Full wwPDB EM Validation Report ⓘ

Sep 16, 2026 – 10:23 PM EDT

PDB ID	:	7N2U / pdb_00007n2u
EMDB ID	:	EMD-24133
Title	:	Elongating 70S ribosome complex in a hybrid-H1 pre-translocation (PRE-H1) conformation
Authors	:	Rundlet, E.J.; Holm, M.; Schacherl, M.; Natchiar, K.S.; Altman, R.B.; Spahn, C.M.T.; Myasnikov, A.G.; Blanchard, S.C.
Deposited on	:	2021-05-29
Resolution	:	2.53 Å(reported)

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

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

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

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

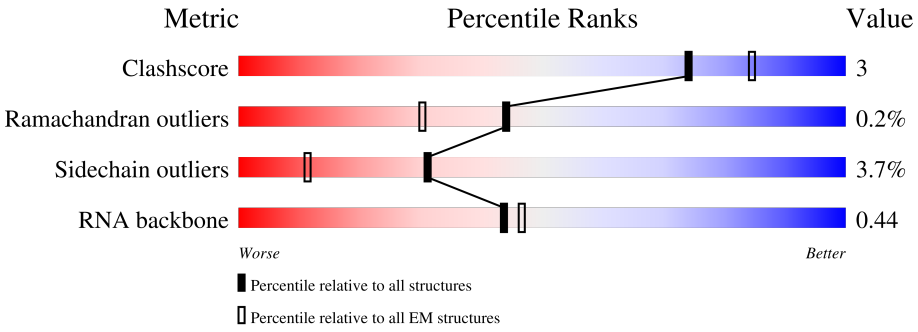
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

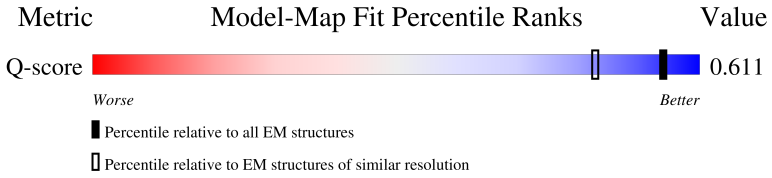
1 Overall quality at a glance

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

The reported resolution of this entry is 2.53 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	7309 (2.03 - 3.03)

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	1534	6% 64% 33% ·
2	SB	241	19% 84% 10% 5%
3	SC	233	11% 79% 11% · 9%

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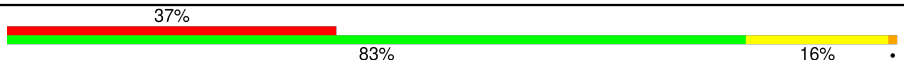
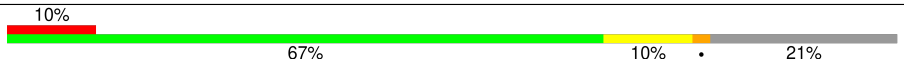
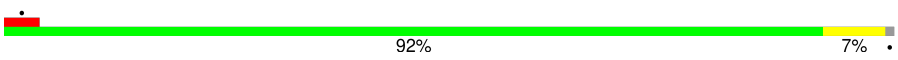
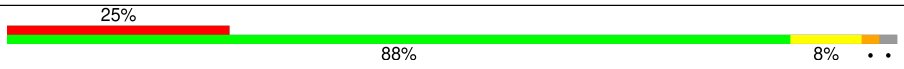
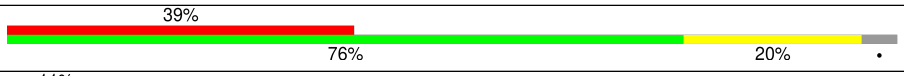
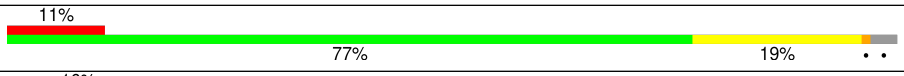
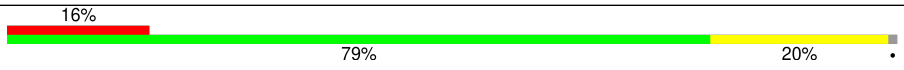
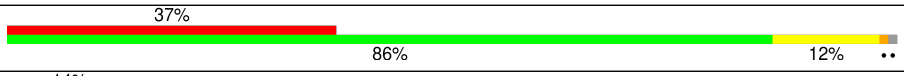
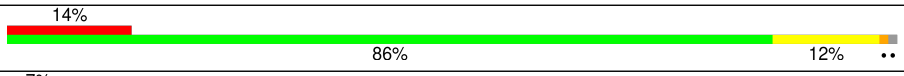
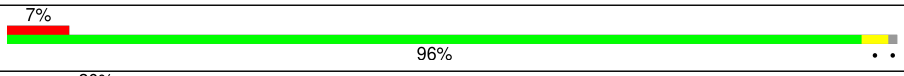
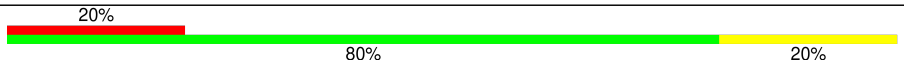
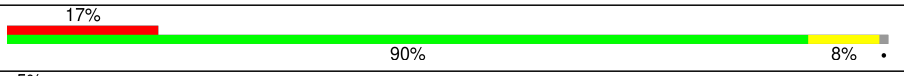
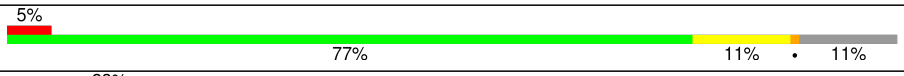
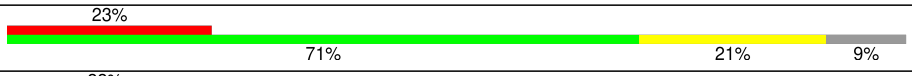
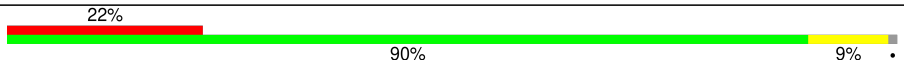
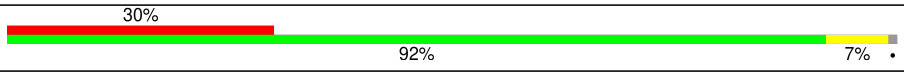
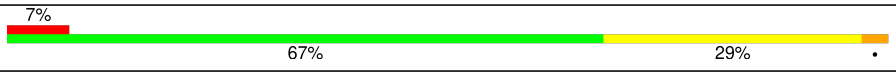
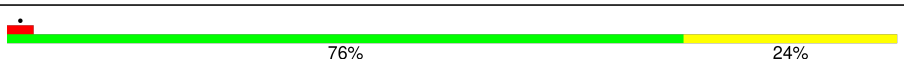
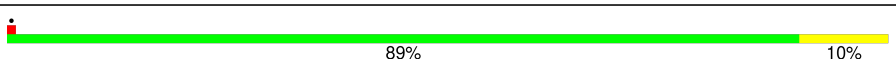
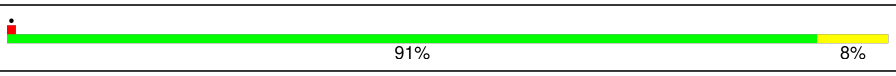
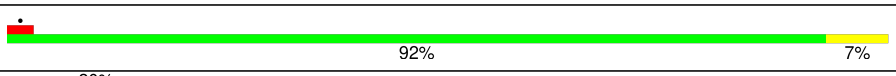
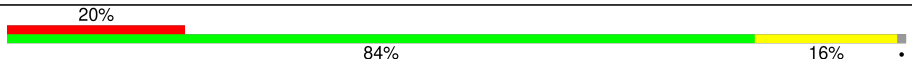
Mol	Chain	Length	Quality of chain
4	SD	206	
5	SE	167	
6	SF	135	
7	SG	179	
8	SH	130	
9	SI	130	
10	SJ	103	
11	SK	129	
12	SL	124	
13	SM	118	
14	SN	101	
15	SO	89	
16	SP	82	
17	SQ	84	
18	SR	75	
19	SS	92	
20	ST	87	
21	SU	71	
22	mR	60	
23	23	2904	
24	5	120	
25	LB	273	
26	LC	209	
27	LD	201	
28	LE	179	

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Mol	Chain	Length	Quality of chain
29	LF	177	10% 82% 16%
30	LI	149	79% 80% 18%
31	LM	142	92% 8%
32	LN	123	83% 16%
33	LO	144	88% 12%
34	LP	136	88% 12%
35	LQ	127	87% 9%
36	LR	117	87% 11%
37	LS	115	8% 92% 6%
38	LT	118	91% 7%
39	LU	103	89% 10%
40	LV	110	93% 7%
41	LW	100	5% 88% 5% 7%
42	LX	104	9% 85% 14%
43	LY	94	80% 20%
44	La	85	79% 8% 12%
45	Lb	78	85% 12%
46	Lc	63	6% 92% 5%
47	Ld	59	83% 14%
48	Le	70	51% 81% 13%
49	Lf	57	82% 16%
50	Lg	55	11% 85% 13%
51	Lh	46	91% 9%
52	Li	65	94% 5%
53	Lj	38	89% 8%

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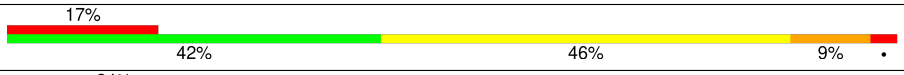
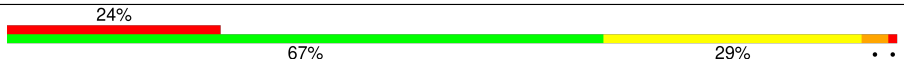
Mol	Chain	Length	Quality of chain
54	Pp	3	
55	Pt	76	
56	Dt	76	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 146877 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	16	1534	32930	14694	6041	10661	1534	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SB	228	1780	1125	319	328	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	1675	1060	314	296	5	2	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	1642	1026	315	297	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	156	1152	717	217	212	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	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SH	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
			1021	634	206	178	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	125	Total	C	N	O	S	0	0
			945	583	192	167	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	117	Total	C	N	O	S	0	0
			910	564	183	160	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
			804	499	164	138	3		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SQ	83	Total	C	N	O	S	1	0
			683	431	128	121	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
			553	350	104	98	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SS	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	ST	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

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

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

- Molecule 22 is a RNA chain called mRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	23	2902	Total	C	N	O	P	0	0
			62315	27806	11465	20142	2902		

- 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	272	Total	C	N	O	S	0	0
			2092	1294	425	366	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
			1551	974	283	289	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	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LI	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LQ	122	Total	C	N	O	S	0	0
			974	602	199	168	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LS	114	Total	C	N	O	S	1	0
			926	579	181	165	1		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
42	LX	103	Total	C	N	O	0	0
			788	498	148	142		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	La	75	Total	C	N	O	S	0	0
			574	356	116	101	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Ld	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	Lg	54	Total	C	N	O	1	0
			452	290	85	77		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Li	64	Total	C	N	O	S	0	0
			503	323	105	73	2		

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

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

- Molecule 54 is a protein called Nascent peptide.

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

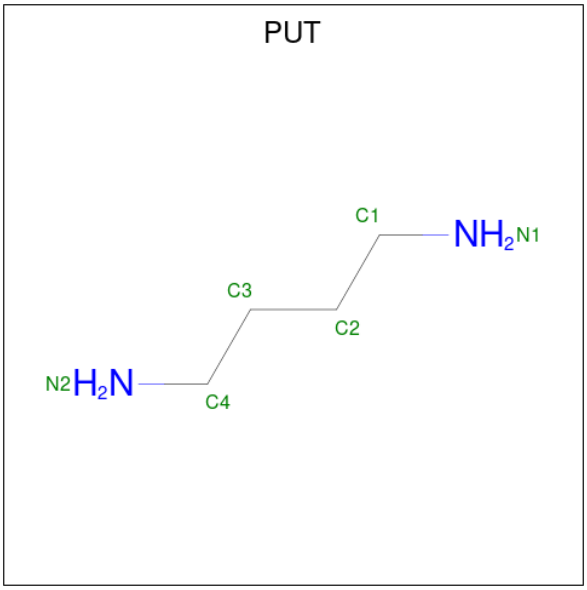
- Molecule 55 is a RNA chain called tRNA.

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

- Molecule 56 is a RNA chain called tRNA.

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

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



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

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

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

Mol	Chain	Residues	Atoms	AltConf
58	16	88	Total Mg 88 88	0
58	SN	1	Total Mg 1 1	0
58	23	267	Total Mg 267 267	0
58	5	5	Total Mg 5 5	0
58	LB	2	Total Mg 2 2	0
58	LC	1	Total Mg 1 1	0
58	LD	1	Total Mg 1 1	0
58	LQ	2	Total Mg 2 2	0
58	Lf	1	Total Mg 1 1	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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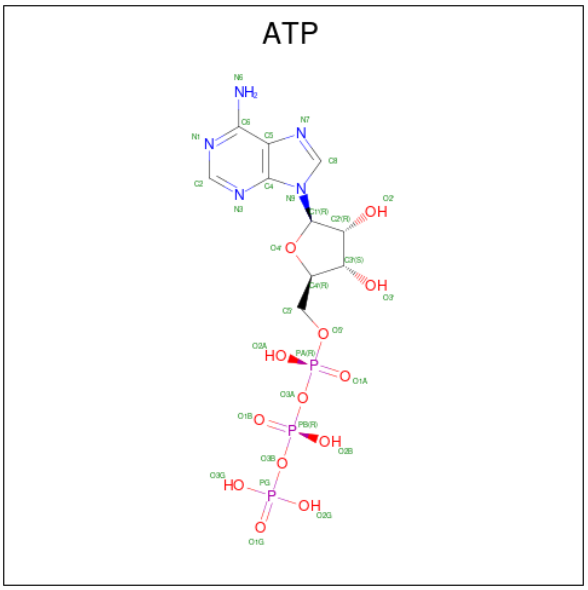
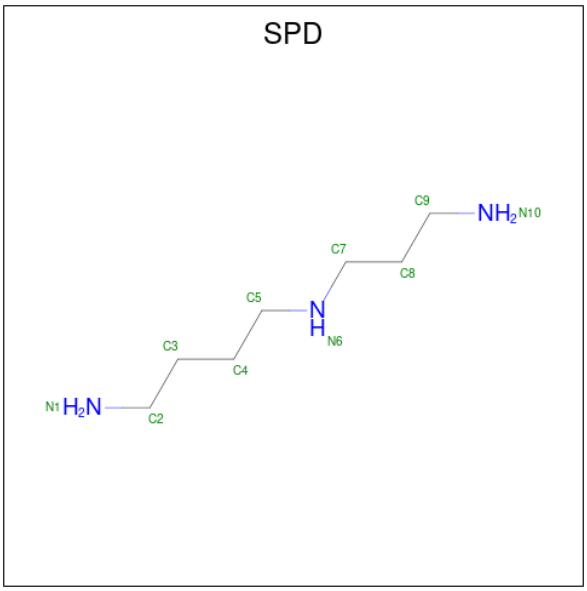
Mol	Chain	Residues	Atoms		AltConf
59	Lj	1	Total	Zn	0
			1	1	

- Molecule 60 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
60	23	1	Total	C	N	O	P	0
			31	10	5	13	3	
60	23	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 61 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



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

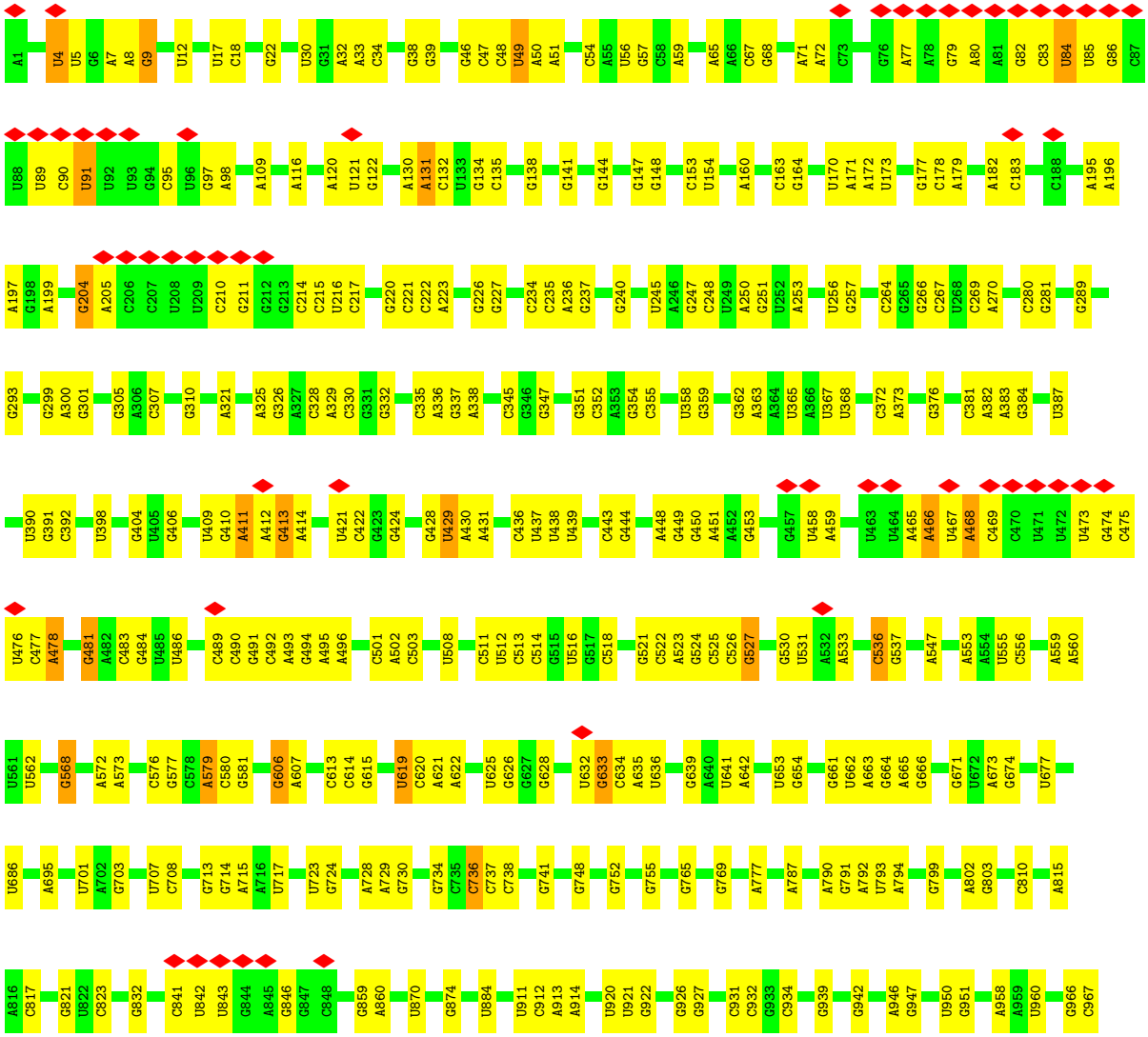
3 Residue-property plots (i)

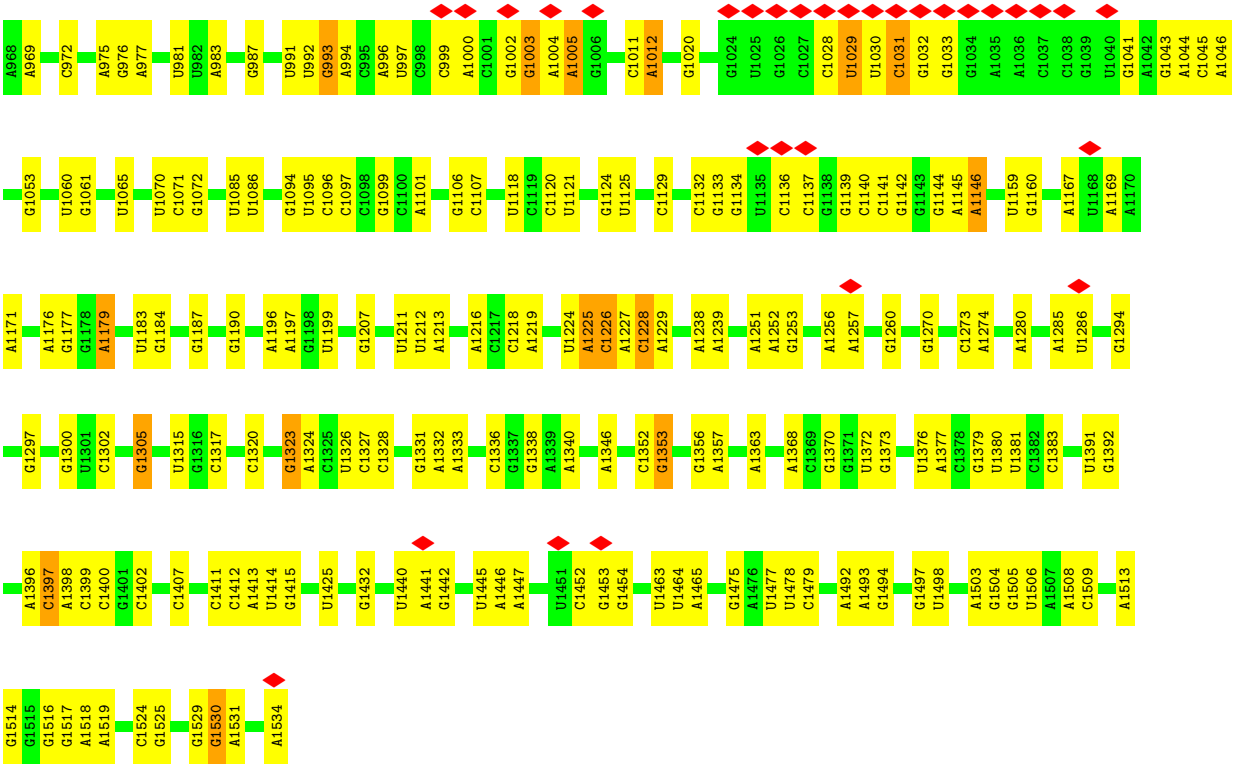
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



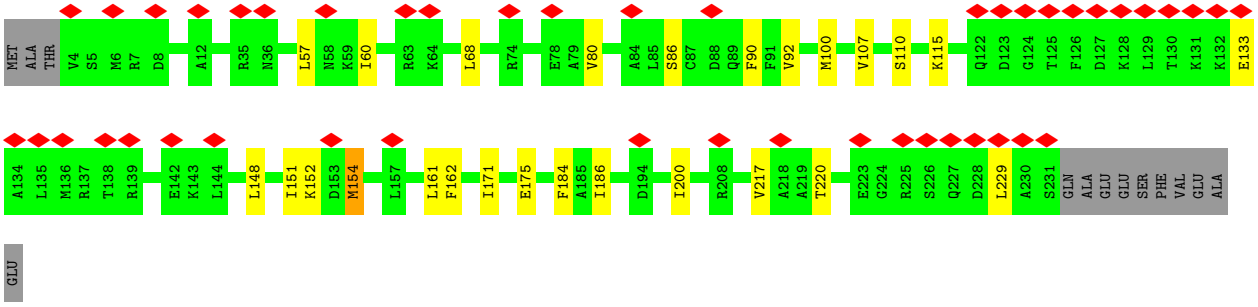




• Molecule 2: 30S ribosomal protein S2

Chain SB:

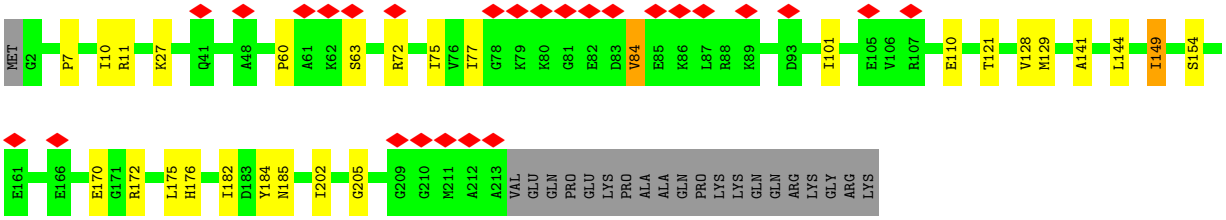




• Molecule 3: 30S ribosomal protein S3

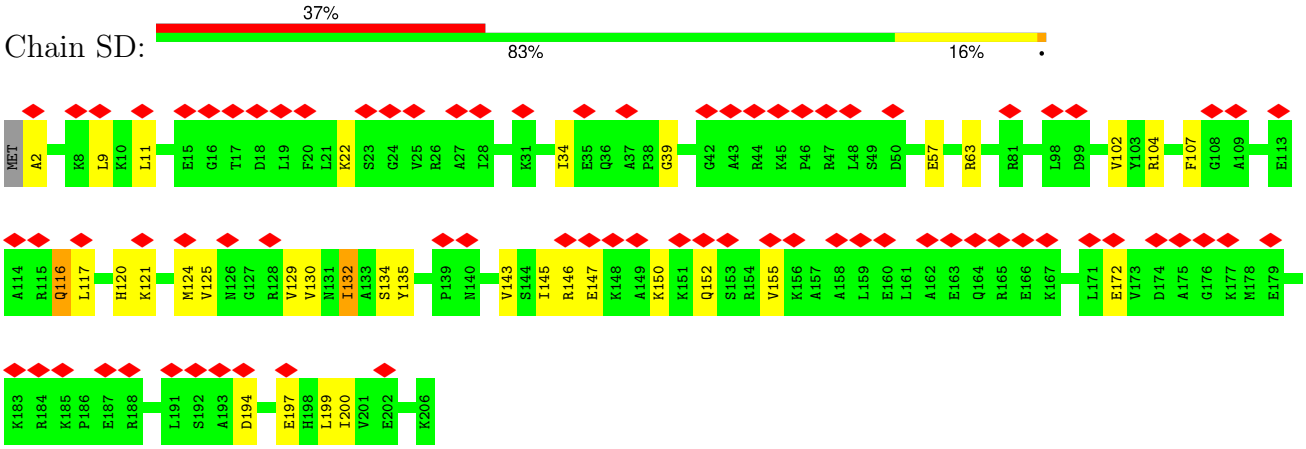
Chain SC:





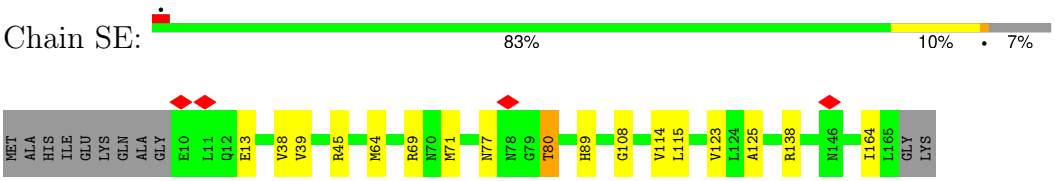
• Molecule 4: 30S ribosomal protein S4

Chain SD:



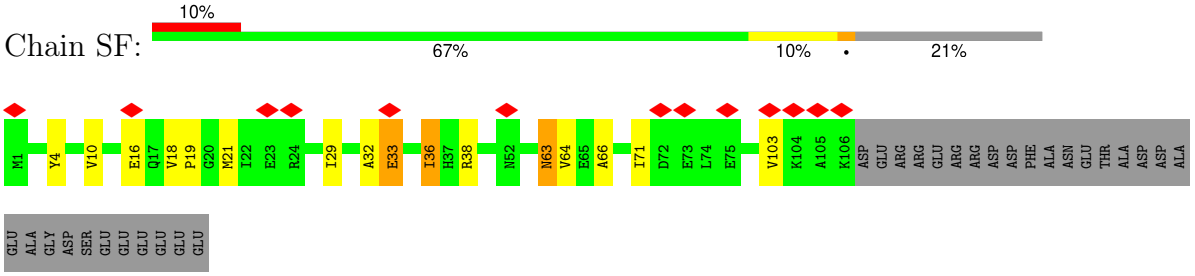
• Molecule 5: 30S ribosomal protein S5

Chain SE:



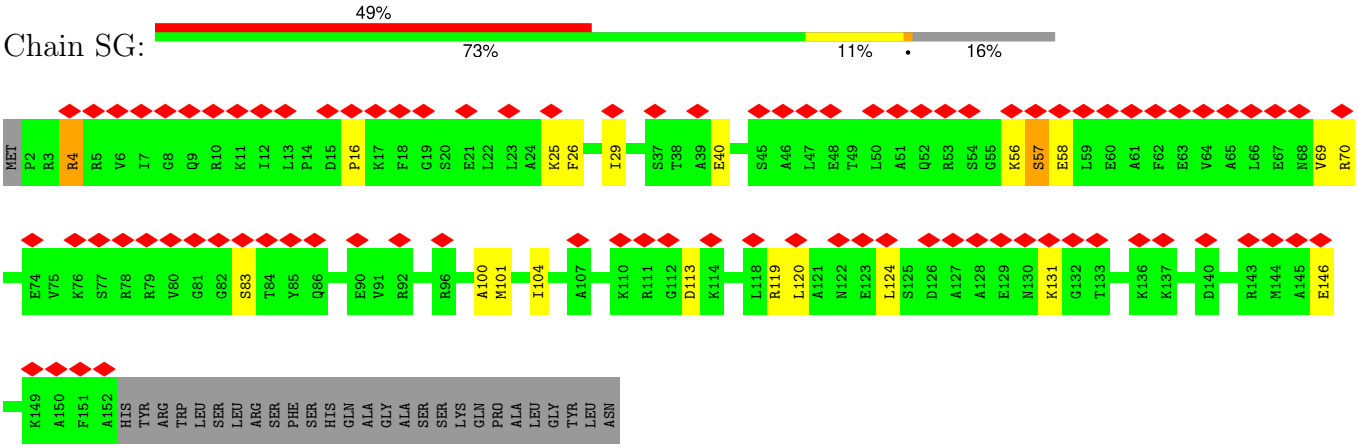
• Molecule 6: 30S ribosomal protein S6

Chain SF:



• Molecule 7: 30S ribosomal protein S7

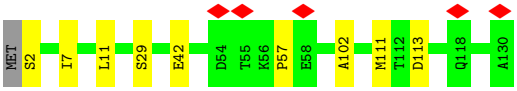
Chain SG:



• Molecule 8: 30S ribosomal protein S8

Chain SH:

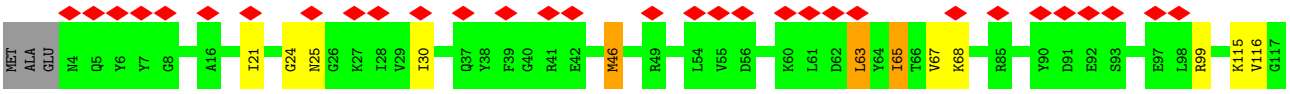




• Molecule 9: 30S ribosomal protein S9

Chain SI:



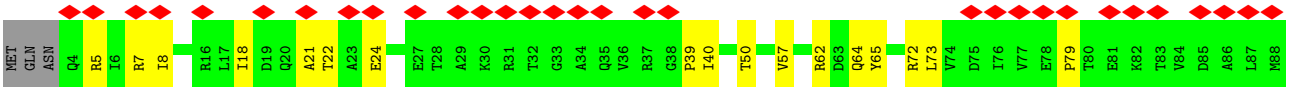


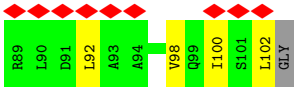


• Molecule 10: 30S ribosomal protein S10

Chain SJ:



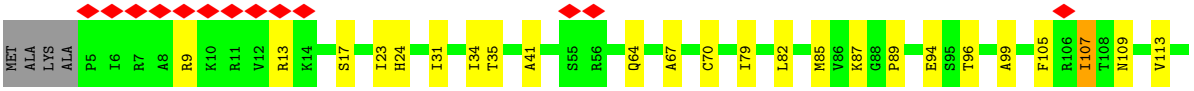


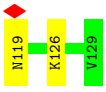


• Molecule 11: 30S ribosomal protein S11

Chain SK:



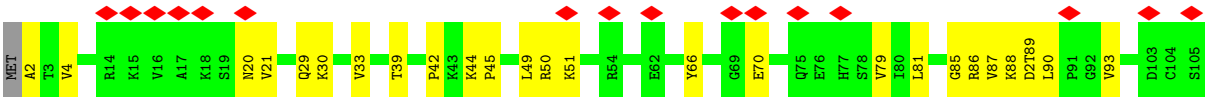


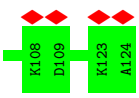


• Molecule 12: 30S ribosomal protein S12

Chain SL:

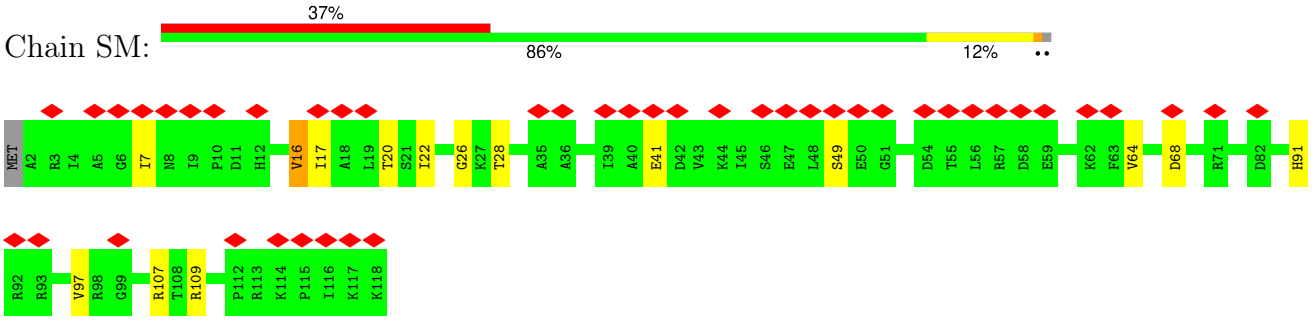






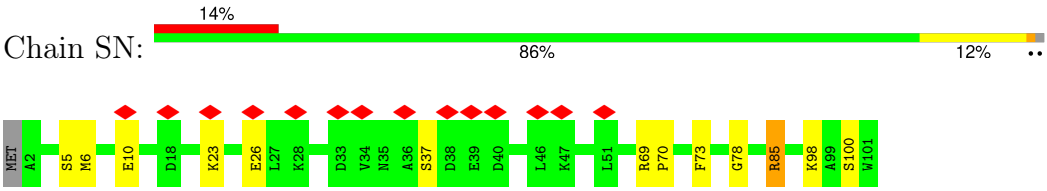
• Molecule 13: 30S ribosomal protein S13

Chain SM:



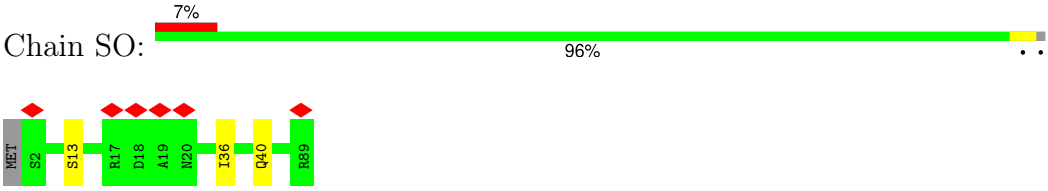
• Molecule 14: 30S ribosomal protein S14

Chain SN:



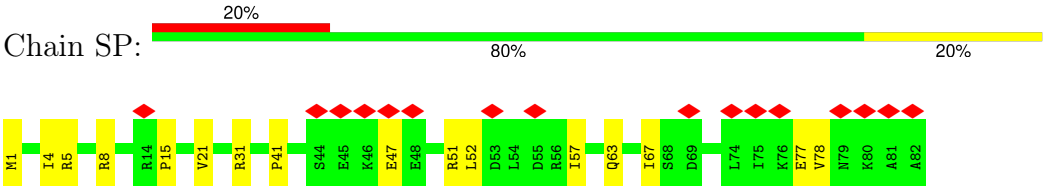
• Molecule 15: 30S ribosomal protein S15

Chain SO:



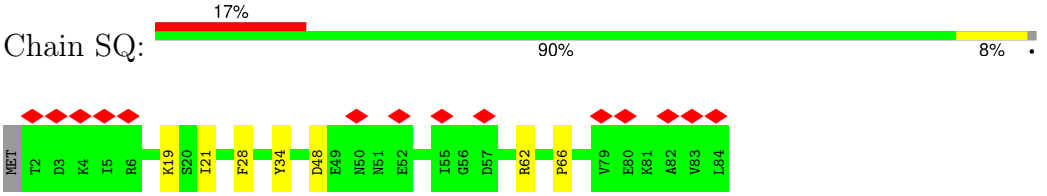
• Molecule 16: 30S ribosomal protein S16

Chain SP:



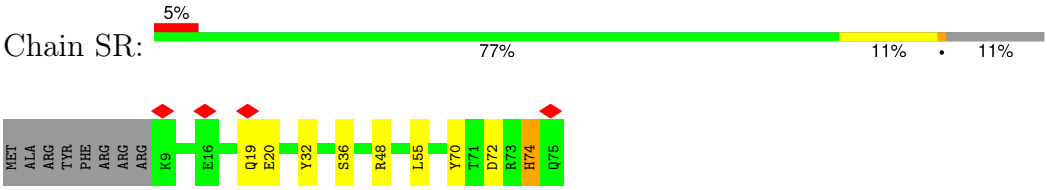
• Molecule 17: 30S ribosomal protein S17

Chain SQ:



• Molecule 18: 30S ribosomal protein S18

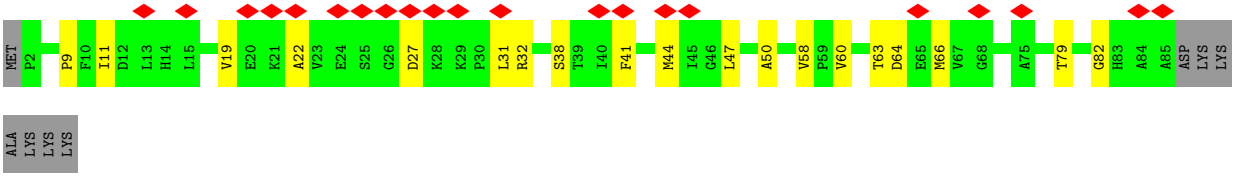
Chain SR:



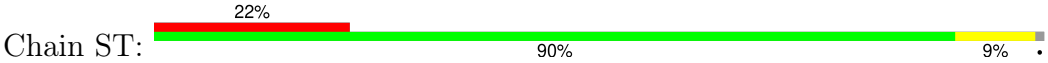
• Molecule 19: 30S ribosomal protein S19

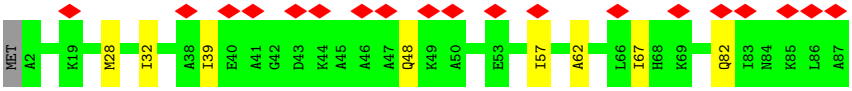
Chain SS:





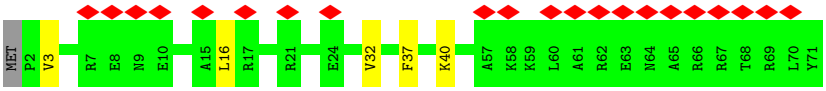
• Molecule 20: 30S ribosomal protein S20





• Molecule 21: 30S ribosomal protein S21





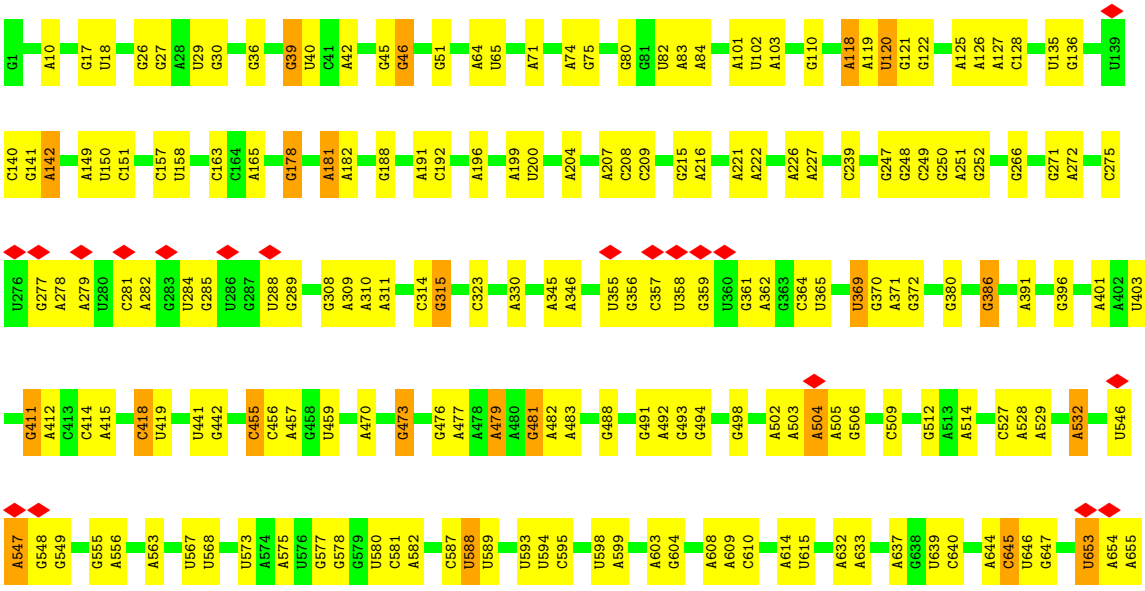
• Molecule 22: mRNA

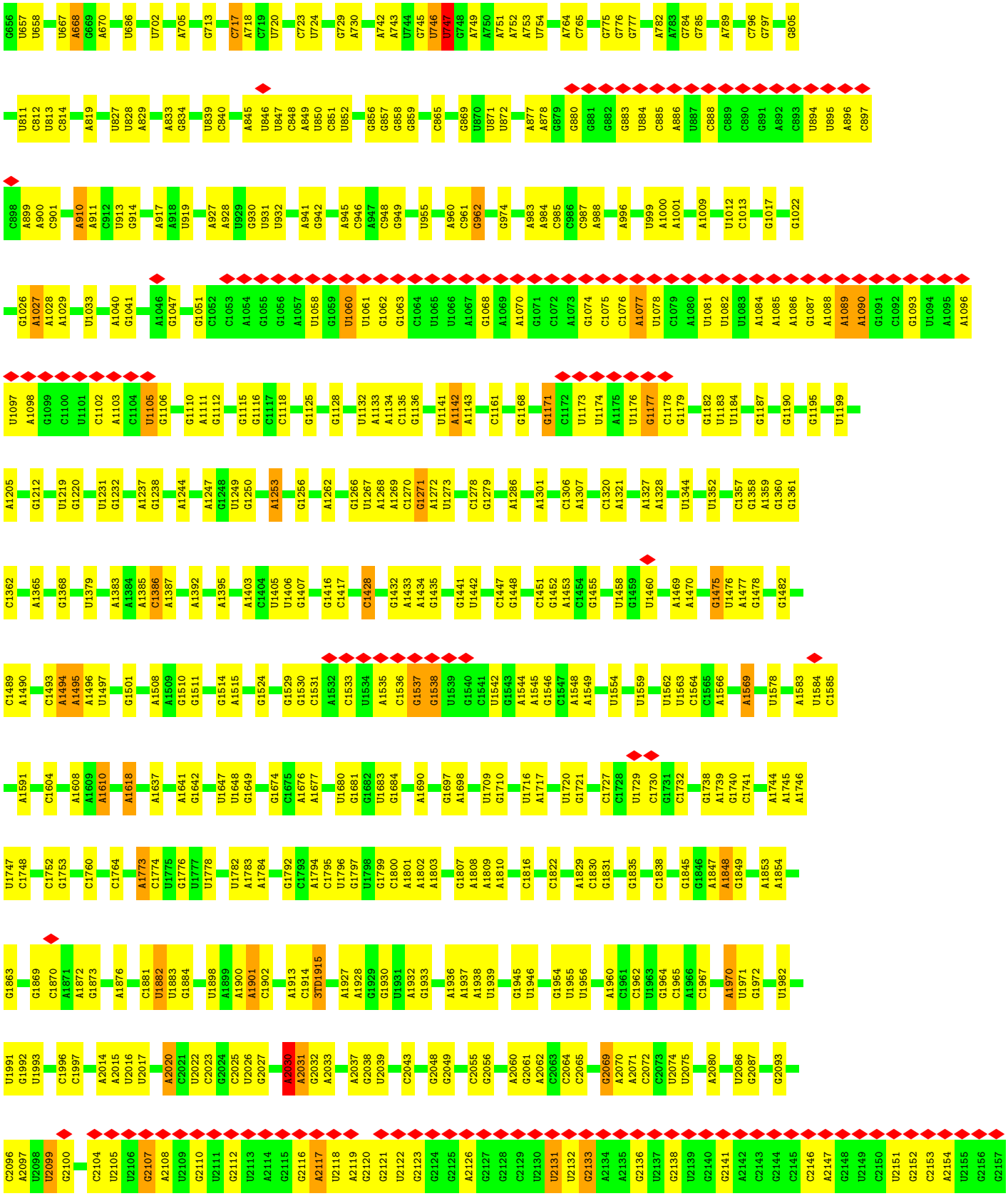


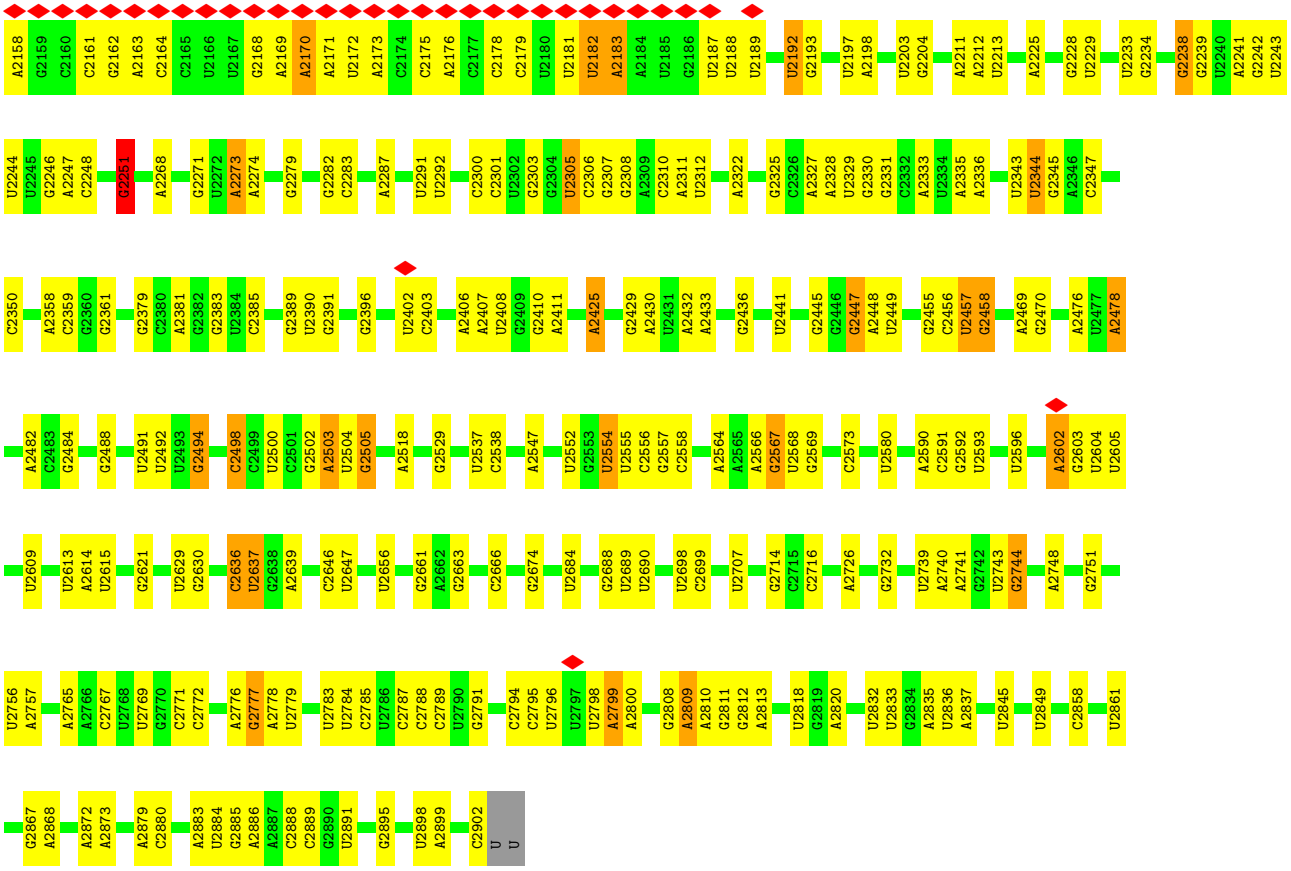


• Molecule 23: 23S rRNA





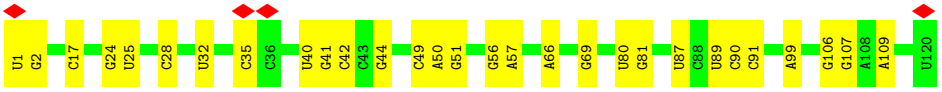




• Molecule 24: 5S rRNA

Chain 5:

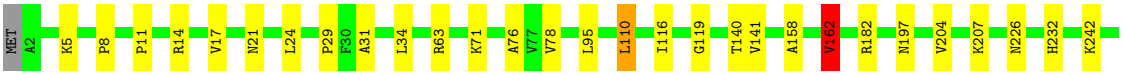




• Molecule 25: 50S ribosomal protein L2

Chain LB:

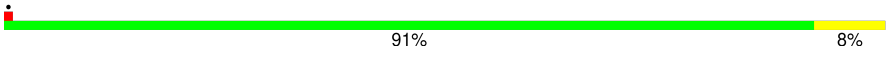


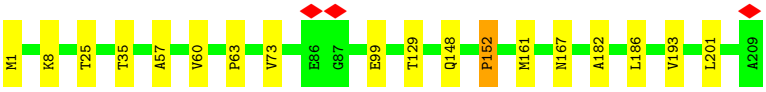




• Molecule 26: 50S ribosomal protein L3

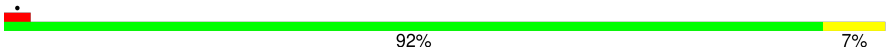
Chain LC:





• Molecule 27: 50S ribosomal protein L4

Chain LD:

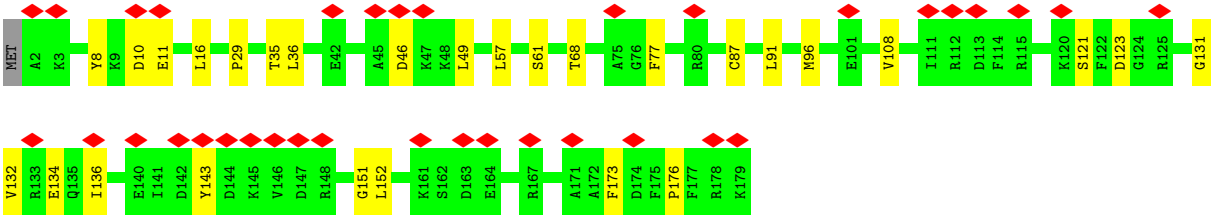




• Molecule 28: 50S ribosomal protein L5

Chain LE:

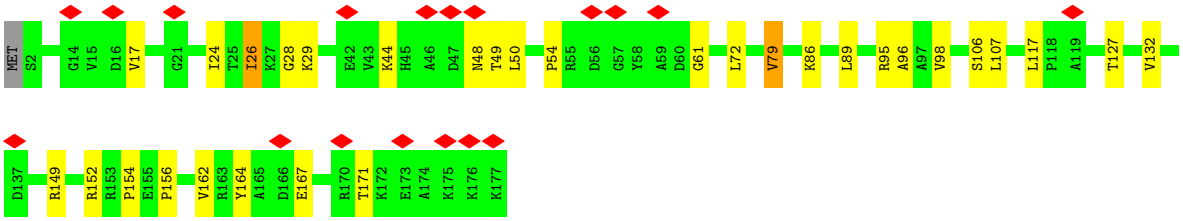




• Molecule 29: 50S ribosomal protein L6

Chain LF:

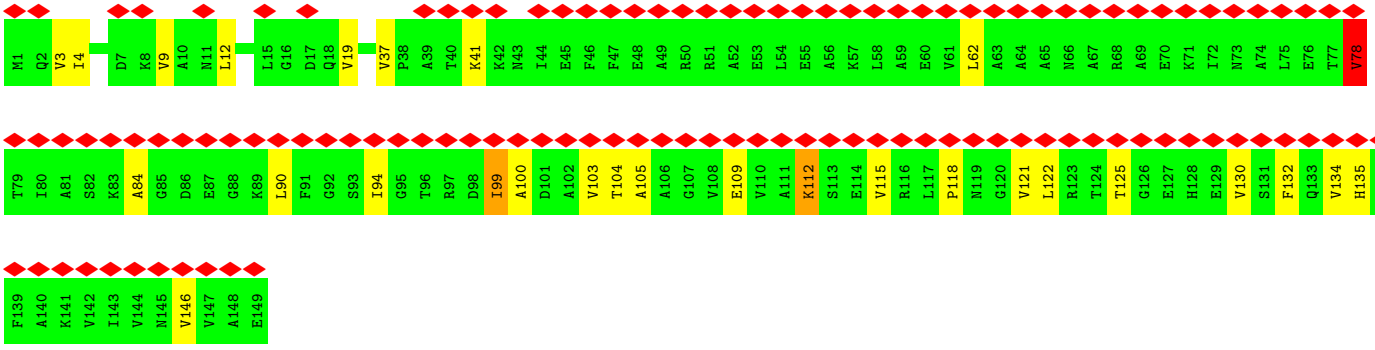




• Molecule 30: 50S ribosomal protein L9

Chain LI:

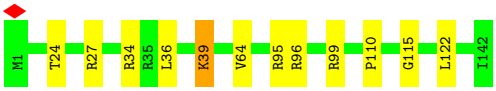




• Molecule 31: 50S ribosomal protein L13

Chain LM:

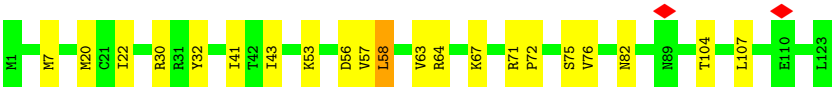




• Molecule 32: 50S ribosomal protein L14

Chain LN:

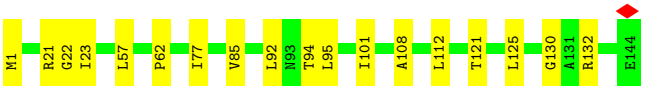




• Molecule 33: 50S ribosomal protein L15

Chain LO:

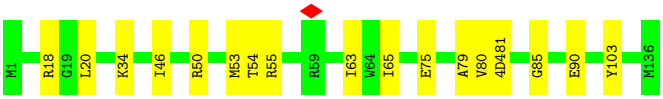




• Molecule 34: 50S ribosomal protein L16

Chain LP:

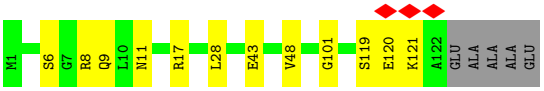




• Molecule 35: 50S ribosomal protein L17

Chain LQ:

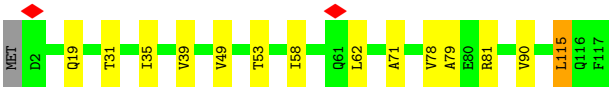




• Molecule 36: 50S ribosomal protein L18

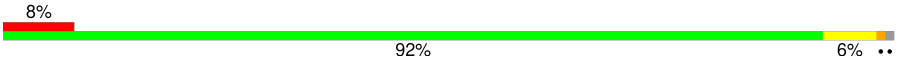
Chain LR:

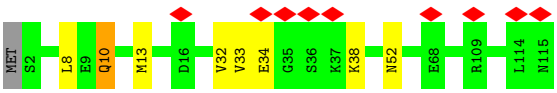




• Molecule 37: 50S ribosomal protein L19

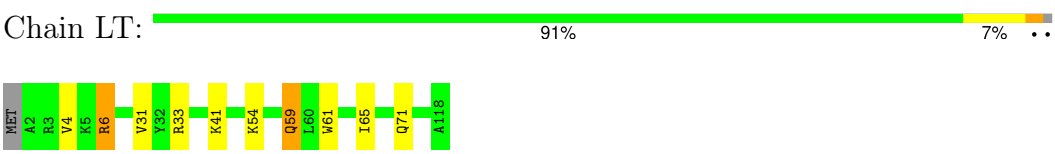
Chain LS:





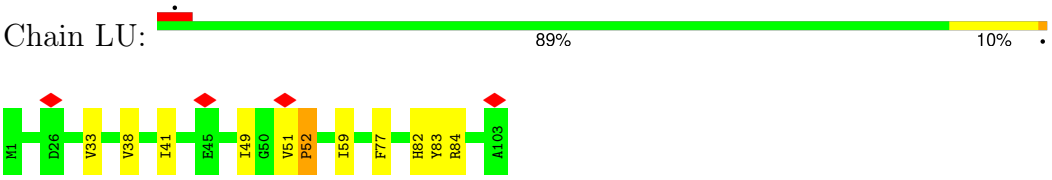
• Molecule 38: 50S ribosomal protein L20

Chain LT:



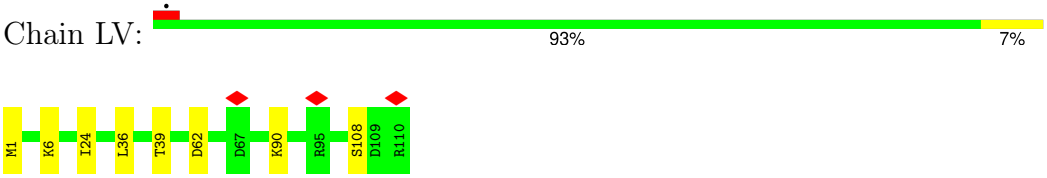
• Molecule 39: 50S ribosomal protein L21

Chain LU:



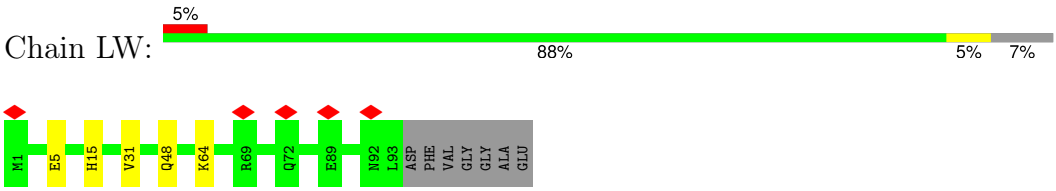
• Molecule 40: 50S ribosomal protein L22

Chain LV:



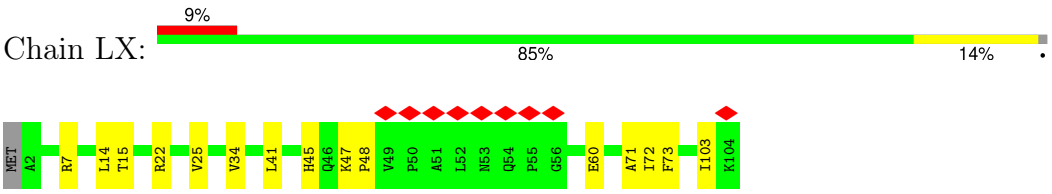
• Molecule 41: 50S ribosomal protein L23

Chain LW:



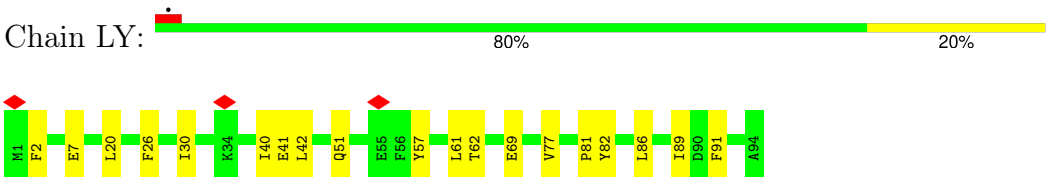
• Molecule 42: 50S ribosomal protein L24

Chain LX:



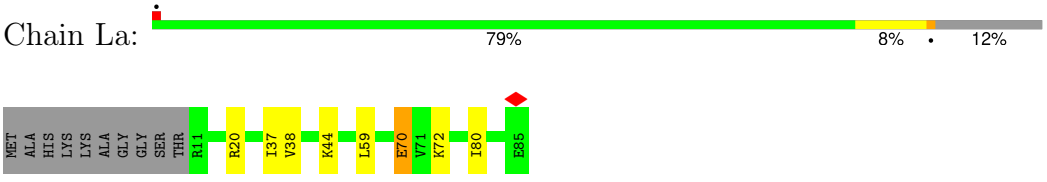
• Molecule 43: 50S ribosomal protein L25

Chain LY:



• Molecule 44: 50S ribosomal protein L27

Chain La:



• Molecule 45: 50S ribosomal protein L28

Chain Lb:

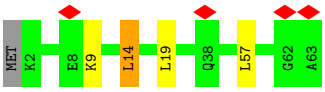




• Molecule 46: 50S ribosomal protein L29

Chain Lc:

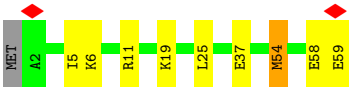




• Molecule 47: 50S ribosomal protein L30

Chain Ld:

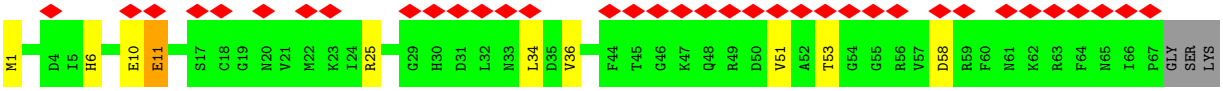




• Molecule 48: 50S ribosomal protein L31

Chain Le:

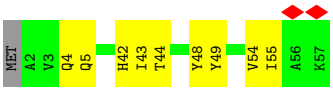




• Molecule 49: 50S ribosomal protein L32

Chain Lf:

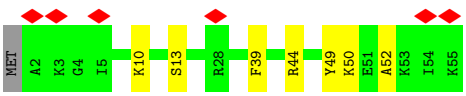




• Molecule 50: 50S ribosomal protein L33

Chain Lg:

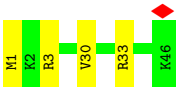




• Molecule 51: 50S ribosomal protein L34

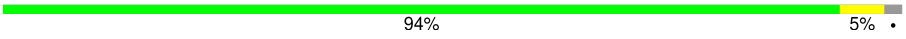
Chain Lh:

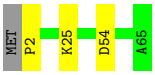




• Molecule 52: 50S ribosomal protein L35

Chain Li:





• Molecule 53: 50S ribosomal protein L36

Chain Lj:





• Molecule 54: Nascent peptide

Chain Pp:

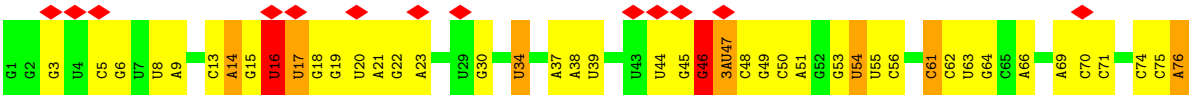




• Molecule 55: tRNA

Chain Pt:

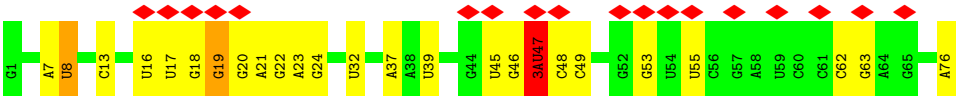




• Molecule 56: tRNA

Chain Dt:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51685	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	0.193	Depositor
Minimum map value	-0.084	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: 1MG, MA6, 6MZ, PSU, 2MA, 2MG, UR3, OMU, 3AU, T6A, MIA, 4D4, ATP, H2U, PUT, 3TD, 4OC, 5MU, 4SU, 5MC, ZN, G7M, OMC, OMG, SPD, U8U, MG, D2T

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	0.37	1/36593 (0.0%)	0.56	1/57081 (0.0%)
2	SB	0.60	0/1811	0.93	0/2440
3	SC	0.62	0/1702	0.95	1/2291 (0.0%)
4	SD	0.71	0/1664	1.04	1/2227 (0.0%)
5	SE	0.62	0/1165	0.98	1/1568 (0.1%)
6	SF	0.69	0/881	0.97	0/1189
7	SG	0.64	0/1195	1.00	1/1602 (0.1%)
8	SH	0.59	0/989	0.90	0/1326
9	SI	0.62	0/1033	0.93	1/1375 (0.1%)
10	SJ	0.73	0/805	1.04	0/1089
11	SK	0.78	0/962	1.12	0/1297
12	SL	0.63	0/960	1.04	2/1286 (0.2%)
13	SM	0.79	0/919	1.15	0/1226
14	SN	0.61	0/816	0.94	0/1088
15	SO	0.50	0/721	0.84	0/964
16	SP	0.71	0/658	1.04	0/884
17	SQ	0.62	0/692	0.88	0/927
18	SR	0.51	0/562	0.81	0/754
19	SS	0.74	0/685	1.02	2/922 (0.2%)
20	ST	0.67	0/675	1.03	0/895
21	SU	0.46	0/597	0.74	0/792
22	mR	0.44	0/261	0.62	0/404
23	23	0.39	0/69262	0.62	15/108048 (0.0%)
24	5	0.32	0/2873	0.50	0/4478
25	LB	0.73	0/2131	1.05	6/2863 (0.2%)
26	LC	0.70	0/1586	1.02	2/2134 (0.1%)
27	LD	0.56	0/1570	0.88	0/2113
28	LE	0.73	0/1444	1.07	0/1937
29	LF	0.50	0/1343	0.81	0/1816
30	LI	0.74	0/1121	1.05	0/1515
31	LM	0.53	0/1152	0.85	2/1551 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LN	0.67	0/956	1.00	0/1279
33	LO	0.72	0/1062	1.06	2/1413 (0.1%)
34	LP	0.60	0/1092	1.00	3/1457 (0.2%)
35	LQ	0.68	0/987	1.02	2/1319 (0.2%)
36	LR	0.59	0/902	0.99	0/1209
37	LS	0.64	0/938	0.97	0/1254
38	LT	0.65	0/960	0.98	0/1278
39	LU	0.59	0/829	0.85	0/1107
40	LV	0.54	0/864	0.88	1/1156 (0.1%)
41	LW	0.54	0/744	0.81	0/994
42	LX	0.57	0/796	0.85	0/1062
43	LY	0.44	0/766	0.72	0/1025
44	La	0.66	0/581	1.08	1/769 (0.1%)
45	Lb	0.63	0/635	0.97	1/848 (0.1%)
46	Lc	0.45	0/502	0.71	0/667
47	Ld	0.81	0/452	1.14	0/605
48	Le	0.76	0/539	1.08	0/721
49	Lf	0.56	0/450	0.89	1/599 (0.2%)
50	Lg	0.36	0/459	0.61	0/608
51	Lh	0.67	0/380	1.10	1/498 (0.2%)
52	Li	0.80	0/512	1.17	0/676
53	Lj	0.64	0/303	1.05	0/397
54	Pp	0.52	0/28	0.35	0/34
55	Pt	0.42	1/1595 (0.1%)	0.61	1/2479 (0.0%)
56	Dt	0.33	1/1650 (0.1%)	0.51	1/2568 (0.0%)
All	All	0.47	3/157810 (0.0%)	0.71	49/236104 (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	4
34	LP	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	Pt	76	A	C4'-O4'	-6.89	1.35	1.45
56	Dt	8	4SU	O3'-P	6.22	1.62	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	1498	UR3	O3'-P	5.44	1.61	1.56

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	LP	79	ALA	CA-C-N	-8.62	106.18	121.70
34	LP	79	ALA	C-N-CA	-8.62	106.18	121.70
23	23	1060	U	C2'-C3'-O3'	8.09	121.63	109.50
33	LO	22	GLY	CA-C-O	-7.30	117.48	122.22
35	LQ	120	GLU	N-CA-C	-7.21	104.22	112.87
23	23	204	A	C2'-C3'-O3'	-7.01	98.99	109.50
23	23	1142	A	C2'-C3'-O3'	-6.90	99.14	109.50
7	SG	4	ARG	CB-CA-C	-6.85	107.91	117.23
34	LP	85	GLY	CA-C-O	-6.55	117.73	122.45
56	Dt	19	G	C2'-C3'-O3'	6.46	119.19	109.50
23	23	2447	G	C2'-C3'-O3'	-6.36	99.96	109.50
23	23	2602	A	C4'-C3'-O3'	-6.26	103.61	113.00
12	SL	20	ASN	N-CA-C	-6.25	105.76	113.19
23	23	1237	A	C2'-C3'-O3'	-6.24	100.14	109.50
25	LB	119	GLY	CA-C-O	-6.14	117.36	122.33
23	23	1783	A	C4'-C3'-O3'	-6.07	103.90	113.00
55	Pt	75	C	O3'-P-O5'	6.04	113.06	104.00
26	LC	167	ASN	CB-CA-C	6.00	120.25	111.73
31	LM	24	THR	CB-CA-C	5.96	119.42	109.89
23	23	1385	A	C4'-C3'-O3'	-5.95	100.47	109.40
23	23	504	A	C2'-C3'-O3'	5.94	118.40	109.50
49	Lf	5	GLN	N-CA-C	-5.93	105.88	113.23
19	SS	82	GLY	CA-C-O	-5.92	118.05	122.37
25	LB	11	PRO	CA-C-N	-5.92	112.79	122.20
25	LB	11	PRO	C-N-CA	-5.92	112.79	122.20
51	Lh	3	ARG	CB-CA-C	5.69	120.29	110.45
23	23	404	A	C2'-C3'-O3'	5.68	118.03	109.50
31	LM	27	ARG	CB-CA-C	5.66	121.10	110.63
44	La	44	LYS	N-CA-C	-5.63	105.14	111.28
3	SC	205	GLY	CA-C-O	-5.60	118.58	122.22
23	23	2494	G	C3'-C2'-O2'	5.45	118.87	110.70
33	LO	22	GLY	N-CA-C	5.38	117.06	111.95
9	SI	24	GLY	CA-C-O	-5.33	117.72	121.88
25	LB	226	ASN	CB-CA-C	5.33	116.76	108.61
5	SE	69	ARG	N-CA-C	-5.33	103.00	110.35
23	23	455	C	C2'-C3'-O3'	5.22	117.33	109.50
40	LV	39	THR	CB-CA-C	5.22	118.65	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	LB	162	VAL	CA-C-N	-5.16	115.71	122.99
25	LB	162	VAL	C-N-CA	-5.16	115.71	122.99
4	SD	39	GLY	CA-C-O	-5.13	118.47	122.52
35	LQ	11	ASN	CB-CA-C	5.12	119.00	111.73
23	23	2637	U	C2'-C3'-O3'	-5.11	106.03	113.70
23	23	2331	G	C2'-C3'-O3'	-5.09	106.06	113.70
45	Lb	17	ASN	N-CA-C	-5.09	101.01	109.46
26	LC	152	PRO	N-CA-C	-5.02	102.12	112.47
23	23	2491	U	C4'-C3'-O3'	-5.02	105.47	113.00
12	SL	85	GLY	CA-C-O	-5.01	116.52	121.48
19	SS	58	VAL	CA-C-O	-5.01	116.19	119.15
1	16	1183	U	C4'-C3'-O3'	-5.01	105.49	113.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	LP	18[A]	ARG	Mainchain
34	LP	18[B]	ARG	Mainchain
3	SC	128	VAL	Mainchain
3	SC	27[A]	LYS	Mainchain
3	SC	27[B]	LYS	Mainchain

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	32930	0	16591	173	0
2	SB	1780	0	1805	10	0
3	SC	1675	0	1752	11	0
4	SD	1642	0	1707	17	0
5	SE	1152	0	1196	9	0
6	SF	862	0	864	9	0
7	SG	1181	0	1238	10	0
8	SH	979	0	1031	5	0
9	SI	1021	0	1070	7	0
10	SJ	795	0	836	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	SK	945	0	972	14	0
12	SL	957	0	1017	14	0
13	SM	910	0	978	6	0
14	SN	804	0	844	6	0
15	SO	713	0	734	1	0
16	SP	648	0	666	7	0
17	SQ	683	0	725	4	0
18	SR	553	0	573	4	0
19	SS	668	0	693	7	0
20	ST	669	0	719	4	0
21	SU	589	0	629	3	0
22	mR	234	0	118	1	0
23	23	62315	0	31365	300	0
24	5	2570	0	1301	7	0
25	LB	2092	0	2167	16	0
26	LC	1565	0	1616	9	0
27	LD	1551	0	1619	11	0
28	LE	1420	0	1457	12	0
29	LF	1323	0	1371	13	0
30	LI	1110	0	1148	18	0
31	LM	1129	0	1162	4	0
32	LN	947	0	1023	12	0
33	LO	1053	0	1129	16	0
34	LP	1086	0	1167	7	0
35	LQ	974	0	1018	6	0
36	LR	892	0	923	8	0
37	LS	926	0	969	5	0
38	LT	947	0	1019	6	0
39	LU	816	0	839	5	0
40	LV	857	0	922	4	0
41	LW	738	0	807	1	0
42	LX	788	0	844	10	0
43	LY	753	0	780	12	0
44	La	574	0	592	4	0
45	Lb	625	0	652	6	0
46	Lc	501	0	531	4	0
47	Ld	448	0	488	3	0
48	Le	529	0	527	2	0
49	Lf	444	0	458	5	0
50	Lg	452	0	494	4	0
51	Lh	377	0	418	3	0
52	Li	503	0	572	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	Lj	302	0	340	3	0
54	Pp	28	0	33	1	0
55	Pt	1636	0	841	12	0
56	Dt	1637	0	844	3	0
57	16	12	0	24	0	0
57	23	84	0	168	1	0
58	16	88	0	0	0	0
58	23	267	0	0	0	0
58	5	5	0	0	0	0
58	LB	2	0	0	0	0
58	LC	1	0	0	0	0
58	LD	1	0	0	0	0
58	LQ	2	0	0	0	0
58	Lf	1	0	0	0	0
58	SN	1	0	0	0	0
59	Le	1	0	0	0	0
59	Lj	1	0	0	0	0
59	SB	1	0	0	0	0
60	23	62	0	24	1	0
61	23	50	0	95	2	0
All	All	146877	0	98505	794	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.

All (794) 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)
27:LD:108:ILE:HA	33:LO:1:MET:HE1	1.56	0.88
7:SG:113:ASP:HB3	7:SG:119:ARG:HG3	1.56	0.87
23:23:2100:G:H1	23:23:2189:U:H3	1.23	0.83
44:La:38:VAL:HG12	44:La:59:LEU:HB2	1.64	0.80
1:16:411:A:H1'	1:16:413:G:H5"	1.63	0.79
23:23:1250:G:H5"	38:LT:6:ARG:HD2	1.64	0.77
55:Pt:8:U:H3	55:Pt:14:A:H2	1.33	0.74
29:LF:28:GLY:HA3	29:LF:79:VAL:HG13	1.69	0.74
23:23:568:U:H1'	23:23:2030:6MZ:H9C1	1.70	0.74
1:16:1086:U:H3	1:16:1099:G:H22	1.38	0.71
10:SJ:7:ARG:HD3	10:SJ:73:LEU:HD11	1.72	0.71
30:LI:104:THR:HG22	30:LI:109:GLU:HA	1.73	0.70
27:LD:181:ILE:HG23	33:LO:1:MET:HG2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SI:21:ILE:HG22	9:SI:63:LEU:HB3	1.73	0.69
25:LB:29:PRO:HG2	25:LB:34:LEU:HD11	1.74	0.69
1:16:664:G:H22	1:16:741:G:H1	1.41	0.69
28:LE:36:LEU:HG	28:LE:152:LEU:HD21	1.75	0.68
12:SL:87:VAL:HB	12:SL:90:LEU:HB2	1.75	0.68
26:LC:148:GLN:HB2	26:LC:152:PRO:HG3	1.76	0.68
28:LE:108:VAL:HG11	28:LE:176:PRO:HG3	1.75	0.68
27:LD:48:THR:HG22	27:LD:86:ALA:HB3	1.76	0.67
1:16:946:A:H2'	1:16:947:G:C8	2.30	0.67
53:Lj:16:ILE:HD13	53:Lj:25:VAL:HG22	1.77	0.67
11:SK:67:ALA:HB2	11:SK:96:THR:HG23	1.75	0.67
23:23:1792:G:H5'	25:LB:204:VAL:HG13	1.77	0.67
30:LI:4:ILE:HG13	30:LI:37:VAL:HG12	1.76	0.66
1:16:299:G:H2'	1:16:300:A:C8	2.31	0.66
1:16:673:A:H2'	1:16:674:G:C8	2.30	0.66
30:LI:4:ILE:HG13	30:LI:37:VAL:CG1	2.26	0.66
23:23:2233:U:H2'	23:23:2234:G:C8	2.30	0.66
23:23:2273:A:H2'	23:23:2274:A:C8	2.31	0.66
33:LO:57:LEU:HD22	52:Li:54:ASP:HB3	1.77	0.65
9:SI:30:ILE:HG12	9:SI:65:ILE:HD11	1.79	0.65
25:LB:232:HIS:HA	25:LB:242:LYS:HD2	1.79	0.65
30:LI:135:HIS:HB3	30:LI:138:VAL:HB	1.78	0.65
1:16:1218:C:H2'	1:16:1219:A:C8	2.31	0.65
23:23:2151:U:H2'	23:23:2152:G:H8	1.62	0.65
1:16:523:A:C2	12:SL:88:LYS:HB3	2.32	0.65
1:16:1356:G:H2'	1:16:1357:A:C8	2.32	0.65
30:LI:84:ALA:HB2	30:LI:90:LEU:HD23	1.79	0.65
23:23:639:U:H2'	23:23:640:C:C6	2.33	0.64
23:23:945:A:H1'	61:23:3017:SPD:H91	1.79	0.64
55:Pt:47:3AU:H5	55:Pt:50:C:H5"	1.78	0.64
3:SC:175:LEU:HD23	3:SC:182:ILE:HD13	1.79	0.64
32:LN:63:VAL:HG12	32:LN:107:LEU:HD11	1.79	0.64
1:16:171:A:H2'	1:16:172:A:C8	2.33	0.63
19:SS:19:VAL:HG11	19:SS:44:MET:HG2	1.80	0.63
23:23:2291:U:H2'	23:23:2292:U:C6	2.33	0.63
23:23:2151:U:H2'	23:23:2152:G:C8	2.34	0.63
1:16:981:U:H5"	14:SN:6:MET:HE1	1.80	0.62
8:SH:29:SER:HB3	8:SH:57:PRO:HB2	1.82	0.62
2:SB:68:LEU:HD11	2:SB:92:VAL:HG23	1.81	0.62
5:SE:13:GLU:HG2	5:SE:39:VAL:HG22	1.81	0.62
4:SD:125:VAL:HG22	4:SD:143:VAL:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:LM:110:PRO:O	31:LM:115:GLY:HA3	1.99	0.62
23:23:742:A:H2'	23:23:743:A:C8	2.35	0.62
1:16:662:U:H2'	1:16:663:A:C8	2.35	0.62
1:16:713:G:H2'	1:16:714:G:C8	2.35	0.62
6:SF:29:ILE:HG23	6:SF:66:ALA:HB2	1.82	0.61
34:LP:20:LEU:HD13	43:LY:81:PRO:HG3	1.82	0.61
10:SJ:22:THR:HG21	10:SJ:39:PRO:HB3	1.81	0.61
24:5:66:A:H61	24:5:107:G:H2'	1.66	0.61
23:23:910:A:H2'	23:23:911:A:C8	2.36	0.61
1:16:606:G:H5"	1:16:606:G:H8	1.65	0.60
23:23:1176:U:H4'	23:23:1177:G:H8	1.64	0.60
1:16:337:G:H2'	1:16:338:A:C8	2.37	0.60
23:23:2014:A:H2'	23:23:2015:A:C8	2.37	0.60
23:23:191:A:H2'	23:23:192:C:C6	2.37	0.60
1:16:1323:G:H2'	1:16:1324:A:C8	2.37	0.59
1:16:1391:U:H2'	1:16:1392:G:C8	2.37	0.59
48:Le:11:GLU:HA	48:Le:25:ARG:HA	1.83	0.59
23:23:1027:A:C2	23:23:2488:G:H5'	2.37	0.59
5:SE:115:LEU:HD13	5:SE:123:VAL:HG11	1.84	0.59
11:SK:94:GLU:HG3	21:SU:16:LEU:HD21	1.84	0.59
23:23:1102:C:H2'	23:23:1103:A:C8	2.37	0.59
23:23:1386:C:H2'	23:23:1387:A:C8	2.37	0.59
1:16:429:U:H3	1:16:431:A:H62	1.48	0.59
23:23:2175:C:H2'	23:23:2176:A:C8	2.38	0.59
42:LX:25:VAL:HG13	42:LX:34:VAL:HG23	1.85	0.59
1:16:79:G:H2'	1:16:80:A:C8	2.38	0.58
6:SF:32:ALA:O	6:SF:33:GLU:C	2.46	0.58
23:23:1434:A:H2'	23:23:1435:G:C8	2.38	0.58
23:23:1809:A:H2'	23:23:1810:A:C8	2.38	0.58
30:LI:90:LEU:HD11	30:LI:146:VAL:HG11	1.85	0.58
12:SL:50:ARG:HB3	12:SL:66:TYR:HE1	1.68	0.58
23:23:796:C:H2'	23:23:797:G:C8	2.38	0.58
26:LC:186:LEU:HD13	37:LS:8:LEU:HD11	1.85	0.58
1:16:1305:G:H21	1:16:1332:A:H2	1.50	0.58
23:23:2800:A:C2	23:23:2895:G:H1'	2.39	0.58
23:23:414:C:H2'	23:23:415:A:C8	2.39	0.58
23:23:2099:U:H2'	23:23:2100:G:C8	2.39	0.58
1:16:465:A:H2'	1:16:466:A:C8	2.39	0.58
1:16:1043:G:H2'	1:16:1044:A:C8	2.38	0.58
3:SC:77:ILE:HA	3:SC:84:VAL:HG23	1.85	0.58
23:23:494:G:H4'	40:LV:6:LYS:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Lg:10:LYS:HG3	50:Lg:52:ALA:HB3	1.86	0.57
1:16:823:C:HO2'	8:SH:2:SER:N	2.02	0.57
31:LM:36:LEU:HD11	31:LM:122:LEU:HD13	1.84	0.57
11:SK:87:LYS:HB2	11:SK:113:VAL:HG23	1.85	0.57
43:LY:40:ILE:HD12	43:LY:42:LEU:HD21	1.86	0.57
23:23:2107:G:H1	23:23:2182:U:H3	1.53	0.57
37:LS:33:VAL:HG22	37:LS:38:LYS:HG3	1.86	0.57
7:SG:26:PHE:HE2	7:SG:120:LEU:HD21	1.70	0.57
25:LB:5:LYS:HG2	25:LB:17:VAL:HG22	1.86	0.57
36:LR:49:VAL:HG21	36:LR:81:ARG:HB3	1.86	0.57
23:23:314:C:H2'	23:23:315:G:H5"	1.86	0.57
46:Lc:14:LEU:HB3	46:Lc:57:LEU:HD21	1.86	0.57
2:SB:100:MET:HA	2:SB:107:VAL:HG21	1.86	0.57
6:SF:38:ARG:HB3	6:SF:63:ASN:HB2	1.85	0.57
23:23:391:A:H1'	23:23:411:G:O4'	2.05	0.57
1:16:1412:C:H2'	1:16:1413:A:C8	2.39	0.57
10:SJ:5:ARG:HG3	10:SJ:5:ARG:HH11	1.69	0.56
3:SC:110:GLU:HB2	3:SC:144:LEU:HD12	1.87	0.56
1:16:56:U:H2'	1:16:57:G:C8	2.41	0.56
6:SF:18:VAL:HA	6:SF:21:MET:HE2	1.86	0.56
23:23:1028:A:N6	23:23:1125:G:H2'	2.20	0.56
11:SK:82:LEU:HG	11:SK:105:PHE:HB3	1.87	0.56
23:23:2305:U:H5"	28:LE:131:GLY:HA3	1.87	0.56
47:Ld:11:ARG:HB3	47:Ld:54:MET:HG2	1.88	0.56
31:LM:96:ARG:HG2	31:LM:99:ARG:HG2	1.87	0.56
33:LO:77:ILE:CD1	33:LO:108:ALA:HB1	2.35	0.56
43:LY:20:LEU:HD21	43:LY:41:GLU:HB3	1.87	0.56
23:23:1495:A:H2'	23:23:1496:A:C8	2.40	0.56
23:23:2329:U:H2'	23:23:2330:G:C8	2.41	0.56
29:LF:86:LYS:HD3	29:LF:132:VAL:HG22	1.87	0.56
3:SC:60:PRO:HG2	3:SC:63:SER:HB2	1.88	0.55
19:SS:11:ILE:HG13	19:SS:38:SER:HB2	1.88	0.55
23:23:813:U:H2'	23:23:814:C:C6	2.41	0.55
23:23:2796:U:H3	23:23:2799:A:H61	1.55	0.55
11:SK:89:PRO:HG3	21:SU:32:VAL:HG11	1.88	0.55
23:23:181:A:H2'	23:23:182:A:C8	2.41	0.55
49:Lf:43:ILE:HG22	49:Lf:49:TYR:HB2	1.88	0.55
4:SD:121:LYS:HB3	4:SD:129:VAL:HG21	1.88	0.55
23:23:1796:U:H2'	23:23:1797:G:C8	2.42	0.55
28:LE:136:ILE:HG21	28:LE:143:TYR:HD1	1.70	0.55
23:23:142:A:H5"	23:23:142:A:H8	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:LO:77:ILE:HD13	33:LO:108:ALA:HB1	1.88	0.55
34:LP:75:GLU:HB2	34:LP:90:GLU:HG3	1.89	0.55
1:16:477:C:H2'	1:16:478:A:C8	2.42	0.55
23:23:1428:C:C5	23:23:1569:A:H5"	2.41	0.55
7:SG:16:PRO:HA	9:SI:46:MET:HE3	1.87	0.55
23:23:2328:A:H2'	23:23:2329:U:C6	2.42	0.55
1:16:1003:G:H21	1:16:1005:A:H5'	1.71	0.55
23:23:851:C:H2'	23:23:852:U:C6	2.41	0.55
1:16:382:A:H2'	1:16:383:A:C8	2.42	0.55
23:23:1548:A:H2'	23:23:1549:A:C8	2.42	0.55
42:LX:14:LEU:HD11	42:LX:71:ALA:HB2	1.89	0.55
23:23:1028:A:H2'	23:23:1029:A:C8	2.42	0.55
1:16:458:U:H2'	1:16:459:A:C8	2.42	0.54
1:16:677:U:H3	1:16:713:G:H22	1.54	0.54
2:SB:90:PHE:CG	2:SB:154:MET:HG2	2.43	0.54
19:SS:22:ALA:HA	19:SS:27:ASP:HB2	1.89	0.54
23:23:247:G:H4'	23:23:386:G:C5	2.42	0.54
23:23:594:U:H2'	23:23:595:C:C6	2.42	0.54
43:LY:26:PHE:HE2	43:LY:89:ILE:HG13	1.70	0.54
1:16:269:C:H2'	1:16:270:A:C8	2.42	0.54
1:16:1216:A:H5"	14:SN:5:SER:HB3	1.88	0.54
10:SJ:8:ILE:HG12	10:SJ:100:ILE:HG22	1.89	0.54
23:23:593:U:H2'	23:23:594:U:C6	2.43	0.54
1:16:17:U:H2'	1:16:18:C:C6	2.42	0.54
23:23:250:G:H2'	23:23:251:A:C8	2.42	0.54
23:23:2327:A:H2'	23:23:2328:A:C8	2.43	0.54
1:16:1190:G:H5'	3:SC:176:HIS:NE2	2.22	0.54
23:23:1927:A:H2'	23:23:1928:A:C8	2.41	0.54
23:23:608:A:H2'	23:23:609:A:C8	2.43	0.54
23:23:833:A:H2'	23:23:834:G:C8	2.42	0.54
55:Pt:63:U:H2'	55:Pt:64:G:C8	2.42	0.54
26:LC:8:LYS:HB2	26:LC:201:LEU:HD11	1.90	0.54
1:16:524:G:H2'	1:16:525:C:C6	2.42	0.54
1:16:568:G:O6	12:SL:2:ALA:HB2	2.08	0.54
1:16:1530:G:H2'	1:16:1531:A:C8	2.43	0.54
23:23:1176:U:H4'	23:23:1177:G:C8	2.43	0.54
30:LI:100:ALA:O	30:LI:104:THR:HG23	2.07	0.54
4:SD:124:MET:HG3	4:SD:146:ARG:HG2	1.90	0.53
4:SD:197:GLU:HA	4:SD:200:ILE:HD12	1.90	0.53
23:23:281:C:H2'	23:23:282:A:C8	2.43	0.53
23:23:1093:G:H21	23:23:1098:A:H62	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1469:A:H2'	23:23:1470:A:C8	2.42	0.53
23:23:2243:U:H2'	23:23:2244:U:C6	2.43	0.53
1:16:790:A:H2'	1:16:791:G:C8	2.43	0.53
23:23:473:G:OP2	61:23:3018:SPD:N1	2.40	0.53
23:23:2016:U:H2'	23:23:2017:U:C6	2.42	0.53
32:LN:43:ILE:HD12	32:LN:56:ASP:HB2	1.88	0.53
1:16:256:U:H2'	1:16:257:G:C8	2.43	0.53
1:16:993:G:N3	1:16:993:G:H2'	2.22	0.53
36:LR:39:VAL:HB	36:LR:49:VAL:HG12	1.90	0.53
23:23:1710:G:H4'	23:23:2858:C:O2	2.09	0.53
23:23:1796:U:H2'	23:23:1797:G:H8	1.72	0.53
23:23:1853:A:N1	23:23:2087:G:H1'	2.24	0.53
16:SP:52:LEU:HD23	16:SP:78:VAL:HG21	1.90	0.53
1:16:109:A:H2'	1:16:326:G:N2	2.24	0.53
1:16:1120:C:H2'	1:16:1121:U:C6	2.44	0.53
7:SG:25:LYS:HG2	7:SG:101:MET:HE1	1.91	0.53
23:23:839:U:H2'	23:23:840:C:C6	2.44	0.53
28:LE:61:SER:HB2	28:LE:91:LEU:HD21	1.91	0.53
29:LF:89:LEU:HD11	29:LF:96:ALA:HB2	1.90	0.53
37:LS:10[B]:GLN:HA	37:LS:13:MET:HE3	1.91	0.53
1:16:59:A:H5"	1:16:387:U:H5"	1.90	0.53
1:16:859:G:H2'	1:16:860:A:C8	2.44	0.53
23:23:2756:U:H1'	23:23:2757:A:H5"	1.90	0.53
36:LR:35:ILE:HG21	36:LR:71:ALA:HA	1.91	0.53
25:LB:8:PRO:HB3	25:LB:14:ARG:HG3	1.91	0.53
25:LB:31:ALA:HA	25:LB:34:LEU:HD12	1.91	0.53
35:LQ:101:GLY:H	49:Lf:42:HIS:HD2	1.57	0.53
23:23:1068:G:H21	23:23:1096:A:H5'	1.74	0.52
23:23:2590:A:H2'	23:23:2591:C:C6	2.43	0.52
23:23:2636:C:H2'	23:23:2637:U:C6	2.44	0.52
23:23:2674:G:H4'	32:LN:30:ARG:HD2	1.91	0.52
34:LP:50:ARG:HD3	34:LP:65:ILE:HD11	1.91	0.52
50:Lg:39:PHE:CZ	50:Lg:44[A]:ARG:HA	2.44	0.52
19:SS:32:ARG:HA	19:SS:50:ALA:HB3	1.90	0.52
23:23:632:A:H2'	23:23:633:A:C8	2.44	0.52
19:SS:63:THR:HG22	19:SS:64:ASP:H	1.75	0.52
23:23:1744:A:H3'	23:23:1745:A:H8	1.74	0.52
23:23:2787:C:H1'	26:LC:63:PRO:HG3	1.90	0.52
37:LS:10[A]:GLN:HA	37:LS:13:MET:HE3	1.91	0.52
13:SM:7:ILE:HD11	13:SM:22:ILE:HG12	1.92	0.52
23:23:948:C:H2'	23:23:949:G:H8	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:1397:C:H42	22:mR:47:U:H5	1.57	0.52
23:23:930:G:H1'	47:Ld:25:LEU:HD11	1.91	0.52
23:23:2567:G:H2'	23:23:2568:U:C6	2.45	0.52
25:LB:78:VAL:HG21	25:LB:110:LEU:HD13	1.90	0.52
4:SD:116:GLN:HG3	4:SD:120:HIS:CD2	2.45	0.52
5:SE:45:ARG:HB3	5:SE:71:MET:HE2	1.90	0.52
23:23:1405:U:H2'	23:23:1406:U:C6	2.44	0.52
23:23:1102:C:H2'	23:23:1103:A:H8	1.74	0.52
1:16:920:U:H2'	1:16:921:U:C6	2.45	0.52
23:23:2788:C:H2'	23:23:2789:C:C6	2.44	0.52
23:23:284:U:H2'	23:23:285:G:C8	2.45	0.52
1:16:1328:C:H5"	13:SM:28:THR:HG21	1.92	0.52
23:23:856:G:H2'	23:23:857:G:C8	2.45	0.52
23:23:2591:C:H2'	23:23:2592:G:C8	2.44	0.52
36:LR:90:VAL:HG22	36:LR:115:LEU:HD22	1.92	0.52
50:Lg:39:PHE:CZ	50:Lg:44[B]:ARG:HA	2.45	0.52
29:LF:164:TYR:HB2	29:LF:167:GLU:HB2	1.91	0.51
10:SJ:21:ALA:HB1	10:SJ:92:LEU:HD12	1.92	0.51
23:23:2537:U:H2'	23:23:2538:C:C6	2.46	0.51
1:16:1071:C:H2'	1:16:1072:G:C8	2.46	0.51
12:SL:66:TYR:HB2	12:SL:93:VAL:HG11	1.92	0.51
23:23:1176:U:H5"	23:23:1177:G:H5'	1.92	0.51
23:23:1901:A:H2'	23:23:1902:C:C6	2.45	0.51
23:23:2271:G:H5'	44:La:20:ARG:HG3	1.91	0.51
4:SD:11:LEU:HB3	4:SD:63:ARG:HD3	1.91	0.51
29:LF:107:LEU:HB3	29:LF:152:ARG:HG3	1.91	0.51
29:LF:54:PRO:HB3	29:LF:61:GLY:HA3	1.93	0.51
24:5:66:A:N6	24:5:107:G:H2'	2.25	0.51
1:16:522:C:H1'	1:16:536:C:H5"	1.93	0.51
1:16:559:A:H4'	1:16:560:A:H3'	1.91	0.51
1:16:1513:A:H2'	1:16:1514:G:C8	2.46	0.51
7:SG:69:VAL:HG23	7:SG:100:ALA:HB1	1.94	0.51
23:23:1357:C:H2'	23:23:1358:G:O4'	2.11	0.51
1:16:413:G:H1'	1:16:428:G:H21	1.75	0.50
23:23:1746:A:H2'	23:23:1747:U:C6	2.47	0.50
43:LY:2:PHE:HB2	43:LY:61:LEU:HD22	1.93	0.50
47:Ld:6:LYS:HB2	47:Ld:58:GLU:HB2	1.93	0.50
49:Lf:44:THR:HG23	49:Lf:48:TYR:O	2.11	0.50
1:16:473:U:H2'	1:16:474:G:C8	2.46	0.50
4:SD:145:ILE:HG23	4:SD:150:LYS:HG2	1.93	0.50
23:23:668:A:H2'	23:23:670:A:H62	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:2025:C:H2'	23:23:2026:U:C6	2.46	0.50
29:LF:17:VAL:HG22	29:LF:26:ILE:HG13	1.92	0.50
1:16:335:C:H2'	1:16:336:A:C8	2.47	0.50
1:16:1326:U:H2'	1:16:1327:C:C6	2.46	0.50
4:SD:145:ILE:HD12	4:SD:155:VAL:HG11	1.93	0.50
23:23:1432:G:H2'	23:23:1433:A:C8	2.47	0.50
23:23:1900:A:H1'	23:23:1970:A:H2'	1.93	0.50
26:LC:35:THR:HG22	26:LC:73:VAL:HG21	1.93	0.50
29:LF:149:ARG:HA	29:LF:162:VAL:HB	1.94	0.50
1:16:1414:U:H2'	1:16:1415:G:H8	1.76	0.50
7:SG:70:ARG:HA	7:SG:100:ALA:HB2	1.92	0.50
25:LB:141:VAL:HG23	25:LB:162:VAL:HG22	1.93	0.50
44:La:70:GLU:HG3	44:La:72:LYS:HD2	1.94	0.50
1:16:1396:A:H4'	1:16:1397:C:H5"	1.94	0.50
27:LD:145:ASP:HA	27:LD:166:LYS:HB3	1.94	0.50
6:SF:16:GLU:O	6:SF:19:PRO:HD2	2.11	0.50
12:SL:44:LYS:HB3	12:SL:45:PRO:HD3	1.93	0.50
23:23:2684:U:H4'	32:LN:76:VAL:HG21	1.93	0.50
23:23:2898:U:H2'	23:23:2899:A:C8	2.47	0.50
28:LE:46:ASP:HB3	28:LE:49:LEU:HG	1.94	0.50
1:16:1251:A:H2'	1:16:1252:A:C8	2.47	0.50
2:SB:115:LYS:HE3	2:SB:152:LYS:HB2	1.93	0.50
23:23:581:C:H2'	23:23:582:A:C8	2.47	0.50
23:23:1187:G:H5"	39:LU:83:TYR:CE1	2.47	0.50
49:Lf:54:VAL:HG23	49:Lf:55:ILE:HG12	1.93	0.49
56:Dt:62:C:H2'	56:Dt:63:G:H8	1.77	0.49
1:16:613:C:H2'	1:16:614:C:C6	2.47	0.49
2:SB:57:LEU:HD13	2:SB:217:VAL:HG13	1.94	0.49
23:23:717:C:H3'	23:23:718:A:H8	1.77	0.49
10:SJ:92:LEU:HG	10:SJ:98:VAL:HG21	1.94	0.49
23:23:1361:G:H2'	23:23:1362:C:C6	2.47	0.49
8:SH:102:ALA:HB3	8:SH:113:ASP:HB3	1.94	0.49
26:LC:57:ALA:HA	26:LC:60:VAL:HG12	1.93	0.49
4:SD:134:SER:O	4:SD:135:TYR:C	2.56	0.49
23:23:441:U:H2'	23:23:442:G:C8	2.48	0.49
1:16:513:C:H2'	1:16:514:C:C6	2.48	0.49
13:SM:17:ILE:H	13:SM:17:ILE:HD12	1.78	0.49
23:23:2776:A:H4'	23:23:2777:G:H5"	1.93	0.49
1:16:950:U:H2'	1:16:951:G:C8	2.48	0.49
44:La:37:ILE:HG21	44:La:80:ILE:HG21	1.93	0.49
1:16:443:C:H2'	1:16:444:G:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:753:A:H2'	23:23:754:U:C6	2.48	0.49
23:23:1802:A:N1	23:23:1822:C:H1'	2.27	0.49
34:LP:46:ILE:HA	34:LP:103:TYR:OH	2.13	0.49
1:16:473:U:H2'	1:16:474:G:H8	1.78	0.49
29:LF:95:ARG:HG2	29:LF:106:SER:HB2	1.93	0.49
1:16:483:C:H2'	1:16:484:G:C8	2.48	0.49
39:LU:38:VAL:HG22	39:LU:59:ILE:HD12	1.94	0.49
1:16:12:U:H4'	1:16:526:C:H4'	1.95	0.48
1:16:376:G:H5"	16:SP:5:ARG:HB2	1.95	0.48
23:23:82:U:H2'	23:23:83:A:C8	2.48	0.48
23:23:580:U:H2'	23:23:581:C:C6	2.48	0.48
23:23:2182:U:H2'	23:23:2183:A:C8	2.47	0.48
26:LC:148:GLN:HB2	26:LC:152:PRO:CG	2.42	0.48
12:SL:39:THR:HG22	12:SL:51:LYS:HD3	1.95	0.48
23:23:479:A:N3	23:23:481:G:H5"	2.28	0.48
32:LN:43:ILE:HD11	32:LN:58:LEU:HD21	1.95	0.48
18:SR:36:SER:HA	18:SR:72:ASP:HB3	1.95	0.48
29:LF:24:ILE:HG21	29:LF:72:LEU:HD21	1.96	0.48
1:16:67:C:H2'	1:16:68:G:C8	2.48	0.48
23:23:1838:C:N4	23:23:1898:U:H2'	2.28	0.48
23:23:1996:C:H5	32:LN:32:TYR:HH	1.62	0.48
23:23:364:C:H2'	23:23:365:U:C6	2.48	0.48
23:23:927:A:H2'	23:23:928:A:C8	2.48	0.48
27:LD:108:ILE:HA	33:LO:1:MET:CE	2.35	0.48
1:16:728:A:H2'	1:16:729:A:C8	2.49	0.48
1:16:999:C:H2'	1:16:1000:A:C8	2.48	0.48
23:23:120:U:H5"	23:23:122:G:OP2	2.13	0.48
23:23:644:A:H2'	23:23:645:C:O4'	2.13	0.48
23:23:1076:C:H2'	23:23:1077:A:O4'	2.13	0.48
23:23:1199:U:H1'	38:LT:4:VAL:HG22	1.94	0.48
23:23:2233:U:H2'	23:23:2234:G:H8	1.76	0.48
27:LD:164:LEU:HB3	27:LD:167:VAL:HG13	1.94	0.48
1:16:769:G:H4'	1:16:1513:A:H4'	1.96	0.48
11:SK:34:ILE:HG12	11:SK:70:CYS:SG	2.53	0.48
23:23:150:U:H2'	23:23:151:C:C6	2.48	0.48
23:23:157:C:H2'	23:23:158:U:O4'	2.14	0.48
1:16:390:U:H2'	1:16:391:G:C8	2.49	0.48
7:SG:26:PHE:HZ	7:SG:120:LEU:HD11	1.79	0.48
23:23:588:U:H2'	23:23:589:U:C6	2.49	0.48
23:23:796:C:H2'	23:23:797:G:H8	1.79	0.48
45:Lb:17:ASN:OD1	45:Lb:27:ARG:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:451:A:H61	1:16:481:G:H5'	1.78	0.48
23:23:127:A:H5"	23:23:128:C:C6	2.48	0.48
18:SR:32:TYR:HB3	18:SR:55:LEU:HD21	1.96	0.47
23:23:2845:U:H5"	37:LS:52:ASN:O	2.13	0.47
8:SH:7:ILE:O	8:SH:11:LEU:HG	2.13	0.47
23:23:609:A:H2'	23:23:610:C:O4'	2.13	0.47
23:23:2074:U:H2'	23:23:2075:U:C6	2.49	0.47
27:LD:41:GLN:HG2	27:LD:43:THR:HG23	1.96	0.47
28:LE:16:LEU:HD13	28:LE:29:PRO:HD2	1.96	0.47
1:16:632:U:H5"	1:16:633:G:C8	2.49	0.47
23:23:849:A:H2'	23:23:850:U:C6	2.49	0.47
23:23:871:U:H2'	23:23:872:U:C6	2.49	0.47
30:LI:9:VAL:HB	30:LI:12:LEU:HB2	1.94	0.47
1:16:1179:A:H5"	9:SI:99:ARG:HH22	1.79	0.47
9:SI:116:VAL:HG11	10:SJ:62:ARG:HB2	1.95	0.47
23:23:752:A:H3'	51:Lh:1:MET:SD	2.53	0.47
23:23:2554:U:H2'	23:23:2555:U:C6	2.49	0.47
1:16:1332:A:H2'	1:16:1333:A:O4'	2.15	0.47
17:SQ:21:ILE:HG12	17:SQ:48:ASP:HB2	1.96	0.47
20:ST:62:ALA:HA	20:ST:67:ILE:O	2.14	0.47
23:23:284:U:H2'	23:23:285:G:H8	1.78	0.47
23:23:2037:A:H2'	23:23:2038:G:C8	2.50	0.47
6:SF:10:VAL:HG21	6:SF:18:VAL:HG22	1.95	0.47
11:SK:24:HIS:HB3	11:SK:31:ILE:HB	1.97	0.47
16:SP:4:ILE:HG12	16:SP:21:VAL:HG22	1.95	0.47
23:23:657:U:H2'	23:23:658:U:C6	2.50	0.47
23:23:2192:U:H2'	23:23:2193:G:H8	1.80	0.47
23:23:2391:G:O6	23:23:2425:A:H8	1.98	0.47
23:23:2812:G:H2'	23:23:2813:A:C8	2.50	0.47
50:Lg:13:SER:HB3	50:Lg:49:TYR:CZ	2.50	0.47
23:23:310:A:H5"	42:LX:15:THR:HG23	1.95	0.47
23:23:948:C:H2'	23:23:949:G:C8	2.50	0.47
23:23:1000:A:H2'	23:23:1001:A:C8	2.50	0.47
23:23:1327:A:H2'	23:23:1328:A:O4'	2.15	0.47
23:23:1792:G:C5'	25:LB:204:VAL:HG13	2.45	0.47
1:16:512:U:H2'	1:16:513:C:C6	2.50	0.47
19:SS:60:VAL:CG1	19:SS:66:MET:HE1	2.45	0.47
23:23:2031:A:C6	23:23:2498:OMC:H1'	2.49	0.47
45:Lb:7:VAL:HG21	45:Lb:59:ILE:HD11	1.95	0.47
1:16:1071:C:H2'	1:16:1072:G:H8	1.80	0.47
28:LE:8:TYR:HB2	28:LE:173:PHE:HZ	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:SB:148:LEU:HD22	2:SB:151:ILE:HD11	1.96	0.46
23:23:2698:U:H2'	23:23:2699:C:C6	2.50	0.46
32:LN:71:ARG:HB2	32:LN:75:SER:OG	2.15	0.46
1:16:450:G:H4'	16:SP:41:PRO:HB2	1.97	0.46
1:16:621:A:H2'	1:16:622:A:C8	2.49	0.46
1:16:1225:A:H2'	1:16:1226:C:C5	2.50	0.46
23:23:1641:A:H2'	23:23:1642:G:O4'	2.15	0.46
40:LV:24:ILE:HD13	40:LV:36:LEU:HD11	1.97	0.46
1:16:490:C:H2'	1:16:491:G:C8	2.50	0.46
23:23:118:A:N3	23:23:178:G:H1'	2.29	0.46
23:23:1683:U:H2'	23:23:1684:G:C8	2.50	0.46
23:23:2615:U:C2	49:Lf:4:GLN:HA	2.50	0.46
31:LM:34:ARG:HG3	31:LM:39:LYS:HB2	1.98	0.46
55:Pt:61:C:H2'	55:Pt:62:C:C6	2.50	0.46
1:16:409:U:H2'	1:16:410:G:O4'	2.16	0.46
1:16:536:C:H2'	1:16:537:G:C8	2.51	0.46
23:23:355:U:H2'	23:23:356:G:C8	2.50	0.46
1:16:493:A:H2'	1:16:494:G:C8	2.51	0.46
25:LB:158:ALA:HB1	25:LB:197:ASN:O	2.16	0.46
23:23:1802:A:H2'	23:23:1803:A:C8	2.51	0.46
23:23:2590:A:H2'	23:23:2591:C:H6	1.80	0.46
23:23:2684:U:H4'	32:LN:76:VAL:CG2	2.45	0.46
1:16:222:C:H2'	1:16:223:A:C8	2.51	0.46
1:16:235:C:H2'	1:16:236:A:C8	2.51	0.46
1:16:436:C:H2'	1:16:437:U:C6	2.51	0.46
1:16:1011:C:H2'	1:16:1012:A:C8	2.50	0.46
1:16:1391:U:H2'	1:16:1392:G:H8	1.78	0.46
4:SD:147:GLU:HA	4:SD:150:LYS:HG3	1.97	0.46
30:LI:99:ILE:HD11	30:LI:130:VAL:HG21	1.98	0.46
1:16:410:G:H2'	1:16:429:U:C4	2.50	0.46
1:16:1376:U:H2'	1:16:1377:A:C8	2.51	0.46
1:16:1463:U:H2'	1:16:1464:U:C6	2.51	0.46
8:SH:111:MET:HE2	8:SH:111:MET:HB3	1.88	0.46
12:SL:29:GLN:HB3	12:SL:81:LEU:HD22	1.97	0.46
23:23:2794:C:H2'	23:23:2795:C:C6	2.50	0.46
24:5:1:U:H2'	24:5:2:G:C8	2.50	0.46
23:23:308:G:H2'	23:23:309:A:C8	2.51	0.46
23:23:355:U:H2'	23:23:356:G:H8	1.80	0.46
43:LY:57:TYR:HE1	43:LY:77:VAL:HG21	1.81	0.46
1:16:358:U:H2'	1:16:359:G:C8	2.51	0.46
1:16:1176:A:H2'	1:16:1177:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:1478:U:H2'	1:16:1479:C:C6	2.50	0.46
23:23:1501:G:H4'	25:LB:95:LEU:HD21	1.97	0.46
55:Pt:47:3AU:H6	55:Pt:47:3AU:H2'	1.41	0.46
1:16:996:A:H2'	1:16:997:U:C6	2.51	0.45
17:SQ:19:LYS:HA	17:SQ:48:ASP:O	2.16	0.45
23:23:1747:U:H2'	23:23:1748:C:C6	2.51	0.45
23:23:2038:G:H2'	23:23:2039:U:O4'	2.16	0.45
30:LI:3:VAL:HG23	30:LI:19:VAL:HG23	1.98	0.45
1:16:8:A:H5'	5:SE:125:ALA:O	2.16	0.45
23:23:749:A:H4'	23:23:1271:G:N3	2.31	0.45
28:LE:57:LEU:HD23	28:LE:57:LEU:HA	1.78	0.45
33:LO:77:ILE:HG12	33:LO:95:LEU:HD13	1.97	0.45
1:16:216:U:H2'	1:16:217:C:C6	2.51	0.45
16:SP:8:ARG:HH21	16:SP:15:PRO:HG3	1.81	0.45
23:23:414:C:H2'	23:23:415:A:H8	1.80	0.45
23:23:2646:C:H2'	23:23:2647:U:O4'	2.15	0.45
55:Pt:62:C:H2'	55:Pt:63:U:C6	2.51	0.45
1:16:49:U:O2	1:16:362:G:H1'	2.16	0.45
1:16:579:A:H2'	1:16:580:C:C6	2.52	0.45
1:16:580:C:H2'	1:16:581:G:O4'	2.17	0.45
10:SJ:40:ILE:HB	10:SJ:73:LEU:HB3	1.98	0.45
42:LX:25:VAL:HG13	42:LX:34:VAL:CG2	2.44	0.45
1:16:492:C:H2'	1:16:493:A:C8	2.51	0.45
1:16:501:C:H2'	1:16:502:A:C8	2.51	0.45
1:16:802:A:H2'	1:16:803:G:O4'	2.15	0.45
1:16:1070:U:H2'	1:16:1071:C:C6	2.51	0.45
1:16:1504:G:H4'	1:16:1505:G:C4	2.51	0.45
23:23:1081:U:H2'	23:23:1082:U:C6	2.52	0.45
23:23:1720:U:H2'	23:23:1721:G:O4'	2.17	0.45
23:23:1830:C:H2'	23:23:1831:G:H8	1.81	0.45
30:LI:78:VAL:HG11	30:LI:103:VAL:HG22	1.99	0.45
30:LI:103:VAL:HG21	30:LI:132:PHE:CZ	2.51	0.45
33:LO:77:ILE:HD11	33:LO:101:ILE:HG21	1.99	0.45
1:16:1508:A:H2'	1:16:1509:C:O4'	2.17	0.45
23:23:1182:G:H2'	23:23:1183:U:O4'	2.17	0.45
23:23:2238:G:H2'	23:23:2238:G:N3	2.32	0.45
30:LI:115:VAL:HG22	30:LI:132:PHE:CE2	2.51	0.45
23:23:288:U:H2'	23:23:289:G:C8	2.52	0.45
23:23:2153:C:H2'	23:23:2154:A:H8	1.81	0.45
30:LI:4:ILE:CG1	30:LI:37:VAL:HG13	2.47	0.45
30:LI:112:LYS:H	30:LI:112:LYS:HG3	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:Lc:14:LEU:HD12	46:Lc:14:LEU:HA	1.78	0.45
1:16:714:G:H2'	1:16:715:A:C8	2.52	0.45
1:16:1225:A:H2'	1:16:1226:C:C6	2.52	0.45
27:LD:41:GLN:HG2	27:LD:43:THR:CG2	2.47	0.45
1:16:234:C:H4'	17:SQ:66:PRO:HG3	1.99	0.45
1:16:489:C:H2'	1:16:490:C:C6	2.51	0.45
23:23:29:U:H2'	23:23:30:G:C8	2.51	0.45
23:23:64:A:H2'	23:23:65:U:C6	2.52	0.45
5:SE:77:ASN:O	5:SE:80:THR:HG22	2.17	0.44
23:23:532:A:N1	23:23:2020:A:H1'	2.32	0.44
23:23:723:C:H2'	23:23:724:U:O4'	2.16	0.44
23:23:1744:A:H3'	23:23:1745:A:C8	2.52	0.44
23:23:2026:U:H2'	23:23:2027:G:O4'	2.18	0.44
23:23:2358:A:H2'	23:23:2359:C:O4'	2.17	0.44
27:LD:111:GLU:HB3	33:LO:1:MET:CE	2.47	0.44
35:LQ:9:GLN:O	35:LQ:17:ARG:HD3	2.18	0.44
43:LY:7:GLU:HB2	43:LY:41:GLU:HG3	1.98	0.44
1:16:429:U:H3'	4:SD:9:LEU:HD12	1.99	0.44
23:23:1716:U:H2'	23:23:1717:A:C8	2.52	0.44
13:SM:20:THR:HG23	13:SM:26:GLY:HA2	1.98	0.44
23:23:1697:G:OP2	23:23:1698:A:O2'	2.34	0.44
23:23:2086:U:H2'	23:23:2087:G:C8	2.53	0.44
45:Lb:31:PRO:HB2	45:Lb:33:LEU:HG	1.99	0.44
55:Pt:50:C:H2'	55:Pt:51:A:C8	2.52	0.44
1:16:404:G:N7	4:SD:2:ALA:HB3	2.33	0.44
23:23:1105:U:H2'	23:23:1106:G:C8	2.52	0.44
23:23:1794:A:H2'	23:23:1795:C:C6	2.52	0.44
33:LO:62:PRO:HG2	52:Li:25:LYS:HB3	1.99	0.44
1:16:448:A:H3'	1:16:449:G:H8	1.81	0.44
5:SE:89:HIS:CE1	5:SE:138:ARG:HD3	2.53	0.44
23:23:885:C:H2'	23:23:886:A:C8	2.52	0.44
25:LB:21:ASN:HB3	25:LB:24:LEU:HG	1.98	0.44
12:SL:66:TYR:CD1	12:SL:87:VAL:HG21	2.52	0.44
13:SM:16:VAL:HG13	13:SM:17:ILE:HD12	2.00	0.44
23:23:577:G:H2'	23:23:578:G:C8	2.53	0.44
23:23:1932:A:H2'	23:23:1933:G:O4'	2.17	0.44
23:23:2407:A:H2'	23:23:2408:U:C6	2.53	0.44
1:16:80:A:H1'	1:16:91:U:C4	2.53	0.44
1:16:1228:C:H2'	1:16:1229:A:C8	2.52	0.44
16:SP:51:ARG:C	16:SP:52:LEU:HD22	2.43	0.44
23:23:747:5MU:O2	23:23:2014:A:H1'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:2783:U:H2'	23:23:2784:U:C6	2.53	0.44
1:16:634:C:H2'	1:16:635:A:C8	2.52	0.44
1:16:950:U:H2'	1:16:951:G:H8	1.83	0.44
10:SJ:50:THR:HG23	10:SJ:64:GLN:HG2	2.00	0.44
11:SK:23:ILE:HD12	11:SK:96:THR:HG21	2.00	0.44
23:23:45:G:H5"	23:23:46:G:H5'	1.99	0.44
23:23:1778:U:H2'	23:23:1784:A:N6	2.33	0.44
51:Lh:1:MET:HE2	51:Lh:1:MET:HB3	1.74	0.44
1:16:730:G:N2	1:16:765:G:H5"	2.33	0.44
23:23:17:G:H2'	23:23:18:U:C6	2.53	0.44
23:23:208:C:H2'	23:23:209:C:C6	2.52	0.44
23:23:482:A:H1'	23:23:498:G:N2	2.33	0.44
23:23:1084:A:H1'	23:23:1106:G:H5'	2.00	0.44
25:LB:34:LEU:HD23	25:LB:63:ARG:HG3	1.99	0.44
42:LX:7:ARG:HA	42:LX:25:VAL:HG12	1.98	0.44
23:23:1074:G:H2'	23:23:1075:C:C6	2.53	0.43
23:23:1231:U:H2'	23:23:1232:G:H8	1.82	0.43
23:23:1278:C:H2'	23:23:1279:G:C8	2.53	0.43
23:23:1563:U:H2'	23:23:1564:C:C6	2.52	0.43
23:23:1680:U:H2'	23:23:1681:G:O4'	2.17	0.43
23:23:2064:C:H2'	23:23:2065:C:C6	2.52	0.43
32:LN:7:MET:SD	32:LN:20:MET:HB2	2.58	0.43
35:LQ:119:SER:C	35:LQ:121:LYS:N	2.75	0.43
43:LY:51:GLN:HG2	43:LY:86:LEU:HD11	2.00	0.43
55:Pt:5:C:H2'	55:Pt:6:G:C8	2.52	0.43
1:16:625:U:H2'	1:16:626:G:C8	2.52	0.43
1:16:1144:G:N2	1:16:1146:A:H62	2.16	0.43
23:23:483:A:C8	42:LX:45:HIS:HD2	2.36	0.43
23:23:1090:A:N1	23:23:1102:C:H1'	2.33	0.43
23:23:1853:A:H2'	23:23:1854:A:C8	2.54	0.43
23:23:2131:U:H4'	23:23:2133:G:H1'	2.00	0.43
23:23:2242:G:H2'	23:23:2243:U:O4'	2.18	0.43
35:LQ:28:LEU:HD23	35:LQ:48:VAL:HG21	2.00	0.43
23:23:2108:A:H2	23:23:2181:U:H3	1.67	0.43
23:23:2740:A:H2'	23:23:2741:A:C8	2.53	0.43
32:LN:22:ILE:HD11	32:LN:57:VAL:HG13	2.01	0.43
35:LQ:8:ARG:HD2	35:LQ:43:GLU:HG2	1.99	0.43
1:16:1106:G:H5"	3:SC:172:ARG:HB3	1.99	0.43
1:16:1524:C:H2'	1:16:1525:G:C8	2.54	0.43
11:SK:126:LYS:HD3	21:SU:37:PHE:HB2	2.01	0.43
23:23:396:G:H1'	45:Lb:29:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1269:A:H2'	23:23:1270:C:C6	2.53	0.43
23:23:1881:C:H2'	23:23:1882:U:O4'	2.18	0.43
23:23:2432:A:H2'	23:23:2433:A:C8	2.53	0.43
55:Pt:16:H2U:H62	55:Pt:16:H2U:H2'	1.20	0.43
14:SN:69:ARG:HA	14:SN:70:PRO:HD3	1.90	0.43
24:5:106:G:H2'	24:5:107:G:O4'	2.18	0.43
30:LI:125:THR:HG23	30:LI:146:VAL:O	2.19	0.43
45:Lb:32:ASN:O	45:Lb:52:SER:HA	2.18	0.43
48:Le:1:MET:HE2	48:Le:6:HIS:CD2	2.53	0.43
3:SC:10:ILE:HG23	3:SC:11:ARG:HG3	2.01	0.43
23:23:357:C:H2'	23:23:358:U:C6	2.53	0.43
23:23:667:U:O2	52:Li:2:PRO:HD2	2.19	0.43
23:23:2251:OMG:HM23	23:23:2251:OMG:H1'	1.66	0.43
23:23:1475:G:H4'	23:23:1476:U:O5'	2.19	0.43
23:23:2310:C:H2'	28:LE:77:PHE:HE2	1.83	0.43
41:LW:15:HIS:HB3	41:LW:31:VAL:HG12	2.01	0.43
1:16:134:G:H1'	1:16:325:A:C5	2.54	0.43
2:SB:186:ILE:HD13	2:SB:200:ILE:HB	2.01	0.43
4:SD:57:GLU:HG2	4:SD:199:LEU:HB2	2.01	0.43
23:23:811:U:H2'	33:LO:21:ARG:HA	1.99	0.43
23:23:1914:C:H2'	23:23:1915:3TD:O4'	2.19	0.43
23:23:2192:U:H2'	23:23:2193:G:C8	2.54	0.43
23:23:2300:C:H2'	23:23:2301:C:C6	2.54	0.43
10:SJ:65:TYR:OH	14:SN:85:ARG:HG2	2.19	0.42
11:SK:82:LEU:HD11	11:SK:107:ILE:HD13	2.00	0.42
23:23:483:A:H5"	42:LX:47:LYS:HG2	2.00	0.42
23:23:488:G:H1'	23:23:492:A:N6	2.33	0.42
33:LO:23:ILE:HG12	39:LU:82:HIS:CD2	2.54	0.42
23:23:492:A:H2'	23:23:493:G:O4'	2.19	0.42
23:23:1545:A:H2'	23:23:1546:G:O4'	2.19	0.42
29:LF:44:LYS:O	29:LF:50:LEU:HA	2.19	0.42
56:Dt:23:A:H2'	56:Dt:24:G:C8	2.54	0.42
1:16:310:G:H5"	16:SP:31:ARG:HB2	2.01	0.42
1:16:413:G:H1'	1:16:428:G:N2	2.34	0.42
1:16:1029:U:H2'	1:16:1031:C:H1'	2.01	0.42
23:23:1084:A:H2'	23:23:1085:A:C8	2.54	0.42
23:23:1562:U:H2'	23:23:1563:U:O4'	2.19	0.42
23:23:1709:U:H2'	23:23:1710:G:C8	2.54	0.42
45:Lb:15:GLY:HA3	45:Lb:29:PHE:HE1	1.83	0.42
1:16:468:A:H3'	1:16:469:C:H6	1.84	0.42
1:16:1477:U:H2'	1:16:1478:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SF:29:ILE:HD13	6:SF:64:VAL:HG11	2.01	0.42
11:SK:64:GLN:HG3	11:SK:99:ALA:HB2	2.01	0.42
23:23:1537:G:C5	23:23:1538:G:H1'	2.54	0.42
23:23:2070:A:H2'	23:23:2071:A:C8	2.55	0.42
23:23:2228:G:H2'	23:23:2229:U:C6	2.55	0.42
23:23:2305:U:C2	28:LE:151:GLY:HA3	2.54	0.42
23:23:2849:U:H4'	23:23:2868:A:C2	2.55	0.42
33:LO:95:LEU:CD1	33:LO:125:LEU:HD21	2.49	0.42
1:16:178:C:H2'	1:16:179:A:C8	2.55	0.42
23:23:598:U:H2'	23:23:599:A:C8	2.54	0.42
23:23:987:C:H2'	23:23:988:A:O4'	2.20	0.42
23:23:1676:A:H2'	23:23:1677:A:O4'	2.20	0.42
40:LV:1:MET:HG2	40:LV:62:ASP:HB3	2.02	0.42
56:Dt:47:3AU:H2'	56:Dt:47:3AU:H6	1.46	0.42
1:16:134:G:H2'	1:16:135:C:O4'	2.18	0.42
23:23:1510:G:H2'	23:23:1511:G:O4'	2.19	0.42
23:23:1683:U:H2'	23:23:1684:G:H8	1.85	0.42
23:23:2505:G:N3	54:Pp:1:MET:HE2	2.35	0.42
23:23:2784:U:H2'	23:23:2785:C:C6	2.55	0.42
23:23:2810:A:H2'	23:23:2811:G:O4'	2.19	0.42
24:5:28:C:H5"	36:LR:31:THR:HG21	2.01	0.42
1:16:46:G:O2'	1:16:365:U:H1'	2.19	0.42
1:16:553:A:H5"	12:SL:21:VAL:HG21	2.01	0.42
1:16:707:U:H2'	1:16:708:C:H6	1.85	0.42
4:SD:102:VAL:HG13	4:SD:107:PHE:HB2	2.00	0.42
23:23:717:C:H3'	23:23:718:A:C8	2.55	0.42
23:23:729:G:C6	25:LB:207:LYS:HB2	2.54	0.42
23:23:1268:A:H2'	23:23:1269:A:O4'	2.20	0.42
23:23:2345:G:N3	23:23:2381:A:H2'	2.35	0.42
14:SN:73:PHE:CZ	14:SN:78:GLY:HA2	2.55	0.42
23:23:476:G:H4'	23:23:502:A:N1	2.35	0.42
23:23:1089:A:H2	23:23:1090:A:H62	1.68	0.42
23:23:2117:A:H61	23:23:2170:A:H61	1.66	0.42
23:23:2187:U:H2'	23:23:2188:U:C6	2.55	0.42
23:23:2469:A:H4'	34:LP:55:ARG:CD	2.49	0.42
25:LB:71:LYS:HB3	25:LB:71:LYS:HE3	1.79	0.42
39:LU:77:PHE:HD1	39:LU:84:ARG:HG2	1.85	0.42
42:LX:41:LEU:HB3	42:LX:60:GLU:HG2	2.01	0.42
1:16:9:G:H5'	5:SE:108:GLY:HA3	2.02	0.42
1:16:1352:C:H2'	1:16:1353:G:C8	2.55	0.42
1:16:1411:C:H2'	1:16:1412:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SD:104:ARG:HD3	4:SD:104:ARG:HA	1.90	0.42
18:SR:19:GLN:C	18:SR:20:GLU:HG3	2.43	0.42
23:23:121:G:H4'	23:23:149:A:H5'	2.01	0.42
23:23:960:A:H2'	23:23:962:G:H5'	2.02	0.42
23:23:1009:A:H5'	38:LT:59:GLN:HG3	2.02	0.42
23:23:1863:G:H4'	23:23:2411:A:H4'	2.02	0.42
23:23:2096:C:H2'	23:23:2097:A:C8	2.54	0.42
26:LC:25:THR:HG21	26:LC:193:VAL:HG22	2.02	0.42
28:LE:36:LEU:HB3	28:LE:57:LEU:HD21	2.02	0.42
53:Lj:15:LYS:HB3	53:Lj:15:LYS:HE2	1.84	0.42
1:16:214:C:H2'	1:16:215:C:C6	2.55	0.42
1:16:381:C:H2'	1:16:382:A:O4'	2.20	0.42
1:16:468:A:H5"	1:16:469:C:H5	1.85	0.42
12:SL:30:LYS:HD3	12:SL:30:LYS:HA	1.92	0.42
23:23:567:U:H2'	23:23:568:U:O4'	2.20	0.42
23:23:1494:A:H3'	23:23:1495:A:H8	1.85	0.42
23:23:2457:PSU:O2'	23:23:2458:G:H5'	2.19	0.42
1:16:222:C:H2'	1:16:223:A:H8	1.83	0.41
23:23:1253:A:OP1	38:LT:33:ARG:NH2	2.53	0.41
23:23:1848:A:H2'	23:23:1849:G:O4'	2.20	0.41
30:LI:4:ILE:CG1	30:LI:37:VAL:CG1	2.96	0.41
1:16:1414:U:H2'	1:16:1415:G:C8	2.55	0.41
3:SC:7:PRO:HD2	3:SC:184:TYR:CD2	2.55	0.41
3:SC:72:ARG:HD2	3:SC:75:ILE:HG13	2.02	0.41
6:SF:36:ILE:HG23	6:SF:64:VAL:HG12	2.02	0.41
10:SJ:18:ILE:HD13	10:SJ:72:ARG:HG2	2.02	0.41
23:23:653:U:H6	23:23:653:U:H2'	1.63	0.41
23:23:2246:G:H2'	23:23:2247:A:C8	2.55	0.41
55:Pt:34:U8U:H6	55:Pt:34:U8U:O5'	2.19	0.41
1:16:195:A:H2'	1:16:196:A:C8	2.56	0.41
1:16:635:A:H2'	1:16:636:U:C6	2.55	0.41
20:ST:28:MET:O	20:ST:32:ILE:HG13	2.21	0.41
23:23:2389:G:H5"	23:23:2390:U:O4'	2.20	0.41
23:23:1183:U:H2'	23:23:1184:U:C6	2.55	0.41
23:23:2636:C:H2'	23:23:2637:U:H6	1.83	0.41
23:23:2809:A:H2'	23:23:2810:A:C8	2.55	0.41
27:LD:108:ILE:HG23	33:LO:1:MET:SD	2.61	0.41
39:LU:51:VAL:HB	39:LU:52:PRO:HD3	2.01	0.41
1:16:619:U:C2	4:SD:132:ILE:HD11	2.55	0.41
7:SG:104:ILE:HD13	7:SG:124:LEU:HD23	2.03	0.41
13:SM:91:HIS:HA	13:SM:109:ARG:HH22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:2030:6MZ:H2	23:23:2500:U:P	2.61	0.41
23:23:2241:A:H2'	23:23:2242:G:C8	2.55	0.41
57:23:3014:PUT:H41	57:23:3014:PUT:H11	1.74	0.41
25:LB:76:ALA:HB3	25:LB:116:ILE:HG13	2.03	0.41
1:16:236:A:H2'	1:16:237:G:C8	2.55	0.41
11:SK:35:THR:HG22	11:SK:41:ALA:HA	2.03	0.41
15:SO:36:ILE:O	15:SO:40:GLN:HG2	2.21	0.41
23:23:1604:C:O2'	23:23:1610:A:N1	2.47	0.41
23:23:1883:U:H2'	23:23:1884:G:O4'	2.20	0.41
1:16:475:C:H2'	1:16:476:U:C6	2.56	0.41
1:16:736:C:H2'	1:16:737:C:C6	2.55	0.41
1:16:1060:U:H2'	1:16:1061:G:H8	1.86	0.41
23:23:26:G:H1'	23:23:514:A:N6	2.36	0.41
23:23:39:G:H2'	23:23:40:U:C6	2.56	0.41
23:23:1171:G:H1	23:23:1178:C:H42	1.68	0.41
23:23:2071:A:H2'	23:23:2072:C:C6	2.56	0.41
23:23:2075:U:H4'	23:23:2596:U:O2	2.20	0.41
23:23:2836:U:H2'	23:23:2837:A:C8	2.56	0.41
29:LF:154:PRO:HD3	29:LF:162:VAL:O	2.19	0.41
1:16:1043:G:H2'	1:16:1044:A:H8	1.86	0.41
5:SE:38:VAL:HG11	5:SE:114:VAL:HG22	2.03	0.41
23:23:885:C:H2'	23:23:886:A:H8	1.86	0.41
23:23:2478:A:H5'	53:Lj:32:LYS:HE2	2.02	0.41
23:23:2557:G:H2'	23:23:2558:C:C6	2.55	0.41
38:LT:61:TRP:O	38:LT:65:ILE:HG13	2.21	0.41
1:16:335:C:H2'	1:16:336:A:H8	1.86	0.41
1:16:502:A:H2'	1:16:503:C:O4'	2.21	0.41
1:16:555:U:H2'	1:16:556:C:C6	2.55	0.41
1:16:606:G:H5"	1:16:606:G:C8	2.51	0.41
1:16:932:C:H5"	7:SG:4:ARG:CZ	2.51	0.41
1:16:1118:U:H1'	1:16:1179:A:C5	2.56	0.41
1:16:1464:U:H2'	1:16:1465:A:C8	2.56	0.41
3:SC:10:ILE:HD12	3:SC:10:ILE:HA	1.92	0.41
6:SF:4:TYR:CD2	6:SF:71:ILE:HG13	2.56	0.41
12:SL:4:VAL:HG23	17:SQ:34:TYR:HB3	2.03	0.41
14:SN:98:LYS:HB3	14:SN:98:LYS:HE2	1.63	0.41
18:SR:70:TYR:HB2	18:SR:74:HIS:NE2	2.35	0.41
19:SS:9:PRO:HB2	19:SS:41:PHE:CZ	2.55	0.41
20:ST:39:ILE:HG21	20:ST:82:GLN:HG2	2.03	0.41
23:23:1219:U:H2'	23:23:1220:G:C8	2.56	0.41
23:23:1306:C:H2'	23:23:1307:A:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:2455:G:H2'	23:23:2456:C:C6	2.56	0.41
23:23:2888:C:H2'	23:23:2889:C:C6	2.56	0.41
26:LC:99:GLU:HG3	26:LC:182:ALA:HB2	2.03	0.41
29:LF:156:PRO:O	29:LF:171:THR:HA	2.21	0.41
30:LI:94:ILE:HB	30:LI:122:LEU:HB2	2.03	0.41
33:LO:112:LEU:HD12	33:LO:130:GLY:HA3	2.02	0.41
34:LP:53:MET:HG3	34:LP:63:ILE:HD13	2.03	0.41
35:LQ:8:ARG:HB2	35:LQ:43:GLU:HG3	2.02	0.41
36:LR:58:ILE:HG22	36:LR:62:LEU:HD12	2.02	0.41
1:16:215:C:H2'	1:16:216:U:C6	2.55	0.41
1:16:737:C:H2'	1:16:738:C:C6	2.56	0.41
1:16:1273:C:H2'	1:16:1274:A:O4'	2.21	0.41
2:SB:100:MET:HE3	2:SB:100:MET:HB2	1.87	0.41
23:23:829:A:N7	23:23:2248:C:H5'	2.36	0.41
1:16:147:G:H2'	1:16:148:G:C8	2.57	0.40
2:SB:171:ILE:O	2:SB:175:GLU:HG3	2.21	0.40
9:SI:30:ILE:HG23	9:SI:65:ILE:HG13	2.02	0.40
11:SK:9:ARG:O	11:SK:13:ARG:HG3	2.21	0.40
20:ST:39:ILE:HD13	20:ST:82:GLN:HB3	2.02	0.40
23:23:135:U:H2'	23:23:136:G:C8	2.56	0.40
23:23:207:A:H2'	23:23:208:C:O4'	2.21	0.40
23:23:751:A:H5'	40:LV:90:LYS:HA	2.02	0.40
23:23:942:G:H4'	23:23:1190:G:H5'	2.02	0.40
23:23:1945:G:H2'	23:23:1946:U:C6	2.56	0.40
32:LN:64:ARG:O	32:LN:82:ASN:HA	2.22	0.40
33:LO:85:VAL:HB	33:LO:94:THR:HG22	2.04	0.40
36:LR:58:ILE:HG22	36:LR:62:LEU:CD1	2.51	0.40
42:LX:22:ARG:HD3	42:LX:73:PHE:CE1	2.56	0.40
43:LY:20:LEU:HD12	43:LY:20:LEU:HA	1.92	0.40
43:LY:30:ILE:HG12	43:LY:91:PHE:HB2	2.03	0.40
55:Pt:46:G7M:H8	55:Pt:46:G7M:H2'	1.65	0.40
1:16:84:U:H6	1:16:84:U:H2'	1.74	0.40
1:16:204:G:H2'	1:16:205:A:N3	2.35	0.40
3:SC:141:ALA:CB	3:SC:149:ILE:HD12	2.51	0.40
11:SK:17:SER:HA	11:SK:79:ILE:HA	2.04	0.40
12:SL:33:VAL:HG22	12:SL:79:VAL:HG22	2.02	0.40
12:SL:81:LEU:HD23	12:SL:81:LEU:HA	1.89	0.40
23:23:1773:A:C2'	23:23:1774:C:H5'	2.52	0.40
23:23:2048:G:H2'	23:23:2049:G:O4'	2.22	0.40
23:23:2175:C:H2'	23:23:2176:A:H8	1.84	0.40
23:23:2743:U:H2'	23:23:2744:G:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:LR:79:ALA:HA	36:LR:115:LEU:HD12	2.02	0.40
38:LT:41:LYS:HA	38:LT:41:LYS:HD3	1.92	0.40
46:Lc:9:LYS:HB2	46:Lc:14:LEU:HD13	2.03	0.40
46:Lc:19:LEU:HD23	46:Lc:19:LEU:HA	1.89	0.40
51:Lh:30:VAL:HG22	51:Lh:33:ARG:NH2	2.37	0.40
1:16:33:A:H2'	1:16:34:C:C6	2.56	0.40
1:16:153:C:H2'	1:16:154:U:C6	2.57	0.40
1:16:911:U:H2'	1:16:912:C:C6	2.57	0.40
1:16:1187:G:H5'	9:SI:115:LYS:HE3	2.03	0.40
2:SB:162:PHE:HA	2:SB:184:PHE:O	2.21	0.40
23:23:493:G:H2'	23:23:494:G:O4'	2.20	0.40
23:23:848:C:H2'	23:23:849:A:C8	2.55	0.40
23:23:1441:G:H2'	23:23:1442:U:C6	2.57	0.40
23:23:1447:C:H2'	23:23:1448:G:C8	2.56	0.40
23:23:1637:A:H5'	23:23:1760:C:O2'	2.22	0.40
23:23:2178:C:H2'	23:23:2179:C:C6	2.56	0.40
23:23:2592:G:H2'	23:23:2593:U:O4'	2.21	0.40
24:5:49:C:H2'	24:5:50:A:C8	2.56	0.40
43:LY:62:THR:HG23	43:LY:69:GLU:HB3	2.04	0.40
1:16:4:U:H6	1:16:4:U:H2'	1.72	0.40
1:16:131:A:H2'	1:16:132:C:C6	2.57	0.40
1:16:449:G:H2'	1:16:450:G:C8	2.56	0.40
1:16:458:U:H2'	1:16:459:A:H8	1.84	0.40
1:16:1372:U:H2'	1:16:1373:G:O4'	2.22	0.40
4:SD:130:VAL:HG13	4:SD:132:ILE:HD12	2.02	0.40
5:SE:13:GLU:HB3	5:SE:64:MET:SD	2.61	0.40
7:SG:56:LYS:HG2	7:SG:57:SER:H	1.87	0.40
23:23:27:G:N2	23:23:512:G:H1'	2.37	0.40
23:23:323:C:H6	23:23:1205:A:C2	2.39	0.40
23:23:369:U:H2'	60:23:3002:ATP:HN62	1.86	0.40
23:23:2306:C:H2'	23:23:2307:G:C8	2.57	0.40
24:5:80:U:H2'	24:5:81:G:C8	2.56	0.40
27:LD:200:LEU:HD23	27:LD:200:LEU:HA	1.88	0.40
32:LN:71:ARG:HB3	32:LN:72:PRO:HD2	2.02	0.40
34:LP:34:LYS:HD3	43:LY:82:TYR:HA	2.03	0.40
42:LX:72:ILE:HD13	42:LX:103:ILE:HD13	2.04	0.40
1:16:1096:C:H2'	1:16:1097:C:C6	2.57	0.40
23:23:418:C:H2'	23:23:419:U:C6	2.56	0.40
23:23:546:U:H2'	23:23:547:A:H4'	2.03	0.40
23:23:1752:C:H2'	23:23:1753:G:C8	2.57	0.40
23:23:2343:U:H2'	23:23:2344:U:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:2771:C:H2'	23:23:2772:C:C6	2.57	0.40
55:Pt:70:C:H2'	55:Pt:71:C:C6	2.57	0.40

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	226/241 (94%)	219 (97%)	7 (3%)	0	100	100
3	SC	212/233 (91%)	210 (99%)	2 (1%)	0	100	100
4	SD	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
5	SE	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
6	SF	104/135 (77%)	100 (96%)	3 (3%)	1 (1%)	12	23
7	SG	149/179 (83%)	145 (97%)	3 (2%)	1 (1%)	18	32
8	SH	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
9	SI	125/130 (96%)	119 (95%)	5 (4%)	1 (1%)	16	29
10	SJ	97/103 (94%)	94 (97%)	1 (1%)	2 (2%)	5	9
11	SK	123/129 (95%)	117 (95%)	6 (5%)	0	100	100
12	SL	120/124 (97%)	111 (92%)	8 (7%)	1 (1%)	16	29
13	SM	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
14	SN	98/101 (97%)	98 (100%)	0	0	100	100
15	SO	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	SP	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
17	SQ	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
18	SR	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
19	SS	82/92 (89%)	80 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	ST	84/87 (97%)	84 (100%)	0	0	100	100
21	SU	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
25	LB	270/273 (99%)	259 (96%)	11 (4%)	0	100	100
26	LC	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
27	LD	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
28	LE	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
29	LF	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
30	LI	147/149 (99%)	130 (88%)	14 (10%)	3 (2%)	6	9
31	LM	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
32	LN	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
33	LO	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
34	LP	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
35	LQ	120/127 (94%)	117 (98%)	3 (2%)	0	100	100
36	LR	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
37	LS	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
38	LT	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
39	LU	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	12	23
40	LV	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	LW	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
42	LX	101/104 (97%)	97 (96%)	3 (3%)	1 (1%)	12	23
43	LY	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
44	La	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
45	Lb	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
46	Lc	60/63 (95%)	60 (100%)	0	0	100	100
47	Ld	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	Le	65/70 (93%)	64 (98%)	1 (2%)	0	100	100
49	Lf	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
50	Lg	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
51	Lh	44/46 (96%)	44 (100%)	0	0	100	100
52	Li	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
53	Lj	36/38 (95%)	36 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
54	Pp	1/3 (33%)	1 (100%)	0	0	100 100
All	All	5644/5916 (95%)	5477 (97%)	156 (3%)	11 (0%)	44 62

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	SJ	57	VAL
6	SF	33	GLU
9	SI	25	ASN
39	LU	52	PRO
42	LX	48	PRO
30	LI	105	ALA
7	SG	57	SER
12	SL	42	PRO
10	SJ	79	PRO
30	LI	78	VAL
30	LI	118	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	SB	189/199 (95%)	180 (95%)	9 (5%)	23 43
3	SC	174/190 (92%)	164 (94%)	10 (6%)	18 36
4	SD	172/173 (99%)	164 (95%)	8 (5%)	23 44
5	SE	119/126 (94%)	117 (98%)	2 (2%)	53 77
6	SF	92/116 (79%)	89 (97%)	3 (3%)	33 58
7	SG	124/147 (84%)	118 (95%)	6 (5%)	23 43
8	SH	104/105 (99%)	103 (99%)	1 (1%)	68 85
9	SI	105/107 (98%)	99 (94%)	6 (6%)	18 36
10	SJ	87/90 (97%)	85 (98%)	2 (2%)	44 70
11	SK	97/99 (98%)	93 (96%)	4 (4%)	27 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	SL	102/103 (99%)	99 (97%)	3 (3%)	37 63
13	SM	95/96 (99%)	88 (93%)	7 (7%)	13 25
14	SN	83/84 (99%)	77 (93%)	6 (7%)	13 26
15	SO	76/77 (99%)	75 (99%)	1 (1%)	61 81
16	SP	65/65 (100%)	59 (91%)	6 (9%)	8 17
17	SQ	78/78 (100%)	76 (97%)	2 (3%)	40 66
18	SR	58/65 (89%)	56 (97%)	2 (3%)	32 57
19	SS	72/79 (91%)	69 (96%)	3 (4%)	26 49
20	ST	65/66 (98%)	63 (97%)	2 (3%)	35 60
21	SU	60/61 (98%)	58 (97%)	2 (3%)	33 58
25	LB	217/218 (100%)	213 (98%)	4 (2%)	51 75
26	LC	164/164 (100%)	161 (98%)	3 (2%)	51 75
27	LD	165/165 (100%)	160 (97%)	5 (3%)	36 62
28	LE	149/150 (99%)	139 (93%)	10 (7%)	15 29
29	LF	137/138 (99%)	129 (94%)	8 (6%)	18 36
30	LI	114/114 (100%)	107 (94%)	7 (6%)	17 33
31	LM	116/116 (100%)	113 (97%)	3 (3%)	40 66
32	LN	104/104 (100%)	99 (95%)	5 (5%)	23 43
33	LO	103/103 (100%)	100 (97%)	3 (3%)	37 63
34	LP	109/108 (101%)	107 (98%)	2 (2%)	51 75
35	LQ	101/103 (98%)	100 (99%)	1 (1%)	68 85
36	LR	86/87 (99%)	82 (95%)	4 (5%)	23 44
37	LS	100/100 (100%)	96 (96%)	4 (4%)	28 51
38	LT	89/90 (99%)	84 (94%)	5 (6%)	19 37
39	LU	84/84 (100%)	81 (96%)	3 (4%)	31 55
40	LV	93/93 (100%)	92 (99%)	1 (1%)	65 83
41	LW	80/84 (95%)	77 (96%)	3 (4%)	29 53
42	LX	84/85 (99%)	84 (100%)	0	100 100
43	LY	78/78 (100%)	78 (100%)	0	100 100
44	La	57/63 (90%)	56 (98%)	1 (2%)	51 75
45	Lb	67/68 (98%)	65 (97%)	2 (3%)	36 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	Lc	54/55 (98%)	53 (98%)	1 (2%)	50 74
47	Ld	48/49 (98%)	43 (90%)	5 (10%)	7 13
48	Le	60/62 (97%)	53 (88%)	7 (12%)	5 10
49	Lf	47/48 (98%)	47 (100%)	0	100 100
50	Lg	49/49 (100%)	48 (98%)	1 (2%)	48 73
51	Lh	38/38 (100%)	38 (100%)	0	100 100
52	Li	51/52 (98%)	51 (100%)	0	100 100
53	Lj	34/34 (100%)	33 (97%)	1 (3%)	37 63
54	Pp	3/3 (100%)	3 (100%)	0	100 100
All	All	4698/4831 (97%)	4524 (96%)	174 (4%)	31 54

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	60	ILE
2	SB	80	VAL
2	SB	86	SER
2	SB	110	SER
2	SB	133	GLU
2	SB	154	MET
2	SB	161	LEU
2	SB	220	THR
2	SB	229	LEU
3	SC	84	VAL
3	SC	101	ILE
3	SC	121	THR
3	SC	129[A]	MET
3	SC	129[B]	MET
3	SC	149	ILE
3	SC	154	SER
3	SC	170	GLU
3	SC	185	ASN
3	SC	202	ILE
4	SD	22	LYS
4	SD	34	ILE
4	SD	116	GLN
4	SD	117	LEU
4	SD	132	ILE
4	SD	152	GLN

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Mol	Chain	Res	Type
4	SD	172	GLU
4	SD	194	ASP
5	SE	80	THR
5	SE	164	ILE
6	SF	36	ILE
6	SF	63	ASN
6	SF	103	VAL
7	SG	29	ILE
7	SG	40	GLU
7	SG	58	GLU
7	SG	83	SER
7	SG	131	LYS
7	SG	146	GLU
8	SH	42	GLU
9	SI	46	MET
9	SI	63	LEU
9	SI	65	ILE
9	SI	67	VAL
9	SI	68	LYS
9	SI	118	LEU
10	SJ	24	GLU
10	SJ	102	LEU
11	SK	85	MET
11	SK	107	ILE
11	SK	109	ASN
11	SK	119	ASN
12	SL	49	LEU
12	SL	70	GLU
12	SL	86	ARG
13	SM	16	VAL
13	SM	41	GLU
13	SM	49	SER
13	SM	64	VAL
13	SM	68	ASP
13	SM	97	VAL
13	SM	107	ARG
14	SN	10	GLU
14	SN	23	LYS
14	SN	26	GLU
14	SN	37	SER
14	SN	85	ARG
14	SN	100	SER

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Mol	Chain	Res	Type
15	SO	13	SER
16	SP	1	MET
16	SP	47	GLU
16	SP	57	ILE
16	SP	63	GLN
16	SP	67	ILE
16	SP	77	GLU
17	SQ	28	PHE
17	SQ	62	ARG
18	SR	48	ARG
18	SR	74	HIS
19	SS	31	LEU
19	SS	47	LEU
19	SS	79	THR
20	ST	48	GLN
20	ST	57	ILE
21	SU	3	VAL
21	SU	40	LYS
25	LB	110	LEU
25	LB	140	THR
25	LB	162	VAL
25	LB	182	ARG
26	LC	1	MET
26	LC	129	THR
26	LC	161	MET
27	LD	2	GLU
27	LD	84	THR
27	LD	90	GLN
27	LD	143	LEU
27	LD	167	VAL
28	LE	10	ASP
28	LE	11	GLU
28	LE	35	THR
28	LE	68	THR
28	LE	87	CYS
28	LE	96	MET
28	LE	121	SER
28	LE	123	ASP
28	LE	132	VAL
28	LE	134	GLU
29	LF	26	ILE
29	LF	29	LYS

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Mol	Chain	Res	Type
29	LF	48	ASN
29	LF	49	THR
29	LF	79	VAL
29	LF	98	VAL
29	LF	117	LEU
29	LF	127	THR
30	LI	41	LYS
30	LI	62	LEU
30	LI	78	VAL
30	LI	99	ILE
30	LI	112	LYS
30	LI	121	VAL
30	LI	134	VAL
31	LM	39	LYS
31	LM	64	VAL
31	LM	95	ARG
32	LN	41	ILE
32	LN	53	LYS
32	LN	58	LEU
32	LN	67	LYS
32	LN	104	THR
33	LO	92	LEU
33	LO	121	THR
33	LO	132	ARG
34	LP	54	THR
34	LP	80	VAL
35	LQ	6	SER
36	LR	19	GLN
36	LR	53	THR
36	LR	78	VAL
36	LR	115	LEU
37	LS	10[A]	GLN
37	LS	10[B]	GLN
37	LS	32	VAL
37	LS	34	GLU
38	LT	6	ARG
38	LT	31	VAL
38	LT	54	LYS
38	LT	59	GLN
38	LT	71	GLN
39	LU	33	VAL
39	LU	41	ILE

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Mol	Chain	Res	Type
39	LU	49	ILE
40	LV	108	SER
41	LW	5	GLU
41	LW	48	GLN
41	LW	64	LYS
44	La	70	GLU
45	Lb	40	VAL
45	Lb	59	ILE
46	Lc	14	LEU
47	Ld	5	ILE
47	Ld	19	LYS
47	Ld	37	GLU
47	Ld	54	MET
47	Ld	59	GLU
48	Le	10	GLU
48	Le	11	GLU
48	Le	34	LEU
48	Le	36	VAL
48	Le	51	VAL
48	Le	53	THR
48	Le	58	ASP
50	Lg	50	LYS
53	Lj	16	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
2	SB	94	HIS
2	SB	177	ASN
2	SB	227	GLN
3	SC	25	ASN
3	SC	185	ASN
4	SD	120	HIS
4	SD	126	ASN
4	SD	152	GLN
5	SE	121	HIS
5	SE	148	ASN
6	SF	3	HIS
6	SF	68	GLN
8	SH	4	GLN
10	SJ	56	HIS
10	SJ	58	ASN

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Mol	Chain	Res	Type
10	SJ	99	GLN
11	SK	81	ASN
11	SK	101	ASN
11	SK	109	ASN
11	SK	119	ASN
12	SL	77	HIS
13	SM	8	ASN
14	SN	49	GLN
16	SP	63	GLN
17	SQ	45	HIS
20	ST	3	ASN
20	ST	48	GLN
20	ST	52	ASN
20	ST	61	GLN
25	LB	90	ASN
26	LC	42	ASN
26	LC	49	GLN
26	LC	94	GLN
26	LC	173	GLN
27	LD	90	GLN
27	LD	94	GLN
27	LD	115	GLN
27	LD	136	GLN
28	LE	5	HIS
28	LE	37	ASN
29	LF	48	ASN
29	LF	104	ASN
30	LI	66	ASN
31	LM	58	ASN
31	LM	86	GLN
33	LO	104	GLN
35	LQ	18	GLN
36	LR	61	GLN
40	LV	9	HIS
41	LW	92	ASN
43	LY	24	ASN
44	La	57	HIS
45	Lb	36	HIS
46	Lc	39	GLN
46	Lc	45	GLN
46	Lc	58	ASN
47	Ld	9	GLN

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Mol	Chain	Res	Type
48	Le	20	ASN
48	Le	48	GLN
49	Lf	42	HIS
51	Lh	26	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1533/1534 (99%)	306 (19%)	26 (1%)
22	mR	10/60 (16%)	0	0
23	23	2901/2904 (99%)	510 (17%)	48 (1%)
24	5	119/120 (99%)	19 (15%)	2 (1%)
55	Pt	75/76 (98%)	28 (37%)	0
56	Dt	75/76 (98%)	16 (21%)	0
All	All	4713/4770 (98%)	879 (18%)	76 (1%)

All (879) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	4	U
1	16	5	U
1	16	7	A
1	16	9	G
1	16	22	G
1	16	30	U
1	16	32	A
1	16	38	G
1	16	39	G
1	16	47	C
1	16	48	C
1	16	49	U
1	16	50	A
1	16	51	A
1	16	54	C
1	16	65	A
1	16	71	A
1	16	72	A
1	16	77	A
1	16	82	G
1	16	83	C
1	16	84	U

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Mol	Chain	Res	Type
1	16	85	U
1	16	86	G
1	16	89	U
1	16	90	C
1	16	91	U
1	16	95	C
1	16	97	G
1	16	98	A
1	16	116	A
1	16	120	A
1	16	121	U
1	16	122	G
1	16	130	A
1	16	131	A
1	16	138	G
1	16	141	G
1	16	144	G
1	16	160	A
1	16	163	C
1	16	164	G
1	16	170	U
1	16	173	U
1	16	177	G
1	16	182	A
1	16	183	C
1	16	197	A
1	16	199	A
1	16	204	G
1	16	210	C
1	16	211	G
1	16	220	G
1	16	221	C
1	16	226	G
1	16	227	G
1	16	240	G
1	16	245	U
1	16	247	G
1	16	248	C
1	16	250	A
1	16	251	G
1	16	253	A
1	16	264	C

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Mol	Chain	Res	Type
1	16	266	G
1	16	267	C
1	16	280	C
1	16	281	G
1	16	289	G
1	16	293	G
1	16	301	G
1	16	305	G
1	16	307	C
1	16	321	A
1	16	328	C
1	16	329	A
1	16	330	C
1	16	332	G
1	16	345	C
1	16	347	G
1	16	351	G
1	16	352	C
1	16	354	G
1	16	355	C
1	16	363	A
1	16	367	U
1	16	368	U
1	16	372	C
1	16	373	A
1	16	384	G
1	16	392	C
1	16	398	U
1	16	406	G
1	16	411	A
1	16	412	A
1	16	413	G
1	16	414	A
1	16	421	U
1	16	422	C
1	16	424	G
1	16	429	U
1	16	430	A
1	16	438	U
1	16	439	U
1	16	453	G
1	16	466	A

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Mol	Chain	Res	Type
1	16	467	U
1	16	468	A
1	16	478	A
1	16	481	G
1	16	486	U
1	16	495	A
1	16	496	A
1	16	508	U
1	16	511	C
1	16	518	C
1	16	521	G
1	16	527	G7M
1	16	530	G
1	16	531	U
1	16	533	A
1	16	536	C
1	16	547	A
1	16	562	U
1	16	568	G
1	16	572	A
1	16	573	A
1	16	576	C
1	16	577	G
1	16	579	A
1	16	606	G
1	16	607	A
1	16	615	G
1	16	619	U
1	16	620	C
1	16	628	G
1	16	633	G
1	16	639	G
1	16	642	A
1	16	653	U
1	16	654	G
1	16	661	G
1	16	665	A
1	16	666	G
1	16	671	G
1	16	686	U
1	16	695	A
1	16	701	U

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Mol	Chain	Res	Type
1	16	703	G
1	16	717	U
1	16	723	U
1	16	724	G
1	16	734	G
1	16	736	C
1	16	748	G
1	16	752	G
1	16	755	G
1	16	777	A
1	16	787	A
1	16	792	A
1	16	793	U
1	16	794	A
1	16	799	G
1	16	810	C
1	16	815	A
1	16	817	C
1	16	821	G
1	16	832	G
1	16	841	C
1	16	842	U
1	16	843	U
1	16	846	G
1	16	870	U
1	16	874	G
1	16	884	U
1	16	913	A
1	16	914	A
1	16	922	G
1	16	926	G
1	16	927	G
1	16	931	C
1	16	934	C
1	16	939	G
1	16	942	G
1	16	958	A
1	16	960	U
1	16	969	A
1	16	972	C
1	16	975	A
1	16	976	G

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Mol	Chain	Res	Type
1	16	977	A
1	16	983	A
1	16	987	G
1	16	991	U
1	16	992	U
1	16	993	G
1	16	994	A
1	16	1002	G
1	16	1003	G
1	16	1004	A
1	16	1005	A
1	16	1012	A
1	16	1020	G
1	16	1028	C
1	16	1029	U
1	16	1030	U
1	16	1031	C
1	16	1032	G
1	16	1033	G
1	16	1041	G
1	16	1045	C
1	16	1046	A
1	16	1053	G
1	16	1065	U
1	16	1085	U
1	16	1094	G
1	16	1095	U
1	16	1101	A
1	16	1107	C
1	16	1124	G
1	16	1125	U
1	16	1129	C
1	16	1132	C
1	16	1133	G
1	16	1134	G
1	16	1136	C
1	16	1137	C
1	16	1139	G
1	16	1140	C
1	16	1141	C
1	16	1142	G
1	16	1145	A

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Mol	Chain	Res	Type
1	16	1146	A
1	16	1159	U
1	16	1160	G
1	16	1167	A
1	16	1169	A
1	16	1171	A
1	16	1179	A
1	16	1184	G
1	16	1196	A
1	16	1197	A
1	16	1199	U
1	16	1212	U
1	16	1213	A
1	16	1224	U
1	16	1225	A
1	16	1226	C
1	16	1227	A
1	16	1228	C
1	16	1238	A
1	16	1253	G
1	16	1256	A
1	16	1257	A
1	16	1260	G
1	16	1270	G
1	16	1280	A
1	16	1285	A
1	16	1286	U
1	16	1294	G
1	16	1297	G
1	16	1300	G
1	16	1302	C
1	16	1305	G
1	16	1315	U
1	16	1317	C
1	16	1320	C
1	16	1323	G
1	16	1331	G
1	16	1336	C
1	16	1338	G
1	16	1340	A
1	16	1346	A
1	16	1353	G

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Mol	Chain	Res	Type
1	16	1363	A
1	16	1368	A
1	16	1370	G
1	16	1379	G
1	16	1380	U
1	16	1381	U
1	16	1383	C
1	16	1397	C
1	16	1398	A
1	16	1399	C
1	16	1400	C
1	16	1425	U
1	16	1432	G
1	16	1440	U
1	16	1441	A
1	16	1442	G
1	16	1445	U
1	16	1446	A
1	16	1452	C
1	16	1453	G
1	16	1454	G
1	16	1475	G
1	16	1492	A
1	16	1493	A
1	16	1494	G
1	16	1497	G
1	16	1503	A
1	16	1506	U
1	16	1517	G
1	16	1529	G
1	16	1530	G
1	16	1534	A
23	23	10	A
23	23	36	G
23	23	39	G
23	23	42	A
23	23	46	G
23	23	51	G
23	23	71	A
23	23	74	A
23	23	75	G
23	23	80	G

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Mol	Chain	Res	Type
23	23	84	A
23	23	101	A
23	23	102	U
23	23	103	A
23	23	110	G
23	23	118	A
23	23	119	A
23	23	120	U
23	23	125	A
23	23	126	A
23	23	140	C
23	23	141	G
23	23	142	A
23	23	163	C
23	23	165	A
23	23	178	G
23	23	181	A
23	23	188	G
23	23	196	A
23	23	199	A
23	23	200	U
23	23	215	G
23	23	216	A
23	23	221	A
23	23	222	A
23	23	226	A
23	23	227	A
23	23	239	C
23	23	248	G
23	23	252	G
23	23	266	G
23	23	271	G
23	23	272	A
23	23	275	C
23	23	278	A
23	23	279	A
23	23	311	A
23	23	315	G
23	23	330	A
23	23	345	A
23	23	346	A
23	23	359	G

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Mol	Chain	Res	Type
23	23	361	G
23	23	362	A
23	23	369	U
23	23	370	G
23	23	371	A
23	23	372	G
23	23	380	G
23	23	386	G
23	23	401	A
23	23	403	U
23	23	404	A
23	23	405	U
23	23	411	G
23	23	412	A
23	23	418	C
23	23	455	C
23	23	456	C
23	23	457	A
23	23	459	U
23	23	470	A
23	23	473	G
23	23	477	A
23	23	481	G
23	23	491	G
23	23	503	A
23	23	504	A
23	23	505	A
23	23	506	G
23	23	509	C
23	23	527	C
23	23	528	A
23	23	529	A
23	23	532	A
23	23	547	A
23	23	548	G
23	23	549	G
23	23	556	A
23	23	563	A
23	23	573	U
23	23	575	A
23	23	587	C
23	23	588	U

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Mol	Chain	Res	Type
23	23	603	A
23	23	604	G
23	23	614	A
23	23	615	U
23	23	637	A
23	23	645	C
23	23	646	U
23	23	647	G
23	23	653	U
23	23	654	A
23	23	655	A
23	23	668	A
23	23	686	U
23	23	702	U
23	23	705	A
23	23	713	G
23	23	717	C
23	23	720	U
23	23	730	A
23	23	746	PSU
23	23	747	5MU
23	23	764	A
23	23	765	C
23	23	775	G
23	23	776	G
23	23	777	G
23	23	782	A
23	23	784	G
23	23	785	G
23	23	789	A
23	23	805	G
23	23	812	C
23	23	819	A
23	23	827	U
23	23	828	U
23	23	845	A
23	23	846	U
23	23	847	U
23	23	858	G
23	23	859	G
23	23	865	C
23	23	869	G

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Mol	Chain	Res	Type
23	23	878	A
23	23	880	G
23	23	883	G
23	23	884	U
23	23	888	C
23	23	894	U
23	23	895	U
23	23	896	A
23	23	897	C
23	23	899	A
23	23	900	A
23	23	901	C
23	23	910	A
23	23	913	U
23	23	914	G
23	23	917	A
23	23	919	U
23	23	931	U
23	23	932	U
23	23	941	A
23	23	946	C
23	23	961	C
23	23	962	G
23	23	974	G
23	23	983	A
23	23	984	A
23	23	985	C
23	23	996	A
23	23	999	U
23	23	1012	U
23	23	1013	C
23	23	1017	G
23	23	1022	G
23	23	1026	G
23	23	1027	A
23	23	1033	U
23	23	1040	A
23	23	1041	G
23	23	1047	G
23	23	1051	G
23	23	1058	U
23	23	1060	U

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Mol	Chain	Res	Type
23	23	1061	U
23	23	1062	G
23	23	1063	G
23	23	1070	A
23	23	1077	A
23	23	1078	U
23	23	1086	A
23	23	1087	G
23	23	1088	A
23	23	1089	A
23	23	1090	A
23	23	1097	U
23	23	1105	U
23	23	1110	G
23	23	1111	A
23	23	1112	G
23	23	1115	G
23	23	1116	G
23	23	1118	C
23	23	1128	G
23	23	1132	U
23	23	1133	A
23	23	1134	A
23	23	1135	C
23	23	1136	G
23	23	1142	A
23	23	1143	A
23	23	1161	C
23	23	1168	G
23	23	1171	G
23	23	1173	U
23	23	1174	U
23	23	1177	G
23	23	1179	G
23	23	1195	G
23	23	1212	G
23	23	1238	G
23	23	1244	A
23	23	1247	A
23	23	1249	U
23	23	1253	A
23	23	1256	G

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Mol	Chain	Res	Type
23	23	1262	A
23	23	1266	G
23	23	1267	U
23	23	1271	G
23	23	1272	A
23	23	1273	U
23	23	1301	A
23	23	1321	A
23	23	1344	U
23	23	1352	U
23	23	1359	A
23	23	1360	G
23	23	1365	A
23	23	1368	G
23	23	1379	U
23	23	1383	A
23	23	1386	C
23	23	1392	A
23	23	1395	A
23	23	1403	A
23	23	1407	G
23	23	1416	G
23	23	1417	C
23	23	1428	C
23	23	1451	C
23	23	1452	G
23	23	1453	A
23	23	1455	G
23	23	1458	U
23	23	1460	U
23	23	1475	G
23	23	1477	A
23	23	1478	G
23	23	1482	G
23	23	1489	C
23	23	1490	A
23	23	1493	C
23	23	1494	A
23	23	1495	A
23	23	1497	U
23	23	1508	A
23	23	1514	G

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Mol	Chain	Res	Type
23	23	1515	A
23	23	1524	G
23	23	1529	G
23	23	1530	G
23	23	1531	C
23	23	1533	C
23	23	1535	A
23	23	1536	C
23	23	1537	G
23	23	1538	G
23	23	1542	U
23	23	1544	A
23	23	1554	U
23	23	1559	U
23	23	1566	A
23	23	1569	A
23	23	1578	U
23	23	1583	A
23	23	1584	U
23	23	1585	C
23	23	1591	A
23	23	1608	A
23	23	1610	A
23	23	1618	6MZ
23	23	1647	U
23	23	1648	U
23	23	1649	G
23	23	1674	G
23	23	1690	A
23	23	1727	C
23	23	1729	U
23	23	1730	C
23	23	1732	C
23	23	1738	G
23	23	1739	A
23	23	1740	G
23	23	1741	C
23	23	1764	C
23	23	1773	A
23	23	1776	G
23	23	1782	U
23	23	1799	G

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Mol	Chain	Res	Type
23	23	1800	C
23	23	1801	A
23	23	1807	G
23	23	1808	A
23	23	1816	C
23	23	1829	A
23	23	1845	G
23	23	1847	A
23	23	1848	A
23	23	1869	G
23	23	1870	C
23	23	1872	A
23	23	1873	G
23	23	1876	A
23	23	1882	U
23	23	1901	A
23	23	1913	A
23	23	1930	G
23	23	1937	A
23	23	1938	A
23	23	1954	G
23	23	1955	U
23	23	1956	U
23	23	1960	A
23	23	1964	G
23	23	1965	C
23	23	1967	C
23	23	1970	A
23	23	1971	U
23	23	1972	G
23	23	1982	U
23	23	1991	U
23	23	1992	G
23	23	1993	U
23	23	1997	C
23	23	2020	A
23	23	2022	U
23	23	2023	C
23	23	2030	6MZ
23	23	2031	A
23	23	2032	G
23	23	2033	A

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Mol	Chain	Res	Type
23	23	2043	C
23	23	2055	C
23	23	2056	G
23	23	2060	A
23	23	2061	G
23	23	2062	A
23	23	2069	G7M
23	23	2080	A
23	23	2093	G
23	23	2099	U
23	23	2104	C
23	23	2105	U
23	23	2107	G
23	23	2110	G
23	23	2112	G
23	23	2116	G
23	23	2117	A
23	23	2118	U
23	23	2119	A
23	23	2120	G
23	23	2121	G
23	23	2122	U
23	23	2123	G
23	23	2126	A
23	23	2131	U
23	23	2132	U
23	23	2133	G
23	23	2136	G
23	23	2138	G
23	23	2141	G
23	23	2146	C
23	23	2147	A
23	23	2158	A
23	23	2161	C
23	23	2162	G
23	23	2163	A
23	23	2164	C
23	23	2168	G
23	23	2169	A
23	23	2170	A
23	23	2171	A
23	23	2172	U

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Mol	Chain	Res	Type
23	23	2173	A
23	23	2182	U
23	23	2183	A
23	23	2192	U
23	23	2197	U
23	23	2198	A
23	23	2203	U
23	23	2204	G
23	23	2211	A
23	23	2212	A
23	23	2213	U
23	23	2225	A
23	23	2238	G
23	23	2239	G
23	23	2251	OMG
23	23	2268	A
23	23	2273	A
23	23	2279	G
23	23	2283	C
23	23	2287	A
23	23	2303	G
23	23	2305	U
23	23	2308	G
23	23	2311	A
23	23	2312	U
23	23	2322	A
23	23	2325	G
23	23	2333	A
23	23	2335	A
23	23	2336	A
23	23	2344	U
23	23	2347	C
23	23	2350	C
23	23	2361	G
23	23	2379	G
23	23	2383	G
23	23	2385	C
23	23	2396	G
23	23	2402	U
23	23	2403	C
23	23	2406	A
23	23	2410	G

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Mol	Chain	Res	Type
23	23	2425	A
23	23	2429	G
23	23	2430	A
23	23	2436	G
23	23	2441	U
23	23	2447	G
23	23	2448	A
23	23	2458	G
23	23	2470	G
23	23	2476	A
23	23	2478	A
23	23	2482	A
23	23	2484	G
23	23	2492	U
23	23	2494	G
23	23	2502	G
23	23	2503	2MA
23	23	2505	G
23	23	2518	A
23	23	2529	G
23	23	2547	A
23	23	2554	U
23	23	2556	C
23	23	2564	A
23	23	2566	A
23	23	2567	G
23	23	2569	G
23	23	2573	C
23	23	2602	A
23	23	2603	G
23	23	2609	U
23	23	2613	U
23	23	2614	A
23	23	2621	G
23	23	2629	U
23	23	2630	G
23	23	2636	C
23	23	2639	A
23	23	2656	U
23	23	2661	G
23	23	2663	G
23	23	2666	C

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Mol	Chain	Res	Type
23	23	2688	G
23	23	2689	U
23	23	2690	U
23	23	2707	U
23	23	2714	G
23	23	2716	C
23	23	2726	A
23	23	2732	G
23	23	2739	U
23	23	2744	G
23	23	2748	A
23	23	2751	G
23	23	2765	A
23	23	2767	C
23	23	2769	U
23	23	2777	G
23	23	2778	A
23	23	2779	U
23	23	2791	G
23	23	2798	U
23	23	2799	A
23	23	2808	G
23	23	2809	A
23	23	2818	U
23	23	2820	A
23	23	2832	U
23	23	2833	U
23	23	2835	A
23	23	2861	U
23	23	2872	A
23	23	2879	A
23	23	2880	C
23	23	2883	A
23	23	2884	U
23	23	2885	G
23	23	2886	A
23	23	2891	U
23	23	2902	C
24	5	17	C
24	5	24	G
24	5	25	U
24	5	32	U

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Mol	Chain	Res	Type
24	5	35	C
24	5	40	U
24	5	41	G
24	5	42	C
24	5	44	G
24	5	51	G
24	5	56	G
24	5	57	A
24	5	69	G
24	5	87	U
24	5	89	U
24	5	90	C
24	5	91	C
24	5	99	A
24	5	109	A
55	Pt	3	G
55	Pt	9	A
55	Pt	13	C
55	Pt	14	A
55	Pt	15	G
55	Pt	16	H2U
55	Pt	17	H2U
55	Pt	18	G
55	Pt	19	G
55	Pt	20	U
55	Pt	21	A
55	Pt	22	G
55	Pt	23	A
55	Pt	30	G
55	Pt	38	A
55	Pt	44	U
55	Pt	45	G
55	Pt	46	G7M
55	Pt	48	C
55	Pt	49	G
55	Pt	53	G
55	Pt	54	5MU
55	Pt	56	C
55	Pt	61	C
55	Pt	66	A
55	Pt	69	A
55	Pt	74	C

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Mol	Chain	Res	Type
55	Pt	76	A
56	Dt	7	A
56	Dt	8	4SU
56	Dt	13	C
56	Dt	16	U
56	Dt	17	U
56	Dt	18	G
56	Dt	19	G
56	Dt	20	G
56	Dt	21	A
56	Dt	22	G
56	Dt	45	U
56	Dt	47	3AU
56	Dt	48	C
56	Dt	49	C
56	Dt	53	G
56	Dt	76	A

All (76) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	16	30	U
1	16	83	C
1	16	90	C
1	16	247	G
1	16	411	A
1	16	429	U
1	16	438	U
1	16	576	C
1	16	606	G
1	16	641	U
1	16	653	U
1	16	793	U
1	16	884	U
1	16	992	U
1	16	993	G
1	16	1094	G
1	16	1124	G
1	16	1129	C
1	16	1145	A
1	16	1211	U
1	16	1225	A

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Mol	Chain	Res	Type
1	16	1239	A
1	16	1257	A
1	16	1432	G
1	16	1445	U
1	16	1447	A
23	23	125	A
23	23	140	C
23	23	199	A
23	23	221	A
23	23	249	C
23	23	277	G
23	23	361	G
23	23	369	U
23	23	404	A
23	23	411	G
23	23	479	A
23	23	503	A
23	23	504	A
23	23	527	C
23	23	555	G
23	23	654	A
23	23	764	A
23	23	776	G
23	23	784	G
23	23	827	U
23	23	877	A
23	23	984	A
23	23	1060	U
23	23	1086	A
23	23	1088	A
23	23	1115	G
23	23	1141	U
23	23	1142	A
23	23	1266	G
23	23	1286	A
23	23	1320	C
23	23	1379	U
23	23	1458	U
23	23	1490	A
23	23	1535	A
23	23	1608	A
23	23	1647	U

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Mol	Chain	Res	Type
23	23	1738	G
23	23	1936	A
23	23	2116	G
23	23	2172	U
23	23	2282	G
23	23	2311	A
23	23	2430	A
23	23	2447	G
23	23	2832	U
23	23	2867	G
23	23	2873	A
24	5	41	G
24	5	56	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	2MA	23	2503	23,58	22,25,26	1.47	4 (18%)	32,37,40	2.45	6 (18%)
55	PSU	Pt	55	55	18,21,22	1.45	3 (16%)	21,30,33	2.14	3 (14%)
1	G7M	16	527	1	23,26,27	2.32	5 (21%)	34,39,42	3.19	14 (41%)
23	6MZ	23	1618	23	22,25,26	1.43	5 (22%)	29,36,39	2.19	10 (34%)
55	H2U	Pt	17	55	18,21,22	1.13	2 (11%)	19,30,33	1.29	3 (15%)
56	G7M	Dt	46	56	23,26,27	2.36	5 (21%)	34,39,42	3.11	12 (35%)
56	3AU	Dt	47	56	24,28,29	1.05	1 (4%)	30,40,43	1.48	3 (10%)
23	H2U	23	2449	23	18,21,22	1.44	2 (11%)	19,30,33	1.32	1 (5%)
1	PSU	16	516	1	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
1	UR3	16	1498	1	19,22,23	0.96	1 (5%)	26,32,35	2.04	3 (11%)
55	H2U	Pt	16	55	18,21,22	1.04	2 (11%)	19,30,33	1.17	1 (5%)
55	U8U	Pt	34	55,22	20,24,25	1.78	4 (20%)	22,34,37	1.56	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	PSU	23	2604	23	18,21,22	1.61	6 (33%)	21,30,33	2.31	7 (33%)
23	1MG	23	745	23	23,26,27	1.25	4 (17%)	33,39,42	1.93	7 (21%)
1	2MG	16	966	1	23,26,27	1.27	4 (17%)	33,38,41	2.43	8 (24%)
1	MA6	16	1519	1	23,26,27	1.56	5 (21%)	33,38,41	2.58	14 (42%)
23	2MG	23	2445	23	23,26,27	1.31	3 (13%)	33,38,41	2.41	8 (24%)
55	3AU	Pt	47	55	24,28,29	1.08	1 (4%)	30,40,43	1.52	5 (16%)
1	MA6	16	1518	1	23,26,27	1.55	5 (21%)	33,38,41	2.41	13 (39%)
55	G7M	Pt	46	55	23,26,27	2.36	5 (21%)	34,39,42	3.08	10 (29%)
56	PSU	Dt	55	56	18,21,22	1.41	2 (11%)	21,30,33	2.24	5 (23%)
56	PSU	Dt	32	56	18,21,22	1.43	3 (16%)	21,30,33	2.15	4 (19%)
23	3TD	23	1915	23	19,22,23	1.25	2 (10%)	23,32,35	2.41	4 (17%)
56	4SU	Dt	8	56	18,21,22	1.85	4 (22%)	25,30,33	2.30	5 (20%)
23	5MU	23	747	23	19,22,23	1.50	5 (26%)	27,32,35	2.33	7 (25%)
56	MIA	Dt	37	56	28,31,32	2.32	6 (21%)	38,44,47	2.93	16 (42%)
23	5MC	23	1962	23	19,22,23	1.51	3 (15%)	26,32,35	1.25	2 (7%)
34	4D4	LP	81	34	9,11,12	2.16	2 (22%)	7,13,15	2.04	3 (42%)
1	2MG	16	1207	1	23,26,27	1.24	3 (13%)	33,38,41	2.24	9 (27%)
23	2MG	23	1835	23	23,26,27	1.26	4 (17%)	33,38,41	2.28	10 (30%)
1	2MG	16	1516	1	23,26,27	1.27	3 (13%)	33,38,41	2.28	10 (30%)
23	PSU	23	2605	23	18,21,22	1.54	3 (16%)	21,30,33	2.21	5 (23%)
55	T6A	Pt	37	55	31,34,35	1.41	6 (19%)	43,49,52	2.14	15 (34%)
23	PSU	23	2580	23	18,21,22	1.54	3 (16%)	21,30,33	2.47	6 (28%)
1	4OC	16	1402	58,1	20,23,24	0.84	0	25,32,35	1.21	2 (8%)
23	G7M	23	2069	23	23,26,27	2.29	6 (26%)	34,39,42	3.03	14 (41%)
23	6MZ	23	2030	23	22,25,26	1.43	5 (22%)	29,36,39	2.39	10 (34%)
55	5MU	Pt	54	55	19,22,23	1.46	6 (31%)	27,32,35	2.13	7 (25%)
23	5MU	23	1939	23	19,22,23	1.48	5 (26%)	27,32,35	2.36	6 (22%)
55	PSU	Pt	39	55	18,21,22	1.37	2 (11%)	21,30,33	2.05	5 (23%)
1	5MC	16	1407	1	19,22,23	1.52	3 (15%)	26,32,35	1.35	5 (19%)
12	D2T	SL	89	12	8,9,10	1.68	2 (25%)	6,11,13	1.52	2 (33%)
23	PSU	23	955	23	18,21,22	1.54	5 (27%)	21,30,33	2.42	6 (28%)
23	OMC	23	2498	23	19,22,23	0.80	0	25,31,34	1.00	2 (8%)
23	PSU	23	2457	23	18,21,22	1.74	3 (16%)	21,30,33	2.38	6 (28%)
23	OMU	23	2552	23	19,22,23	1.33	3 (15%)	25,31,34	2.06	6 (24%)
23	OMG	23	2251	55,23	23,26,27	1.23	3 (13%)	32,38,41	2.18	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	PSU	23	2504	23,58	18,21,22	1.39	3 (16%)	21,30,33	2.14	5 (23%)
23	PSU	23	746	23,58	18,21,22	1.46	4 (22%)	21,30,33	2.30	5 (23%)
56	PSU	Dt	39	56	18,21,22	1.40	3 (16%)	21,30,33	2.04	3 (14%)
1	5MC	16	967	1	19,22,23	1.42	3 (15%)	26,32,35	1.18	2 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	2MA	23	2503	23,58	-	2/7/25/26	0/3/3/3
55	PSU	Pt	55	55	-	0/7/25/26	0/2/2/2
1	G7M	16	527	1	-	2/7/25/26	0/3/3/3
23	6MZ	23	1618	23	-	2/9/27/28	0/3/3/3
55	H2U	Pt	17	55	-	3/7/38/39	0/2/2/2
56	G7M	Dt	46	56	-	0/7/25/26	0/3/3/3
56	3AU	Dt	47	56	-	6/16/34/35	0/2/2/2
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2
1	PSU	16	516	1	-	0/7/25/26	0/2/2/2
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
55	H2U	Pt	16	55	-	5/7/38/39	0/2/2/2
55	U8U	Pt	34	55,22	-	0/10/28/29	0/2/2/2
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
23	1MG	23	745	23	-	0/7/25/26	0/3/3/3
1	2MG	16	966	1	-	2/9/27/28	0/3/3/3
1	MA6	16	1519	1	-	5/11/29/30	0/3/3/3
23	2MG	23	2445	23	-	0/9/27/28	0/3/3/3
55	3AU	Pt	47	55	-	7/16/34/35	0/2/2/2
1	MA6	16	1518	1	-	1/11/29/30	0/3/3/3
55	G7M	Pt	46	55	-	0/7/25/26	0/3/3/3
56	PSU	Dt	55	56	-	0/7/25/26	0/2/2/2
56	PSU	Dt	32	56	-	0/7/25/26	0/2/2/2
23	3TD	23	1915	23	-	4/7/25/26	0/2/2/2
56	4SU	Dt	8	56	-	0/7/25/26	0/2/2/2
23	5MU	23	747	23	-	0/7/25/26	0/2/2/2
56	MIA	Dt	37	56	-	1/15/33/34	0/3/3/3
23	5MC	23	1962	23	-	0/7/25/26	0/2/2/2
34	4D4	LP	81	34	-	3/11/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	16	1207	1	-	0/9/27/28	0/3/3/3
23	2MG	23	1835	23	-	0/9/27/28	0/3/3/3
1	2MG	16	1516	1	-	0/9/27/28	0/3/3/3
23	PSU	23	2605	23	-	0/7/25/26	0/2/2/2
55	T6A	Pt	37	55	-	0/23/41/42	0/3/3/3
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
1	4OC	16	1402	58,1	-	1/9/29/30	0/2/2/2
23	G7M	23	2069	23	-	0/7/25/26	0/3/3/3
23	6MZ	23	2030	23	-	2/9/27/28	0/3/3/3
55	5MU	Pt	54	55	-	1/7/25/26	0/2/2/2
23	5MU	23	1939	23	-	0/7/25/26	0/2/2/2
55	PSU	Pt	39	55	-	0/7/25/26	0/2/2/2
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
12	D2T	SL	89	12	-	3/7/12/14	-
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
23	OMC	23	2498	23	-	0/9/27/28	0/2/2/2
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
23	OMU	23	2552	23	-	0/9/27/28	0/2/2/2
23	OMG	23	2251	55,23	-	3/9/27/28	0/3/3/3
23	PSU	23	2504	23,58	-	0/7/25/26	0/2/2/2
23	PSU	23	746	23,58	-	1/7/25/26	0/2/2/2
56	PSU	Dt	39	56	-	1/7/25/26	0/2/2/2
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Dt	46	G7M	C8-N7	7.68	1.46	1.33
55	Pt	46	G7M	C8-N7	7.61	1.46	1.33
1	16	527	G7M	C8-N7	7.47	1.45	1.33
56	Dt	37	MIA	C2-S10	-7.33	1.69	1.75
23	23	2069	G7M	C8-N7	7.31	1.45	1.33
56	Dt	37	MIA	C13-C14	6.78	1.52	1.32
55	Pt	34	U8U	C2-S2	-5.55	1.58	1.67
1	16	1407	5MC	C5-C4	5.29	1.48	1.44
23	23	1962	5MC	C5-C4	5.24	1.48	1.44
34	LP	81	4D4	CZ-NE	5.03	1.43	1.33
56	Dt	8	4SU	C4-S4	-5.03	1.59	1.68
23	23	2069	G7M	C5-N7	-4.81	1.33	1.39
1	16	967	5MC	C5-C4	4.77	1.47	1.44
55	Pt	46	G7M	C5-N7	-4.50	1.34	1.39
56	Dt	46	G7M	C5-N7	-4.48	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	527	G7M	C5-N7	-4.45	1.34	1.39
23	23	2503	2MA	C5-C4	4.36	1.46	1.39
23	23	1618	6MZ	C5-C4	4.28	1.46	1.39
1	16	1518	MA6	C5-C4	4.28	1.46	1.39
1	16	1519	MA6	C5-C4	4.23	1.46	1.39
23	23	2030	6MZ	C5-C4	4.18	1.46	1.39
1	16	527	G7M	C8-N9	4.11	1.46	1.35
55	Pt	46	G7M	C8-N9	4.08	1.46	1.35
56	Dt	46	G7M	C8-N9	4.04	1.46	1.35
55	Pt	37	T6A	C5-C4	4.03	1.46	1.39
56	Dt	37	MIA	C5-C4	4.03	1.46	1.39
55	Pt	46	G7M	C5-C4	3.83	1.47	1.38
23	23	2069	G7M	C8-N9	3.81	1.46	1.35
56	Dt	46	G7M	C5-C4	3.80	1.47	1.38
23	23	2457	PSU	C6-C5	3.73	1.39	1.35
23	23	2457	PSU	C4-N3	-3.70	1.31	1.38
23	23	2605	PSU	C4-N3	-3.53	1.32	1.38
23	23	2604	PSU	C4-N3	-3.51	1.32	1.38
55	Pt	55	PSU	C6-C5	3.50	1.39	1.35
23	23	2449	H2U	C2-N3	-3.49	1.31	1.38
55	Pt	34	U8U	C6-N1	-3.47	1.32	1.38
1	16	527	G7M	C5-C4	3.45	1.46	1.38
23	23	2580	PSU	C4-N3	-3.43	1.32	1.38
23	23	747	5MU	C4-N3	-3.43	1.32	1.38
34	LP	81	4D4	CZ-NH2	3.42	1.44	1.32
23	23	747	5MU	C2-N3	-3.37	1.32	1.38
56	Dt	8	4SU	C4-N3	-3.36	1.34	1.37
23	23	2449	H2U	C4-N3	-3.35	1.32	1.37
23	23	955	PSU	C4-N3	-3.34	1.32	1.38
55	Pt	39	PSU	C6-C5	3.33	1.39	1.35
23	23	2552	OMU	C4-N3	-3.30	1.33	1.38
56	Dt	55	PSU	C6-C5	3.29	1.38	1.35
23	23	1939	5MU	C4-N3	-3.28	1.32	1.38
1	16	516	PSU	C6-C5	3.22	1.38	1.35
23	23	2504	PSU	C6-C5	3.21	1.38	1.35
23	23	1915	3TD	C6-C5	3.16	1.38	1.35
1	16	1519	MA6	C5-C6	3.13	1.49	1.41
56	Dt	39	PSU	C6-C5	3.10	1.38	1.35
23	23	745	1MG	C5-N7	-3.09	1.32	1.39
56	Dt	32	PSU	C4-N3	-3.04	1.33	1.38
23	23	2069	G7M	C5-C4	3.02	1.45	1.38
1	16	1516	2MG	C5-C4	3.01	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	2605	PSU	C2-N3	-3.01	1.32	1.37
1	16	1207	2MG	C5-C4	2.99	1.46	1.38
12	SL	89	D2T	CB-CA	-2.99	1.53	1.54
23	23	746	PSU	C4-N3	-2.98	1.33	1.38
23	23	2251	OMG	C6-N1	-2.98	1.33	1.38
55	Pt	54	5MU	C4-N3	-2.96	1.33	1.38
23	23	2445	2MG	C6-N1	-2.95	1.33	1.38
23	23	2605	PSU	C6-C5	2.94	1.38	1.35
55	Pt	34	U8U	C4-N3	-2.92	1.33	1.38
55	Pt	55	PSU	C4-N3	-2.91	1.33	1.38
55	Pt	17	H2U	C2-N3	-2.89	1.32	1.38
23	23	2580	PSU	C6-C5	2.89	1.38	1.35
23	23	2504	PSU	C4-N3	-2.86	1.33	1.38
23	23	746	PSU	C2-N3	-2.86	1.32	1.37
23	23	955	PSU	C2-N3	-2.85	1.32	1.37
23	23	1915	3TD	C2-N1	-2.83	1.33	1.37
56	Dt	39	PSU	C4-N3	-2.82	1.33	1.38
1	16	1518	MA6	C5-N7	-2.82	1.33	1.39
23	23	1939	5MU	C2-N3	-2.81	1.33	1.38
55	Pt	37	T6A	C5-N7	-2.78	1.34	1.39
56	Dt	55	PSU	C4-N3	-2.77	1.33	1.38
23	23	1835	2MG	C6-N1	-2.77	1.33	1.38
23	23	746	PSU	C6-C5	2.77	1.38	1.35
23	23	745	1MG	C5-C4	2.76	1.46	1.38
23	23	1939	5MU	C6-C5	2.76	1.39	1.34
23	23	2251	OMG	C5-C4	2.73	1.46	1.38
23	23	2503	2MA	C5-N7	-2.73	1.34	1.39
23	23	2445	2MG	C5-C4	2.73	1.46	1.38
55	Pt	16	H2U	C2-N3	-2.73	1.33	1.38
23	23	2457	PSU	C2-N3	-2.70	1.33	1.37
56	Dt	8	4SU	C5-C4	-2.70	1.39	1.42
55	Pt	39	PSU	C4-N3	-2.68	1.33	1.38
1	16	966	2MG	C5-C4	2.65	1.46	1.38
23	23	1835	2MG	C5-C4	2.64	1.46	1.38
55	Pt	17	H2U	C4-N3	-2.62	1.33	1.37
1	16	966	2MG	C6-N1	-2.62	1.33	1.38
1	16	527	G7M	C6-N1	-2.61	1.34	1.38
23	23	2030	6MZ	C5-C6	2.60	1.48	1.41
23	23	2604	PSU	C2-N3	-2.59	1.33	1.37
56	Dt	32	PSU	C6-C5	2.59	1.38	1.35
56	Dt	37	MIA	C5-N7	-2.59	1.34	1.39
23	23	745	1MG	C2-N1	2.57	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	1207	2MG	C6-N1	-2.57	1.34	1.38
23	23	2580	PSU	C2-N3	-2.56	1.33	1.37
1	16	1519	MA6	C4-N9	-2.56	1.32	1.37
1	16	1518	MA6	C8-N9	-2.56	1.33	1.37
23	23	2503	2MA	C5-C6	2.55	1.48	1.41
1	16	1518	MA6	C5-C6	2.53	1.47	1.41
55	Pt	54	5MU	C2-N3	-2.52	1.33	1.38
1	16	516	PSU	C4-N3	-2.52	1.34	1.38
23	23	2552	OMU	C2-N3	-2.52	1.33	1.38
23	23	1618	6MZ	C5-C6	2.52	1.48	1.41
1	16	1519	MA6	C5-N7	-2.52	1.34	1.39
56	Dt	32	PSU	C2-N3	-2.52	1.33	1.37
1	16	967	5MC	C6-N1	-2.52	1.33	1.38
23	23	1618	6MZ	C5-N7	-2.51	1.34	1.39
1	16	1516	2MG	C6-N1	-2.50	1.34	1.38
23	23	2030	6MZ	C5-N7	-2.48	1.34	1.39
23	23	1835	2MG	C5-N7	-2.44	1.34	1.39
23	23	2552	OMU	C5-C4	-2.44	1.38	1.43
23	23	1962	5MC	C6-N1	-2.44	1.33	1.38
23	23	1962	5MC	C6-C5	2.44	1.38	1.34
1	16	1407	5MC	C6-C5	2.43	1.38	1.34
55	Pt	46	G7M	C6-N1	-2.43	1.34	1.38
23	23	2251	OMG	C5-N7	-2.42	1.34	1.39
23	23	747	5MU	C6-N1	-2.41	1.33	1.38
23	23	2604	PSU	C6-N1	-2.39	1.32	1.36
55	Pt	54	5MU	C6-N1	-2.39	1.33	1.38
23	23	2604	PSU	C6-C5	2.37	1.37	1.35
23	23	2069	G7M	C6-N1	-2.35	1.34	1.38
23	23	2445	2MG	C5-N7	-2.35	1.34	1.39
55	Pt	16	H2U	C4-N3	-2.35	1.33	1.37
23	23	955	PSU	C2-N1	-2.34	1.33	1.36
55	Pt	54	5MU	C6-C5	2.33	1.38	1.34
23	23	2069	G7M	C4-N9	-2.32	1.32	1.38
55	Pt	37	T6A	C5-C6	2.31	1.47	1.41
56	Dt	37	MIA	C5-C6	2.31	1.47	1.41
1	16	966	2MG	C5-N7	-2.30	1.34	1.39
1	16	1518	MA6	C4-N9	-2.28	1.32	1.37
55	Pt	54	5MU	C4-C5	2.26	1.48	1.44
56	Dt	46	G7M	C6-N1	-2.23	1.34	1.38
23	23	2030	6MZ	C8-N7	2.23	1.36	1.31
23	23	2030	6MZ	C4-N9	-2.22	1.33	1.37
56	Dt	8	4SU	C2-N3	-2.22	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	745	1MG	C4-N9	-2.22	1.32	1.38
23	23	1939	5MU	C6-N1	-2.22	1.34	1.38
55	Pt	47	3AU	C2-N1	2.20	1.41	1.38
56	Dt	37	MIA	C4-N9	-2.20	1.33	1.37
23	23	955	PSU	C6-C5	2.20	1.37	1.35
23	23	746	PSU	C2-N1	-2.18	1.33	1.36
1	16	967	5MC	C6-C5	2.18	1.38	1.34
23	23	2503	2MA	C8-N7	2.17	1.35	1.31
56	Dt	47	3AU	C2-N1	2.16	1.41	1.38
23	23	2504	PSU	C2-N3	-2.15	1.33	1.37
23	23	2604	PSU	C2-N1	-2.14	1.33	1.36
23	23	747	5MU	C6-C5	2.14	1.38	1.34
1	16	1516	2MG	C5-N7	-2.14	1.34	1.39
23	23	955	PSU	C6-N1	-2.13	1.32	1.36
23	23	2604	PSU	C2'-C1'	-2.12	1.50	1.53
1	16	1407	5MC	C6-N1	-2.12	1.34	1.38
23	23	1835	2MG	C4-N9	-2.12	1.32	1.38
23	23	747	5MU	C2-N1	2.12	1.41	1.38
1	16	1207	2MG	C5-N7	-2.12	1.34	1.39
23	23	1618	6MZ	C8-N7	2.12	1.35	1.31
55	Pt	37	T6A	C4-N9	-2.12	1.33	1.37
12	SL	89	D2T	CB1-SB	-2.11	1.75	1.79
55	Pt	34	U8U	C-N	-2.09	1.43	1.46
55	Pt	55	PSU	C2-N3	-2.06	1.34	1.37
23	23	1618	6MZ	C4-N9	-2.05	1.33	1.37
1	16	966	2MG	C4-N9	-2.05	1.32	1.38
56	Dt	39	PSU	C2-N3	-2.04	1.34	1.37
55	Pt	37	T6A	C8-N9	-2.04	1.34	1.37
1	16	1498	UR3	C6-N1	-2.04	1.33	1.38
1	16	1519	MA6	C8-N9	-2.03	1.34	1.37
55	Pt	37	T6A	C10-N6	-2.01	1.33	1.37
23	23	1939	5MU	C2-N1	2.00	1.41	1.38
55	Pt	54	5MU	C2-N1	2.00	1.41	1.38

All (330) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2503	2MA	C5-C4-N3	-9.21	117.48	127.18
56	Dt	37	MIA	C12-C13-C14	-8.79	111.24	127.01
1	16	527	G7M	CN7-N7-C8	-8.68	111.64	124.79
55	Pt	46	G7M	CN7-N7-C8	-8.37	112.11	124.79
56	Dt	46	G7M	CN7-N7-C8	-8.36	112.13	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2069	G7M	CN7-N7-C8	-8.04	112.61	124.79
1	16	1498	UR3	C4-N3-C2	-8.03	118.11	124.58
23	23	2445	2MG	C2-N3-C4	7.99	122.00	112.00
1	16	966	2MG	C2-N3-C4	7.73	121.67	112.00
23	23	2457	PSU	N1-C2-N3	7.65	123.23	115.17
56	Dt	37	MIA	C5-C4-N3	-7.62	119.16	127.18
23	23	2580	PSU	N1-C2-N3	7.43	123.00	115.17
23	23	955	PSU	N1-C2-N3	7.38	122.96	115.17
23	23	1915	3TD	N1-C2-N3	7.33	121.46	116.13
23	23	1835	2MG	C2-N3-C4	7.23	121.05	112.00
23	23	2605	PSU	N1-C2-N3	7.19	122.75	115.17
1	16	1207	2MG	C2-N3-C4	7.12	120.91	112.00
23	23	2604	PSU	N1-C2-N3	7.11	122.67	115.17
1	16	1516	2MG	C2-N3-C4	7.09	120.87	112.00
56	Dt	8	4SU	C4-N3-C2	-6.98	120.62	127.31
23	23	2503	2MA	N3-C4-N9	6.97	135.84	126.99
23	23	2069	G7M	N9-C8-N7	-6.90	95.72	112.48
55	Pt	46	G7M	N9-C8-N7	-6.89	95.74	112.48
1	16	527	G7M	N9-C8-N7	-6.89	95.76	112.48
56	Dt	46	G7M	N9-C8-N7	-6.80	95.98	112.48
23	23	2504	PSU	N1-C2-N3	6.63	122.17	115.17
1	16	527	G7M	C8-N7-C5	6.63	116.07	107.78
55	Pt	55	PSU	N1-C2-N3	6.58	122.11	115.17
23	23	2069	G7M	C8-N7-C5	6.51	115.92	107.78
56	Dt	55	PSU	N1-C2-N3	6.51	122.03	115.17
56	Dt	46	G7M	C8-N7-C5	6.50	115.91	107.78
23	23	2445	2MG	C5-C4-N3	-6.47	118.09	128.39
56	Dt	39	PSU	N1-C2-N3	6.45	121.97	115.17
55	Pt	46	G7M	C8-N7-C5	6.40	115.79	107.78
56	Dt	32	PSU	N1-C2-N3	6.35	121.86	115.17
1	16	516	PSU	N1-C2-N3	6.30	121.82	115.17
55	Pt	39	PSU	N1-C2-N3	6.28	121.79	115.17
55	Pt	46	G7M	N9-C4-N3	6.21	138.37	125.95
23	23	746	PSU	N1-C2-N3	6.21	121.72	115.17
56	Dt	37	MIA	N3-C4-N9	6.09	134.71	126.99
23	23	2251	OMG	C5-C4-N3	-6.09	118.70	128.39
23	23	1939	5MU	N3-C2-N1	6.03	122.74	114.89
56	Dt	46	G7M	N9-C4-N3	6.01	137.97	125.95
1	16	1516	2MG	C5-C4-N3	-6.01	118.83	128.39
1	16	1207	2MG	C5-C4-N3	-5.96	118.91	128.39
55	Pt	37	T6A	C5-C4-N3	-5.95	118.52	126.72
1	16	966	2MG	C5-C4-N3	-5.94	118.94	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	1835	2MG	C5-C4-N3	-5.91	118.98	128.39
23	23	1915	3TD	C1'-C5-C4	5.87	126.51	117.61
1	16	527	G7M	N9-C4-N3	5.82	137.59	125.95
56	Dt	8	4SU	C5-C4-N3	5.80	120.15	114.75
23	23	1618	6MZ	C5-C4-N3	-5.72	118.84	126.72
23	23	2030	6MZ	C5-C4-N3	-5.66	118.92	126.72
23	23	1939	5MU	C4-N3-C2	-5.58	120.02	127.34
23	23	2251	OMG	C2-N3-C4	5.49	121.76	112.30
23	23	747	5MU	N3-C2-N1	5.47	122.01	114.89
1	16	1518	MA6	C5-C4-N3	-5.47	119.19	126.72
23	23	955	PSU	C4-N3-C2	-5.34	119.02	126.37
1	16	1519	MA6	C10-N6-C6	-5.30	107.03	120.52
23	23	747	5MU	C4-N3-C2	-5.29	120.40	127.34
23	23	2251	OMG	N9-C4-N3	5.26	136.47	125.95
23	23	2030	6MZ	C9-N6-C6	-5.22	118.00	122.85
56	Dt	46	G7M	C5-C4-N3	-5.21	118.30	128.15
1	16	1519	MA6	C5-C4-N3	-5.19	119.57	126.72
1	16	527	G7M	C5-C4-N3	-5.18	118.36	128.15
23	23	746	PSU	C4-N3-C2	-5.04	119.43	126.37
55	Pt	46	G7M	C5-C4-N3	-5.04	118.63	128.15
23	23	1915	3TD	C4-N3-C2	-4.97	119.35	124.61
23	23	745	1MG	C5-C4-N3	-4.96	120.50	128.39
56	Dt	47	3AU	C4-N3-C2	-4.95	118.85	124.66
23	23	2552	OMU	C4-N3-C2	-4.91	120.52	126.61
23	23	2445	2MG	N9-C4-N3	4.90	135.75	125.95
23	23	2069	G7M	N9-C4-N3	4.88	135.72	125.95
55	Pt	54	5MU	C4-N3-C2	-4.88	120.94	127.34
55	Pt	37	T6A	N3-C4-N9	4.87	135.45	127.17
1	16	1519	MA6	C2'-C1'-N9	-4.86	101.24	113.30
55	Pt	47	3AU	C4-N3-C2	-4.83	118.98	124.66
23	23	2552	OMU	N3-C2-N1	4.78	121.12	114.89
55	Pt	54	5MU	N3-C2-N1	4.76	121.09	114.89
56	Dt	37	MIA	C11-S10-C2	-4.74	98.69	102.25
23	23	1939	5MU	C5-C4-N3	4.69	119.40	115.32
1	16	1519	MA6	C4-C5-N7	-4.67	105.24	110.58
23	23	747	5MU	C5-C4-N3	4.66	119.38	115.32
1	16	1518	MA6	N3-C4-N9	4.65	135.07	127.17
23	23	2580	PSU	C4-N3-C2	-4.64	119.98	126.37
23	23	2069	G7M	C2-N3-C4	4.64	120.29	112.30
23	23	2504	PSU	C4-N3-C2	-4.63	120.00	126.37
23	23	745	1MG	C2-N3-C4	4.62	122.36	111.98
23	23	1835	2MG	N9-C4-N3	4.61	135.17	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	Pt	46	G7M	C8-N9-C4	4.59	118.46	107.09
23	23	1618	6MZ	N3-C4-N9	4.58	134.96	127.17
1	16	1518	MA6	C2-N1-C6	4.57	122.99	111.83
56	Dt	32	PSU	C4-N3-C2	-4.56	120.08	126.37
1	16	527	G7M	C2-N3-C4	4.52	120.09	112.30
23	23	2604	PSU	C4-N3-C2	-4.49	120.19	126.37
23	23	2605	PSU	C4-N3-C2	-4.46	120.23	126.37
55	Pt	54	5MU	C5-C4-N3	4.44	119.19	115.32
23	23	2069	G7M	C5-C4-N3	-4.43	119.77	128.15
23	23	2457	PSU	C4-N3-C2	-4.43	120.27	126.37
1	16	1519	MA6	C2-N1-C6	4.42	122.62	111.83
56	Dt	55	PSU	C4-N3-C2	-4.41	120.29	126.37
56	Dt	46	G7M	C2-N3-C4	4.41	119.89	112.30
55	Pt	37	T6A	N6-C10-N11	4.41	119.83	113.77
1	16	527	G7M	CN7-N7-C5	4.40	132.29	126.80
56	Dt	46	G7M	C8-N9-C4	4.36	117.88	107.09
23	23	1939	5MU	O4-C4-C5	-4.32	119.97	124.92
1	16	527	G7M	C8-N9-C4	4.30	117.73	107.09
1	16	1516	2MG	N9-C4-N3	4.29	134.54	125.95
23	23	2030	6MZ	N3-C4-N9	4.29	134.46	127.17
56	Dt	8	4SU	N3-C2-N1	4.27	120.45	114.89
23	23	2069	G7M	C8-N9-C4	4.27	117.66	107.09
1	16	1207	2MG	N9-C4-N3	4.26	134.48	125.95
55	Pt	46	G7M	C1'-N9-C8	-4.26	112.34	126.74
23	23	747	5MU	C5-C6-N1	-4.26	118.69	123.31
55	Pt	46	G7M	CN7-N7-C5	4.25	132.10	126.80
1	16	966	2MG	N9-C4-N3	4.15	134.26	125.95
56	Dt	46	G7M	CN7-N7-C5	4.14	131.96	126.80
55	Pt	55	PSU	C4-N3-C2	-4.13	120.67	126.37
55	Pt	46	G7M	C2-N3-C4	4.12	119.40	112.30
56	Dt	37	MIA	C15-C14-C13	-4.12	110.31	122.66
55	Pt	39	PSU	C4-N3-C2	-4.11	120.71	126.37
23	23	2030	6MZ	C6-C5-N7	4.05	136.84	132.43
56	Dt	39	PSU	C4-N3-C2	-4.02	120.84	126.37
56	Dt	46	G7M	C1'-N9-C8	-4.00	113.23	126.74
23	23	745	1MG	N9-C4-N3	3.94	133.83	125.95
56	Dt	8	4SU	C5-C4-S4	-3.94	119.81	124.31
23	23	1939	5MU	C5-C6-N1	-3.93	119.05	123.31
23	23	2449	H2U	O4'-C1'-N1	3.90	114.61	109.30
1	16	1518	MA6	N1-C6-N6	3.88	121.59	116.86
23	23	2580	PSU	O2-C2-N1	-3.86	118.80	122.79
1	16	516	PSU	C4-N3-C2	-3.86	121.05	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Dt	37	MIA	C6-C5-N7	3.85	136.63	132.43
55	Pt	37	T6A	C2-N3-C4	3.84	121.22	111.83
1	16	966	2MG	C6-C5-N7	3.83	137.26	130.29
23	23	2030	6MZ	C4-C5-N7	-3.83	106.21	110.58
23	23	2552	OMU	C5-C4-N3	3.83	120.16	114.80
23	23	1962	5MC	C5-C6-N1	-3.80	119.18	123.31
1	16	516	PSU	O2-C2-N1	-3.80	118.87	122.79
1	16	1518	MA6	C10-N6-C6	-3.80	110.86	120.52
23	23	2445	2MG	C6-C5-N7	3.76	137.14	130.29
1	16	1498	UR3	C5-C4-N3	3.76	119.99	115.04
23	23	2030	6MZ	C2-N3-C4	3.74	120.98	111.83
23	23	2069	G7M	CN7-N7-C5	3.74	131.46	126.80
23	23	747	5MU	O4-C4-C5	-3.70	120.68	124.92
23	23	955	PSU	O2-C2-N1	-3.70	118.97	122.79
23	23	1618	6MZ	C2-N3-C4	3.70	120.86	111.83
1	16	966	2MG	N1-C2-N2	3.69	120.33	116.56
56	Dt	55	PSU	O2-C2-N1	-3.69	118.99	122.79
1	16	1519	MA6	C2-N3-C4	3.65	120.75	111.83
56	Dt	37	MIA	C16-C14-C13	-3.65	111.70	122.66
55	Pt	37	T6A	N3-C2-N1	-3.63	123.08	128.58
56	Dt	37	MIA	C2-N3-C4	3.61	121.75	112.29
1	16	1518	MA6	C2-N3-C4	3.60	120.63	111.83
55	Pt	39	PSU	O2-C2-N1	-3.60	119.08	122.79
1	16	1518	MA6	N1-C2-N3	-3.60	123.14	128.58
56	Dt	39	PSU	O2-C2-N1	-3.59	119.08	122.79
1	16	1519	MA6	N3-C4-N9	3.59	133.27	127.17
34	LP	81	4D4	NE-CZ-NH2	-3.57	114.54	120.67
23	23	2503	2MA	C4-C5-N7	-3.54	106.53	110.58
55	Pt	54	5MU	C5-C6-N1	-3.54	119.47	123.31
55	Pt	34	U8U	C1'-N1-C6	-3.53	115.33	121.15
55	Pt	55	PSU	O2-C2-N1	-3.53	119.15	122.79
56	Dt	32	PSU	O2-C2-N1	-3.52	119.16	122.79
55	Pt	54	5MU	O4-C4-C5	-3.52	120.89	124.92
1	16	1207	2MG	C6-C5-N7	3.51	136.68	130.29
23	23	1618	6MZ	C9-N6-C6	-3.51	119.59	122.85
23	23	2604	PSU	O2-C2-N1	-3.51	119.17	122.79
1	16	1518	MA6	C4-C5-N7	-3.47	106.62	110.58
23	23	2457	PSU	O2-C2-N1	-3.46	119.22	122.79
23	23	745	1MG	C2'-C1'-N9	-3.45	103.65	113.25
23	23	2251	OMG	C2'-C1'-N9	-3.44	107.70	114.24
23	23	2580	PSU	C3'-C2'-C1'	3.42	105.72	101.69
1	16	1516	2MG	C6-C5-N7	3.39	136.46	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Dt	37	MIA	C4-C5-N7	-3.39	106.71	110.58
23	23	2552	OMU	C2'-C1'-N1	-3.36	107.86	114.24
23	23	1618	6MZ	N1-C2-N3	-3.34	123.52	128.58
23	23	2030	6MZ	N1-C2-N3	-3.34	123.52	128.58
55	Pt	34	U8U	C-C5-C6	-3.32	116.22	121.21
23	23	1618	6MZ	C4-C5-N7	-3.32	106.78	110.58
23	23	1618	6MZ	C6-C5-N7	3.32	136.04	132.43
55	Pt	37	T6A	C2'-C1'-N9	-3.31	105.09	113.30
34	LP	81	4D4	NH1-CZ-NE	3.27	126.70	119.27
23	23	1835	2MG	C6-C5-N7	3.27	136.23	130.29
1	16	967	5MC	C5-C6-N1	-3.26	119.77	123.31
1	16	1519	MA6	C6-C5-N7	3.25	138.62	133.43
1	16	1519	MA6	C5-N7-C8	3.25	108.55	103.45
1	16	1519	MA6	N1-C2-N3	-3.23	123.69	128.58
55	Pt	37	T6A	C4-C5-N7	-3.20	106.92	110.58
23	23	2504	PSU	O2-C2-N1	-3.17	119.52	122.79
56	Dt	55	PSU	C3'-C2'-C1'	3.16	105.42	101.69
1	16	527	G7M	C2'-C1'-N9	-3.14	104.51	113.25
56	Dt	37	MIA	C2'-C1'-N9	-3.12	105.55	113.30
1	16	1402	4OC	O2-C2-N3	-3.09	117.46	122.33
23	23	2503	2MA	N6-C6-N1	3.08	121.18	117.03
23	23	2069	G7M	C6-C5-N7	3.06	136.01	132.17
1	16	527	G7M	C1'-N9-C8	-3.05	116.44	126.74
55	Pt	47	3AU	C10-N3-C2	3.04	122.13	117.64
23	23	2069	G7M	O6-C6-C5	-3.04	121.22	128.01
23	23	746	PSU	O2-C2-N1	-3.03	119.66	122.79
23	23	747	5MU	C3'-C2'-C1'	3.01	107.16	101.46
56	Dt	37	MIA	C4-N9-C8	3.00	108.88	105.74
1	16	1407	5MC	C5-C6-N1	-2.95	120.11	123.31
23	23	746	PSU	O3'-C3'-C4'	-2.95	102.61	111.08
55	Pt	37	T6A	O4'-C1'-N9	2.93	113.72	108.09
23	23	2030	6MZ	C4-N9-C8	2.92	108.81	105.74
23	23	2445	2MG	C2'-C1'-N9	-2.92	105.12	113.25
56	Dt	47	3AU	C5-C4-N3	2.91	119.67	115.64
23	23	746	PSU	C5-C6-N1	-2.89	118.13	122.14
56	Dt	37	MIA	N3-C2-N1	-2.88	121.74	127.00
55	Pt	37	T6A	C6-C5-N7	2.86	135.55	132.43
55	Pt	34	U8U	O4-C4-C5	-2.86	119.90	124.71
23	23	2457	PSU	C5-C6-N1	-2.85	118.18	122.14
23	23	2251	OMG	C6-C5-N7	2.85	135.47	130.29
1	16	1519	MA6	C10-N6-C9	-2.84	107.05	116.18
23	23	2445	2MG	C4-C5-N7	-2.83	106.18	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2030	6MZ	C5-N7-C8	2.83	107.89	103.45
55	Pt	47	3AU	C5-C4-N3	2.81	119.52	115.64
55	Pt	37	T6A	C4-N9-C8	2.80	108.68	105.74
1	16	1519	MA6	C4-N9-C8	2.79	108.67	105.74
1	16	1516	2MG	N1-C2-N2	2.77	119.39	116.56
23	23	745	1MG	C6-C5-N7	2.77	135.51	129.36
23	23	1962	5MC	C5-C4-N3	-2.76	118.93	121.75
1	16	1518	MA6	C4-N9-C8	2.76	108.63	105.74
23	23	1618	6MZ	C4-N9-C8	2.75	108.63	105.74
1	16	966	2MG	C4-C5-N7	-2.75	106.31	110.67
1	16	1516	2MG	C4-C5-N7	-2.75	106.31	110.67
23	23	955	PSU	C5-C6-N1	-2.73	118.35	122.14
23	23	2605	PSU	O2-C2-N3	-2.73	117.01	121.86
23	23	2251	OMG	O6-C6-C5	-2.72	119.34	126.53
1	16	527	G7M	O4'-C1'-N9	2.72	114.52	108.36
1	16	1207	2MG	C4-C5-N7	-2.71	106.38	110.67
23	23	2069	G7M	N2-C2-N1	2.67	122.39	116.76
23	23	2552	OMU	O4-C4-C5	-2.66	120.58	125.16
55	Pt	17	H2U	C5-C6-N1	-2.66	103.47	111.52
23	23	1939	5MU	O2-C2-N1	-2.64	119.36	122.80
55	Pt	37	T6A	N6-C6-N1	2.64	124.37	117.54
1	16	1407	5MC	C5-C4-N3	-2.64	119.05	121.75
23	23	2069	G7M	N2-C2-N3	-2.63	114.53	119.67
23	23	2498	OMC	C2'-C1'-N1	-2.63	109.25	114.24
55	Pt	47	3AU	C3'-C2'-C1'	2.63	106.43	101.46
56	Dt	37	MIA	C5-N7-C8	2.61	107.56	103.45
23	23	2552	OMU	O2-C2-N1	-2.61	119.40	122.80
1	16	1207	2MG	N1-C2-N2	2.60	119.22	116.56
23	23	2503	2MA	C5-N7-C8	2.60	107.53	103.45
56	Dt	47	3AU	C10-N3-C2	2.60	121.47	117.64
1	16	1519	MA6	C9-N6-C6	-2.58	113.97	120.52
23	23	1835	2MG	N1-C2-N2	2.57	119.19	116.56
55	Pt	54	5MU	C2'-C1'-N1	-2.56	106.12	113.25
1	16	967	5MC	C5-C4-N3	-2.56	119.13	121.75
1	16	1518	MA6	C9-N6-C6	-2.56	114.01	120.52
1	16	966	2MG	N2-C2-N3	-2.53	117.28	120.51
23	23	1835	2MG	O6-C6-C5	-2.52	119.88	126.53
1	16	1519	MA6	N9-C8-N7	-2.51	110.37	113.94
23	23	747	5MU	O2-C2-N3	-2.49	116.90	121.49
23	23	1618	6MZ	C5-N7-C8	2.49	107.36	103.45
23	23	2604	PSU	C3'-C2'-C1'	2.49	104.62	101.69
56	Dt	37	MIA	C2-N1-C6	2.49	122.26	117.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	23	2580	PSU	C5-C6-N1	-2.48	118.70	122.14
1	16	1407	5MC	O2-C2-N3	-2.48	118.42	122.33
23	23	2605	PSU	O2-C2-N1	-2.48	120.23	122.79
55	Pt	37	T6A	C5-N7-C8	2.48	107.34	103.45
1	16	1518	MA6	C5-N7-C8	2.45	107.31	103.45
23	23	2030	6MZ	N9-C8-N7	-2.44	110.48	113.94
1	16	527	G7M	O6-C6-C5	-2.43	122.58	128.01
23	23	2457	PSU	C3'-C2'-C1'	2.43	104.56	101.69
23	23	2457	PSU	O2-C2-N3	-2.43	117.54	121.86
56	Dt	46	G7M	O6-C6-C5	-2.43	122.58	128.01
23	23	1835	2MG	CM2-N2-C2	-2.43	118.44	123.65
56	Dt	32	PSU	C6-C5-C4	-2.42	116.54	118.17
1	16	1518	MA6	C2'-C1'-N9	-2.41	107.31	113.30
23	23	2069	G7M	C1'-N9-C8	-2.41	118.59	126.74
23	23	2069	G7M	C2'-C1'-N9	-2.39	106.60	113.25
55	Pt	17	H2U	O4'-C1'-N1	2.35	112.50	109.30
23	23	2445	2MG	C8-N7-C5	2.34	108.43	104.26
1	16	1516	2MG	CM2-N2-C2	-2.33	118.64	123.65
55	Pt	46	G7M	O6-C6-C5	-2.33	122.81	128.01
23	23	745	1MG	C6-C5-C4	-2.33	117.33	119.97
23	23	1835	2MG	C2-N1-C6	-2.31	121.75	124.55
55	Pt	47	3AU	C1'-N1-C2	2.31	120.82	117.04
55	Pt	37	T6A	O10-C10-N6	-2.31	119.54	123.64
23	23	2605	PSU	C5-C6-N1	-2.30	118.94	122.14
1	16	1498	UR3	C3U-N3-C2	2.28	121.31	117.33
1	16	1407	5MC	O2'-C2'-C3'	-2.27	104.55	111.82
56	Dt	37	MIA	N9-C8-N7	-2.27	110.72	113.94
23	23	2604	PSU	C5-C6-N1	-2.26	119.00	122.14
1	16	1518	MA6	C5-C6-N6	-2.23	121.80	125.33
23	23	745	1MG	C4-C5-N7	-2.22	107.16	110.67
55	Pt	39	PSU	O4'-C1'-C2'	2.21	108.21	105.15
23	23	1835	2MG	C4-C5-N7	-2.21	107.16	110.67
23	23	2604	PSU	C2'-C3'-C4'	-2.21	98.35	102.61
23	23	1835	2MG	C5-C6-N1	2.18	118.81	113.25
55	Pt	16	H2U	C5-C6-N1	-2.17	104.95	111.52
1	16	1516	2MG	N2-C2-N3	-2.17	117.75	120.51
23	23	2445	2MG	C5-C6-N1	2.16	118.76	113.25
56	Dt	55	PSU	C5-C6-N1	-2.16	119.14	122.14
23	23	955	PSU	C3'-C2'-C1'	2.16	104.24	101.69
56	Dt	46	G7M	C3'-C2'-C1'	2.15	105.54	101.46
55	Pt	54	5MU	C3'-C2'-C1'	2.15	105.52	101.46
56	Dt	46	G7M	O4'-C1'-N9	2.14	113.21	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	Pt	17	H2U	O3'-C3'-C2'	-2.14	104.95	111.82
1	16	1207	2MG	CM2-N2-C2	-2.14	119.05	123.65
23	23	955	PSU	O2-C2-N3	-2.13	118.07	121.86
1	16	1207	2MG	N2-C2-N3	-2.13	117.79	120.51
23	23	1915	3TD	O4'-C4'-C3'	-2.13	100.92	105.15
12	SL	89	D2T	CB-CA-N	2.12	113.39	109.10
34	LP	81	4D4	O-C-CA	-2.12	119.32	124.77
23	23	2503	2MA	C2-N1-C6	2.12	121.36	118.10
55	Pt	39	PSU	C5-C6-N1	-2.11	119.21	122.14
55	Pt	37	T6A	C2-N1-C6	2.11	122.23	115.24
23	23	2251	OMG	C5-C6-N1	2.10	118.61	113.25
1	16	527	G7M	C5-C6-N1	2.10	116.18	111.84
1	16	1207	2MG	O6-C6-C5	-2.10	120.99	126.53
23	23	2604	PSU	O2-C2-N3	-2.08	118.16	121.86
1	16	1402	4OC	C6-C5-C4	2.07	119.50	117.00
23	23	2580	PSU	O2-C2-N3	-2.07	118.19	121.86
23	23	2504	PSU	C5-C6-N1	-2.06	119.28	122.14
55	Pt	37	T6A	N9-C8-N7	-2.06	111.02	113.94
1	16	516	PSU	O4'-C1'-C2'	2.06	108.00	105.15
1	16	966	2MG	O6-C6-C5	-2.05	121.11	126.53
23	23	1618	6MZ	N9-C8-N7	-2.05	111.03	113.94
56	Dt	8	4SU	O2-C2-N1	-2.05	120.13	122.80
1	16	1516	2MG	O6-C6-C5	-2.04	121.16	126.53
12	SL	89	D2T	O-C-CA	-2.04	119.54	124.77
1	16	527	G7M	C6-C5-N7	2.03	134.72	132.17
1	16	1407	5MC	C2'-C1'-N1	-2.03	107.61	113.25
56	Dt	37	MIA	N6-C6-N1	2.02	121.05	118.33
23	23	2498	OMC	O2-C2-N3	-2.02	119.15	122.33
55	Pt	34	U8U	C3'-C2'-C1'	2.01	105.26	101.46
1	16	1516	2MG	C2'-C1'-N9	-2.00	107.68	113.25
23	23	2504	PSU	O2-C2-N3	-2.00	118.31	121.86

There are no chirality outliers.

All (55) 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'
1	16	966	2MG	N1-C2-N2-CM2
1	16	966	2MG	N3-C2-N2-CM2
1	16	1519	MA6	C5-C6-N6-C10
12	SL	89	D2T	SB-CB-CG-OD2

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Mol	Chain	Res	Type	Atoms
23	23	1618	6MZ	O4'-C4'-C5'-O5'
23	23	1915	3TD	C2'-C1'-C5-C4
23	23	1915	3TD	O4'-C1'-C5-C4
23	23	1915	3TD	O4'-C1'-C5-C6
23	23	2251	OMG	O4'-C4'-C5'-O5'
23	23	2251	OMG	C1'-C2'-O2'-CM2
55	Pt	16	H2U	O4'-C1'-N1-C6
55	Pt	16	H2U	C2'-C1'-N1-C2
55	Pt	16	H2U	C2'-C1'-N1-C6
55	Pt	47	3AU	C2'-C1'-N1-C2
55	Pt	47	3AU	C2'-C1'-N1-C6
56	Dt	37	MIA	C12-C13-C14-C16
56	Dt	47	3AU	C2'-C1'-N1-C2
56	Dt	47	3AU	C2'-C1'-N1-C6
23	23	2251	OMG	C3'-C4'-C5'-O5'
23	23	2030	6MZ	O4'-C4'-C5'-O5'
1	16	1519	MA6	N1-C6-N6-C10
23	23	2030	6MZ	C3'-C4'-C5'-O5'
23	23	2503	2MA	O4'-C4'-C5'-O5'
23	23	1618	6MZ	C3'-C4'-C5'-O5'
23	23	1915	3TD	O4'-C4'-C5'-O5'
1	16	1519	MA6	O4'-C4'-C5'-O5'
23	23	2503	2MA	C3'-C4'-C5'-O5'
56	Dt	47	3AU	C4'-C5'-O5'-P
56	Dt	47	3AU	O4'-C1'-N1-C6
34	LP	81	4D4	OB-CB-CG-CD
56	Dt	47	3AU	O4'-C1'-N1-C2
34	LP	81	4D4	CA-CB-CG-CD
55	Pt	16	H2U	O4'-C1'-N1-C2
55	Pt	16	H2U	C4'-C5'-O5'-P
55	Pt	17	H2U	C4'-C5'-O5'-P
55	Pt	47	3AU	O4'-C1'-N1-C6
1	16	1518	MA6	C5-C6-N6-C9
1	16	1402	4OC	O4'-C4'-C5'-O5'
55	Pt	47	3AU	C11-C12-C13-O31
56	Dt	39	PSU	O4'-C4'-C5'-O5'
55	Pt	47	3AU	O4'-C4'-C5'-O5'
12	SL	89	D2T	CA-CB-SB-CB1
55	Pt	47	3AU	O4'-C1'-N1-C2
55	Pt	54	5MU	C3'-C4'-C5'-O5'
23	23	746	PSU	O4'-C1'-C5-C6
56	Dt	47	3AU	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
55	Pt	47	3AU	C11-C12-C13-O30
1	16	1519	MA6	C5-C6-N6-C9
55	Pt	17	H2U	O4'-C4'-C5'-O5'
12	SL	89	D2T	CG-CB-SB-CB1
1	16	1519	MA6	C3'-C4'-C5'-O5'
55	Pt	17	H2U	C2'-C1'-N1-C2
34	LP	81	4D4	CG-CD-NE-CZ

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	Dt	47	3AU	1	0
55	Pt	16	H2U	1	0
55	Pt	34	U8U	1	0
55	Pt	47	3AU	2	0
55	Pt	46	G7M	1	0
23	23	1915	3TD	1	0
23	23	747	5MU	1	0
23	23	2030	6MZ	2	0
23	23	2498	OMC	1	0
23	23	2457	PSU	1	0
23	23	2251	OMG	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 394 ligands modelled in this entry, 371 are monoatomic - leaving 23 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	$\#\|Z\|>2$
60	ATP	23	3001	-	32,33,33	0.55	0	48,52,52	0.58	0
57	PUT	23	3009	-	5,5,5	0.13	0	4,4,4	0.18	0
57	PUT	23	3006	-	5,5,5	0.11	0	4,4,4	0.18	0
57	PUT	23	3015	-	5,5,5	0.15	0	4,4,4	0.26	0
57	PUT	16	1601	-	5,5,5	0.13	0	4,4,4	0.16	0
61	SPD	23	3020	-	9,9,9	0.17	0	8,8,8	0.39	0
57	PUT	23	3011	-	5,5,5	0.14	0	4,4,4	0.22	0
57	PUT	23	3014	-	5,5,5	0.16	0	4,4,4	0.29	0
61	SPD	23	3021	-	9,9,9	0.34	0	8,8,8	1.09	0
60	ATP	23	3002	-	32,33,33	0.55	0	48,52,52	0.57	0
61	SPD	23	3017	-	9,9,9	0.21	0	8,8,8	0.47	0
57	PUT	16	1602	-	5,5,5	0.16	0	4,4,4	0.27	0
61	SPD	23	3019	-	9,9,9	0.17	0	8,8,8	0.24	0
61	SPD	23	3018	-	9,9,9	0.33	0	8,8,8	0.72	0
57	PUT	23	3008	-	5,5,5	0.12	0	4,4,4	0.30	0
57	PUT	23	3012	-	5,5,5	0.16	0	4,4,4	0.23	0
57	PUT	23	3005	-	5,5,5	0.09	0	4,4,4	0.13	0
57	PUT	23	3007	-	5,5,5	0.13	0	4,4,4	0.24	0
57	PUT	23	3003	-	5,5,5	0.11	0	4,4,4	0.19	0
57	PUT	23	3016	-	5,5,5	0.15	0	4,4,4	0.26	0
57	PUT	23	3013	-	5,5,5	0.15	0	4,4,4	0.30	0
57	PUT	23	3004	-	5,5,5	0.14	0	4,4,4	0.23	0
57	PUT	23	3010	-	5,5,5	0.12	0	4,4,4	0.27	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
60	ATP	23	3001	-	-	1/22/38/38	0/3/3/3
57	PUT	23	3009	-	-	0/3/3/3	-
57	PUT	23	3006	-	-	1/3/3/3	-
57	PUT	23	3015	-	-	0/3/3/3	-
57	PUT	16	1601	-	-	0/3/3/3	-
61	SPD	23	3020	-	-	1/7/7/7	-
57	PUT	23	3011	-	-	1/3/3/3	-
57	PUT	23	3014	-	-	2/3/3/3	-
61	SPD	23	3021	-	-	3/7/7/7	-
60	ATP	23	3002	-	-	2/22/38/38	0/3/3/3
61	SPD	23	3017	-	-	0/7/7/7	-
57	PUT	16	1602	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SPD	23	3019	-	-	2/7/7/7	-
61	SPD	23	3018	-	-	2/7/7/7	-
57	PUT	23	3008	-	-	2/3/3/3	-
57	PUT	23	3012	-	-	1/3/3/3	-
57	PUT	23	3005	-	-	3/3/3/3	-
57	PUT	23	3007	-	-	0/3/3/3	-
57	PUT	23	3003	-	-	1/3/3/3	-
57	PUT	23	3016	-	-	0/3/3/3	-
57	PUT	23	3013	-	-	1/3/3/3	-
57	PUT	23	3004	-	-	0/3/3/3	-
57	PUT	23	3010	-	-	0/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	23	3014	PUT	C1-C2-C3-C4
61	23	3021	SPD	N6-C7-C8-C9
61	23	3019	SPD	C3-C4-C5-N6
61	23	3021	SPD	C3-C4-C5-N6
61	23	3018	SPD	C3-C4-C5-N6
60	23	3002	ATP	C3'-C4'-C5'-O5'
57	23	3008	PUT	C1-C2-C3-C4
57	23	3008	PUT	C2-C3-C4-N2
57	23	3005	PUT	C1-C2-C3-C4
57	23	3005	PUT	C2-C3-C4-N2
57	23	3005	PUT	N1-C1-C2-C3
60	23	3001	ATP	C5'-O5'-PA-O1A
60	23	3002	ATP	O4'-C4'-C5'-O5'
57	23	3011	PUT	N1-C1-C2-C3
57	23	3014	PUT	N1-C1-C2-C3
61	23	3018	SPD	N1-C2-C3-C4
57	23	3013	PUT	C1-C2-C3-C4
61	23	3020	SPD	C3-C4-C5-N6
61	23	3021	SPD	N1-C2-C3-C4
61	23	3019	SPD	C4-C5-N6-C7
57	23	3012	PUT	C1-C2-C3-C4
57	23	3003	PUT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
57	23	3006	PUT	N1-C1-C2-C3

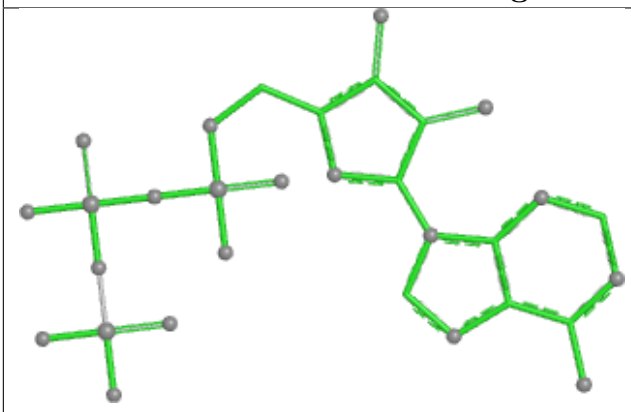
There are no ring outliers.

4 monomers are involved in 4 short contacts:

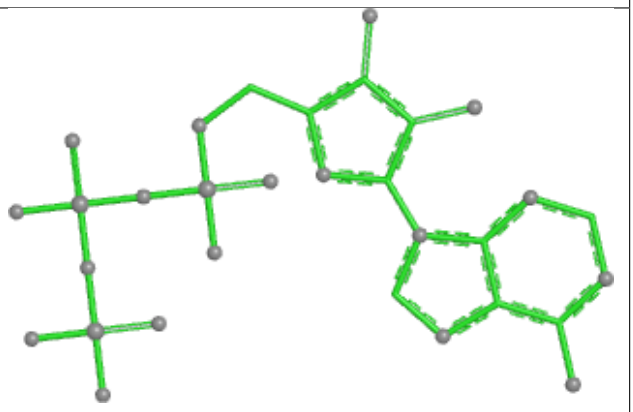
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	23	3014	PUT	1	0
60	23	3002	ATP	1	0
61	23	3017	SPD	1	0
61	23	3018	SPD	1	0

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.

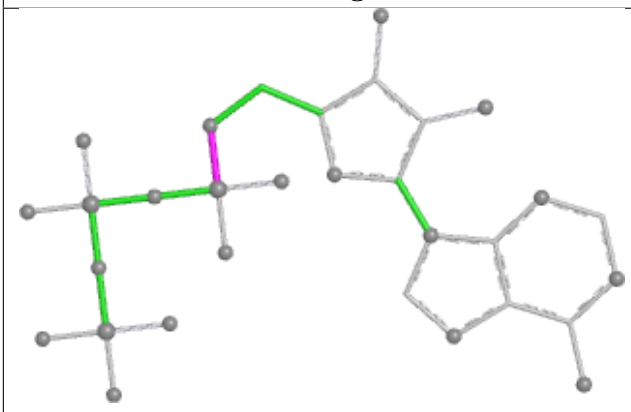
Ligand ATP 23 3001



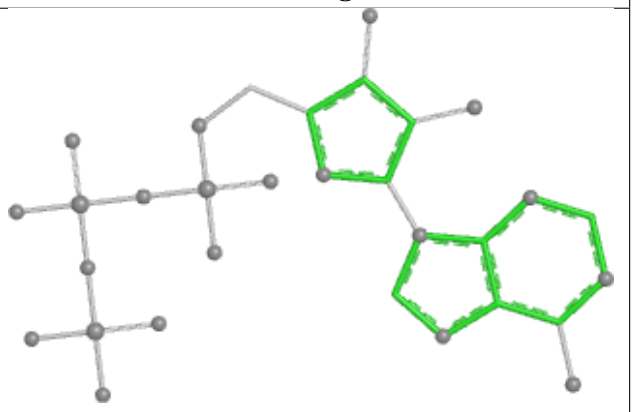
Bond lengths



Bond angles

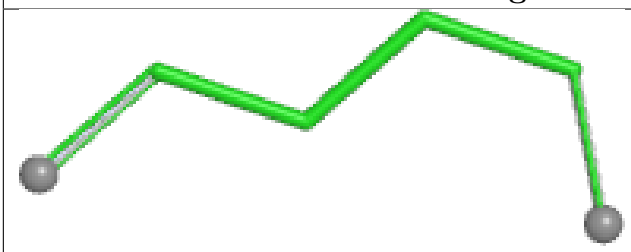


Torsions

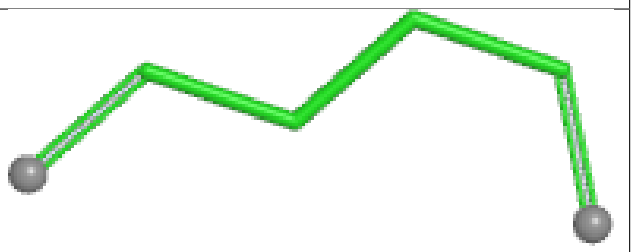


Rings

Ligand PUT 23 3009



Bond lengths



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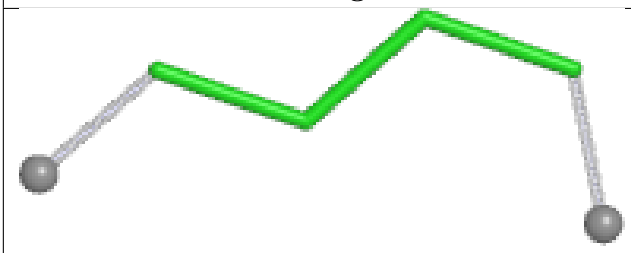
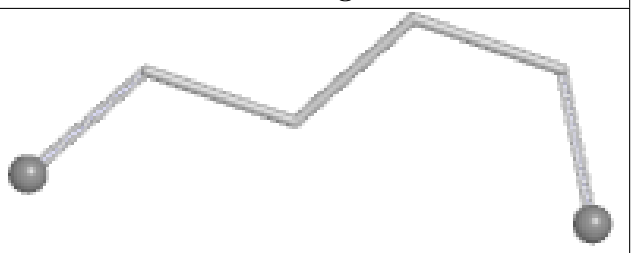
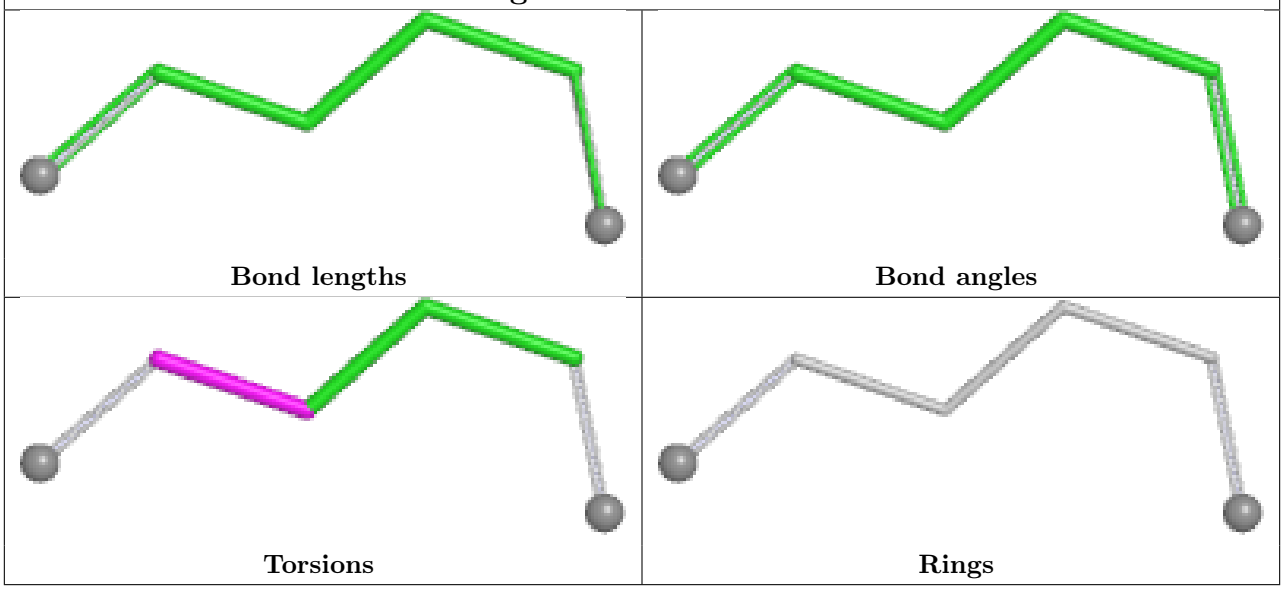


Torsions



Rings

Ligand PUT 23 3006



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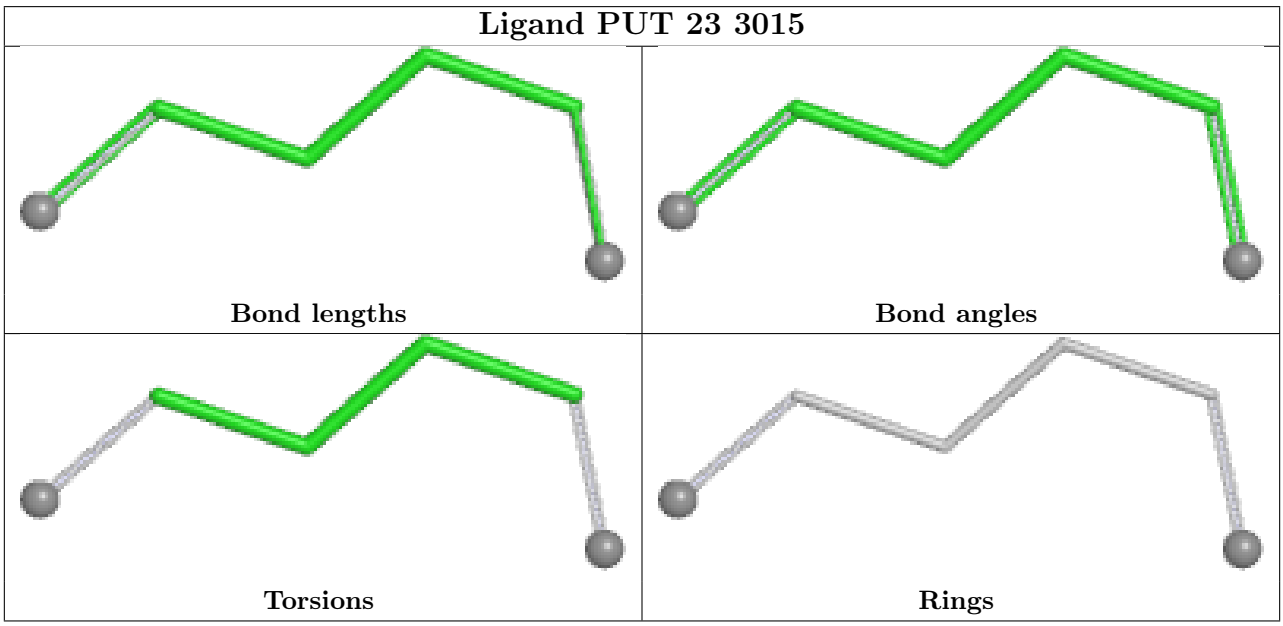
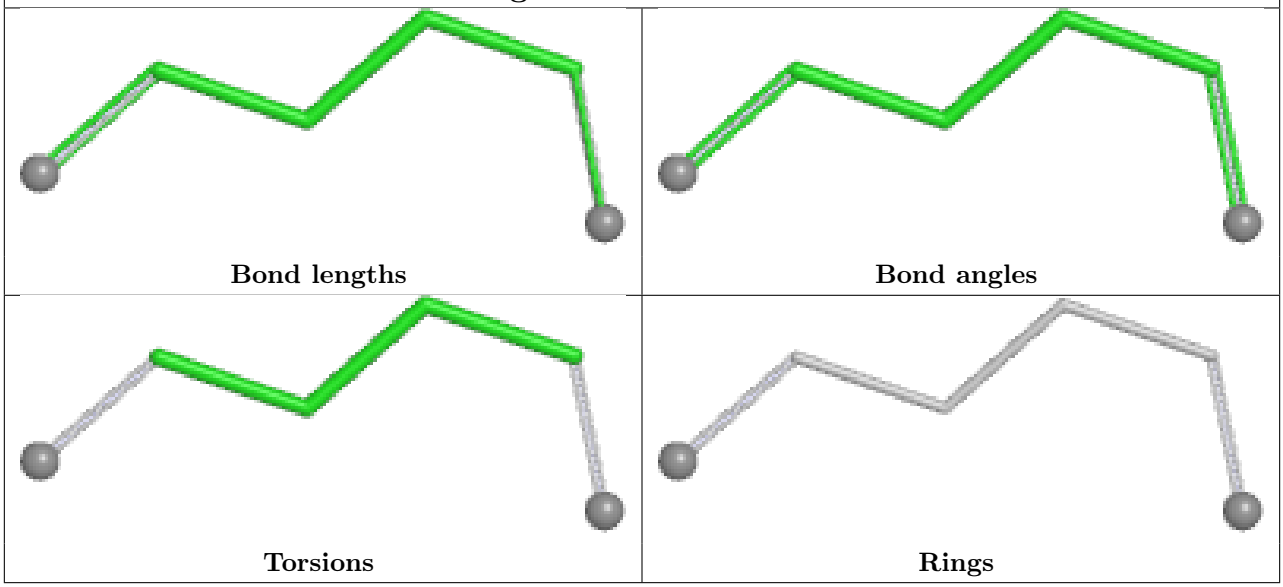


Ligand PUT 16 1601



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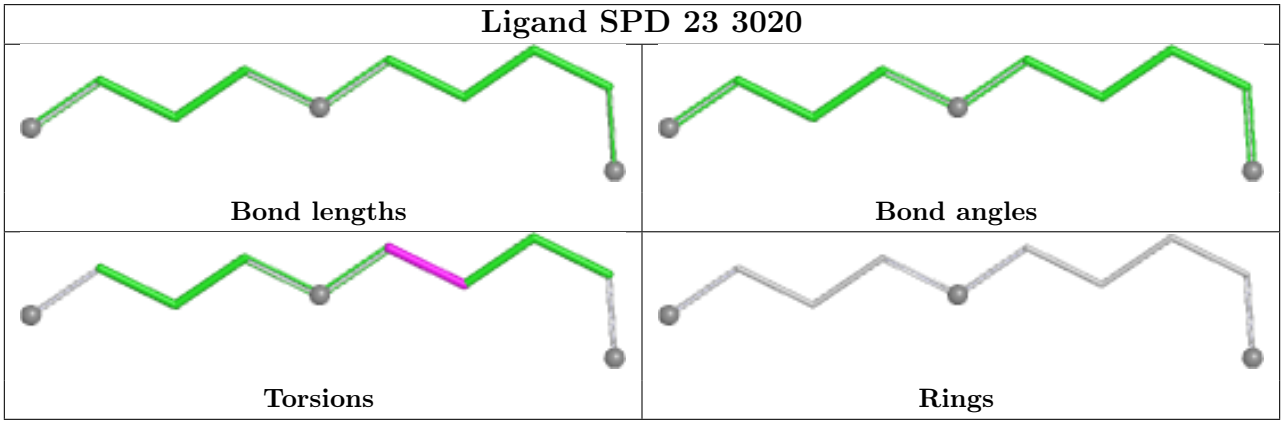

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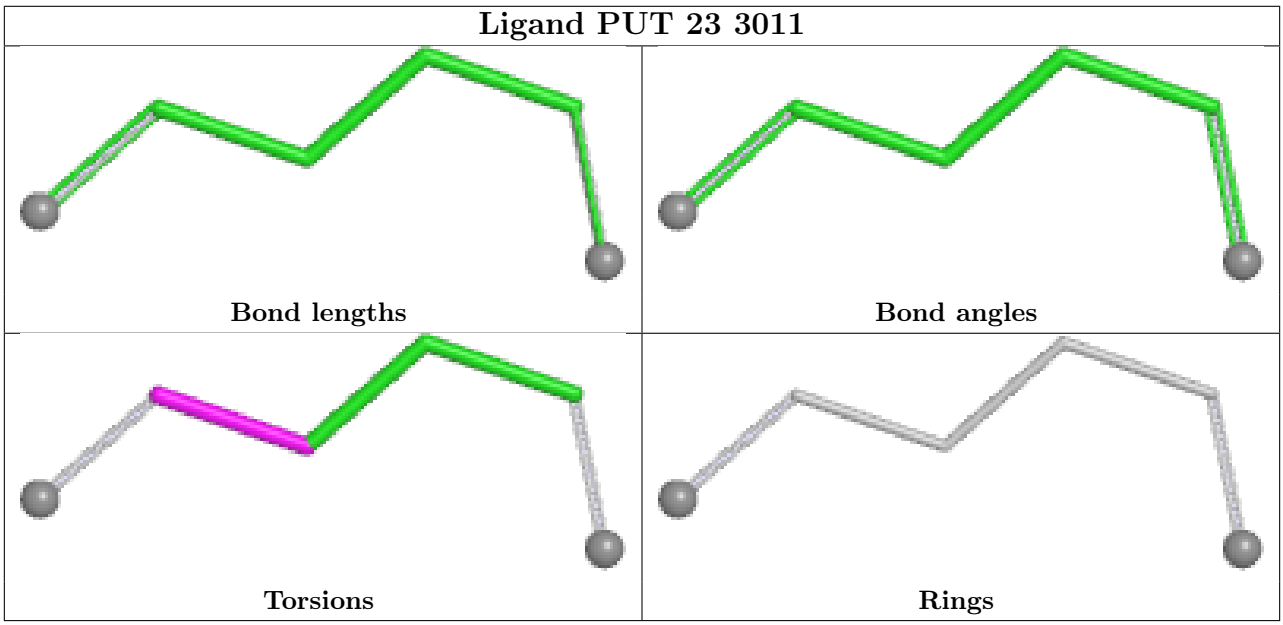

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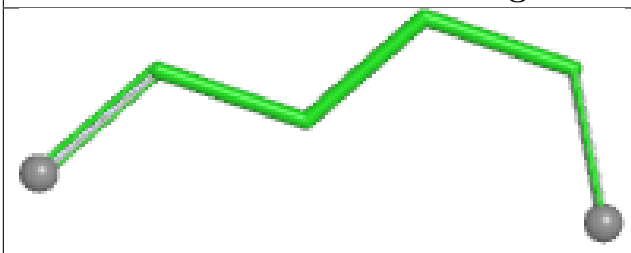
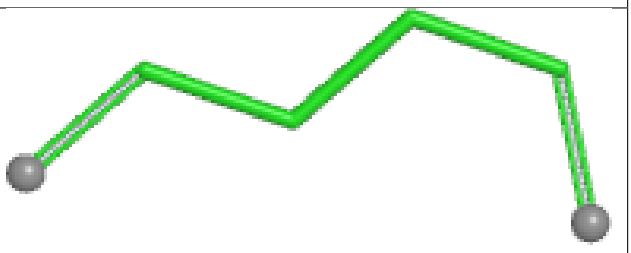
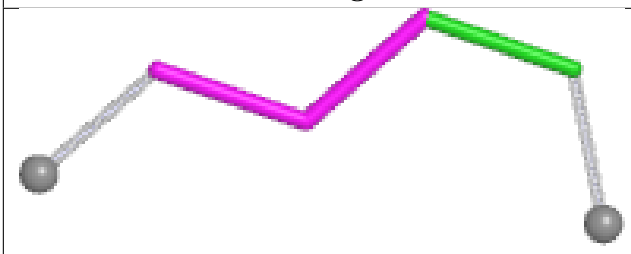


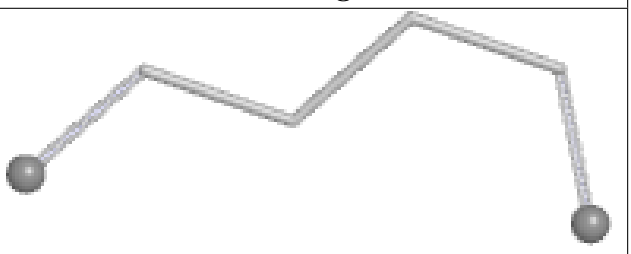
Bond lengths



Bond angles

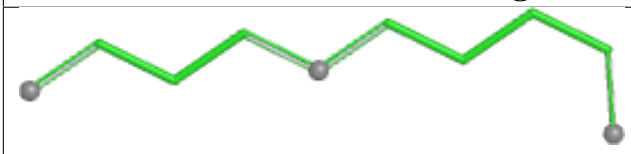


Torsions



Rings

Ligand SPD 23 3021



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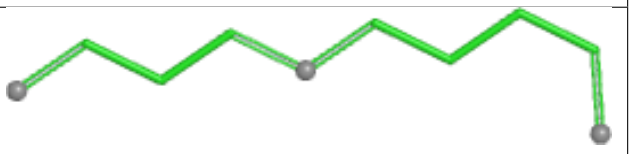

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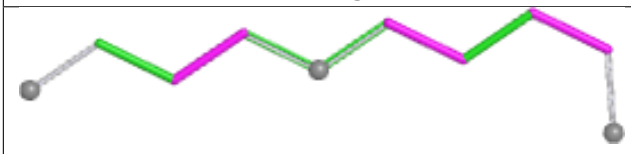

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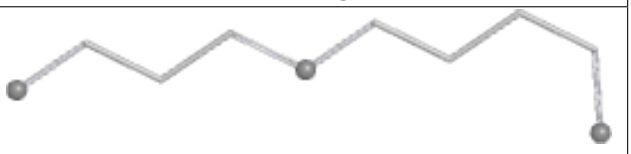
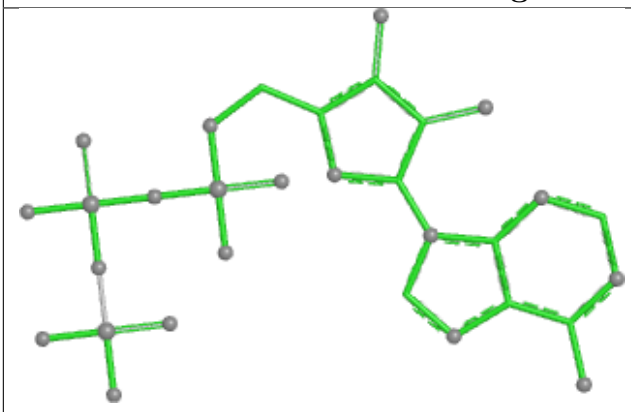


Rings

Ligand ATP 23 3002



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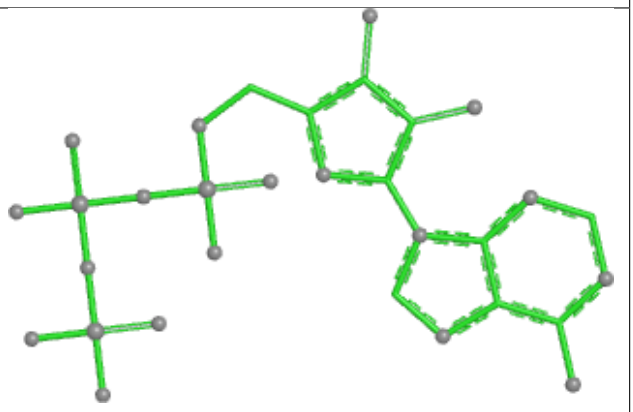
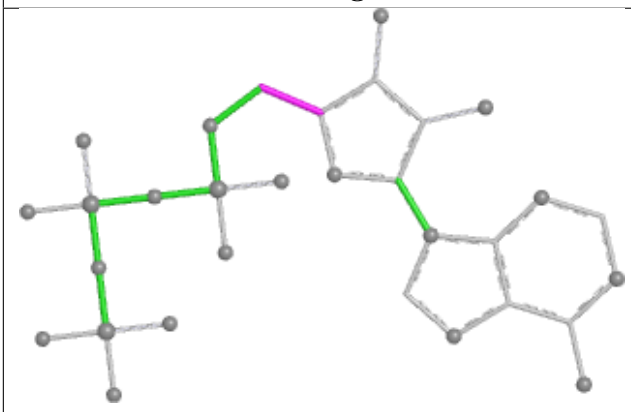


Bond angles



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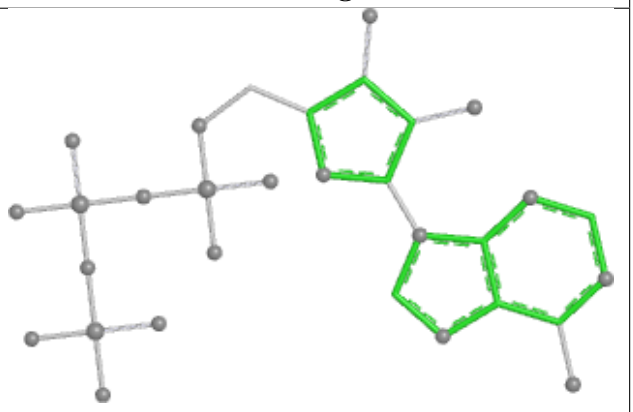

Rings

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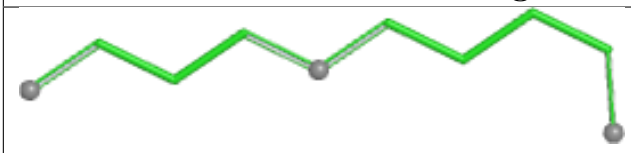

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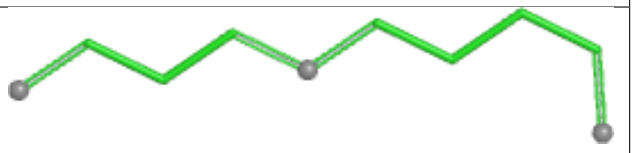
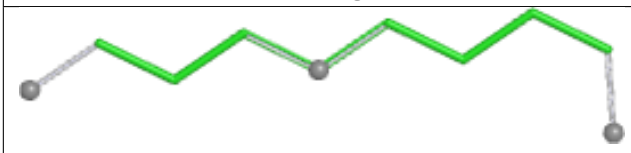


Bond angles



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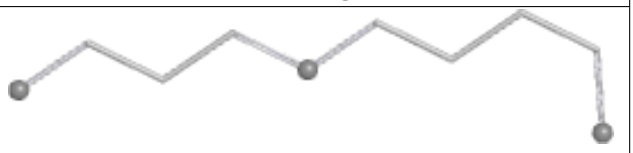
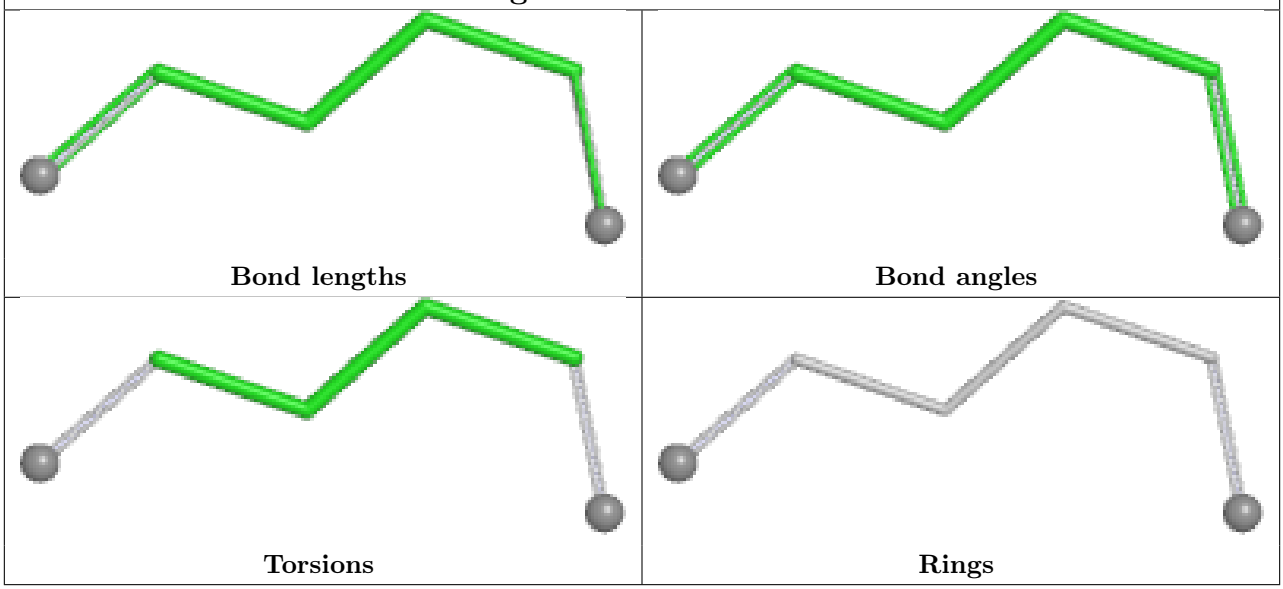


Rings

Ligand PUT 16 1602



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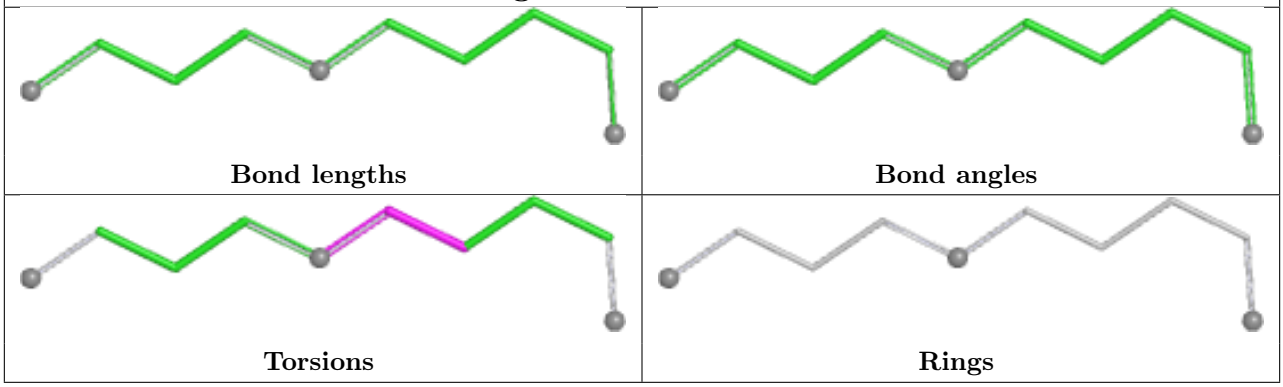

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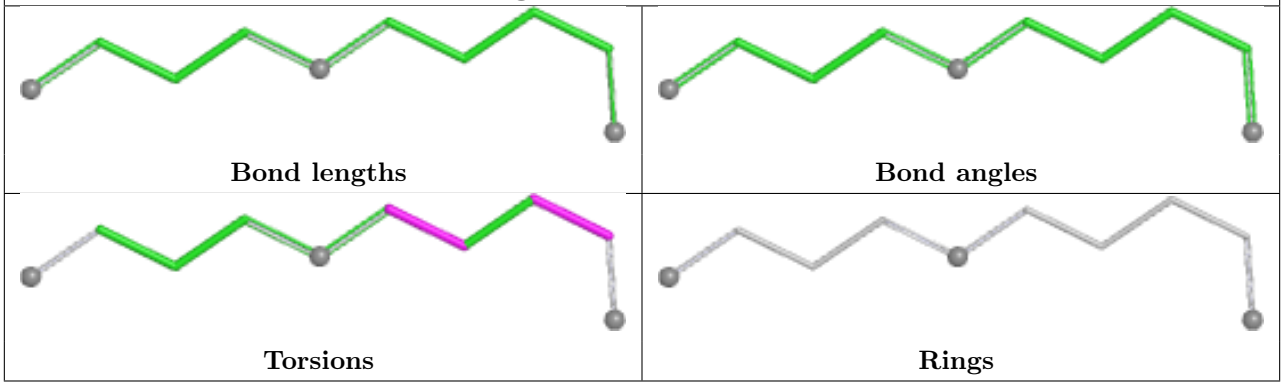

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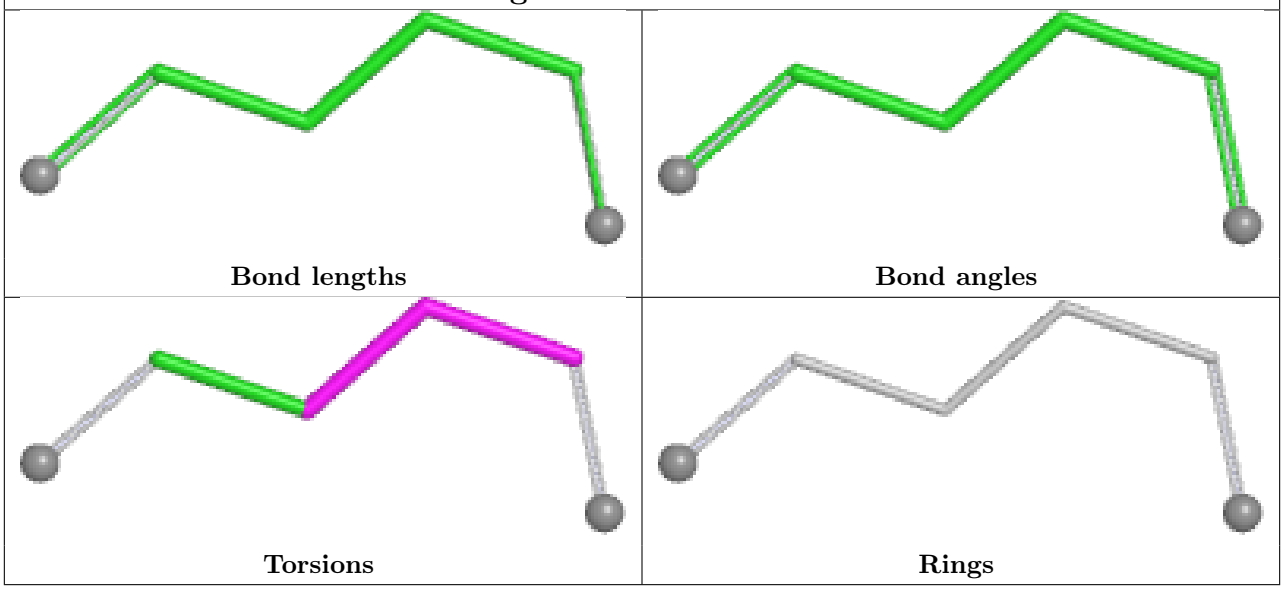

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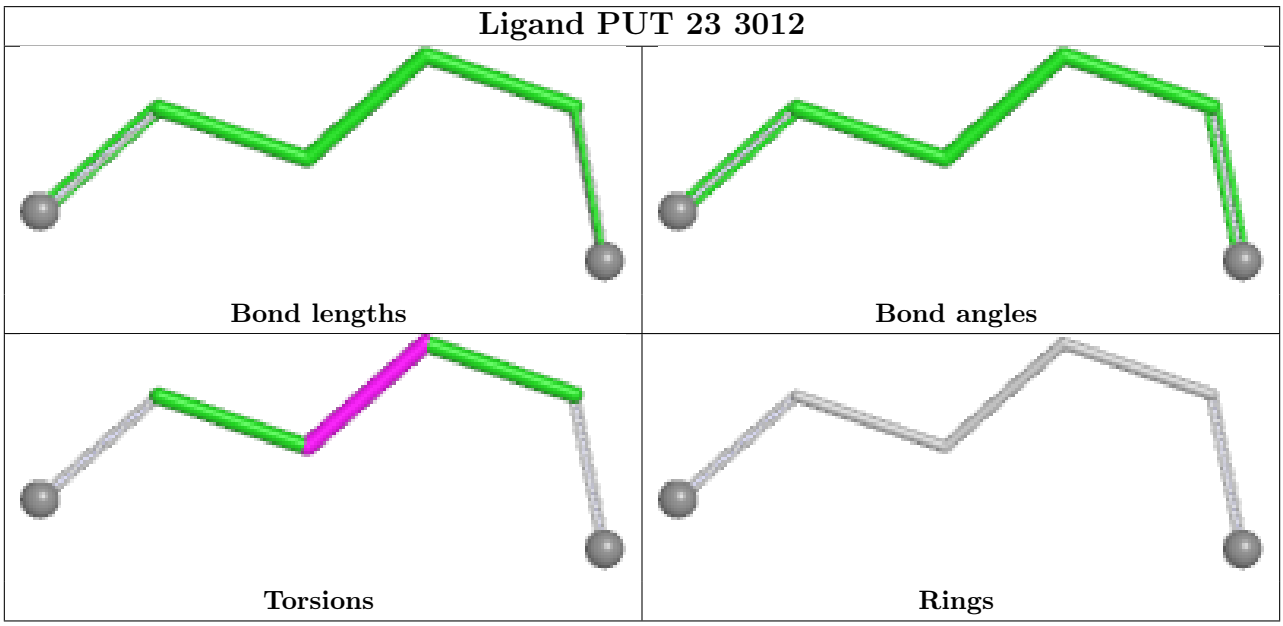

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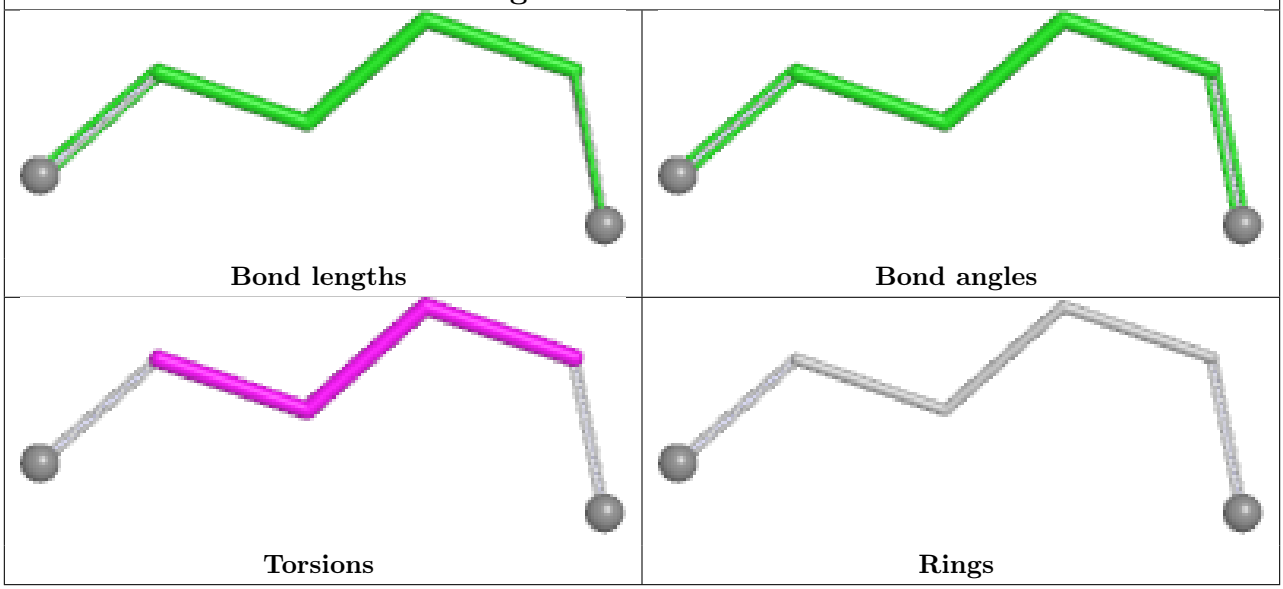
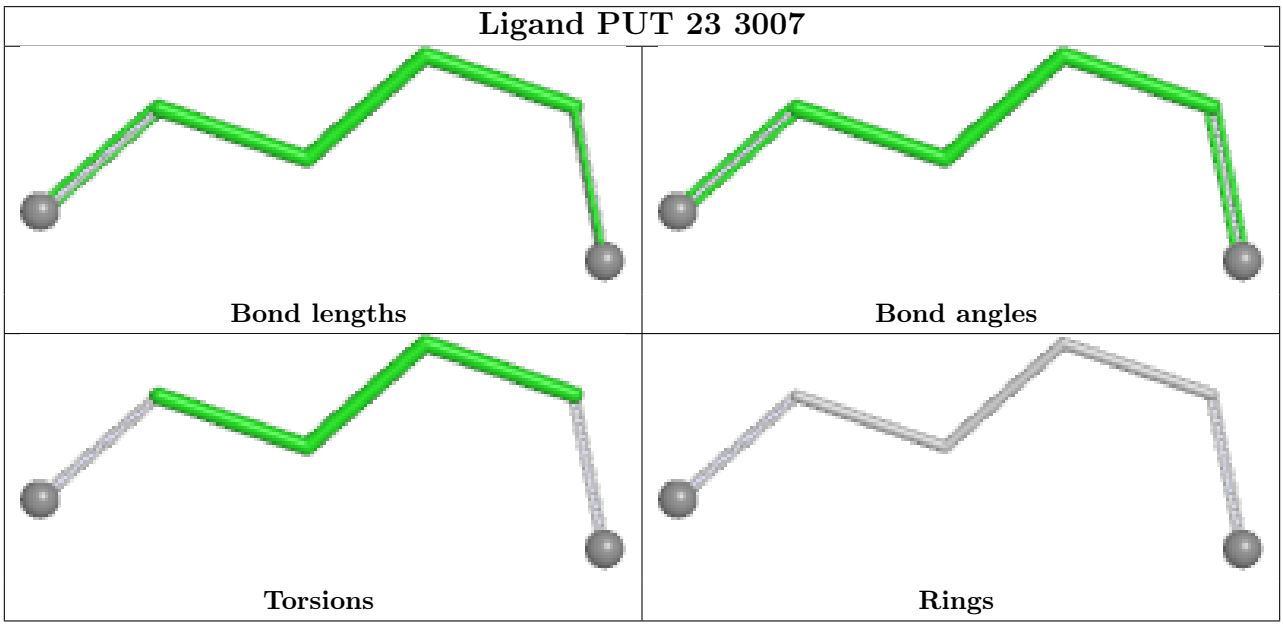
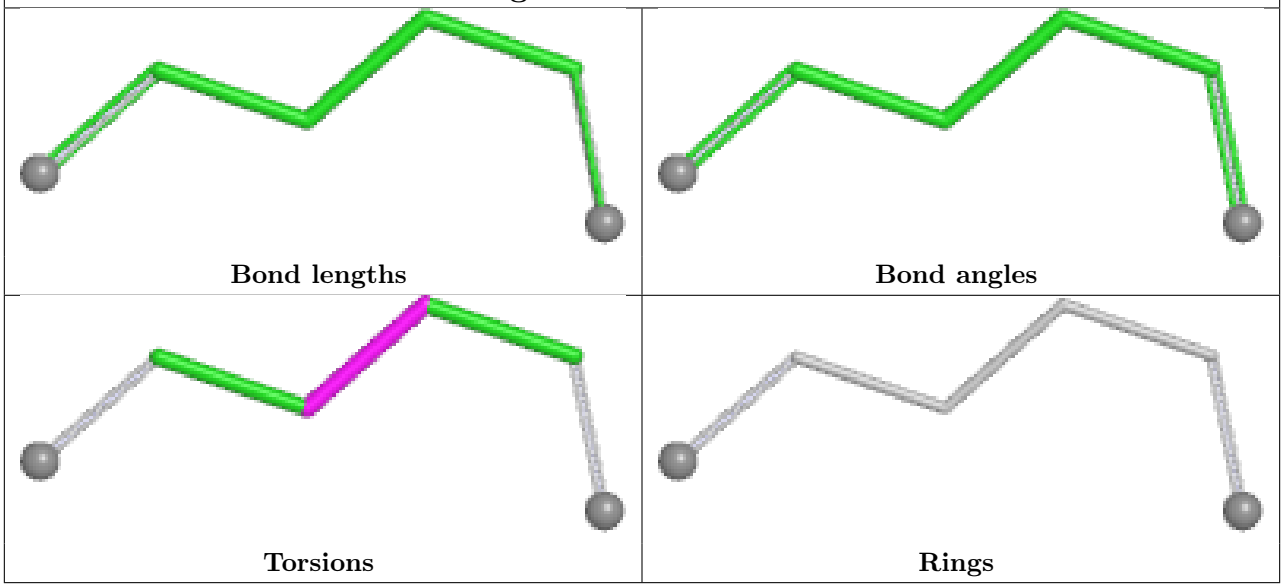


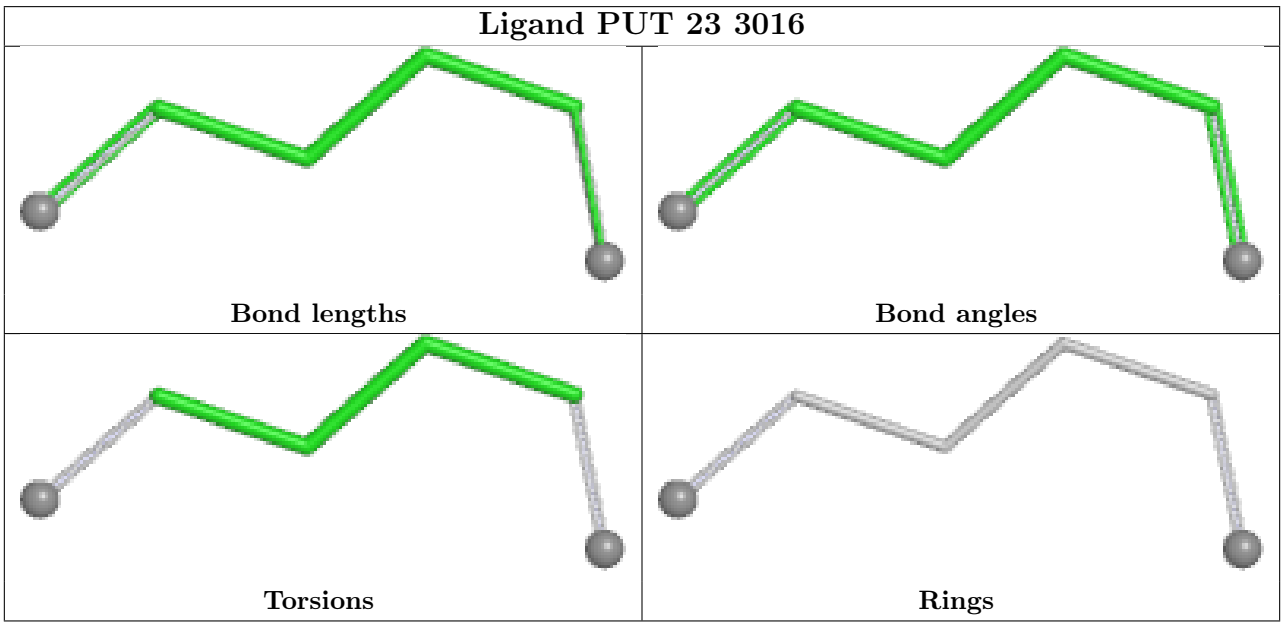
Ligand PUT 23 3007



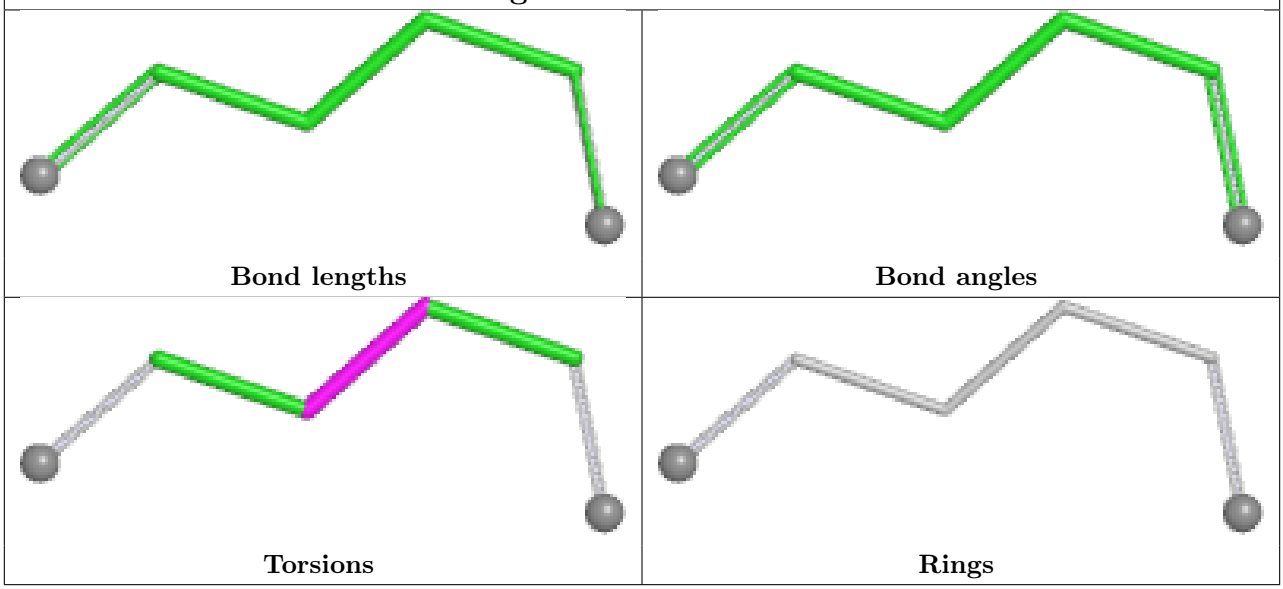
Ligand PUT 23 3003



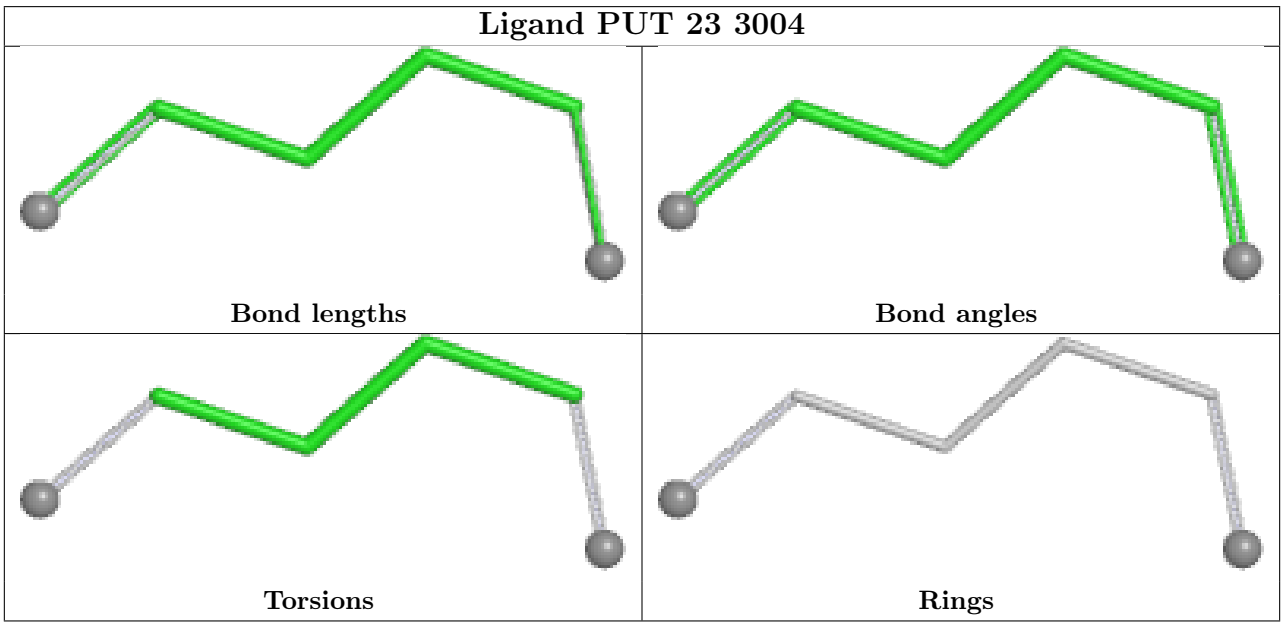
Ligand PUT 23 3016



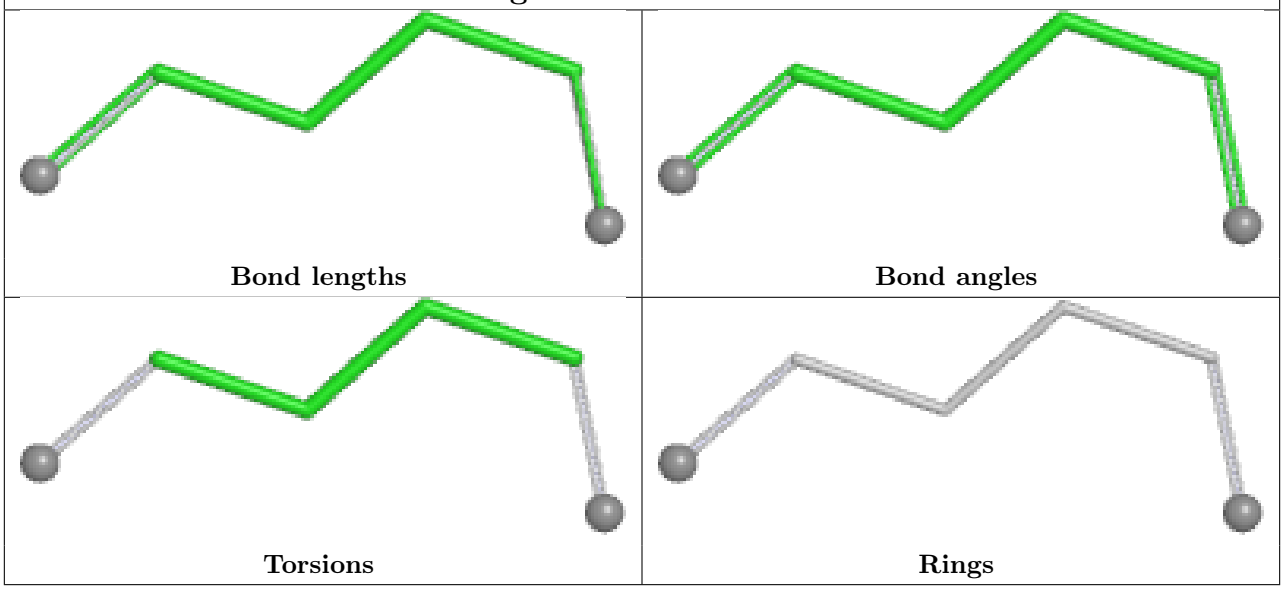
Ligand PUT 23 3013



Ligand PUT 23 3004



Ligand PUT 23 3010



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.

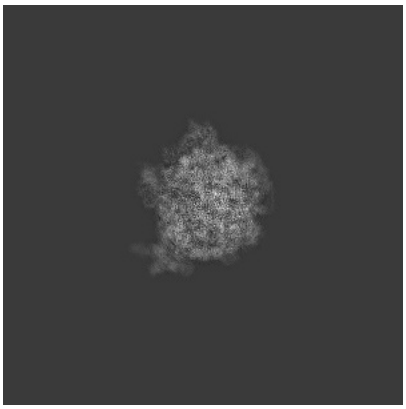
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24133. These allow visual inspection of the internal detail of the map and identification of artifacts.

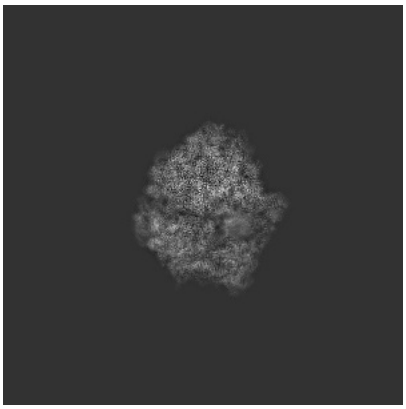
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

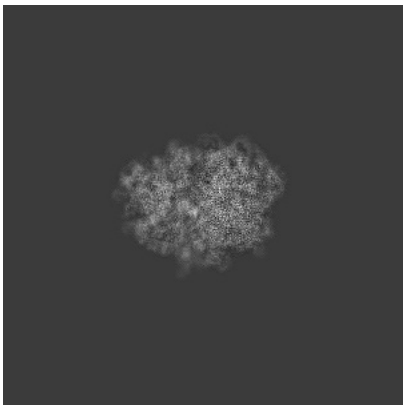
6.1.1 Primary map



X

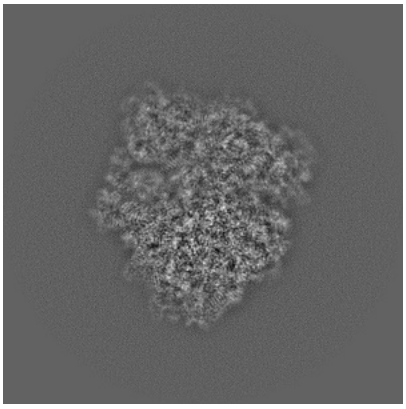


Y

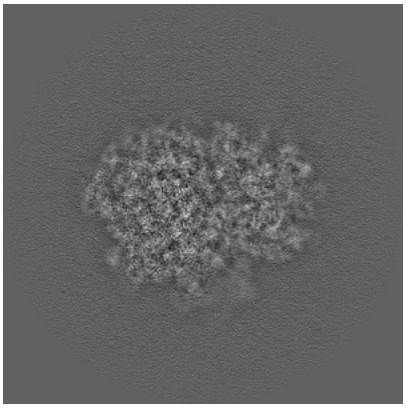


Z

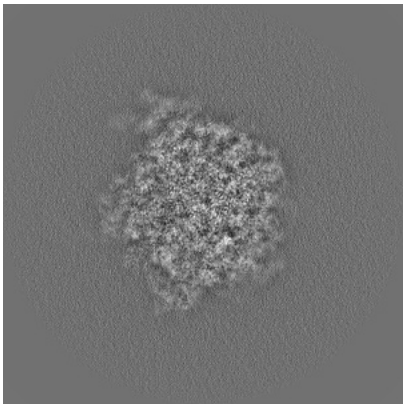
6.1.2 Raw map



X



Y

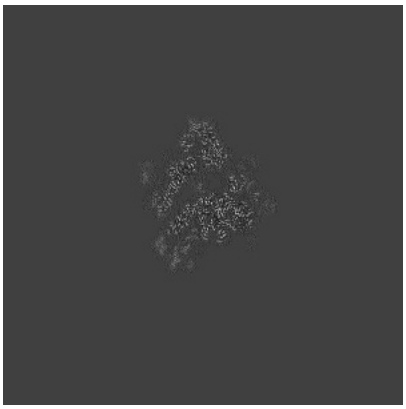


Z

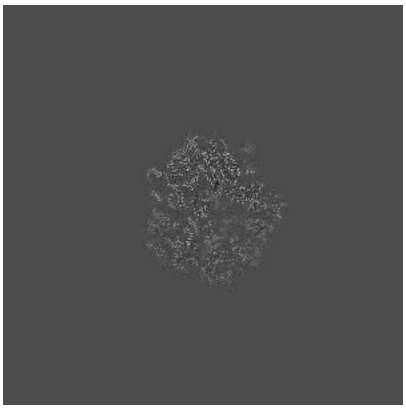
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

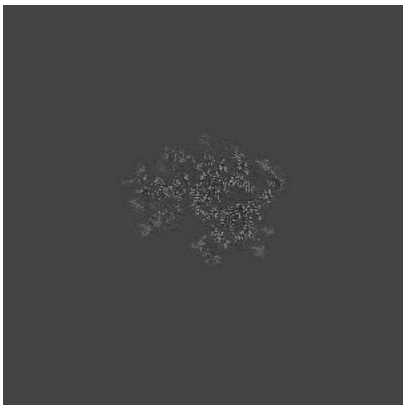
6.2.1 Primary map



X Index: 288

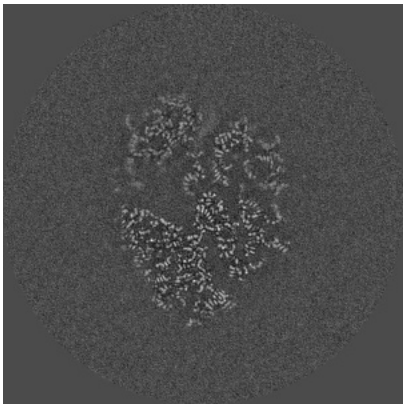


Y Index: 288

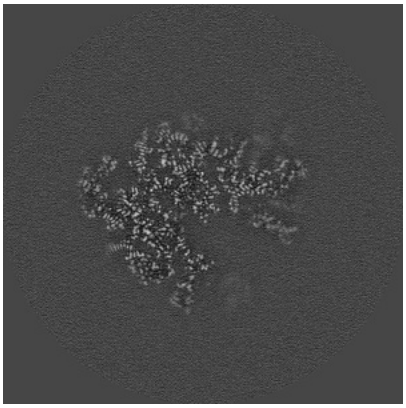


Z Index: 288

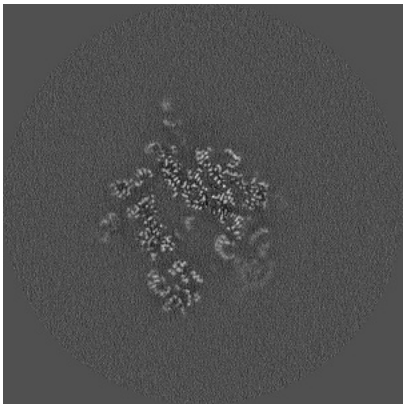
6.2.2 Raw map



X Index: 256



Y Index: 256

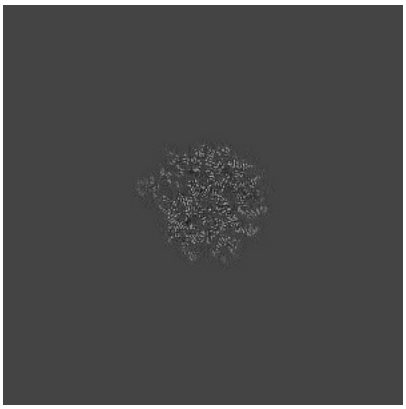


Z Index: 256

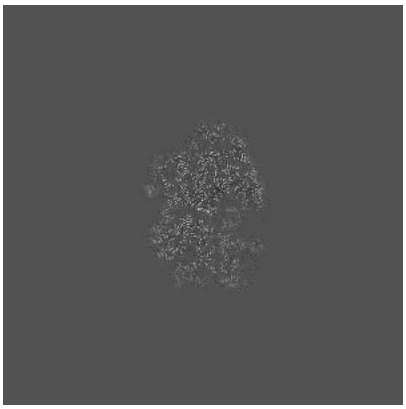
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

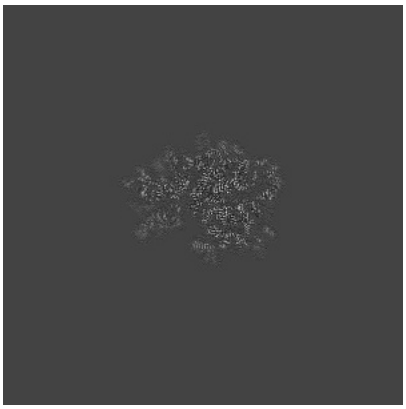
6.3.1 Primary map



X Index: 316

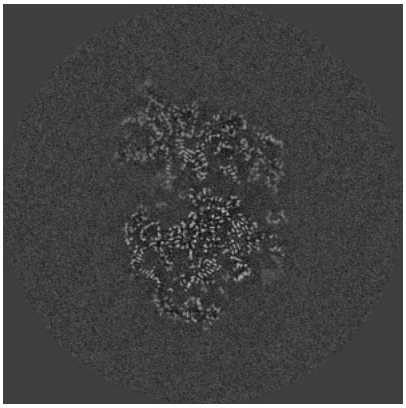


Y Index: 316

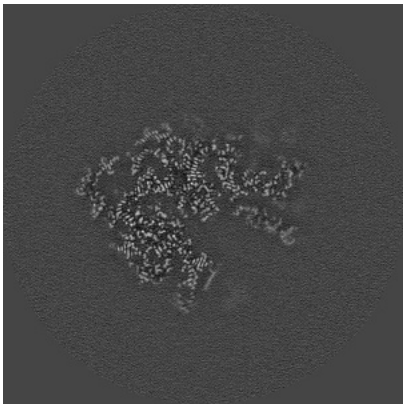


Z Index: 283

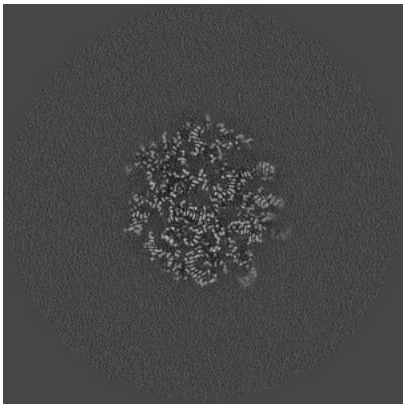
6.3.2 Raw map



X Index: 271



Y Index: 260

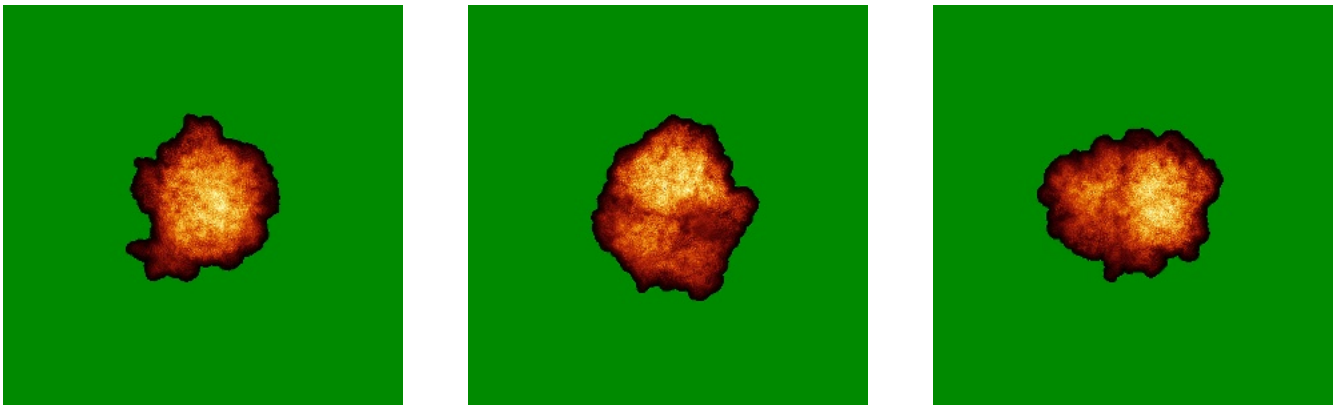


Z Index: 211

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

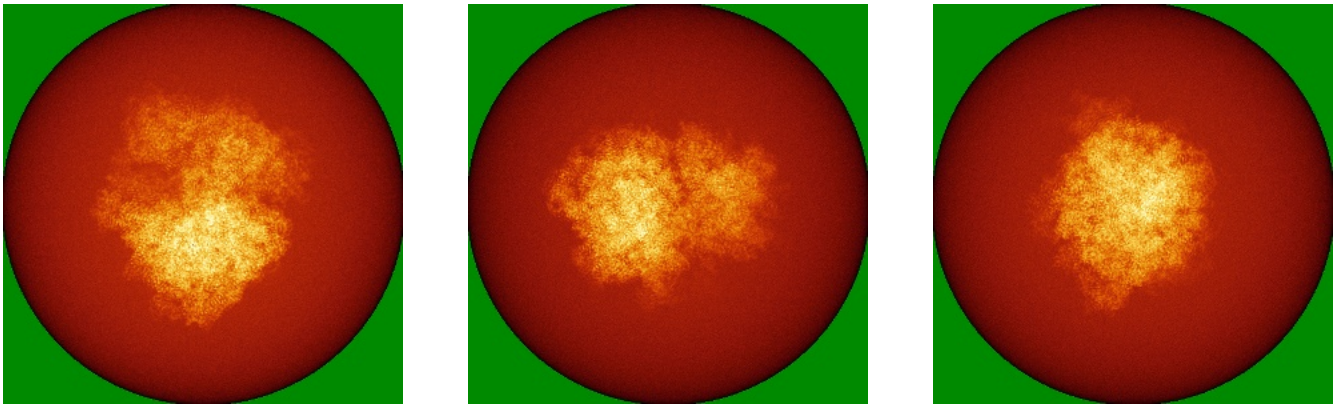
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

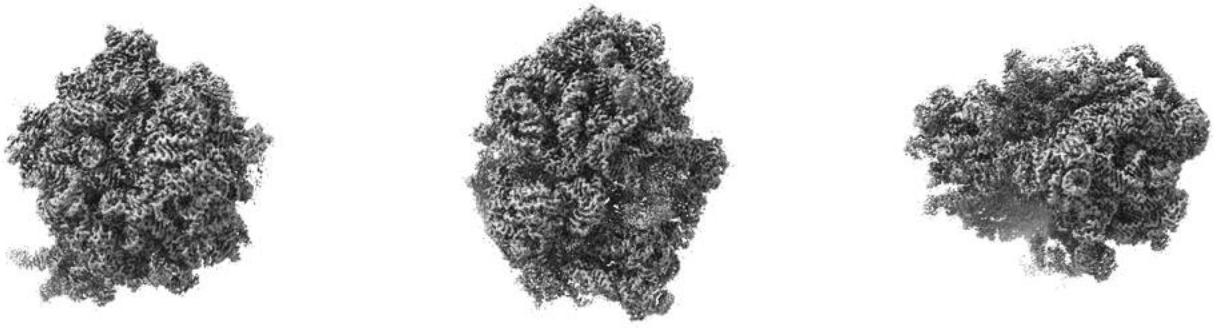


X Y Z

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.

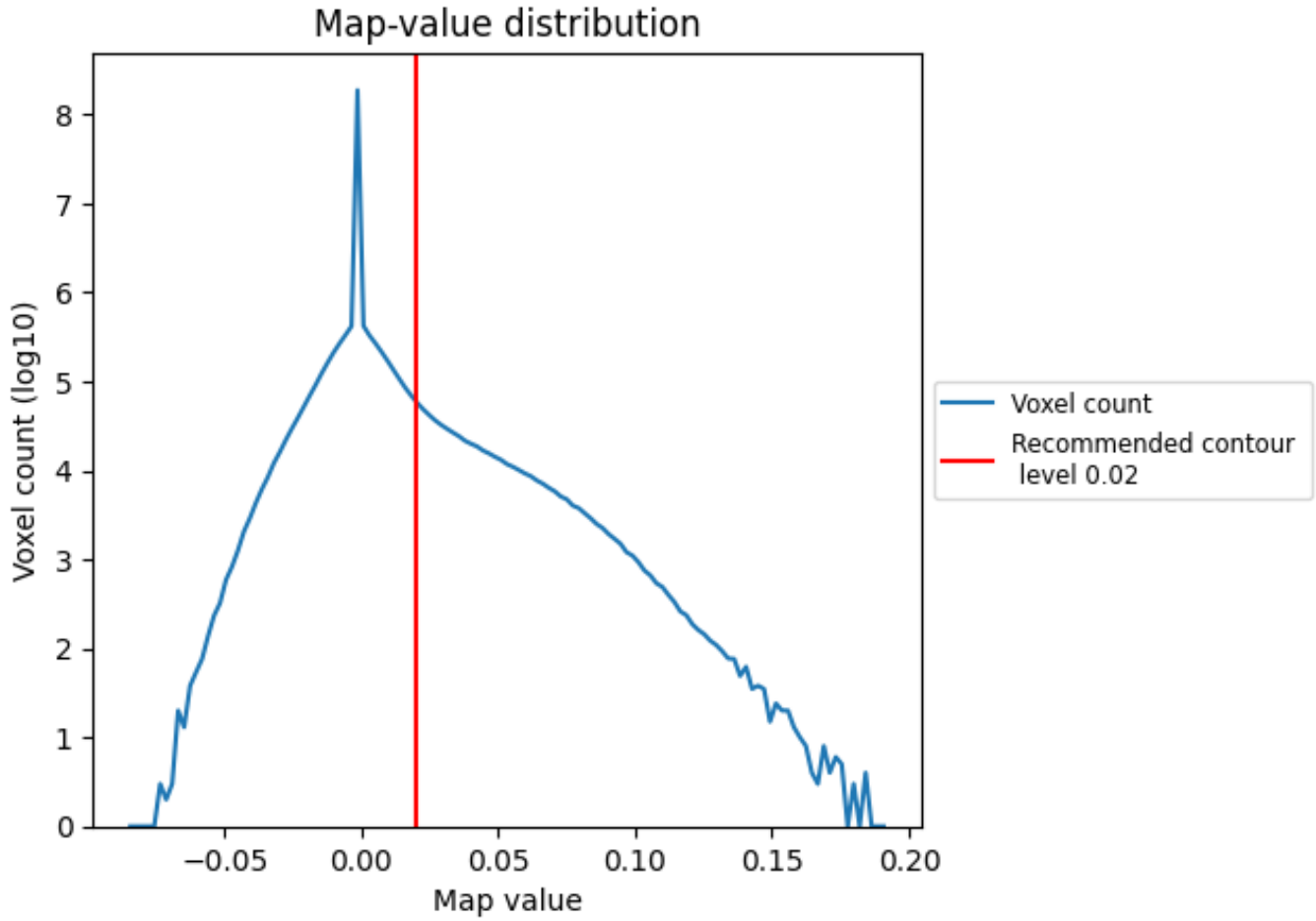
6.6 Mask visualisation (i)

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

7 Map analysis

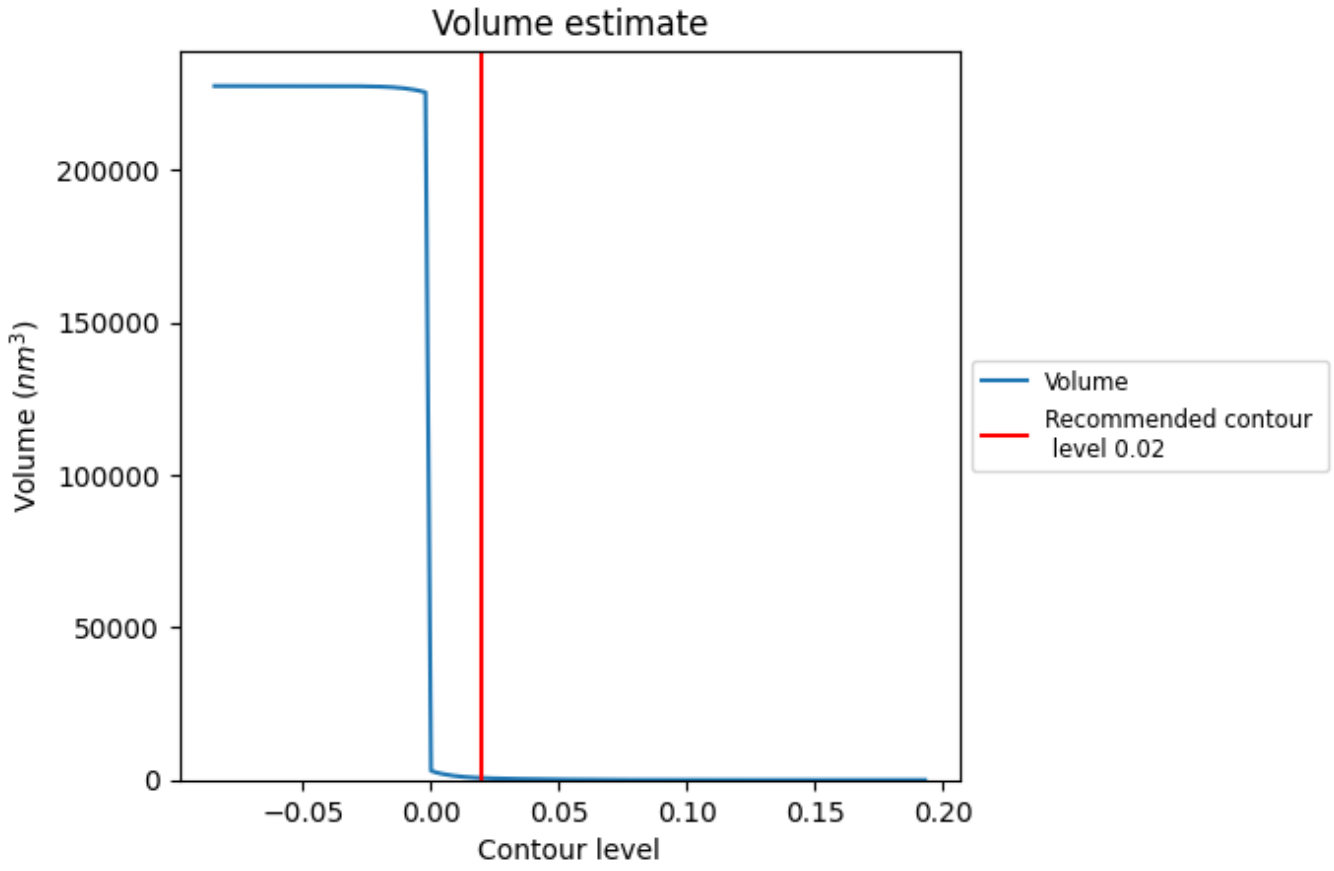
This section contains the results of statistical analysis of the map.

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.

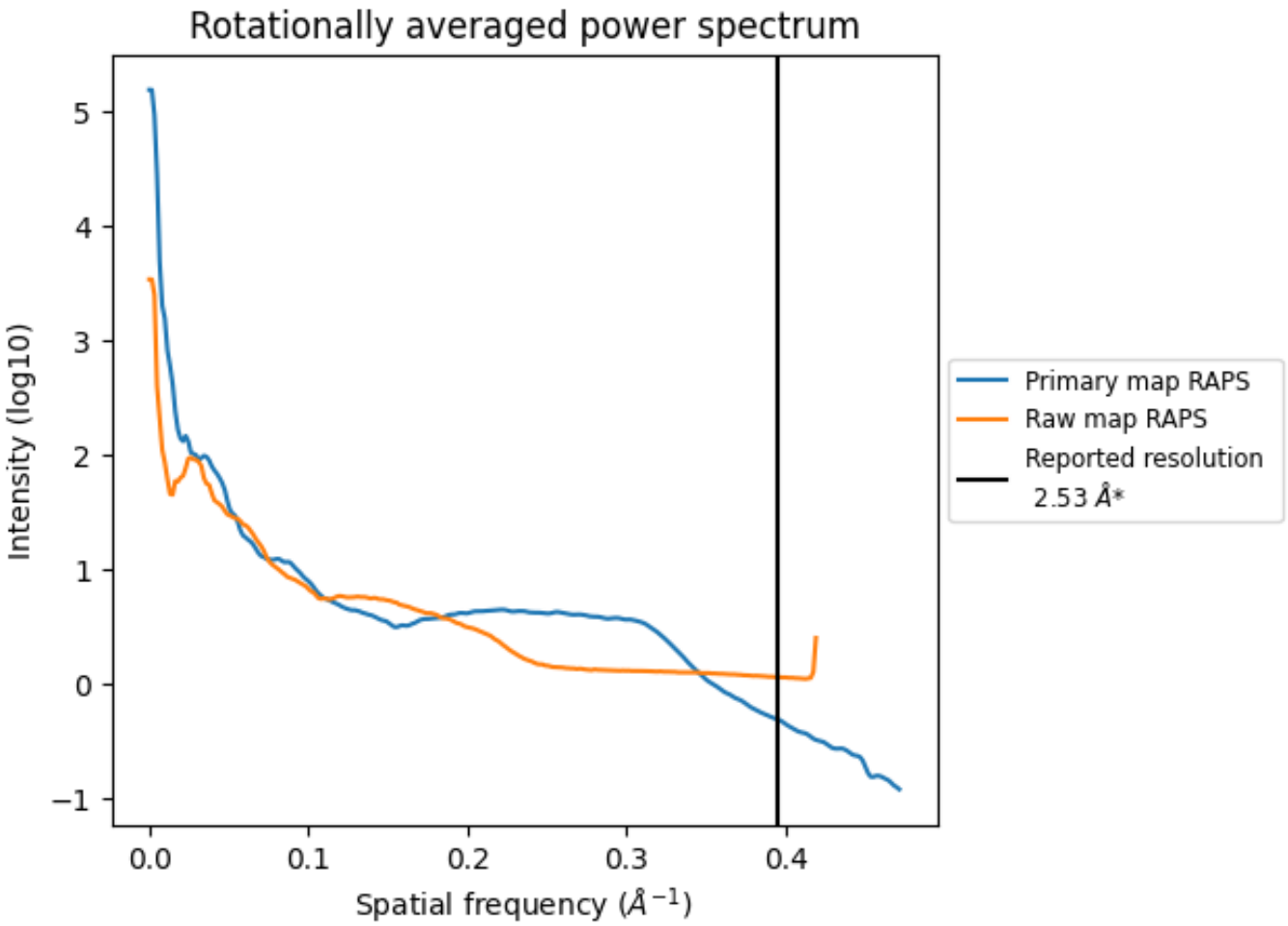
7.2 Volume estimate



The volume at the recommended contour level is 652 nm^3; this corresponds to an approximate mass of 589 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)

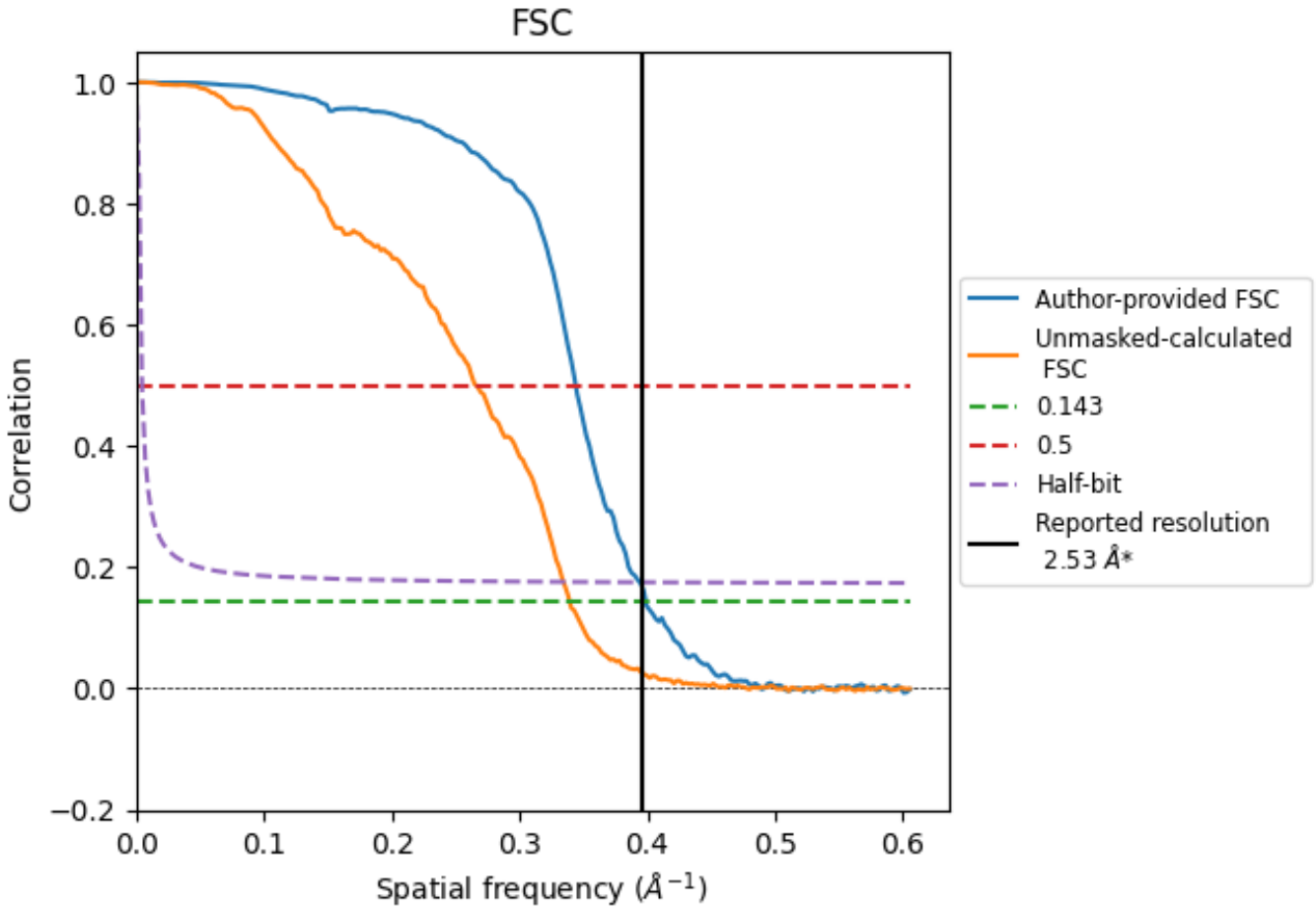


*Reported resolution corresponds to spatial frequency of 0.395 Å^{-1}

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 0.395 Å^{-1}

8.2 Resolution estimates (i)

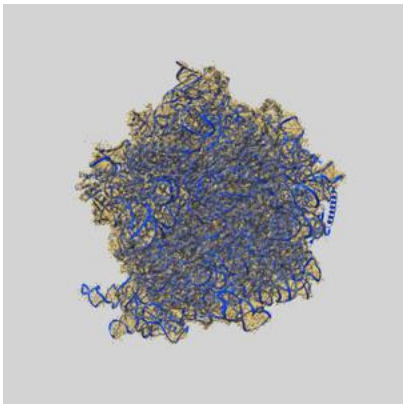
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.53	-	-
Author-provided FSC curve	2.51	2.91	2.54
Unmasked-calculated*	2.95	3.76	2.99

*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 2.95 differs from the reported value 2.53 by more than 10 %

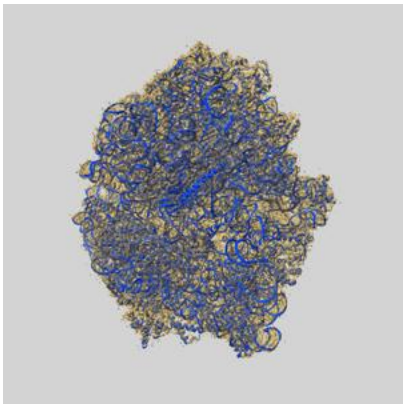
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24133 and PDB model 7N2U. Per-residue inclusion information can be found in section 3 on page 18.

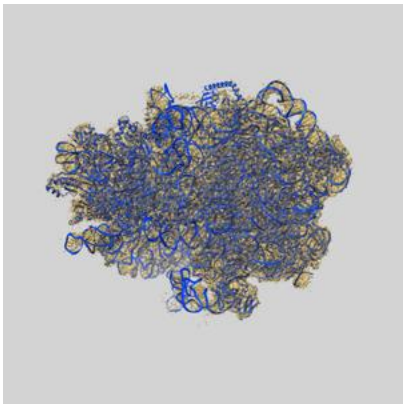
9.1 Map-model overlay



X



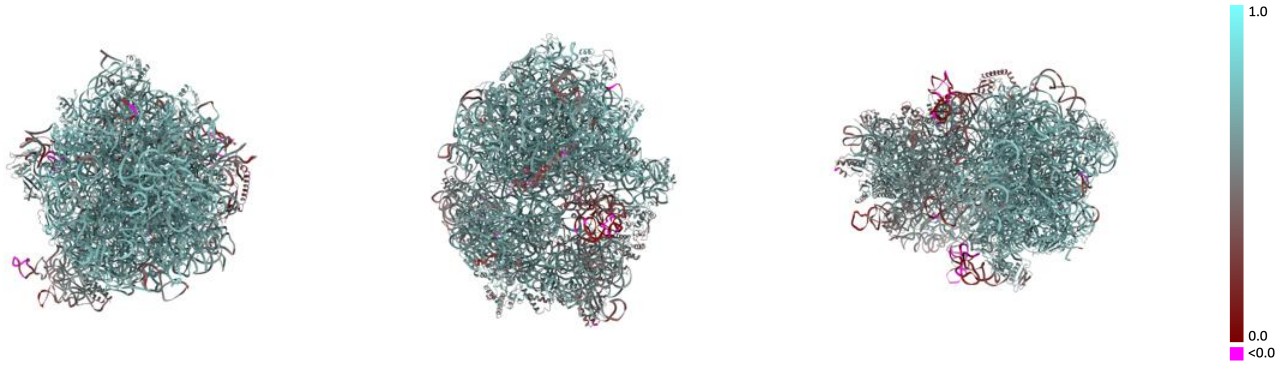
Y



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.

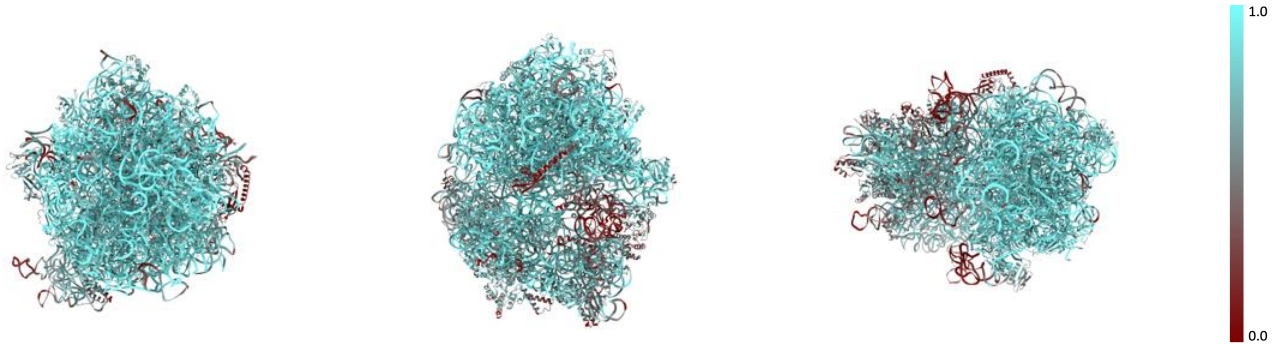
9.2 Q-score mapped to coordinate model (i)



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.

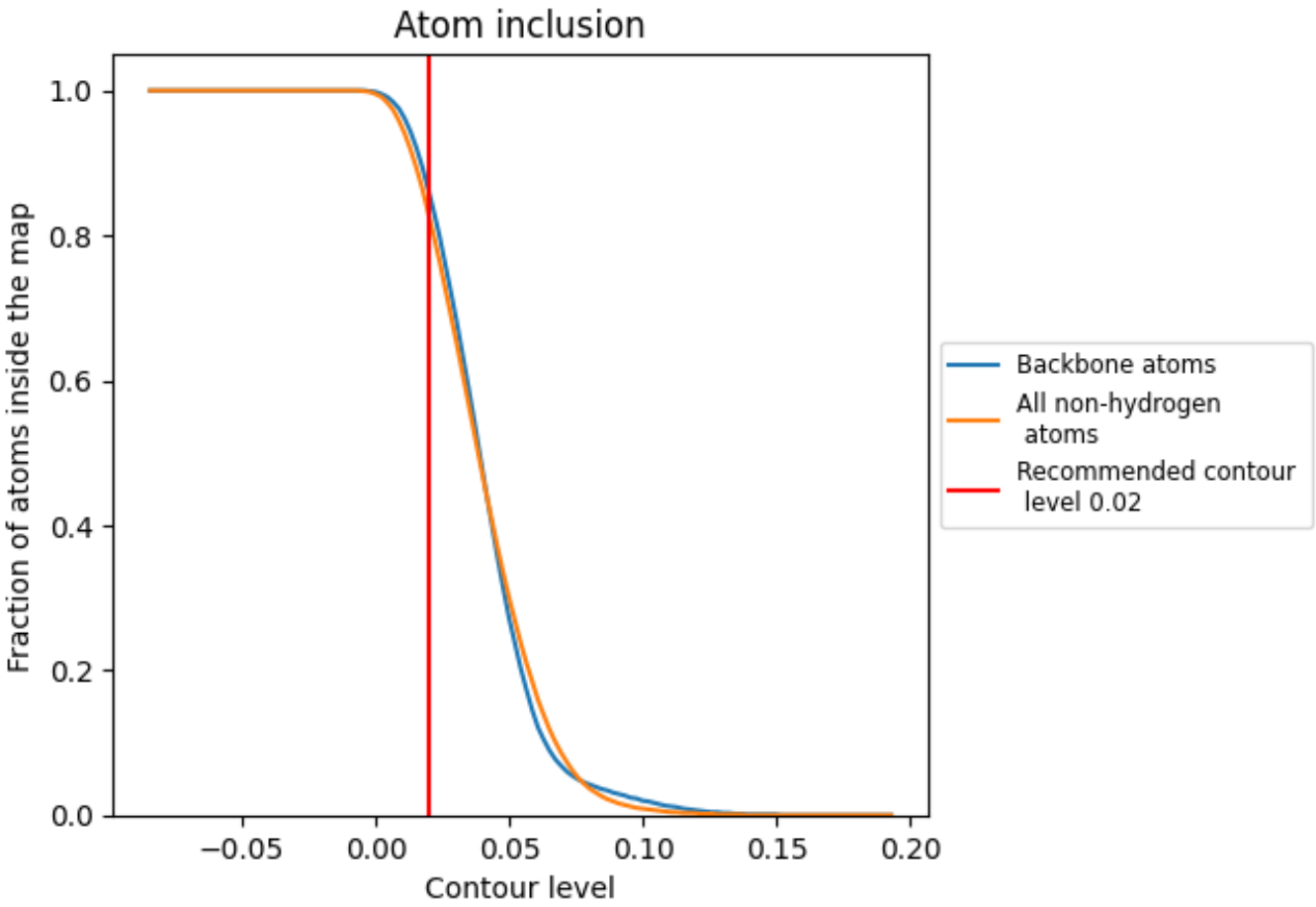
9.3 Atom inclusion mapped to coordinate model (i)



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, 86% of all backbone atoms, 83% 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	0.8260	0.6110
16	0.8340	0.5850
23	0.9010	0.6360
5	0.9120	0.6330
Dt	0.6600	0.5060
LB	0.9190	0.6980
LC	0.9040	0.6840
LD	0.8380	0.6450
LE	0.5930	0.5490
LF	0.6620	0.5650
LI	0.2060	0.3450
LM	0.9150	0.6860
LN	0.8810	0.6780
LO	0.8810	0.6780
LP	0.8880	0.6780
LQ	0.9300	0.6960
LR	0.8010	0.6230
LS	0.8120	0.6400
LT	0.9550	0.7040
LU	0.8460	0.6580
LV	0.8860	0.6860
LW	0.8100	0.6480
LX	0.7540	0.6000
LY	0.7980	0.6280
La	0.9070	0.6910
Lb	0.8850	0.6720
Lc	0.7320	0.6160
Ld	0.8760	0.6750
Le	0.3950	0.4400
Lf	0.8720	0.6720
Lg	0.7370	0.6320
Lh	0.9380	0.7040
Li	0.9350	0.7070
Lj	0.8870	0.6760
Pp	0.7860	0.6600



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Pt	0.5760	0.4740
SB	0.5870	0.5390
SC	0.6770	0.5830
SD	0.4870	0.4970
SE	0.7960	0.6380
SF	0.6290	0.5490
SG	0.3730	0.4470
SH	0.7970	0.6380
SI	0.5780	0.5260
SJ	0.5140	0.5030
SK	0.7300	0.5910
SL	0.6220	0.5750
SM	0.5150	0.5100
SN	0.6870	0.5870
SO	0.7810	0.6260
SP	0.6070	0.5510
SQ	0.6300	0.5700
SR	0.7460	0.6190
SS	0.5640	0.5370
ST	0.5780	0.5440
SU	0.5510	0.5530
mR	0.8080	0.6120