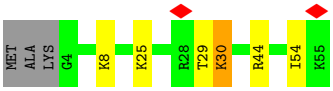




• Molecule 52: 50S ribosomal protein L33

Chain Lg:

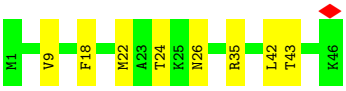




• Molecule 53: 50S ribosomal protein L34

Chain Lh:





• Molecule 54: 50S ribosomal protein L35

Chain Li:

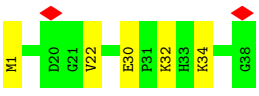




• Molecule 55: 50S ribosomal protein L36

Chain Lj:

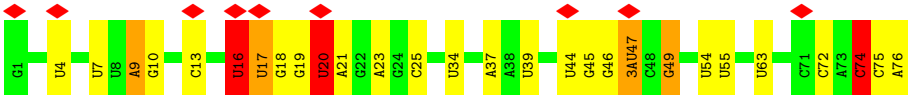




• Molecule 56: tRNA

Chain Pt:





- Molecule 57: Chains: Pp

Chain Pp:

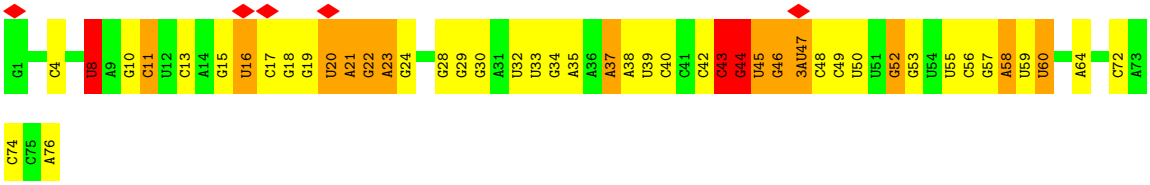




- Molecule 58: tRNA

Chain Dt:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109769	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 ($e^-/Å^2$)	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	0.235	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	610.55994, 610.55994, 610.55994	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.23	0/36772	0.30	3/57358 (0.0%)
2	SB	0.43	0/1818	0.73	0/2450
3	SC	0.51	2/1696 (0.1%)	0.74	7/2284 (0.3%)
4	SD	0.33	0/1665	0.58	0/2227
5	SE	0.38	0/1179	0.55	0/1584
6	SF	0.30	0/881	0.52	0/1189
7	SG	0.72	2/1257 (0.2%)	0.93	3/1686 (0.2%)
8	SH	0.30	0/989	0.55	0/1326
9	SI	0.46	0/1034	0.84	4/1375 (0.3%)
10	SJ	0.53	0/805	0.86	1/1089 (0.1%)
11	SK	0.36	0/904	0.54	0/1219
12	SL	0.42	0/960	0.64	0/1286
13	SM	0.57	0/892	0.92	0/1193
14	SN	0.38	0/817	0.61	0/1088
15	SO	0.32	0/740	0.64	0/986
16	SP	0.36	0/659	0.53	0/884
17	SQ	0.32	0/657	0.56	0/881
18	SR	0.67	2/564 (0.4%)	0.91	1/756 (0.1%)
19	SS	0.47	0/680	0.78	1/915 (0.1%)
20	ST	0.21	0/676	0.40	0/895
21	SU	0.78	4/610 (0.7%)	0.95	4/808 (0.5%)
22	mR	0.41	0/716	0.83	3/1113 (0.3%)
23	23	0.25	0/69305	0.31	11/108114 (0.0%)
24	5	0.22	0/2873	0.26	0/4478
25	LB	0.31	0/2121	0.47	1/2852 (0.0%)
26	LC	0.38	0/1586	0.60	0/2134
27	LD	0.32	0/1571	0.49	2/2113 (0.1%)
28	LE	0.44	0/1444	0.78	3/1937 (0.2%)
29	LF	0.21	0/1333	0.44	0/1805
30	LI	0.62	0/1122	1.01	1/1515 (0.1%)
31	LJ	0.52	0/1037	0.78	0/1400

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LK	0.57	0/993	0.82	1/1341 (0.1%)
33	LM	0.35	0/1152	0.52	0/1551
34	LN	0.42	0/956	0.63	0/1279
35	LO	0.29	0/1062	0.50	0/1413
36	LP	0.21	0/1092	0.32	0/1457
37	LQ	0.34	0/973	0.46	0/1301
38	LR	0.38	0/902	0.67	0/1209
39	LS	0.34	0/929	0.53	0/1242
40	LT	0.33	0/960	0.45	0/1278
41	LU	0.40	0/829	0.65	0/1107
42	LV	0.33	0/864	0.47	1/1156 (0.1%)
43	LW	0.38	0/744	0.60	0/994
44	LX	0.39	0/787	0.65	2/1051 (0.2%)
45	LY	0.38	0/766	0.60	0/1025
46	La	0.37	0/642	0.59	1/848 (0.1%)
47	Lb	0.30	0/646	0.50	0/863
48	Lc	0.42	0/502	0.73	2/667 (0.3%)
49	Ld	0.29	0/453	0.51	0/605
50	Le	0.65	0/543	1.07	1/726 (0.1%)
51	Lf	0.31	0/450	0.56	0/599
52	Lg	0.66	0/434	0.97	1/576 (0.2%)
53	Lh	0.31	0/380	0.46	0/498
54	Li	0.38	0/513	0.60	0/676
55	Lj	0.20	0/303	0.31	0/397
56	Pt	0.32	1/1599 (0.1%)	0.45	1/2486 (0.0%)
57	Pp	0.43	0/28	0.78	0/34
58	Dt	0.75	2/1628 (0.1%)	0.99	19/2531 (0.8%)
All	All	0.32	13/160493 (0.0%)	0.44	74/239850 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	SC	0	1
4	SD	0	1
5	SE	0	1
10	SJ	0	2
11	SK	0	1
15	SO	0	4
16	SP	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
20	ST	0	2
25	LB	0	1
27	LD	0	1
29	LF	0	1
34	LN	0	1
35	LO	0	1
44	LX	0	1
46	La	0	1
50	Le	0	1
All	All	0	21

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	SG	78[A]	ARG	C-O	11.55	1.37	1.24
7	SG	78[B]	ARG	C-O	11.55	1.37	1.24
3	SC	132[A]	ARG	C-O	8.81	1.34	1.24
3	SC	132[B]	ARG	C-O	8.81	1.34	1.24
21	SU	37[A]	PHE	C-O	8.70	1.35	1.23

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	SC	132[A]	ARG	CA-C-O	11.16	132.38	120.55
3	SC	132[B]	ARG	CA-C-O	11.16	132.38	120.55
1	16	252	U	C2'-C3'-O3'	9.76	128.34	113.70
21	SU	37[A]	PHE	CA-C-O	9.41	131.74	121.11
21	SU	37[B]	PHE	CA-C-O	9.41	131.74	121.11

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	SC	107	ARG	Sidechain
4	SD	104	ARG	Sidechain
5	SE	54	ARG	Sidechain
10	SJ	37	ARG	Sidechain
10	SJ	48	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	16	33092	0	16676	126	0
2	SB	1787	0	1812	27	0
3	SC	1666	0	1745	22	0
4	SD	1643	0	1707	9	0
5	SE	1166	0	1212	16	0
6	SF	862	0	864	14	0
7	SG	1236	0	1290	9	0
8	SH	979	0	1031	9	0
9	SI	1022	0	1070	17	0
10	SJ	795	0	836	21	0
11	SK	888	0	899	10	0
12	SL	957	0	1017	10	0
13	SM	883	0	941	14	0
14	SN	805	0	844	8	0
15	SO	730	0	759	8	0
16	SP	649	0	666	4	0
17	SQ	648	0	691	0	0
18	SR	555	0	578	7	0
19	SS	663	0	688	10	0
20	ST	670	0	719	17	0
21	SU	598	0	638	12	0
22	mR	640	0	323	13	0
23	23	62354	0	31384	212	0
24	5	2570	0	1301	6	0
25	LB	2082	0	2154	20	0
26	LC	1565	0	1616	13	0
27	LD	1552	0	1619	21	0
28	LE	1420	0	1457	25	0
29	LF	1313	0	1358	20	0
30	LI	1111	0	1148	26	0
31	LJ	1023	0	1050	21	0
32	LK	979	0	1028	21	0
33	LM	1129	0	1162	8	0
34	LN	947	0	1023	14	0
35	LO	1053	0	1129	21	0
36	LP	1086	0	1167	15	0
37	LQ	960	0	1000	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	LR	892	0	923	11	0
39	LS	917	0	962	9	0
40	LT	947	0	1019	3	0
41	LU	816	0	839	8	0
42	LV	857	0	922	8	0
43	LW	738	0	807	2	0
44	LX	779	0	831	3	0
45	LY	753	0	780	11	0
46	La	634	0	653	4	0
47	Lb	632	0	659	5	0
48	Lc	501	0	531	1	0
49	Ld	449	0	488	3	0
50	Le	533	0	530	14	0
51	Lf	444	0	458	6	0
52	Lg	427	0	464	4	0
53	Lh	377	0	418	5	0
54	Li	504	0	572	4	0
55	Lj	302	0	340	3	0
56	Pt	1635	0	840	13	0
57	Pp	28	0	33	0	0
58	Dt	1638	0	844	8	0
59	16	18	0	36	0	0
59	23	90	0	180	0	0
60	16	113	0	0	0	0
60	23	275	0	0	0	0
60	5	5	0	0	0	0
60	Dt	3	0	0	0	0
60	LB	1	0	0	0	0
60	LC	1	0	0	0	0
60	LD	1	0	0	0	0
60	LE	1	0	0	0	0
60	Ld	1	0	0	0	0
60	Lf	1	0	0	0	0
60	Pt	1	0	0	0	0
60	SD	1	0	0	0	0
60	mR	1	0	0	0	0
61	Le	1	0	0	0	0
61	Lj	1	0	0	0	0
61	SB	1	0	0	0	0
62	23	93	0	36	0	0
63	23	50	0	95	2	0
64	16	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	23	41	0	0	0	0
64	LB	3	0	0	0	0
64	LC	1	0	0	0	0
64	LT	1	0	0	0	0
64	LY	1	0	0	0	0
All	All	149590	0	100862	843	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 843 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:Pt:20:H2U:H4'	56:Pt:20:H2U:OP1	1.56	1.05
56:Pt:25:C:H5"	56:Pt:25:C:H6	1.32	0.95
34:LN:123:LEU:HD12	34:LN:123:LEU:OXT	1.74	0.87
35:LO:92:LEU:HD21	35:LO:106:GLU:HA	1.60	0.83
23:23:2377:A:O2'	38:LR:117:PHE:OXT	1.97	0.82

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SB	227/241 (94%)	217 (96%)	10 (4%)	0	100	100
3	SC	211/233 (91%)	208 (99%)	3 (1%)	0	100	100
4	SD	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
5	SE	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
6	SF	104/135 (77%)	102 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	SG	154/179 (86%)	150 (97%)	4 (3%)	0	100	100
8	SH	127/130 (98%)	127 (100%)	0	0	100	100
9	SI	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
10	SJ	97/103 (94%)	93 (96%)	4 (4%)	0	100	100
11	SK	116/129 (90%)	110 (95%)	6 (5%)	0	100	100
12	SL	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
13	SM	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
14	SN	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	SO	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
16	SP	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
17	SQ	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
18	SR	65/75 (87%)	63 (97%)	2 (3%)	0	100	100
19	SS	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
20	ST	84/87 (97%)	84 (100%)	0	0	100	100
21	SU	69/71 (97%)	69 (100%)	0	0	100	100
25	LB	269/273 (98%)	265 (98%)	4 (2%)	0	100	100
26	LC	207/209 (99%)	205 (99%)	2 (1%)	0	100	100
27	LD	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
28	LE	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
29	LF	173/177 (98%)	169 (98%)	4 (2%)	0	100	100
30	LI	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
31	LJ	133/165 (81%)	123 (92%)	10 (8%)	0	100	100
32	LK	132/142 (93%)	123 (93%)	9 (7%)	0	100	100
33	LM	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
34	LN	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
35	LO	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
36	LP	134/136 (98%)	134 (100%)	0	0	100	100
37	LQ	118/127 (93%)	115 (98%)	3 (2%)	0	100	100
38	LR	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
39	LS	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
40	LT	115/118 (98%)	115 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	LU	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
42	LV	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
43	LW	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
44	LX	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
45	LY	92/94 (98%)	92 (100%)	0	0	100	100
46	La	82/85 (96%)	81 (99%)	1 (1%)	0	100	100
47	Lb	76/78 (97%)	74 (97%)	2 (3%)	0	100	100
48	Lc	60/63 (95%)	60 (100%)	0	0	100	100
49	Ld	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	Le	66/70 (94%)	61 (92%)	5 (8%)	0	100	100
51	Lf	54/57 (95%)	54 (100%)	0	0	100	100
52	Lg	50/55 (91%)	50 (100%)	0	0	100	100
53	Lh	44/46 (96%)	44 (100%)	0	0	100	100
54	Li	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
55	Lj	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
57	Pp	1/3 (33%)	1 (100%)	0	0	100	100
All	All	5905/6223 (95%)	5741 (97%)	164 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SB	190/199 (96%)	187 (98%)	3 (2%)	55	67
3	SC	173/190 (91%)	166 (96%)	7 (4%)	28	36
4	SD	172/173 (99%)	170 (99%)	2 (1%)	63	75
5	SE	120/126 (95%)	115 (96%)	5 (4%)	26	34
6	SF	92/116 (79%)	87 (95%)	5 (5%)	20	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	SG	129/147 (88%)	113 (88%)	16 (12%)	4 3
8	SH	104/105 (99%)	103 (99%)	1 (1%)	68 79
9	SI	105/107 (98%)	96 (91%)	9 (9%)	10 10
10	SJ	87/90 (97%)	83 (95%)	4 (5%)	24 31
11	SK	91/99 (92%)	85 (93%)	6 (7%)	15 17
12	SL	102/103 (99%)	95 (93%)	7 (7%)	14 15
13	SM	92/96 (96%)	85 (92%)	7 (8%)	12 13
14	SN	83/84 (99%)	79 (95%)	4 (5%)	23 29
15	SO	78/77 (101%)	75 (96%)	3 (4%)	29 38
16	SP	65/65 (100%)	65 (100%)	0	100 100
17	SQ	74/78 (95%)	72 (97%)	2 (3%)	39 51
18	SR	58/65 (89%)	51 (88%)	7 (12%)	5 4
19	SS	72/79 (91%)	71 (99%)	1 (1%)	59 71
20	ST	65/66 (98%)	64 (98%)	1 (2%)	57 69
21	SU	61/61 (100%)	55 (90%)	6 (10%)	7 7
25	LB	216/218 (99%)	214 (99%)	2 (1%)	70 80
26	LC	164/164 (100%)	161 (98%)	3 (2%)	51 64
27	LD	165/165 (100%)	160 (97%)	5 (3%)	36 47
28	LE	149/150 (99%)	146 (98%)	3 (2%)	48 61
29	LF	136/138 (99%)	130 (96%)	6 (4%)	25 33
30	LI	114/114 (100%)	96 (84%)	18 (16%)	2 2
31	LJ	103/123 (84%)	90 (87%)	13 (13%)	4 3
32	LK	104/110 (94%)	100 (96%)	4 (4%)	29 38
33	LM	116/116 (100%)	114 (98%)	2 (2%)	53 66
34	LN	104/104 (100%)	101 (97%)	3 (3%)	37 48
35	LO	103/103 (100%)	100 (97%)	3 (3%)	37 48
36	LP	109/108 (101%)	107 (98%)	2 (2%)	51 64
37	LQ	100/103 (97%)	98 (98%)	2 (2%)	48 61
38	LR	86/87 (99%)	80 (93%)	6 (7%)	14 15
39	LS	99/100 (99%)	96 (97%)	3 (3%)	36 47
40	LT	89/90 (99%)	88 (99%)	1 (1%)	65 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
41	LU	84/84 (100%)	80 (95%)	4 (5%)	23 29
42	LV	93/93 (100%)	92 (99%)	1 (1%)	65 77
43	LW	80/84 (95%)	77 (96%)	3 (4%)	29 38
44	LX	83/85 (98%)	82 (99%)	1 (1%)	63 75
45	LY	78/78 (100%)	74 (95%)	4 (5%)	21 26
46	La	62/63 (98%)	61 (98%)	1 (2%)	55 67
47	Lb	68/68 (100%)	66 (97%)	2 (3%)	37 48
48	Lc	54/55 (98%)	54 (100%)	0	100 100
49	Ld	48/49 (98%)	48 (100%)	0	100 100
50	Le	60/62 (97%)	55 (92%)	5 (8%)	10 11
51	Lf	47/48 (98%)	46 (98%)	1 (2%)	47 60
52	Lg	47/49 (96%)	46 (98%)	1 (2%)	47 60
53	Lh	38/38 (100%)	37 (97%)	1 (3%)	40 53
54	Li	51/52 (98%)	51 (100%)	0	100 100
55	Lj	34/34 (100%)	33 (97%)	1 (3%)	37 48
57	Pp	3/3 (100%)	2 (67%)	1 (33%)	0 0
All	All	4900/5064 (97%)	4702 (96%)	198 (4%)	29 36

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	LI	21	VAL
31	LJ	56	ARG
30	LI	72	ILE
30	LI	145	ASN
33	LM	2	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
27	LD	9	GLN
47	Lb	36	HIS
29	LF	45	HIS
46	La	57	HIS
40	LT	44	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1541/1542 (99%)	224 (14%)	13 (0%)
22	mR	23/60 (38%)	12 (52%)	0
23	23	2903/2904 (99%)	447 (15%)	27 (0%)
24	5	119/120 (99%)	14 (11%)	1 (0%)
56	Pt	75/76 (98%)	16 (21%)	0
58	Dt	75/76 (98%)	31 (41%)	0
All	All	4736/4778 (99%)	744 (15%)	41 (0%)

5 of 744 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	4	U
1	16	9	G
1	16	22	G
1	16	32	A
1	16	39	G

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	23	1379	U
23	23	2491	U
23	23	1416	G
23	23	2116	G
23	23	2581	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	PSU	Pt	39	56	18,21,22	1.37	3 (16%)	21,30,33	2.09	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	PSU	23	2605	23	18,21,22	1.38	3 (16%)	21,30,33	2.07	4 (19%)
58	PSU	Dt	39	58	18,21,22	2.79	7 (38%)	21,30,33	3.07	10 (47%)
58	4SU	Dt	8	58	18,21,22	1.85	4 (22%)	25,30,33	2.30	5 (20%)
23	PSU	23	746	23,60	18,21,22	1.41	3 (16%)	21,30,33	1.98	4 (19%)
23	3TD	23	1915	23	19,22,23	1.21	2 (10%)	23,32,35	2.10	3 (13%)
23	PSU	23	2580	23	18,21,22	1.42	4 (22%)	21,30,33	2.08	5 (23%)
58	H2U	Dt	16	58	18,21,22	1.43	3 (16%)	19,30,33	1.86	4 (21%)
56	PSU	Pt	55	56	18,21,22	1.39	2 (11%)	21,30,33	2.08	4 (19%)
23	5MC	23	1962	23	19,22,23	1.51	3 (15%)	26,32,35	1.11	2 (7%)
58	MIA	Dt	37	58	28,31,32	2.34	6 (21%)	38,44,47	3.25	19 (50%)
1	2MG	16	1207	1,60	23,26,27	1.26	4 (17%)	33,38,41	2.18	6 (18%)
1	5MC	16	967	1	19,22,23	1.55	3 (15%)	26,32,35	1.12	2 (7%)
56	U8U	Pt	34	56,22	20,24,25	1.51	3 (15%)	22,34,37	1.06	3 (13%)
56	3AU	Pt	47	56	24,28,29	1.04	0	30,40,43	1.62	4 (13%)
58	PSU	Dt	55	58	18,21,22	2.23	6 (33%)	21,30,33	2.93	9 (42%)
1	4OC	16	1402	1,60	20,23,24	0.74	0	25,32,35	0.93	1 (4%)
23	G7M	23	2069	23	23,26,27	2.25	6 (26%)	34,39,42	3.19	17 (50%)
23	OMU	23	2552	23	19,22,23	4.23	13 (68%)	25,31,34	2.29	6 (24%)
56	H2U	Pt	17	56	18,21,22	1.06	2 (11%)	19,30,33	1.15	2 (10%)
23	2MG	23	2445	23	23,26,27	1.24	3 (13%)	33,38,41	2.24	10 (30%)
1	PSU	16	516	1,60	18,21,22	1.41	3 (16%)	21,30,33	2.14	5 (23%)
23	5MU	23	1939	23	19,22,23	1.39	5 (26%)	27,32,35	2.14	6 (22%)
23	2MG	23	1835	23	23,26,27	1.27	3 (13%)	33,38,41	2.19	6 (18%)
23	PSU	23	955	23	18,21,22	1.38	3 (16%)	21,30,33	2.13	4 (19%)
56	5MU	Pt	54	56	19,22,23	1.36	5 (26%)	27,32,35	2.11	7 (25%)
1	G7M	16	527	1	23,26,27	2.37	5 (21%)	34,39,42	2.99	10 (29%)
1	UR3	16	1498	1	19,22,23	0.93	0	26,32,35	1.76	3 (11%)
23	OMC	23	2498	23,60	19,22,23	1.01	2 (10%)	25,31,34	1.13	1 (4%)
23	2MA	23	2503	23,60	22,25,26	1.44	5 (22%)	32,37,40	2.29	9 (28%)
1	5MC	16	1407	1	19,22,23	1.52	3 (15%)	26,32,35	1.10	3 (11%)
23	1MG	23	745	23	23,26,27	1.18	3 (13%)	33,39,42	1.68	5 (15%)
23	PSU	23	2504	23	18,21,22	1.42	3 (16%)	21,30,33	2.08	4 (19%)
58	3AU	Dt	47	58	24,28,29	0.98	0	30,40,43	1.49	5 (16%)
23	H2U	23	2449	23	18,21,22	4.32	13 (72%)	19,30,33	1.72	4 (21%)
1	MA6	16	1519	1	23,26,27	1.47	5 (21%)	33,38,41	2.11	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
58	G7M	Dt	46	58	23,26,27	2.34	5 (21%)	34,39,42	3.37	11 (32%)
58	PSU	Dt	32	58	18,21,22	3.22	9 (50%)	21,30,33	3.06	6 (28%)
12	D2T	SL	89	12	8,9,10	1.65	2 (25%)	6,11,13	1.52	2 (33%)
56	H2U	Pt	16	56	18,21,22	1.10	2 (11%)	19,30,33	1.22	1 (5%)
23	PSU	23	2457	23	18,21,22	1.41	3 (16%)	21,30,33	2.16	4 (19%)
56	H2U	Pt	20	56	18,21,22	4.44	12 (66%)	19,30,33	1.63	5 (26%)
56	T6A	Pt	37	56	31,34,35	1.47	6 (19%)	43,49,52	2.10	12 (27%)
1	2MG	16	1516	1	23,26,27	1.25	4 (17%)	33,38,41	2.23	9 (27%)
1	2MG	16	966	1	23,26,27	1.25	4 (17%)	33,38,41	2.17	7 (21%)
1	MA6	16	1518	1	23,26,27	1.48	5 (21%)	33,38,41	2.12	10 (30%)
23	OMG	23	2251	23,58	23,26,27	0.52	0	32,38,41	0.47	0
23	6MZ	23	2030	23	22,25,26	1.43	5 (22%)	29,36,39	2.39	10 (34%)
23	PSU	23	2604	23	18,21,22	1.84	6 (33%)	21,30,33	2.32	9 (42%)
23	6MZ	23	1618	23	22,25,26	1.43	5 (22%)	29,36,39	2.19	10 (34%)
36	4D4	LP	81	36	9,11,12	2.16	2 (22%)	7,13,15	2.04	3 (42%)
23	5MU	23	747	23	19,22,23	1.41	6 (31%)	27,32,35	2.11	6 (22%)

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
56	PSU	Pt	39	56	-	0/7/25/26	0/2/2/2
23	PSU	23	2605	23	-	0/7/25/26	0/2/2/2
58	PSU	Dt	39	58	-	0/7/25/26	0/2/2/2
58	4SU	Dt	8	58	-	2/7/25/26	0/2/2/2
23	PSU	23	746	23,60	-	2/7/25/26	0/2/2/2
23	3TD	23	1915	23	-	2/7/25/26	0/2/2/2
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
58	H2U	Dt	16	58	-	0/7/38/39	0/2/2/2
56	PSU	Pt	55	56	-	0/7/25/26	0/2/2/2
23	5MC	23	1962	23	-	0/7/25/26	0/2/2/2
58	MIA	Dt	37	58	-	8/15/33/34	0/3/3/3
1	2MG	16	1207	1,60	-	0/9/27/28	0/3/3/3
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
56	U8U	Pt	34	56,22	-	0/10/28/29	0/2/2/2
56	3AU	Pt	47	56	-	7/16/34/35	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PSU	Dt	55	58	-	0/7/25/26	0/2/2/2
1	4OC	16	1402	1,60	-	0/9/29/30	0/2/2/2
23	G7M	23	2069	23	-	1/7/25/26	0/3/3/3
23	OMU	23	2552	23	-	1/9/27/28	0/2/2/2
56	H2U	Pt	17	56	-	3/7/38/39	0/2/2/2
23	2MG	23	2445	23	-	1/9/27/28	0/3/3/3
1	PSU	16	516	1,60	-	0/7/25/26	0/2/2/2
23	5MU	23	1939	23	-	0/7/25/26	0/2/2/2
23	2MG	23	1835	23	-	0/9/27/28	0/3/3/3
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
56	5MU	Pt	54	56	-	0/7/25/26	0/2/2/2
1	G7M	16	527	1	-	2/7/25/26	0/3/3/3
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
23	OMC	23	2498	23,60	-	2/9/27/28	0/2/2/2
23	2MA	23	2503	23,60	-	2/7/25/26	0/3/3/3
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
23	1MG	23	745	23	-	0/7/25/26	0/3/3/3
23	PSU	23	2504	23	-	2/7/25/26	0/2/2/2
58	3AU	Dt	47	58	-	6/16/34/35	0/2/2/2
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2
1	MA6	16	1519	1	-	2/11/29/30	0/3/3/3
58	G7M	Dt	46	58	-	2/7/25/26	0/3/3/3
58	PSU	Dt	32	58	-	0/7/25/26	0/2/2/2
12	D2T	SL	89	12	-	3/7/12/14	-
56	H2U	Pt	16	56	-	7/7/38/39	0/2/2/2
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
56	H2U	Pt	20	56	-	2/7/38/39	0/2/2/2
56	T6A	Pt	37	56	-	10/23/41/42	0/3/3/3
1	2MG	16	1516	1	-	0/9/27/28	0/3/3/3
1	2MG	16	966	1	-	0/9/27/28	0/3/3/3
1	MA6	16	1518	1	-	0/11/29/30	0/3/3/3
23	OMG	23	2251	23,58	-	3/9/27/28	0/3/3/3
23	6MZ	23	2030	23	-	2/9/27/28	0/3/3/3
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
23	6MZ	23	1618	23	-	2/9/27/28	0/3/3/3
36	4D4	LP	81	36	-	3/11/12/14	-
23	5MU	23	747	23	-	0/7/25/26	0/2/2/2

The worst 5 of 214 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	2552	OMU	C3'-C2'	-10.60	1.29	1.53
23	23	2449	H2U	C2'-C3'	-10.18	1.25	1.53
56	Pt	20	H2U	C2'-C3'	-10.02	1.26	1.53
56	Pt	20	H2U	C2-N1	9.59	1.48	1.35
23	23	2449	H2U	C2-N1	8.93	1.48	1.35

The worst 5 of 311 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	Dt	46	G7M	CN7-N7-C8	-9.39	110.57	124.79
58	Dt	37	MIA	C12-C13-C14	-9.35	110.23	127.01
58	Dt	32	PSU	N1-C2-N3	9.22	124.89	115.17
23	23	2069	G7M	CN7-N7-C8	-8.58	111.80	124.79
23	23	2503	2MA	C5-C4-N3	-8.07	118.68	127.18

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	527	G7M	O4'-C4'-C5'-O5'
1	16	527	G7M	C3'-C4'-C5'-O5'
12	SL	89	D2T	SB-CB-CG-OD2
23	23	1618	6MZ	O4'-C4'-C5'-O5'
23	23	2251	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	Dt	8	4SU	1	0
1	16	967	5MC	1	0
23	23	2552	OMU	2	0
23	23	2449	H2U	1	0
56	Pt	16	H2U	1	0
56	Pt	20	H2U	3	0
1	16	966	2MG	1	0
23	23	2251	OMG	1	0
23	23	2030	6MZ	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 434 ligands modelled in this entry, 408 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
59	PUT	16	1601	-	5,5,5	0.09	0	4,4,4	0.13	0
59	PUT	23	3015	-	5,5,5	0.10	0	4,4,4	0.13	0
59	PUT	23	3011	-	5,5,5	0.09	0	4,4,4	0.13	0
59	PUT	23	3013	-	5,5,5	0.10	0	4,4,4	0.13	0
59	PUT	23	3016	-	5,5,5	0.10	0	4,4,4	0.13	0
59	PUT	23	3006	-	5,5,5	0.10	0	4,4,4	0.13	0
63	SPD	23	3023	-	9,9,9	0.31	0	8,8,8	0.92	0
59	PUT	23	3014	-	5,5,5	0.11	0	4,4,4	0.13	0
59	PUT	23	3007	-	5,5,5	0.08	0	4,4,4	0.14	0
59	PUT	23	3004	-	5,5,5	0.11	0	4,4,4	0.12	0
59	PUT	23	3005	-	5,5,5	0.09	0	4,4,4	0.13	0
59	PUT	23	3017	-	5,5,5	0.11	0	4,4,4	0.12	0
62	ATP	23	3002	-	32,33,33	0.54	0	48,52,52	0.57	0
63	SPD	23	3022	-	9,9,9	0.32	0	8,8,8	0.90	0
62	ATP	23	3001	-	32,33,33	0.27	0	48,52,52	0.29	0
59	PUT	23	3012	-	5,5,5	0.10	0	4,4,4	0.12	0
59	PUT	23	3008	-	5,5,5	0.09	0	4,4,4	0.13	0
59	PUT	23	3018	-	5,5,5	0.10	0	4,4,4	0.12	0
63	SPD	23	3019	-	9,9,9	0.32	0	8,8,8	0.95	0
59	PUT	23	3009	-	5,5,5	0.09	0	4,4,4	0.13	0
63	SPD	23	3021	-	9,9,9	0.31	0	8,8,8	0.87	0
62	ATP	23	3003	-	32,33,33	0.25	0	48,52,52	0.27	0
59	PUT	16	1603	-	5,5,5	0.12	0	4,4,4	0.13	0
63	SPD	23	3020	-	9,9,9	0.31	0	8,8,8	0.91	0
59	PUT	16	1602	-	5,5,5	0.10	0	4,4,4	0.13	0
59	PUT	23	3010	-	5,5,5	0.12	0	4,4,4	0.19	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
59	PUT	16	1601	-	-	0/3/3/3	-
59	PUT	23	3015	-	-	1/3/3/3	-
59	PUT	23	3011	-	-	0/3/3/3	-
59	PUT	23	3013	-	-	0/3/3/3	-
59	PUT	23	3016	-	-	0/3/3/3	-
59	PUT	23	3006	-	-	1/3/3/3	-
63	SPD	23	3023	-	-	3/7/7/7	-
59	PUT	23	3014	-	-	0/3/3/3	-
59	PUT	23	3007	-	-	1/3/3/3	-
59	PUT	23	3004	-	-	1/3/3/3	-
59	PUT	23	3005	-	-	0/3/3/3	-
59	PUT	23	3017	-	-	1/3/3/3	-
62	ATP	23	3002	-	-	4/22/38/38	0/3/3/3
63	SPD	23	3022	-	-	1/7/7/7	-
62	ATP	23	3001	-	-	10/22/38/38	0/3/3/3
59	PUT	23	3012	-	-	0/3/3/3	-
59	PUT	23	3008	-	-	1/3/3/3	-
59	PUT	23	3018	-	-	0/3/3/3	-
63	SPD	23	3019	-	-	0/7/7/7	-
59	PUT	23	3009	-	-	3/3/3/3	-
63	SPD	23	3021	-	-	5/7/7/7	-
62	ATP	23	3003	-	-	6/22/38/38	0/3/3/3
59	PUT	16	1603	-	-	1/3/3/3	-
63	SPD	23	3020	-	-	2/7/7/7	-
59	PUT	16	1602	-	-	1/3/3/3	-
59	PUT	23	3010	-	-	1/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

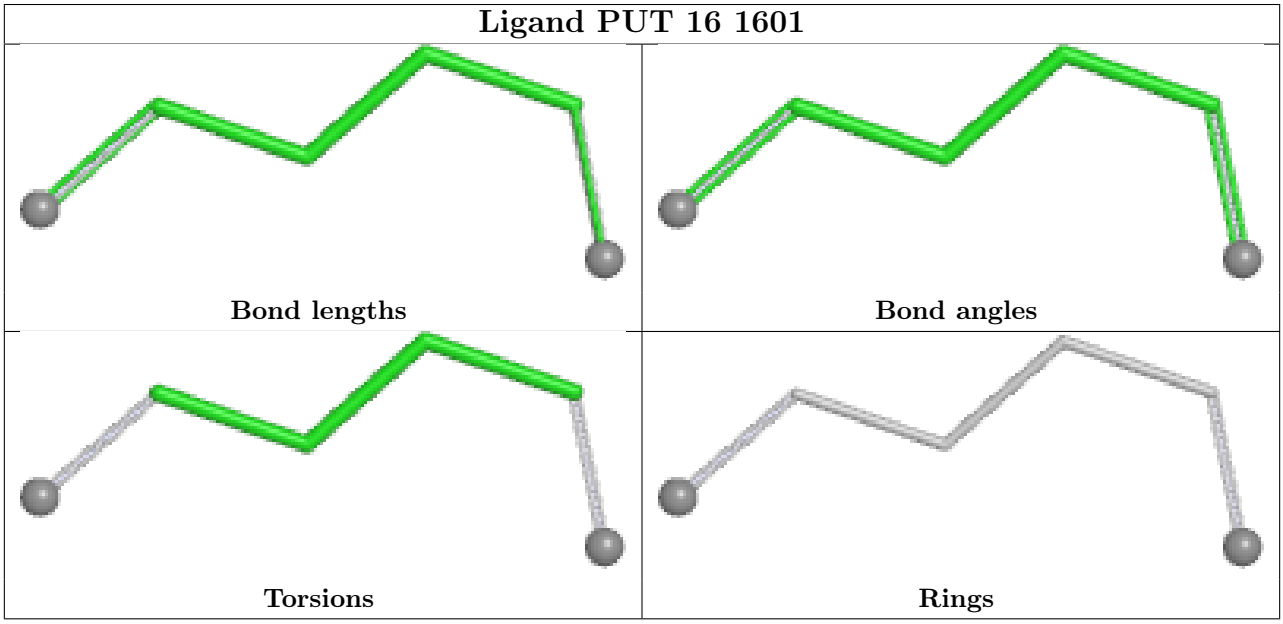
Mol	Chain	Res	Type	Atoms
62	23	3001	ATP	C5'-O5'-PA-O2A
62	23	3002	ATP	C5'-O5'-PA-O3A
62	23	3002	ATP	O4'-C4'-C5'-O5'
62	23	3003	ATP	C5'-O5'-PA-O1A
62	23	3003	ATP	C5'-O5'-PA-O2A

There are no ring outliers.

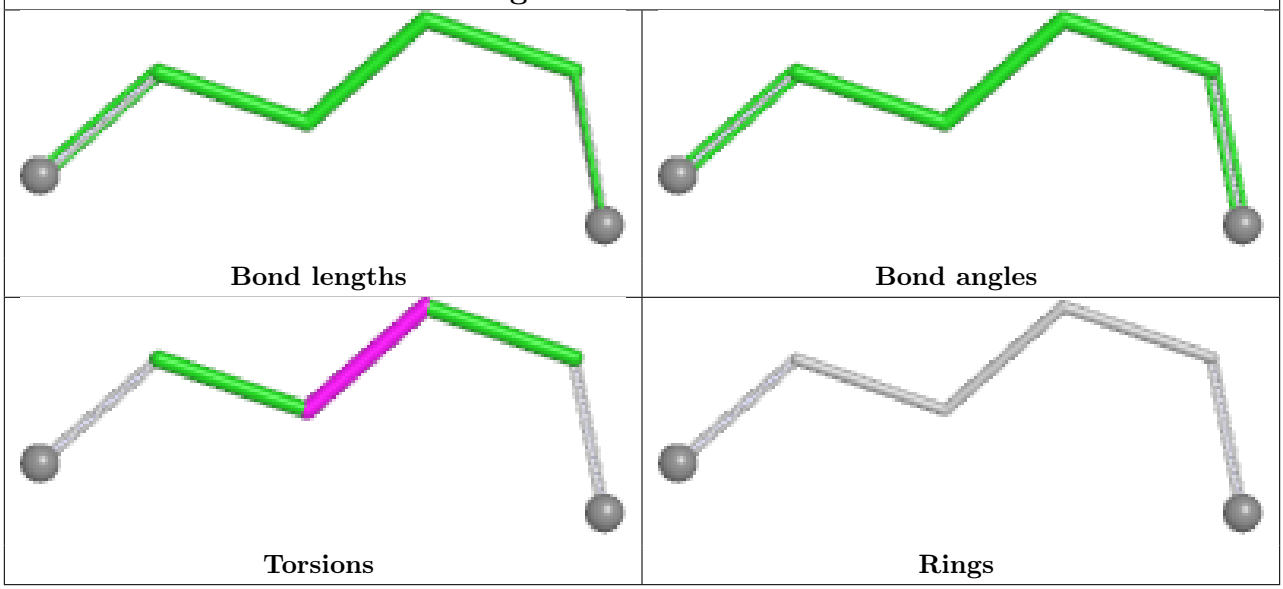
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	23	3019	SPD	1	0
63	23	3020	SPD	1	0

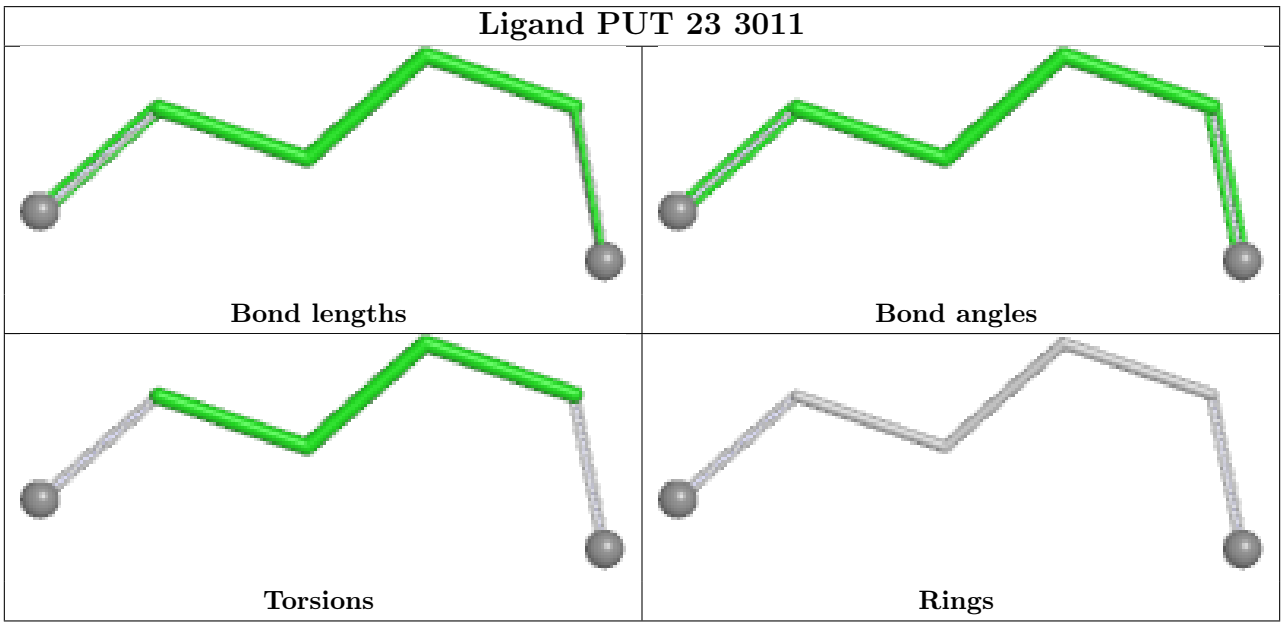
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



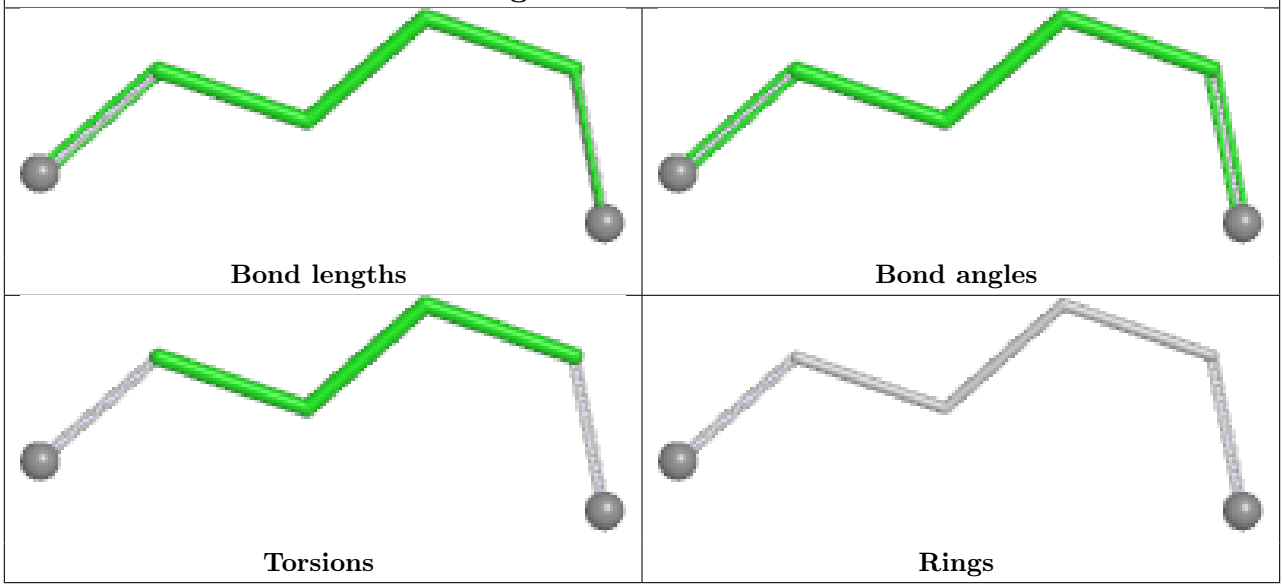
Ligand PUT 23 3015



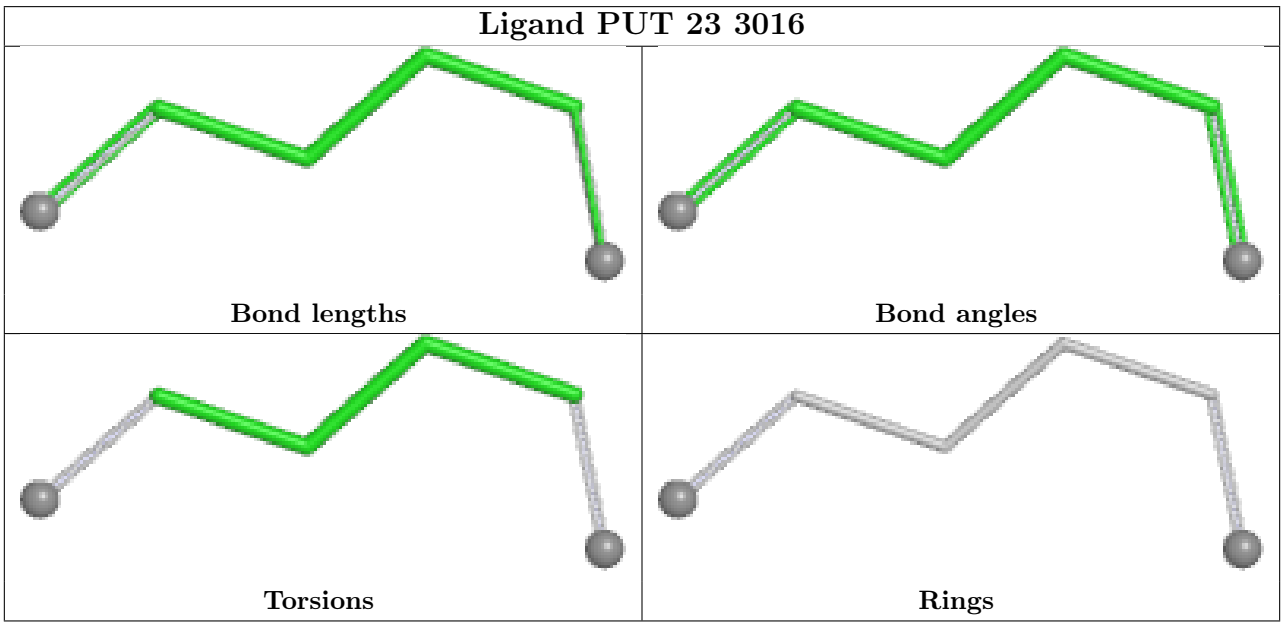
Ligand PUT 23 3011



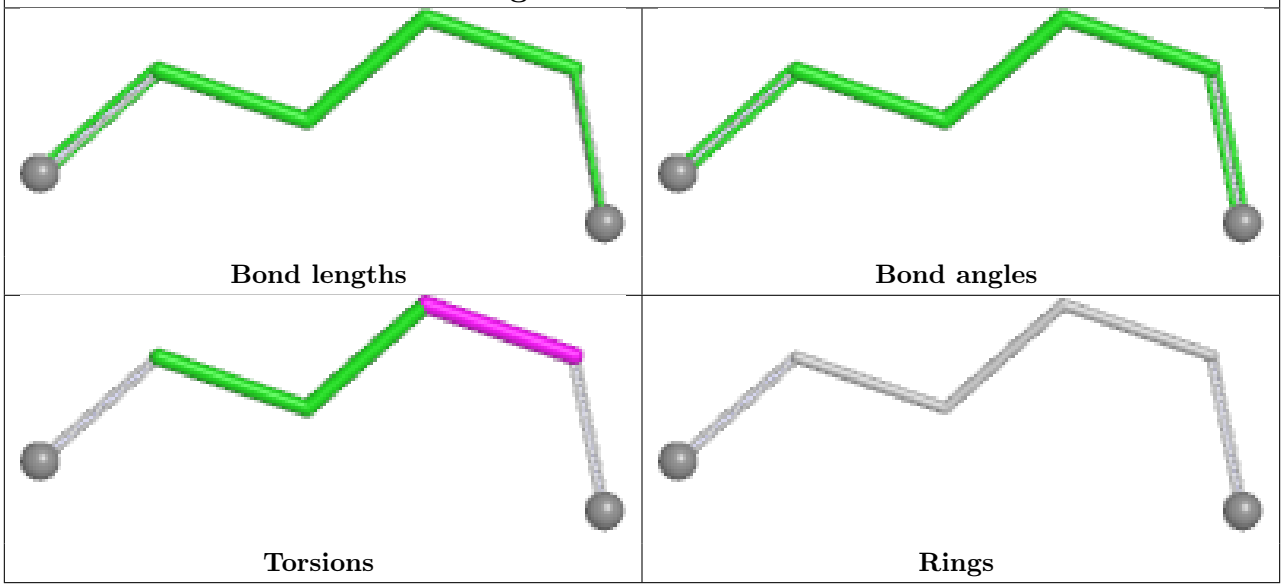
Ligand PUT 23 3013



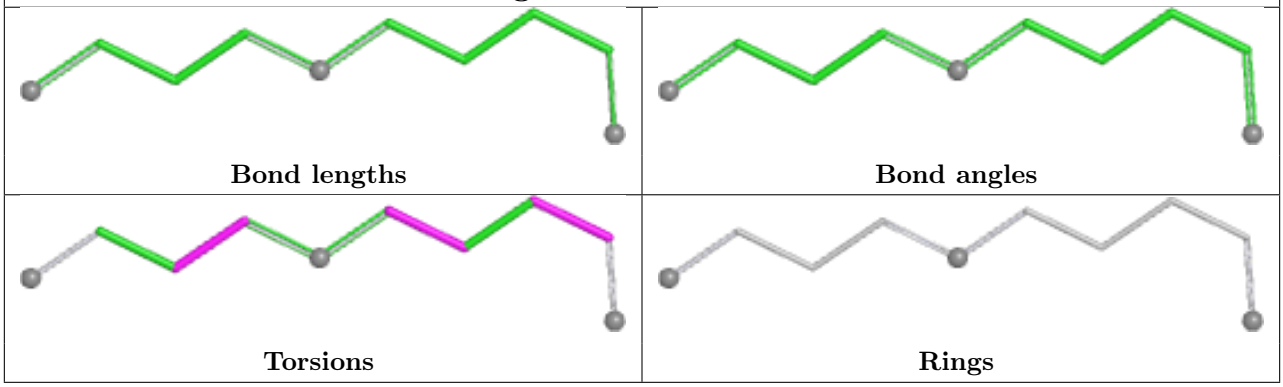
Ligand PUT 23 3016



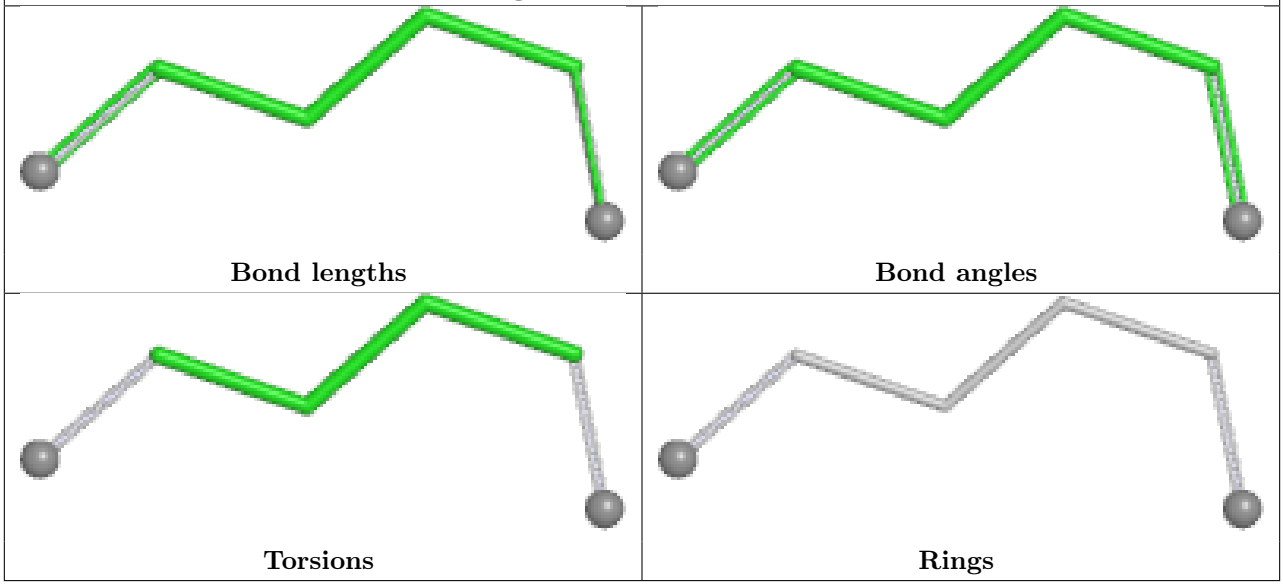
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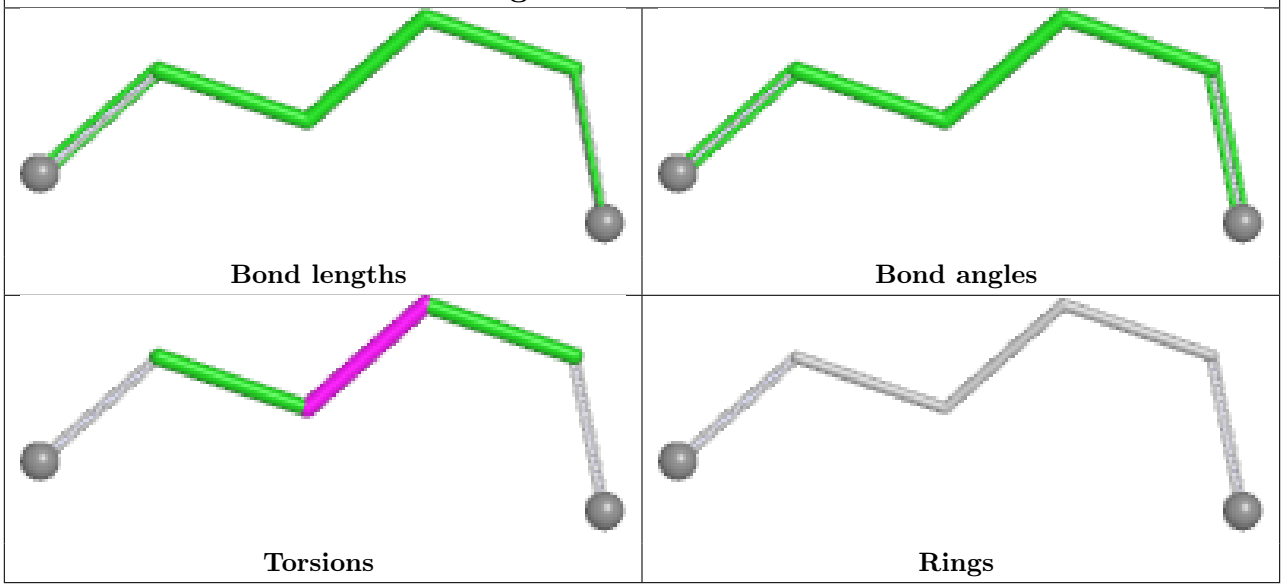
Ligand SPD 23 3023



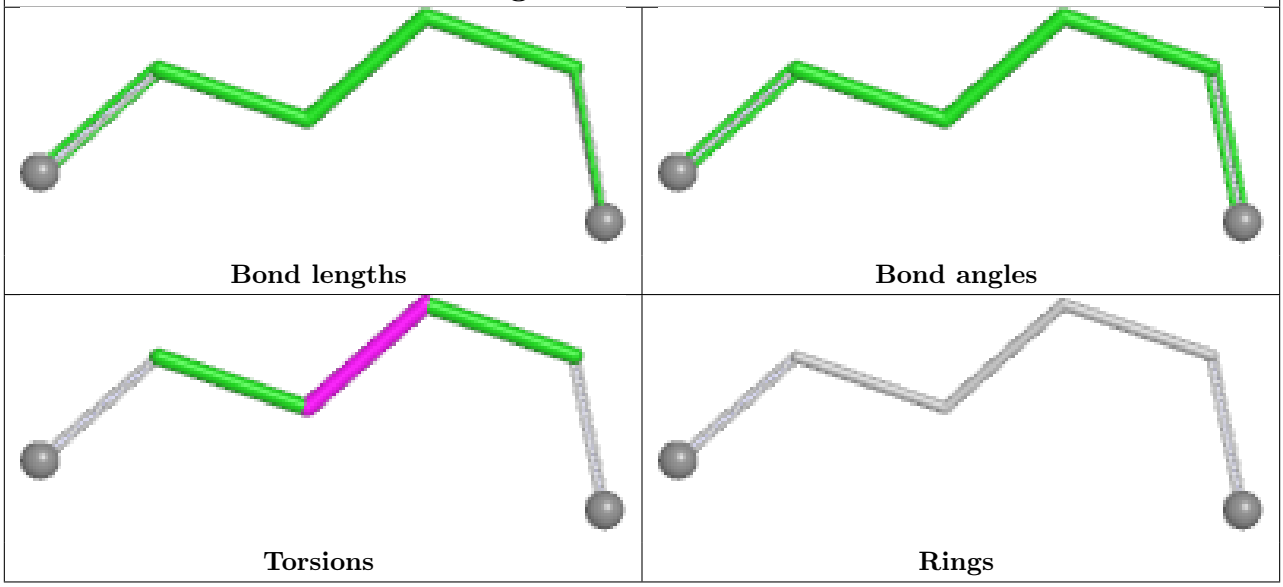
Ligand PUT 23 3014



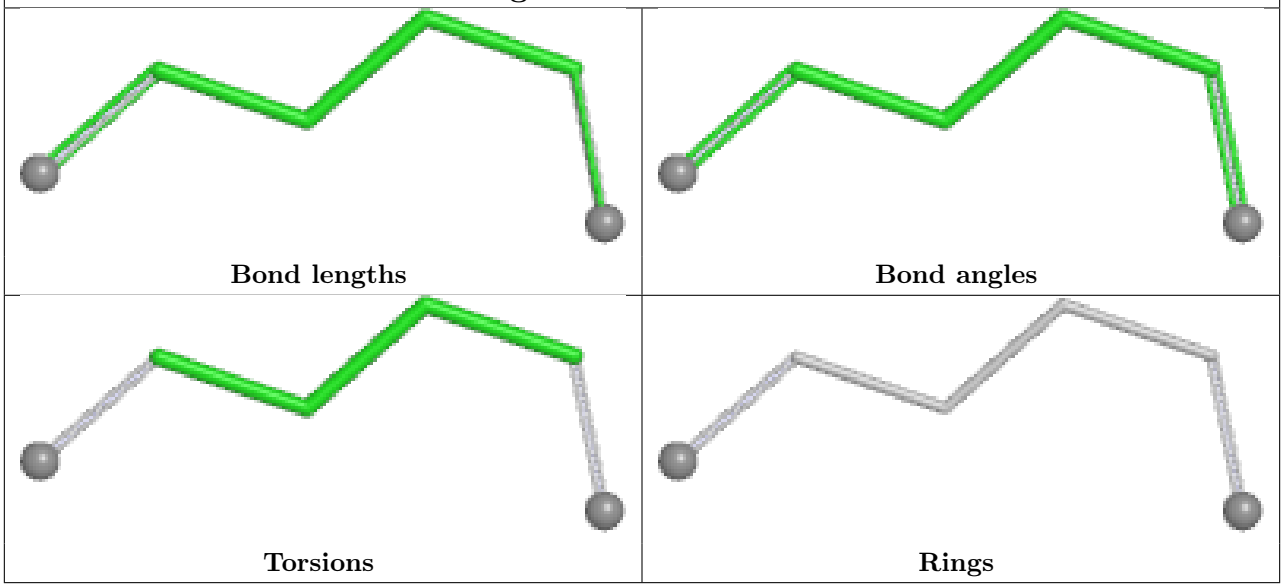
Ligand PUT 23 3007



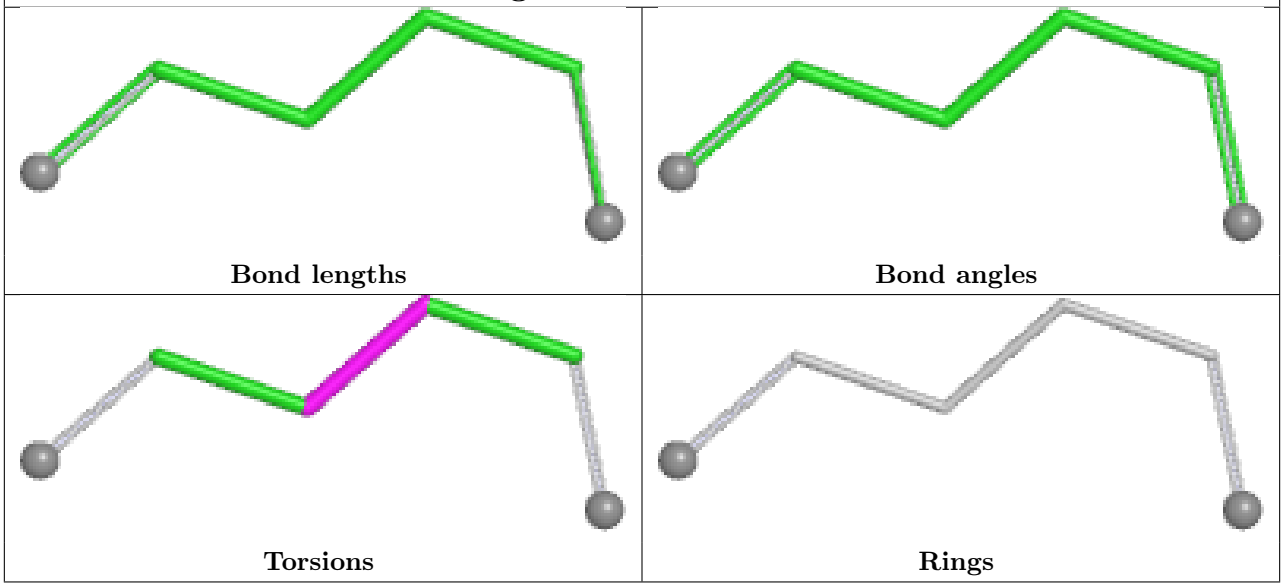
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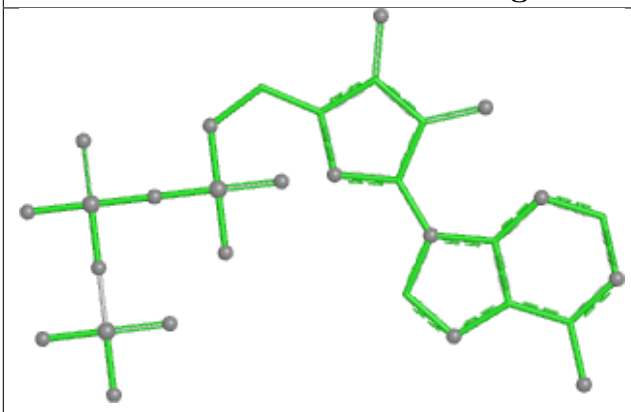
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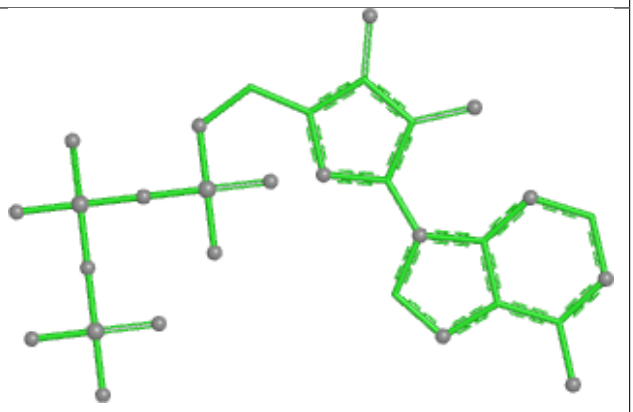
Ligand PUT 23 3017



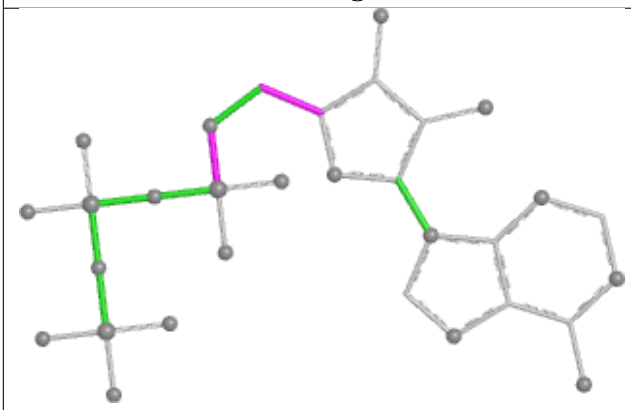
Ligand ATP 23 3002



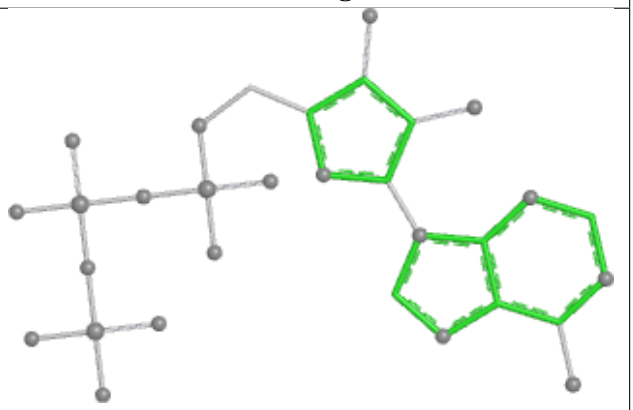
Bond lengths



Bond angles

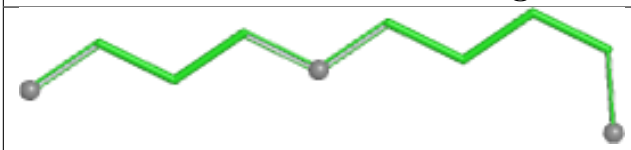


Torsions

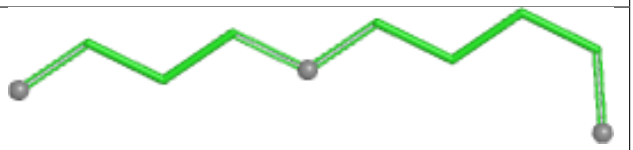


Rings

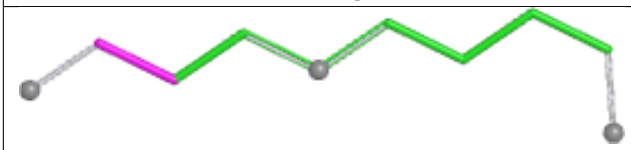
Ligand SPD 23 3022



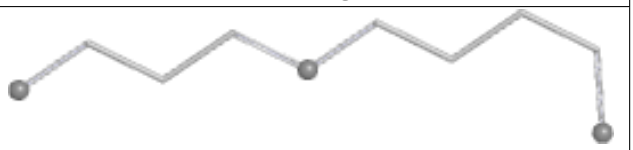
Bond lengths



Bond angles

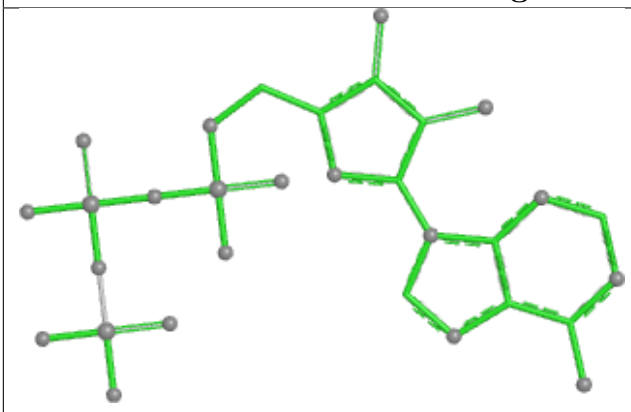


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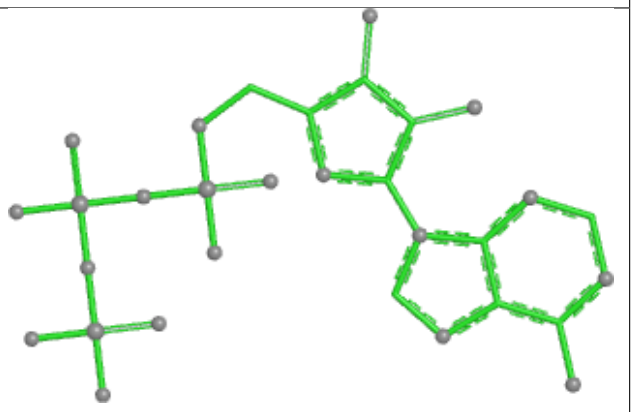


Rings

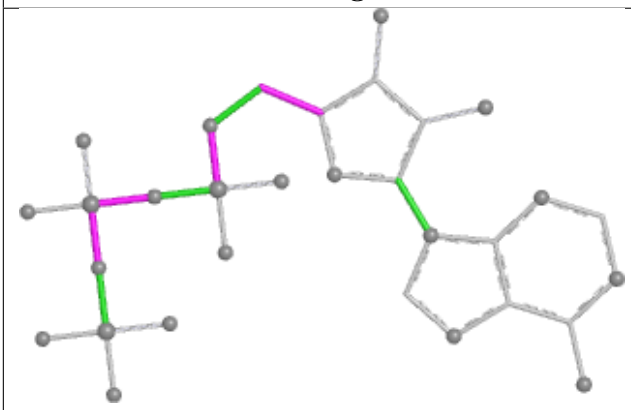
Ligand ATP 23 3001



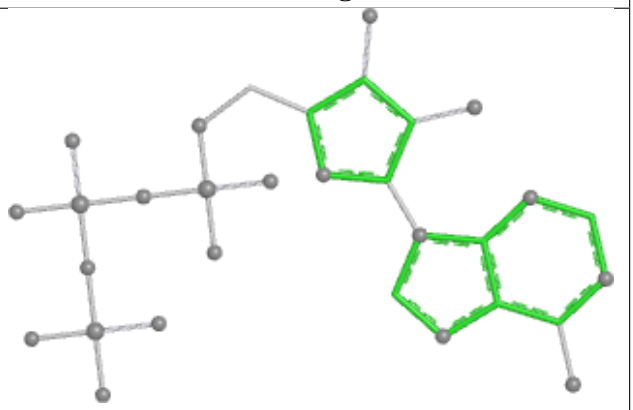
Bond lengths



Bond angles

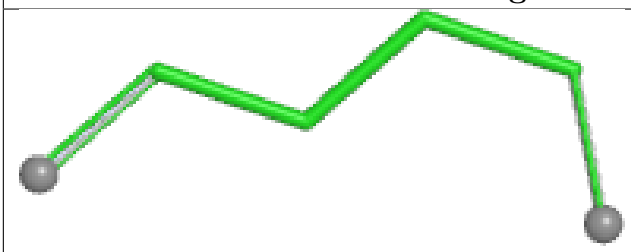


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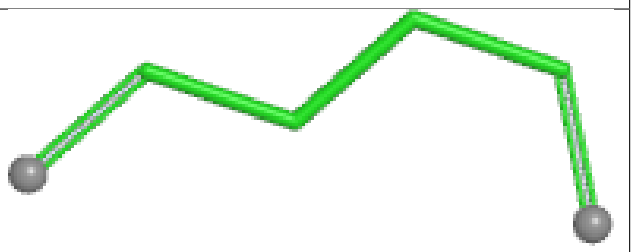


Rings

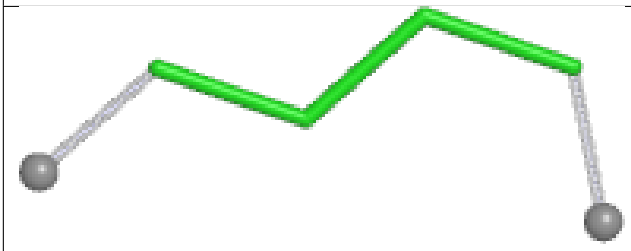
Ligand PUT 23 3012



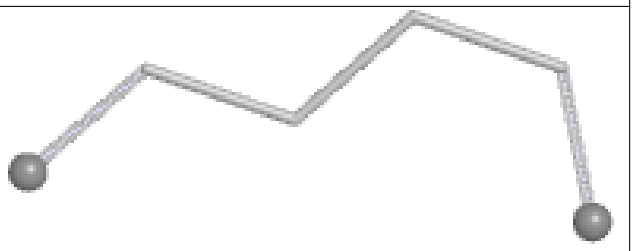
Bond lengths



Bond angles

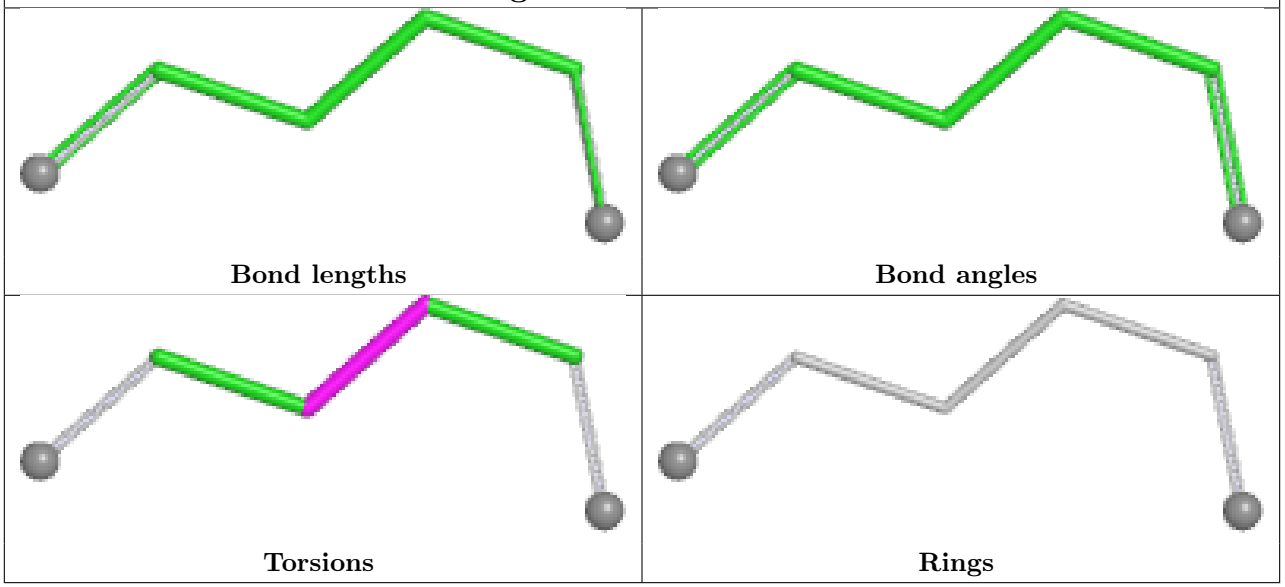


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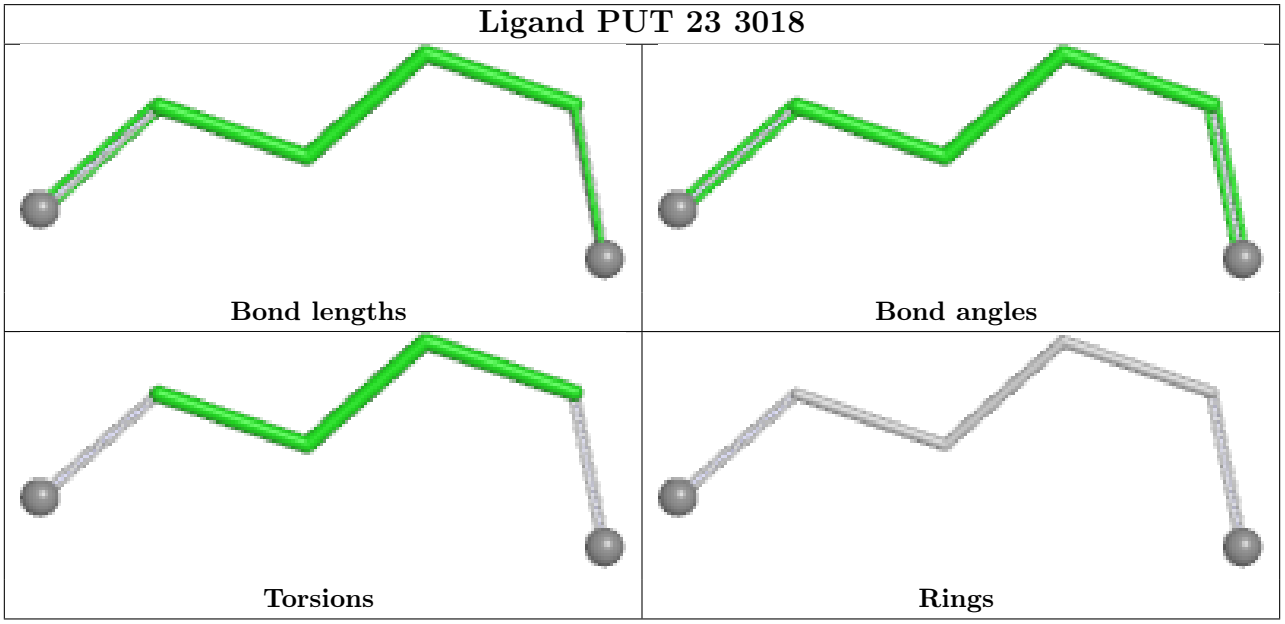


Rings

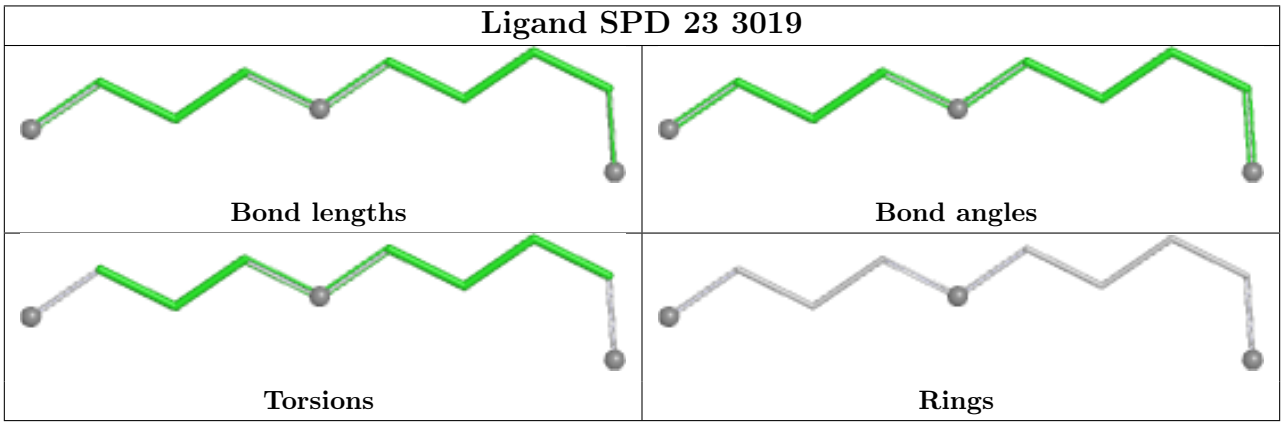
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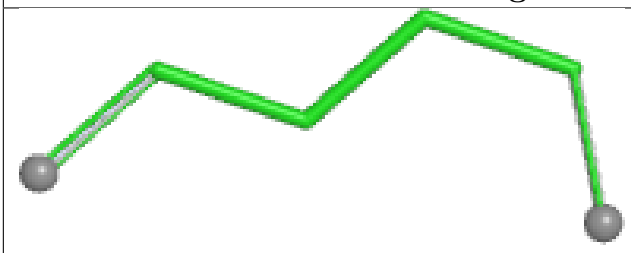
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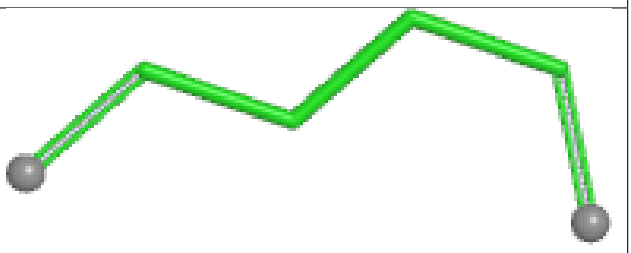
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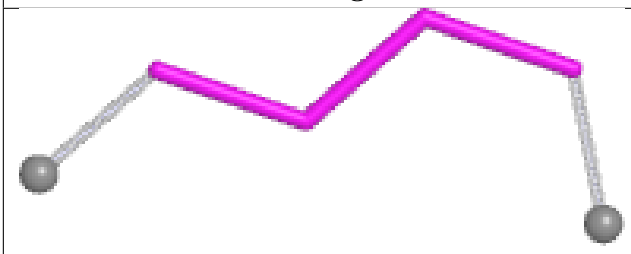
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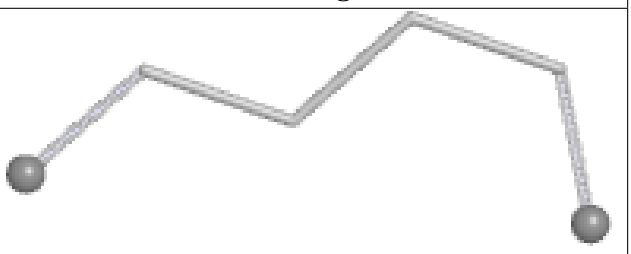
Bond lengths



Bond angles

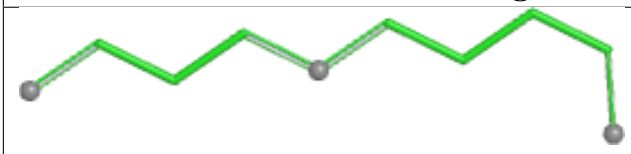


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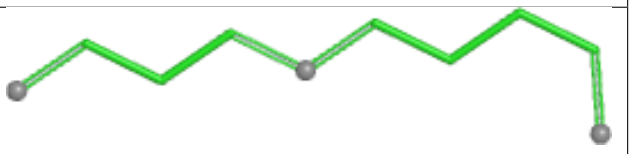


Rings

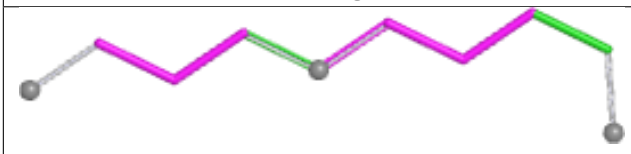
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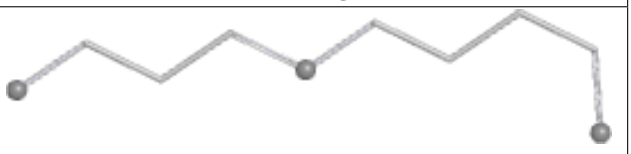
Bond lengths



Bond angles

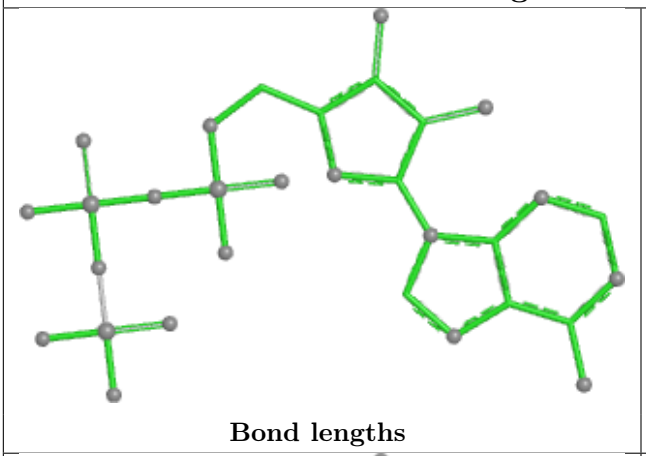


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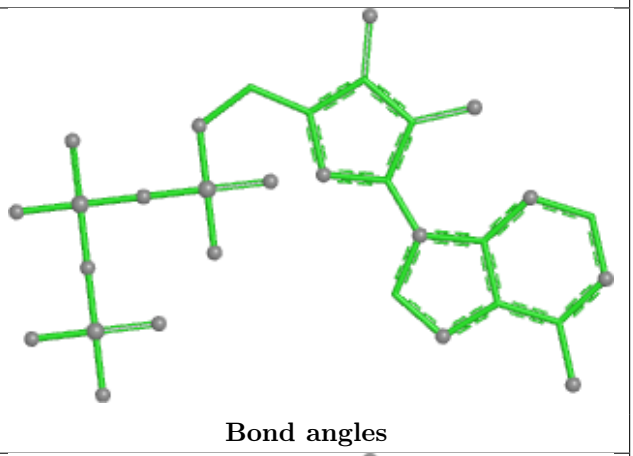


Rings

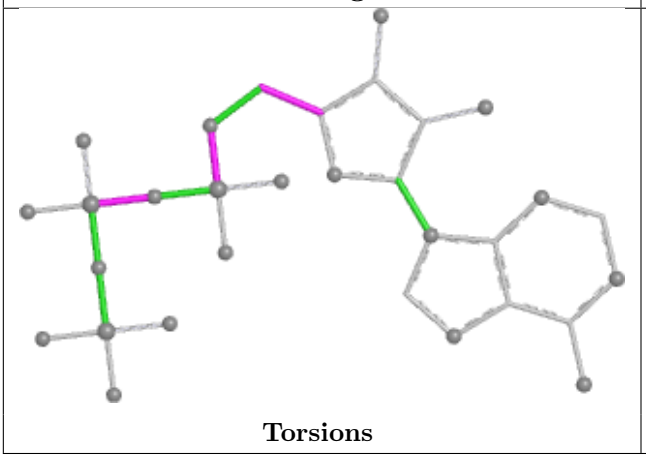
Ligand ATP 23 3003



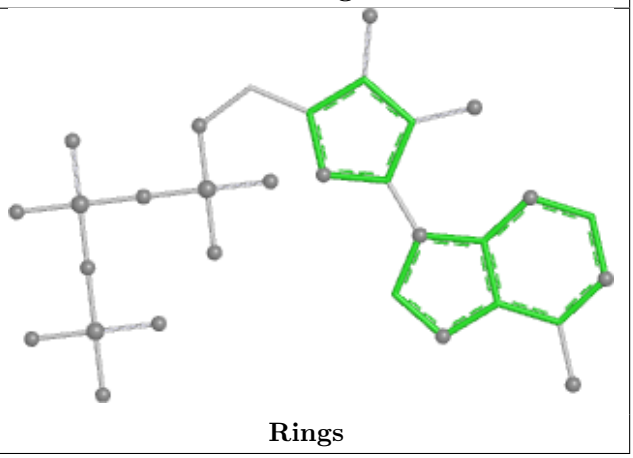
Bond lengths



Bond angles

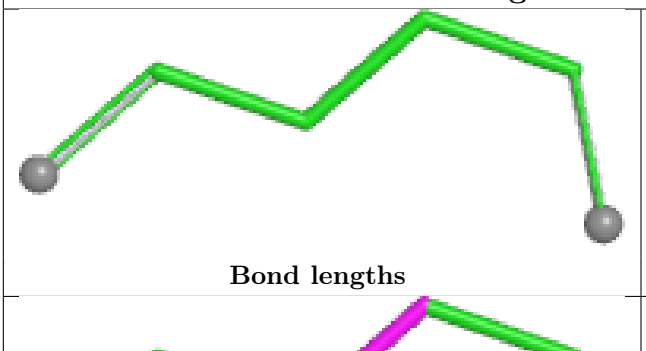


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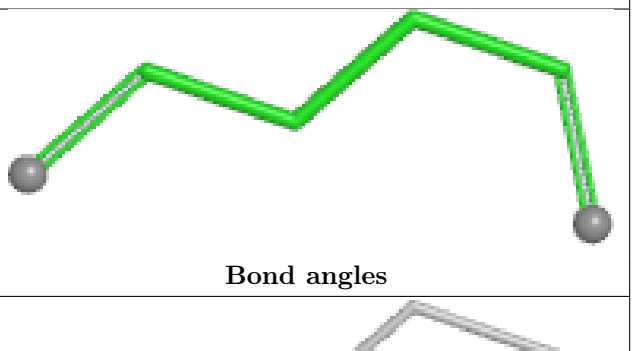


Rings

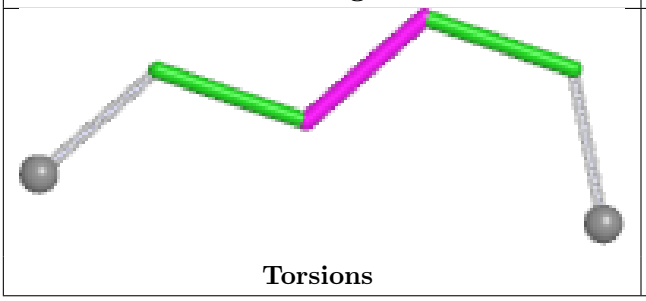
Ligand PUT 16 1603



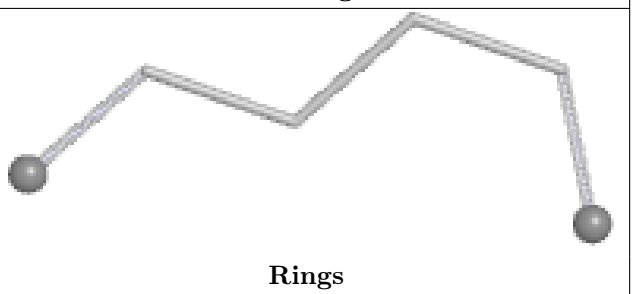
Bond lengths



Bond angles

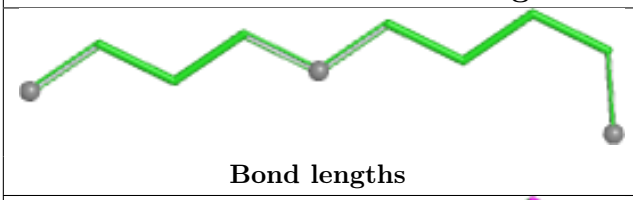


Torsions

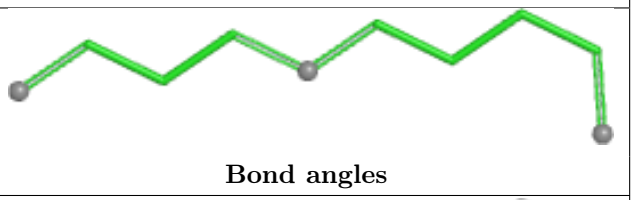


Rings

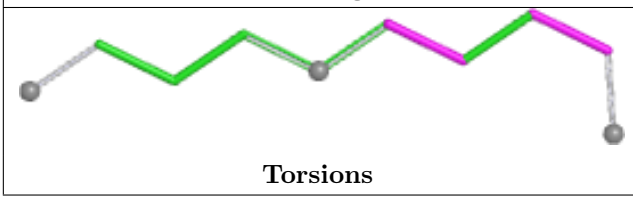
Ligand SPD 23 3020



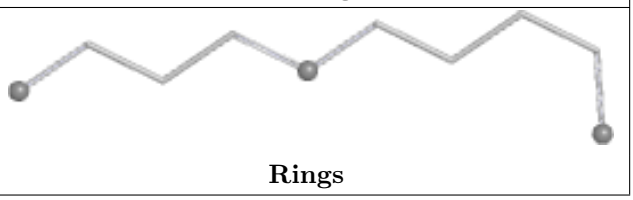
Bond lengths



Bond angles

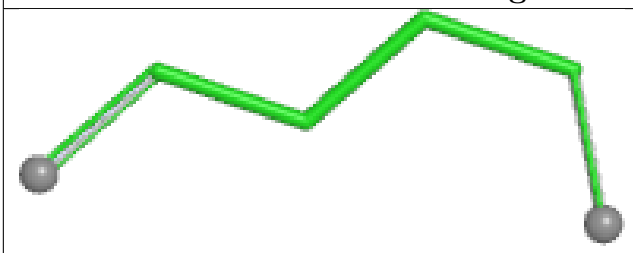


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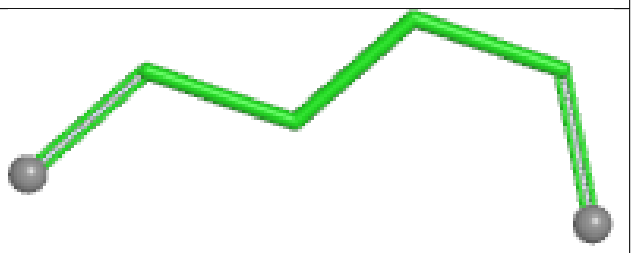


Rings

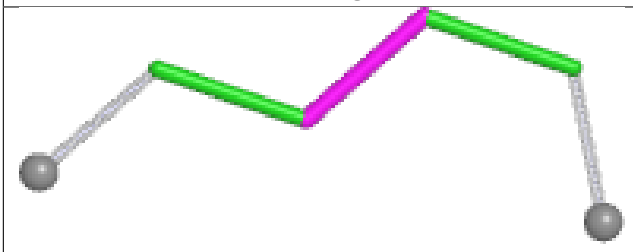
Ligand PUT 16 1602



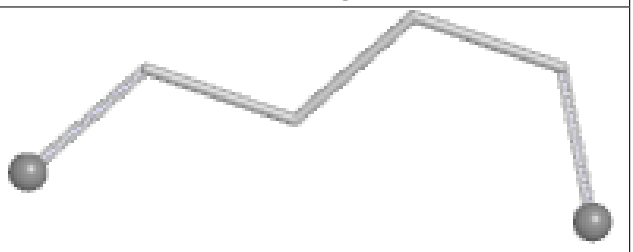
Bond lengths



Bond angles

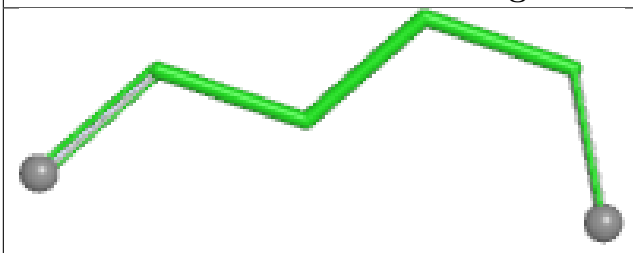


Torsions

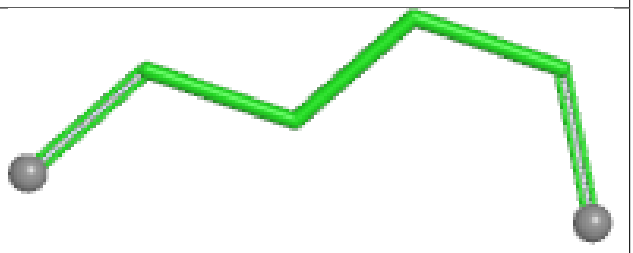


Rings

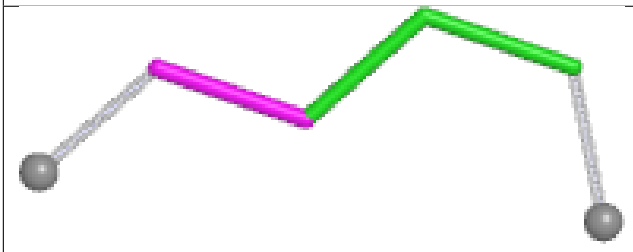
Ligand PUT 23 3010



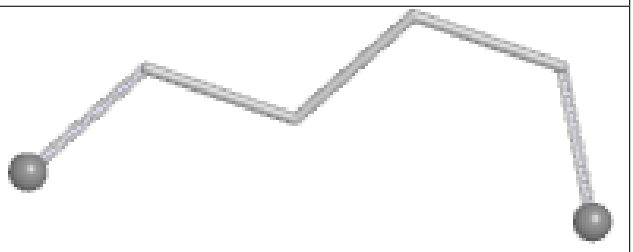
Bond lengths



Bond angles



Torsions



Rings

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.

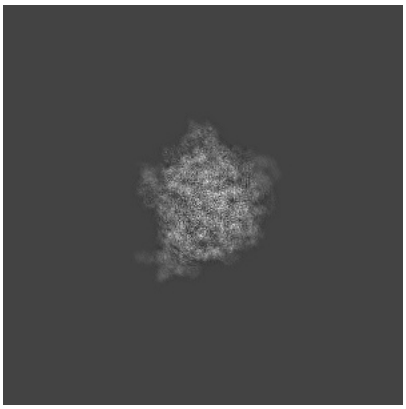
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24120. These allow visual inspection of the internal detail of the map and identification of artifacts.

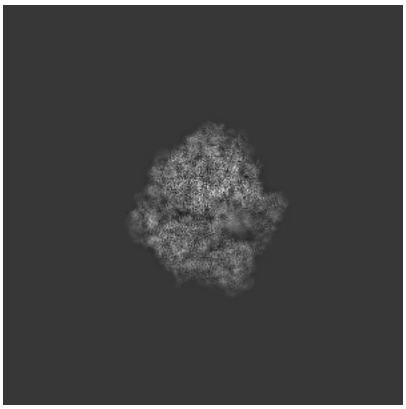
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

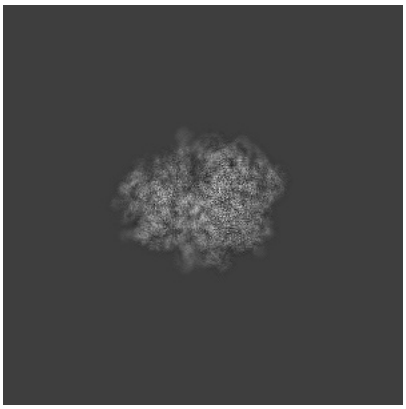
6.1.1 Primary map



X

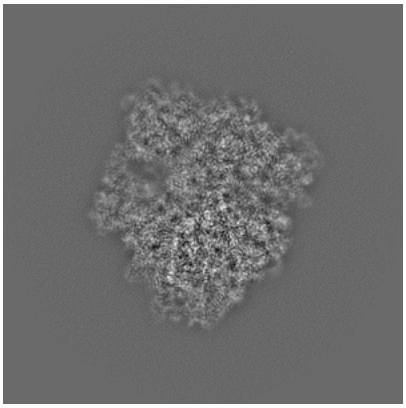


Y

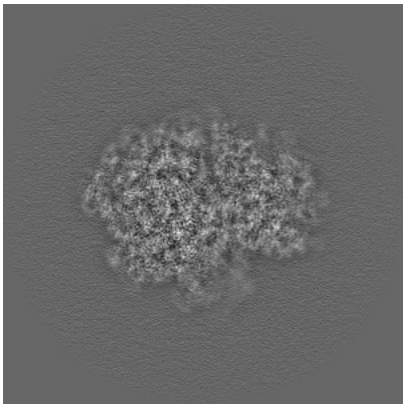


Z

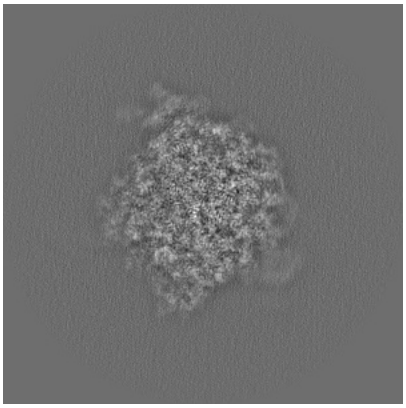
6.1.2 Raw map



X



Y

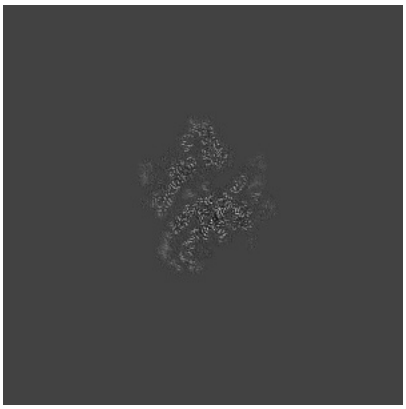


Z

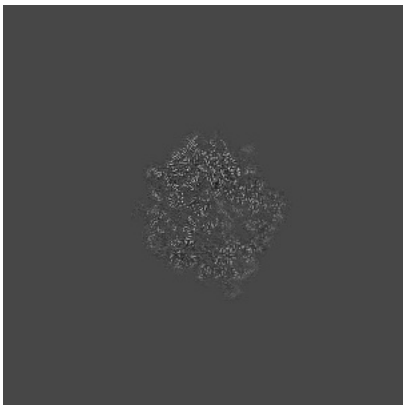
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

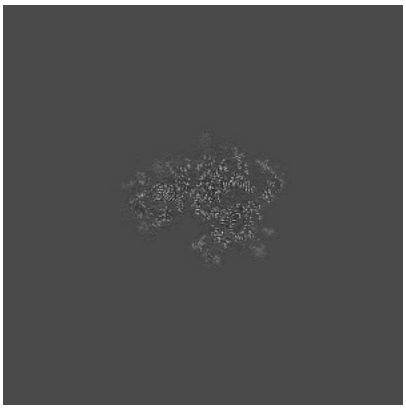
6.2.1 Primary map



X Index: 288

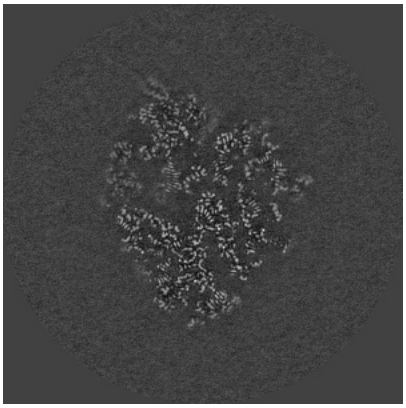


Y Index: 288

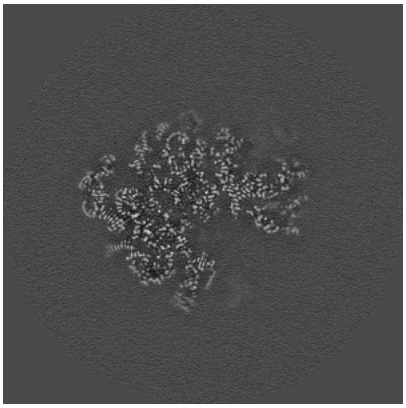


Z Index: 288

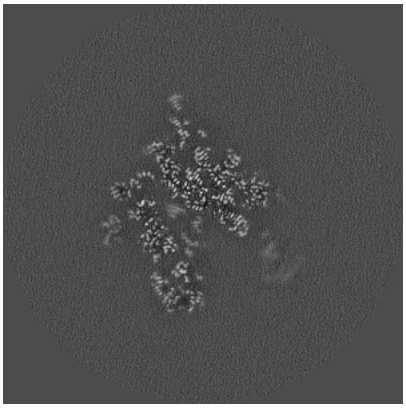
6.2.2 Raw map



X Index: 256



Y Index: 256

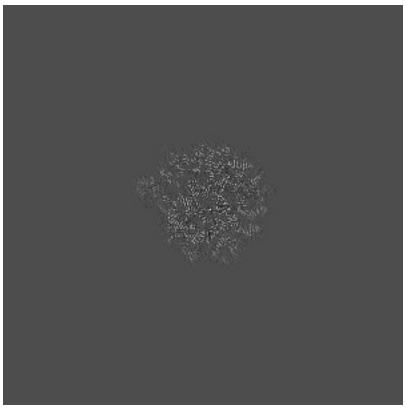


Z Index: 256

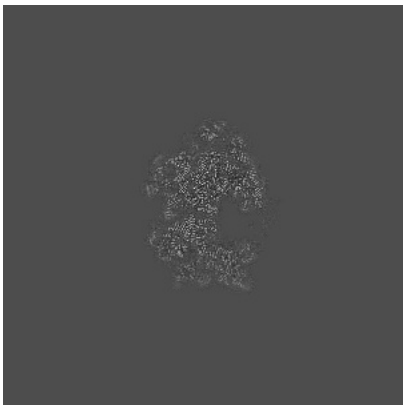
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

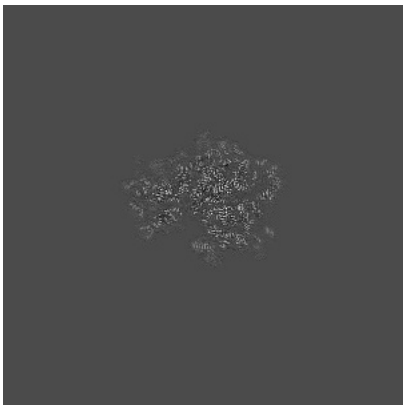
6.3.1 Primary map



X Index: 316

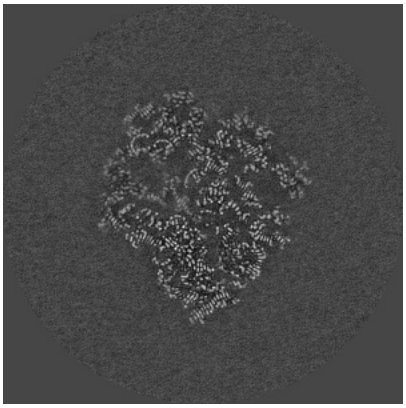


Y Index: 315

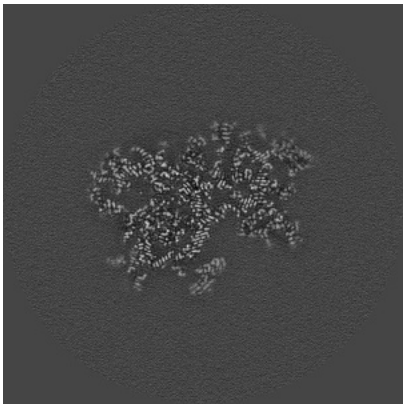


Z Index: 283

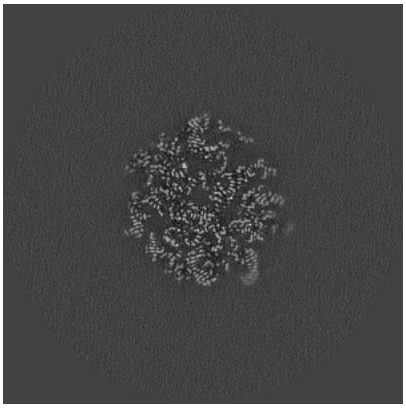
6.3.2 Raw map



X Index: 247



Y Index: 280

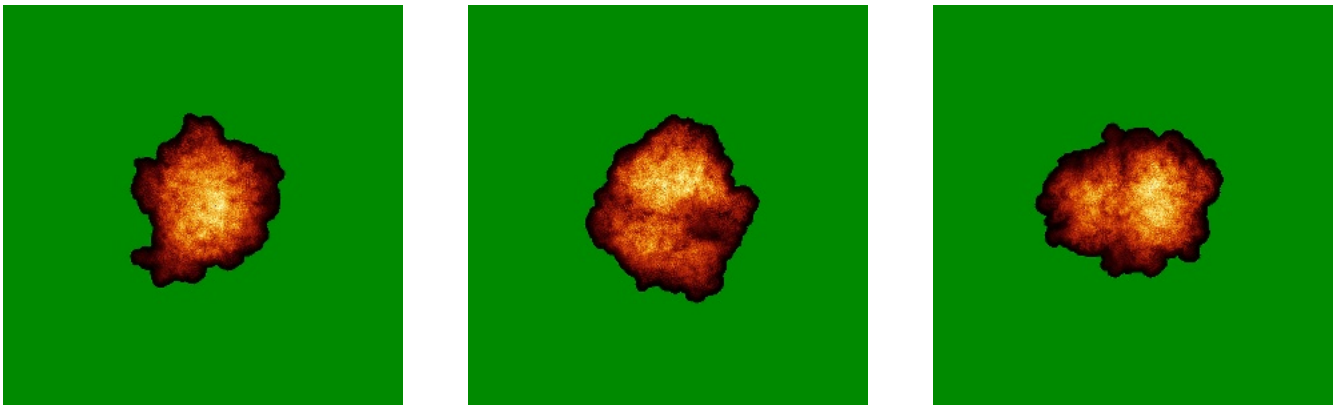


Z Index: 210

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

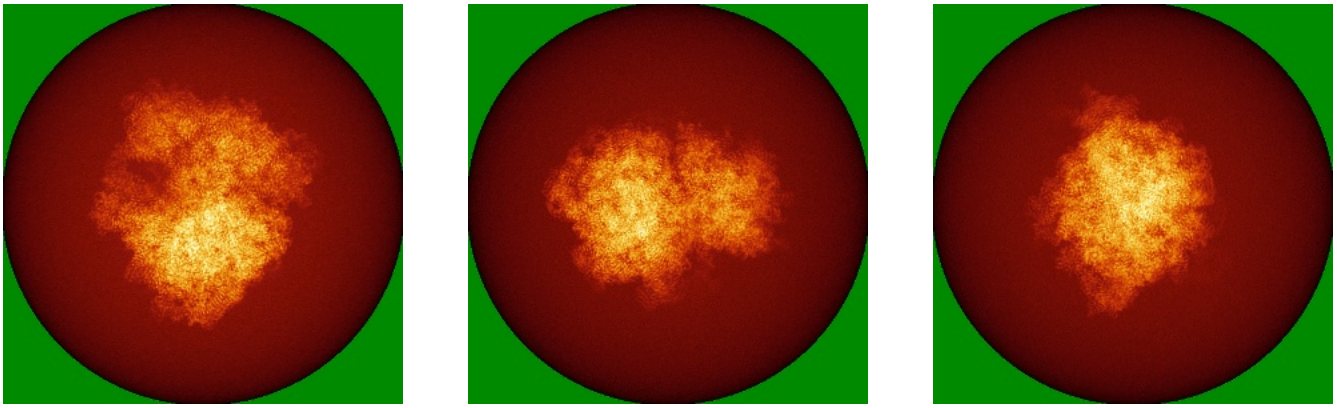
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

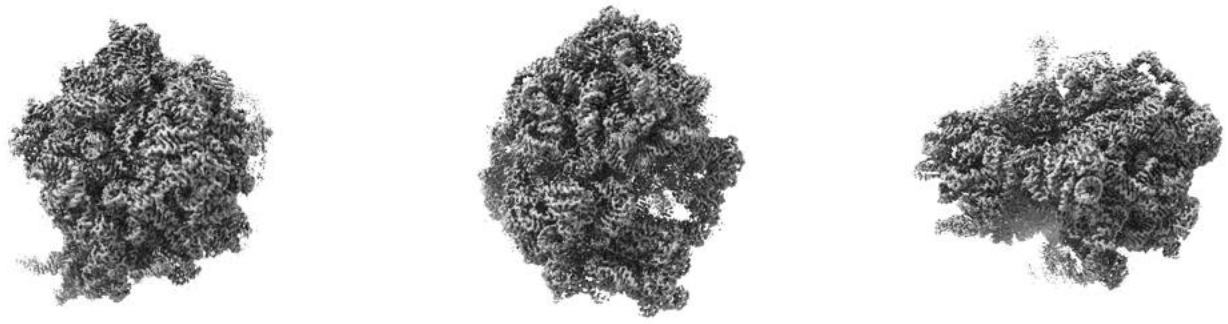


X Y Z

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)

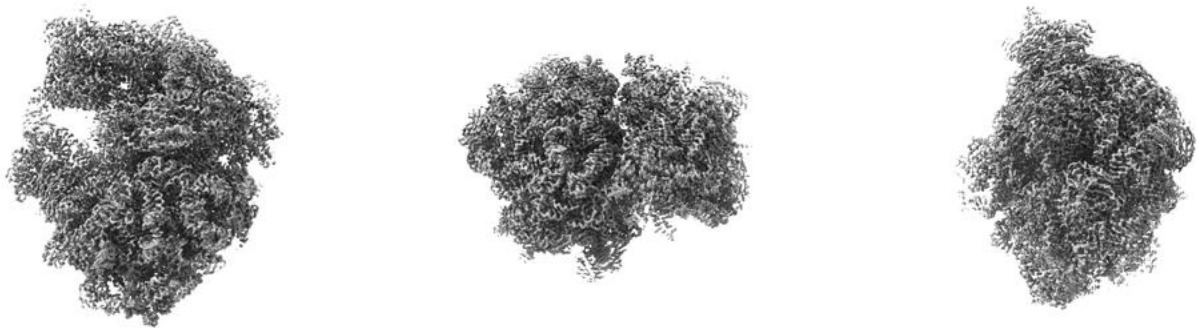
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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



X Y Z

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.

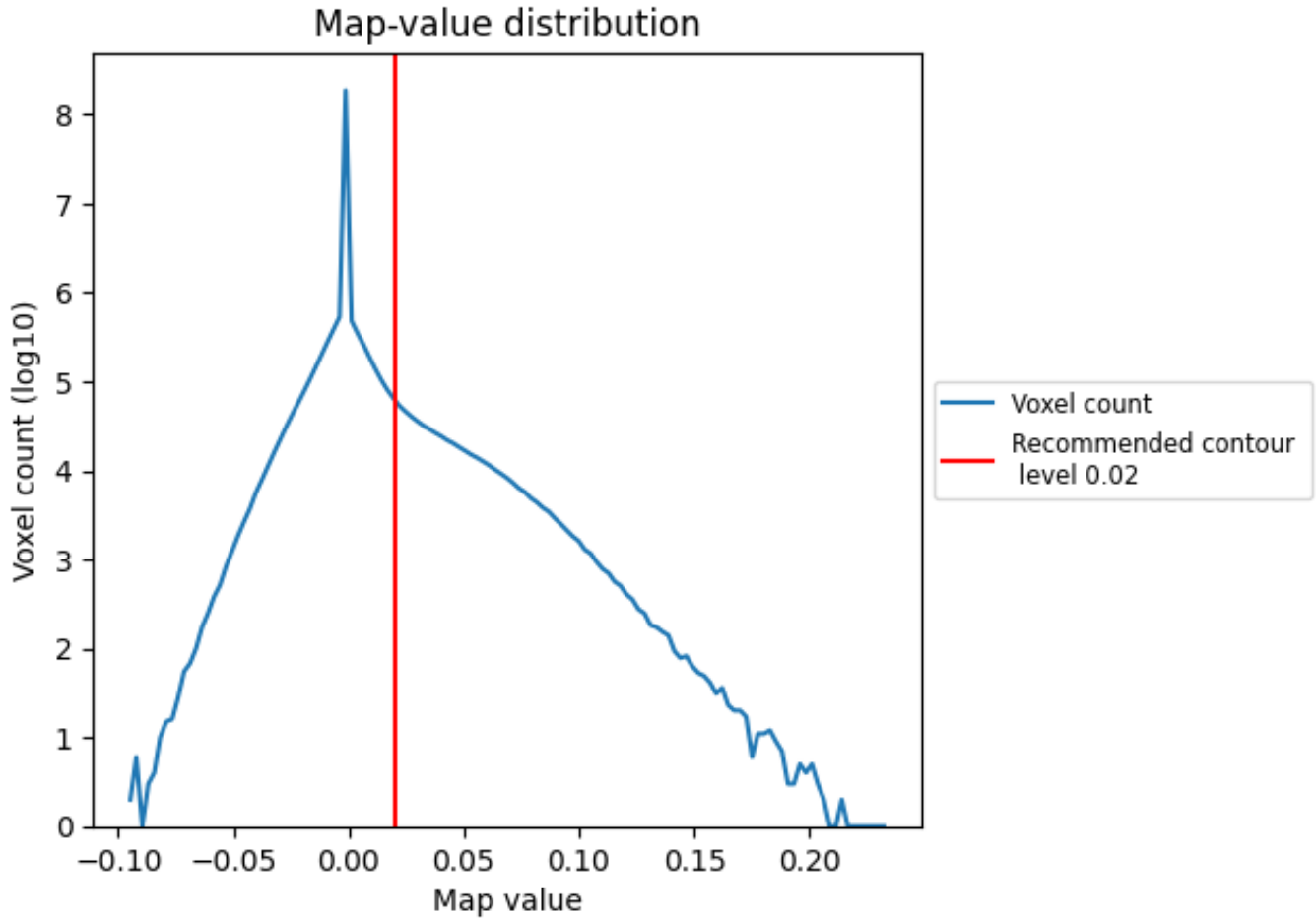
6.6 Mask visualisation (i)

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

7 Map analysis

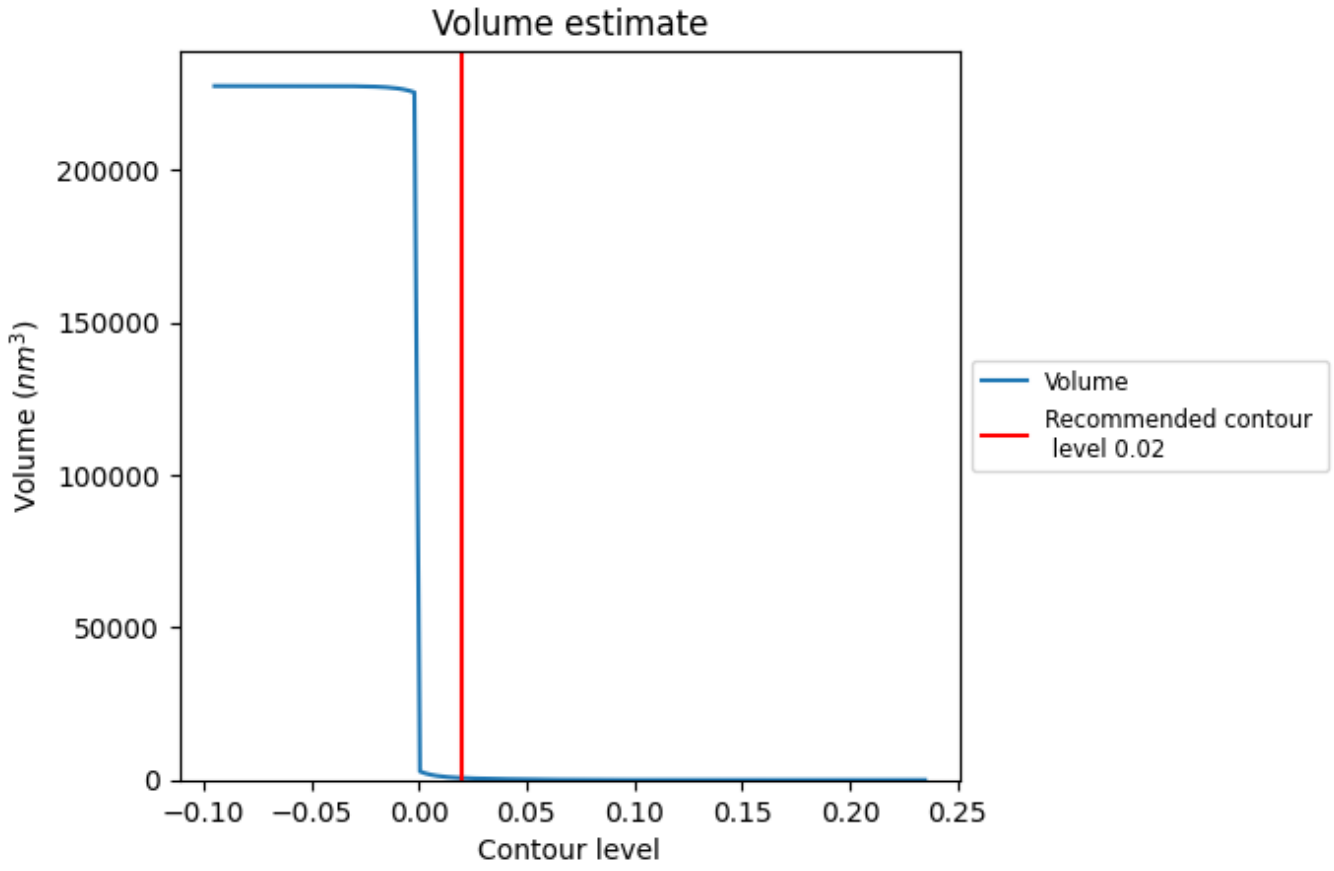
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

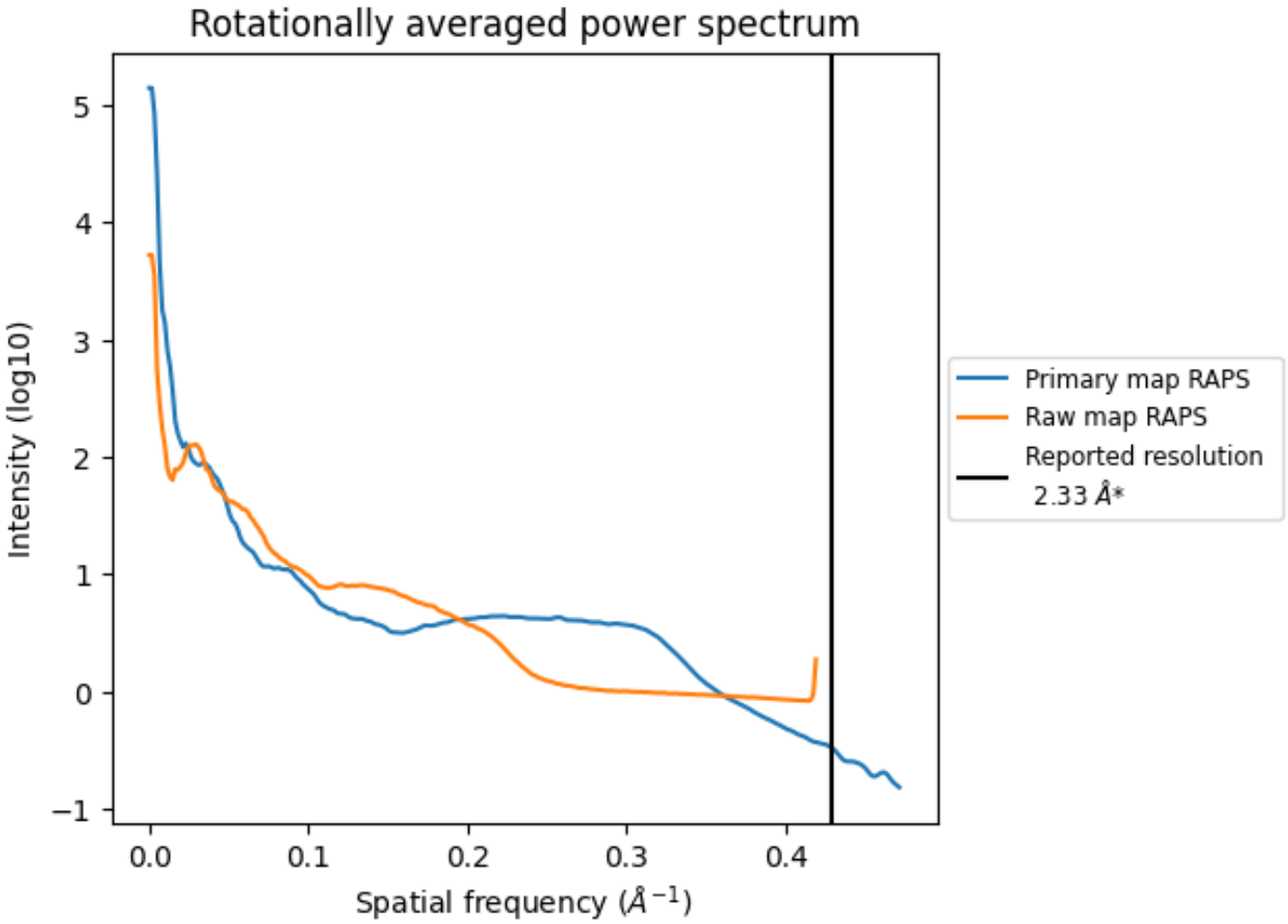
7.2 Volume estimate (i)



The volume at the recommended contour level is 657 nm^3; this corresponds to an approximate mass of 593 kDa.

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

7.3 Rotationally averaged power spectrum (i)

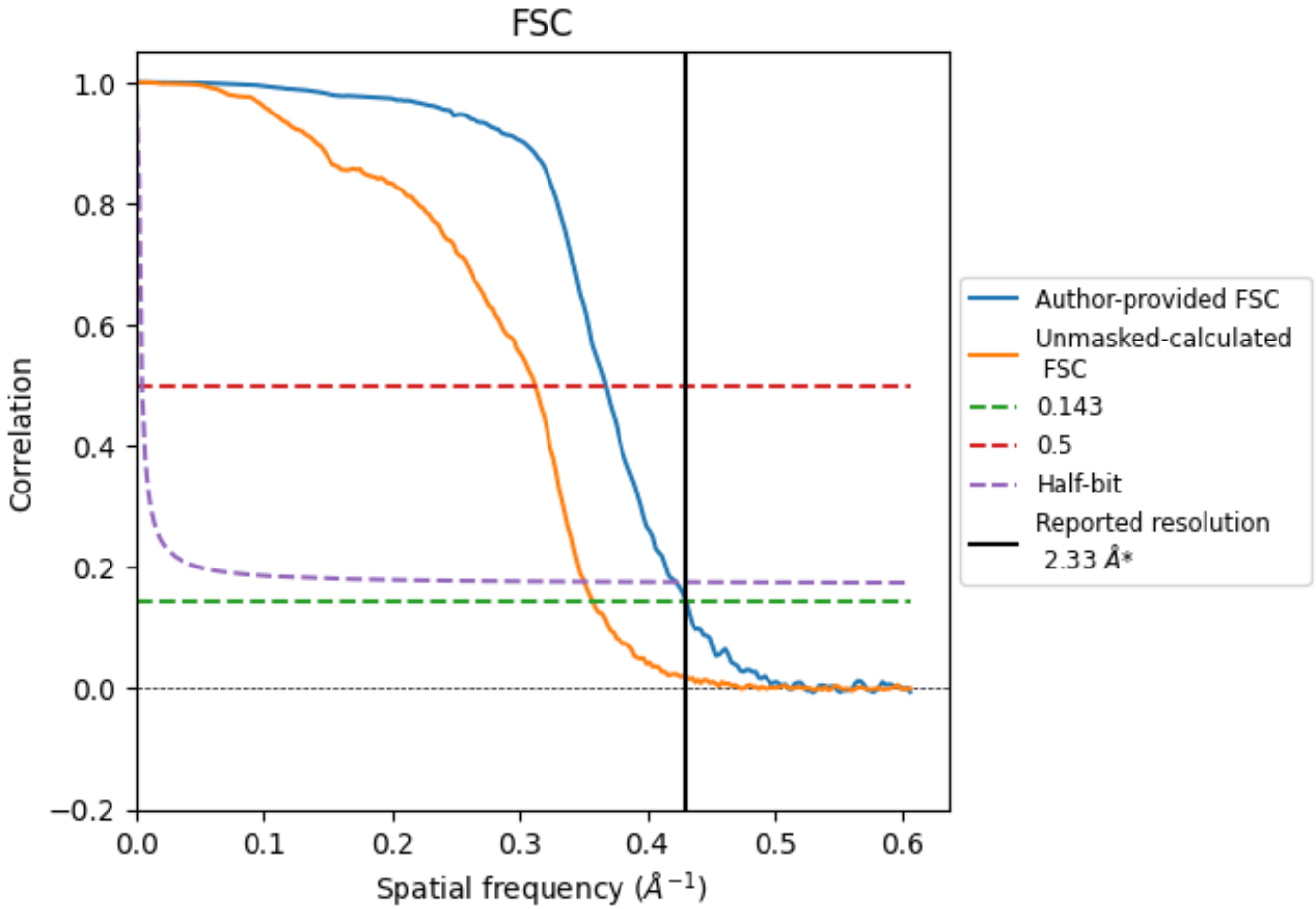


*Reported resolution corresponds to spatial frequency of 0.429 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.429 $Å^{-1}$

8.2 Resolution estimates (i)

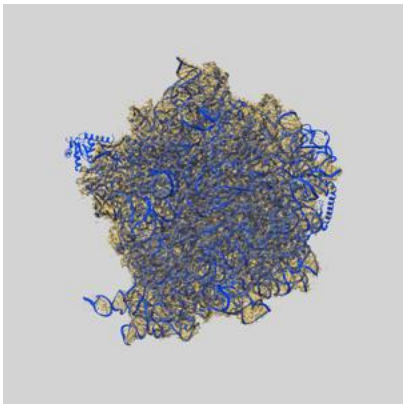
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.33	-	-
Author-provided FSC curve	2.32	2.72	2.37
Unmasked-calculated*	2.80	3.20	2.85

*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 2.80 differs from the reported value 2.33 by more than 10 %

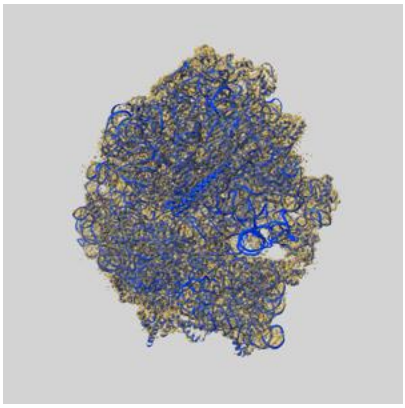
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24120 and PDB model 7N1P. Per-residue inclusion information can be found in section 3 on page 19.

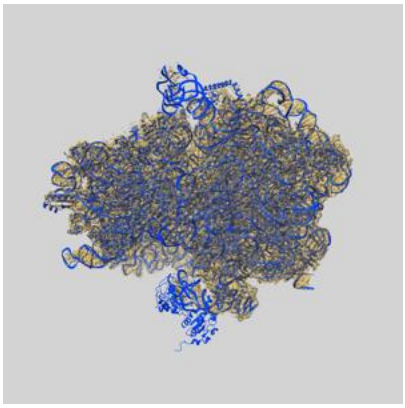
9.1 Map-model overlay



X



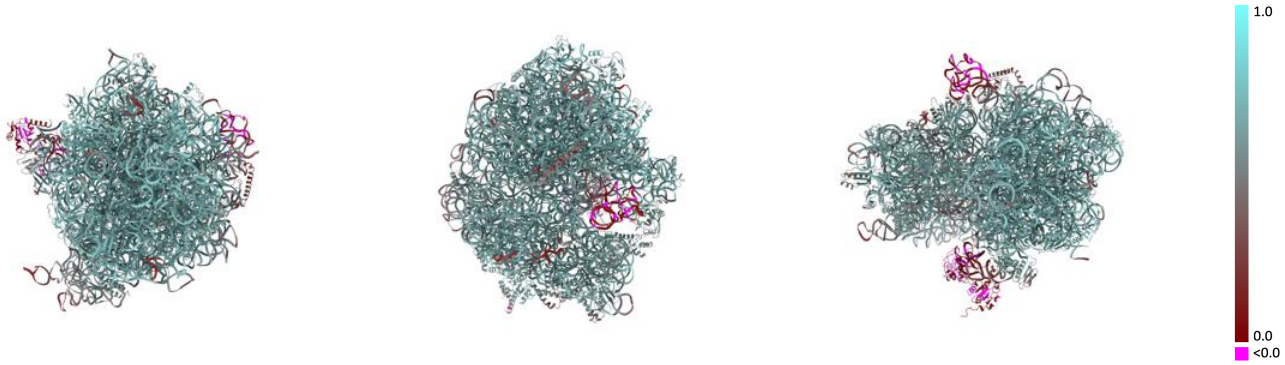
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

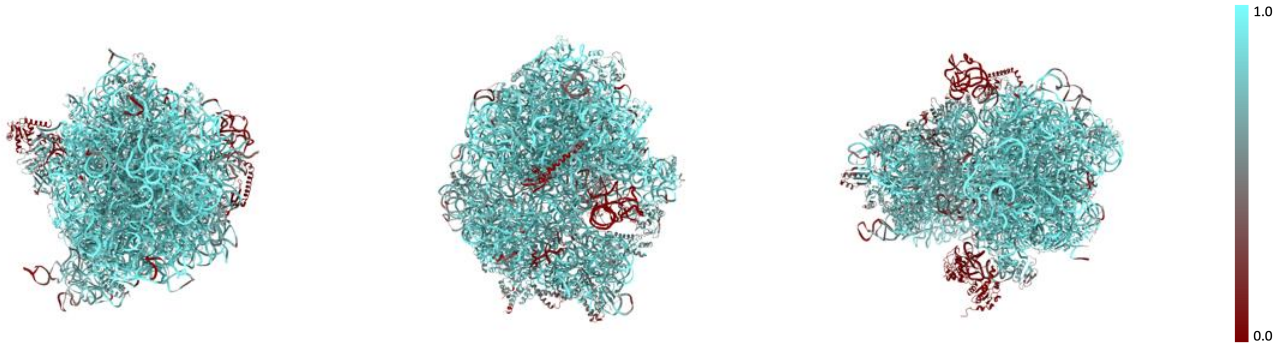
9.2 Q-score mapped to coordinate model



X Y Z

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

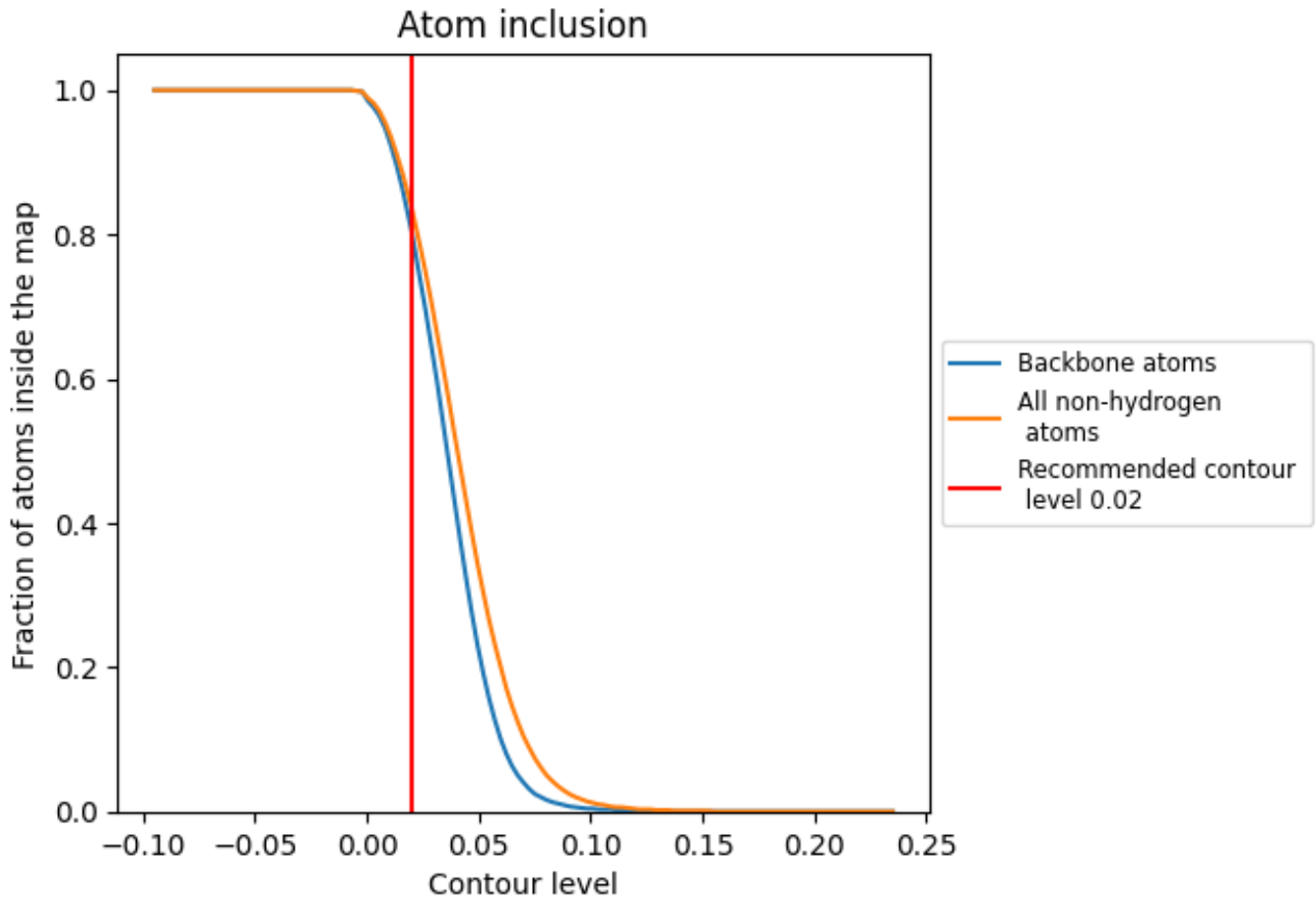
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 84% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8380	0.6240
16	0.8870	0.6290
23	0.8930	0.6400
5	0.9020	0.6400
Dt	0.7420	0.5980
LB	0.9210	0.6960
LC	0.9110	0.6790
LD	0.8380	0.6570
LE	0.6320	0.5760
LF	0.6830	0.5700
LI	0.2340	0.4160
LJ	0.0040	0.0320
LK	0.0010	0.0320
LM	0.9010	0.6870
LN	0.8660	0.6810
LO	0.9000	0.6740
LP	0.9100	0.6950
LQ	0.9340	0.7020
LR	0.7900	0.6220
LS	0.8550	0.6650
LT	0.9360	0.7080
LU	0.8290	0.6630
LV	0.8760	0.6790
LW	0.7880	0.6490
LX	0.7840	0.6170
LY	0.8270	0.6400
La	0.8590	0.6790
Lb	0.8850	0.6800
Lc	0.7120	0.6220
Ld	0.8580	0.6540
Le	0.5030	0.5010
Lf	0.8650	0.6800
Lg	0.8110	0.6540
Lh	0.9470	0.7100
Li	0.9490	0.7090



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lj	0.8800	0.6670
Pp	0.3210	0.4120
Pt	0.7090	0.5670
SB	0.6120	0.5660
SC	0.7470	0.6340
SD	0.7400	0.6140
SE	0.8610	0.6490
SF	0.6580	0.5790
SG	0.6700	0.5560
SH	0.8560	0.6560
SI	0.7300	0.6160
SJ	0.5810	0.5580
SK	0.7690	0.6220
SL	0.8600	0.6630
SM	0.7240	0.5910
SN	0.7620	0.6330
SO	0.7980	0.6360
SP	0.7540	0.5970
SQ	0.7930	0.6410
SR	0.7410	0.6090
SS	0.7250	0.5890
ST	0.7600	0.6130
SU	0.5320	0.5550
mR	0.3630	0.3990