



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 01:33 PM EDT

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

This is a 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:

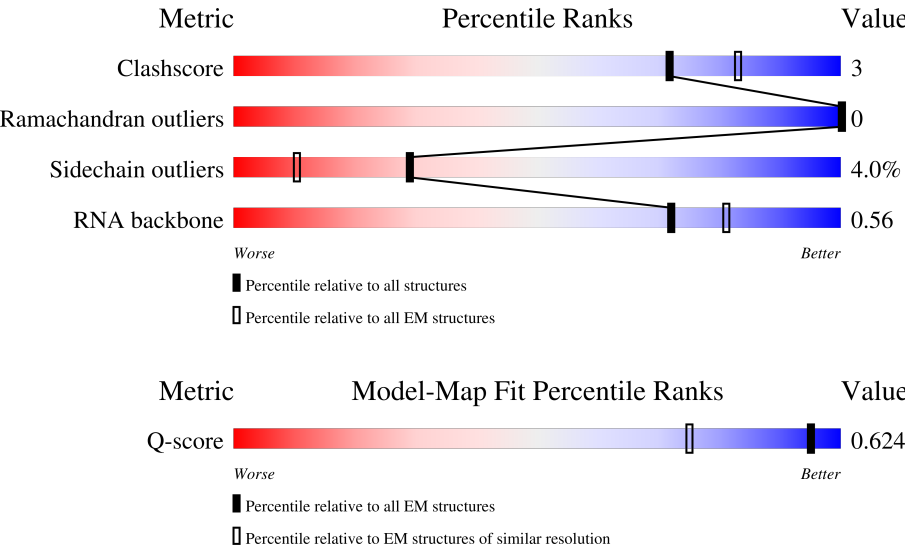
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.33 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	16	1542	5% 75% 23% •
2	SB	241	20% 79% 15% • 5%
3	SC	233	7% 75% 15% • 9%

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

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

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Mol	Chain	Length	Quality of chain
54	Li	65	91% 8%
55	Lj	38	5% 87% 13%
56	Pt	76	12% 63% 28% 5%
57	Pp	3	67% 33%
58	Dt	76	7% 38% 41% 17%

2 Entry composition [i](#)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SS	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	ST	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	SU	70	Total	C	N	O	S	1	0
			598	374	125	98	1		

- Molecule 22 is a RNA chain called mRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LF	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

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

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

- Molecule 31 is a protein called 50S ribosomal protein L10.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is a RNA chain called tRNA.

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

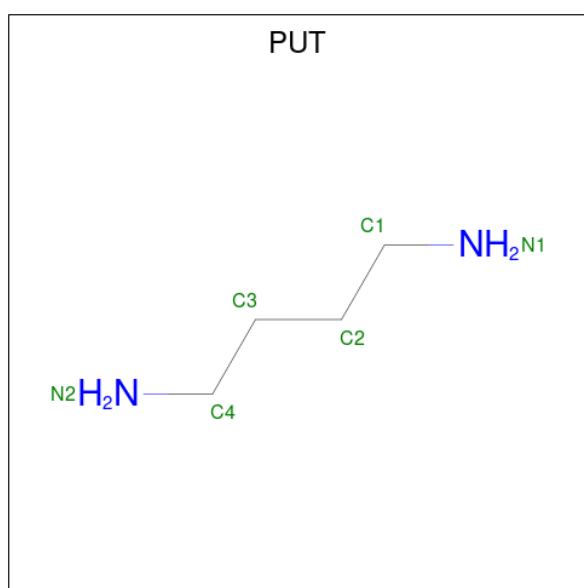
- Molecule 57 is a protein called Chains: Pp.

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

- Molecule 58 is a RNA chain called tRNA.

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

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



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

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

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

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

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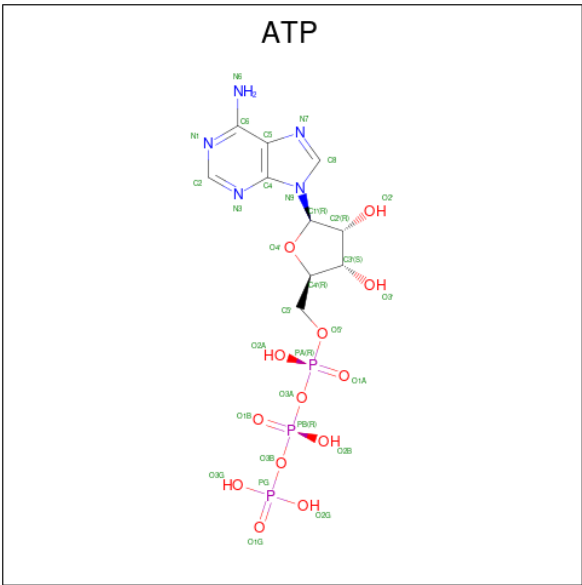
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Mol	Chain	Residues	Atoms		AltConf
60	LB	1	Total 1	Mg 1	0
60	LC	1	Total 1	Mg 1	0
60	LD	1	Total 1	Mg 1	0
60	LE	1	Total 1	Mg 1	0
60	Ld	1	Total 1	Mg 1	0
60	Lf	1	Total 1	Mg 1	0
60	Pt	1	Total 1	Mg 1	0
60	Dt	3	Total 3	Mg 3	0

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

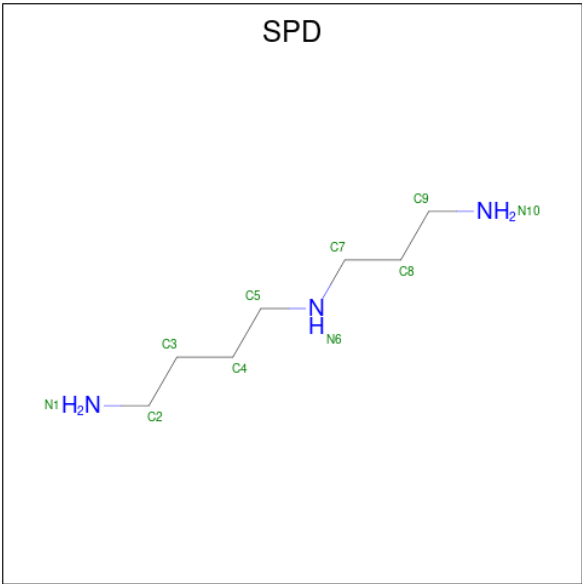
Mol	Chain	Residues	Atoms		AltConf
61	SB	1	Total 1	Zn 1	0
61	Le	1	Total 1	Zn 1	0
61	Lj	1	Total 1	Zn 1	0

- Molecule 62 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 63 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 64 is water.

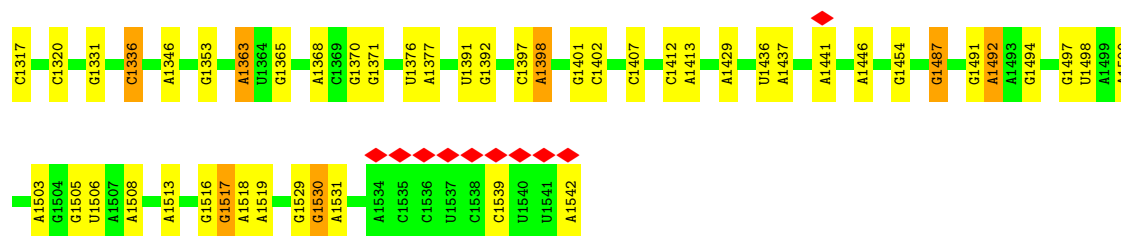
Mol	Chain	Residues	Atoms		AltConf
64	16	3	Total	O	0
			3	3	
64	23	41	Total	O	0
			41	41	
64	LB	3	Total	O	0
			3	3	
64	LC	1	Total	O	0
			1	1	
64	LT	1	Total	O	0
			1	1	
64	LY	1	Total	O	0
			1	1	

3 Residue-property plots

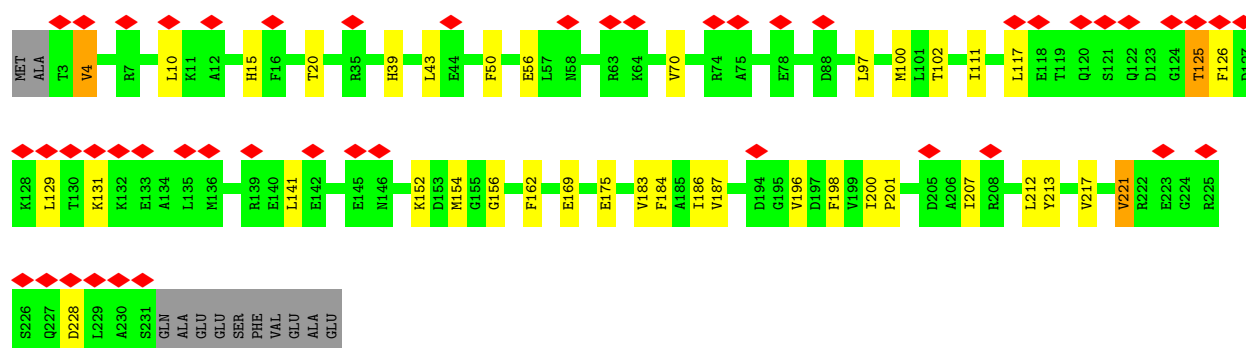
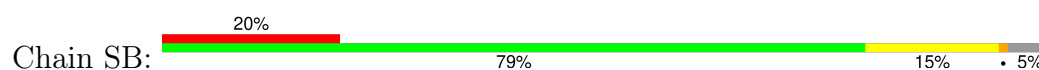
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

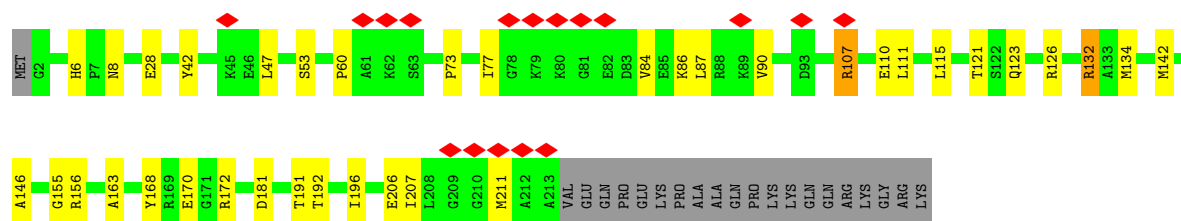
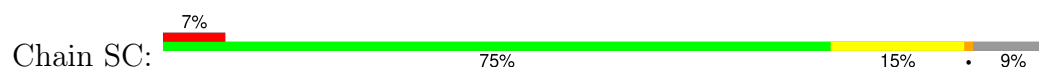




• Molecule 2: 30S ribosomal protein S2



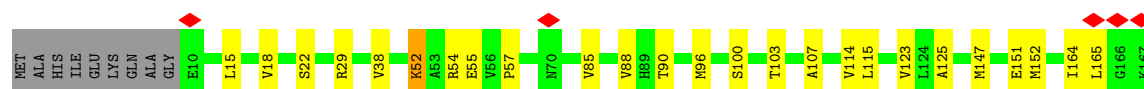
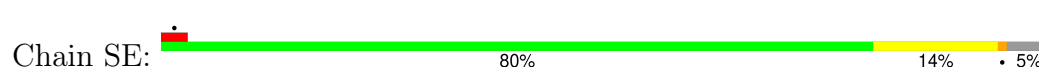
• Molecule 3: 30S ribosomal protein S3



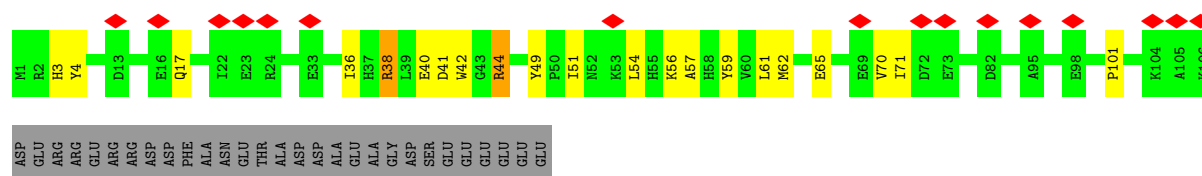
• Molecule 4: 30S ribosomal protein S4



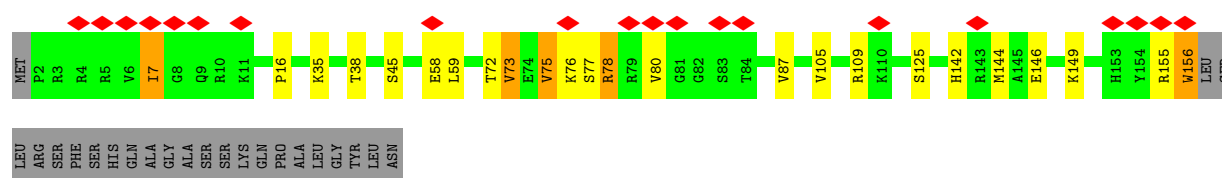
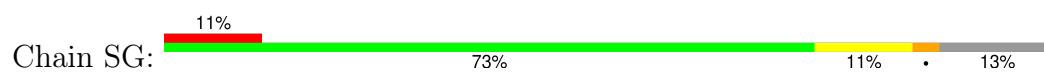
• Molecule 5: 30S ribosomal protein S5



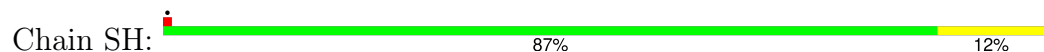
• Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7



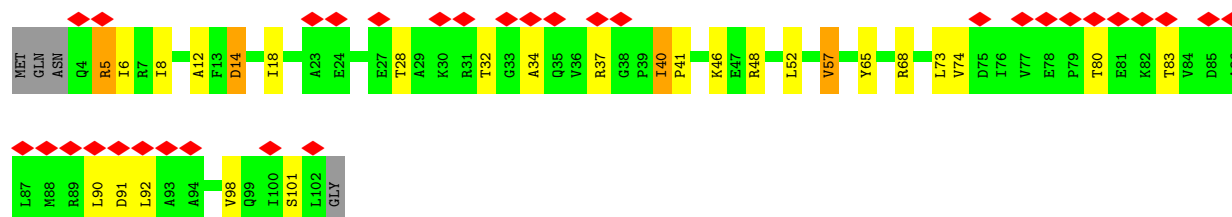
- Molecule 8: 30S ribosomal protein S8



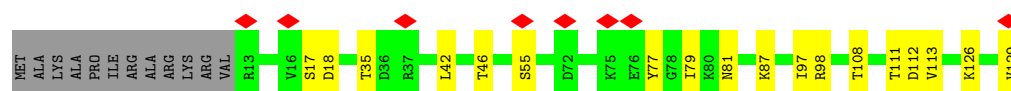
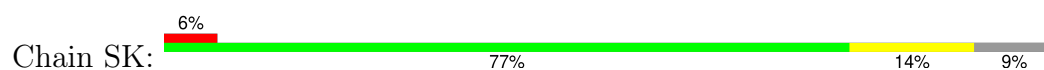
- Molecule 9: 30S ribosomal protein S9



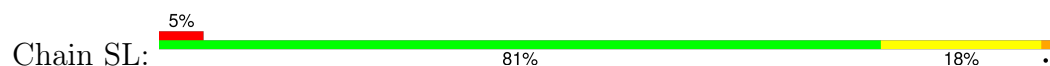
- Molecule 10: 30S ribosomal protein S10



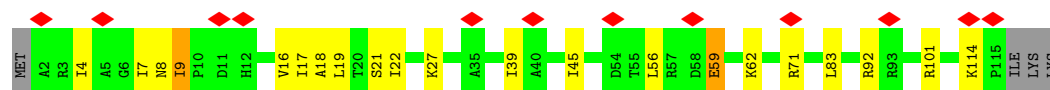
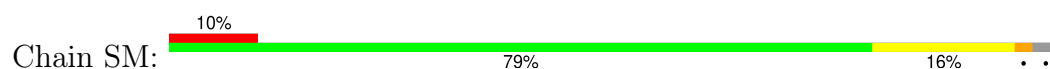
- Molecule 11: 30S ribosomal protein S11



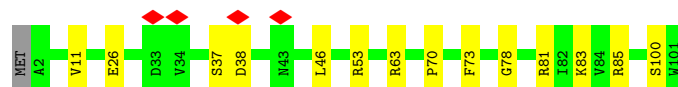
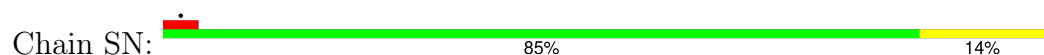
- Molecule 12: 30S ribosomal protein S12



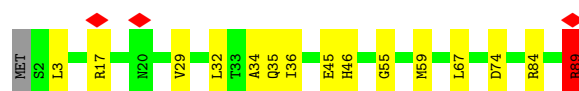
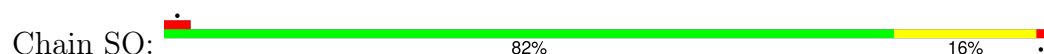
- Molecule 13: 30S ribosomal protein S13



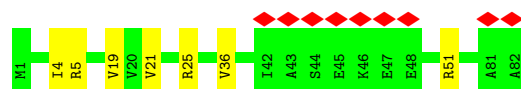
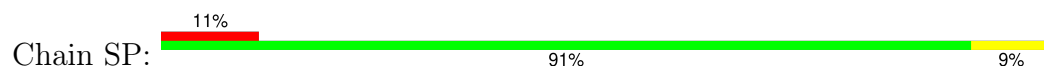
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16

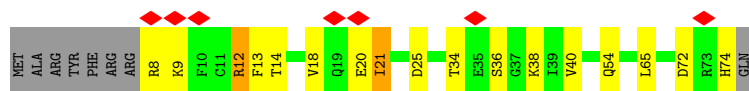


- Molecule 17: 30S ribosomal protein S17

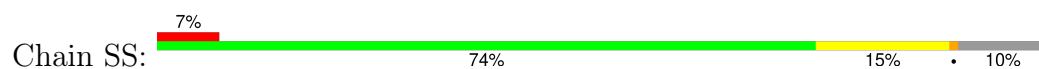




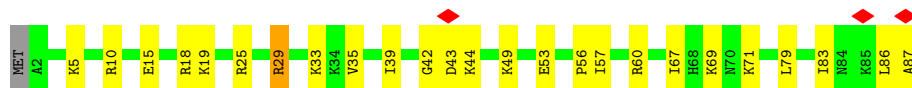
- Molecule 18: 30S ribosomal protein S18



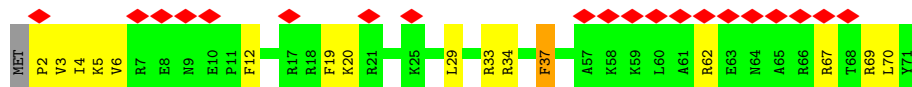
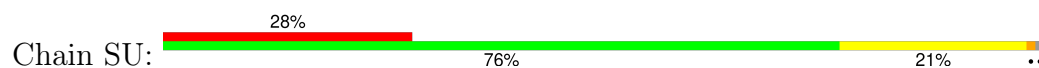
- Molecule 19: 30S ribosomal protein S19



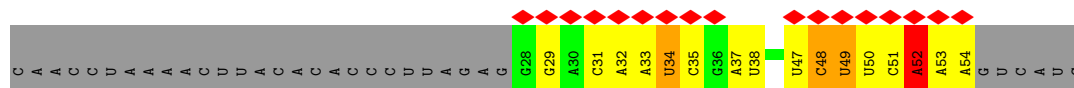
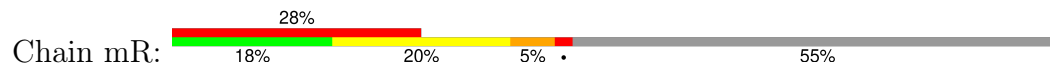
- Molecule 20: 30S ribosomal protein S20



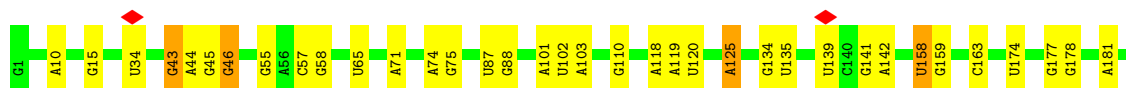
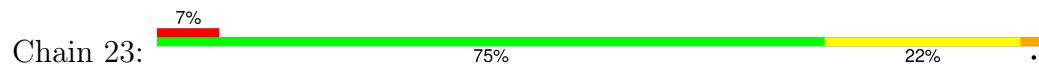
- Molecule 21: 30S ribosomal protein S21

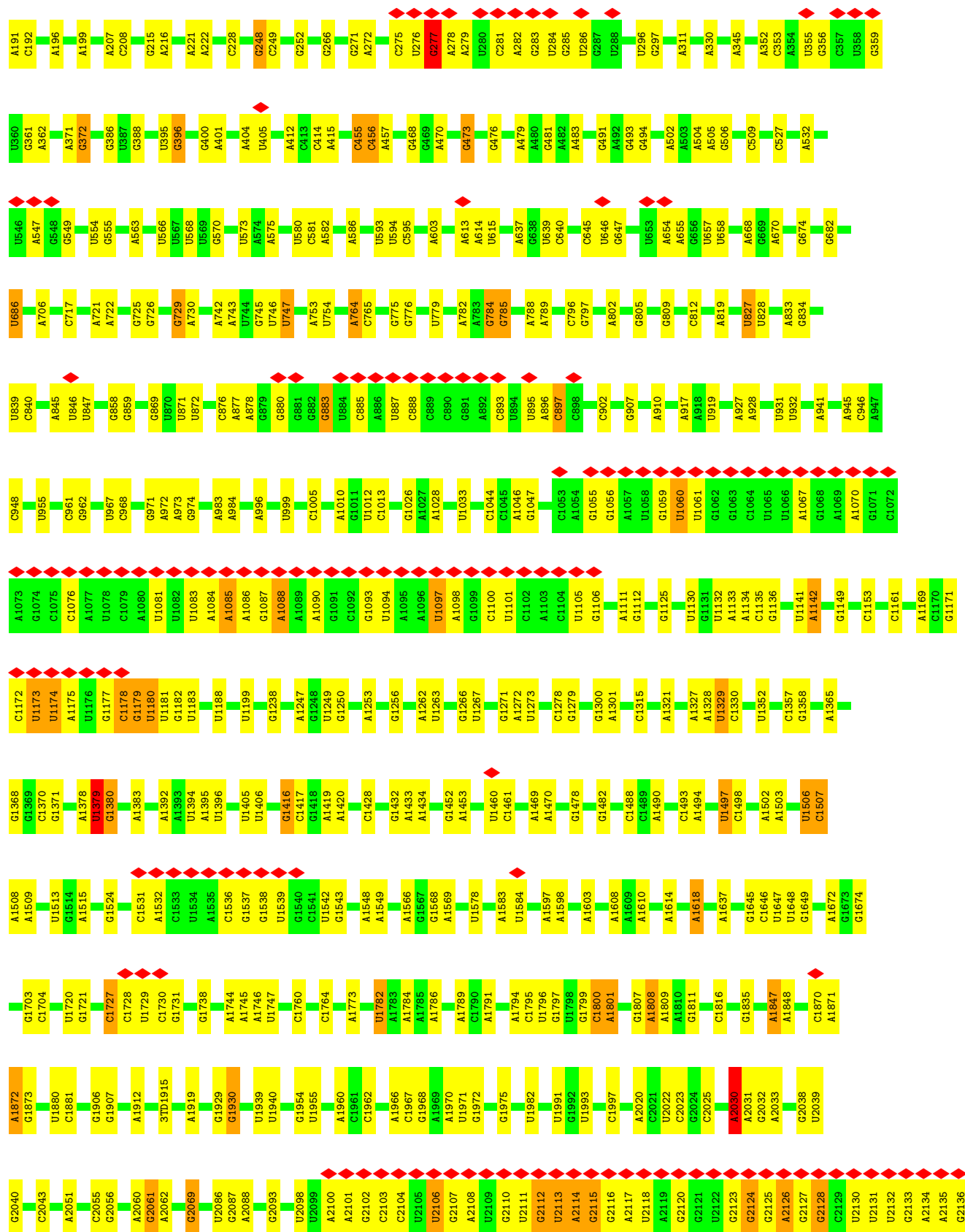


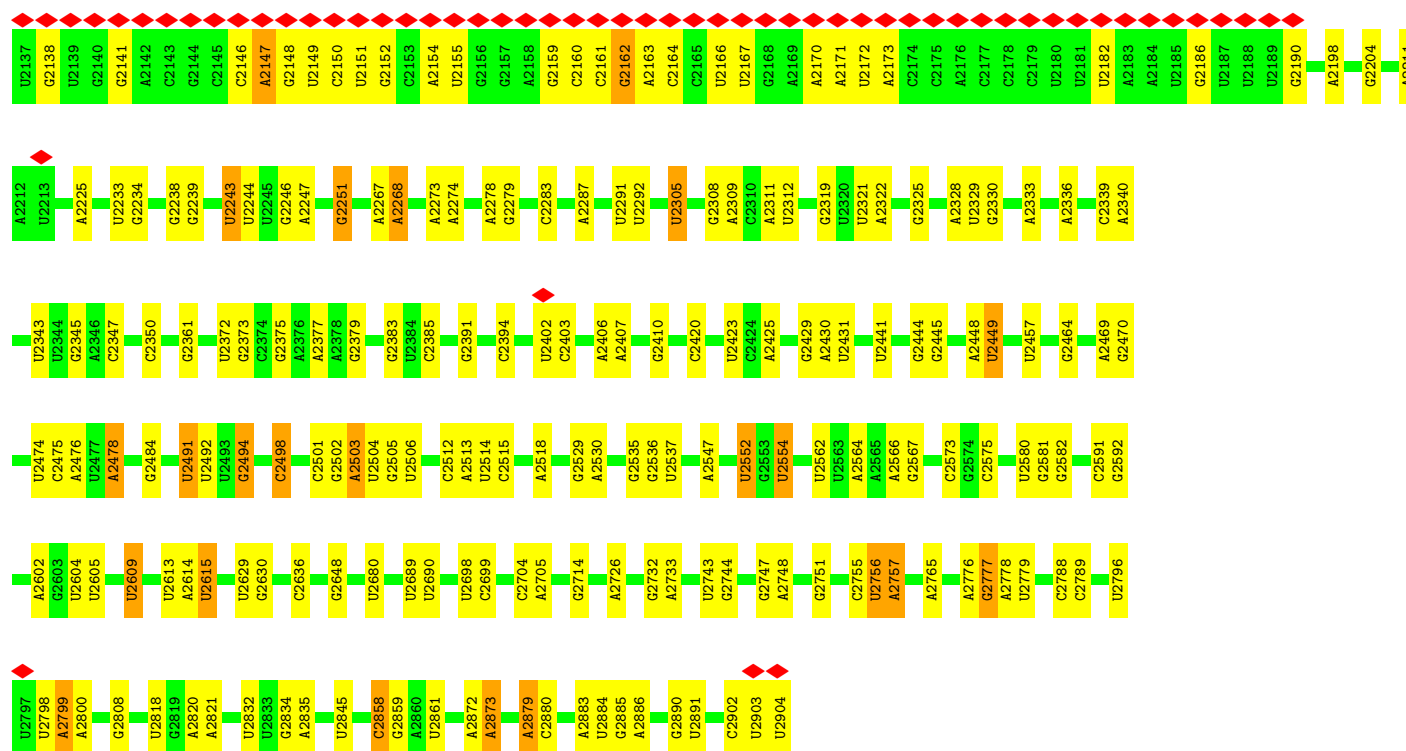
- Molecule 22: mRNA



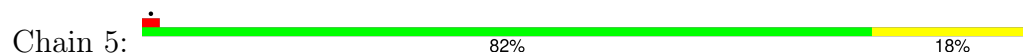
- Molecule 23: 23S rRNA



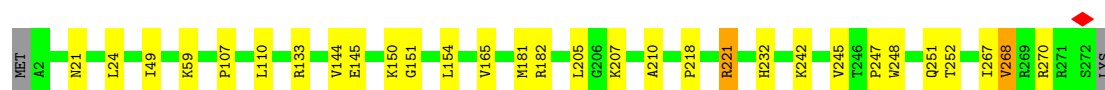




• Molecule 24: 5S rRNA



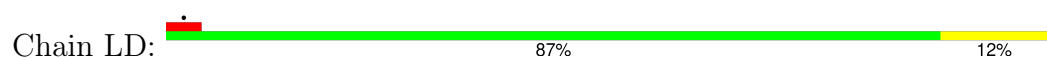
• Molecule 25: 50S ribosomal protein L2



• Molecule 26: 50S ribosomal protein L3

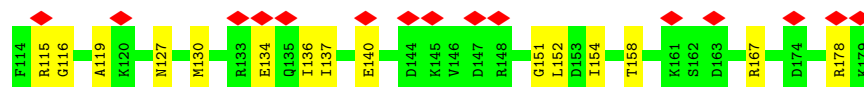
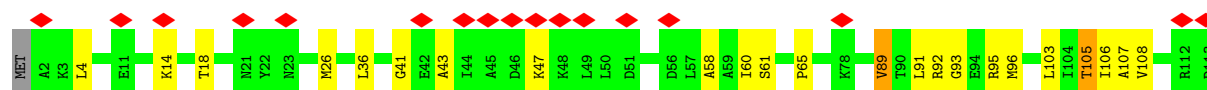
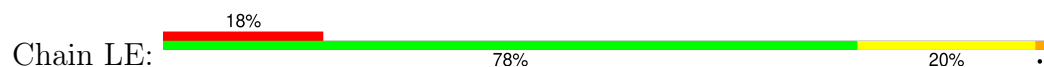


• Molecule 27: 50S ribosomal protein L4

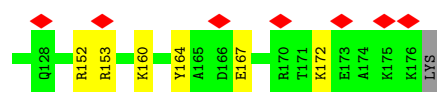
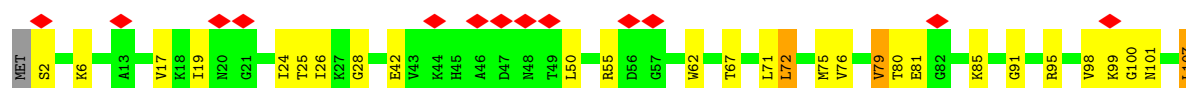
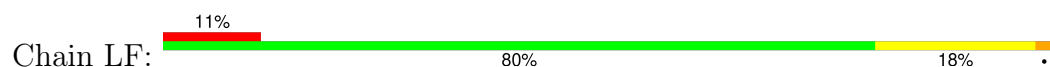




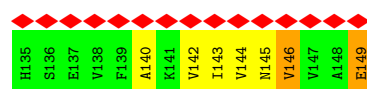
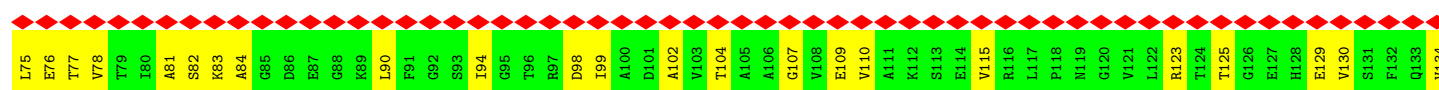
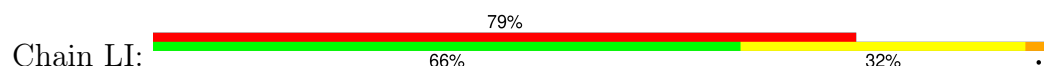
- Molecule 28: 50S ribosomal protein L5



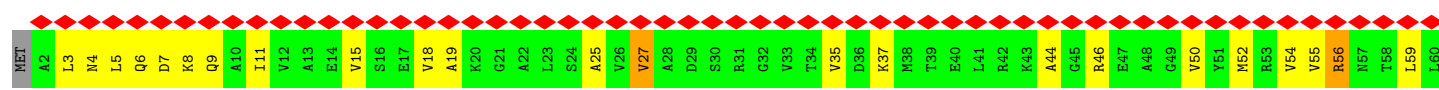
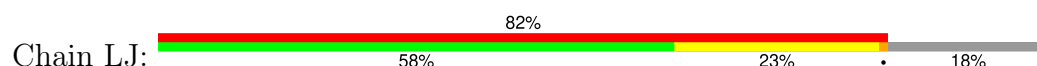
- Molecule 29: 50S ribosomal protein L6

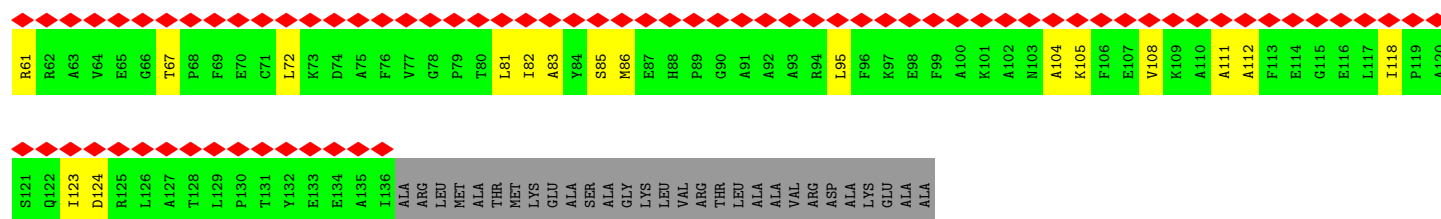


- Molecule 30: 50S ribosomal protein L9

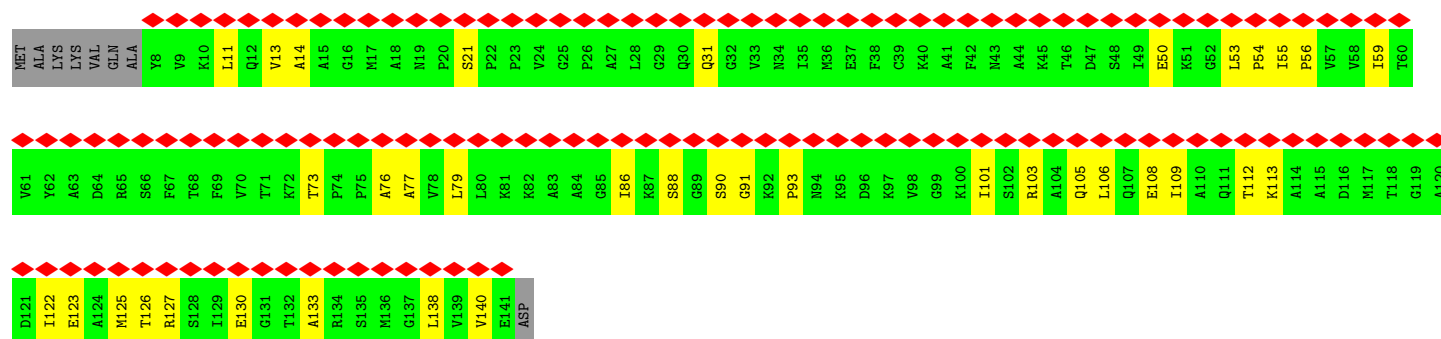


- Molecule 31: 50S ribosomal protein L10

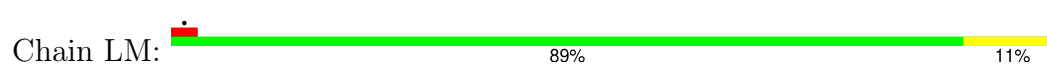




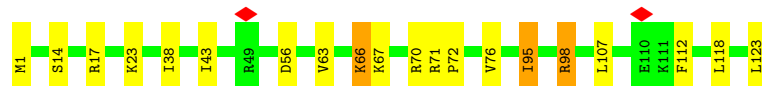
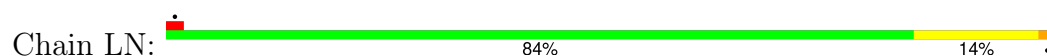
• Molecule 32: 50S ribosomal protein L11



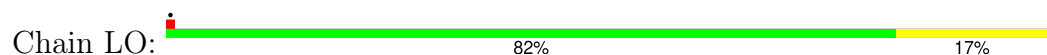
• Molecule 33: 50S ribosomal protein L13



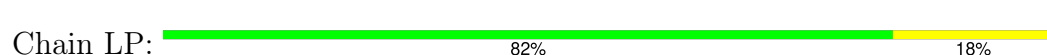
• Molecule 34: 50S ribosomal protein L14



• Molecule 35: 50S ribosomal protein L15

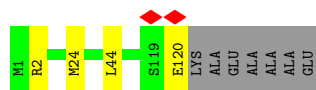


• Molecule 36: 50S ribosomal protein L16

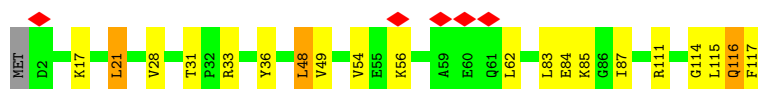
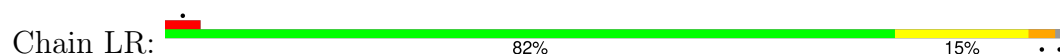




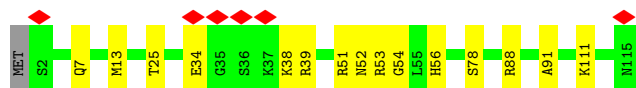
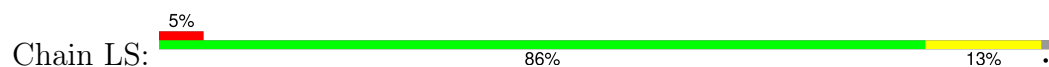
- Molecule 37: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L18



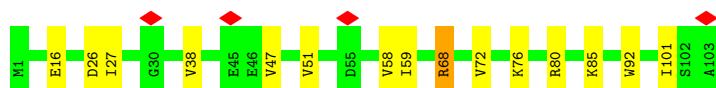
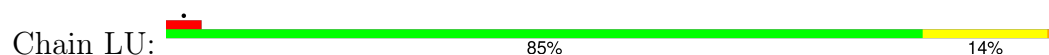
- Molecule 39: 50S ribosomal protein L19



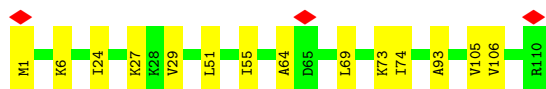
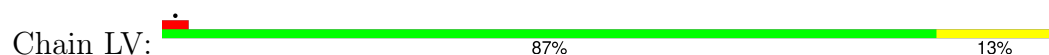
- Molecule 40: 50S ribosomal protein L20



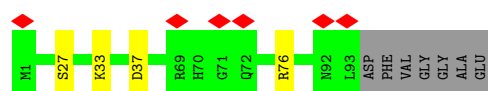
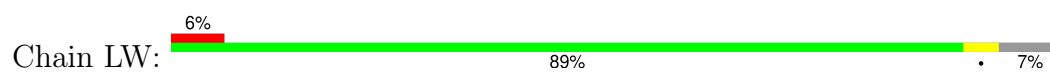
- Molecule 41: 50S ribosomal protein L21



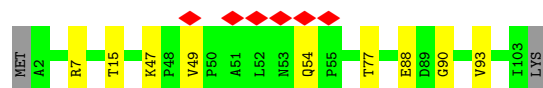
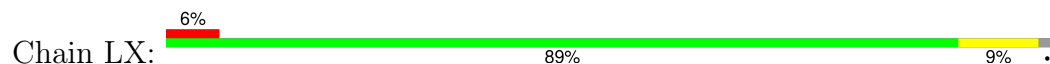
- Molecule 42: 50S ribosomal protein L22



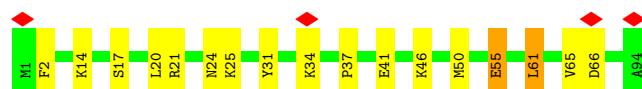
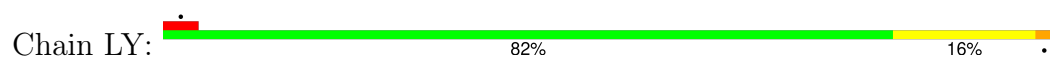
- Molecule 43: 50S ribosomal protein L23



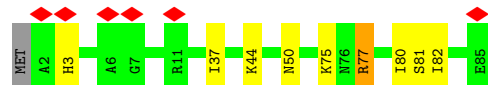
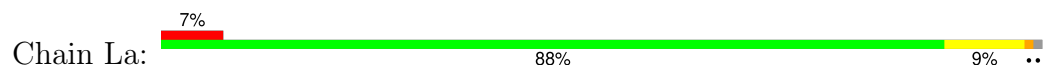
- Molecule 44: 50S ribosomal protein L24



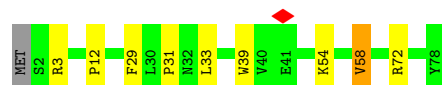
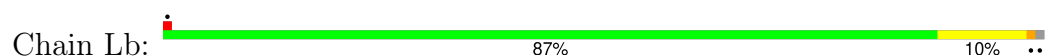
- Molecule 45: 50S ribosomal protein L25



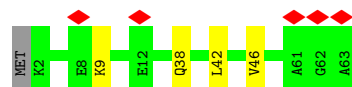
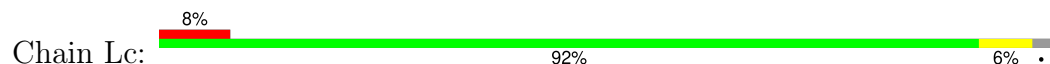
- Molecule 46: 50S ribosomal protein L27



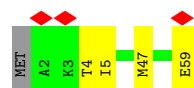
- Molecule 47: 50S ribosomal protein L28



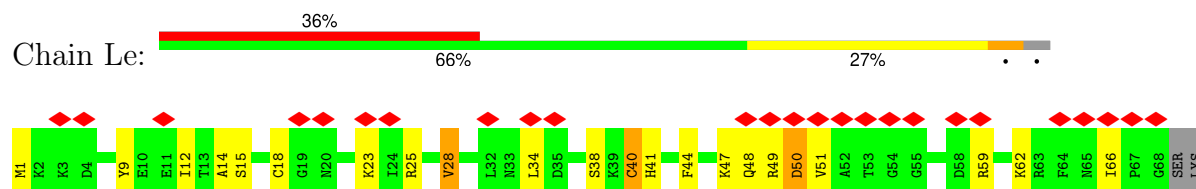
- Molecule 48: 50S ribosomal protein L29



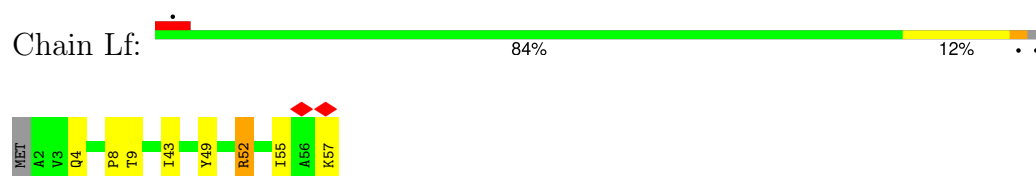
- Molecule 49: 50S ribosomal protein L30



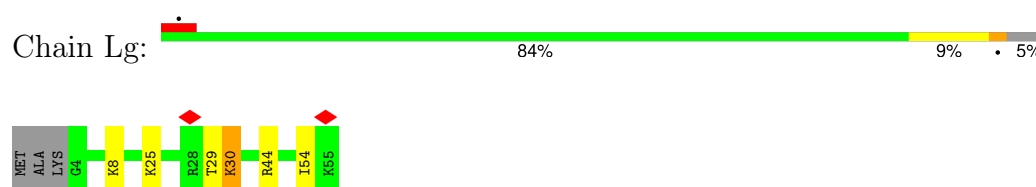
- Molecule 50: 50S ribosomal protein L31



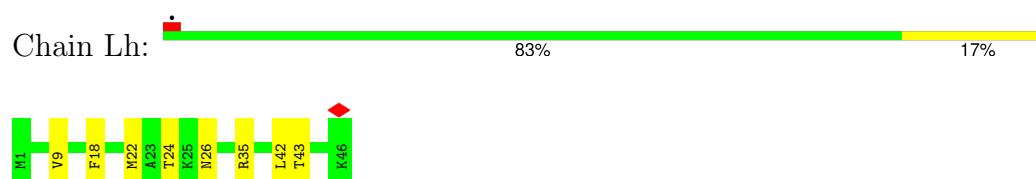
- Molecule 51: 50S ribosomal protein L32



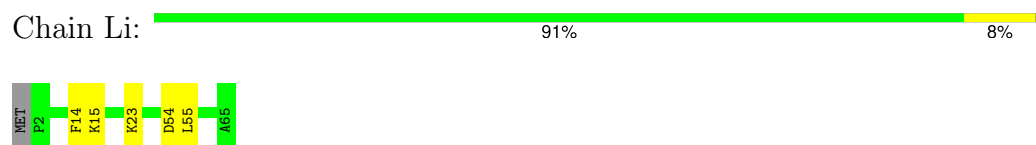
- Molecule 52: 50S ribosomal protein L33



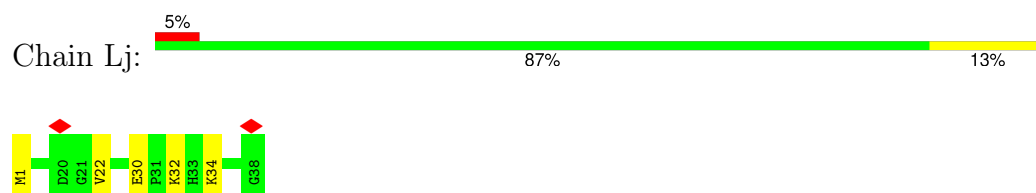
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35

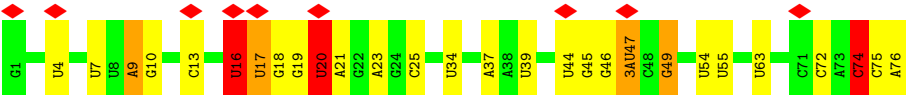


- Molecule 55: 50S ribosomal protein L36



- Molecule 56: tRNA

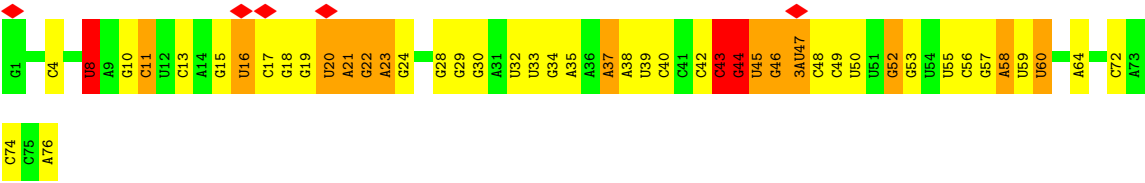




• Molecule 57: Chains: Pp



• Molecule 58: tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109769	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	87	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.235	Depositor
Minimum map value	-0.095	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	610.55994, 610.55994, 610.55994	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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

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

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

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

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	SG	78[A]	ARG	C-O	11.55	1.37	1.24
7	SG	78[B]	ARG	C-O	11.55	1.37	1.24
3	SC	132[A]	ARG	C-O	8.81	1.34	1.24
3	SC	132[B]	ARG	C-O	8.81	1.34	1.24
21	SU	37[A]	PHE	C-O	8.70	1.35	1.23
21	SU	37[B]	PHE	C-O	8.70	1.35	1.23
18	SR	13	PHE	C-O	-8.00	1.14	1.24
18	SR	12	ARG	C-O	-7.06	1.15	1.24
58	Dt	34	G	O3'-P	-6.38	1.51	1.61
58	Dt	30	G	O3'-P	-5.58	1.52	1.61
56	Pt	37	T6A	O3'-P	5.21	1.61	1.56
21	SU	37[A]	PHE	CA-C	5.10	1.58	1.52
21	SU	37[B]	PHE	CA-C	5.10	1.58	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	SC	132[A]	ARG	CA-C-O	11.16	132.38	120.55
3	SC	132[B]	ARG	CA-C-O	11.16	132.38	120.55
1	16	252	U	C2'-C3'-O3'	9.76	128.34	113.70
21	SU	37[A]	PHE	CA-C-O	9.41	131.74	121.11
21	SU	37[B]	PHE	CA-C-O	9.41	131.74	121.11
58	Dt	58	A	C1'-C2'-O2'	-8.99	98.31	111.80
23	23	158	U	C2'-C3'-O3'	8.52	126.47	113.70
58	Dt	45	U	C4'-C3'-O3'	8.49	125.74	113.00
9	SI	23	PRO	N-CA-C	-8.48	97.97	111.03
7	SG	78[A]	ARG	CA-C-O	8.12	130.81	120.57
7	SG	78[B]	ARG	CA-C-O	8.12	130.81	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	1847	A	C2'-C3'-O3'	8.00	125.70	113.70
58	Dt	43	C	C2'-C3'-O3'	7.91	125.56	113.70
58	Dt	34	G	C2'-C3'-O3'	-7.88	101.87	113.70
3	SC	60	PRO	N-CA-C	-7.56	100.07	111.41
22	mR	52	A	C2'-C3'-O3'	-7.52	98.22	109.50
23	23	2491	U	C2'-C3'-O3'	7.19	124.49	113.70
23	23	2858	C	C2'-C3'-O3'	7.09	124.33	113.70
23	23	827	U	C1'-C2'-O2'	-7.00	101.31	111.80
58	Dt	38	A	C2'-C3'-O3'	-6.94	103.28	113.70
58	Dt	45	U	C2'-C3'-O3'	6.94	124.10	113.70
23	23	1847	A	C3'-C2'-O2'	6.83	120.95	110.70
58	Dt	43	C	C4'-C3'-O3'	6.75	123.12	113.00
58	Dt	28	G	C2'-C3'-O3'	-6.45	104.02	113.70
58	Dt	60	U	C3'-C2'-O2'	-6.40	105.00	114.60
58	Dt	59	U	C4'-C3'-O3'	-6.25	103.62	113.00
23	23	43	G	P-O3'-C3'	6.20	129.50	120.20
58	Dt	52	G	C3'-C2'-O2'	6.17	119.96	110.70
58	Dt	35	A	C4'-C3'-O3'	-6.13	103.80	113.00
56	Pt	74	C	C3'-C2'-O2'	6.04	119.75	110.70
58	Dt	33	U	C3'-C2'-O2'	5.91	119.56	110.70
58	Dt	42	C	C2'-C3'-O3'	-5.91	104.84	113.70
23	23	1416	G	C2'-C3'-O3'	5.89	118.34	109.50
18	SR	13	PHE	CB-CA-C	5.85	120.50	110.79
58	Dt	53	G	C3'-C2'-O2'	5.76	119.34	110.70
10	SJ	57	VAL	N-CA-C	5.72	121.25	109.34
58	Dt	43	C	O4'-C4'-C3'	-5.65	98.35	104.00
28	LE	92	ARG	CA-C-O	-5.62	115.76	122.27
52	Lg	30	LYS	CA-C-O	-5.62	115.77	120.26
9	SI	12	ARG	CA-C-N	-5.61	115.76	122.44
9	SI	12	ARG	C-N-CA	-5.61	115.76	122.44
23	23	1379	U	C2'-C3'-O3'	-5.59	105.31	113.70
46	La	3	HIS	N-CA-C	5.58	117.05	111.07
23	23	277	G	C4'-C3'-O3'	5.57	117.76	109.40
22	mR	34	U	C2'-C3'-O3'	5.56	117.84	109.50
19	SS	7	LYS	N-CA-C	-5.53	106.58	113.38
3	SC	132[A]	ARG	O-C-N	-5.50	116.29	122.12
3	SC	132[B]	ARG	O-C-N	-5.50	116.29	122.12
30	LI	33	GLN	N-CA-C	-5.48	103.15	110.55
23	23	1416	G	C4'-C3'-O3'	5.47	117.61	109.40
22	mR	49	U	C4'-C3'-O3'	5.45	121.18	113.00
9	SI	93	SER	N-CA-C	-5.44	106.69	113.38
21	SU	37[A]	PHE	O-C-N	-5.43	116.13	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	SU	37[B]	PHE	O-C-N	-5.43	116.13	123.19
25	LB	133	ARG	N-CA-C	-5.43	105.91	112.54
28	LE	92	ARG	N-CA-C	5.41	118.80	111.17
44	LX	77	THR	N-CA-C	-5.38	106.72	113.28
3	SC	132[A]	ARG	N-CA-C	5.35	117.11	111.28
3	SC	132[B]	ARG	N-CA-C	5.35	117.11	111.28
1	16	572	A	C4'-C3'-O3'	-5.34	104.99	113.00
7	SG	146	GLU	N-CA-C	-5.33	106.91	113.41
32	LK	91	GLY	N-CA-C	-5.28	106.40	112.73
27	LD	172	ALA	CA-C-N	-5.23	113.97	122.65
27	LD	172	ALA	C-N-CA	-5.23	113.97	122.65
42	LV	64	ALA	N-CA-C	5.21	114.71	107.73
58	Dt	44	G	C2'-C3'-O3'	-5.19	105.92	113.70
48	Lc	38	GLN	N-CA-C	-5.11	107.22	113.50
50	Le	40	CYS	CB-CA-C	-5.09	100.48	110.11
44	LX	90	GLY	N-CA-C	-5.09	108.30	115.32
28	LE	60	ILE	N-CA-C	-5.08	105.37	110.30
48	Lc	9	LYS	N-CA-C	5.07	116.64	110.41
58	Dt	35	A	C1'-C2'-O2'	-5.04	100.84	108.40
58	Dt	45	U	O4'-C4'-C3'	-5.02	98.98	104.00
1	16	457	G	P-O3'-C3'	5.01	127.72	120.20

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	LB	221	ARG	Sidechain
27	LD	114	ARG	Sidechain
29	LF	153	ARG	Sidechain
34	LN	98	ARG	Sidechain
35	LO	69	ARG	Sidechain
44	LX	7	ARG	Sidechain
46	La	77	ARG	Sidechain
50	Le	62	LYS	Mainchain
3	SC	107	ARG	Sidechain
4	SD	104	ARG	Sidechain
5	SE	54	ARG	Sidechain
10	SJ	37	ARG	Sidechain
10	SJ	48	ARG	Sidechain
11	SK	98	ARG	Sidechain
15	SO	17	ARG	Sidechain
15	SO	84	ARG	Sidechain

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Mol	Chain	Res	Type	Group
15	SO	89[A]	ARG	Sidechain
15	SO	89[B]	ARG	Sidechain
16	SP	51	ARG	Sidechain
20	ST	29	ARG	Sidechain
20	ST	60	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	16	33092	0	16676	126	0
2	SB	1787	0	1812	27	0
3	SC	1666	0	1745	22	0
4	SD	1643	0	1707	9	0
5	SE	1166	0	1212	16	0
6	SF	862	0	864	14	0
7	SG	1236	0	1290	9	0
8	SH	979	0	1031	9	0
9	SI	1022	0	1070	17	0
10	SJ	795	0	836	21	0
11	SK	888	0	899	10	0
12	SL	957	0	1017	10	0
13	SM	883	0	941	14	0
14	SN	805	0	844	8	0
15	SO	730	0	759	8	0
16	SP	649	0	666	4	0
17	SQ	648	0	691	0	0
18	SR	555	0	578	7	0
19	SS	663	0	688	10	0
20	ST	670	0	719	17	0
21	SU	598	0	638	12	0
22	mR	640	0	323	13	0
23	23	62354	0	31384	212	0
24	5	2570	0	1301	6	0
25	LB	2082	0	2154	20	0
26	LC	1565	0	1616	13	0
27	LD	1552	0	1619	21	0
28	LE	1420	0	1457	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	LF	1313	0	1358	20	0
30	LI	1111	0	1148	26	0
31	LJ	1023	0	1050	21	0
32	LK	979	0	1028	21	0
33	LM	1129	0	1162	8	0
34	LN	947	0	1023	14	0
35	LO	1053	0	1129	21	0
36	LP	1086	0	1167	15	0
37	LQ	960	0	1000	3	0
38	LR	892	0	923	11	0
39	LS	917	0	962	9	0
40	LT	947	0	1019	3	0
41	LU	816	0	839	8	0
42	LV	857	0	922	8	0
43	LW	738	0	807	2	0
44	LX	779	0	831	3	0
45	LY	753	0	780	11	0
46	La	634	0	653	4	0
47	Lb	632	0	659	5	0
48	Lc	501	0	531	1	0
49	Ld	449	0	488	3	0
50	Le	533	0	530	14	0
51	Lf	444	0	458	6	0
52	Lg	427	0	464	4	0
53	Lh	377	0	418	5	0
54	Li	504	0	572	4	0
55	Lj	302	0	340	3	0
56	Pt	1635	0	840	13	0
57	Pp	28	0	33	0	0
58	Dt	1638	0	844	8	0
59	16	18	0	36	0	0
59	23	90	0	180	0	0
60	16	113	0	0	0	0
60	23	275	0	0	0	0
60	5	5	0	0	0	0
60	Dt	3	0	0	0	0
60	LB	1	0	0	0	0
60	LC	1	0	0	0	0
60	LD	1	0	0	0	0
60	LE	1	0	0	0	0
60	Ld	1	0	0	0	0
60	Lf	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	Pt	1	0	0	0	0
60	SD	1	0	0	0	0
60	mR	1	0	0	0	0
61	Le	1	0	0	0	0
61	Lj	1	0	0	0	0
61	SB	1	0	0	0	0
62	23	93	0	36	0	0
63	23	50	0	95	2	0
64	16	3	0	0	0	0
64	23	41	0	0	0	0
64	LB	3	0	0	0	0
64	LC	1	0	0	0	0
64	LT	1	0	0	0	0
64	LY	1	0	0	0	0
All	All	149590	0	100862	843	0

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

All (843) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:Pt:20:H2U:H4'	56:Pt:20:H2U:OP1	1.56	1.05
56:Pt:25:C:H5''	56:Pt:25:C:H6	1.32	0.95
34:LN:123:LEU:HD12	34:LN:123:LEU:OXT	1.74	0.87
35:LO:92:LEU:HD21	35:LO:106:GLU:HA	1.60	0.83
23:23:2377:A:O2'	38:LR:117:PHE:OXT	1.97	0.82
56:Pt:25:C:H5''	56:Pt:25:C:C6	2.14	0.82
32:LK:14:ALA:H	32:LK:54:PRO:HA	1.46	0.80
23:23:568:U:H1'	23:23:2030:6MZ:H9C1	1.70	0.73
22:mR:47[B]:U:H3'	22:mR:47[B]:U:C6	2.24	0.73
2:SB:207:ILE:HD12	2:SB:207:ILE:H	1.54	0.72
1:16:664:G:H22	1:16:741:G:H1	1.38	0.72
1:16:1086:U:H3	1:16:1099:G:H22	1.37	0.72
30:LI:78:VAL:HG11	30:LI:102:ALA:HB1	1.75	0.68
30:LI:149:GLU:OXT	30:LI:149:GLU:HG2	1.92	0.68
30:LI:90:LEU:HD11	30:LI:146:VAL:HG11	1.75	0.68
23:23:1178:C:OP2	23:23:1178:C:H6	1.77	0.68
3:SC:132[A]:ARG:NH1	22:mR:54:A:H62	1.91	0.68
38:LR:31:THR:HG22	38:LR:33:ARG:H	1.58	0.67
23:23:1093:G:H21	23:23:1098:A:H2	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LI:75:LEU:HD11	30:LI:107:GLY:HA3	1.77	0.66
36:LP:53:MET:HG3	36:LP:120:ALA:HB2	1.76	0.66
58:Dt:43:C:H2'	58:Dt:44:G:C8	2.31	0.66
23:23:2112:G:H5''	23:23:2115:G:H22	1.59	0.66
5:SE:15:LEU:HD11	5:SE:18:VAL:HG23	1.76	0.66
7:SG:75:VAL:HG21	7:SG:144:MET:HG2	1.78	0.66
1:16:1494:G:HO2'	23:23:1912:A:HO2'	1.39	0.66
50:Le:66:ILE:HD12	50:Le:66:ILE:O	1.96	0.66
2:SB:15:HIS:HB3	2:SB:43:LEU:HD21	1.77	0.65
8:SH:41:LYS:HD2	8:SH:48:ASP:HA	1.77	0.65
31:LJ:56:ARG:HB2	31:LJ:59:LEU:HD12	1.78	0.65
36:LP:64:TRP:HB2	36:LP:104:GLU:HB2	1.79	0.65
6:SF:40:GLU:HB2	6:SF:61:LEU:HB3	1.78	0.65
3:SC:132[A]:ARG:HH11	22:mR:54:A:H62	1.45	0.65
1:16:823:C:HO2'	8:SH:2:SER:N	1.96	0.63
7:SG:72:THR:HG23	7:SG:73:VAL:HG22	1.80	0.63
1:16:1238:A:H5'	1:16:1336:C:H41	1.63	0.63
23:23:2343:U:HO2'	23:23:2373:G:HO2'	1.44	0.63
25:LB:107:PRO:HD2	25:LB:110:LEU:HD22	1.81	0.63
35:LO:81:ASP:HB3	35:LO:100:ILE:HD12	1.81	0.62
10:SJ:32:THR:HG23	10:SJ:83:THR:HG22	1.79	0.62
23:23:2552:OMU:O5'	23:23:2552:OMU:H6	2.00	0.62
1:16:6:G:H1	5:SE:103:THR:HG21	1.64	0.62
23:23:1105:U:H2'	23:23:1106:G:C8	2.35	0.62
31:LJ:111:ALA:HB3	31:LJ:118:ILE:HB	1.81	0.62
23:23:1568:G:H4'	25:LB:59:LYS:HG2	1.82	0.62
51:Lf:43:ILE:HG22	51:Lf:49:TYR:HB2	1.82	0.62
2:SB:102:THR:HG23	2:SB:175:GLU:HB3	1.82	0.61
28:LE:65:PRO:HA	28:LE:89:VAL:HG23	1.82	0.61
31:LJ:61:ARG:NE	31:LJ:61:ARG:HA	2.15	0.61
1:16:209:U:H5'	1:16:210:C:H5	1.64	0.61
27:LD:111:GLU:HG2	35:LO:1:MET:HG2	1.83	0.61
1:16:1182:G:H5'	1:16:1184:G:H5''	1.83	0.61
29:LF:91:GLY:HA2	29:LF:160:LYS:HD2	1.83	0.61
1:16:376:G:H5''	16:SP:5:ARG:HB2	1.83	0.60
22:mR:47[B]:U:C6	22:mR:47[B]:U:C3'	2.84	0.60
19:SS:32:ARG:HA	19:SS:50:ALA:HB3	1.84	0.60
34:LN:1:MET:HG3	34:LN:67:LYS:HG2	1.83	0.60
41:LU:76:LYS:HB2	41:LU:85:LYS:HB3	1.84	0.60
1:16:1080:A:OP1	5:SE:52:LYS:HD2	2.02	0.60
2:SB:97:LEU:H	2:SB:100:MET:HE3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SI:47:VAL:HA	9:SI:50:GLN:HG3	1.82	0.59
23:23:1329:U:H5''	23:23:1330:C:H5	1.67	0.59
23:23:883:G:H1	23:23:893:C:H42	1.50	0.59
32:LK:106:LEU:HA	32:LK:109:ILE:HD12	1.84	0.59
11:SK:126:LYS:HG3	21:SU:37[B]:PHE:CD1	2.37	0.59
29:LF:107:LEU:HB3	29:LF:152:ARG:HD3	1.83	0.59
5:SE:38:VAL:HG11	5:SE:114:VAL:HG22	1.85	0.59
10:SJ:57:VAL:HG23	10:SJ:57:VAL:O	2.01	0.59
28:LE:36:LEU:HB3	28:LE:152:LEU:HD11	1.84	0.59
1:16:108:G:C6	20:ST:10:ARG:HD2	2.38	0.59
2:SB:111:ILE:HD12	2:SB:152:LYS:HA	1.85	0.59
23:23:682:G:H5'	53:Lh:26:ASN:ND2	2.17	0.59
40:LT:49:ASP:HA	40:LT:52:GLN:HB2	1.85	0.59
7:SG:16:PRO:HB2	9:SI:42:GLU:HG3	1.85	0.58
23:23:880:G:H1	23:23:897:C:H42	1.51	0.58
3:SC:110:GLU:CD	3:SC:110:GLU:H	2.12	0.58
19:SS:30:PRO:HA	19:SS:48:THR:HG22	1.84	0.58
1:16:677:U:H3	1:16:713:G:H22	1.51	0.58
20:ST:25:ARG:HG2	20:ST:29:ARG:NH2	2.18	0.58
35:LO:77:ILE:HD13	35:LO:108:ALA:HB1	1.85	0.58
2:SB:70:VAL:HG12	2:SB:169:GLU:CD	2.27	0.58
23:23:455:C:H3'	23:23:456:C:H5''	1.85	0.58
23:23:2788:C:H2'	23:23:2789:C:C6	2.38	0.58
30:LI:82:SER:HB2	30:LI:94:ILE:HD11	1.86	0.58
23:23:494:G:H4'	42:LV:6:LYS:HB2	1.86	0.58
45:LY:20:LEU:HD21	45:LY:41:GLU:HB2	1.86	0.58
1:16:83:C:H4'	1:16:84:U:H6	1.69	0.57
11:SK:87:LYS:HB2	11:SK:113:VAL:HG23	1.86	0.57
30:LI:78:VAL:CG1	30:LI:102:ALA:HB1	2.34	0.57
23:23:1178:C:HO2'	23:23:1179:G:H5''	1.68	0.57
30:LI:84:ALA:HB2	30:LI:90:LEU:HD23	1.86	0.57
55:Lj:1:MET:HE2	55:Lj:34:LYS:HG2	1.86	0.57
28:LE:105:THR:HA	50:Le:38:SER:HB3	1.87	0.57
36:LP:46:ILE:HD12	36:LP:69:PRO:HG3	1.87	0.57
20:ST:18:ARG:HH11	20:ST:18:ARG:HG2	1.70	0.56
2:SB:50:PHE:HA	2:SB:200:ILE:HD12	1.87	0.56
23:23:2135:A:H4'	23:23:2160:C:H4'	1.87	0.56
56:Pt:25:C:H6	56:Pt:25:C:C5'	2.11	0.56
2:SB:207:ILE:HD12	2:SB:207:ILE:N	2.19	0.56
10:SJ:52:LEU:HB2	14:SN:81:ARG:HD2	1.87	0.56
20:ST:57:ILE:HD12	20:ST:57:ILE:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LF:17:VAL:HG22	29:LF:26:ILE:HD12	1.86	0.56
36:LP:111:GLU:CD	36:LP:111:GLU:H	2.14	0.56
30:LI:6:LEU:HD21	30:LI:37:VAL:HG23	1.88	0.56
22:mR:37[B]:A:H2'	22:mR:38:U:C6	2.41	0.56
53:Lh:18:PHE:HA	53:Lh:43:THR:HG21	1.87	0.56
8:SH:75:ILE:HG13	8:SH:129:VAL:HG22	1.88	0.56
2:SB:217:VAL:O	2:SB:221:VAL:HG12	2.06	0.55
9:SI:65:ILE:HG21	9:SI:79:ILE:HG12	1.86	0.55
28:LE:106:ILE:HG13	50:Le:34:LEU:HD21	1.88	0.55
31:LJ:54:VAL:HG22	31:LJ:81:LEU:HA	1.88	0.55
19:SS:50:ALA:HB1	19:SS:57:HIS:HB3	1.88	0.55
46:La:75:LYS:HB2	46:La:77:ARG:HG3	1.88	0.55
33:LM:98:GLU:H	33:LM:98:GLU:CD	2.14	0.55
1:16:523:A:C2	12:SL:88:LYS:HB3	2.42	0.55
23:23:2575:C:H5'	26:LC:149:ASN:HB2	1.88	0.55
35:LO:57:LEU:HD22	54:Li:54:ASP:HB3	1.89	0.55
42:LV:73:LYS:HB2	42:LV:106:VAL:HB	1.88	0.55
25:LB:107:PRO:HG2	25:LB:110:LEU:HB2	1.88	0.55
23:23:1105:U:H2'	23:23:1106:G:H8	1.70	0.55
1:16:769:G:H4'	1:16:1513:A:H4'	1.88	0.55
4:SD:147:GLU:HA	4:SD:150:LYS:HG3	1.88	0.55
28:LE:61:SER:HB2	28:LE:91:LEU:HD21	1.89	0.55
23:23:2113:U:H2'	23:23:2114:A:H8	1.73	0.54
27:LD:184:ASP:HA	35:LO:2:ARG:HH12	1.72	0.54
23:23:2845:U:H5''	39:LS:52:ASN:O	2.07	0.54
5:SE:115:LEU:HD13	5:SE:123:VAL:HG11	1.88	0.54
6:SF:38:ARG:HD3	6:SF:40:GLU:HG3	1.89	0.54
23:23:2680:U:H5'	26:LC:194:PRO:HA	1.90	0.54
32:LK:101:ILE:HD11	32:LK:105:GLN:HG2	1.89	0.54
23:23:742:A:H2'	23:23:743:A:C8	2.42	0.54
1:16:216:U:H4'	1:16:463:U:H4'	1.90	0.54
9:SI:88:MET:O	9:SI:92:GLU:HG3	2.07	0.54
18:SR:36:SER:HA	18:SR:72:ASP:HB3	1.89	0.54
23:23:674:G:H1'	27:LD:69:ARG:HD2	1.89	0.54
27:LD:21:ARG:HD3	27:LD:106:LYS:HB3	1.90	0.54
27:LD:108:ILE:HG23	35:LO:1:MET:HE1	1.88	0.54
32:LK:31:GLN:HG2	32:LK:59:ILE:HD11	1.90	0.54
38:LR:54:VAL:HG23	38:LR:54:VAL:O	2.08	0.54
15:SO:32:LEU:O	15:SO:36:ILE:HG13	2.08	0.54
23:23:473:G:OP2	63:23:3020:SPD:N1	2.41	0.54
23:23:945:A:H1'	63:23:3019:SPD:H91	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:1038:C:H2'	1:16:1039:G:H8	1.73	0.54
2:SB:4:VAL:HG21	2:SB:212:LEU:HD21	1.89	0.54
20:ST:18:ARG:HG2	20:ST:18:ARG:NH1	2.23	0.54
2:SB:70:VAL:HG12	2:SB:169:GLU:OE2	2.08	0.53
9:SI:84:THR:HG23	9:SI:98:LEU:HD13	1.90	0.53
19:SS:30:PRO:HA	19:SS:48:THR:CG2	2.39	0.53
21:SU:34:ARG:HH11	21:SU:34:ARG:HB3	1.73	0.53
22:mR:48:C:H6	22:mR:48:C:O5'	1.91	0.53
30:LI:41:LYS:HA	30:LI:44:ILE:HD12	1.89	0.53
58:Dt:43:C:H2'	58:Dt:44:G:H8	1.71	0.53
50:Le:18:CYS:HB3	50:Le:40:CYS:SG	2.47	0.53
1:16:1078:U:C2	5:SE:90:THR:HG21	2.43	0.53
27:LD:1:MET:HG3	27:LD:14:VAL:HG23	1.91	0.53
23:23:476:G:H22	23:23:479:A:C5'	2.22	0.53
29:LF:25:THR:C	29:LF:26:ILE:HD13	2.33	0.53
1:16:160:A:H2'	1:16:161:A:O4'	2.09	0.53
23:23:2267:A:H5''	23:23:2268:A:H5'	1.91	0.53
32:LK:76:ALA:O	32:LK:79:LEU:HB2	2.08	0.53
45:LY:2:PHE:HB2	45:LY:61:LEU:HD12	1.90	0.53
23:23:1094:U:H1'	23:23:1097:U:H5	1.74	0.53
23:23:1478:G:H1	23:23:1513:U:H3	1.55	0.53
27:LD:119:ILE:HB	27:LD:187:VAL:HG22	1.91	0.53
47:Lb:31:PRO:HB2	47:Lb:33:LEU:HG	1.89	0.53
3:SC:142:MET:HG3	3:SC:170:GLU:HG2	1.91	0.53
58:Dt:50:U:H3	58:Dt:64:A:H61	1.56	0.53
3:SC:155:GLY:HA2	3:SC:163:ALA:HB1	1.91	0.53
52:Lg:44:ARG:HG3	52:Lg:44:ARG:HH11	1.74	0.53
1:16:404:G:N7	4:SD:2:ALA:HB3	2.24	0.53
31:LJ:27:VAL:HG13	31:LJ:82:ILE:HB	1.90	0.53
36:LP:53:MET:HE3	36:LP:63:ILE:HD13	1.90	0.52
23:23:2149:U:H2'	23:23:2150:C:C6	2.45	0.52
1:16:439:U:H4'	4:SD:121:LYS:HD2	1.92	0.52
1:16:640:A:HO2'	8:SH:107:SER:HG	1.57	0.52
20:ST:29:ARG:O	20:ST:33:LYS:HG3	2.10	0.52
1:16:337:G:H2'	1:16:338:A:C8	2.44	0.52
10:SJ:46:LYS:HG2	10:SJ:68:ARG:HG2	1.91	0.52
16:SP:4:ILE:HG12	16:SP:21:VAL:HG22	1.92	0.52
34:LN:123:LEU:OXT	34:LN:123:LEU:CD1	2.54	0.52
1:16:966:2MG:HM23	1:16:967:5MC:H1'	1.92	0.52
35:LO:132:ARG:O	35:LO:136:GLU:HG2	2.10	0.52
10:SJ:8:ILE:HB	10:SJ:74:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:SO:35:GLN:HB3	15:SO:59:MET:HE1	1.91	0.52
45:LY:20:LEU:HG	45:LY:25:LYS:HB2	1.91	0.52
1:16:1009:U:H3	1:16:1020:G:H1	1.59	0.51
25:LB:21:ASN:HB3	25:LB:24:LEU:HG	1.92	0.51
45:LY:46:LYS:O	45:LY:50:MET:HG3	2.10	0.51
54:Li:15:LYS:HB2	54:Li:23:LYS:HE2	1.92	0.51
23:23:2552:OMU:H2'	23:23:2554:U:OP2	2.10	0.51
25:LB:181:MET:HB2	25:LB:268:VAL:HG22	1.91	0.51
25:LB:232:HIS:HA	25:LB:242:LYS:HD2	1.93	0.51
1:16:82:G:H2'	1:16:84:U:H5	1.75	0.51
9:SI:40:GLY:HA2	9:SI:45:ARG:HH21	1.76	0.51
20:ST:35:VAL:O	20:ST:39:ILE:HG13	2.11	0.51
23:23:476:G:H22	23:23:479:A:H5''	1.76	0.51
25:LB:245:VAL:HG12	25:LB:251:GLN:HA	1.93	0.51
3:SC:73:PRO:O	3:SC:77:ILE:HG12	2.11	0.51
19:SS:15:LEU:O	19:SS:19:VAL:HG13	2.10	0.51
23:23:674:G:H1'	27:LD:69:ARG:CD	2.41	0.51
23:23:45:G:H5'	23:23:46:G:H5'	1.92	0.51
31:LJ:55:VAL:HB	31:LJ:59:LEU:HB2	1.91	0.51
2:SB:213:TYR:O	2:SB:217:VAL:HG12	2.09	0.51
22:mR:47[B]:U:H3'	22:mR:47[B]:U:H6	1.73	0.51
42:LV:74:ILE:HD12	42:LV:105:VAL:HG22	1.93	0.51
13:SM:71:ARG:CZ	28:LE:115:ARG:HD2	2.40	0.51
21:SU:5:LYS:HB2	21:SU:5:LYS:NZ	2.25	0.51
22:mR:47[B]:U:H2'	22:mR:48:C:H5	1.75	0.51
23:23:586:A:N1	23:23:809:G:O2'	2.39	0.51
34:LN:38:ILE:HD11	34:LN:112:PHE:HZ	1.75	0.51
10:SJ:92:LEU:HD12	10:SJ:98:VAL:HG21	1.93	0.51
1:16:56:U:H2'	1:16:57:G:C8	2.46	0.50
10:SJ:6:ILE:HD12	10:SJ:101:SER:O	2.11	0.50
31:LJ:61:ARG:HA	31:LJ:61:ARG:HE	1.74	0.50
1:16:1143:G:H2'	1:16:1144:G:H8	1.75	0.50
1:16:67:C:H2'	1:16:68:G:C8	2.45	0.50
1:16:1398:A:H5'	1:16:1401:G:H4'	1.93	0.50
23:23:2233:U:H2'	23:23:2234:G:C8	2.47	0.50
28:LE:58:ALA:HB2	28:LE:65:PRO:HD3	1.94	0.50
51:Lf:52:ARG:CZ	51:Lf:52:ARG:HB3	2.41	0.50
23:23:1789:A:OP1	25:LB:221:ARG:HG3	2.11	0.50
32:LK:13:VAL:HB	32:LK:54:PRO:HB3	1.94	0.50
50:Le:23:LYS:HA	50:Le:23:LYS:HE2	1.93	0.50
20:ST:42:GLY:HA2	20:ST:86:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:2151:U:H2'	23:23:2152:G:H8	1.77	0.50
1:16:1218:C:H2'	1:16:1219:A:C8	2.45	0.50
23:23:414:C:H2'	23:23:415:A:C8	2.47	0.50
23:23:1796:U:H2'	23:23:1797:G:C8	2.47	0.50
26:LC:184:ARG:NH1	39:LS:7:GLN:HE21	2.09	0.50
33:LM:98:GLU:O	33:LM:102:GLU:HG3	2.12	0.50
35:LO:81:ASP:HA	35:LO:84:LYS:HD2	1.92	0.50
1:16:652:U:O4	1:16:752:G:O2'	2.30	0.50
5:SE:151:GLU:H	5:SE:151:GLU:CD	2.19	0.50
23:23:1432:G:H2'	23:23:1433:A:C8	2.46	0.50
36:LP:108:VAL:HB	36:LP:112:LEU:HD23	1.93	0.50
18:SR:21:ILE:HG12	18:SR:54:GLN:HB3	1.93	0.49
39:LS:34:GLU:HA	39:LS:34:GLU:OE1	2.10	0.49
48:Lc:42:LEU:O	48:Lc:46:VAL:HG12	2.12	0.49
1:16:465:A:H1'	1:16:467:U:H1'	1.94	0.49
2:SB:207:ILE:H	2:SB:207:ILE:CD1	2.25	0.49
23:23:228:C:N4	23:23:2407:A:N3	2.60	0.49
23:23:1028:A:N6	23:23:1125:G:H2'	2.27	0.49
34:LN:14:SER:HB2	34:LN:95:ILE:HD11	1.94	0.49
23:23:2126:A:H61	23:23:2162:G:H1'	1.77	0.49
34:LN:17:ARG:HG3	34:LN:17:ARG:HH11	1.77	0.49
56:Pt:7:U:O2'	56:Pt:49:G:OP2	2.22	0.49
20:ST:44:LYS:NZ	20:ST:87:ALA:H	2.11	0.49
41:LU:16:GLU:HG2	41:LU:101:ILE:HD12	1.95	0.49
20:ST:53:GLU:O	20:ST:56:PRO:HD2	2.13	0.49
23:23:2159:G:H2'	23:23:2160:C:C6	2.48	0.49
23:23:468:G:H5''	27:LD:55:SER:HB2	1.94	0.49
32:LK:106:LEU:H	32:LK:106:LEU:HD23	1.78	0.49
42:LV:29:VAL:HB	42:LV:55:ILE:HD11	1.95	0.49
12:SL:114:ARG:HB3	12:SL:119:VAL:HB	1.95	0.49
47:Lb:3:ARG:O	47:Lb:12:PRO:HD3	2.12	0.49
26:LC:113:SER:HB3	26:LC:170:VAL:HG11	1.95	0.49
27:LD:122:GLU:HG3	27:LD:123:LYS:HG3	1.94	0.49
1:16:559:A:H4'	1:16:560:A:H3'	1.95	0.49
2:SB:129:LEU:C	2:SB:131:LYS:H	2.20	0.49
23:23:1801:A:OP2	25:LB:150:LYS:NZ	2.39	0.49
39:LS:25:THR:HB	39:LS:88:ARG:HB3	1.93	0.49
23:23:2394:C:H5''	35:LO:63:LYS:HD3	1.94	0.49
28:LE:134:GLU:HG3	28:LE:137:ILE:HG23	1.95	0.49
1:16:501:C:H2'	1:16:502:A:C8	2.48	0.48
1:16:1302:C:C6	13:SM:17:ILE:HG12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SC:155:GLY:O	3:SC:196:ILE:HG12	2.13	0.48
23:23:1199:U:H1'	40:LT:4:VAL:HG22	1.95	0.48
23:23:2530:A:N7	29:LF:172:LYS:NZ	2.61	0.48
28:LE:107:ALA:HB1	28:LE:137:ILE:HD12	1.95	0.48
28:LE:127:ASN:HD22	28:LE:158:THR:H	1.61	0.48
22:mR:47[B]:U:H6	22:mR:47[B]:U:O5'	1.95	0.48
23:23:355:U:H2'	23:23:356:G:H8	1.78	0.48
23:23:2420:C:H5''	52:Lg:8:LYS:HE2	1.95	0.48
37:LQ:24:MET:HG2	37:LQ:44:LEU:HD13	1.95	0.48
10:SJ:65:TYR:OH	14:SN:85:ARG:HG3	2.14	0.48
30:LI:4:ILE:HA	30:LI:17:ASP:O	2.12	0.48
23:23:2514:U:H2'	23:23:2515:C:C6	2.49	0.48
1:16:94:G:H4'	1:16:95:C:H5'	1.94	0.48
1:16:382:A:H2'	1:16:383:A:C8	2.48	0.48
13:SM:92:ARG:HG2	23:23:888:C:C6	2.49	0.48
23:23:1808:A:H3'	23:23:1809:A:C8	2.48	0.48
24:5:66:A:H61	24:5:107:G:H2'	1.77	0.48
1:16:222:C:H2'	1:16:223:A:H8	1.77	0.48
6:SF:101:PRO:HG2	18:SR:25:ASP:HB2	1.96	0.48
28:LE:119:ALA:HB1	28:LE:167:ARG:HE	1.79	0.48
8:SH:47:GLU:HG2	8:SH:64:LYS:HG3	1.96	0.48
9:SI:91:ASP:HB3	9:SI:94:LEU:HG	1.95	0.48
23:23:1357:C:H2'	23:23:1358:G:O4'	2.14	0.48
28:LE:26:MET:HE3	28:LE:26:MET:HB3	1.80	0.48
29:LF:2:SER:O	29:LF:6:LYS:HG2	2.14	0.48
29:LF:71:LEU:O	29:LF:75:MET:HG3	2.14	0.48
36:LP:49:ALA:HB1	36:LP:120:ALA:HB1	1.96	0.48
46:La:37:ILE:HG21	46:La:80:ILE:HG21	1.96	0.48
53:Lh:22:MET:HE3	53:Lh:22:MET:HB3	1.77	0.48
1:16:1220:G:P	14:SN:53:ARG:HH12	2.37	0.48
26:LC:184:ARG:HH12	39:LS:7:GLN:HE21	1.61	0.48
30:LI:9:VAL:O	30:LI:9:VAL:HG12	2.12	0.48
1:16:56:U:H2'	1:16:57:G:H8	1.79	0.48
1:16:689:C:OP1	11:SK:46:THR:OG1	2.30	0.48
13:SM:9:ILE:HG23	13:SM:18:ALA:HB1	1.96	0.48
23:23:1059:G:H3'	23:23:1060:U:H2'	1.96	0.48
30:LI:67:ALA:O	30:LI:70:GLU:HG3	2.12	0.48
1:16:1391:U:H2'	1:16:1392:G:C8	2.49	0.47
23:23:833:A:H2'	23:23:834:G:C8	2.49	0.47
23:23:2251:OMG:H1'	23:23:2251:OMG:HM23	1.68	0.47
23:23:2328:A:H2'	23:23:2329:U:C6	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:1225:A:N3	1:16:1225:A:H2'	2.28	0.47
10:SJ:28:THR:O	10:SJ:32:THR:HG22	2.14	0.47
22:mR:37[A]:A:H2'	22:mR:38:U:C6	2.49	0.47
41:LU:51:VAL:HG23	41:LU:51:VAL:O	2.13	0.47
49:Ld:5:ILE:CD1	49:Ld:59:GLU:HB3	2.45	0.47
11:SK:17:SER:HA	11:SK:79:ILE:HA	1.95	0.47
23:23:1180:U:H2'	23:23:1181:U:O4'	2.15	0.47
23:23:2478:A:H5'	55:Lj:32:LYS:HE2	1.95	0.47
1:16:147:G:H2'	1:16:148:G:C8	2.50	0.47
1:16:1225:A:H5''	1:16:1226:C:OP2	2.15	0.47
14:SN:63:ARG:NH2	14:SN:70:PRO:HG3	2.29	0.47
16:SP:19:VAL:HG12	16:SP:36:VAL:HG23	1.97	0.47
23:23:784:G:H5'	23:23:785:G:OP1	2.13	0.47
23:23:1141:U:H4'	23:23:1142:A:O4'	2.15	0.47
23:23:2106:U:H2'	23:23:2107:G:C8	2.50	0.47
56:Pt:20:H2U:H62	56:Pt:20:H2U:H5''	1.97	0.47
6:SF:51:ILE:O	6:SF:54:LEU:HB2	2.15	0.47
20:ST:49:LYS:O	20:ST:53:GLU:HG3	2.15	0.47
23:23:1263:U:O2'	51:Lf:8:PRO:HD2	2.14	0.47
33:LM:114:LEU:O	33:LM:118:MET:HG3	2.14	0.47
34:LN:66:LYS:HE2	34:LN:66:LYS:HB3	1.38	0.47
1:16:963:G:H21	10:SJ:57:VAL:CG1	2.28	0.47
23:23:779:U:OP1	25:LB:49:ILE:HG13	2.14	0.47
23:23:1542:U:H2'	23:23:1543:G:O4'	2.15	0.47
1:16:1106:G:H5''	3:SC:172:ARG:HG3	1.96	0.47
9:SI:6:TYR:HB2	9:SI:21:ILE:HB	1.96	0.47
23:23:2151:U:H2'	23:23:2152:G:C8	2.49	0.47
23:23:2291:U:H2'	23:23:2292:U:C6	2.49	0.47
28:LE:130:MET:HE3	28:LE:130:MET:HB2	1.82	0.47
37:LQ:24:MET:HG2	37:LQ:44:LEU:CD1	2.45	0.47
54:Li:14:PHE:O	54:Li:15:LYS:HD3	2.14	0.47
27:LD:111:GLU:O	27:LD:115:GLN:HG3	2.15	0.47
31:LJ:86:MET:HB3	31:LJ:86:MET:HE3	1.83	0.47
32:LK:50:GLU:HB3	32:LK:53:LEU:HG	1.97	0.47
49:Ld:4:THR:HG23	49:Ld:4:THR:O	2.15	0.47
58:Dt:23:A:H2'	58:Dt:24:G:C8	2.49	0.47
1:16:1144:G:N2	1:16:1146:A:H62	2.12	0.46
1:16:1187:G:H5'	9:SI:115:LYS:HE2	1.96	0.46
23:23:566:U:H5''	35:LO:29:LYS:HE3	1.96	0.46
31:LJ:56:ARG:H	31:LJ:59:LEU:HD12	1.79	0.46
1:16:946:A:H2'	1:16:947:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:2469:A:H4'	36:LP:55:ARG:HD3	1.96	0.46
56:Pt:75:C:H2'	56:Pt:76:A:C8	2.50	0.46
13:SM:83:LEU:HD11	19:SS:66:MET:HG2	1.98	0.46
28:LE:140:GLU:HG3	50:Le:28:VAL:HG22	1.96	0.46
30:LI:81:ALA:HB1	30:LI:149:GLU:HB2	1.97	0.46
35:LO:77:ILE:HD12	35:LO:77:ILE:N	2.30	0.46
41:LU:26:ASP:C	41:LU:27:ILE:HD13	2.40	0.46
1:16:662:U:H2'	1:16:663:A:C8	2.51	0.46
10:SJ:40:ILE:HD12	10:SJ:40:ILE:O	2.16	0.46
23:23:729:G:C6	25:LB:207:LYS:HB2	2.51	0.46
32:LK:55:ILE:HD12	32:LK:56:PRO:HD2	1.98	0.46
23:23:396:G:H1'	47:Lb:29:PHE:HB3	1.98	0.46
23:23:2799:A:O2'	23:23:2800:A:H5''	2.15	0.46
32:LK:127:ARG:O	32:LK:130:GLU:HG3	2.15	0.46
2:SB:183:VAL:HG12	2:SB:196:VAL:HG13	1.97	0.46
3:SC:156:ARG:H	3:SC:163:ALA:HA	1.81	0.46
23:23:1178:C:O2'	23:23:1179:G:H5''	2.15	0.46
23:23:1327:A:H2'	23:23:1328:A:O4'	2.16	0.46
23:23:1379:U:H6	23:23:1379:U:H5'	1.80	0.46
23:23:1720:U:H2'	23:23:1721:G:O4'	2.15	0.46
23:23:1800:C:P	25:LB:182:ARG:HH12	2.39	0.46
23:23:2494:G:O2'	36:LP:79:ALA:HA	2.16	0.46
23:23:2615:U:C2	51:Lf:4:GLN:HA	2.51	0.46
29:LF:28:GLY:HA3	29:LF:79:VAL:HG13	1.98	0.46
31:LJ:108:VAL:HG11	31:LJ:123:ILE:HD13	1.97	0.46
6:SF:4:TYR:CD2	6:SF:71:ILE:HG13	2.51	0.46
23:23:1672:A:C2	23:23:2582:G:H5'	2.51	0.46
28:LE:116:GLY:HA3	28:LE:178:ARG:HG2	1.98	0.46
29:LF:42:GLU:HB3	29:LF:55:ARG:NE	2.31	0.46
24:5:28:C:OP1	38:LR:36:TYR:OH	2.33	0.46
24:5:98:G:H1	45:LY:14:LYS:HB2	1.80	0.46
1:16:335:C:H2'	1:16:336:A:C8	2.51	0.46
6:SF:61:LEU:HD12	6:SF:62:MET:N	2.31	0.46
15:SO:32:LEU:HD22	15:SO:59:MET:HB3	1.97	0.46
23:23:1597:A:H5''	23:23:1598:A:H5'	1.97	0.46
23:23:1614:A:C2	42:LV:93:ALA:HB2	2.51	0.46
58:Dt:8:4SU:O2'	58:Dt:21:A:N1	2.45	0.46
1:16:384:G:H2'	1:16:385:C:C6	2.50	0.45
30:LI:72:ILE:HG23	30:LI:142:VAL:HG23	1.98	0.45
46:La:44:LYS:HE2	46:La:44:LYS:HB2	1.60	0.45
1:16:1038:C:H2'	1:16:1039:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SG:7:ILE:HD13	7:SG:7:ILE:HA	1.81	0.45
13:SM:59:GLU:HA	13:SM:62:LYS:HD2	1.98	0.45
23:23:668:A:H2'	23:23:670:A:H62	1.80	0.45
23:23:1727:C:H2'	23:23:1728:C:C6	2.51	0.45
23:23:1871:A:O2'	23:23:1872:A:H8	2.00	0.45
23:23:2233:U:H2'	23:23:2234:G:H8	1.81	0.45
30:LI:149:GLU:OXT	30:LI:149:GLU:CG	2.61	0.45
1:16:169:C:H2'	1:16:170:U:C6	2.51	0.45
23:23:593:U:H2'	23:23:594:U:C6	2.51	0.45
29:LF:24:ILE:HG21	29:LF:72:LEU:HD11	1.97	0.45
43:LW:76:ARG:HG2	43:LW:76:ARG:HH11	1.81	0.45
45:LY:55:GLU:CD	45:LY:55:GLU:H	2.25	0.45
10:SJ:34:ALA:HB2	10:SJ:83:THR:HG21	1.99	0.45
25:LB:267:ILE:HG21	25:LB:270:ARG:HD2	1.99	0.45
26:LC:3:GLY:HA3	26:LC:204:LYS:HG2	1.98	0.45
1:16:381:C:H2'	1:16:382:A:O4'	2.16	0.45
1:16:721:G:H4'	1:16:722:G:O4'	2.17	0.45
1:16:1004:A:H2'	1:16:1005:A:O4'	2.16	0.45
2:SB:117:LEU:HB3	2:SB:141:LEU:HD23	1.98	0.45
30:LI:72:ILE:HG23	30:LI:142:VAL:CG2	2.46	0.45
31:LJ:104:ALA:O	31:LJ:105:LYS:HD3	2.16	0.45
44:LX:49:VAL:O	44:LX:54:GLN:HA	2.17	0.45
3:SC:123:GLN:HG2	3:SC:126:ARG:HH22	1.80	0.45
11:SK:126:LYS:HE2	21:SU:37[B]:PHE:CZ	2.51	0.45
19:SS:17:LYS:HA	19:SS:17:LYS:HE3	1.99	0.45
23:23:281:C:H2'	23:23:282:A:C8	2.52	0.45
32:LK:73:THR:HG21	32:LK:113:LYS:HD3	1.99	0.45
32:LK:109:ILE:HG22	32:LK:113:LYS:HG3	1.98	0.45
50:Le:9:TYR:CE2	50:Le:25:ARG:HG2	2.52	0.45
1:16:1228:C:H5'	13:SM:114:LYS:O	2.16	0.45
5:SE:57:PRO:HD3	22:mR:52:A:H2	1.81	0.45
11:SK:42:LEU:HB3	11:SK:77:TYR:CE2	2.52	0.45
23:23:2134:A:H2'	23:23:2135:A:O4'	2.17	0.45
30:LI:104:THR:HG22	30:LI:109:GLU:HA	1.98	0.45
35:LO:132:ARG:HG3	35:LO:142:ILE:HD12	1.98	0.45
46:La:50:ASN:HB2	46:La:82:ILE:HB	1.97	0.45
1:16:665:A:H1'	1:16:733:G:H5'	1.98	0.45
23:23:87:U:H5'	23:23:88:G:H5''	1.99	0.45
25:LB:181:MET:HE3	25:LB:181:MET:HB3	1.92	0.45
30:LI:4:ILE:HD12	30:LI:4:ILE:O	2.16	0.45
31:LJ:25:ALA:HB3	31:LJ:112:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:LU:68:ARG:HD3	41:LU:92:TRP:CE2	2.52	0.45
43:LW:76:ARG:HG2	43:LW:76:ARG:NH1	2.32	0.45
1:16:1305:G:N2	1:16:1331:G:H1'	2.32	0.45
3:SC:134:MET:HE2	3:SC:168:TYR:CD1	2.52	0.45
11:SK:112:ASP:HB3	21:SU:2:PRO:HG2	1.98	0.45
23:23:191:A:H2'	23:23:192:C:C6	2.52	0.45
23:23:1067:A:O5'	23:23:1067:A:H8	1.99	0.45
45:LY:31:TYR:HB3	45:LY:37:PRO:HB3	1.98	0.45
6:SF:44:ARG:HG3	6:SF:44:ARG:HH11	1.82	0.45
31:LJ:52:MET:HE3	31:LJ:83:ALA:HB2	1.99	0.45
32:LK:86:ILE:HG22	32:LK:88:SER:H	1.82	0.45
45:LY:21:ARG:HA	45:LY:25:LYS:O	2.17	0.45
1:16:983:A:H5''	1:16:984:C:OP2	2.16	0.44
1:16:1371:G:O3'	9:SI:71:GLY:HA3	2.17	0.44
4:SD:107:PHE:CG	4:SD:145:ILE:HD11	2.52	0.44
9:SI:119:ARG:NH1	9:SI:119:ARG:HG2	2.33	0.44
23:23:2329:U:H2'	23:23:2330:G:C8	2.52	0.44
55:Lj:30:GLU:HG3	55:Lj:32:LYS:HB2	1.99	0.44
5:SE:85:VAL:HG11	5:SE:147:MET:HB2	1.99	0.44
23:23:372:G:O2'	23:23:400:G:O6	2.34	0.44
23:23:797:G:OP1	27:LD:55:SER:OG	2.31	0.44
23:23:1088:A:H2'	23:23:1088:A:N3	2.32	0.44
23:23:2127:G:H2'	23:23:2128:G:C8	2.53	0.44
23:23:2512:C:H2'	23:23:2513:A:O4'	2.17	0.44
29:LF:164:TYR:HB2	29:LF:167:GLU:HB2	1.99	0.44
30:LI:99:ILE:HG21	30:LI:115:VAL:HG11	1.99	0.44
56:Pt:25:C:C6	56:Pt:25:C:C5'	2.93	0.44
3:SC:181:ASP:HB2	3:SC:207:ILE:HG13	1.99	0.44
11:SK:97:ILE:HG22	21:SU:12:PHE:HZ	1.82	0.44
21:SU:4:ILE:HG12	21:SU:19:PHE:HD1	1.81	0.44
23:23:570:G:H2'	23:23:2030:6MZ:N7	2.32	0.44
25:LB:165:VAL:HG21	25:LB:181:MET:HE1	1.99	0.44
32:LK:122:ILE:O	32:LK:126:THR:HG23	2.17	0.44
1:16:109:A:C6	1:16:326:G:C6	3.05	0.44
5:SE:85:VAL:HG23	5:SE:96:MET:HE3	1.99	0.44
7:SG:72:THR:HG22	7:SG:142:HIS:CE1	2.52	0.44
23:23:796:C:H2'	23:23:797:G:C8	2.52	0.44
23:23:876:C:H2'	23:23:877:A:O4'	2.18	0.44
23:23:2698:U:H2'	23:23:2699:C:C6	2.53	0.44
29:LF:98:VAL:HG22	29:LF:100:GLY:H	1.83	0.44
30:LI:77:THR:HA	30:LI:143:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:LY:34:LYS:HA	45:LY:34:LYS:HD3	1.85	0.44
10:SJ:40:ILE:HD11	10:SJ:73:LEU:HD23	1.99	0.44
21:SU:3:VAL:C	21:SU:4:ILE:HD13	2.43	0.44
23:23:2757:A:N1	29:LF:67:THR:OG1	2.47	0.44
27:LD:145:ASP:HB3	27:LD:184:ASP:HB2	2.00	0.44
38:LR:111:ARG:HA	38:LR:115:LEU:O	2.18	0.44
1:16:68:G:H5'	1:16:171:A:O2'	2.17	0.44
1:16:162:A:C5	1:16:163:C:H1'	2.53	0.44
6:SF:41:ASP:OD1	6:SF:41:ASP:C	2.61	0.44
23:23:657:U:H2'	23:23:658:U:C6	2.52	0.44
23:23:2747:G:O6	23:23:2755:C:H5''	2.18	0.44
30:LI:74:ALA:O	30:LI:75:LEU:C	2.60	0.44
1:16:881:G:P	12:SL:9:ARG:HH22	2.41	0.44
1:16:1074:G:O2'	1:16:1101:A:N1	2.41	0.44
23:23:248:G:OP2	23:23:249:C:H5''	2.17	0.44
23:23:296:U:H2'	23:23:297:G:C8	2.52	0.44
27:LD:29:HIS:CE1	35:LO:8:PRO:HG3	2.52	0.44
28:LE:95:ARG:CZ	50:Le:1:MET:HE1	2.47	0.44
29:LF:2:SER:HB2	29:LF:62:TRP:CE3	2.52	0.44
31:LJ:9:GLN:HA	31:LJ:9:GLN:NE2	2.33	0.44
33:LM:110:PRO:O	33:LM:115:GLY:HA3	2.17	0.44
44:LX:88:GLU:HG3	44:LX:93:VAL:HG21	1.99	0.44
1:16:714:G:H2'	1:16:715:A:C8	2.53	0.44
1:16:1187:G:N3	14:SN:100:SER:OG	2.50	0.44
2:SB:20:THR:HA	2:SB:39:HIS:CD2	2.52	0.44
23:23:2273:A:H2'	23:23:2274:A:C8	2.53	0.44
28:LE:41:GLY:C	28:LE:43:ALA:H	2.24	0.44
28:LE:130:MET:HG3	28:LE:154:ILE:HB	1.99	0.44
40:LT:58:ARG:HA	40:LT:61:TRP:CE3	2.52	0.44
53:Lh:35:ARG:HG3	53:Lh:42:LEU:HD11	2.00	0.44
1:16:154:U:H2'	1:16:155:A:C8	2.53	0.44
1:16:335:C:H2'	1:16:336:A:H8	1.83	0.44
12:SL:73:ASN:HD21	12:SL:105:SER:HB3	1.83	0.44
50:Le:12:ILE:C	50:Le:12:ILE:HD12	2.43	0.44
51:Lf:55:ILE:HG22	51:Lf:57:LYS:H	1.82	0.44
1:16:6:G:H4'	1:16:298:A:H4'	1.99	0.43
16:SP:25:ARG:HE	16:SP:25:ARG:HB2	1.55	0.43
23:23:743:A:OP1	26:LC:135:GLY:HA2	2.18	0.43
28:LE:103:LEU:O	28:LE:108:VAL:HG23	2.18	0.43
34:LN:71:ARG:HB3	34:LN:72:PRO:HD2	1.99	0.43
35:LO:77:ILE:CD1	35:LO:108:ALA:HB1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Le:14:ALA:HB1	50:Le:34:LEU:HD11	2.00	0.43
50:Le:41:HIS:HB3	50:Le:44:PHE:CD1	2.53	0.43
1:16:477:C:H2'	1:16:478:A:C8	2.54	0.43
6:SF:44:ARG:HA	6:SF:57:ALA:O	2.18	0.43
9:SI:19:VAL:HG22	9:SI:65:ILE:HD13	2.00	0.43
15:SO:89[B]:ARG:HE	15:SO:89[B]:ARG:HB2	1.33	0.43
23:23:1405:U:H2'	23:23:1406:U:C6	2.53	0.43
23:23:1794:A:H2'	23:23:1795:C:C6	2.53	0.43
23:23:2038:G:H2'	23:23:2039:U:O4'	2.18	0.43
23:23:2086:U:H2'	23:23:2087:G:C8	2.53	0.43
38:LR:83:LEU:HD11	38:LR:114:GLY:HA3	2.00	0.43
1:16:542:G:H5'	4:SD:39:GLY:HA3	2.00	0.43
1:16:1034:G:H2'	1:16:1035:A:H8	1.83	0.43
12:SL:76:GLU:HG3	12:SL:77:HIS:CE1	2.53	0.43
23:23:57:C:H2'	23:23:58:G:O4'	2.19	0.43
26:LC:13:ARG:HH21	39:LS:56:HIS:HA	1.83	0.43
31:LJ:72:LEU:HD23	31:LJ:72:LEU:H	1.83	0.43
45:LY:65:VAL:HG13	45:LY:65:VAL:O	2.17	0.43
50:Le:47:LYS:HA	50:Le:49:ARG:HH11	1.83	0.43
56:Pt:20:H2U:H61	56:Pt:20:H2U:H3'	2.00	0.43
1:16:95:C:H2'	1:16:96:U:C6	2.52	0.43
2:SB:70:VAL:CG1	2:SB:169:GLU:CD	2.90	0.43
27:LD:111:GLU:CG	35:LO:1:MET:HG2	2.47	0.43
1:16:1308:U:H2'	1:16:1309:G:H8	1.84	0.43
2:SB:187:VAL:O	2:SB:201:PRO:HA	2.19	0.43
3:SC:47:LEU:HD21	3:SC:87:LEU:HD11	1.99	0.43
7:SG:59:LEU:HD12	7:SG:59:LEU:HA	1.89	0.43
7:SG:87:VAL:HG11	7:SG:156:TRP:HA	2.01	0.43
7:SG:105:VAL:O	7:SG:109:ARG:HG3	2.19	0.43
8:SH:108:LYS:HG2	8:SH:121:LEU:HD11	2.00	0.43
9:SI:12:ARG:HD3	9:SI:107:ASP:HB3	2.01	0.43
14:SN:83:LYS:HD3	14:SN:83:LYS:HA	1.80	0.43
21:SU:34:ARG:HB3	21:SU:34:ARG:NH1	2.33	0.43
23:23:2756:U:H1'	23:23:2757:A:H5''	2.01	0.43
52:Lg:25:LYS:HE2	52:Lg:30:LYS:O	2.17	0.43
1:16:122:G:OP2	1:16:122:G:H8	2.01	0.43
1:16:473:U:H2'	1:16:474:G:C8	2.53	0.43
1:16:792:A:O2'	1:16:794:A:N7	2.45	0.43
27:LD:127:GLU:H	27:LD:127:GLU:CD	2.26	0.43
32:LK:123:GLU:C	32:LK:123:GLU:CD	2.87	0.43
35:LO:76:GLU:C	35:LO:77:ILE:HD12	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Lg:29:THR:O	52:Lg:30:LYS:C	2.61	0.43
1:16:1070:U:H2'	1:16:1071:C:C6	2.54	0.43
1:16:1144:G:H21	1:16:1146:A:H62	1.67	0.43
12:SL:87:VAL:HB	12:SL:90:LEU:HB2	2.00	0.43
23:23:594:U:H2'	23:23:595:C:C6	2.54	0.43
23:23:1637:A:H5'	23:23:1760:C:O2'	2.19	0.43
28:LE:14:LYS:O	28:LE:18:THR:HG23	2.18	0.43
39:LS:51:ARG:CZ	39:LS:53:ARG:HG3	2.49	0.43
7:SG:144:MET:HE2	7:SG:144:MET:HB2	1.78	0.43
23:23:87:U:H5'	23:23:88:G:C5'	2.49	0.43
23:23:2039:U:H2'	23:23:2040:G:C8	2.54	0.43
23:23:2124:G:H3'	23:23:2125:G:C8	2.52	0.43
23:23:2147:A:C5	23:23:2148:G:H1'	2.53	0.43
38:LR:56:LYS:NZ	38:LR:56:LYS:HB3	2.33	0.43
3:SC:207:ILE:O	3:SC:207:ILE:HG22	2.19	0.43
23:23:1796:U:H2'	23:23:1797:G:H8	1.84	0.43
26:LC:150:GLN:O	26:LC:150:GLN:HG2	2.18	0.43
39:LS:13:MET:HE3	39:LS:54:GLY:C	2.42	0.43
3:SC:111:LEU:HD21	3:SC:146:ALA:HB2	2.01	0.43
15:SO:45:GLU:HG2	15:SO:46:HIS:CD2	2.54	0.43
20:ST:67:ILE:HD12	20:ST:71:LYS:HB3	2.01	0.43
23:23:276:U:H2'	23:23:277:G:C2	2.54	0.43
23:23:2243:U:H2'	23:23:2244:U:C6	2.54	0.43
27:LD:49:ARG:HE	27:LD:49:ARG:HB2	1.64	0.43
32:LK:133:ALA:HB1	32:LK:138:LEU:HB2	2.01	0.43
34:LN:17:ARG:HG3	34:LN:17:ARG:NH1	2.33	0.43
42:LV:1:MET:HE3	42:LV:1:MET:HB2	1.93	0.43
1:16:150:U:H2'	1:16:151:A:H8	1.84	0.42
6:SF:3:HIS:HD2	6:SF:65:GLU:HB2	1.83	0.42
12:SL:43:LYS:HB2	12:SL:43:LYS:HE3	1.60	0.42
23:23:566:U:H5	41:LU:80:ARG:HG2	1.84	0.42
23:23:871:U:H2'	23:23:872:U:C6	2.53	0.42
23:23:2776:A:H4'	23:23:2777:G:H5''	2.01	0.42
25:LB:247:PRO:HG2	25:LB:248:TRP:CZ3	2.54	0.42
29:LF:76:VAL:O	29:LF:80:THR:HG23	2.19	0.42
30:LI:32:PRO:HA	47:Lb:39:TRP:CD1	2.54	0.42
36:LP:41:LEU:HD23	36:LP:41:LEU:HA	1.79	0.42
58:Dt:10:G:H2'	58:Dt:11:C:C6	2.54	0.42
1:16:17:U:H2'	1:16:18:C:C6	2.53	0.42
5:SE:107:ALA:HB2	5:SE:125:ALA:HB3	2.01	0.42
15:SO:29:VAL:HG11	15:SO:67:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1085:A:N6	31:LJ:35:VAL:HG21	2.34	0.42
23:23:2020:A:H5'	51:Lf:9:THR:CG2	2.49	0.42
24:5:76:G:H5'	45:LY:17:SER:OG	2.19	0.42
27:LD:118:LEU:HD11	27:LD:188:MET:SD	2.59	0.42
31:LJ:44:ALA:HB1	31:LJ:95:LEU:HD11	2.01	0.42
15:SO:55:GLY:O	15:SO:59:MET:HG3	2.18	0.42
23:23:971:G:H2'	23:23:972:A:O4'	2.19	0.42
23:23:1548:A:H2'	23:23:1549:A:C8	2.55	0.42
23:23:1645:G:H5''	23:23:1646:C:H5'	2.01	0.42
23:23:1703:G:H2'	23:23:1704:C:C6	2.54	0.42
23:23:2872:A:H2'	23:23:2873:A:H5''	2.01	0.42
28:LE:4:LEU:HD23	28:LE:4:LEU:HA	1.78	0.42
1:16:448:A:H3'	1:16:449:G:C8	2.54	0.42
1:16:579:A:H2'	1:16:580:C:C6	2.54	0.42
4:SD:192:SER:OG	4:SD:194:ASP:OD1	2.28	0.42
6:SF:42:TRP:HZ2	6:SF:61:LEU:HD22	1.83	0.42
11:SK:108:THR:O	21:SU:6:VAL:HG23	2.19	0.42
23:23:948:C:H1'	23:23:984:A:C8	2.55	0.42
23:23:1746:A:H2'	23:23:1747:U:C6	2.55	0.42
58:Dt:20:U:O2'	58:Dt:21:A:H5'	2.20	0.42
1:16:911:U:H2'	1:16:912:C:C6	2.54	0.42
2:SB:186:ILE:HD13	2:SB:200:ILE:HB	2.02	0.42
9:SI:88:MET:SD	9:SI:95:ARG:HD3	2.60	0.42
10:SJ:5:ARG:HE	10:SJ:5:ARG:HB3	1.58	0.42
23:23:2449:H2U:O5'	23:23:2449:H2U:H2'	2.20	0.42
31:LJ:19:ALA:HB3	31:LJ:67:THR:HG21	2.01	0.42
41:LU:26:ASP:O	41:LU:27:ILE:HD13	2.19	0.42
3:SC:53:SER:HB2	3:SC:115:LEU:HG	2.00	0.42
23:23:192:C:O2'	23:23:802:A:N3	2.48	0.42
23:23:2834:G:H2'	23:23:2879:A:H61	1.84	0.42
29:LF:99:LYS:HE3	29:LF:99:LYS:HB2	1.92	0.42
1:16:131:A:H2'	1:16:132:C:C6	2.55	0.42
1:16:719:C:H1'	18:SR:38:LYS:HG2	2.01	0.42
20:ST:79:LEU:O	20:ST:83:ILE:HG13	2.20	0.42
32:LK:103:ARG:HG2	32:LK:140:VAL:HG22	2.01	0.42
56:Pt:74:C:H2'	56:Pt:75:C:H5'	2.01	0.42
1:16:222:C:H2'	1:16:223:A:C8	2.55	0.42
1:16:404:G:O2'	1:16:498:A:N1	2.51	0.42
1:16:1412:C:H2'	1:16:1413:A:C8	2.55	0.42
8:SH:29:SER:HB2	8:SH:59:LEU:HB2	2.02	0.42
23:23:554:U:H2'	23:23:555:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1076:C:O2	32:LK:93:PRO:HD2	2.20	0.42
23:23:2591:C:H2'	23:23:2592:G:C8	2.53	0.42
30:LI:72:ILE:HG21	30:LI:140:ALA:HB1	2.02	0.42
32:LK:109:ILE:HA	32:LK:112:THR:HB	2.02	0.42
42:LV:51:LEU:O	42:LV:55:ILE:HG13	2.19	0.42
1:16:1491:G:H5'	1:16:1492:A:OP1	2.20	0.42
12:SL:100:GLY:HA3	12:SL:118:GLY:HA3	2.02	0.42
13:SM:9:ILE:HD11	13:SM:22:ILE:HG12	2.01	0.42
23:23:2339:C:H2'	23:23:2340:A:H8	1.85	0.42
25:LB:144:VAL:HB	25:LB:154:LEU:HB2	2.02	0.42
29:LF:19:ILE:HG12	29:LF:24:ILE:CD1	2.50	0.42
33:LM:34:ARG:HG3	33:LM:39:LYS:HB2	2.02	0.42
36:LP:12:MET:HE3	36:LP:12:MET:HB2	1.93	0.42
36:LP:44:ARG:HH11	36:LP:44:ARG:HG2	1.85	0.42
37:LQ:24:MET:CG	37:LQ:44:LEU:HD13	2.50	0.42
1:16:7:A:H5'	1:16:298:A:O4'	2.19	0.42
2:SB:212:LEU:HD23	2:SB:212:LEU:C	2.44	0.42
2:SB:228:ASP:OD1	2:SB:228:ASP:C	2.61	0.42
4:SD:48:LEU:HD21	4:SD:56:ARG:HG3	2.01	0.42
23:23:483:A:H5''	44:LX:47:LYS:HG3	2.01	0.42
23:23:1044:C:O2'	23:23:1111:A:N1	2.48	0.42
23:23:2305:U:C2	28:LE:151:GLY:HA3	2.55	0.42
29:LF:95:ARG:NH1	29:LF:95:ARG:HB3	2.35	0.42
3:SC:6:HIS:CE1	3:SC:8:ASN:HB3	2.55	0.41
10:SJ:90:LEU:HD22	10:SJ:91:ASP:H	1.84	0.41
23:23:65:U:O2'	23:23:456:C:N3	2.51	0.41
23:23:476:G:H4'	23:23:502:A:N1	2.35	0.41
23:23:1010:A:N3	23:23:1153:C:H1'	2.35	0.41
23:23:1059:G:H2'	23:23:1060:U:C5	2.55	0.41
23:23:2339:C:H2'	23:23:2340:A:C8	2.55	0.41
31:LJ:61:ARG:NE	31:LJ:61:ARG:CA	2.80	0.41
34:LN:63:VAL:HG12	34:LN:107:LEU:HD11	2.02	0.41
1:16:339:C:H5	34:LN:98:ARG:NH1	2.18	0.41
5:SE:100:SER:O	5:SE:103:THR:HG23	2.20	0.41
18:SR:34:THR:HG22	18:SR:40:VAL:HG22	2.01	0.41
20:ST:25:ARG:O	20:ST:29:ARG:HG3	2.19	0.41
23:23:581:C:H2'	23:23:582:A:C8	2.55	0.41
23:23:706:A:H61	23:23:725:G:C2'	2.33	0.41
23:23:721:A:H2'	23:23:722:A:C8	2.55	0.41
23:23:1100:C:H2'	23:23:1101:U:O4'	2.20	0.41
23:23:1173:U:H2'	23:23:1174:U:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1497:U:H5''	23:23:1498:C:H5	1.85	0.41
25:LB:145:GLU:HG2	25:LB:151:GLY:C	2.45	0.41
34:LN:70:ARG:HG2	34:LN:76:VAL:HG22	2.02	0.41
1:16:269:C:H2'	1:16:270:A:C8	2.55	0.41
1:16:467:U:H6	1:16:467:U:H2'	1.67	0.41
1:16:558:G:OP2	1:16:559:A:O2'	2.36	0.41
1:16:950:U:H2'	1:16:951:G:C8	2.55	0.41
1:16:1413:A:H2	1:16:1487:G:H22	1.68	0.41
6:SF:56:LYS:HE2	6:SF:56:LYS:HB3	1.78	0.41
9:SI:11:ARG:HA	9:SI:15:SER:O	2.20	0.41
13:SM:19:LEU:HD23	13:SM:19:LEU:HA	1.90	0.41
23:23:207:A:H2'	23:23:208:C:O4'	2.20	0.41
23:23:973:A:H5'	23:23:1188:U:H1'	2.02	0.41
23:23:2808:G:O2'	23:23:2890:G:O6	2.36	0.41
32:LK:90:SER:HB3	32:LK:93:PRO:HA	2.01	0.41
33:LM:36:LEU:HD11	33:LM:122:LEU:HD13	2.01	0.41
35:LO:131:ALA:O	35:LO:135:ILE:HG13	2.20	0.41
56:Pt:9:A:H2	56:Pt:23:A:H62	1.68	0.41
3:SC:132[A]:ARG:CZ	22:mR:54:A:N7	2.84	0.41
26:LC:121:THR:HB	26:LC:127:PHE:CD2	2.56	0.41
28:LE:136:ILE:H	28:LE:136:ILE:HG12	1.67	0.41
30:LI:46:PHE:HD1	30:LI:46:PHE:O	2.03	0.41
31:LJ:7:ASP:O	31:LJ:11:ILE:HG12	2.20	0.41
34:LN:43:ILE:HD12	34:LN:56:ASP:HB2	2.01	0.41
56:Pt:16:H2U:H62	56:Pt:16:H2U:H2'	1.21	0.41
1:16:1022:A:H2'	1:16:1023:U:O4'	2.20	0.41
2:SB:56:GLU:HG2	2:SB:198:PHE:CZ	2.56	0.41
3:SC:42:TYR:OH	3:SC:90:VAL:HG11	2.21	0.41
5:SE:151:GLU:CD	5:SE:151:GLU:N	2.78	0.41
14:SN:73:PHE:CZ	14:SN:78:GLY:HA2	2.55	0.41
23:23:1378:A:O2'	23:23:1380:G:N7	2.51	0.41
36:LP:38:ARG:HB2	36:LP:98:PRO:HD3	2.02	0.41
38:LR:17:LYS:O	38:LR:21:LEU:HD22	2.20	0.41
1:16:1151:A:N3	10:SJ:41:PRO:HG2	2.36	0.41
6:SF:59:TYR:OH	18:SR:65:LEU:O	2.34	0.41
10:SJ:14:ASP:O	10:SJ:18:ILE:HG22	2.20	0.41
10:SJ:90:LEU:HD22	10:SJ:91:ASP:N	2.35	0.41
23:23:639:U:H2'	23:23:640:C:C6	2.55	0.41
23:23:1278:C:H2'	23:23:1279:G:C8	2.56	0.41
23:23:1394:U:H4'	23:23:1603:A:H4'	2.00	0.41
26:LC:35:THR:HG22	26:LC:73:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Le:49:ARG:HB3	50:Le:50:ASP:H	1.72	0.41
1:16:343:U:H2'	1:16:345:C:C5	2.56	0.41
1:16:693:G:C5	22:mR:37[A]:A:H1'	2.55	0.41
6:SF:49:TYR:HB3	18:SR:74:HIS:CD2	2.56	0.41
13:SM:39:ILE:HD12	13:SM:56:LEU:HD21	2.02	0.41
23:23:674:G:H5''	27:LD:71:GLY:N	2.36	0.41
23:23:833:A:H2'	23:23:834:G:H8	1.85	0.41
23:23:880:G:H1	23:23:897:C:N4	2.18	0.41
23:23:2154:A:H2'	23:23:2155:U:O4'	2.21	0.41
23:23:2246:G:H2'	23:23:2247:A:C8	2.55	0.41
26:LC:25:THR:HG21	26:LC:193:VAL:HG22	2.02	0.41
28:LE:41:GLY:C	28:LE:43:ALA:N	2.77	0.41
29:LF:19:ILE:HG12	29:LF:24:ILE:HD12	2.01	0.41
36:LP:35:ALA:HB2	36:LP:102:LEU:HD11	2.02	0.41
50:Le:59:ARG:HB3	50:Le:59:ARG:CZ	2.51	0.41
56:Pt:44:U:H2'	56:Pt:45:G:O4'	2.21	0.41
1:16:219:U:H2'	1:16:220:G:C8	2.55	0.41
1:16:568:G:O6	12:SL:2:ALA:HB2	2.21	0.41
1:16:1530:G:H2'	1:16:1531:A:C8	2.56	0.41
13:SM:7:ILE:HD12	13:SM:7:ILE:HA	1.95	0.41
21:SU:33:ARG:NH1	21:SU:33:ARG:HG3	2.36	0.41
23:23:1329:U:H5''	23:23:1330:C:C5	2.52	0.41
23:23:2087:G:H2'	23:23:2088:A:C8	2.55	0.41
23:23:2796:U:H3	23:23:2799:A:N6	2.18	0.41
30:LI:56:ALA:O	30:LI:60:GLU:HB2	2.21	0.41
35:LO:77:ILE:HG12	35:LO:95:LEU:HD13	2.02	0.41
38:LR:116:GLN:H	38:LR:116:GLN:HG2	1.36	0.41
39:LS:91:ALA:HB3	39:LS:111:LYS:HG3	2.03	0.41
1:16:219:U:H2'	1:16:220:G:H8	1.86	0.41
1:16:563:A:H2'	1:16:563:A:N3	2.35	0.41
1:16:736:C:H2'	1:16:737:C:C6	2.55	0.41
1:16:1314:C:H2'	1:16:1315:U:C6	2.56	0.41
1:16:1376:U:H2'	1:16:1377:A:C8	2.56	0.41
1:16:1517:G:N3	23:23:1919:A:O2'	2.49	0.41
4:SD:62:ARG:HE	4:SD:62:ARG:HB3	1.61	0.41
5:SE:164:ILE:HG13	5:SE:165:LEU:N	2.35	0.41
13:SM:101:ARG:O	13:SM:101:ARG:HG3	2.21	0.41
20:ST:43:ASP:OD1	20:ST:43:ASP:C	2.64	0.41
23:23:125:A:H2	53:Lh:9:VAL:HG12	1.86	0.41
23:23:493:G:H2'	23:23:494:G:O4'	2.21	0.41
23:23:927:A:H2'	23:23:928:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:928:A:H2	49:Ld:47:MET:HE1	1.85	0.41
23:23:1315:C:O2'	23:23:1392:A:N3	2.48	0.41
23:23:1782:U:H1'	23:23:2609:U:H5''	2.03	0.41
23:23:1930:G:O2'	23:23:1968:G:O6	2.33	0.41
24:5:48:U:H2'	24:5:49:C:C6	2.56	0.41
28:LE:93:GLY:H	28:LE:96:MET:HB3	1.84	0.41
31:LJ:11:ILE:O	31:LJ:15:VAL:HG22	2.20	0.41
35:LO:77:ILE:HD11	35:LO:101:ILE:HG21	2.03	0.41
38:LR:49:VAL:HG12	38:LR:85:LYS:HD2	2.02	0.41
47:Lb:54:LYS:O	47:Lb:58:VAL:HG13	2.20	0.41
1:16:973:G:H5''	10:SJ:52:LEU:HD11	2.02	0.41
1:16:1273:C:H2'	1:16:1274:A:O4'	2.21	0.41
2:SB:162:PHE:HA	2:SB:184:PHE:O	2.21	0.41
10:SJ:12:ALA:HB3	10:SJ:18:ILE:HB	2.03	0.41
14:SN:46:LEU:HD12	19:SS:13:LEU:HB2	2.03	0.41
20:ST:15:GLU:OE1	20:ST:19:LYS:HE2	2.21	0.41
20:ST:69:LYS:HB2	20:ST:69:LYS:HE3	1.96	0.41
23:23:1178:C:O2'	23:23:1179:G:H8	2.04	0.41
23:23:1744:A:H3'	23:23:1745:A:H8	1.86	0.41
58:Dt:22:G:H2'	58:Dt:23:A:C8	2.56	0.41
1:16:6:G:N1	5:SE:103:THR:HG21	2.35	0.40
1:16:1162:C:H2'	1:16:1163:A:C8	2.57	0.40
1:16:1436:U:H2'	1:16:1437:A:C8	2.56	0.40
2:SB:125:THR:O	2:SB:126:PHE:C	2.64	0.40
13:SM:71:ARG:CZ	13:SM:71:ARG:HB2	2.50	0.40
23:23:2636:C:HO2'	26:LC:45:TYR:HH	1.59	0.40
25:LB:205:LEU:HB3	25:LB:210:ALA:HB3	2.02	0.40
30:LI:45:GLU:HA	30:LI:48:GLU:OE1	2.20	0.40
32:LK:77:ALA:C	32:LK:79:LEU:N	2.79	0.40
34:LN:118:LEU:HD23	34:LN:118:LEU:HA	1.86	0.40
35:LO:82:LEU:HD22	35:LO:90:VAL:HG21	2.02	0.40
1:16:1180:A:P	9:SI:99:ARG:HH12	2.45	0.40
1:16:1363:A:O2'	1:16:1365:G:N7	2.53	0.40
3:SC:86:LYS:O	3:SC:90:VAL:HG12	2.20	0.40
4:SD:105:MET:HG2	4:SD:173:VAL:HG22	2.02	0.40
19:SS:37:ARG:O	19:SS:70:LYS:NZ	2.43	0.40
23:23:45:G:H5'	23:23:46:G:OP1	2.20	0.40
23:23:1056:G:H4'	23:23:1086:A:H8	1.86	0.40
23:23:1182:G:H2'	23:23:1183:U:O4'	2.21	0.40
23:23:1469:A:H2'	23:23:1470:A:C8	2.56	0.40
23:23:1880:U:H2'	23:23:1881:C:C6	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:2061:G:H2'	23:23:2501:C:O2'	2.21	0.40
27:LD:21:ARG:HD3	27:LD:106:LYS:CB	2.52	0.40
29:LF:81:GLU:OE1	29:LF:81:GLU:HA	2.22	0.40
33:LM:37:ARG:HB3	33:LM:39:LYS:HG2	2.03	0.40
1:16:160:A:H1'	1:16:344:A:C5	2.57	0.40
2:SB:10:LEU:HD13	2:SB:10:LEU:HA	1.97	0.40
2:SB:154:MET:HG2	2:SB:156:GLY:O	2.21	0.40
8:SH:111:MET:HB2	8:SH:115:ALA:HB3	2.04	0.40
9:SI:17:ALA:HB2	9:SI:67:VAL:HG23	2.03	0.40
10:SJ:32:THR:CG2	10:SJ:83:THR:HG22	2.48	0.40
11:SK:126:LYS:HG3	21:SU:37[B]:PHE:CE1	2.56	0.40
23:23:686:U:H6	23:23:788:A:N1	2.19	0.40
23:23:753:A:H2'	23:23:754:U:C6	2.57	0.40
23:23:839:U:H2'	23:23:840:C:C6	2.56	0.40
23:23:1490:A:N3	23:23:1490:A:H2'	2.36	0.40
23:23:1506:U:H2'	23:23:1507:C:C6	2.56	0.40
23:23:2469:A:H2'	23:23:2470:G:O4'	2.21	0.40
23:23:2704:C:H2'	23:23:2705:A:O4'	2.22	0.40
33:LM:97:PRO:O	33:LM:100:VAL:HG22	2.20	0.40
36:LP:10:ARG:NH2	36:LP:11:LYS:HE3	2.36	0.40
38:LR:48:LEU:HD23	38:LR:87:ILE:HD13	2.04	0.40
42:LV:24:ILE:HA	42:LV:27:LYS:HD2	2.03	0.40
1:16:299:G:H2'	1:16:300:A:C8	2.56	0.40
1:16:1034:G:H2'	1:16:1035:A:C8	2.56	0.40
1:16:1500:A:H5''	1:16:1508:A:H5''	2.03	0.40
3:SC:168:TYR:HE2	5:SE:55:GLU:OE2	2.03	0.40
3:SC:191:THR:HG21	3:SC:196:ILE:HD12	2.02	0.40
8:SH:3:MET:HE2	8:SH:3:MET:HB2	1.78	0.40
12:SL:53:CYS:HB3	12:SL:67:ILE:HD11	2.03	0.40
13:SM:45:ILE:HD13	13:SM:45:ILE:HA	1.91	0.40
15:SO:3:LEU:HD11	15:SO:34:ALA:HB3	2.04	0.40
19:SS:11:ILE:HA	19:SS:38:SER:HB3	2.03	0.40
23:23:580:U:H2'	23:23:581:C:C6	2.56	0.40
23:23:858:G:N3	23:23:2268:A:H2'	2.37	0.40
23:23:967:U:H2'	23:23:968:C:C6	2.57	0.40
23:23:1370:C:H2'	23:23:1371:G:O4'	2.22	0.40
23:23:2444:G:P	27:LD:63:LYS:HD3	2.62	0.40
23:23:2564:A:OP1	23:23:2648:G:H4'	2.22	0.40
23:23:764:A:H2	25:LB:218:PRO:HG3	1.86	0.40
23:23:1130:U:C2	23:23:2025:C:H5''	2.57	0.40
23:23:2051:A:OP2	23:23:2051:A:H8	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:2902:C:H2'	23:23:2903:U:O4'	2.22	0.40
24:5:106:G:H2'	24:5:107:G:O4'	2.22	0.40
41:LU:38:VAL:HG22	41:LU:59:ILE:HD12	2.02	0.40
54:Li:55:LEU:HA	54:Li:55:LEU:HD12	1.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SB	227/241 (94%)	217 (96%)	10 (4%)	0	100	100
3	SC	211/233 (91%)	208 (99%)	3 (1%)	0	100	100
4	SD	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
5	SE	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
6	SF	104/135 (77%)	102 (98%)	2 (2%)	0	100	100
7	SG	154/179 (86%)	150 (97%)	4 (3%)	0	100	100
8	SH	127/130 (98%)	127 (100%)	0	0	100	100
9	SI	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
10	SJ	97/103 (94%)	93 (96%)	4 (4%)	0	100	100
11	SK	116/129 (90%)	110 (95%)	6 (5%)	0	100	100
12	SL	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
13	SM	112/118 (95%)	109 (97%)	3 (3%)	0	100	100
14	SN	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	SO	87/89 (98%)	85 (98%)	2 (2%)	0	100	100
16	SP	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
17	SQ	78/84 (93%)	77 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	SR	65/75 (87%)	63 (97%)	2 (3%)	0	100	100
19	SS	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
20	ST	84/87 (97%)	84 (100%)	0	0	100	100
21	SU	69/71 (97%)	69 (100%)	0	0	100	100
25	LB	269/273 (98%)	265 (98%)	4 (2%)	0	100	100
26	LC	207/209 (99%)	205 (99%)	2 (1%)	0	100	100
27	LD	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
28	LE	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
29	LF	173/177 (98%)	169 (98%)	4 (2%)	0	100	100
30	LI	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
31	LJ	133/165 (81%)	123 (92%)	10 (8%)	0	100	100
32	LK	132/142 (93%)	123 (93%)	9 (7%)	0	100	100
33	LM	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
34	LN	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
35	LO	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
36	LP	134/136 (98%)	134 (100%)	0	0	100	100
37	LQ	118/127 (93%)	115 (98%)	3 (2%)	0	100	100
38	LR	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
39	LS	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
40	LT	115/118 (98%)	115 (100%)	0	0	100	100
41	LU	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
42	LV	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
43	LW	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
44	LX	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
45	LY	92/94 (98%)	92 (100%)	0	0	100	100
46	La	82/85 (96%)	81 (99%)	1 (1%)	0	100	100
47	Lb	76/78 (97%)	74 (97%)	2 (3%)	0	100	100
48	Lc	60/63 (95%)	60 (100%)	0	0	100	100
49	Ld	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	Le	66/70 (94%)	61 (92%)	5 (8%)	0	100	100
51	Lf	54/57 (95%)	54 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	Lg	50/55 (91%)	50 (100%)	0	0	100	100
53	Lh	44/46 (96%)	44 (100%)	0	0	100	100
54	Li	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
55	Lj	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
57	Pp	1/3 (33%)	1 (100%)	0	0	100	100
All	All	5905/6223 (95%)	5741 (97%)	164 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SB	190/199 (96%)	187 (98%)	3 (2%)	55	67
3	SC	173/190 (91%)	166 (96%)	7 (4%)	28	36
4	SD	172/173 (99%)	170 (99%)	2 (1%)	63	75
5	SE	120/126 (95%)	115 (96%)	5 (4%)	26	34
6	SF	92/116 (79%)	87 (95%)	5 (5%)	20	24
7	SG	129/147 (88%)	113 (88%)	16 (12%)	4	3
8	SH	104/105 (99%)	103 (99%)	1 (1%)	68	79
9	SI	105/107 (98%)	96 (91%)	9 (9%)	10	10
10	SJ	87/90 (97%)	83 (95%)	4 (5%)	24	31
11	SK	91/99 (92%)	85 (93%)	6 (7%)	15	17
12	SL	102/103 (99%)	95 (93%)	7 (7%)	14	15
13	SM	92/96 (96%)	85 (92%)	7 (8%)	12	13
14	SN	83/84 (99%)	79 (95%)	4 (5%)	23	29
15	SO	78/77 (101%)	75 (96%)	3 (4%)	29	38
16	SP	65/65 (100%)	65 (100%)	0	100	100
17	SQ	74/78 (95%)	72 (97%)	2 (3%)	39	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	SR	58/65 (89%)	51 (88%)	7 (12%)	5	4
19	SS	72/79 (91%)	71 (99%)	1 (1%)	59	71
20	ST	65/66 (98%)	64 (98%)	1 (2%)	57	69
21	SU	61/61 (100%)	55 (90%)	6 (10%)	7	7
25	LB	216/218 (99%)	214 (99%)	2 (1%)	70	80
26	LC	164/164 (100%)	161 (98%)	3 (2%)	51	64
27	LD	165/165 (100%)	160 (97%)	5 (3%)	36	47
28	LE	149/150 (99%)	146 (98%)	3 (2%)	48	61
29	LF	136/138 (99%)	130 (96%)	6 (4%)	25	33
30	LI	114/114 (100%)	96 (84%)	18 (16%)	2	2
31	LJ	103/123 (84%)	90 (87%)	13 (13%)	4	3
32	LK	104/110 (94%)	100 (96%)	4 (4%)	29	38
33	LM	116/116 (100%)	114 (98%)	2 (2%)	53	66
34	LN	104/104 (100%)	101 (97%)	3 (3%)	37	48
35	LO	103/103 (100%)	100 (97%)	3 (3%)	37	48
36	LP	109/108 (101%)	107 (98%)	2 (2%)	51	64
37	LQ	100/103 (97%)	98 (98%)	2 (2%)	48	61
38	LR	86/87 (99%)	80 (93%)	6 (7%)	14	15
39	LS	99/100 (99%)	96 (97%)	3 (3%)	36	47
40	LT	89/90 (99%)	88 (99%)	1 (1%)	65	77
41	LU	84/84 (100%)	80 (95%)	4 (5%)	23	29
42	LV	93/93 (100%)	92 (99%)	1 (1%)	65	77
43	LW	80/84 (95%)	77 (96%)	3 (4%)	29	38
44	LX	83/85 (98%)	82 (99%)	1 (1%)	63	75
45	LY	78/78 (100%)	74 (95%)	4 (5%)	21	26
46	La	62/63 (98%)	61 (98%)	1 (2%)	55	67
47	Lb	68/68 (100%)	66 (97%)	2 (3%)	37	48
48	Lc	54/55 (98%)	54 (100%)	0	100	100
49	Ld	48/49 (98%)	48 (100%)	0	100	100
50	Le	60/62 (97%)	55 (92%)	5 (8%)	10	11
51	Lf	47/48 (98%)	46 (98%)	1 (2%)	47	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	Lg	47/49 (96%)	46 (98%)	1 (2%)	47	60
53	Lh	38/38 (100%)	37 (97%)	1 (3%)	40	53
54	Li	51/52 (98%)	51 (100%)	0	100	100
55	Lj	34/34 (100%)	33 (97%)	1 (3%)	37	48
57	Pp	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	4900/5064 (97%)	4702 (96%)	198 (4%)	29	36

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	4	VAL
2	SB	125	THR
2	SB	221	VAL
3	SC	28	GLU
3	SC	84	VAL
3	SC	107	ARG
3	SC	121	THR
3	SC	192	THR
3	SC	206	GLU
3	SC	211	MET
4	SD	30	THR
4	SD	91	LEU
5	SE	22	SER
5	SE	29	ARG
5	SE	52	LYS
5	SE	88	VAL
5	SE	152	MET
6	SF	17	GLN
6	SF	36	ILE
6	SF	38	ARG
6	SF	44	ARG
6	SF	70	VAL
7	SG	7	ILE
7	SG	35	LYS
7	SG	38	THR
7	SG	45	SER
7	SG	58	GLU
7	SG	73	VAL
7	SG	75	VAL
7	SG	76	LYS

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Mol	Chain	Res	Type
7	SG	77	SER
7	SG	78[A]	ARG
7	SG	78[B]	ARG
7	SG	80	VAL
7	SG	125	SER
7	SG	149	LYS
7	SG	155	ARG
7	SG	156	TRP
8	SH	74	SER
9	SI	4	ASN
9	SI	12	ARG
9	SI	14	SER
9	SI	32	GLN
9	SI	36	GLU
9	SI	52	LEU
9	SI	58	VAL
9	SI	61	LEU
9	SI	130	ARG
10	SJ	5	ARG
10	SJ	14	ASP
10	SJ	40	ILE
10	SJ	80	THR
11	SK	18	ASP
11	SK	35	THR
11	SK	55	SER
11	SK	81	ASN
11	SK	111	THR
11	SK	129	VAL
12	SL	15	LYS
12	SL	35	THR
12	SL	43	LYS
12	SL	62	GLU
12	SL	82	ILE
12	SL	110	ARG
12	SL	115	SER
13	SM	4	ILE
13	SM	8	ASN
13	SM	9	ILE
13	SM	16	VAL
13	SM	21	SER
13	SM	27	LYS
13	SM	59	GLU

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Mol	Chain	Res	Type
14	SN	11	VAL
14	SN	26	GLU
14	SN	37	SER
14	SN	38	ASP
15	SO	74	ASP
15	SO	89[A]	ARG
15	SO	89[B]	ARG
17	SQ	27	ARG
17	SQ	83	VAL
18	SR	8	ARG
18	SR	9	LYS
18	SR	12	ARG
18	SR	14	THR
18	SR	18	VAL
18	SR	20	GLU
18	SR	21	ILE
19	SS	48	THR
20	ST	5	LYS
21	SU	20	LYS
21	SU	29	LEU
21	SU	62	ARG
21	SU	67	ARG
21	SU	69	ARG
21	SU	70	LEU
25	LB	252	THR
25	LB	268	VAL
26	LC	18	ASP
26	LC	95	SER
26	LC	170	VAL
27	LD	1	MET
27	LD	2	GLU
27	LD	17	THR
27	LD	49	ARG
27	LD	167	VAL
28	LE	47	LYS
28	LE	89	VAL
28	LE	105	THR
29	LF	50	LEU
29	LF	72	LEU
29	LF	79	VAL
29	LF	85	LYS
29	LF	101	ASN

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Mol	Chain	Res	Type
29	LF	107	LEU
30	LI	21	VAL
30	LI	37	VAL
30	LI	40	THR
30	LI	66	ASN
30	LI	72	ILE
30	LI	76	GLU
30	LI	83	LYS
30	LI	98	ASP
30	LI	110	VAL
30	LI	123	ARG
30	LI	125	THR
30	LI	129	GLU
30	LI	130	VAL
30	LI	134	VAL
30	LI	144	VAL
30	LI	145	ASN
30	LI	146	VAL
30	LI	149	GLU
31	LJ	3	LEU
31	LJ	4	ASN
31	LJ	5	LEU
31	LJ	6	GLN
31	LJ	8	LYS
31	LJ	18	VAL
31	LJ	27	VAL
31	LJ	37	LYS
31	LJ	46	ARG
31	LJ	50	VAL
31	LJ	56	ARG
31	LJ	85	SER
31	LJ	124	ASP
32	LK	11	LEU
32	LK	21	SER
32	LK	108	GLU
32	LK	125	MET
33	LM	2	LYS
33	LM	142	ILE
34	LN	23	LYS
34	LN	66	LYS
34	LN	95	ILE
35	LO	1	MET

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Mol	Chain	Res	Type
35	LO	30	THR
35	LO	121	THR
36	LP	80	VAL
36	LP	135	VAL
37	LQ	2	ARG
37	LQ	120	GLU
38	LR	21	LEU
38	LR	28	VAL
38	LR	48	LEU
38	LR	62	LEU
38	LR	84	GLU
38	LR	116	GLN
39	LS	38	LYS
39	LS	39	ARG
39	LS	78	SER
40	LT	74	ILE
41	LU	47	VAL
41	LU	58	VAL
41	LU	68	ARG
41	LU	72	VAL
42	LV	69	LEU
43	LW	27	SER
43	LW	33	LYS
43	LW	37	ASP
44	LX	15	THR
45	LY	24	ASN
45	LY	55	GLU
45	LY	61	LEU
45	LY	66	ASP
46	La	81	SER
47	Lb	58	VAL
47	Lb	72	ARG
50	Le	15	SER
50	Le	28	VAL
50	Le	48	GLN
50	Le	50	ASP
50	Le	51	VAL
51	Lf	52	ARG
52	Lg	54	ILE
53	Lh	24	THR
55	Lj	22	VAL
57	Pp	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
2	SB	93	ASN
3	SC	8	ASN
3	SC	69	HIS
4	SD	71	GLN
4	SD	152	GLN
5	SE	12	GLN
6	SF	37	HIS
6	SF	68	GLN
7	SG	130	ASN
8	SH	67	GLN
10	SJ	4	GLN
10	SJ	15	HIS
10	SJ	56	HIS
10	SJ	58	ASN
11	SK	118	HIS
11	SK	119	ASN
13	SM	8	ASN
15	SO	40	GLN
15	SO	50	HIS
16	SP	63	GLN
18	SR	54	GLN
19	SS	56	GLN
20	ST	20	HIS
20	ST	61	GLN
25	LB	134	ASN
25	LB	239	ASN
26	LC	42	ASN
26	LC	150	GLN
27	LD	9	GLN
27	LD	92	HIS
27	LD	163	ASN
28	LE	21	ASN
28	LE	63	GLN
28	LE	127	ASN
29	LF	38	ASN
29	LF	45	HIS
29	LF	48	ASN
30	LI	33	GLN
30	LI	66	ASN
31	LJ	122	GLN
33	LM	80	HIS

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Mol	Chain	Res	Type
33	LM	138	GLN
36	LP	13	HIS
37	LQ	9	GLN
38	LR	38	GLN
38	LR	98	GLN
38	LR	116	GLN
39	LS	7	GLN
40	LT	20	GLN
40	LT	44	GLN
40	LT	52	GLN
43	LW	59	ASN
46	La	3	HIS
46	La	50	ASN
46	La	57	HIS
47	Lb	36	HIS
48	Lc	15	ASN
48	Lc	38	GLN
52	Lg	45	GLN

5.3.3 RNA ⓘ

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

All (744) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	4	U
1	16	9	G
1	16	22	G
1	16	32	A
1	16	39	G
1	16	47	C
1	16	48	C
1	16	50	A

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Mol	Chain	Res	Type
1	16	51	A
1	16	65	A
1	16	71	A
1	16	72	A
1	16	73	C
1	16	74	A
1	16	75	G
1	16	76	G
1	16	78	A
1	16	79	G
1	16	82	G
1	16	83	C
1	16	84	U
1	16	85	U
1	16	86	G
1	16	88	U
1	16	91	U
1	16	92	U
1	16	95	C
1	16	131	A
1	16	137	U
1	16	141	G
1	16	143	A
1	16	144	G
1	16	159	G
1	16	163	C
1	16	171	A
1	16	174	A
1	16	192	A
1	16	193	C
1	16	197	A
1	16	204	G
1	16	208	U
1	16	209	U
1	16	210	C
1	16	215	C
1	16	226	G
1	16	245	U
1	16	247	G
1	16	250	A
1	16	251	G
1	16	252	U

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Mol	Chain	Res	Type
1	16	253	A
1	16	266	G
1	16	267	C
1	16	281	G
1	16	289	G
1	16	300	A
1	16	321	A
1	16	328	C
1	16	329	A
1	16	332	G
1	16	345	C
1	16	348	G
1	16	351	G
1	16	352	C
1	16	354	G
1	16	367	U
1	16	372	C
1	16	388	G
1	16	398	U
1	16	406	G
1	16	411	A
1	16	412	A
1	16	413	G
1	16	421	U
1	16	424	G
1	16	429	U
1	16	458	U
1	16	459	A
1	16	460	A
1	16	462	G
1	16	463	U
1	16	464	U
1	16	465	A
1	16	466	A
1	16	467	U
1	16	468	A
1	16	469	C
1	16	479	U
1	16	484	G
1	16	485	U
1	16	486	U
1	16	509	A

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Mol	Chain	Res	Type
1	16	511	C
1	16	518	C
1	16	527	G7M
1	16	531	U
1	16	532	A
1	16	533	A
1	16	535	A
1	16	547	A
1	16	559	A
1	16	562	U
1	16	564	C
1	16	572	A
1	16	573	A
1	16	576	C
1	16	577	G
1	16	633	G
1	16	634	C
1	16	653	U
1	16	665	A
1	16	703	G
1	16	718	A
1	16	721	G
1	16	723	U
1	16	734	G
1	16	755	G
1	16	777	A
1	16	793	U
1	16	794	A
1	16	815	A
1	16	817	C
1	16	821	G
1	16	828	U
1	16	829	G
1	16	841	C
1	16	842	U
1	16	843	U
1	16	844	G
1	16	845	A
1	16	846	G
1	16	902	G
1	16	914	A
1	16	926	G

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Mol	Chain	Res	Type
1	16	927	G
1	16	933	G
1	16	934	C
1	16	935	A
1	16	960	U
1	16	969	A
1	16	971	G
1	16	975	A
1	16	976	G
1	16	977	A
1	16	983	A
1	16	993	G
1	16	994	A
1	16	1004	A
1	16	1008	U
1	16	1016	A
1	16	1024	G
1	16	1026	G
1	16	1029	U
1	16	1031	C
1	16	1032	G
1	16	1033	G
1	16	1035	A
1	16	1043	G
1	16	1044	A
1	16	1045	C
1	16	1065	U
1	16	1085	U
1	16	1094	G
1	16	1095	U
1	16	1101	A
1	16	1124	G
1	16	1125	U
1	16	1133	G
1	16	1135	U
1	16	1136	C
1	16	1137	C
1	16	1138	G
1	16	1139	G
1	16	1140	C
1	16	1141	C
1	16	1152	A

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Mol	Chain	Res	Type
1	16	1154	G
1	16	1158	C
1	16	1159	U
1	16	1168	U
1	16	1169	A
1	16	1183	U
1	16	1184	G
1	16	1196	A
1	16	1197	A
1	16	1212	U
1	16	1213	A
1	16	1227	A
1	16	1228	C
1	16	1238	A
1	16	1239	A
1	16	1258	G
1	16	1260	G
1	16	1280	A
1	16	1286	U
1	16	1287	A
1	16	1300	G
1	16	1302	C
1	16	1305	G
1	16	1317	C
1	16	1320	C
1	16	1336	C
1	16	1346	A
1	16	1353	G
1	16	1363	A
1	16	1368	A
1	16	1370	G
1	16	1397	C
1	16	1398	A
1	16	1429	A
1	16	1441	A
1	16	1446	A
1	16	1454	G
1	16	1487	G
1	16	1492	A
1	16	1497	G
1	16	1503	A
1	16	1505	G

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Mol	Chain	Res	Type
1	16	1506	U
1	16	1517	G
1	16	1529	G
1	16	1530	G
1	16	1539	C
1	16	1542	A
22	mR	29	G
22	mR	31	C
22	mR	32	A
22	mR	33	A
22	mR	34	U
22	mR	35	C
22	mR	48	C
22	mR	49	U
22	mR	50	U
22	mR	51	C
22	mR	52	A
22	mR	53	A
23	23	10	A
23	23	15	G
23	23	34	U
23	23	44	A
23	23	46	G
23	23	55	G
23	23	71	A
23	23	74	A
23	23	75	G
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	135	U
23	23	139	U
23	23	141	G
23	23	142	A
23	23	158	U
23	23	159	G
23	23	163	C

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Mol	Chain	Res	Type
23	23	174	U
23	23	177	G
23	23	178	G
23	23	181	A
23	23	196	A
23	23	199	A
23	23	215	G
23	23	216	A
23	23	221	A
23	23	222	A
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	277	G
23	23	278	A
23	23	279	A
23	23	283	G
23	23	284	U
23	23	285	G
23	23	286	U
23	23	311	A
23	23	330	A
23	23	345	A
23	23	353	C
23	23	359	G
23	23	361	G
23	23	362	A
23	23	371	A
23	23	372	G
23	23	386	G
23	23	388	G
23	23	395	U
23	23	396	G
23	23	401	A
23	23	405	U
23	23	412	A
23	23	455	C
23	23	456	C
23	23	457	A

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Mol	Chain	Res	Type
23	23	470	A
23	23	473	G
23	23	481	G
23	23	491	G
23	23	504	A
23	23	505	A
23	23	506	G
23	23	509	C
23	23	527	C
23	23	532	A
23	23	547	A
23	23	549	G
23	23	563	A
23	23	573	U
23	23	575	A
23	23	603	A
23	23	613	A
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	654	A
23	23	655	A
23	23	686	U
23	23	717	C
23	23	726	G
23	23	729	G
23	23	730	A
23	23	747	5MU
23	23	764	A
23	23	765	C
23	23	775	G
23	23	776	G
23	23	782	A
23	23	784	G
23	23	785	G
23	23	789	A
23	23	805	G
23	23	812	C
23	23	819	A

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Mol	Chain	Res	Type
23	23	827	U
23	23	828	U
23	23	845	A
23	23	846	U
23	23	847	U
23	23	859	G
23	23	869	G
23	23	878	A
23	23	883	G
23	23	885	C
23	23	887	U
23	23	895	U
23	23	896	A
23	23	897	C
23	23	902	C
23	23	907	G
23	23	910	A
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	996	A
23	23	999	U
23	23	1005	C
23	23	1012	U
23	23	1013	C
23	23	1026	G
23	23	1033	U
23	23	1046	A
23	23	1047	G
23	23	1055	G
23	23	1060	U
23	23	1061	U
23	23	1070	A
23	23	1081	U
23	23	1083	U

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Mol	Chain	Res	Type
23	23	1084	A
23	23	1085	A
23	23	1087	G
23	23	1088	A
23	23	1090	A
23	23	1097	U
23	23	1112	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	1149	G
23	23	1161	C
23	23	1169	A
23	23	1171	G
23	23	1172	C
23	23	1173	U
23	23	1174	U
23	23	1175	A
23	23	1177	G
23	23	1178	C
23	23	1179	G
23	23	1180	U
23	23	1238	G
23	23	1247	A
23	23	1249	U
23	23	1250	G
23	23	1253	A
23	23	1256	G
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	1300	G
23	23	1301	A
23	23	1321	A
23	23	1329	U
23	23	1352	U

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Mol	Chain	Res	Type
23	23	1365	A
23	23	1368	G
23	23	1379	U
23	23	1380	G
23	23	1383	A
23	23	1395	A
23	23	1396	U
23	23	1416	G
23	23	1417	C
23	23	1419	A
23	23	1420	A
23	23	1428	C
23	23	1434	A
23	23	1452	G
23	23	1453	A
23	23	1460	U
23	23	1461	C
23	23	1482	G
23	23	1488	C
23	23	1493	C
23	23	1494	A
23	23	1497	U
23	23	1502	A
23	23	1503	A
23	23	1506	U
23	23	1507	C
23	23	1508	A
23	23	1509	A
23	23	1515	A
23	23	1524	G
23	23	1531	C
23	23	1532	A
23	23	1536	C
23	23	1537	G
23	23	1538	G
23	23	1539	U
23	23	1566	A
23	23	1569	A
23	23	1578	U
23	23	1583	A
23	23	1584	U
23	23	1608	A

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Mol	Chain	Res	Type
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	1727	C
23	23	1729	U
23	23	1730	C
23	23	1731	G
23	23	1738	G
23	23	1764	C
23	23	1773	A
23	23	1782	U
23	23	1784	A
23	23	1786	A
23	23	1791	A
23	23	1799	G
23	23	1800	C
23	23	1801	A
23	23	1807	G
23	23	1808	A
23	23	1811	G
23	23	1816	C
23	23	1848	A
23	23	1870	C
23	23	1872	A
23	23	1873	G
23	23	1906	G
23	23	1907	G
23	23	1929	G
23	23	1930	G
23	23	1940	U
23	23	1954	G
23	23	1955	U
23	23	1960	A
23	23	1966	A
23	23	1967	C
23	23	1970	A
23	23	1971	U
23	23	1972	G
23	23	1975	G

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Mol	Chain	Res	Type
23	23	1982	U
23	23	1991	U
23	23	1993	U
23	23	1997	C
23	23	2022	U
23	23	2023	C
23	23	2030	6MZ
23	23	2031	A
23	23	2032	G
23	23	2033	A
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	2093	G
23	23	2098	U
23	23	2100	A
23	23	2101	A
23	23	2102	G
23	23	2103	C
23	23	2104	C
23	23	2106	U
23	23	2108	A
23	23	2110	G
23	23	2111	U
23	23	2112	G
23	23	2113	U
23	23	2114	A
23	23	2115	G
23	23	2116	G
23	23	2117	A
23	23	2118	U
23	23	2120	G
23	23	2123	G
23	23	2124	G
23	23	2126	A
23	23	2128	G
23	23	2130	U
23	23	2131	U

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Mol	Chain	Res	Type
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	2161	C
23	23	2162	G
23	23	2163	A
23	23	2164	C
23	23	2166	U
23	23	2167	U
23	23	2170	A
23	23	2171	A
23	23	2172	U
23	23	2173	A
23	23	2182	U
23	23	2186	G
23	23	2190	G
23	23	2198	A
23	23	2204	G
23	23	2211	A
23	23	2225	A
23	23	2238	G
23	23	2239	G
23	23	2243	U
23	23	2251	OMG
23	23	2268	A
23	23	2278	A
23	23	2279	G
23	23	2283	C
23	23	2287	A
23	23	2305	U
23	23	2308	G
23	23	2309	A
23	23	2311	A
23	23	2312	U
23	23	2319	G
23	23	2321	U
23	23	2322	A
23	23	2325	G

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Mol	Chain	Res	Type
23	23	2333	A
23	23	2336	A
23	23	2345	G
23	23	2347	C
23	23	2350	C
23	23	2361	G
23	23	2372	U
23	23	2375	G
23	23	2379	G
23	23	2383	G
23	23	2385	C
23	23	2391	G
23	23	2402	U
23	23	2403	C
23	23	2406	A
23	23	2410	G
23	23	2423	U
23	23	2425	A
23	23	2429	G
23	23	2430	A
23	23	2431	U
23	23	2441	U
23	23	2448	A
23	23	2464	G
23	23	2475	C
23	23	2476	A
23	23	2478	A
23	23	2484	G
23	23	2491	U
23	23	2492	U
23	23	2494	G
23	23	2498	OMC
23	23	2502	G
23	23	2503	2MA
23	23	2505	G
23	23	2506	U
23	23	2518	A
23	23	2529	G
23	23	2535	G
23	23	2537	U
23	23	2547	A
23	23	2554	U

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Mol	Chain	Res	Type
23	23	2562	U
23	23	2566	A
23	23	2567	G
23	23	2573	C
23	23	2602	A
23	23	2609	U
23	23	2613	U
23	23	2614	A
23	23	2615	U
23	23	2629	U
23	23	2630	G
23	23	2689	U
23	23	2690	U
23	23	2714	G
23	23	2726	A
23	23	2732	G
23	23	2733	A
23	23	2743	U
23	23	2744	G
23	23	2748	A
23	23	2751	G
23	23	2757	A
23	23	2765	A
23	23	2777	G
23	23	2778	A
23	23	2779	U
23	23	2798	U
23	23	2799	A
23	23	2818	U
23	23	2820	A
23	23	2821	A
23	23	2832	U
23	23	2835	A
23	23	2858	C
23	23	2859	G
23	23	2861	U
23	23	2873	A
23	23	2879	A
23	23	2880	C
23	23	2883	A
23	23	2884	U
23	23	2885	G

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Mol	Chain	Res	Type
23	23	2886	A
23	23	2891	U
23	23	2904	U
24	5	9	G
24	5	13	G
24	5	15	A
24	5	16	G
24	5	35	C
24	5	50	A
24	5	51	G
24	5	67	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
56	Pt	4	U
56	Pt	9	A
56	Pt	10	G
56	Pt	13	C
56	Pt	16	H2U
56	Pt	17	H2U
56	Pt	18	G
56	Pt	19	G
56	Pt	20	H2U
56	Pt	21	A
56	Pt	46	G
56	Pt	47	3AU
56	Pt	49	G
56	Pt	63	U
56	Pt	72	C
56	Pt	74	C
58	Dt	4	C
58	Dt	8	4SU
58	Dt	11	C
58	Dt	13	C
58	Dt	15	G
58	Dt	16	H2U
58	Dt	17	C
58	Dt	18	G
58	Dt	19	G

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Mol	Chain	Res	Type
58	Dt	20	U
58	Dt	21	A
58	Dt	22	G
58	Dt	23	A
58	Dt	29	G
58	Dt	37	MIA
58	Dt	40	C
58	Dt	43	C
58	Dt	44	G
58	Dt	45	U
58	Dt	46	G7M
58	Dt	47	3AU
58	Dt	48	C
58	Dt	49	C
58	Dt	52	G
58	Dt	56	C
58	Dt	57	G
58	Dt	58	A
58	Dt	60	U
58	Dt	72	C
58	Dt	74	C
58	Dt	76	A

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	16	72	A
1	16	84	U
1	16	85	U
1	16	251	G
1	16	252	U
1	16	428	G
1	16	457	G
1	16	633	G
1	16	845	A
1	16	1025	U
1	16	1124	G
1	16	1137	C
1	16	1505	G
23	23	43	G
23	23	134	G
23	23	158	U

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Mol	Chain	Res	Type
23	23	177	G
23	23	277	G
23	23	285	G
23	23	352	A
23	23	404	A
23	23	613	A
23	23	784	G
23	23	827	U
23	23	1046	A
23	23	1060	U
23	23	1087	G
23	23	1266	G
23	23	1379	U
23	23	1416	G
23	23	1506	U
23	23	1847	A
23	23	2116	G
23	23	2430	A
23	23	2474	U
23	23	2491	U
23	23	2536	G
23	23	2581	G
23	23	2756	U
23	23	2858	C
24	5	15	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	PSU	23	2504	23	18,21,22	1.42	3 (16%)	21,30,33	2.08	4 (19%)
23	H2U	23	2449	23	18,21,22	4.32	13 (72%)	19,30,33	1.72	4 (21%)
23	OMG	23	2251	58,23	23,26,27	0.52	0	32,38,41	0.47	0

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	1.84	6 (33%)	21,30,33	2.32	9 (42%)
58	PSU	Dt	39	58	18,21,22	2.79	7 (38%)	21,30,33	3.07	10 (47%)
56	H2U	Pt	16	56	18,21,22	1.10	2 (11%)	19,30,33	1.22	1 (5%)
58	G7M	Dt	46	58	23,26,27	2.34	5 (21%)	34,39,42	3.37	11 (32%)
56	3AU	Pt	47	56	24,28,29	1.04	0	30,40,43	1.62	4 (13%)
56	PSU	Pt	55	56	18,21,22	1.39	2 (11%)	21,30,33	2.08	4 (19%)
23	OMC	23	2498	23,60	19,22,23	1.01	2 (10%)	25,31,34	1.13	1 (4%)
23	3TD	23	1915	23	19,22,23	1.21	2 (10%)	23,32,35	2.10	3 (13%)
56	H2U	Pt	17	56	18,21,22	1.06	2 (11%)	19,30,33	1.15	2 (10%)
23	6MZ	23	1618	23	22,25,26	1.43	5 (22%)	29,36,39	2.19	10 (34%)
23	6MZ	23	2030	23	22,25,26	1.43	5 (22%)	29,36,39	2.39	10 (34%)
36	4D4	LP	81	36	9,11,12	2.16	2 (22%)	7,13,15	2.04	3 (42%)
12	D2T	SL	89	12	8,9,10	1.65	2 (25%)	6,11,13	1.52	2 (33%)
56	5MU	Pt	54	56	19,22,23	1.36	5 (26%)	27,32,35	2.11	7 (25%)
23	OMU	23	2552	23	19,22,23	4.23	13 (68%)	25,31,34	2.29	6 (24%)
58	PSU	Dt	32	58	18,21,22	3.22	9 (50%)	21,30,33	3.06	6 (28%)
1	PSU	16	516	60,1	18,21,22	1.41	3 (16%)	21,30,33	2.14	5 (23%)
1	2MG	16	1207	60,1	23,26,27	1.26	4 (17%)	33,38,41	2.18	6 (18%)
23	2MG	23	2445	23	23,26,27	1.24	3 (13%)	33,38,41	2.24	10 (30%)
1	5MC	16	967	1	19,22,23	1.55	3 (15%)	26,32,35	1.12	2 (7%)
23	PSU	23	2605	23	18,21,22	1.38	3 (16%)	21,30,33	2.07	4 (19%)
23	PSU	23	746	23,60	18,21,22	1.41	3 (16%)	21,30,33	1.98	4 (19%)
58	H2U	Dt	16	58	18,21,22	1.43	3 (16%)	19,30,33	1.86	4 (21%)
56	T6A	Pt	37	56	31,34,35	1.47	6 (19%)	43,49,52	2.10	12 (27%)
58	3AU	Dt	47	58	24,28,29	0.98	0	30,40,43	1.49	5 (16%)
23	5MC	23	1962	23	19,22,23	1.51	3 (15%)	26,32,35	1.11	2 (7%)
1	MA6	16	1518	1	23,26,27	1.48	5 (21%)	33,38,41	2.12	10 (30%)
1	UR3	16	1498	1	19,22,23	0.93	0	26,32,35	1.76	3 (11%)
23	PSU	23	955	23	18,21,22	1.38	3 (16%)	21,30,33	2.13	4 (19%)
1	2MG	16	1516	1	23,26,27	1.25	4 (17%)	33,38,41	2.23	9 (27%)
58	4SU	Dt	8	58	18,21,22	1.85	4 (22%)	25,30,33	2.30	5 (20%)
58	MIA	Dt	37	58	28,31,32	2.34	6 (21%)	38,44,47	3.25	19 (50%)
1	4OC	16	1402	60,1	20,23,24	0.74	0	25,32,35	0.93	1 (4%)
1	2MG	16	966	1	23,26,27	1.25	4 (17%)	33,38,41	2.17	7 (21%)
23	5MU	23	1939	23	19,22,23	1.39	5 (26%)	27,32,35	2.14	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PSU	23	2580	23	18,21,22	1.42	4 (22%)	21,30,33	2.08	5 (23%)
1	MA6	16	1519	1	23,26,27	1.47	5 (21%)	33,38,41	2.11	10 (30%)
23	1MG	23	745	23	23,26,27	1.18	3 (13%)	33,39,42	1.68	5 (15%)
56	H2U	Pt	20	56	18,21,22	4.44	12 (66%)	19,30,33	1.63	5 (26%)
56	PSU	Pt	39	56	18,21,22	1.37	3 (16%)	21,30,33	2.09	4 (19%)
23	PSU	23	2457	23	18,21,22	1.41	3 (16%)	21,30,33	2.16	4 (19%)
23	2MA	23	2503	23,60	22,25,26	1.44	5 (22%)	32,37,40	2.29	9 (28%)
1	5MC	16	1407	1	19,22,23	1.52	3 (15%)	26,32,35	1.10	3 (11%)
23	G7M	23	2069	23	23,26,27	2.25	6 (26%)	34,39,42	3.19	17 (50%)
58	PSU	Dt	55	58	18,21,22	2.23	6 (33%)	21,30,33	2.93	9 (42%)
23	5MU	23	747	23	19,22,23	1.41	6 (31%)	27,32,35	2.11	6 (22%)
56	U8U	Pt	34	56,22	20,24,25	1.51	3 (15%)	22,34,37	1.06	3 (13%)
23	2MG	23	1835	23	23,26,27	1.27	3 (13%)	33,38,41	2.19	6 (18%)
1	G7M	16	527	1	23,26,27	2.37	5 (21%)	34,39,42	2.99	10 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	23	2504	23	-	2/7/25/26	0/2/2/2
23	H2U	23	2449	23	-	0/7/38/39	0/2/2/2
23	OMG	23	2251	58,23	-	3/9/27/28	0/3/3/3
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
58	PSU	Dt	39	58	-	0/7/25/26	0/2/2/2
56	H2U	Pt	16	56	-	7/7/38/39	0/2/2/2
58	G7M	Dt	46	58	-	2/7/25/26	0/3/3/3
56	3AU	Pt	47	56	-	7/16/34/35	0/2/2/2
56	PSU	Pt	55	56	-	0/7/25/26	0/2/2/2
23	OMC	23	2498	23,60	-	2/9/27/28	0/2/2/2
23	3TD	23	1915	23	-	2/7/25/26	0/2/2/2
56	H2U	Pt	17	56	-	3/7/38/39	0/2/2/2
23	6MZ	23	1618	23	-	2/9/27/28	0/3/3/3
23	6MZ	23	2030	23	-	2/9/27/28	0/3/3/3
36	4D4	LP	81	36	-	3/11/12/14	-
12	D2T	SL	89	12	-	3/7/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	5MU	Pt	54	56	-	0/7/25/26	0/2/2/2
23	OMU	23	2552	23	-	1/9/27/28	0/2/2/2
58	PSU	Dt	32	58	-	0/7/25/26	0/2/2/2
1	PSU	16	516	60,1	-	0/7/25/26	0/2/2/2
1	2MG	16	1207	60,1	-	0/9/27/28	0/3/3/3
23	2MG	23	2445	23	-	1/9/27/28	0/3/3/3
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
23	PSU	23	2605	23	-	0/7/25/26	0/2/2/2
23	PSU	23	746	23,60	-	2/7/25/26	0/2/2/2
58	H2U	Dt	16	58	-	0/7/38/39	0/2/2/2
56	T6A	Pt	37	56	-	10/23/41/42	0/3/3/3
58	3AU	Dt	47	58	-	6/16/34/35	0/2/2/2
23	5MC	23	1962	23	-	0/7/25/26	0/2/2/2
1	MA6	16	1518	1	-	0/11/29/30	0/3/3/3
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
1	2MG	16	1516	1	-	0/9/27/28	0/3/3/3
58	4SU	Dt	8	58	-	2/7/25/26	0/2/2/2
58	MIA	Dt	37	58	-	8/15/33/34	0/3/3/3
1	4OC	16	1402	60,1	-	0/9/29/30	0/2/2/2
1	2MG	16	966	1	-	0/9/27/28	0/3/3/3
23	5MU	23	1939	23	-	0/7/25/26	0/2/2/2
23	PSU	23	2580	23	-	0/7/25/26	0/2/2/2
1	MA6	16	1519	1	-	2/11/29/30	0/3/3/3
23	1MG	23	745	23	-	0/7/25/26	0/3/3/3
56	H2U	Pt	20	56	-	2/7/38/39	0/2/2/2
56	PSU	Pt	39	56	-	0/7/25/26	0/2/2/2
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
23	2MA	23	2503	23,60	-	2/7/25/26	0/3/3/3
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
23	G7M	23	2069	23	-	1/7/25/26	0/3/3/3
58	PSU	Dt	55	58	-	0/7/25/26	0/2/2/2
23	5MU	23	747	23	-	0/7/25/26	0/2/2/2
56	U8U	Pt	34	56,22	-	0/10/28/29	0/2/2/2
23	2MG	23	1835	23	-	0/9/27/28	0/3/3/3
1	G7M	16	527	1	-	2/7/25/26	0/3/3/3

All (214) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	2552	OMU	C3'-C2'	-10.60	1.29	1.53
23	23	2449	H2U	C2'-C3'	-10.18	1.25	1.53
56	Pt	20	H2U	C2'-C3'	-10.02	1.26	1.53
56	Pt	20	H2U	C2-N1	9.59	1.48	1.35
23	23	2449	H2U	C2-N1	8.93	1.48	1.35
58	Dt	37	MIA	C2-S10	-7.57	1.69	1.75
1	16	527	G7M	C8-N7	7.57	1.46	1.33
23	23	2069	G7M	C8-N7	7.04	1.45	1.33
58	Dt	46	G7M	C8-N7	6.91	1.44	1.33
58	Dt	37	MIA	C13-C14	6.58	1.52	1.32
23	23	2552	OMU	C2-N1	6.01	1.47	1.38
58	Dt	32	PSU	C2-N1	-5.97	1.28	1.36
56	Pt	20	H2U	C2-N3	5.95	1.48	1.38
23	23	2552	OMU	C2-N3	5.80	1.48	1.38
58	Dt	32	PSU	C6-N1	-5.73	1.26	1.36
58	Dt	32	PSU	C4-N3	-5.64	1.28	1.38
23	23	2552	OMU	O4'-C1'	-5.60	1.29	1.42
56	Pt	20	H2U	C4-N3	5.50	1.46	1.37
1	16	967	5MC	C5-C4	5.50	1.48	1.44
58	Dt	39	PSU	C4-N3	-5.48	1.28	1.38
1	16	1407	5MC	C5-C4	5.36	1.48	1.44
23	23	1962	5MC	C5-C4	5.35	1.48	1.44
58	Dt	32	PSU	C2-N3	-5.34	1.28	1.37
23	23	2552	OMU	C6-C5	5.17	1.47	1.35
23	23	2449	H2U	C2-N3	5.16	1.46	1.38
58	Dt	46	G7M	C5-N7	-5.09	1.33	1.39
58	Dt	8	4SU	C4-S4	-5.04	1.59	1.68
36	LP	81	4D4	CZ-NE	5.03	1.43	1.33
56	Pt	34	U8U	C2-S2	-4.97	1.59	1.67
1	16	527	G7M	C5-N7	-4.97	1.33	1.39
58	Dt	39	PSU	C2-N3	-4.94	1.29	1.37
23	23	2449	H2U	O4'-C1'	-4.84	1.30	1.42
58	Dt	55	PSU	C2-N1	-4.82	1.30	1.36
58	Dt	55	PSU	C4-N3	-4.81	1.29	1.38
58	Dt	39	PSU	C2-N1	-4.80	1.30	1.36
23	23	2069	G7M	C5-N7	-4.66	1.33	1.39
1	16	1518	MA6	C5-C4	4.53	1.47	1.39
58	Dt	39	PSU	C2'-C1'	-4.47	1.47	1.53
1	16	1519	MA6	C5-C4	4.47	1.47	1.39
56	Pt	20	H2U	O4'-C1'	-4.46	1.31	1.42
23	23	2449	H2U	C4-N3	4.37	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	Dt	39	PSU	C6-N1	-4.29	1.29	1.36
23	23	1618	6MZ	C5-C4	4.28	1.46	1.39
23	23	2503	2MA	C5-C4	4.20	1.46	1.39
23	23	2030	6MZ	C5-C4	4.18	1.46	1.39
1	16	527	G7M	C8-N9	4.09	1.46	1.35
23	23	2552	OMU	O4'-C4'	3.97	1.53	1.45
23	23	2449	H2U	C5'-C4'	-3.96	1.39	1.51
56	Pt	20	H2U	C5'-C4'	-3.92	1.39	1.51
23	23	2552	OMU	C5'-C4'	-3.92	1.39	1.51
23	23	2069	G7M	C8-N9	3.88	1.46	1.35
58	Dt	55	PSU	C2-N3	-3.85	1.31	1.37
58	Dt	46	G7M	C8-N9	3.84	1.46	1.35
56	Pt	37	T6A	C5-C4	3.84	1.45	1.39
23	23	2449	H2U	O4-C4	-3.82	1.15	1.23
58	Dt	16	H2U	C2-N3	-3.71	1.31	1.38
23	23	2604	PSU	C4-N3	-3.69	1.31	1.38
23	23	2552	OMU	O4-C4	-3.65	1.17	1.24
1	16	527	G7M	C5-C4	3.61	1.47	1.38
56	Pt	20	H2U	C2'-C1'	3.60	1.64	1.53
58	Dt	46	G7M	C5-C4	3.55	1.47	1.38
23	23	2552	OMU	O2-C2	-3.49	1.16	1.23
36	LP	81	4D4	CZ-NH2	3.42	1.44	1.32
58	Dt	32	PSU	C2'-C1'	-3.41	1.49	1.53
58	Dt	37	MIA	C5-C4	3.40	1.45	1.39
23	23	1915	3TD	C6-C5	3.40	1.39	1.35
23	23	2552	OMU	C4-N3	3.37	1.44	1.38
58	Dt	8	4SU	C4-N3	-3.36	1.34	1.37
23	23	2449	H2U	O2-C2	-3.33	1.17	1.23
23	23	2069	G7M	C5-C4	3.27	1.46	1.38
58	Dt	32	PSU	O4'-C1'	-3.26	1.39	1.43
56	Pt	55	PSU	C6-C5	3.23	1.38	1.35
23	23	2504	PSU	C6-C5	3.19	1.38	1.35
23	23	2552	OMU	C2'-C1'	3.15	1.60	1.53
58	Dt	32	PSU	C1'-C5	-3.14	1.43	1.50
23	23	746	PSU	C6-C5	3.13	1.38	1.35
23	23	2457	PSU	C6-C5	3.12	1.38	1.35
23	23	2449	H2U	O3'-C3'	3.08	1.50	1.43
56	Pt	37	T6A	C5-N7	-3.08	1.33	1.39
56	Pt	20	H2U	O3'-C3'	3.08	1.50	1.43
23	23	745	1MG	C5-C4	3.06	1.47	1.38
56	Pt	39	PSU	C6-C5	3.05	1.38	1.35
1	16	516	PSU	C6-C5	3.05	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	2604	PSU	C2'-C1'	-3.01	1.49	1.53
58	Dt	46	G7M	C6-N1	-2.99	1.33	1.38
23	23	1835	2MG	C5-C4	2.98	1.46	1.38
1	16	1207	2MG	C5-C4	2.97	1.46	1.38
23	23	2580	PSU	C6-C5	2.97	1.38	1.35
23	23	2605	PSU	C6-C5	2.95	1.38	1.35
1	16	966	2MG	C5-C4	2.94	1.46	1.38
58	Dt	37	MIA	C5-N7	-2.94	1.33	1.39
23	23	2605	PSU	C4-N3	-2.93	1.33	1.38
56	Pt	16	H2U	C2-N3	-2.93	1.32	1.38
23	23	1939	5MU	C4-N3	-2.92	1.33	1.38
23	23	2604	PSU	C2-N3	-2.92	1.32	1.37
58	Dt	16	H2U	C4-N3	-2.92	1.32	1.37
23	23	2457	PSU	C4-N3	-2.92	1.33	1.38
23	23	2504	PSU	C4-N3	-2.92	1.33	1.38
1	16	1518	MA6	C5-C6	2.91	1.48	1.41
23	23	2449	H2U	C2'-C1'	2.91	1.62	1.53
23	23	2580	PSU	C4-N3	-2.91	1.33	1.38
56	Pt	20	H2U	O4-C4	-2.91	1.17	1.23
58	Dt	16	H2U	C2-N1	-2.90	1.31	1.35
1	16	1516	2MG	C5-C4	2.89	1.46	1.38
1	16	1519	MA6	C5-C6	2.88	1.48	1.41
12	SL	89	D2T	CB-CA	-2.88	1.53	1.54
56	Pt	17	H2U	C2-N3	-2.88	1.32	1.38
23	23	2445	2MG	C5-C4	2.88	1.46	1.38
23	23	747	5MU	C4-N3	-2.87	1.33	1.38
58	Dt	8	4SU	C5-C4	-2.86	1.39	1.42
1	16	516	PSU	C4-N3	-2.86	1.33	1.38
23	23	955	PSU	C4-N3	-2.83	1.33	1.38
23	23	955	PSU	C6-C5	2.81	1.38	1.35
56	Pt	39	PSU	C4-N3	-2.81	1.33	1.38
23	23	2604	PSU	C2-N1	-2.79	1.33	1.36
58	Dt	55	PSU	C6-N1	-2.78	1.31	1.36
23	23	746	PSU	C4-N3	-2.78	1.33	1.38
56	Pt	55	PSU	C4-N3	-2.77	1.33	1.38
56	Pt	54	5MU	C4-N3	-2.77	1.33	1.38
56	Pt	34	U8U	C4-N3	-2.76	1.33	1.38
23	23	1835	2MG	C6-N1	-2.73	1.33	1.38
56	Pt	16	H2U	C4-N3	-2.66	1.33	1.37
58	Dt	39	PSU	C6-C5	-2.66	1.32	1.35
1	16	1207	2MG	C6-N1	-2.64	1.33	1.38
56	Pt	37	T6A	C4-N9	-2.64	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	1516	2MG	C6-N1	-2.63	1.33	1.38
1	16	967	5MC	C6-C5	2.60	1.38	1.34
23	23	2030	6MZ	C5-C6	2.60	1.48	1.41
58	Dt	37	MIA	C4-N9	-2.59	1.32	1.37
23	23	1939	5MU	C6-C5	2.58	1.38	1.34
23	23	2445	2MG	C6-N1	-2.58	1.34	1.38
56	Pt	20	H2U	O2-C2	-2.57	1.18	1.23
23	23	1962	5MC	C6-C5	2.56	1.38	1.34
1	16	527	G7M	C6-N1	-2.55	1.34	1.38
58	Dt	32	PSU	C6-C5	-2.55	1.32	1.35
23	23	2503	2MA	C5-C6	2.54	1.48	1.41
58	Dt	55	PSU	O4'-C1'	-2.53	1.40	1.43
1	16	1407	5MC	C6-C5	2.53	1.38	1.34
1	16	966	2MG	C6-N1	-2.53	1.34	1.38
23	23	1618	6MZ	C5-C6	2.52	1.48	1.41
56	Pt	54	5MU	C6-C5	2.52	1.38	1.34
23	23	2604	PSU	C6-C5	2.51	1.38	1.35
23	23	1618	6MZ	C5-N7	-2.51	1.34	1.39
23	23	747	5MU	C6-N1	-2.49	1.33	1.38
23	23	2030	6MZ	C5-N7	-2.48	1.34	1.39
56	Pt	20	H2U	C3'-C4'	2.48	1.59	1.53
23	23	747	5MU	C6-C5	2.48	1.38	1.34
23	23	2503	2MA	C5-N7	-2.47	1.34	1.39
23	23	1939	5MU	C2-N3	-2.44	1.33	1.38
56	Pt	20	H2U	O4'-C4'	2.43	1.50	1.45
23	23	1939	5MU	C6-N1	-2.43	1.33	1.38
56	Pt	34	U8U	C6-N1	-2.43	1.33	1.38
56	Pt	17	H2U	C4-N3	-2.42	1.33	1.37
23	23	1915	3TD	C2-N1	-2.41	1.34	1.37
23	23	2552	OMU	O3'-C3'	2.40	1.48	1.43
23	23	747	5MU	C2-N3	-2.40	1.33	1.38
1	16	967	5MC	C6-N1	-2.39	1.33	1.38
23	23	1962	5MC	C6-N1	-2.39	1.33	1.38
56	Pt	54	5MU	C6-N1	-2.38	1.34	1.38
1	16	1518	MA6	C5-N7	-2.36	1.34	1.39
1	16	1407	5MC	C6-N1	-2.36	1.34	1.38
23	23	745	1MG	C2-N1	2.33	1.41	1.37
58	Dt	37	MIA	C8-N9	-2.32	1.33	1.37
23	23	2552	OMU	C6-N1	2.31	1.43	1.38
23	23	1835	2MG	C5-N7	-2.31	1.34	1.39
23	23	745	1MG	C5-N7	-2.29	1.34	1.39
23	23	2069	G7M	C4-N9	-2.26	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	1519	MA6	C5-N7	-2.25	1.35	1.39
23	23	2449	H2U	O4'-C4'	2.25	1.50	1.45
23	23	2445	2MG	C5-N7	-2.24	1.34	1.39
23	23	2030	6MZ	C8-N7	2.23	1.36	1.31
23	23	2030	6MZ	C4-N9	-2.22	1.33	1.37
1	16	1519	MA6	C4-N9	-2.22	1.33	1.37
1	16	1207	2MG	C5-N7	-2.21	1.34	1.39
23	23	2069	G7M	C6-N1	-2.21	1.34	1.38
23	23	2498	OMC	C6-N1	-2.21	1.32	1.38
58	Dt	8	4SU	C2-N3	-2.21	1.34	1.38
1	16	1516	2MG	C5-N7	-2.20	1.34	1.39
1	16	966	2MG	C5-N7	-2.19	1.34	1.39
56	Pt	54	5MU	C2-N3	-2.18	1.34	1.38
23	23	2503	2MA	C8-N7	2.18	1.35	1.31
1	16	1519	MA6	C8-N7	2.18	1.35	1.31
23	23	2457	PSU	C2-N3	-2.17	1.33	1.37
56	Pt	37	T6A	C6-N6	-2.17	1.34	1.39
23	23	2504	PSU	C2-N3	-2.16	1.33	1.37
58	Dt	39	PSU	O2'-C2'	-2.15	1.37	1.43
23	23	747	5MU	C4-C5	2.15	1.48	1.44
23	23	2449	H2U	C3'-C4'	2.14	1.58	1.53
23	23	2604	PSU	C6-N1	-2.13	1.32	1.36
23	23	1618	6MZ	C8-N7	2.12	1.35	1.31
56	Pt	54	5MU	C4-C5	2.11	1.48	1.44
23	23	955	PSU	C2-N3	-2.11	1.34	1.37
1	16	1518	MA6	C4-N9	-2.11	1.33	1.37
23	23	2580	PSU	O4'-C1'	-2.11	1.40	1.43
23	23	2498	OMC	C5-C4	-2.10	1.38	1.42
12	SL	89	D2T	CB1-SB	-2.10	1.75	1.79
58	Dt	32	PSU	C3'-C2'	-2.07	1.47	1.53
23	23	2605	PSU	C2-N3	-2.07	1.34	1.37
23	23	1939	5MU	C4-C5	2.07	1.48	1.44
23	23	2503	2MA	C4-N9	-2.06	1.33	1.37
23	23	746	PSU	C2-N3	-2.06	1.34	1.37
56	Pt	37	T6A	C10-N6	-2.05	1.32	1.37
23	23	1618	6MZ	C4-N9	-2.05	1.33	1.37
23	23	2449	H2U	C1'-N1	-2.05	1.43	1.46
1	16	1516	2MG	C4-N9	-2.05	1.32	1.38
1	16	516	PSU	C2-N3	-2.04	1.34	1.37
1	16	1518	MA6	C8-N7	2.04	1.35	1.31
58	Dt	55	PSU	C1'-C5	-2.04	1.45	1.50
56	Pt	39	PSU	C2-N3	-2.02	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	747	5MU	C2-N1	2.02	1.41	1.38
1	16	1207	2MG	C2-N3	2.02	1.35	1.32
56	Pt	37	T6A	C8-N9	-2.02	1.34	1.37
1	16	966	2MG	C2-N3	2.01	1.35	1.32
23	23	2580	PSU	C2-N3	-2.01	1.34	1.37

All (311) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Dt	46	G7M	CN7-N7-C8	-9.39	110.57	124.79
58	Dt	37	MIA	C12-C13-C14	-9.35	110.23	127.01
58	Dt	32	PSU	N1-C2-N3	9.22	124.89	115.17
23	23	2069	G7M	CN7-N7-C8	-8.58	111.80	124.79
23	23	2503	2MA	C5-C4-N3	-8.07	118.68	127.18
1	16	527	G7M	CN7-N7-C8	-7.96	112.73	124.79
58	Dt	55	PSU	N1-C2-N3	7.71	123.31	115.17
58	Dt	37	MIA	C5-C4-N3	-7.62	119.15	127.18
23	23	2445	2MG	C2-N3-C4	7.22	121.03	112.00
23	23	1915	3TD	N1-C2-N3	7.21	121.37	116.13
58	Dt	32	PSU	C4-N3-C2	-7.19	116.47	126.37
23	23	1835	2MG	C2-N3-C4	7.18	120.98	112.00
1	16	1207	2MG	C2-N3-C4	7.18	120.98	112.00
1	16	966	2MG	C2-N3-C4	7.12	120.91	112.00
1	16	1516	2MG	C2-N3-C4	7.11	120.89	112.00
58	Dt	8	4SU	C4-N3-C2	-6.98	120.62	127.31
1	16	1498	UR3	C4-N3-C2	-6.90	119.02	124.58
1	16	527	G7M	N9-C8-N7	-6.84	95.86	112.48
23	23	2604	PSU	N1-C2-N3	6.83	122.38	115.17
23	23	2457	PSU	N1-C2-N3	6.81	122.35	115.17
58	Dt	46	G7M	N9-C8-N7	-6.79	95.99	112.48
58	Dt	46	G7M	N9-C4-N3	6.68	139.31	125.95
1	16	516	PSU	N1-C2-N3	6.68	122.22	115.17
23	23	955	PSU	N1-C2-N3	6.66	122.19	115.17
23	23	2069	G7M	N9-C8-N7	-6.60	96.45	112.48
23	23	2504	PSU	N1-C2-N3	6.58	122.11	115.17
1	16	527	G7M	C8-N7-C5	6.57	115.99	107.78
23	23	2580	PSU	N1-C2-N3	6.56	122.09	115.17
23	23	2552	OMU	C4-N3-C2	-6.56	118.47	126.61
56	Pt	39	PSU	N1-C2-N3	6.52	122.05	115.17
56	Pt	55	PSU	N1-C2-N3	6.49	122.02	115.17
23	23	2605	PSU	N1-C2-N3	6.43	121.96	115.17
58	Dt	39	PSU	N1-C2-N3	6.30	121.82	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	746	PSU	N1-C2-N3	6.30	121.81	115.17
58	Dt	39	PSU	O2-C2-N1	-6.24	116.36	122.79
1	16	527	G7M	N9-C4-N3	6.24	138.42	125.95
58	Dt	37	MIA	N3-C4-N9	6.22	134.89	126.99
23	23	2503	2MA	N3-C4-N9	6.22	134.89	126.99
58	Dt	46	G7M	C8-N7-C5	6.21	115.55	107.78
23	23	1835	2MG	C5-C4-N3	-6.19	118.55	128.39
23	23	2069	G7M	C8-N7-C5	6.17	115.49	107.78
23	23	2445	2MG	C5-C4-N3	-6.08	118.72	128.39
1	16	1207	2MG	C5-C4-N3	-6.04	118.78	128.39
58	Dt	37	MIA	C11-S10-C2	-6.03	97.72	102.25
1	16	966	2MG	C5-C4-N3	-6.00	118.84	128.39
1	16	1516	2MG	C5-C4-N3	-5.95	118.92	128.39
58	Dt	8	4SU	C5-C4-N3	5.83	120.17	114.75
23	23	1618	6MZ	C5-C4-N3	-5.72	118.84	126.72
58	Dt	39	PSU	C6-C5-C4	-5.70	114.33	118.17
56	Pt	47	3AU	C4-N3-C2	-5.69	117.98	124.66
58	Dt	55	PSU	C4-N3-C2	-5.69	118.54	126.37
58	Dt	46	G7M	CN7-N7-C5	5.68	133.88	126.80
23	23	2030	6MZ	C5-C4-N3	-5.66	118.92	126.72
56	Pt	37	T6A	C5-C4-N3	-5.62	118.98	126.72
1	16	1518	MA6	C5-C4-N3	-5.57	119.05	126.72
23	23	2069	G7M	N9-C4-N3	5.41	136.78	125.95
1	16	527	G7M	C5-C4-N3	-5.36	118.01	128.15
58	Dt	46	G7M	C5-C4-N3	-5.36	118.03	128.15
1	16	1519	MA6	C5-C4-N3	-5.33	119.38	126.72
23	23	1939	5MU	C4-N3-C2	-5.31	120.38	127.34
23	23	2030	6MZ	C9-N6-C6	-5.22	118.00	122.85
23	23	2069	G7M	C2-N3-C4	5.20	121.25	112.30
23	23	1939	5MU	N3-C2-N1	5.16	121.61	114.89
56	Pt	54	5MU	C4-N3-C2	-5.15	120.59	127.34
58	Dt	39	PSU	C4-N3-C2	-5.15	119.28	126.37
23	23	1915	3TD	C4-N3-C2	-5.13	119.18	124.61
23	23	745	1MG	C5-C4-N3	-5.13	120.23	128.39
23	23	747	5MU	C4-N3-C2	-5.10	120.65	127.34
58	Dt	46	G7M	C1'-N9-C8	-5.06	109.65	126.74
58	Dt	55	PSU	O2-C2-N1	-5.05	117.58	122.79
23	23	747	5MU	N3-C2-N1	5.02	121.42	114.89
56	Pt	54	5MU	N3-C2-N1	5.00	121.41	114.89
23	23	2069	G7M	C5-C4-N3	-4.94	118.82	128.15
56	Pt	37	T6A	N3-C4-N9	4.92	135.53	127.17
58	Dt	47	3AU	C4-N3-C2	-4.82	119.00	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	2069	G7M	CN7-N7-C5	4.74	132.71	126.80
58	Dt	46	G7M	C2-N3-C4	4.63	120.27	112.30
23	23	1835	2MG	N9-C4-N3	4.61	135.17	125.95
23	23	1939	5MU	C5-C4-N3	4.61	119.33	115.32
56	Pt	37	T6A	N6-C10-N11	4.61	120.10	113.77
23	23	1618	6MZ	N3-C4-N9	4.58	134.96	127.17
58	Dt	46	G7M	C8-N9-C4	4.57	118.41	107.09
56	Pt	54	5MU	C5-C4-N3	4.50	119.24	115.32
1	16	966	2MG	N9-C4-N3	4.43	134.81	125.95
1	16	1207	2MG	N9-C4-N3	4.41	134.78	125.95
23	23	2457	PSU	C4-N3-C2	-4.41	120.30	126.37
58	Dt	16	H2U	C3'-C2'-C1'	4.40	109.78	101.46
23	23	747	5MU	C5-C4-N3	4.38	119.13	115.32
23	23	2552	OMU	C5-C4-N3	4.36	120.90	114.80
1	16	1518	MA6	C2-N1-C6	4.35	122.45	111.83
1	16	1519	MA6	C2-N1-C6	4.34	122.43	111.83
23	23	2445	2MG	N9-C4-N3	4.34	134.62	125.95
1	16	527	G7M	C2-N3-C4	4.33	119.76	112.30
23	23	2552	OMU	N3-C2-N1	4.32	120.52	114.89
23	23	745	1MG	C2-N3-C4	4.31	121.67	111.98
1	16	527	G7M	C8-N9-C4	4.31	117.76	107.09
23	23	2552	OMU	C2'-C1'-N1	-4.30	106.07	114.24
1	16	516	PSU	C4-N3-C2	-4.30	120.45	126.37
23	23	2030	6MZ	N3-C4-N9	4.29	134.46	127.17
23	23	955	PSU	C4-N3-C2	-4.29	120.47	126.37
1	16	1518	MA6	N3-C4-N9	4.28	134.45	127.17
1	16	1516	2MG	N9-C4-N3	4.25	134.45	125.95
56	Pt	39	PSU	C4-N3-C2	-4.24	120.53	126.37
23	23	2449	H2U	N3-C2-N1	4.23	120.90	116.65
1	16	1519	MA6	C4-C5-N7	-4.21	105.77	110.58
23	23	2605	PSU	C4-N3-C2	-4.20	120.58	126.37
56	Pt	55	PSU	C4-N3-C2	-4.20	120.59	126.37
58	Dt	8	4SU	N3-C2-N1	4.20	120.35	114.89
23	23	2504	PSU	C4-N3-C2	-4.19	120.60	126.37
58	Dt	37	MIA	N6-C6-N1	4.17	123.93	118.33
23	23	746	PSU	C4-N3-C2	-4.17	120.63	126.37
23	23	2069	G7M	C8-N9-C4	4.09	117.23	107.09
58	Dt	37	MIA	C16-C14-C13	-4.08	110.41	122.66
58	Dt	8	4SU	C5-C4-S4	-4.08	119.65	124.31
23	23	2498	OMC	C2'-C1'-N1	-4.07	106.51	114.24
1	16	1518	MA6	C4-C5-N7	-4.05	105.95	110.58
23	23	2030	6MZ	C6-C5-N7	4.05	136.84	132.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	2580	PSU	C4-N3-C2	-4.04	120.81	126.37
56	Pt	37	T6A	N3-C2-N1	-4.04	122.47	128.58
58	Dt	16	H2U	O3'-C3'-C2'	-4.03	98.89	111.82
23	23	2604	PSU	C4-N3-C2	-4.02	120.83	126.37
56	Pt	54	5MU	O4-C4-C5	-4.02	120.32	124.92
23	23	955	PSU	O2-C2-N1	-4.01	118.65	122.79
58	Dt	55	PSU	C2'-C3'-C4'	-4.01	94.87	102.61
58	Dt	37	MIA	C15-C14-C13	-4.00	110.66	122.66
23	23	1939	5MU	C5-C6-N1	-3.92	119.06	123.31
23	23	745	1MG	N9-C4-N3	3.92	133.78	125.95
23	23	1939	5MU	O4-C4-C5	-3.90	120.46	124.92
58	Dt	32	PSU	O2-C2-N1	-3.89	118.77	122.79
1	16	1519	MA6	N3-C4-N9	3.89	133.78	127.17
23	23	747	5MU	O4-C4-C5	-3.87	120.50	124.92
1	16	516	PSU	O2-C2-N1	-3.84	118.83	122.79
23	23	2030	6MZ	C4-C5-N7	-3.83	106.21	110.58
58	Dt	37	MIA	C2-N3-C4	3.77	122.17	112.29
23	23	2030	6MZ	C2-N3-C4	3.74	120.98	111.83
56	Pt	37	T6A	C2-N3-C4	3.74	120.97	111.83
1	16	1518	MA6	C2-N3-C4	3.71	120.89	111.83
56	Pt	55	PSU	O2-C2-N1	-3.70	118.97	122.79
23	23	1618	6MZ	C2-N3-C4	3.70	120.86	111.83
58	Dt	39	PSU	C3'-C2'-C1'	3.70	106.05	101.69
23	23	2580	PSU	O2-C2-N1	-3.68	118.99	122.79
23	23	2457	PSU	O2-C2-N1	-3.68	118.99	122.79
1	16	1519	MA6	C2-N3-C4	3.68	120.81	111.83
58	Dt	37	MIA	C2'-C1'-N9	-3.63	104.29	113.30
1	16	527	G7M	C1'-N9-C8	-3.62	114.53	126.74
23	23	747	5MU	C5-C6-N1	-3.61	119.40	123.31
56	Pt	39	PSU	O2-C2-N1	-3.60	119.07	122.79
1	16	527	G7M	CN7-N7-C5	3.60	131.28	126.80
56	Pt	47	3AU	C10-N3-C2	3.59	122.94	117.64
36	LP	81	4D4	NE-CZ-NH2	-3.57	114.54	120.67
58	Dt	37	MIA	C4-N9-C8	3.54	109.46	105.74
23	23	2503	2MA	C4-C5-N7	-3.52	106.56	110.58
23	23	1618	6MZ	C9-N6-C6	-3.51	119.59	122.85
58	Dt	37	MIA	C6-C5-N7	3.50	136.25	132.43
1	16	1519	MA6	N1-C2-N3	-3.48	123.31	128.58
1	16	1498	UR3	C5-C4-N3	3.48	119.62	115.04
1	16	1516	2MG	C6-C5-N7	3.46	136.58	130.29
23	23	746	PSU	O2-C2-N1	-3.45	119.23	122.79
58	Dt	55	PSU	C5-C6-N1	-3.43	117.37	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16	1518	MA6	N1-C2-N3	-3.43	123.39	128.58
23	23	2605	PSU	O2-C2-N1	-3.43	119.25	122.79
23	23	2449	H2U	C5-C4-N3	3.42	120.32	116.69
56	Pt	54	5MU	C5-C6-N1	-3.41	119.61	123.31
23	23	1962	5MC	C5-C6-N1	-3.41	119.61	123.31
23	23	2504	PSU	O2-C2-N1	-3.40	119.28	122.79
1	16	967	5MC	C5-C6-N1	-3.39	119.63	123.31
56	Pt	20	H2U	N3-C2-N1	3.39	120.05	116.65
23	23	2445	2MG	C6-C5-N7	3.37	136.42	130.29
56	Pt	47	3AU	C5-C4-N3	3.36	120.28	115.64
1	16	1207	2MG	C6-C5-N7	3.36	136.40	130.29
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
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
36	LP	81	4D4	NH1-CZ-NE	3.27	126.70	119.27
1	16	966	2MG	C6-C5-N7	3.26	136.22	130.29
58	Dt	37	MIA	C4-C5-N7	-3.26	106.86	110.58
58	Dt	32	PSU	C3'-C2'-C1'	3.16	105.42	101.69
23	23	1835	2MG	C6-C5-N7	3.16	136.04	130.29
23	23	2604	PSU	O2-C2-N1	-3.15	119.53	122.79
1	16	1407	5MC	C5-C6-N1	-3.14	119.90	123.31
58	Dt	32	PSU	O2-C2-N3	-3.12	116.31	121.86
56	Pt	37	T6A	C12-N11-C10	3.11	127.15	121.99
58	Dt	39	PSU	C4'-O4'-C1'	3.04	116.06	108.44
58	Dt	32	PSU	C5-C6-N1	-3.04	117.92	122.14
56	Pt	37	T6A	N6-C6-N1	3.03	125.38	117.54
56	Pt	20	H2U	C5-C4-N3	3.00	119.88	116.69
23	23	2552	OMU	O4-C4-C5	-2.97	120.05	125.16
58	Dt	37	MIA	N3-C2-N1	-2.96	121.60	127.00
23	23	2069	G7M	O4'-C1'-N9	2.95	115.03	108.36
56	Pt	37	T6A	O10-C10-N6	-2.93	118.43	123.64
23	23	2449	H2U	C5-C6-N1	2.93	120.37	111.52
58	Dt	37	MIA	O3'-C3'-C2'	-2.92	102.44	111.82
23	23	2030	6MZ	C4-N9-C8	2.92	108.81	105.74
1	16	1519	MA6	C5-N7-C8	2.92	108.04	103.45
1	16	1518	MA6	C5-N7-C8	2.92	108.03	103.45
23	23	2069	G7M	C2'-C1'-N9	-2.91	105.15	113.25
23	23	1915	3TD	C1'-C5-C4	2.91	122.02	117.61
23	23	1939	5MU	O2-C2-N1	-2.91	119.01	122.80
56	Pt	37	T6A	C4-N9-C8	2.90	108.78	105.74
1	16	1518	MA6	C4-N9-C8	2.89	108.77	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	2069	G7M	C6-C5-N7	2.85	135.75	132.17
23	23	2503	2MA	N6-C6-N1	2.83	120.85	117.03
23	23	2069	G7M	O6-C6-C5	-2.83	121.70	128.01
23	23	2030	6MZ	C5-N7-C8	2.83	107.89	103.45
1	16	1519	MA6	C4-N9-C8	2.81	108.69	105.74
56	Pt	20	H2U	C5-C6-N1	2.79	119.97	111.52
56	Pt	20	H2U	O2-C2-N1	-2.76	119.79	123.10
58	Dt	47	3AU	C5-C4-N3	2.75	119.45	115.64
23	23	1618	6MZ	C4-N9-C8	2.75	108.63	105.74
58	Dt	37	MIA	N9-C8-N7	-2.73	110.07	113.94
23	23	2503	2MA	C4-N9-C8	2.72	108.59	105.74
58	Dt	55	PSU	O4'-C4'-C3'	-2.72	99.75	105.15
23	23	2445	2MG	C4-C5-N7	-2.70	106.39	110.67
23	23	2069	G7M	N2-C2-N1	2.69	122.44	116.76
56	Pt	16	H2U	C3'-C2'-C1'	2.68	106.54	101.46
23	23	745	1MG	C6-C5-N7	2.68	135.31	129.36
58	Dt	37	MIA	C5-N7-C8	2.68	107.66	103.45
1	16	1516	2MG	C4-C5-N7	-2.67	106.44	110.67
58	Dt	55	PSU	C3'-C2'-C1'	2.65	104.81	101.69
58	Dt	39	PSU	O2'-C2'-C1'	-2.64	104.95	111.21
23	23	2503	2MA	C5-N7-C8	2.63	107.58	103.45
1	16	1407	5MC	C5-C4-N3	-2.61	119.08	121.75
1	16	1519	MA6	C6-C5-N7	2.60	137.59	133.43
23	23	2503	2MA	C2-N1-C6	2.60	122.10	118.10
56	Pt	54	5MU	O2-C2-N1	-2.60	119.41	122.80
23	23	2604	PSU	O2'-C2'-C3'	-2.60	103.50	111.82
1	16	967	5MC	C5-C4-N3	-2.59	119.10	121.75
23	23	1962	5MC	C5-C4-N3	-2.59	119.10	121.75
58	Dt	37	MIA	O4'-C4'-C3'	-2.58	100.04	105.15
1	16	1207	2MG	C4-C5-N7	-2.58	106.59	110.67
58	Dt	46	G7M	C5-C6-N1	2.56	117.14	111.84
1	16	527	G7M	O6-C6-C5	-2.55	122.31	128.01
23	23	2445	2MG	N1-C2-N2	2.54	119.15	116.56
23	23	2069	G7M	N2-C2-N3	-2.53	114.74	119.67
56	Pt	20	H2U	C3'-C2'-C1'	2.51	106.22	101.46
58	Dt	55	PSU	O2'-C2'-C3'	-2.51	103.78	111.82
58	Dt	39	PSU	O4'-C1'-C2'	-2.50	101.69	105.15
56	Pt	17	H2U	C5-C6-N1	-2.50	103.95	111.52
1	16	966	2MG	C4-C5-N7	-2.50	106.71	110.67
23	23	1618	6MZ	C5-N7-C8	2.49	107.36	103.45
56	Pt	34	U8U	O4-C4-C5	-2.49	120.53	124.71
23	23	745	1MG	C4-C5-N7	-2.48	106.74	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	1835	2MG	C4-C5-N7	-2.47	106.75	110.67
56	Pt	34	U8U	C1'-N1-C6	-2.47	117.08	121.15
56	Pt	37	T6A	C4-C5-N7	-2.47	107.76	110.58
56	Pt	34	U8U	C5-C4-N3	2.46	118.96	115.21
23	23	2030	6MZ	N9-C8-N7	-2.44	110.48	113.94
58	Dt	46	G7M	O6-C6-C5	-2.42	122.61	128.01
23	23	2457	PSU	C5-C6-N1	-2.39	118.83	122.14
56	Pt	37	T6A	C2-N1-C6	2.35	123.02	115.24
58	Dt	37	MIA	C2-N1-C6	2.34	121.99	117.54
23	23	2552	OMU	O2-C2-N1	-2.34	119.75	122.80
58	Dt	39	PSU	O4'-C4'-C3'	-2.34	100.51	105.15
23	23	2069	G7M	C5'-C4'-C3'	-2.34	106.80	115.21
23	23	2069	G7M	C1'-N9-C8	-2.33	118.87	126.74
58	Dt	55	PSU	O4'-C1'-C2'	-2.33	101.94	105.15
56	Pt	17	H2U	N3-C2-N1	-2.32	114.31	116.65
1	16	1519	MA6	N9-C8-N7	-2.31	110.66	113.94
1	16	1402	4OC	C6-C5-C4	2.29	119.76	117.00
23	23	2503	2MA	C6-C5-N7	2.27	136.47	132.09
23	23	747	5MU	O2-C2-N1	-2.26	119.86	122.80
1	16	1518	MA6	N9-C8-N7	-2.25	110.75	113.94
23	23	2604	PSU	C3'-C2'-C1'	2.24	104.33	101.69
1	16	1516	2MG	N1-C2-N2	2.24	118.84	116.56
1	16	1518	MA6	C6-C5-N7	2.23	136.99	133.43
58	Dt	16	H2U	O4'-C1'-N1	2.22	112.33	109.30
56	Pt	37	T6A	C6-C5-N7	2.22	134.85	132.43
58	Dt	8	4SU	O2-C2-N1	-2.21	119.92	122.80
1	16	516	PSU	C5-C6-N1	-2.21	119.08	122.14
23	23	2503	2MA	N9-C8-N7	-2.19	110.83	113.94
23	23	2580	PSU	O4'-C1'-C2'	2.19	108.18	105.15
56	Pt	39	PSU	C5-C6-N1	-2.19	119.10	122.14
58	Dt	47	3AU	C2'-C3'-C4'	2.18	106.81	102.61
58	Dt	16	H2U	O2'-C2'-C3'	-2.17	104.85	111.82
23	23	2445	2MG	O6-C6-C5	-2.16	120.83	126.53
58	Dt	37	MIA	C5-C6-N6	-2.16	117.86	122.03
23	23	2069	G7M	C5-C6-N1	2.16	116.31	111.84
1	16	516	PSU	O4'-C1'-C2'	2.16	108.14	105.15
58	Dt	47	3AU	C3'-C2'-C1'	2.15	105.54	101.46
1	16	966	2MG	O6-C6-C5	-2.15	120.85	126.53
1	16	1498	UR3	C1'-N1-C2	2.15	120.55	117.04
56	Pt	54	5MU	C5M-C5-C4	2.13	121.06	118.78
12	SL	89	D2T	CB-CA-N	2.13	113.42	109.10
23	23	2604	PSU	O4'-C4'-C3'	-2.13	100.92	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	2445	2MG	CM2-N2-C2	-2.13	119.07	123.65
23	23	1835	2MG	O6-C6-C5	-2.13	120.91	126.53
23	23	2604	PSU	O2-C2-N3	-2.12	118.09	121.86
23	23	2605	PSU	C5-C6-N1	-2.12	119.20	122.14
23	23	2604	PSU	C5-C6-N1	-2.12	119.20	122.14
36	LP	81	4D4	O-C-CA	-2.12	119.32	124.77
23	23	2449	H2U	O2-C2-N1	-2.11	120.56	123.10
58	Dt	47	3AU	C10-N3-C4	2.10	121.17	117.10
23	23	2604	PSU	O2'-C2'-C1'	-2.10	106.22	111.21
1	16	1407	5MC	O2-C2-N3	-2.10	119.02	122.33
1	16	1516	2MG	CM2-N2-C2	-2.10	119.14	123.65
23	23	746	PSU	C5-C6-N1	-2.10	119.23	122.14
1	16	1516	2MG	O6-C6-C5	-2.09	121.01	126.53
1	16	1207	2MG	O6-C6-C5	-2.08	121.03	126.53
58	Dt	39	PSU	O4-C4-C5	-2.08	118.85	124.01
1	16	966	2MG	N1-C2-N2	2.07	118.68	116.56
56	Pt	55	PSU	C5-C6-N1	-2.06	119.28	122.14
23	23	2445	2MG	C2-N1-C6	-2.06	122.06	124.55
23	23	2504	PSU	C5-C6-N1	-2.05	119.29	122.14
23	23	2445	2MG	N2-C2-N3	-2.05	117.89	120.51
56	Pt	47	3AU	O2-C2-N1	-2.05	118.21	122.78
1	16	1516	2MG	C2-N1-C6	-2.05	122.07	124.55
23	23	1618	6MZ	N9-C8-N7	-2.05	111.03	113.94
23	23	955	PSU	C5-C6-N1	-2.04	119.31	122.14
12	SL	89	D2T	O-C-CA	-2.04	119.53	124.77
23	23	2580	PSU	C5-C6-N1	-2.00	119.36	122.14

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	527	G7M	O4'-C4'-C5'-O5'
1	16	527	G7M	C3'-C4'-C5'-O5'
12	SL	89	D2T	SB-CB-CG-OD2
23	23	1618	6MZ	O4'-C4'-C5'-O5'
23	23	2251	OMG	O4'-C4'-C5'-O5'
23	23	2251	OMG	C1'-C2'-O2'-CM2
56	Pt	16	H2U	O4'-C4'-C5'-O5'
56	Pt	16	H2U	O4'-C1'-N1-C2
56	Pt	16	H2U	O4'-C1'-N1-C6
56	Pt	20	H2U	C4'-C5'-O5'-P
58	Dt	37	MIA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
58	Dt	37	MIA	C5-C6-N6-C12
58	Dt	37	MIA	N1-C2-S10-C11
58	Dt	37	MIA	N3-C2-S10-C11
58	Dt	37	MIA	C12-C13-C14-C16
1	16	1519	MA6	O4'-C4'-C5'-O5'
23	23	2251	OMG	C3'-C4'-C5'-O5'
23	23	2498	OMC	C3'-C4'-C5'-O5'
56	Pt	16	H2U	C3'-C4'-C5'-O5'
23	23	1915	3TD	C3'-C4'-C5'-O5'
23	23	1915	3TD	O4'-C4'-C5'-O5'
23	23	2030	6MZ	O4'-C4'-C5'-O5'
23	23	2498	OMC	O4'-C4'-C5'-O5'
23	23	2503	2MA	O4'-C4'-C5'-O5'
58	Dt	8	4SU	C3'-C4'-C5'-O5'
58	Dt	8	4SU	O4'-C4'-C5'-O5'
23	23	2030	6MZ	C3'-C4'-C5'-O5'
56	Pt	37	T6A	N11-C12-C14-O14
56	Pt	16	H2U	C2'-C1'-N1-C6
56	Pt	37	T6A	N11-C10-N6-C6
56	Pt	37	T6A	C14-C12-C13-ODA
23	23	1618	6MZ	C3'-C4'-C5'-O5'
23	23	2503	2MA	C3'-C4'-C5'-O5'
56	Pt	47	3AU	C3'-C4'-C5'-O5'
58	Dt	37	MIA	C3'-C4'-C5'-O5'
58	Dt	37	MIA	C12-C13-C14-C15
56	Pt	37	T6A	N11-C12-C13-ODA
1	16	1519	MA6	C3'-C4'-C5'-O5'
23	23	2504	PSU	O4'-C4'-C5'-O5'
56	Pt	47	3AU	O4'-C4'-C5'-O5'
58	Dt	37	MIA	N1-C6-N6-C12
56	Pt	17	H2U	C4'-C5'-O5'-P
56	Pt	37	T6A	C13-C12-C14-C15
56	Pt	47	3AU	C2'-C1'-N1-C6
58	Dt	47	3AU	C2'-C1'-N1-C6
56	Pt	37	T6A	C14-C12-C13-ODB
56	Pt	37	T6A	N11-C12-C13-ODB
56	Pt	16	H2U	C4'-C5'-O5'-P
58	Dt	46	G7M	C2'-C1'-N9-C4
23	23	2445	2MG	C3'-C4'-C5'-O5'
36	LP	81	4D4	OB-CB-CG-CD
58	Dt	47	3AU	O4'-C4'-C5'-O5'
56	Pt	16	H2U	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
36	LP	81	4D4	CA-CB-CG-CD
56	Pt	17	H2U	C2'-C1'-N1-C2
58	Dt	47	3AU	O4'-C1'-N1-C6
56	Pt	37	T6A	N11-C12-C14-C15
56	Pt	47	3AU	O4'-C1'-N1-C6
56	Pt	37	T6A	C13-C12-C14-O14
56	Pt	20	H2U	C3'-C4'-C5'-O5'
58	Dt	47	3AU	C3'-C4'-C5'-O5'
56	Pt	17	H2U	C2'-C1'-N1-C6
58	Dt	46	G7M	C2'-C1'-N9-C8
23	23	2552	OMU	C3'-C2'-O2'-CM2
56	Pt	47	3AU	C11-C10-N3-C4
23	23	2069	G7M	C4'-C5'-O5'-P
58	Dt	47	3AU	O4'-C1'-N1-C2
12	SL	89	D2T	CA-CB-SB-CB1
58	Dt	47	3AU	C2'-C1'-N1-C2
23	23	746	PSU	O4'-C1'-C5-C6
56	Pt	47	3AU	C2'-C1'-N1-C2
56	Pt	47	3AU	O4'-C1'-N1-C2
23	23	2504	PSU	C3'-C4'-C5'-O5'
12	SL	89	D2T	CG-CB-SB-CB1
23	23	746	PSU	C2'-C1'-C5-C6
56	Pt	37	T6A	O10-C10-N6-C6
36	LP	81	4D4	CG-CD-NE-CZ

There are no ring outliers.

9 monomers are involved in 12 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 434 ligands modelled in this entry, 408 are monoatomic - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	PUT	23	3011	-	5,5,5	0.09	0	4,4,4	0.13	0
59	PUT	23	3007	-	5,5,5	0.08	0	4,4,4	0.14	0
59	PUT	23	3008	-	5,5,5	0.09	0	4,4,4	0.13	0
59	PUT	23	3009	-	5,5,5	0.09	0	4,4,4	0.13	0
59	PUT	16	1602	-	5,5,5	0.10	0	4,4,4	0.13	0
63	SPD	23	3020	-	9,9,9	0.31	0	8,8,8	0.91	0
59	PUT	23	3010	-	5,5,5	0.12	0	4,4,4	0.19	0
63	SPD	23	3023	-	9,9,9	0.31	0	8,8,8	0.92	0
63	SPD	23	3019	-	9,9,9	0.32	0	8,8,8	0.95	0
59	PUT	23	3004	-	5,5,5	0.11	0	4,4,4	0.12	0
59	PUT	23	3016	-	5,5,5	0.10	0	4,4,4	0.13	0
59	PUT	23	3005	-	5,5,5	0.09	0	4,4,4	0.13	0
59	PUT	16	1603	-	5,5,5	0.12	0	4,4,4	0.13	0
59	PUT	23	3018	-	5,5,5	0.10	0	4,4,4	0.12	0
63	SPD	23	3021	-	9,9,9	0.31	0	8,8,8	0.87	0
59	PUT	23	3013	-	5,5,5	0.10	0	4,4,4	0.13	0
59	PUT	23	3006	-	5,5,5	0.10	0	4,4,4	0.13	0
59	PUT	23	3014	-	5,5,5	0.11	0	4,4,4	0.13	0
62	ATP	23	3001	-	32,33,33	0.27	0	48,52,52	0.29	0
59	PUT	16	1601	-	5,5,5	0.09	0	4,4,4	0.13	0
62	ATP	23	3003	-	32,33,33	0.25	0	48,52,52	0.27	0
59	PUT	23	3012	-	5,5,5	0.10	0	4,4,4	0.12	0
59	PUT	23	3017	-	5,5,5	0.11	0	4,4,4	0.12	0
62	ATP	23	3002	-	32,33,33	0.54	0	48,52,52	0.57	0
63	SPD	23	3022	-	9,9,9	0.32	0	8,8,8	0.90	0
59	PUT	23	3015	-	5,5,5	0.10	0	4,4,4	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	PUT	23	3011	-	-	0/3/3/3	-
59	PUT	23	3007	-	-	1/3/3/3	-
59	PUT	23	3008	-	-	1/3/3/3	-
59	PUT	23	3009	-	-	3/3/3/3	-
59	PUT	16	1602	-	-	1/3/3/3	-
63	SPD	23	3020	-	-	2/7/7/7	-
59	PUT	23	3010	-	-	1/3/3/3	-
63	SPD	23	3023	-	-	3/7/7/7	-
63	SPD	23	3019	-	-	0/7/7/7	-
59	PUT	23	3004	-	-	1/3/3/3	-
59	PUT	23	3016	-	-	0/3/3/3	-
59	PUT	23	3005	-	-	0/3/3/3	-
59	PUT	16	1603	-	-	1/3/3/3	-
59	PUT	23	3018	-	-	0/3/3/3	-
63	SPD	23	3021	-	-	5/7/7/7	-
59	PUT	23	3013	-	-	0/3/3/3	-
59	PUT	23	3006	-	-	1/3/3/3	-
59	PUT	23	3014	-	-	0/3/3/3	-
62	ATP	23	3001	-	-	10/22/38/38	0/3/3/3
59	PUT	16	1601	-	-	0/3/3/3	-
62	ATP	23	3003	-	-	6/22/38/38	0/3/3/3
59	PUT	23	3012	-	-	0/3/3/3	-
59	PUT	23	3017	-	-	1/3/3/3	-
62	ATP	23	3002	-	-	4/22/38/38	0/3/3/3
63	SPD	23	3022	-	-	1/7/7/7	-
59	PUT	23	3015	-	-	1/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (43) torsion outliers are listed below:

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

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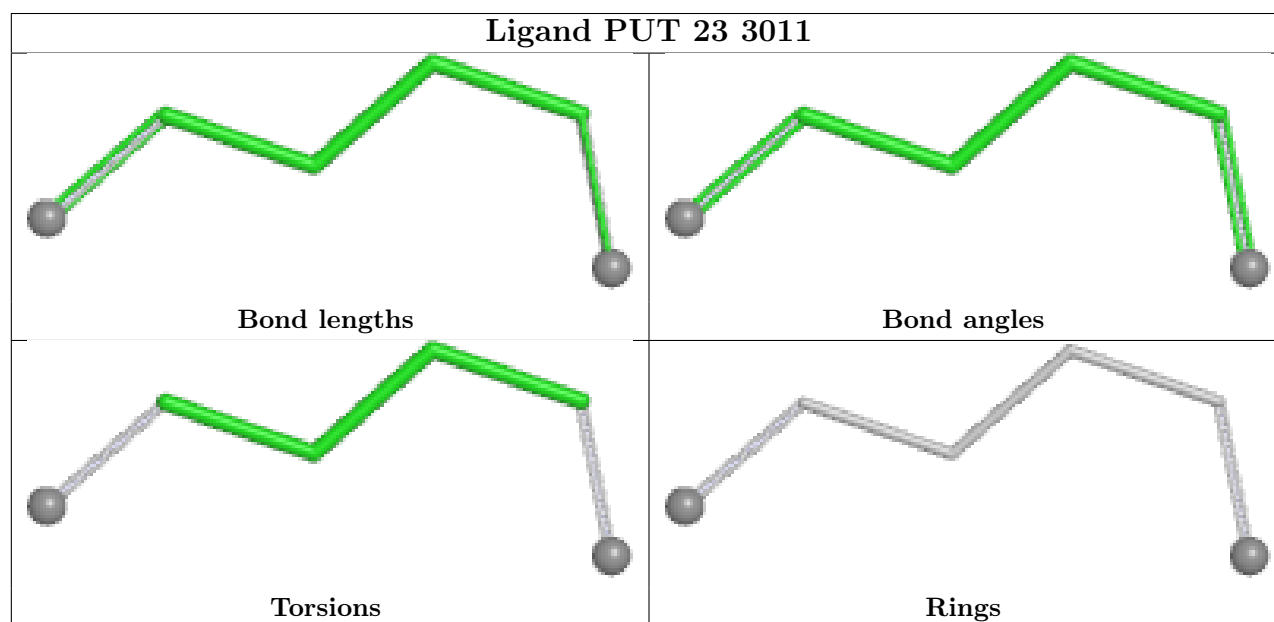
Mol	Chain	Res	Type	Atoms
62	23	3003	ATP	C5'-O5'-PA-O1A
62	23	3003	ATP	C5'-O5'-PA-O2A
62	23	3003	ATP	C5'-O5'-PA-O3A
62	23	3002	ATP	C3'-C4'-C5'-O5'
62	23	3003	ATP	O4'-C4'-C5'-O5'
62	23	3003	ATP	C3'-C4'-C5'-O5'
63	23	3021	SPD	N6-C7-C8-C9
63	23	3023	SPD	N6-C7-C8-C9
63	23	3023	SPD	C3-C4-C5-N6
63	23	3020	SPD	C3-C4-C5-N6
59	23	3007	PUT	C1-C2-C3-C4
62	23	3001	ATP	O4'-C4'-C5'-O5'
62	23	3001	ATP	C3'-C4'-C5'-O5'
59	23	3015	PUT	C1-C2-C3-C4
59	23	3009	PUT	C1-C2-C3-C4
63	23	3021	SPD	C3-C4-C5-N6
62	23	3001	ATP	PG-O3B-PB-O3A
59	23	3009	PUT	C2-C3-C4-N2
59	23	3009	PUT	N1-C1-C2-C3
63	23	3021	SPD	C2-C3-C4-C5
59	16	1603	PUT	C1-C2-C3-C4
62	23	3001	ATP	C5'-O5'-PA-O1A
62	23	3001	ATP	C5'-O5'-PA-O3A
62	23	3002	ATP	C5'-O5'-PA-O1A
63	23	3021	SPD	C7-C8-C9-N10
59	23	3006	PUT	C2-C3-C4-N2
63	23	3020	SPD	N1-C2-C3-C4
63	23	3023	SPD	N1-C2-C3-C4
63	23	3021	SPD	C4-C5-N6-C7
59	23	3004	PUT	C1-C2-C3-C4
59	23	3008	PUT	C1-C2-C3-C4
59	23	3017	PUT	C1-C2-C3-C4
59	16	1602	PUT	C1-C2-C3-C4
62	23	3001	ATP	PG-O3B-PB-O1B
62	23	3001	ATP	PA-O3A-PB-O1B
62	23	3001	ATP	PA-O3A-PB-O2B
62	23	3003	ATP	PA-O3A-PB-O2B
59	23	3010	PUT	N1-C1-C2-C3
63	23	3022	SPD	C7-C8-C9-N10
62	23	3001	ATP	PG-O3B-PB-O2B

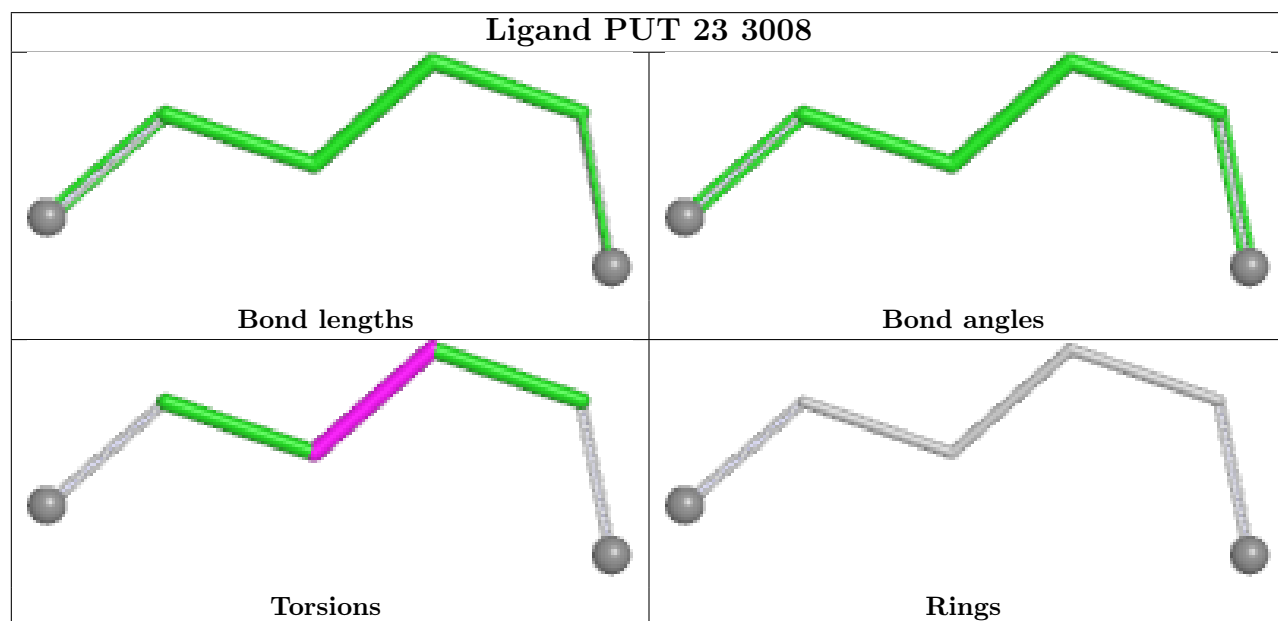
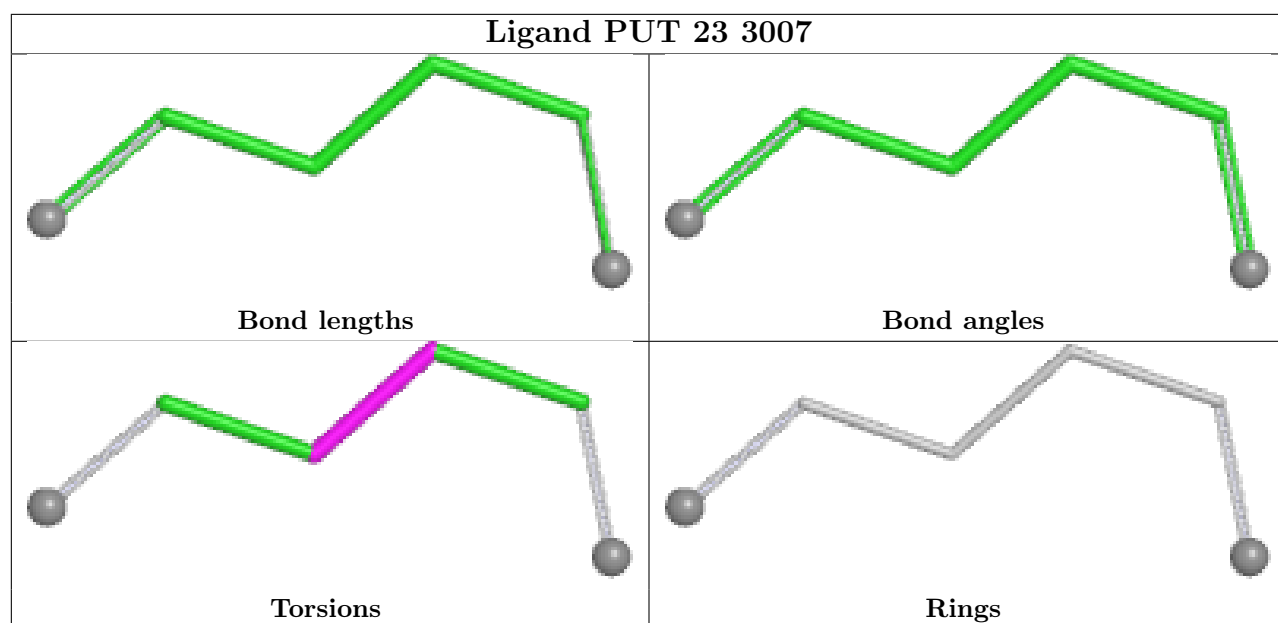
There are no ring outliers.

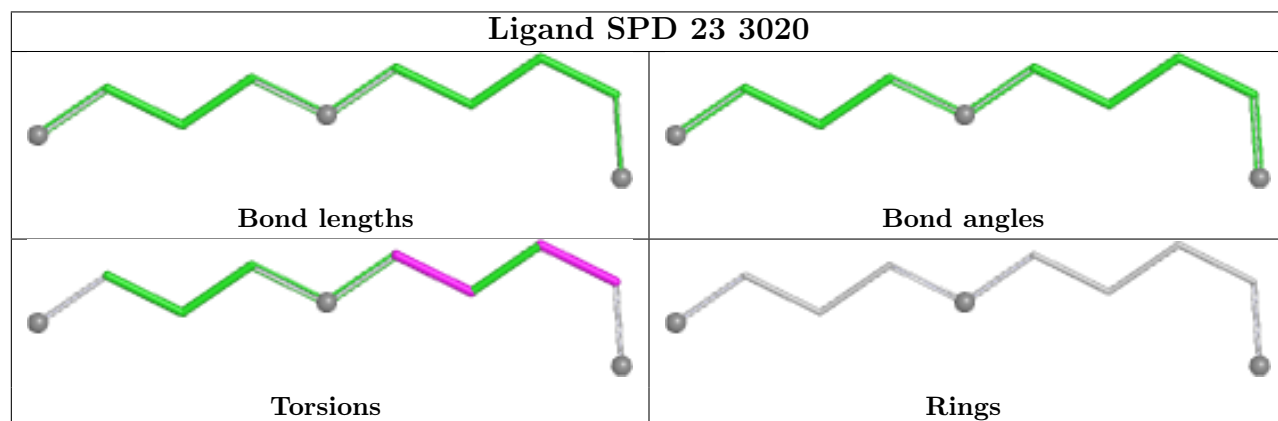
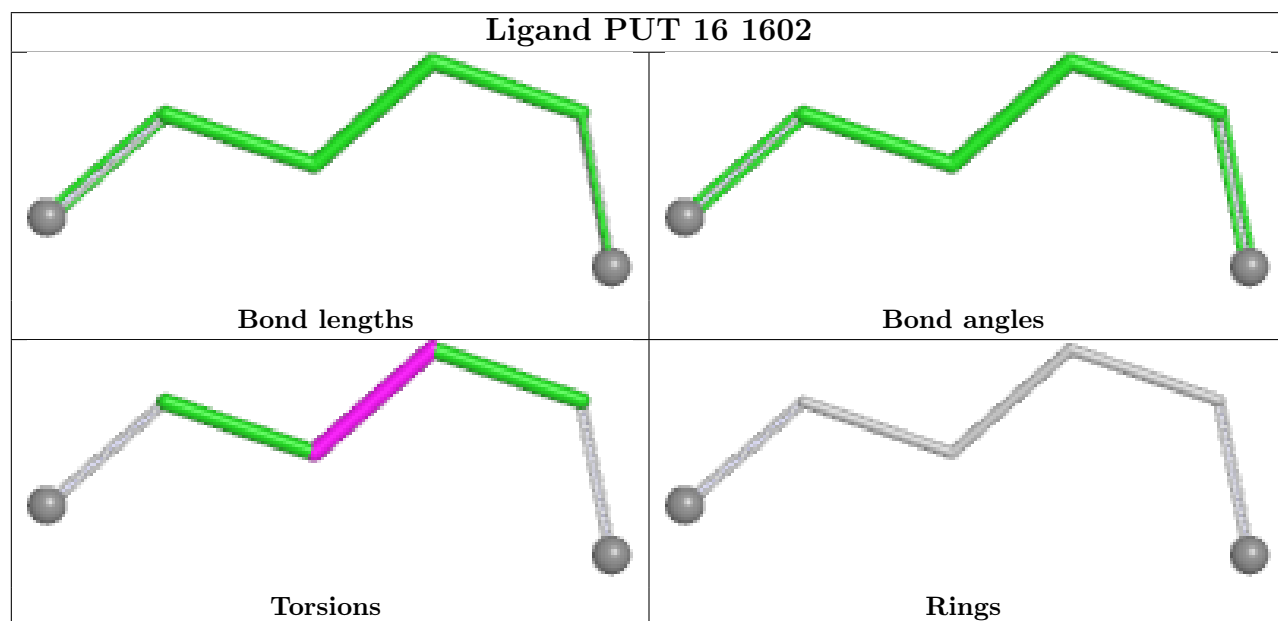
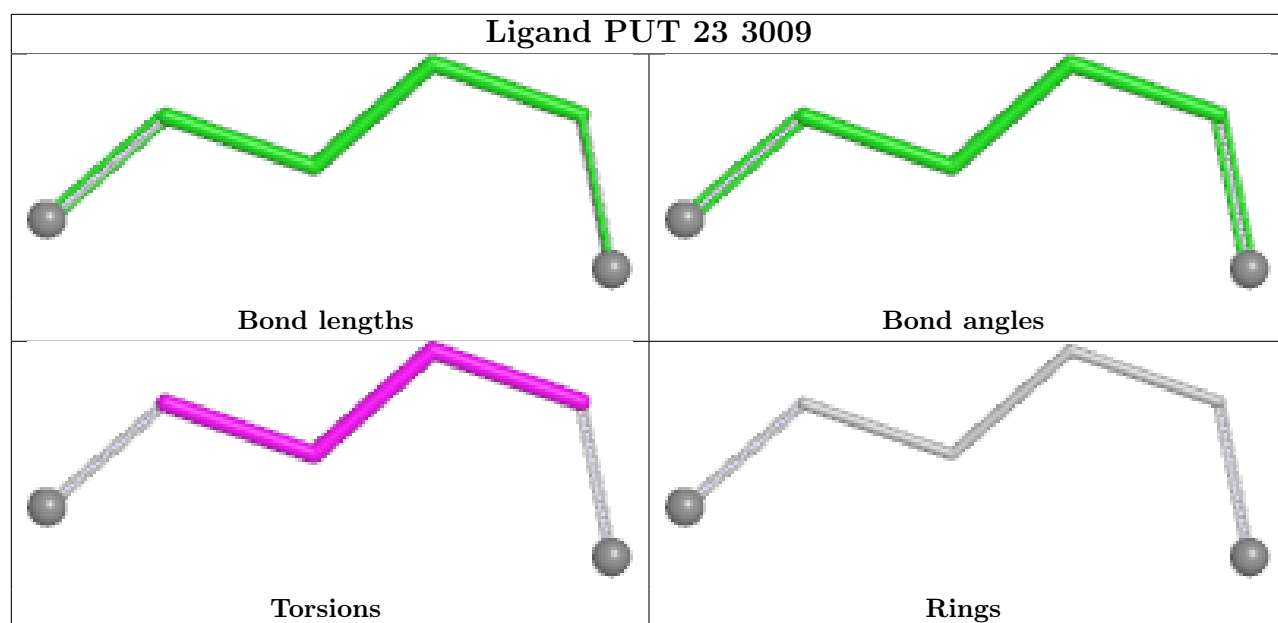
2 monomers are involved in 2 short contacts:

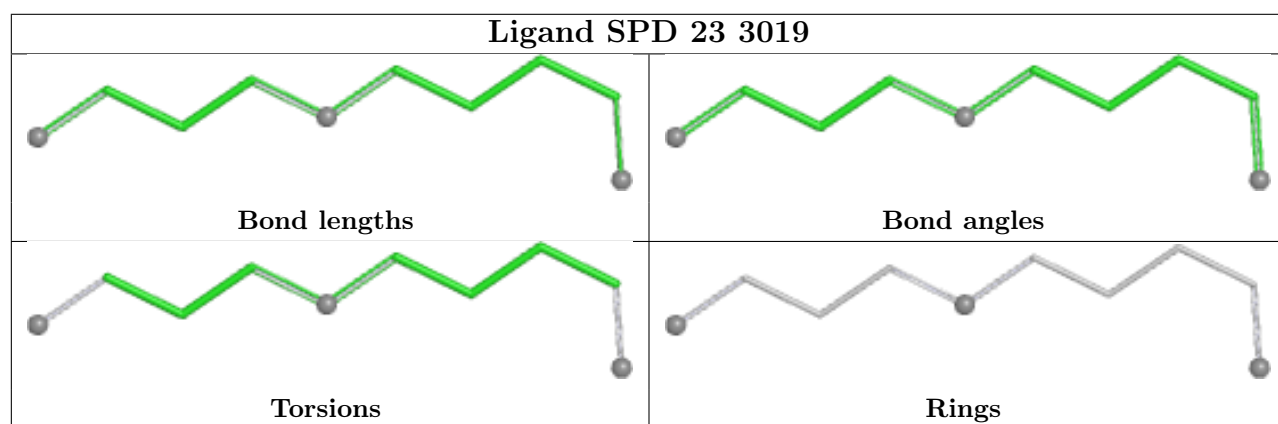
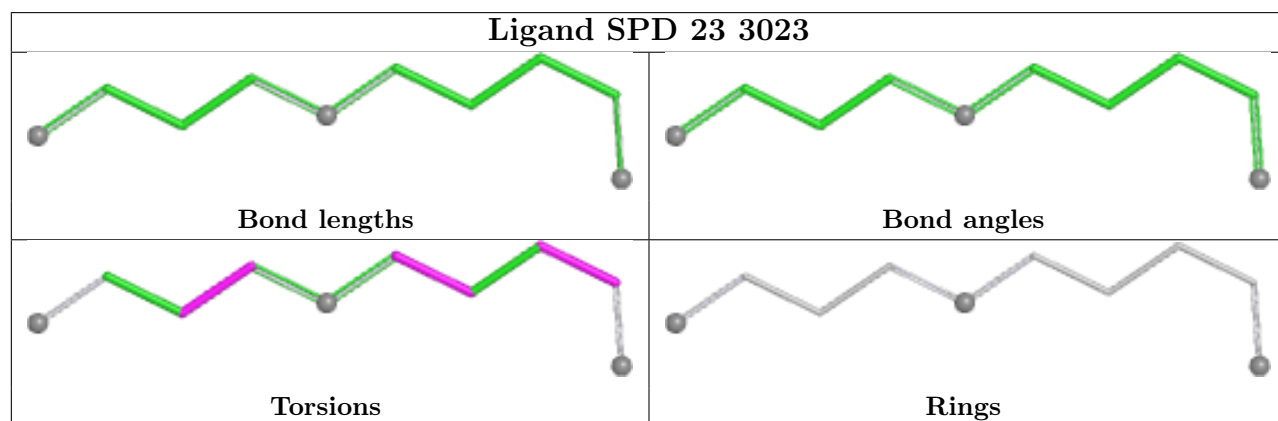
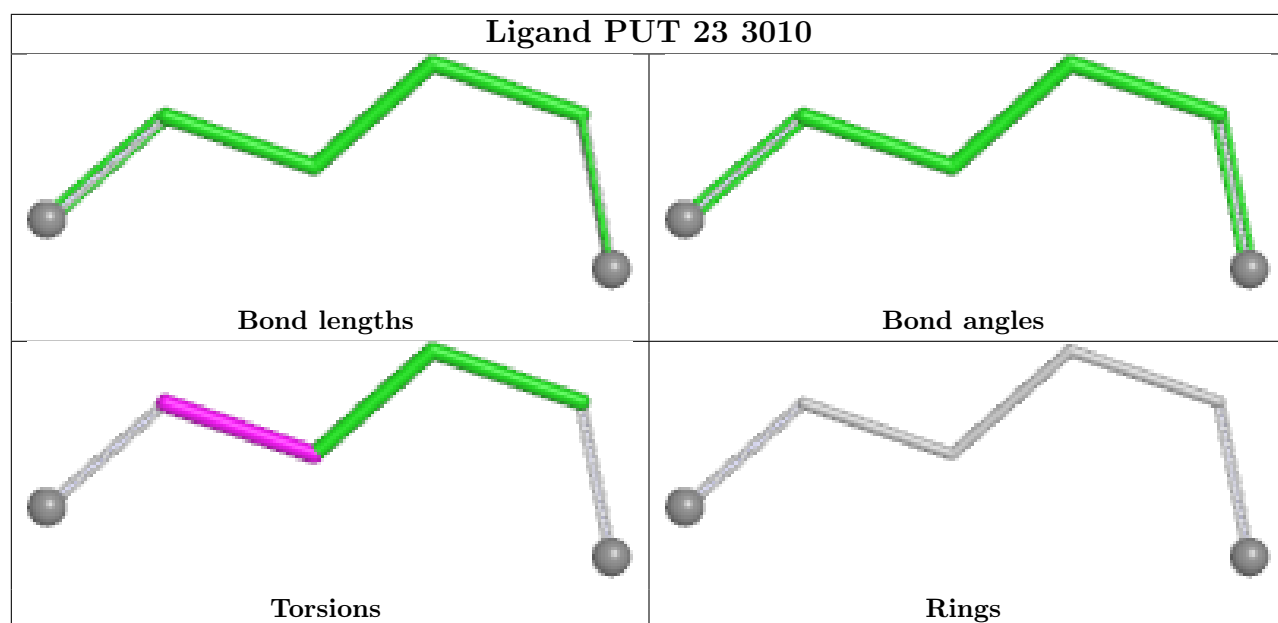
Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	23	3020	SPD	1	0
63	23	3019	SPD	1	0

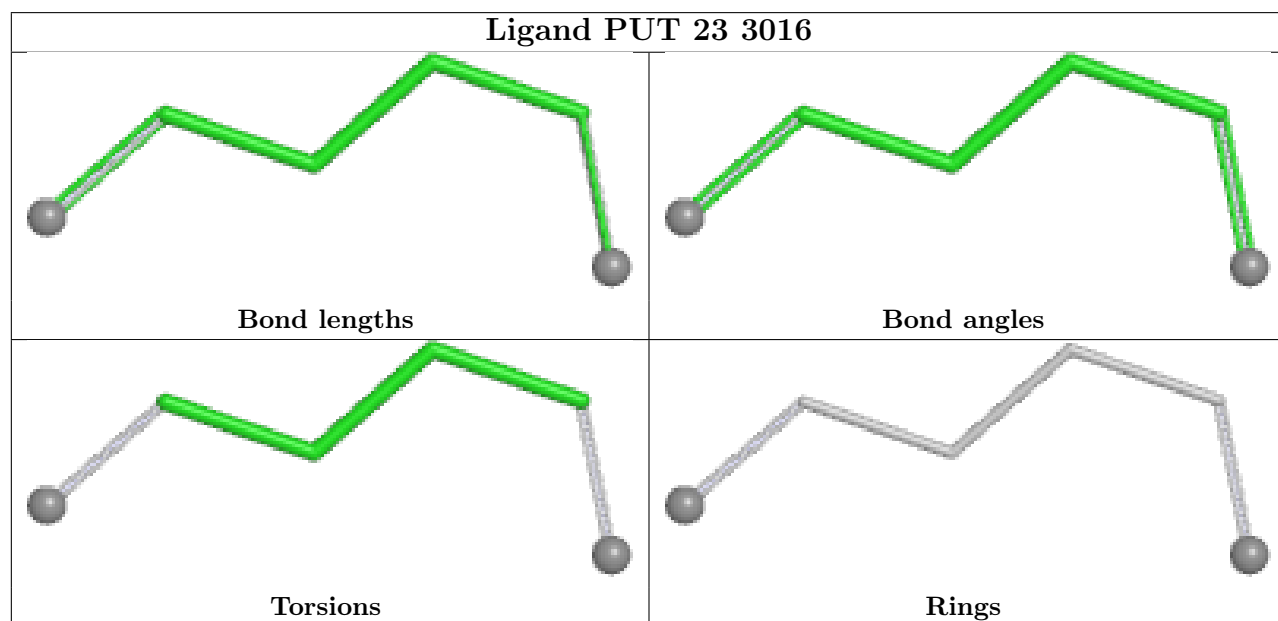
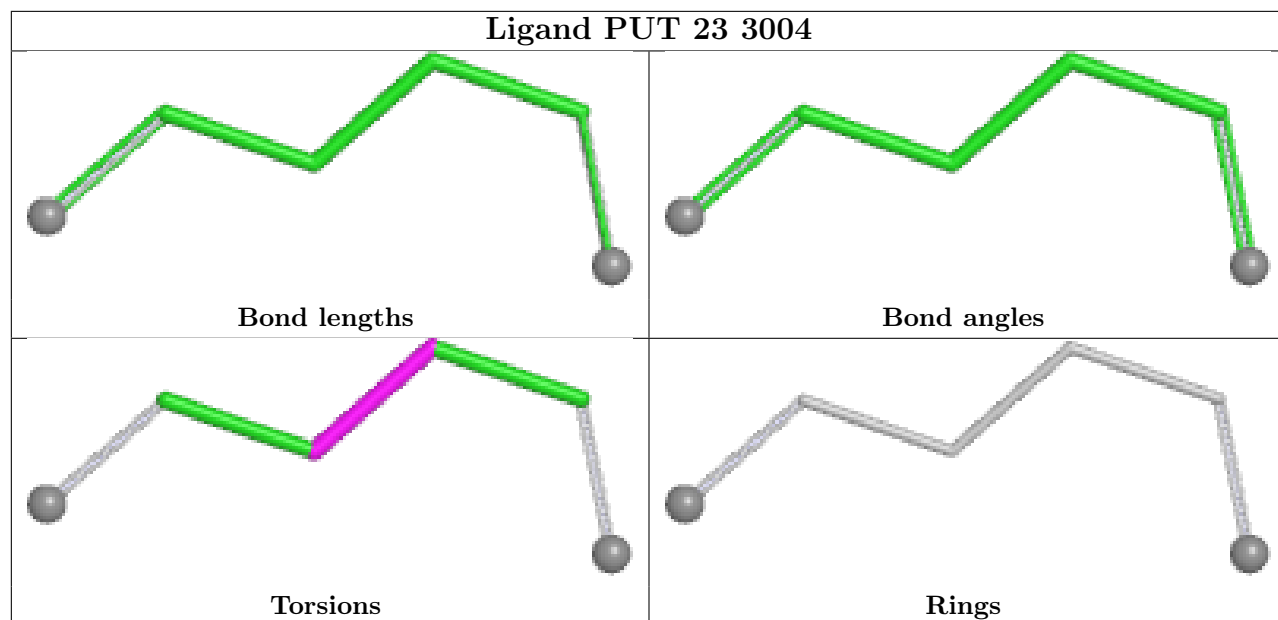
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

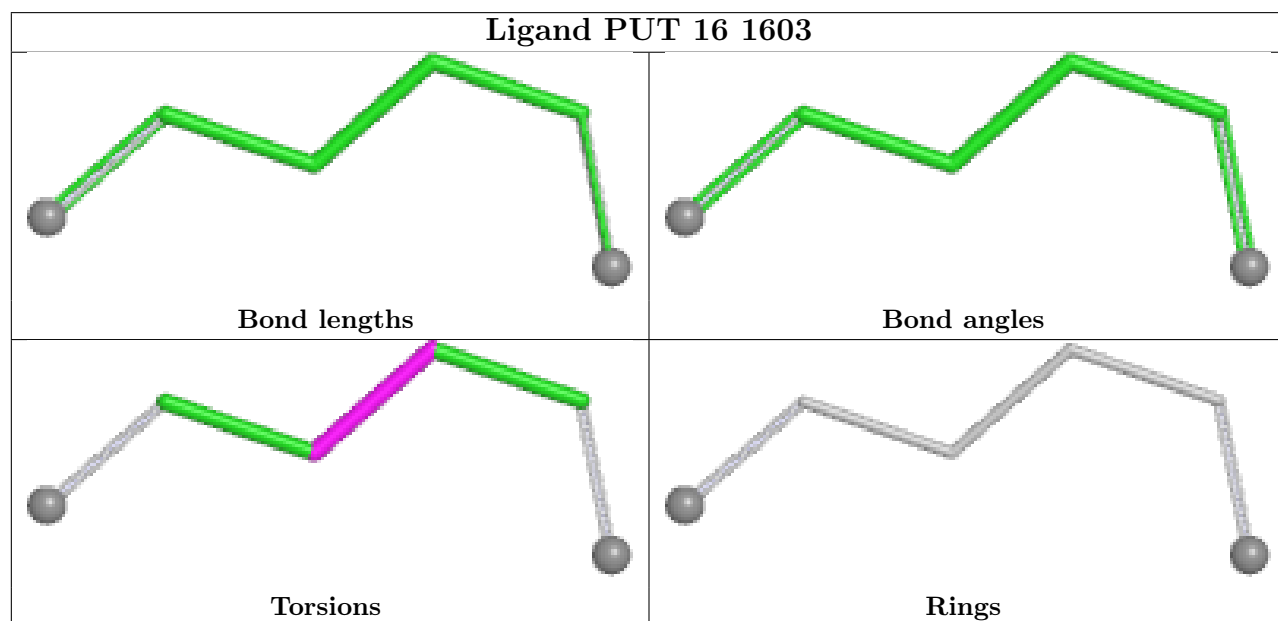
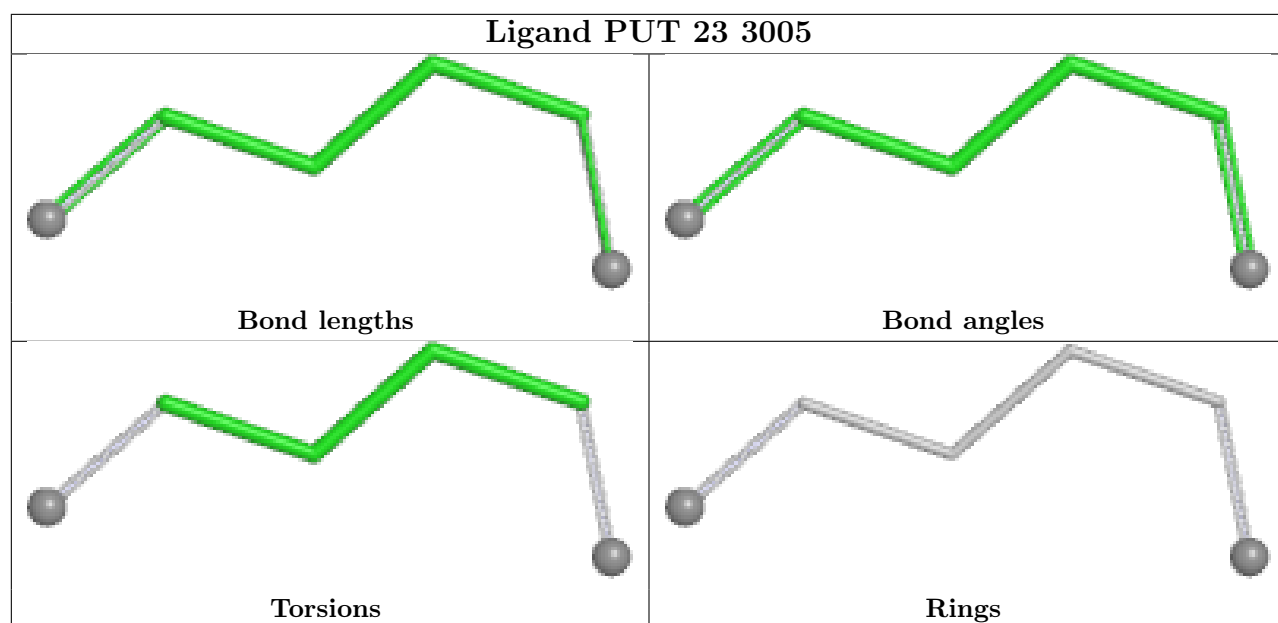


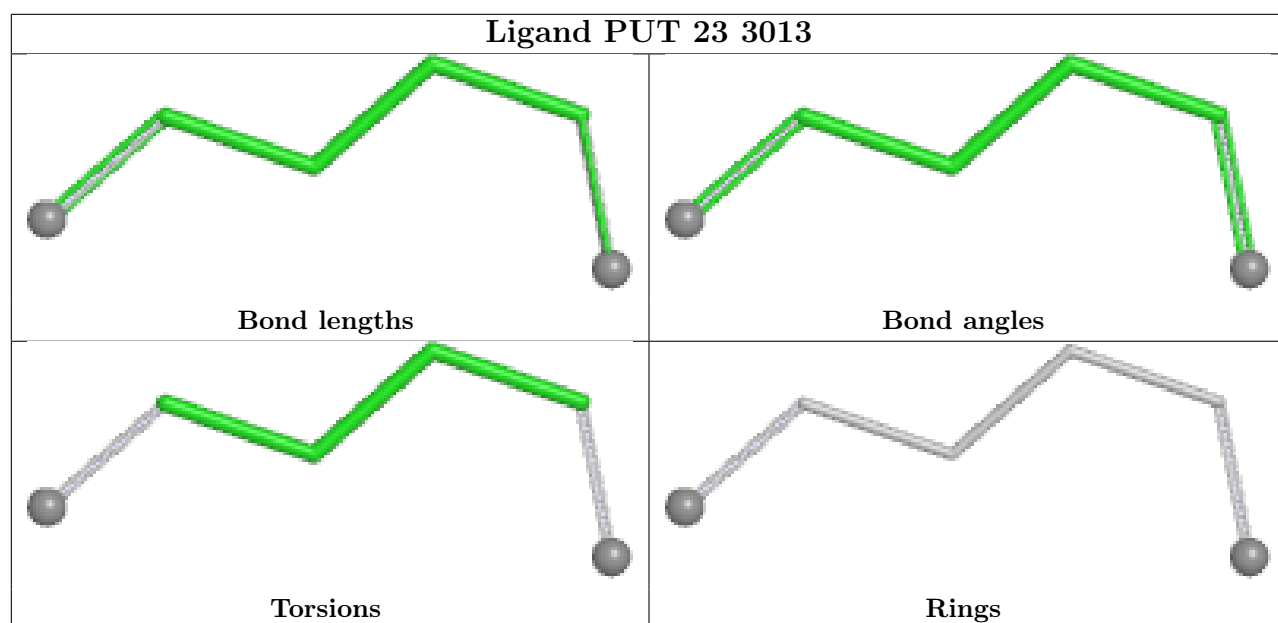
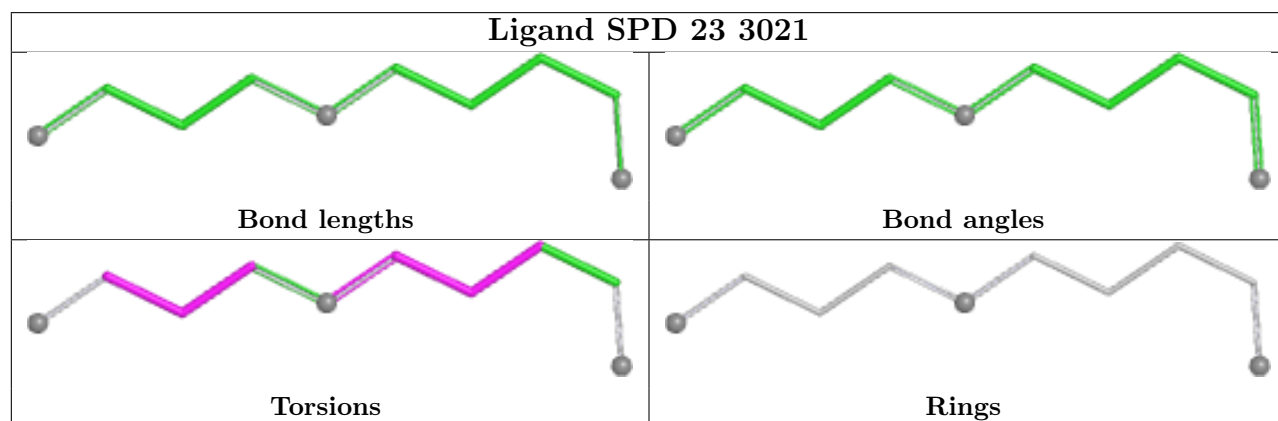
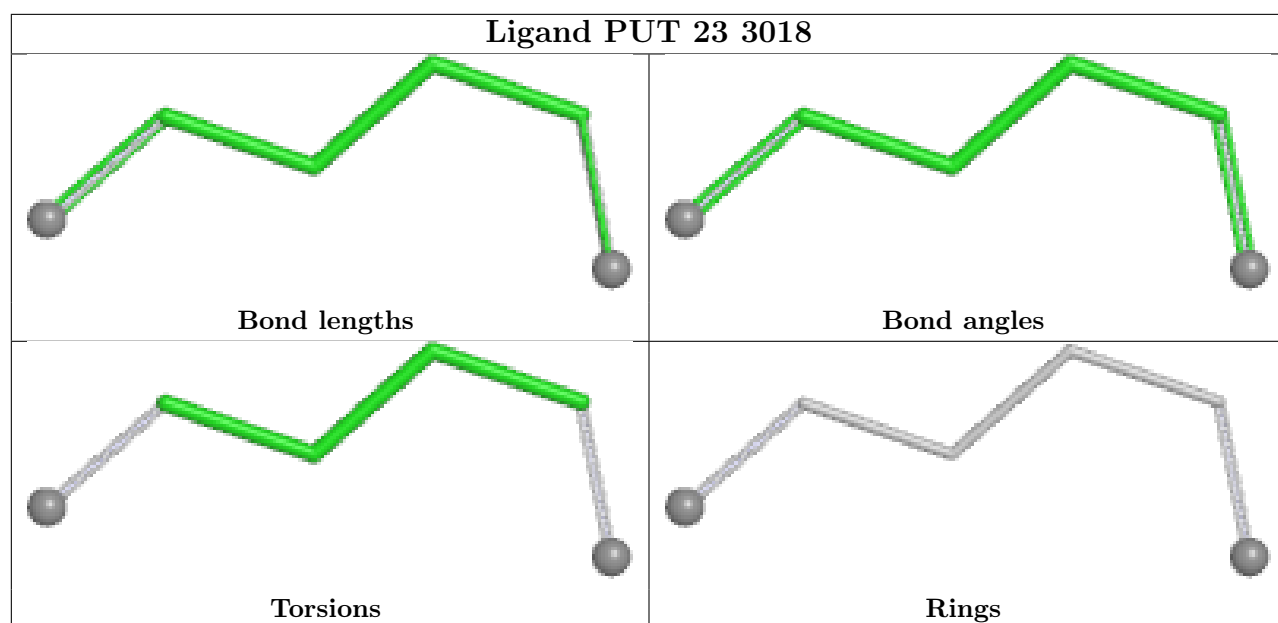


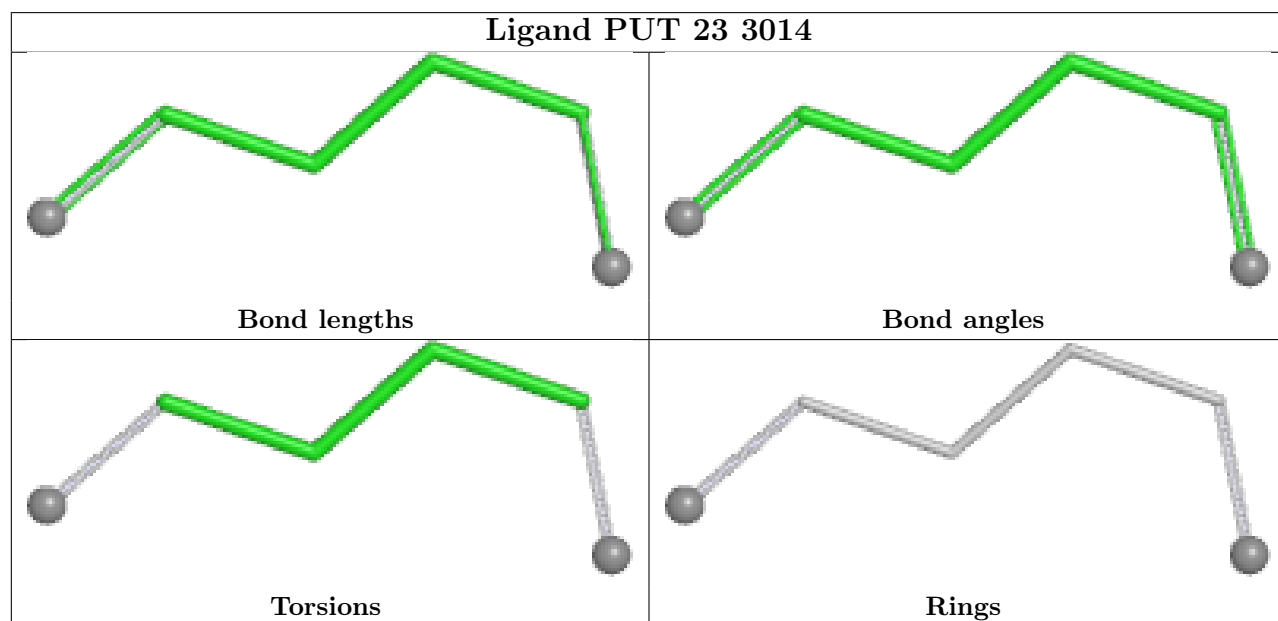
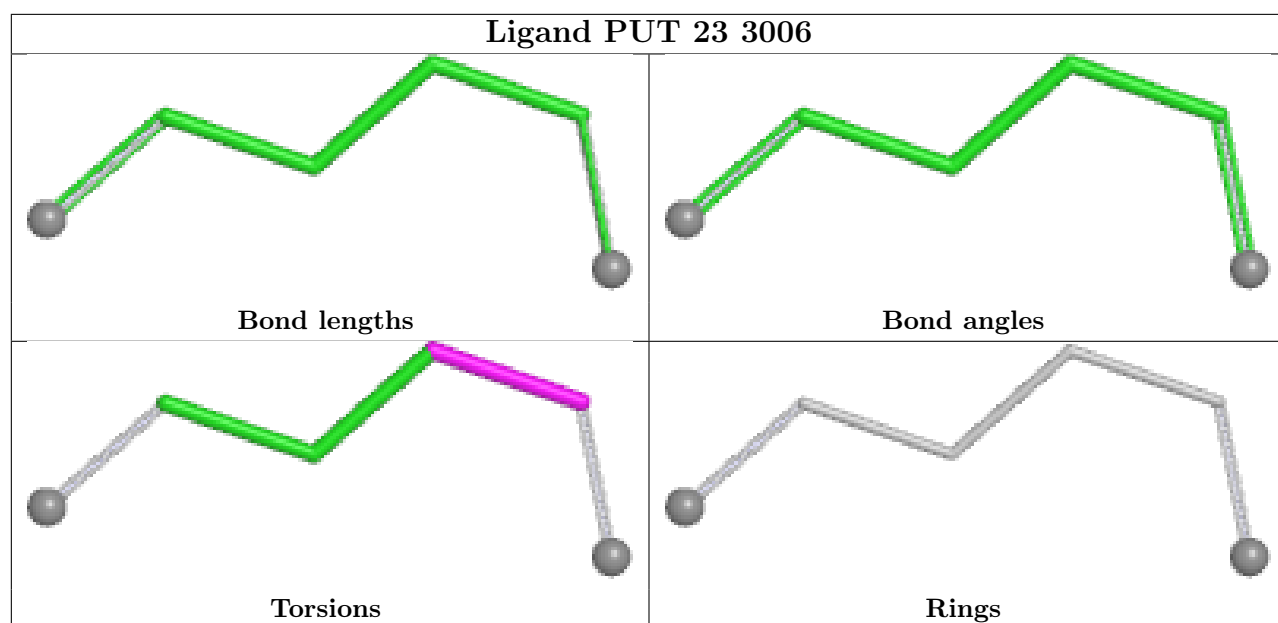




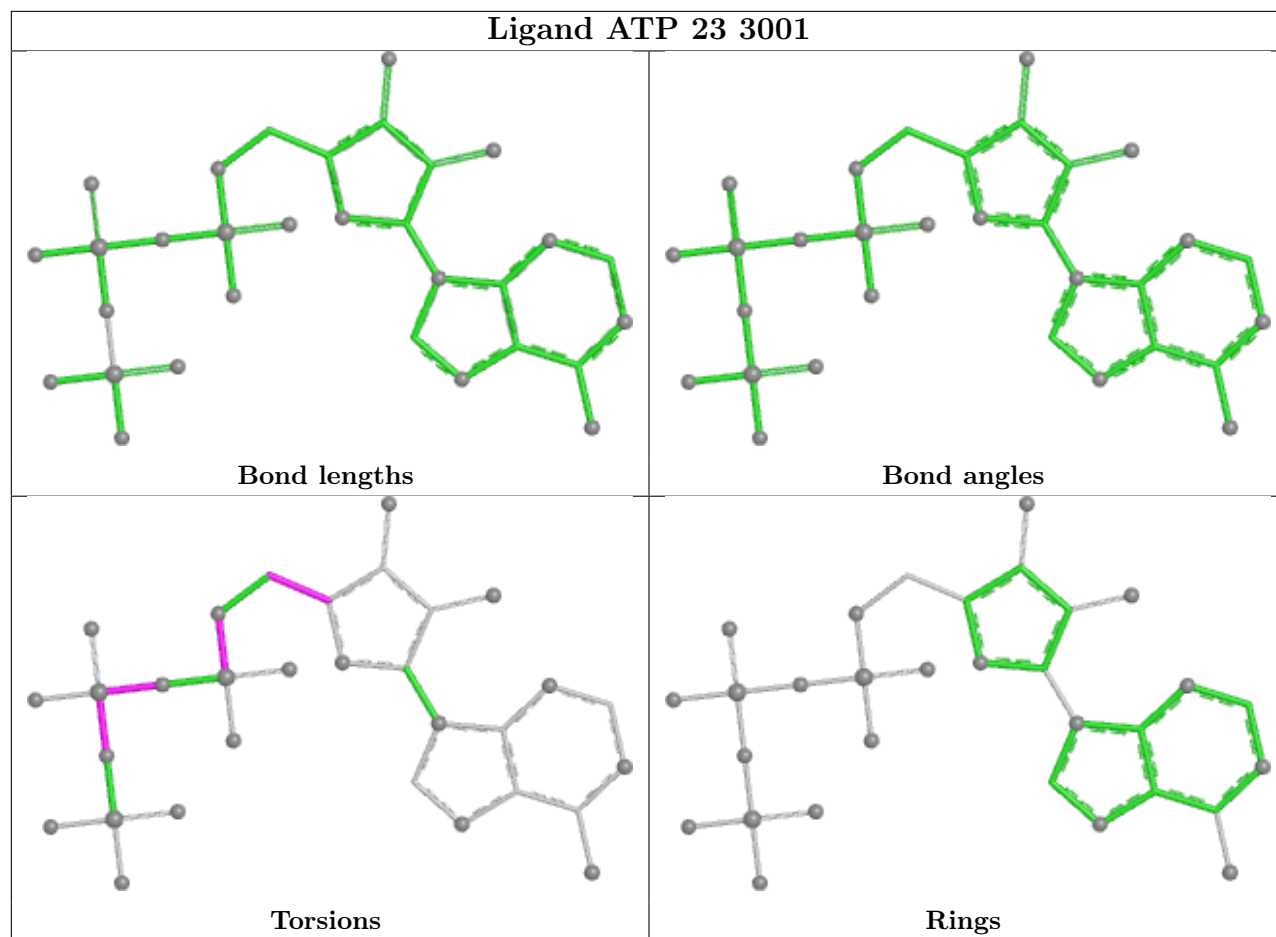




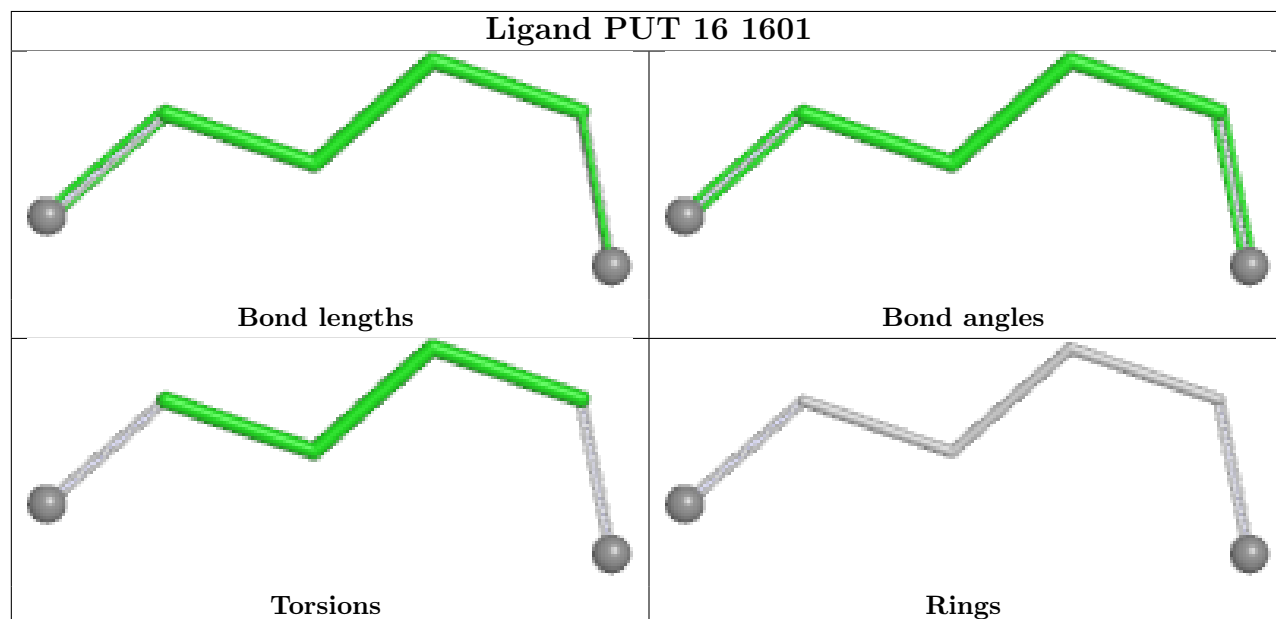




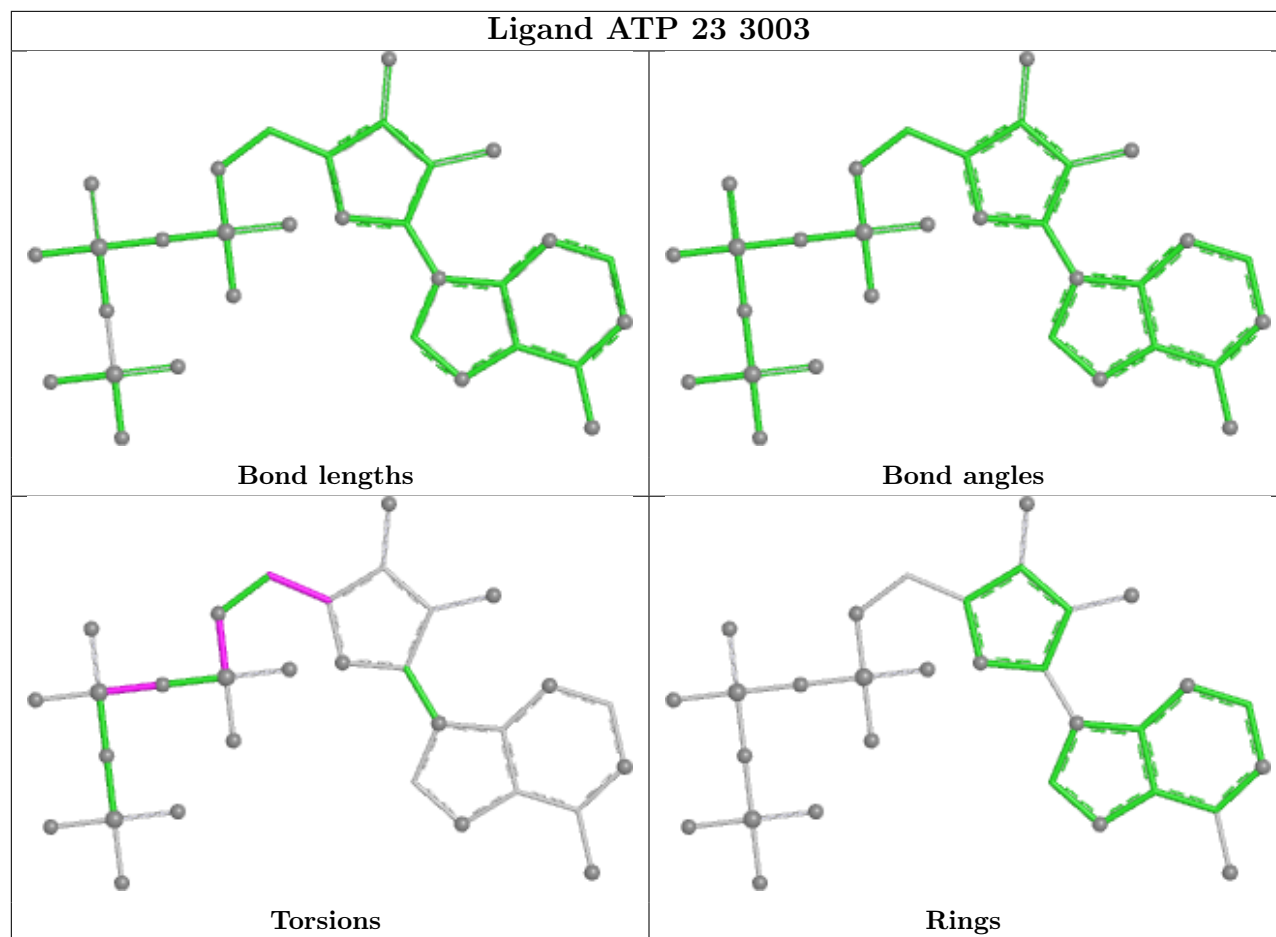
Ligand ATP 23 3001



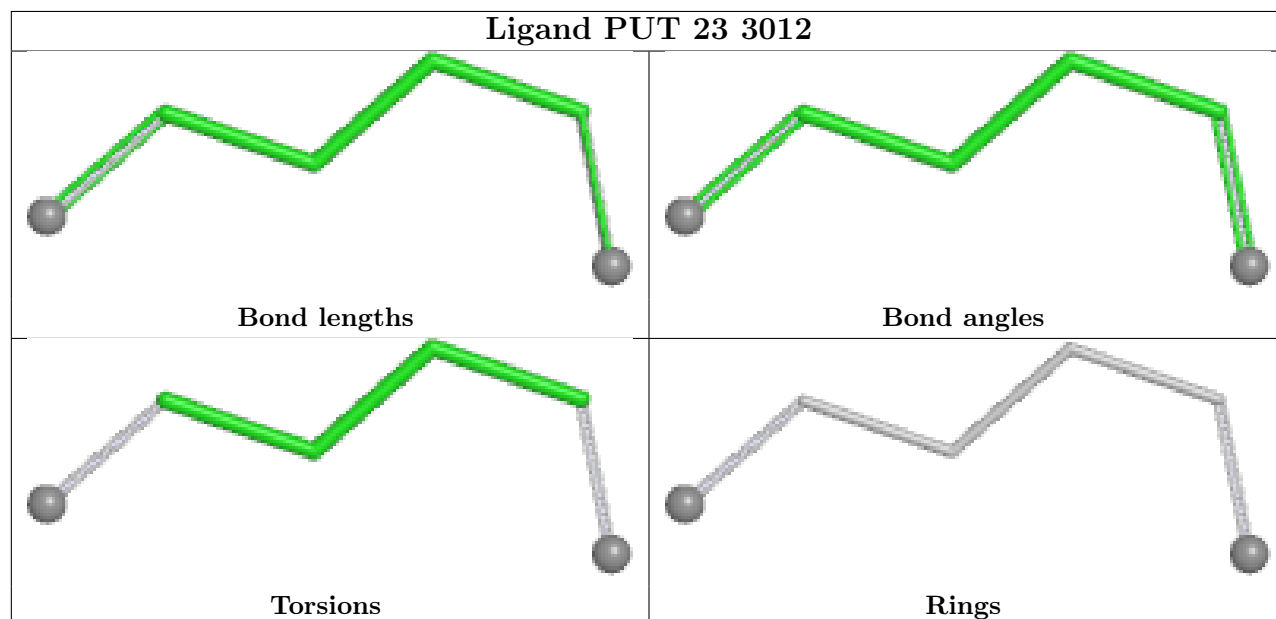
Ligand PUT 16 1601



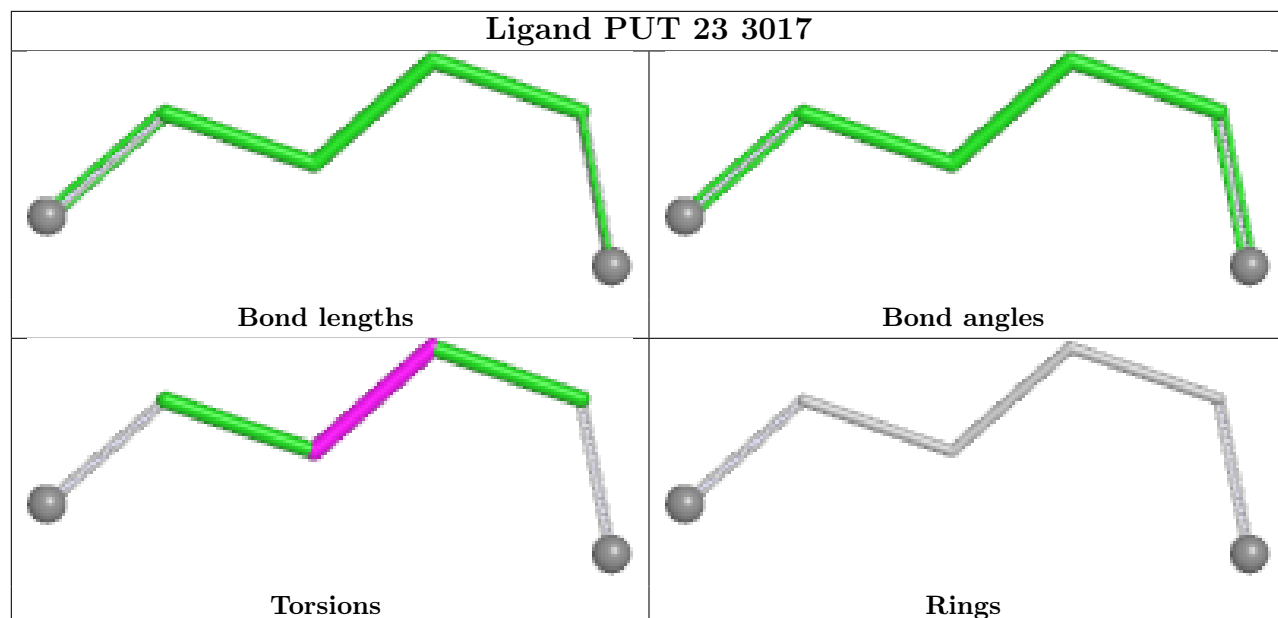
Ligand ATP 23 3003



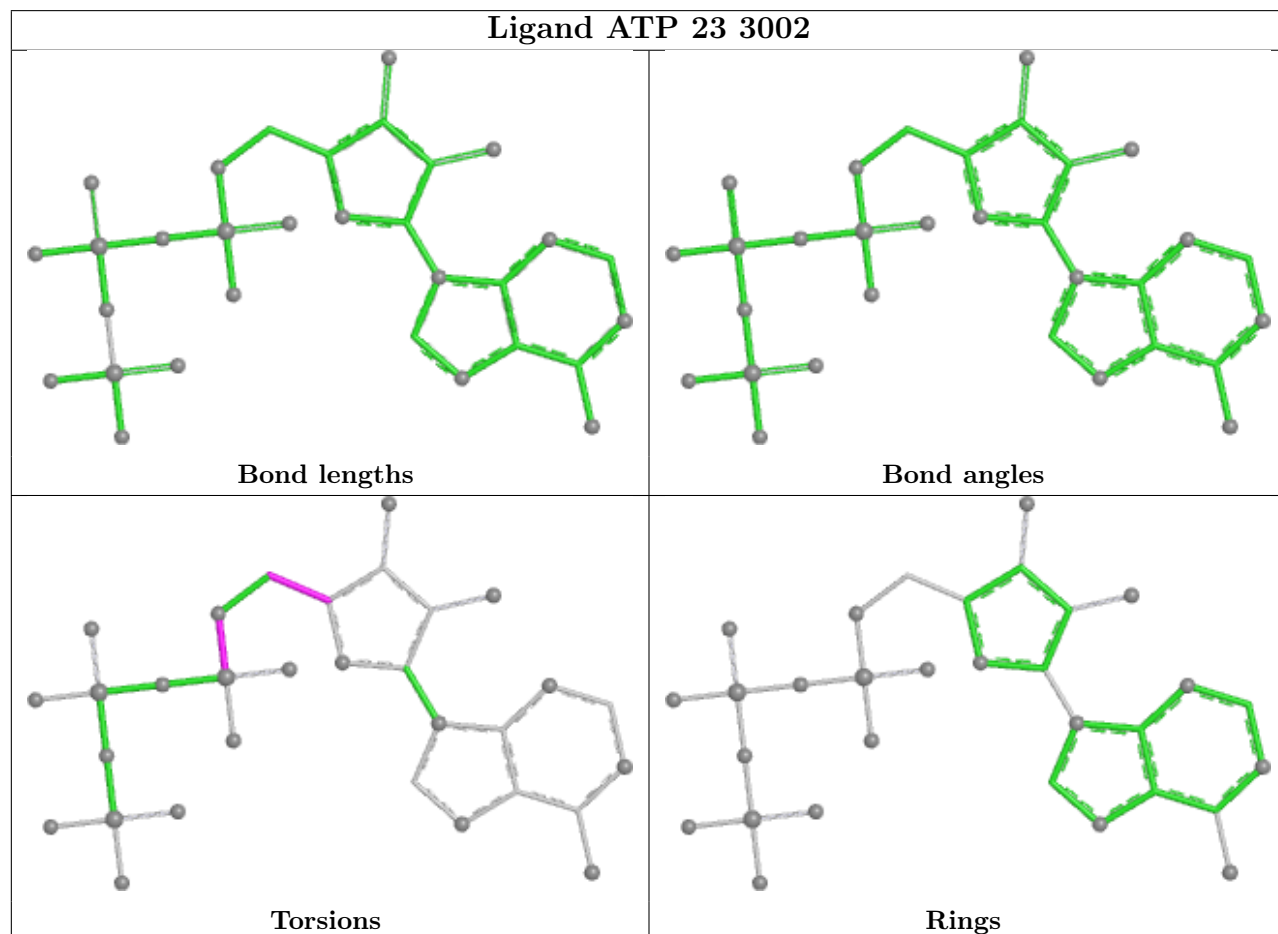
Ligand PUT 23 3012

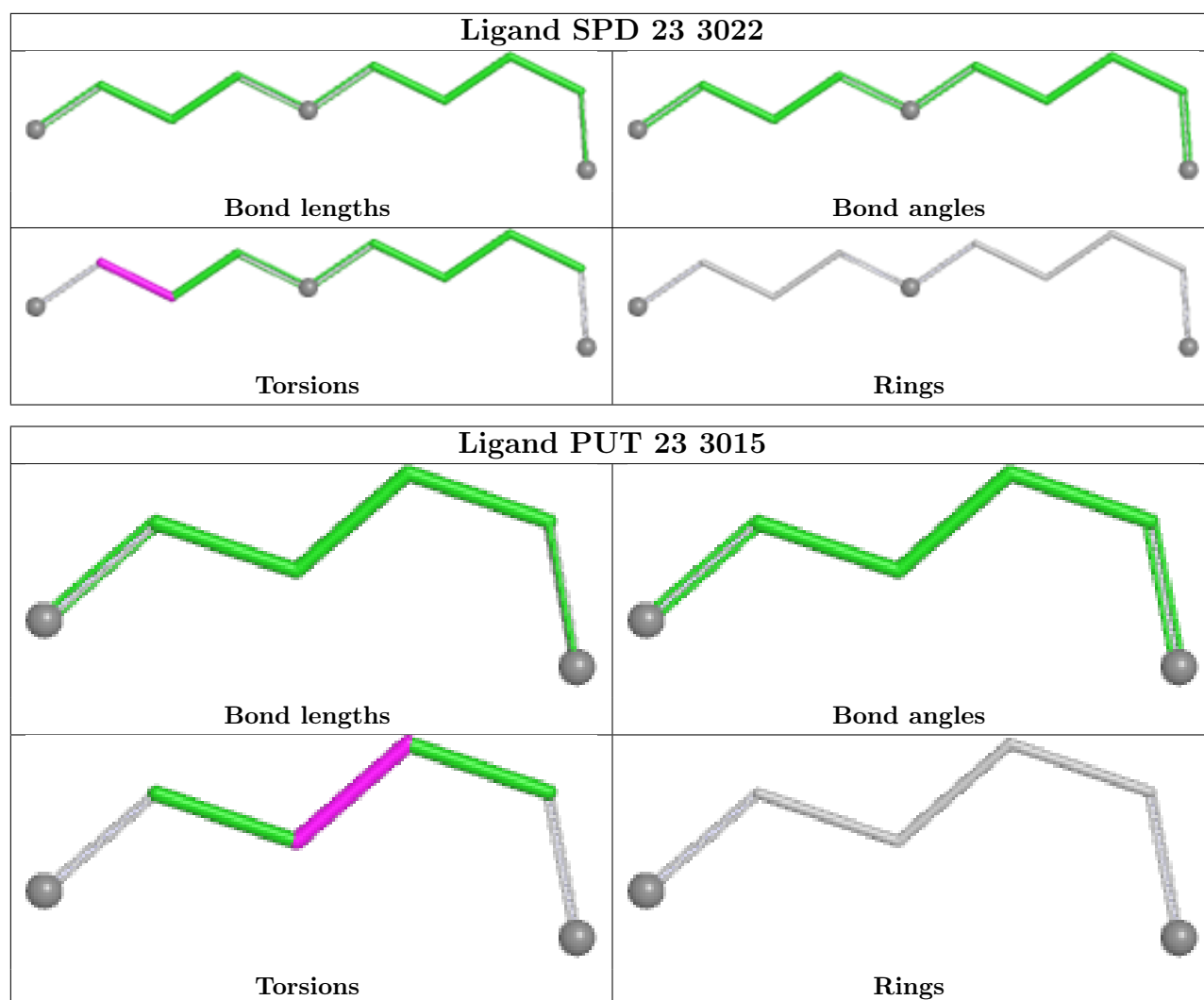


Ligand PUT 23 3017



Ligand ATP 23 3002





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

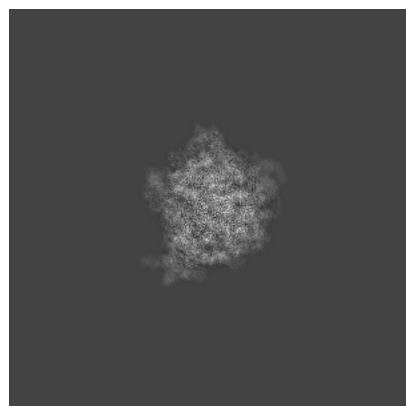
6 Map visualisation [i](#)

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

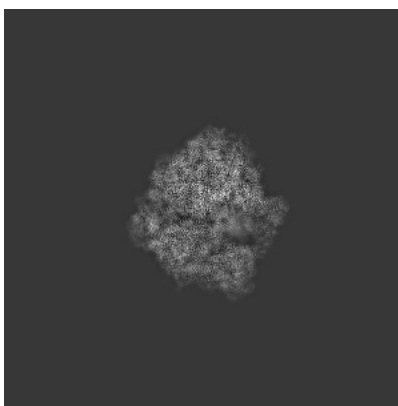
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

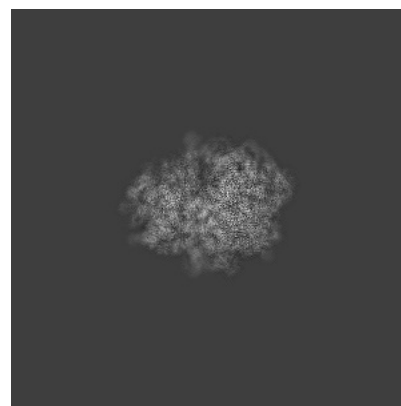
6.1.1 Primary map



X

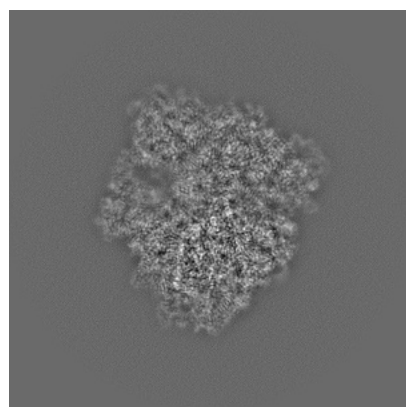


Y

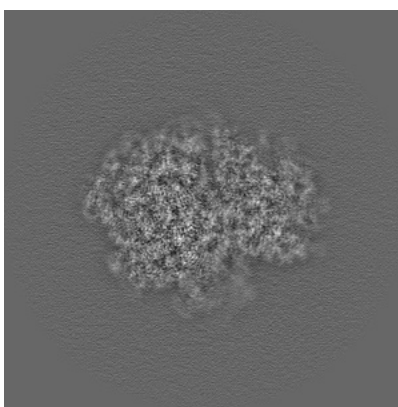


Z

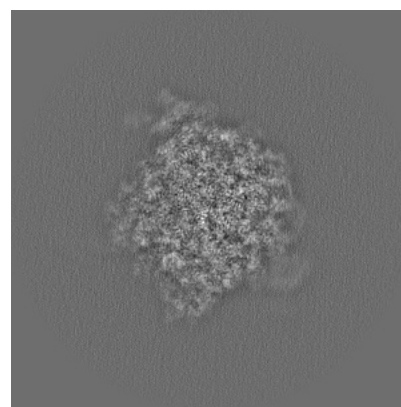
6.1.2 Raw map



X



Y



Z

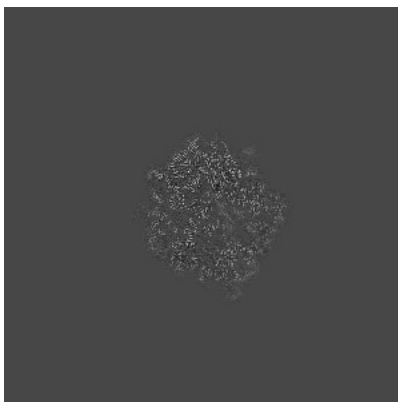
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

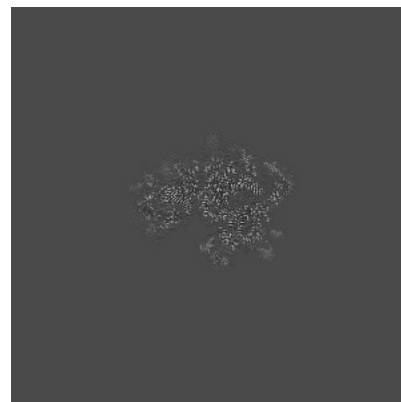
6.2.1 Primary map



X Index: 288

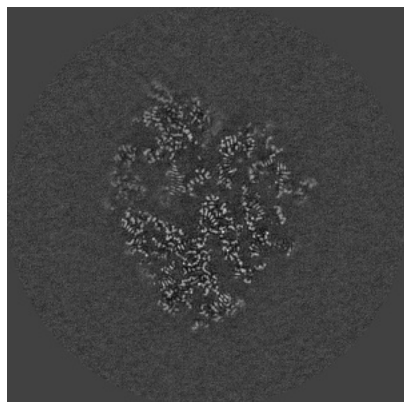


Y Index: 288

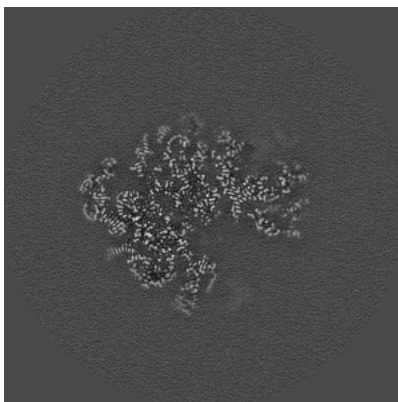


Z Index: 288

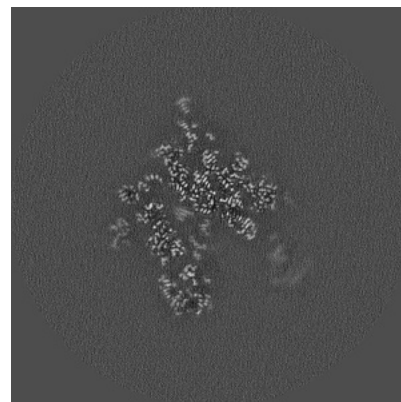
6.2.2 Raw map



X Index: 256



Y Index: 256

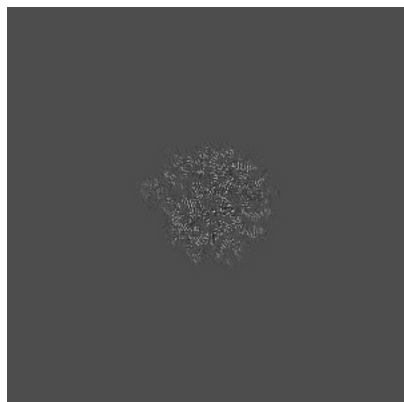


Z Index: 256

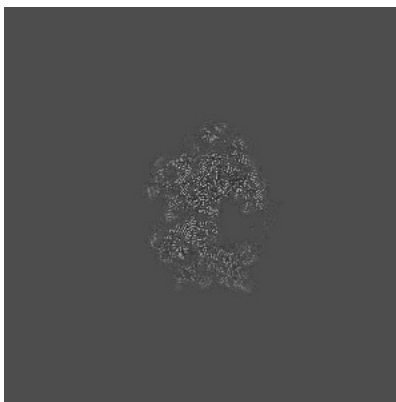
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

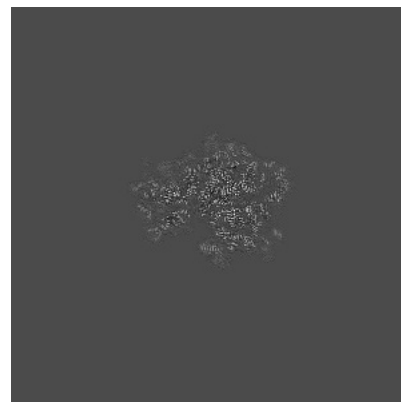
6.3.1 Primary map



X Index: 316

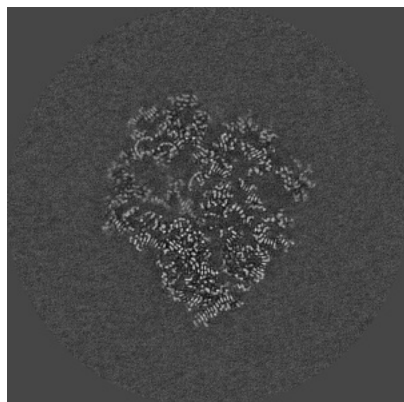


Y Index: 315

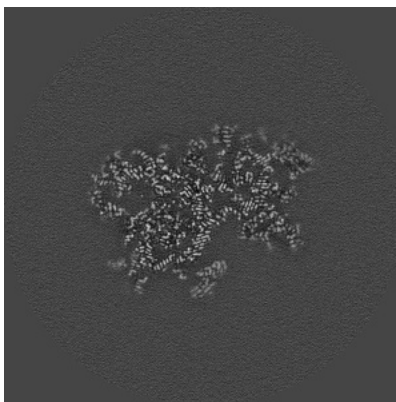


Z Index: 283

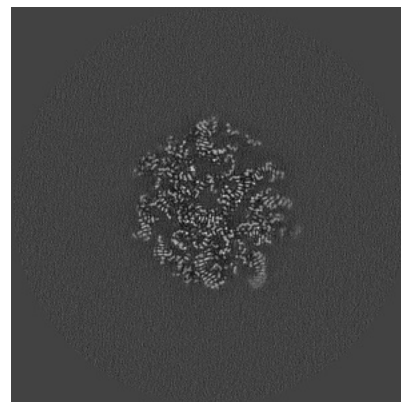
6.3.2 Raw map



X Index: 247



Y Index: 280

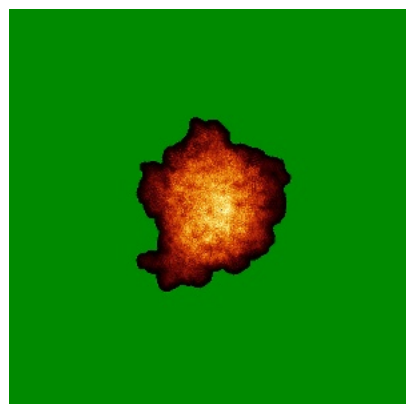


Z Index: 210

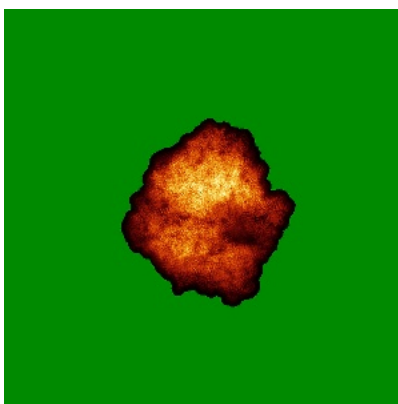
The images above show the largest variance slices of the map in three orthogonal directions.

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

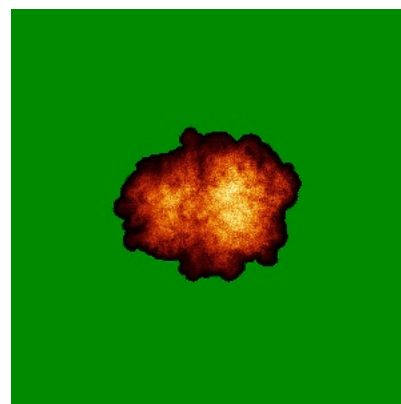
6.4.1 Primary map



X

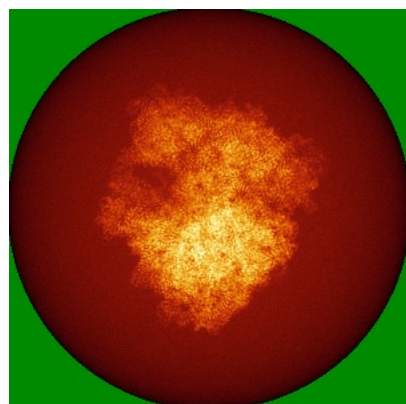


Y

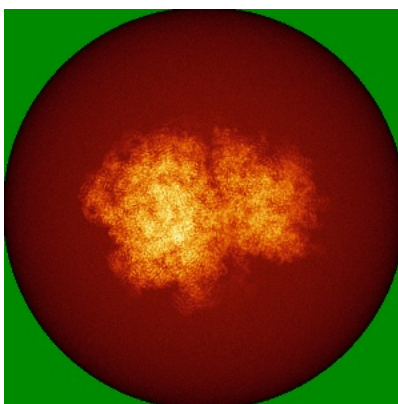


Z

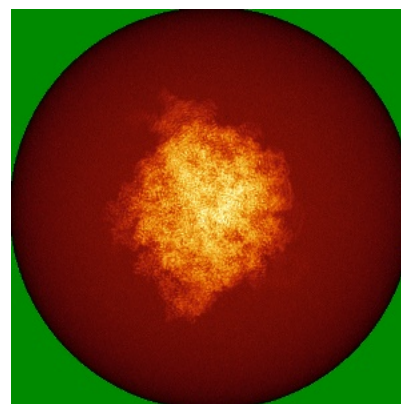
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

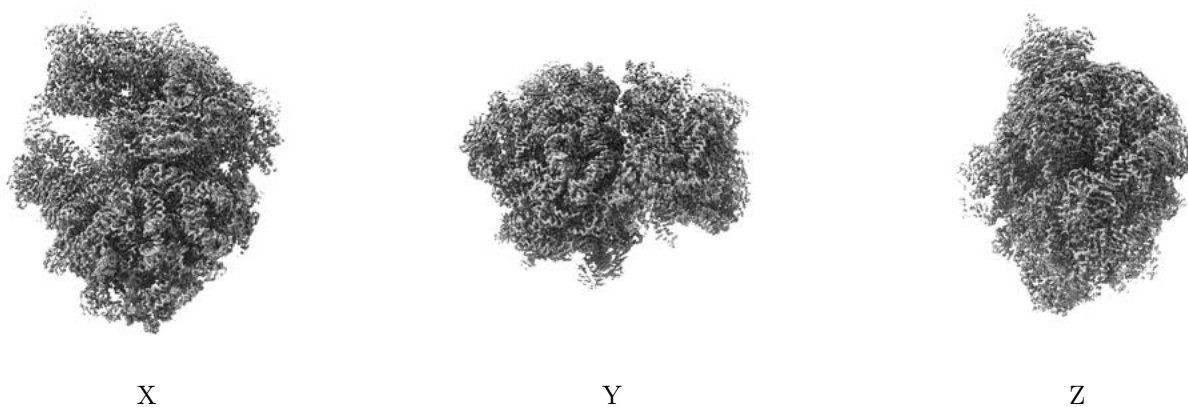
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

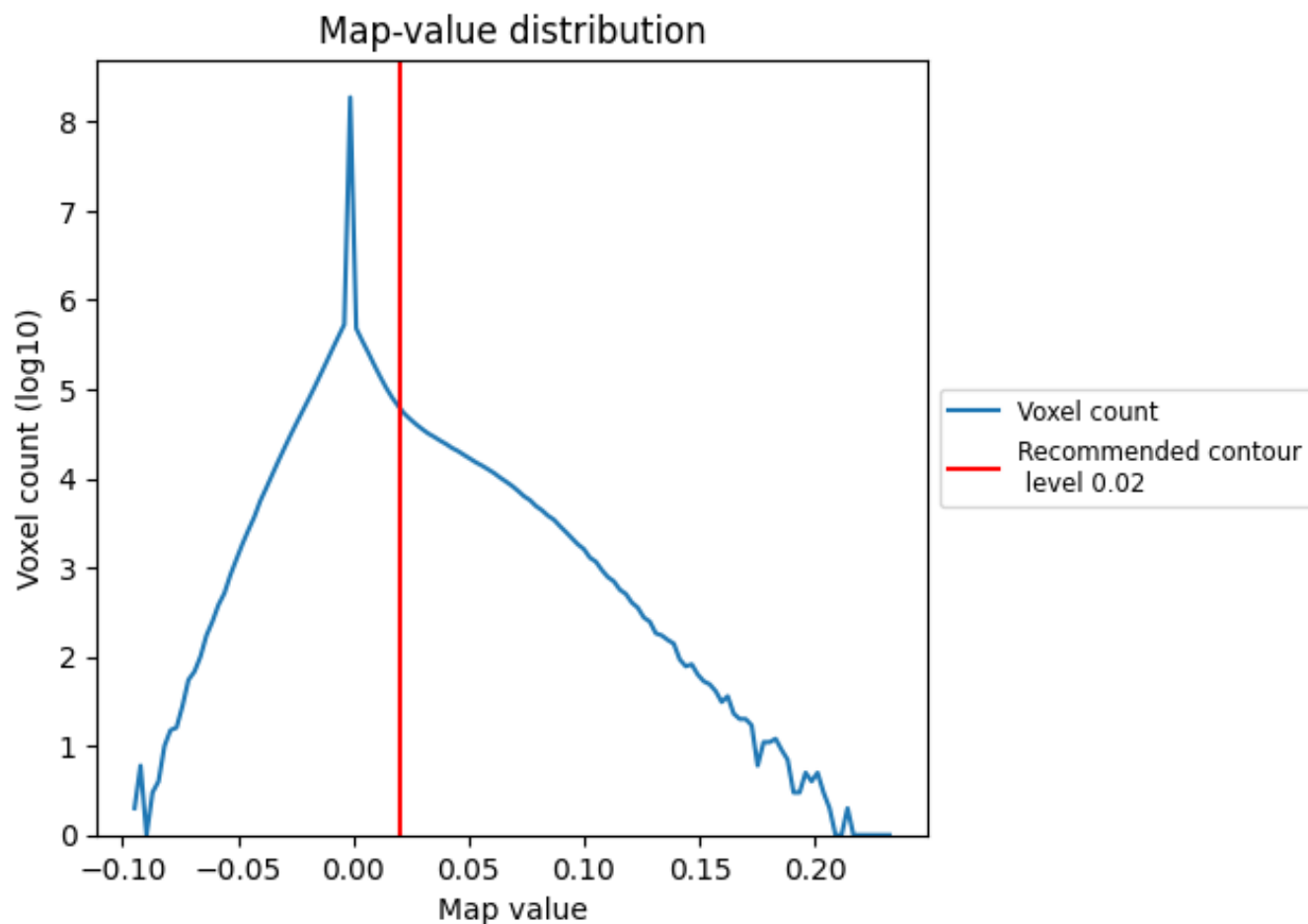
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

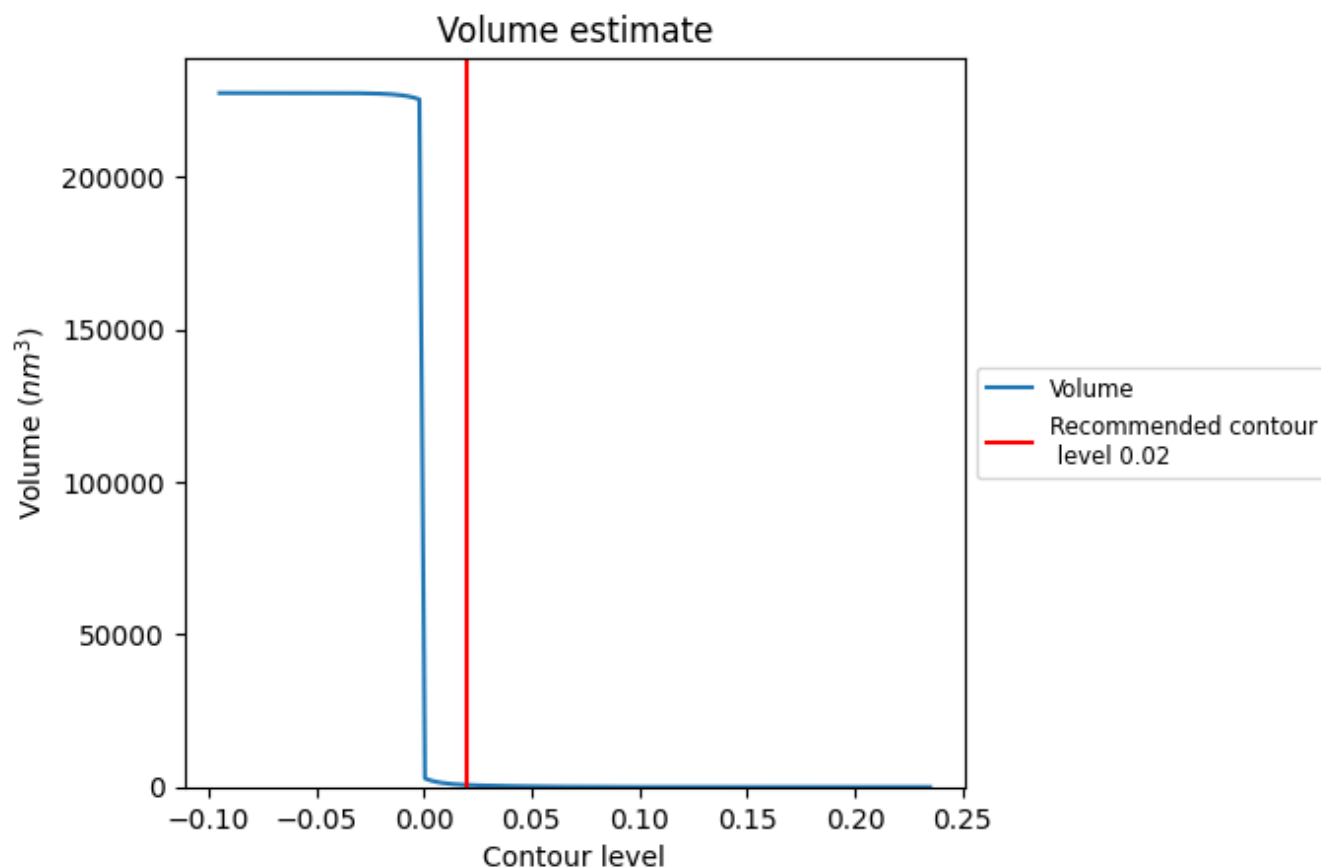
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

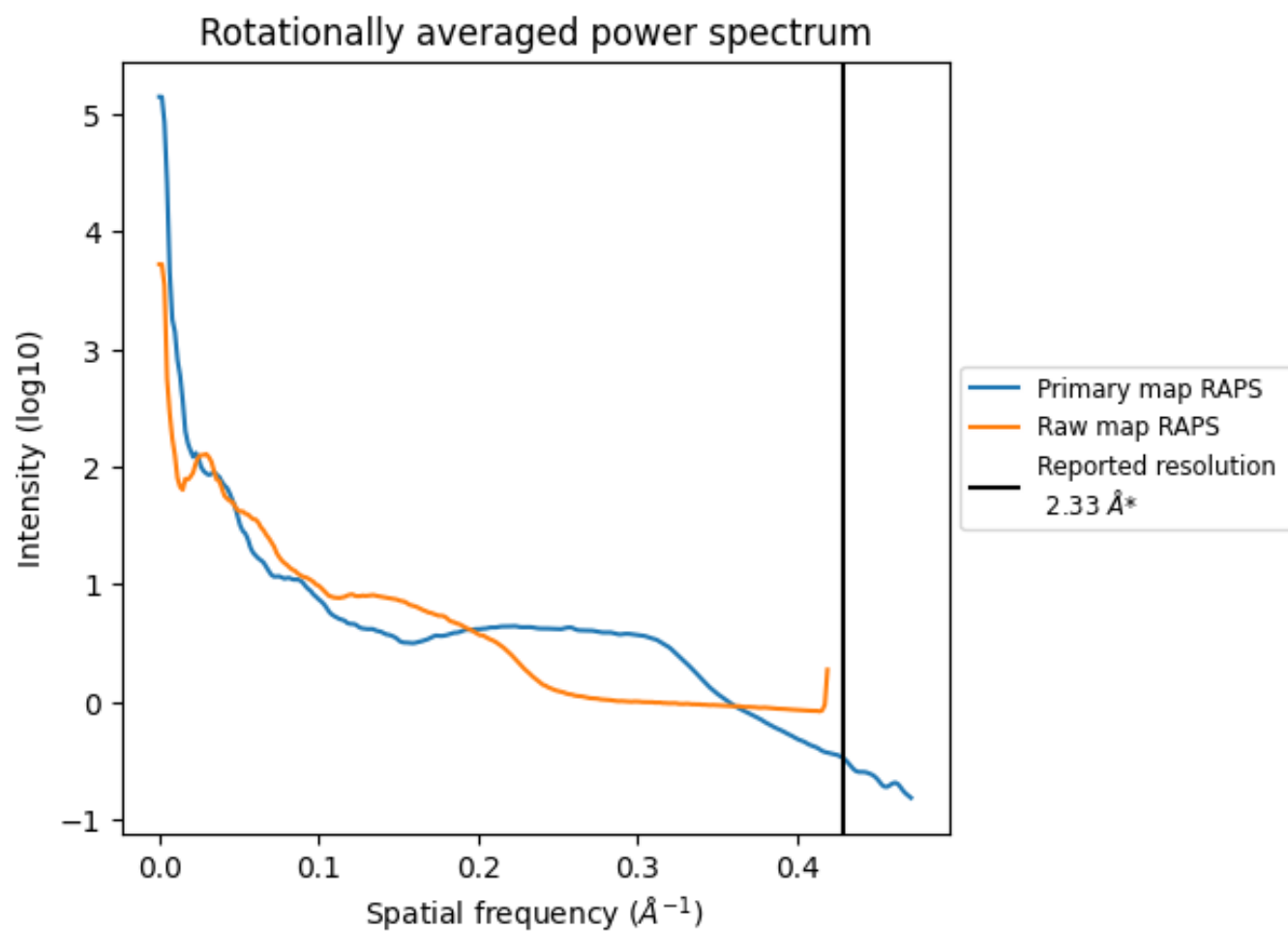
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

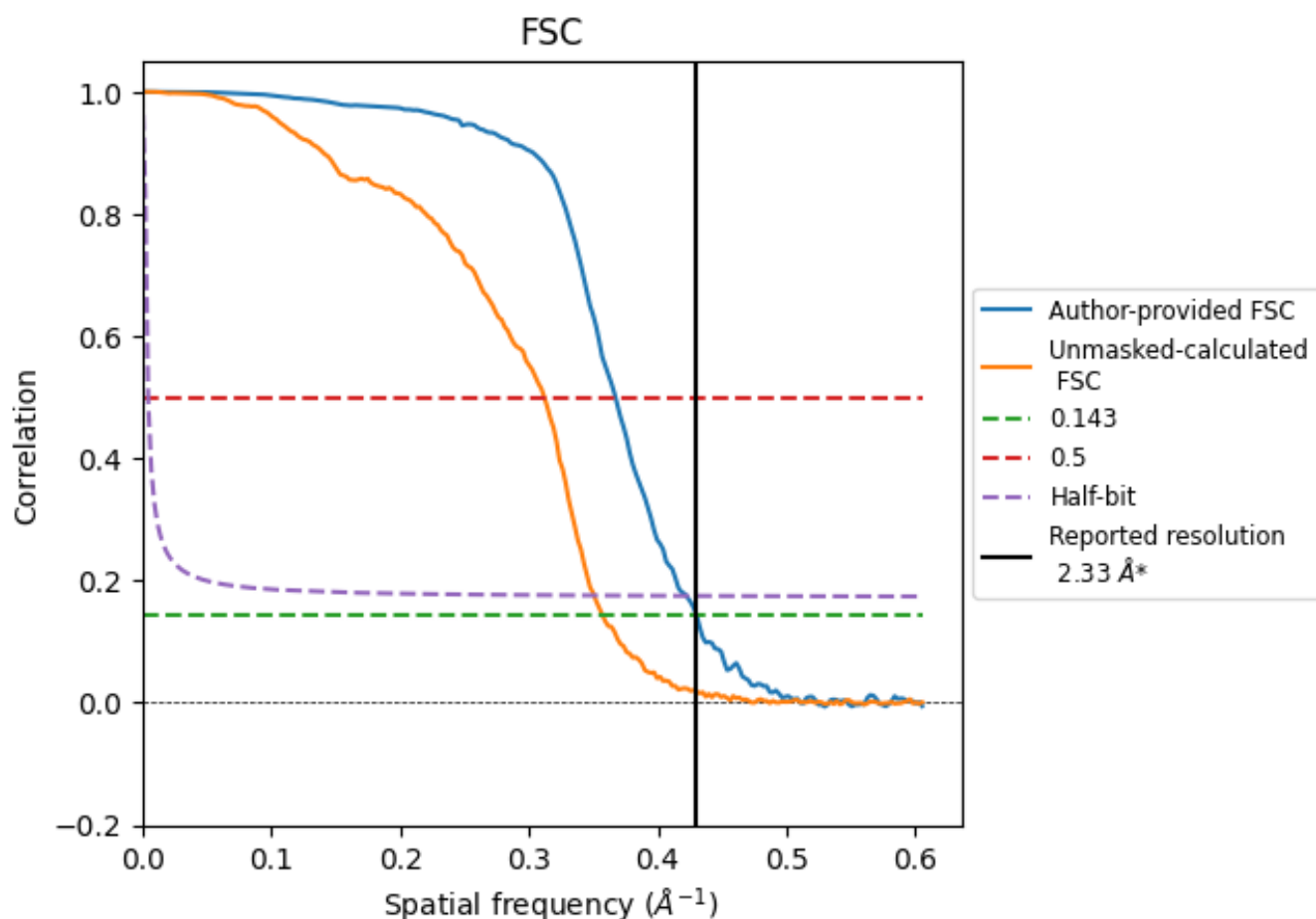


*Reported resolution corresponds to spatial frequency of 0.429 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.429 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

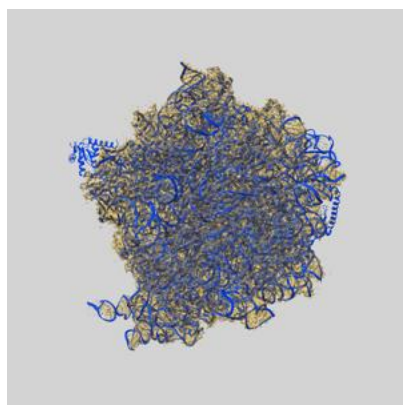
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.33	-	-
Author-provided FSC curve	2.32	2.72	2.37
Unmasked-calculated*	2.80	3.20	2.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.80 differs from the reported value 2.33 by more than 10 %

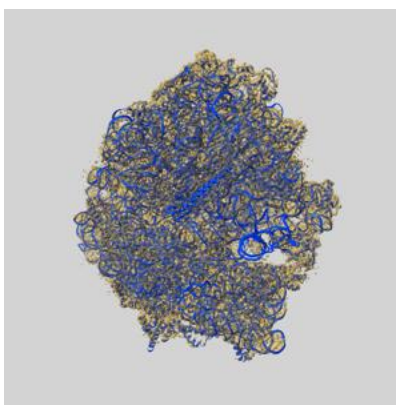
9 Map-model fit [i](#)

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

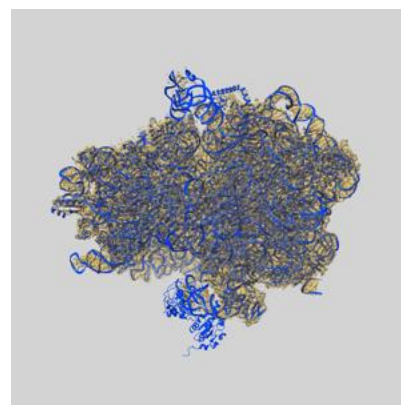
9.1 Map-model overlay [i](#)



X



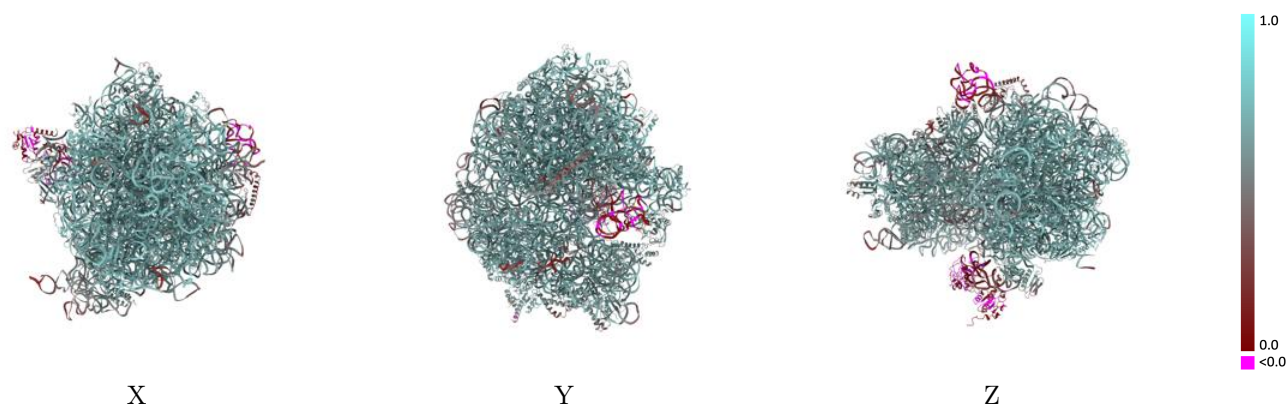
Y



Z

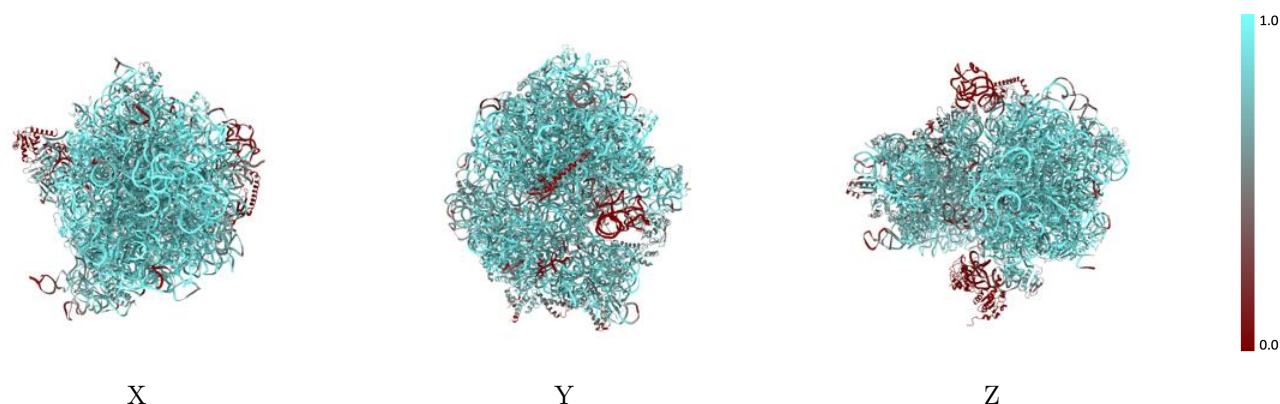
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



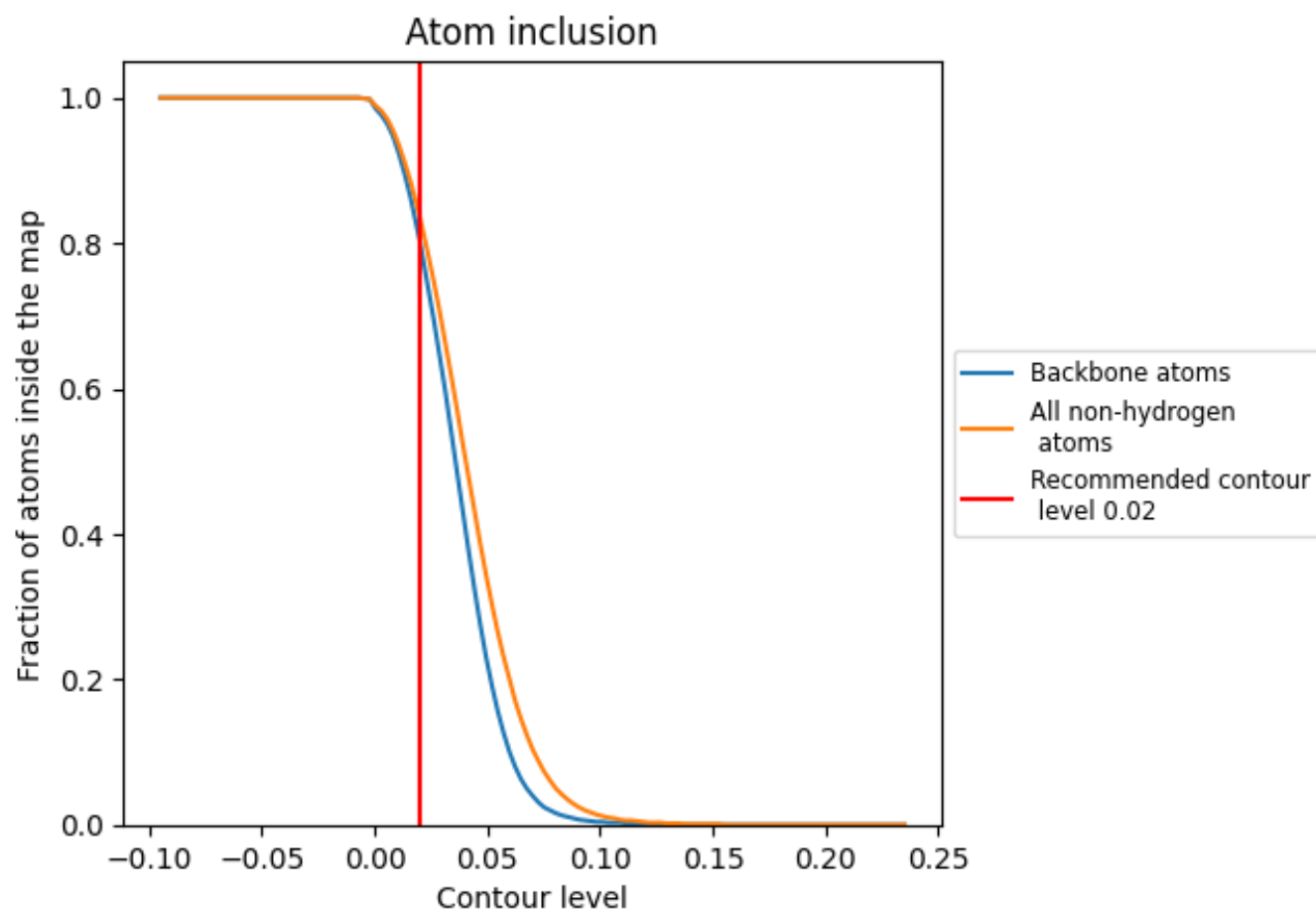
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

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



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