



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 11:06 PM EDT

PDB ID : 7N2V / pdb_00007n2v
EMDB ID : EMD-24134
Title : Elongating 70S ribosome complex in a spectinomycin-stalled intermediate state of translocation bound to EF-G in an active, GTP conformation (INT1)
Authors : Rundlet, E.J.; Holm, M.; Schacherl, M.; Natchiar, K.S.; Altman, R.B.; Spahn, C.M.T.; Myasnikov, A.G.; Blanchard, S.C.
Deposited on : 2021-05-29
Resolution : 2.54 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:

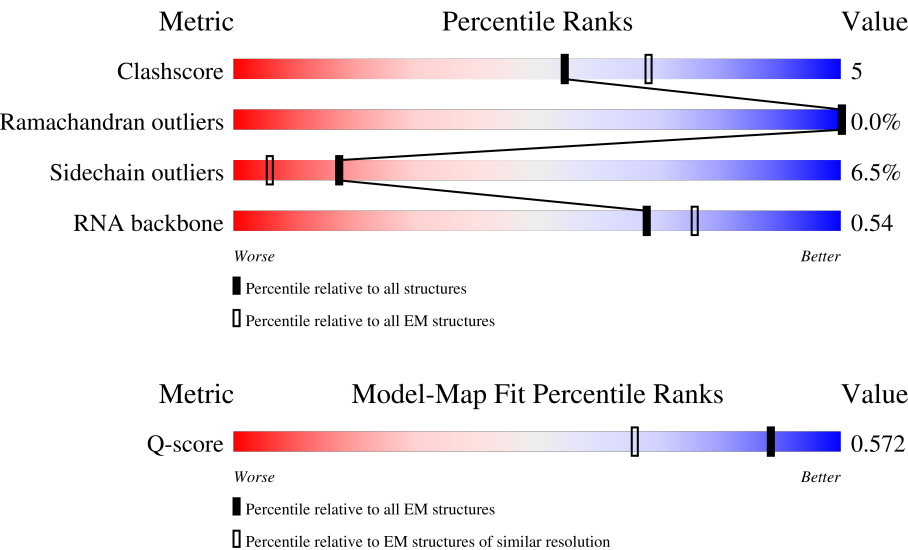
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 2.54 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.



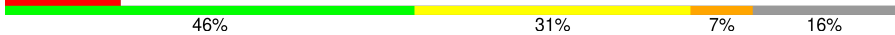
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7403 (2.04 - 3.04)

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	1534	72%25%
2	SB	241	70%23%7%
3	SC	233	64%25%9%

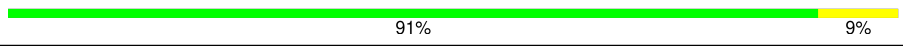
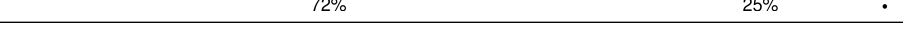
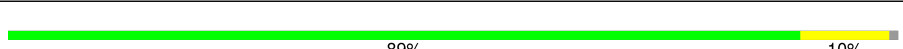
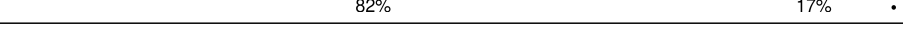
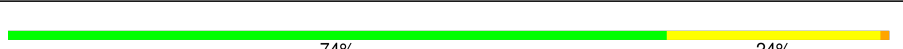
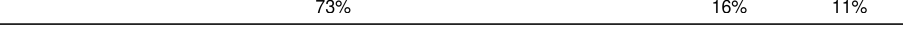
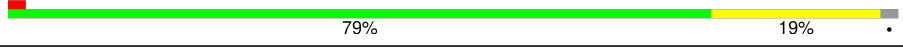
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Mol	Chain	Length	Quality of chain
4	SD	206	
5	SE	167	
6	SF	135	
7	SG	179	
8	SH	130	
9	SI	130	
10	SJ	103	
11	SK	129	
12	SL	124	
13	SM	118	
14	SN	101	
15	SO	89	
16	SP	82	
17	SQ	84	
18	SR	75	
19	SS	92	
20	ST	87	
21	SU	71	
22	mR	60	
23	23	2904	
24	5	120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

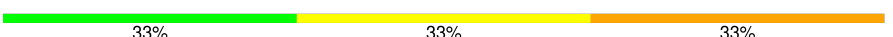
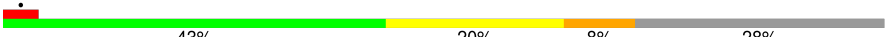
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Mol	Chain	Length	Quality of chain
29	LF	177	
30	LI	149	
31	LJ	165	
32	LK	142	
33	LM	142	
34	LN	123	
35	LO	144	
36	LP	136	
37	LQ	127	
38	LR	117	
39	LS	115	
40	LT	118	
41	LU	103	
42	LV	110	
43	LW	100	
44	LX	104	
45	LY	94	
46	La	85	
47	Lb	78	
48	Lc	63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

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Mol	Chain	Length	Quality of chain
54	Li	65	
55	Lj	38	
56	EF	704	
57	Pp	3	
58	Pt	106	
59	Dt	106	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
64	ATP	23	3003	X	-	-	-

2 Entry composition [i](#)

There are 67 unique types of molecules in this entry. The entry contains 154120 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	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SC	211	Total	C	N	O	S	0	0
			1653	1046	310	293	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	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SH	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	119	Total	C	N	O	S	0	0
			895	551	179	162	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	0	0
			714	439	144	130	1		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	ST	85	Total	C	N	O	S	0	0
			664	411	137	113	3		

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

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	mR	12	Total	C	N	O	P	0	0
			254	114	44	84	12		

- 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
			62355	27824	11469	20158	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	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LI	148	Total	C	N	O	S	0	0
			1101	694	196	210	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LJ	131	Total	C	N	O	S	0	0
			992	629	175	184	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	122	Total	C	N	O	S	0	0
			938	587	180	165	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	0	0
			1075	686	205	178	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	76	Total	C	N	O	S	0	0
			582	360	117	104	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	0	0
			625	388	129	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 protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	EF	704	Total	C	N	O	S	0	0
			5388	3395	938	1033	22		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EF	1	SER	-	expression tag	UNP A0A0H3PU63

- Molecule 57 is a protein called Nascent peptide.

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

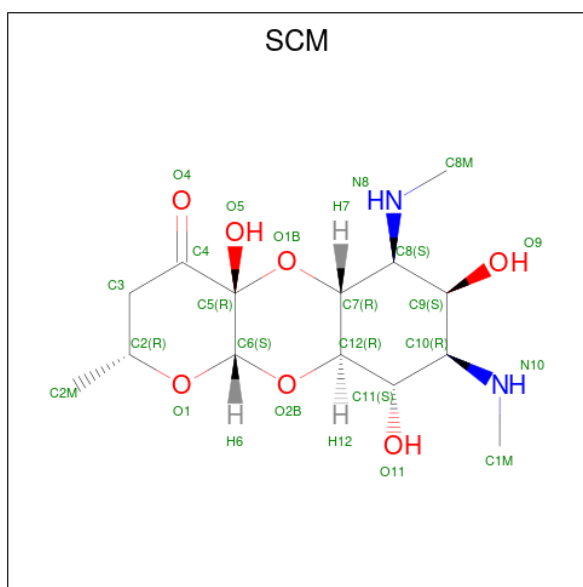
- Molecule 58 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
58	Pt	76	Total	C	N	O	P	S	0	0
			1636	733	284	542	76	1		

- Molecule 59 is a RNA chain called tRNA.

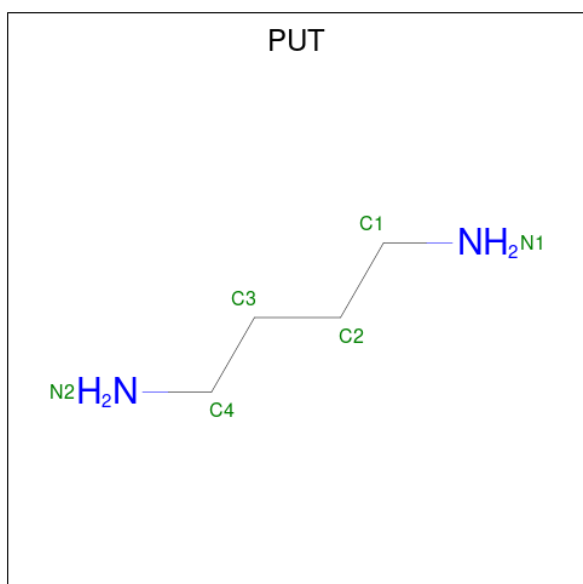
Mol	Chain	Residues	Atoms					AltConf	Trace	
59	Dt	76	Total	C	N	O	P	S	0	0
			1641	735	294	534	76	2		

- Molecule 60 is SPECTINOMYCIN (CCD ID: SCM) (formula: $C_{14}H_{24}N_2O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
60	16	1	Total	C	N	O	0
			23	14	2	7	
60	16	1	Total	C	N	O	0
			23	14	2	7	
60	23	1	Total	C	N	O	0
			23	14	2	7	

- Molecule 61 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
61	16	1	Total	C	N	0
			6	4	2	
61	16	1	Total	C	N	0
			6	4	2	
61	16	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	23	1	Total	C	N	0
			6	4	2	
61	LC	1	Total	C	N	0
			6	4	2	

- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
62	16	63	Total	Mg	0
			63	63	
62	SK	1	Total	Mg	0
			1	1	

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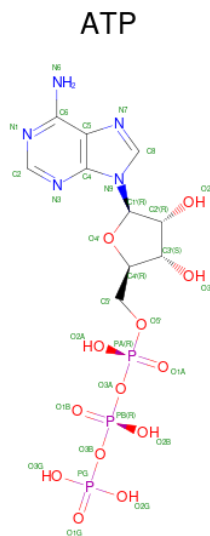
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Mol	Chain	Residues	Atoms		AltConf
62	SN	1	Total 1	Mg 1	0
62	SR	1	Total 1	Mg 1	0
62	23	264	Total 264	Mg 264	0
62	5	6	Total 6	Mg 6	0
62	LB	1	Total 1	Mg 1	0
62	LC	1	Total 1	Mg 1	0
62	LD	1	Total 1	Mg 1	0
62	LO	1	Total 1	Mg 1	0
62	LQ	1	Total 1	Mg 1	0
62	Lf	1	Total 1	Mg 1	0
62	EF	1	Total 1	Mg 1	0
62	Pt	1	Total 1	Mg 1	0

- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

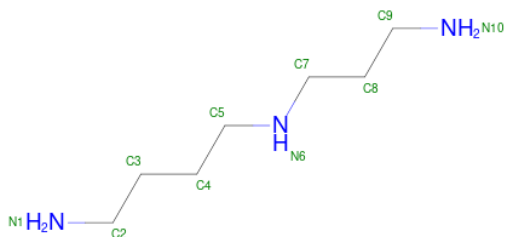
Mol	Chain	Residues	Atoms		AltConf
63	SB	1	Total 1	Zn 1	0
63	Le	1	Total 1	Zn 1	0
63	Lj	1	Total 1	Zn 1	0

- Molecule 64 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
64	23	1	Total 31	C 10	N 5	O 13	P 3	0
64	23	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 65 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



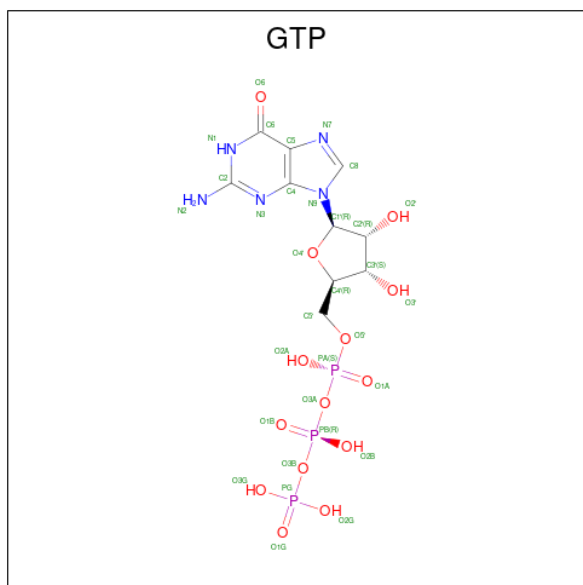
Mol	Chain	Residues	Atoms			AltConf
65	23	1	Total	C	N	0
			10	7	3	

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Mol	Chain	Residues	Atoms			AltConf
65	23	1	Total	C	N	0
			10	7	3	

- Molecule 66 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
66	EF	1	Total	C	N	O	P	0
			32	10	5	14	3	

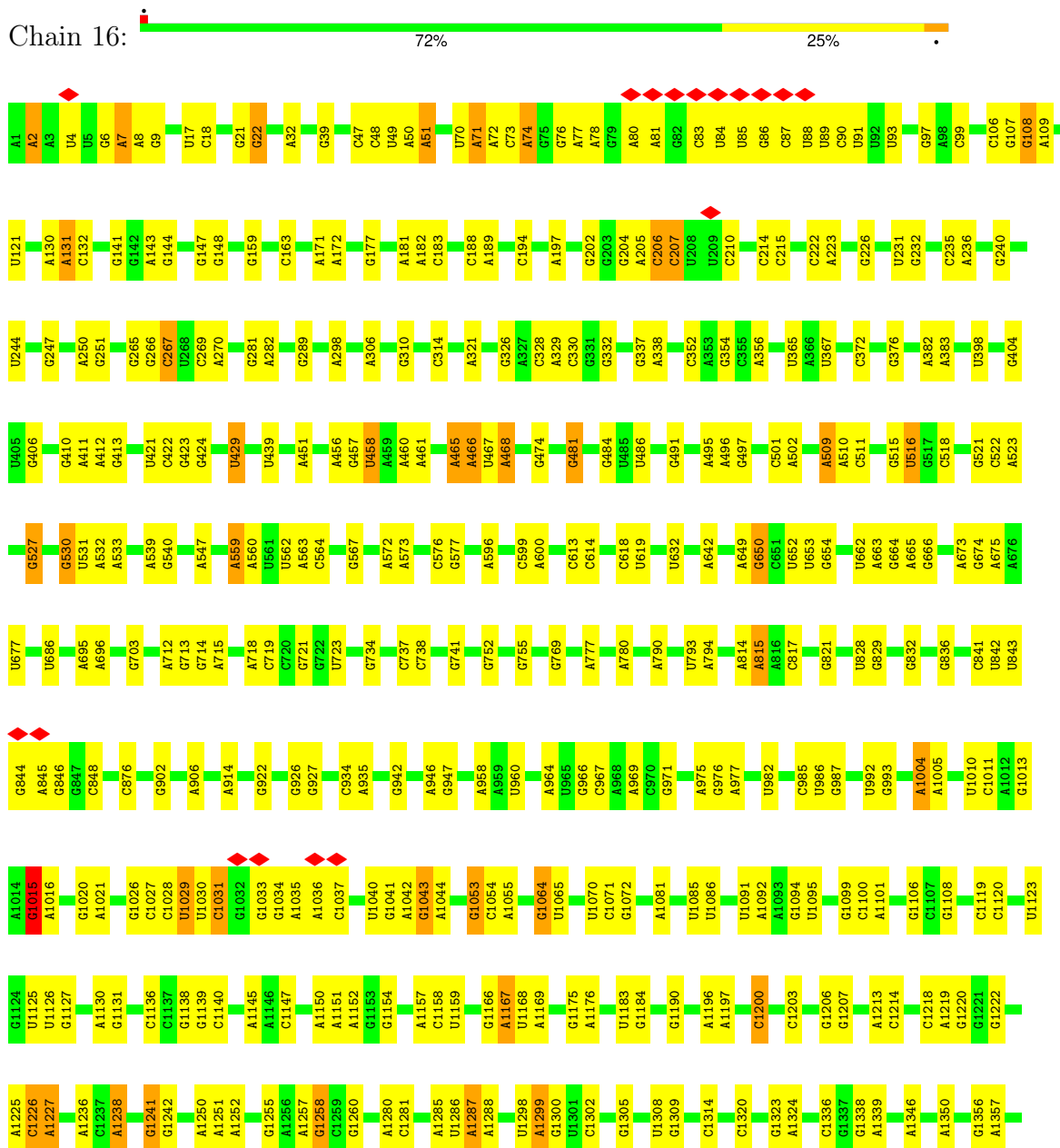
- Molecule 67 is water.

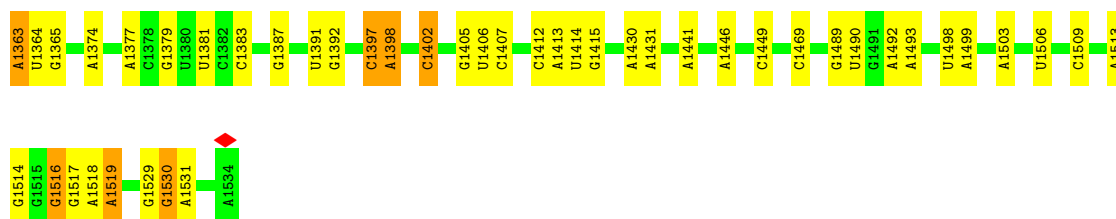
Mol	Chain	Residues	Atoms		AltConf
67	16	1	Total	O	0
			1	1	
67	SB	1	Total	O	0
			1	1	
67	23	22	Total	O	0
			22	22	
67	LB	1	Total	O	0
			1	1	
67	EF	1	Total	O	0
			1	1	

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.

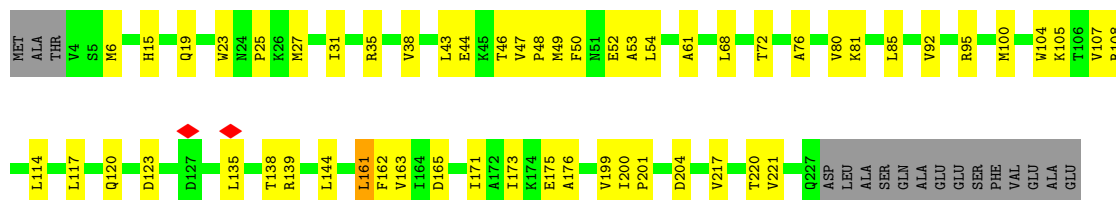
• Molecule 1: 16S rRNA





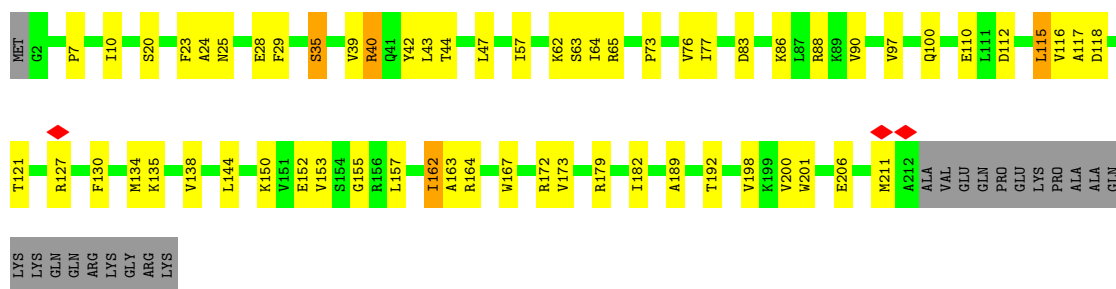
• Molecule 2: 30S ribosomal protein S2

Chain SB: 70% 23% 7%



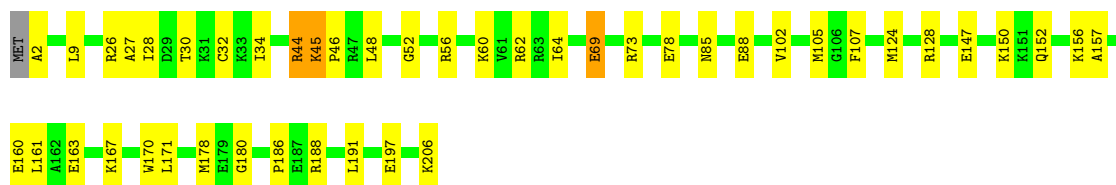
• Molecule 3: 30S ribosomal protein S3

Chain SC: 64% 25% 9%



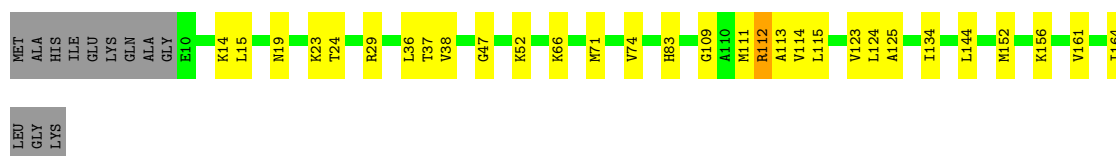
• Molecule 4: 30S ribosomal protein S4

Chain SD: 78% 20% 2%



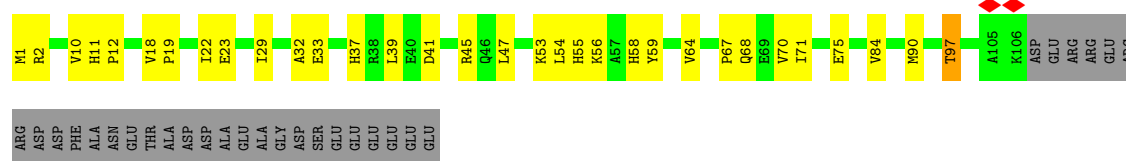
• Molecule 5: 30S ribosomal protein S5

Chain SE: 75% 17% 7%

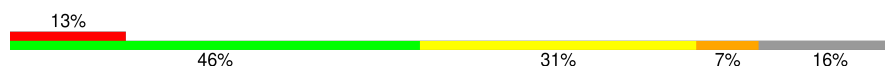


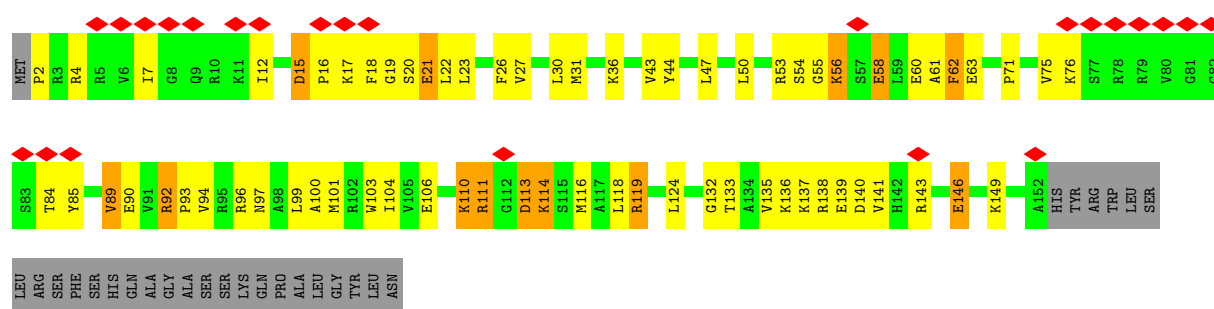
- Molecule 6: 30S ribosomal protein S6

Chain SF: 



- Molecule 7: 30S ribosomal protein S7

Chain SG: 



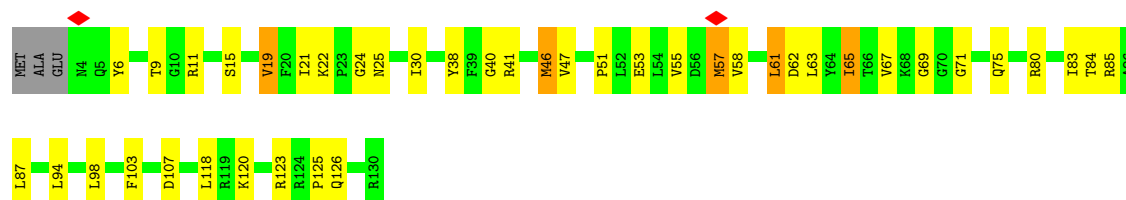
- Molecule 8: 30S ribosomal protein S8

Chain SH: 



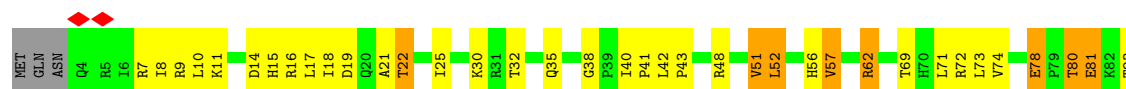
- Molecule 9: 30S ribosomal protein S9

Chain SI: 



- Molecule 10: 30S ribosomal protein S10

Chain SJ: 

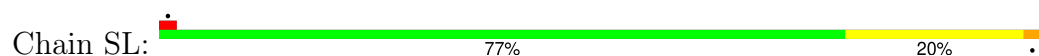




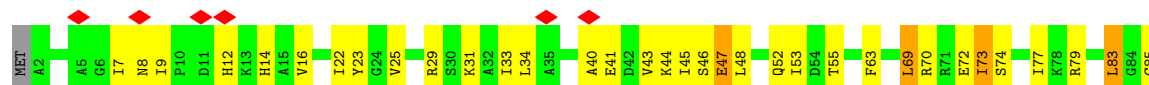
- Molecule 11: 30S ribosomal protein S11



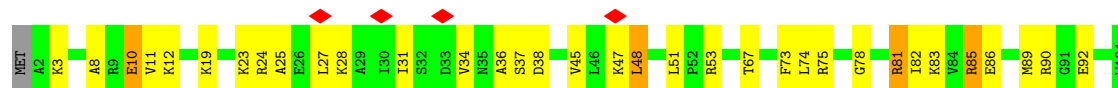
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14

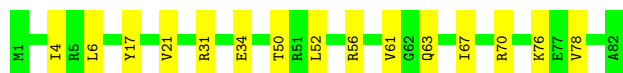


- Molecule 15: 30S ribosomal protein S15



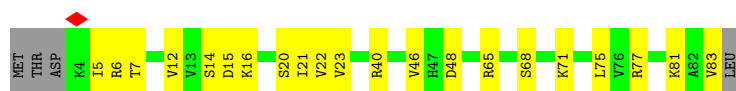
- Molecule 16: 30S ribosomal protein S16

Chain SP:  82% 18%



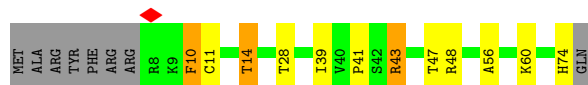
- Molecule 17: 30S ribosomal protein S17

Chain SQ:  70% 25% 5%



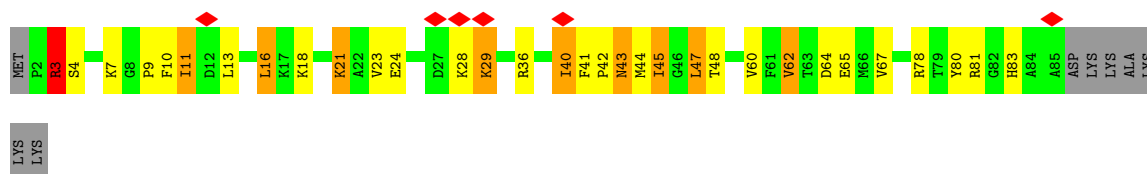
- Molecule 18: 30S ribosomal protein S18

Chain SR:  73% 12% 11%



- Molecule 19: 30S ribosomal protein S19

Chain SS:  7% 57% 24% 10% 9%



- Molecule 20: 30S ribosomal protein S20

Chain ST:  80% 16% ..



- Molecule 21: 30S ribosomal protein S21

Chain SU:  79% 18% ..

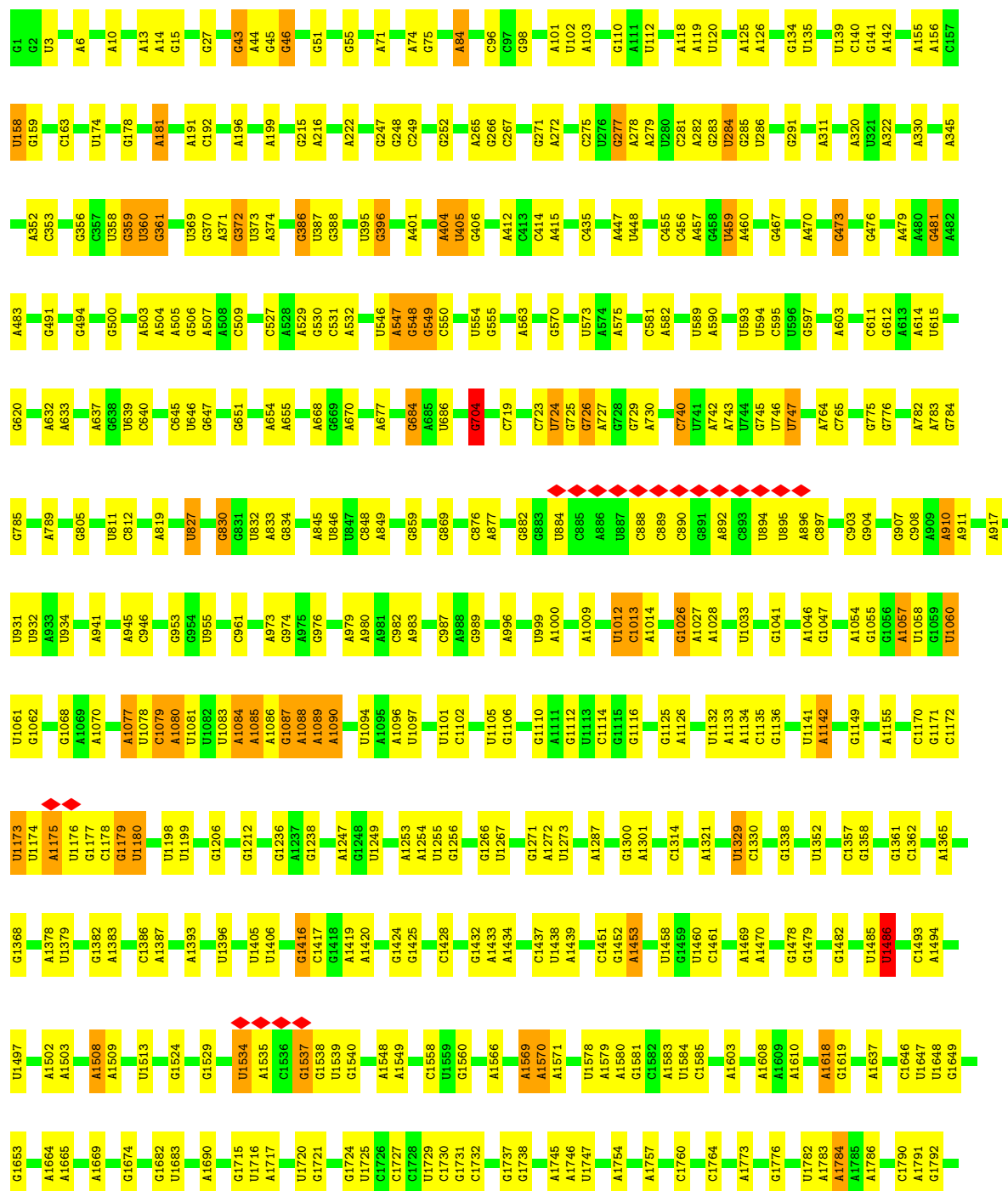


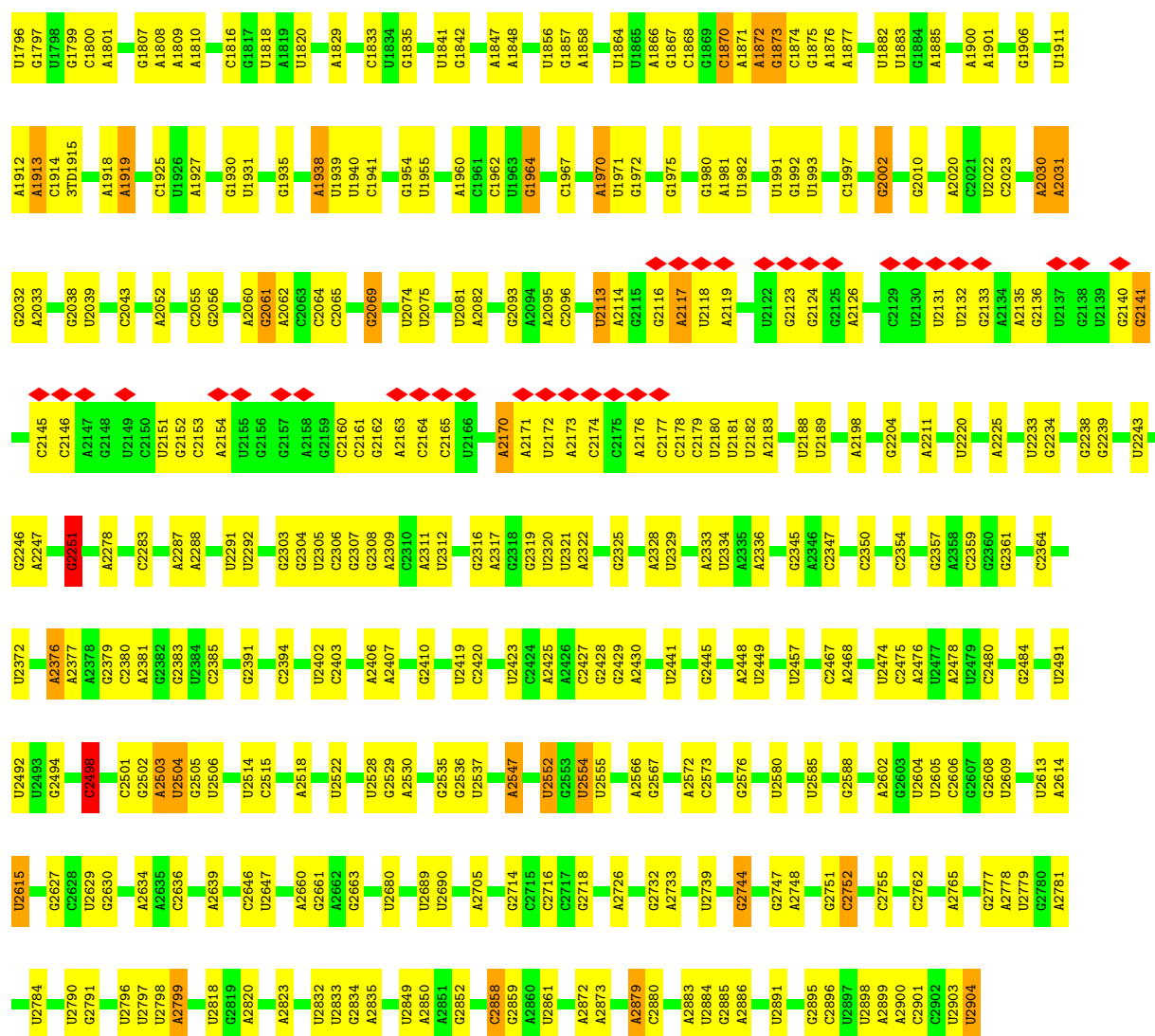
- Molecule 22: mRNA

Chain mR:  15% 80%



• Molecule 23: 23S rRNA





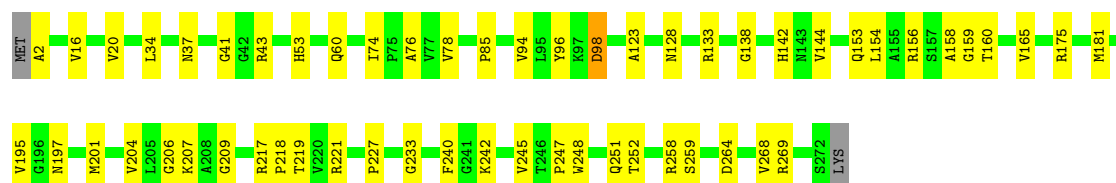
• Molecule 24: 5S rRNA

Chain 5: 79% 19%



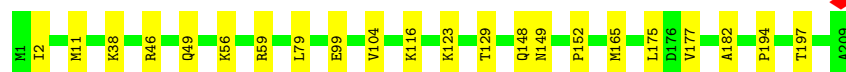
• Molecule 25: 50S ribosomal protein L2

Chain LB: 79% 20%



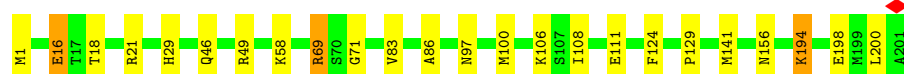
• Molecule 26: 50S ribosomal protein L3

Chain LC:  89% 11%



- Molecule 27: 50S ribosomal protein L4

Chain LD:  88% 10%



- Molecule 28: 50S ribosomal protein L5

Chain LE:  66% 27% 6%



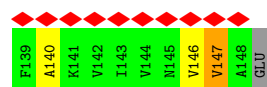
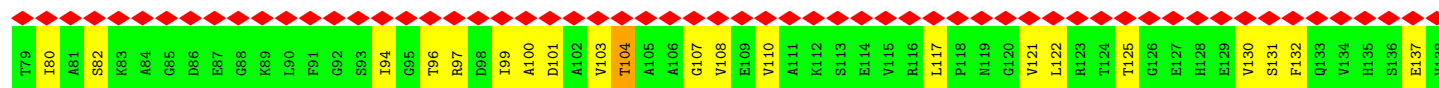
- Molecule 29: 50S ribosomal protein L6

Chain LF:  73% 25%

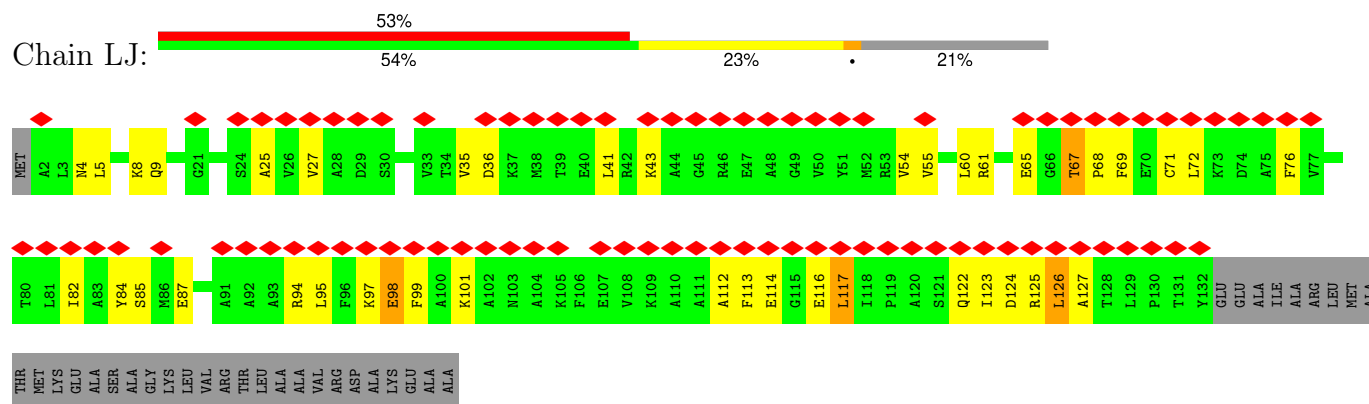


- Molecule 30: 50S ribosomal protein L9

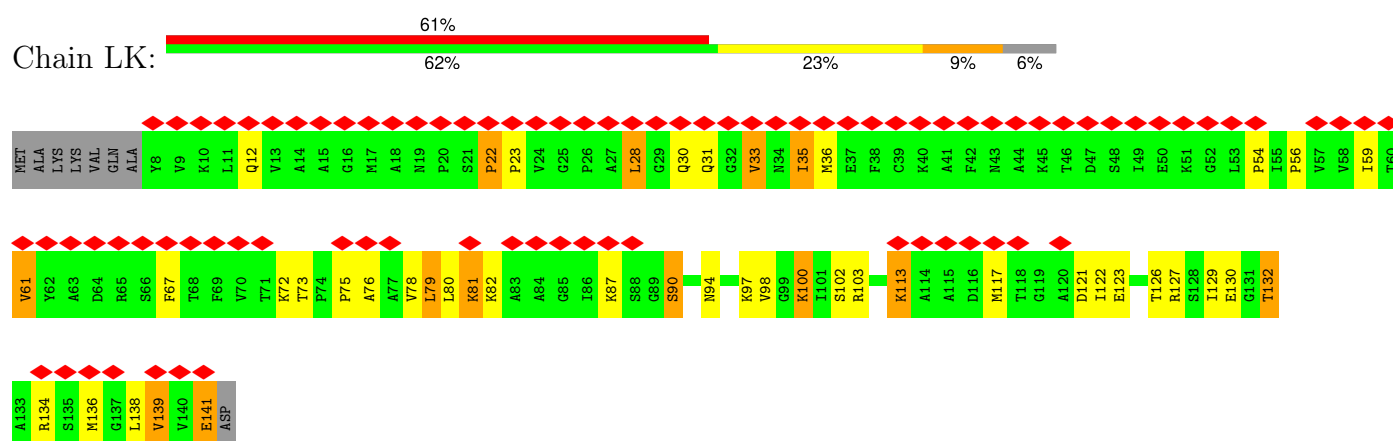
Chain LI:  66% 61% 36%



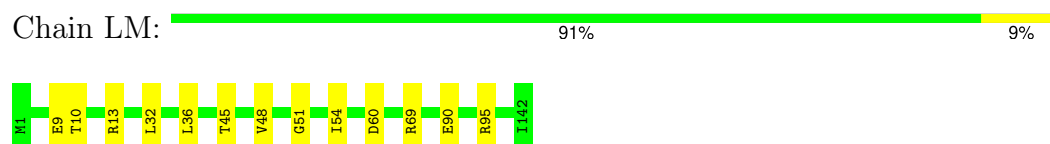
- Molecule 31: 50S ribosomal protein L10



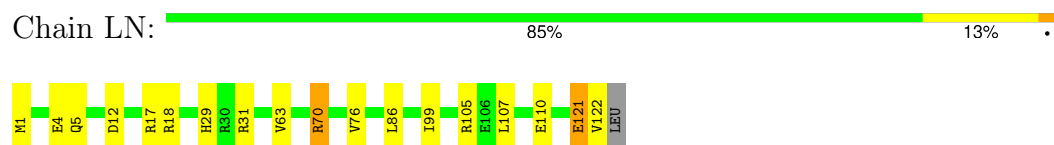
- Molecule 32: 50S ribosomal protein L11



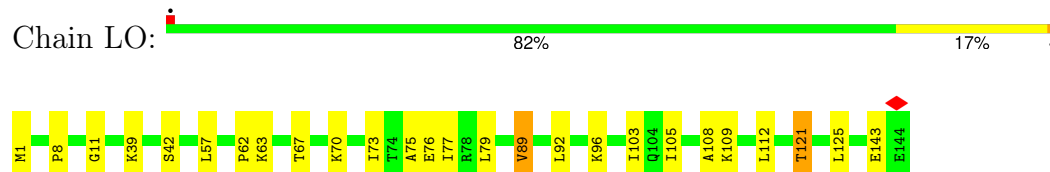
- Molecule 33: 50S ribosomal protein L13



- Molecule 34: 50S ribosomal protein L14

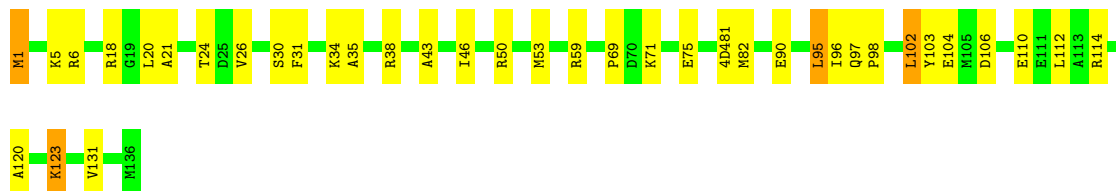


- Molecule 35: 50S ribosomal protein L15



- Molecule 36: 50S ribosomal protein L16

Chain LP:  72% 25%



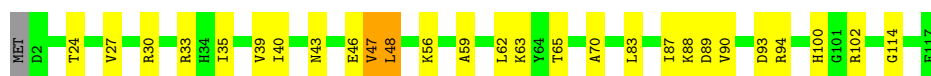
- Molecule 37: 50S ribosomal protein L17

Chain LQ:  75% 19% 6%



- Molecule 38: 50S ribosomal protein L18

Chain LR:  76% 21%



- Molecule 39: 50S ribosomal protein L19

Chain LS:  83% 16%



- Molecule 40: 50S ribosomal protein L20

Chain LT:  89% 10%



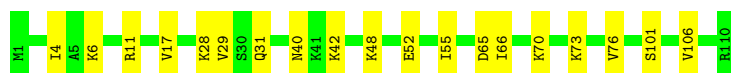
- Molecule 41: 50S ribosomal protein L21

Chain LU:  82% 17%

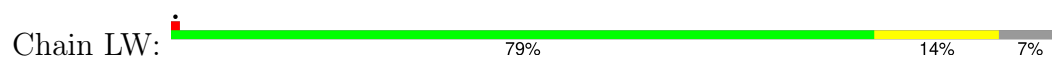


- Molecule 42: 50S ribosomal protein L22

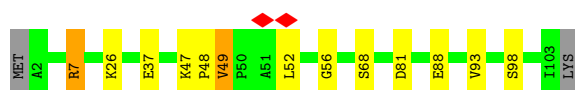
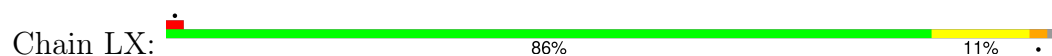
Chain LV:  83% 17%



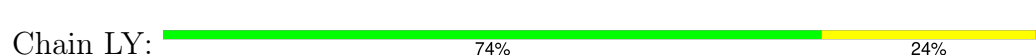
- Molecule 43: 50S ribosomal protein L23



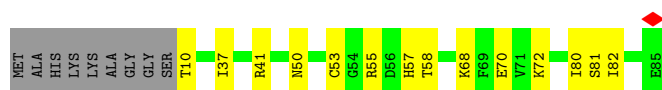
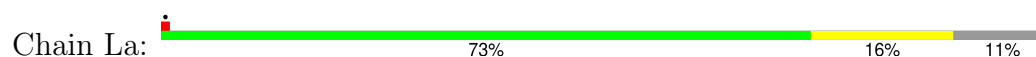
- Molecule 44: 50S ribosomal protein L24



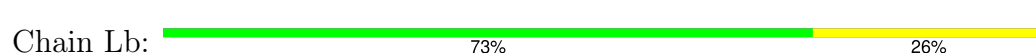
- Molecule 45: 50S ribosomal protein L25



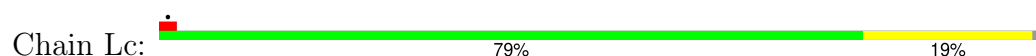
- Molecule 46: 50S ribosomal protein L27



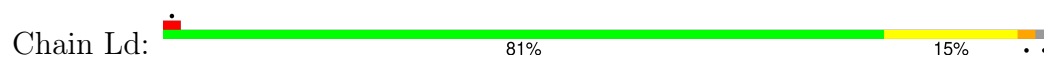
- Molecule 47: 50S ribosomal protein L28



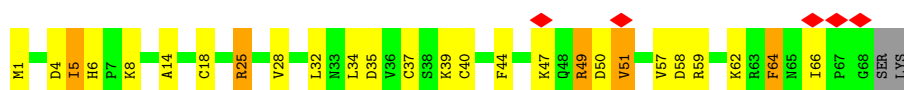
- Molecule 48: 50S ribosomal protein L29



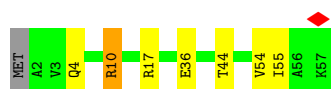
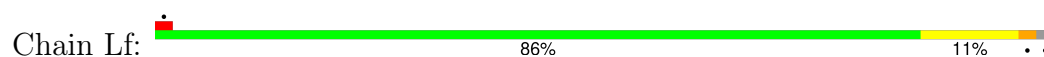
- Molecule 49: 50S ribosomal protein L30



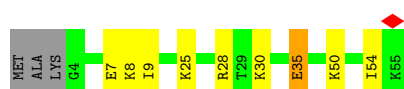
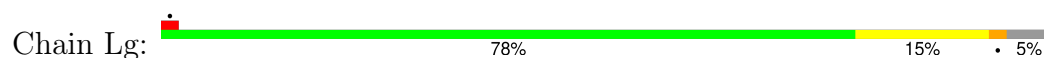
- Molecule 50: 50S ribosomal protein L31



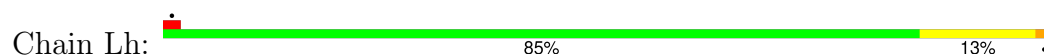
- Molecule 51: 50S ribosomal protein L32



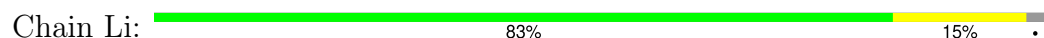
- Molecule 52: 50S ribosomal protein L33



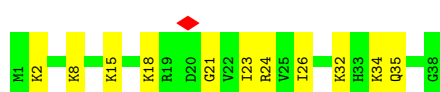
- Molecule 53: 50S ribosomal protein L34



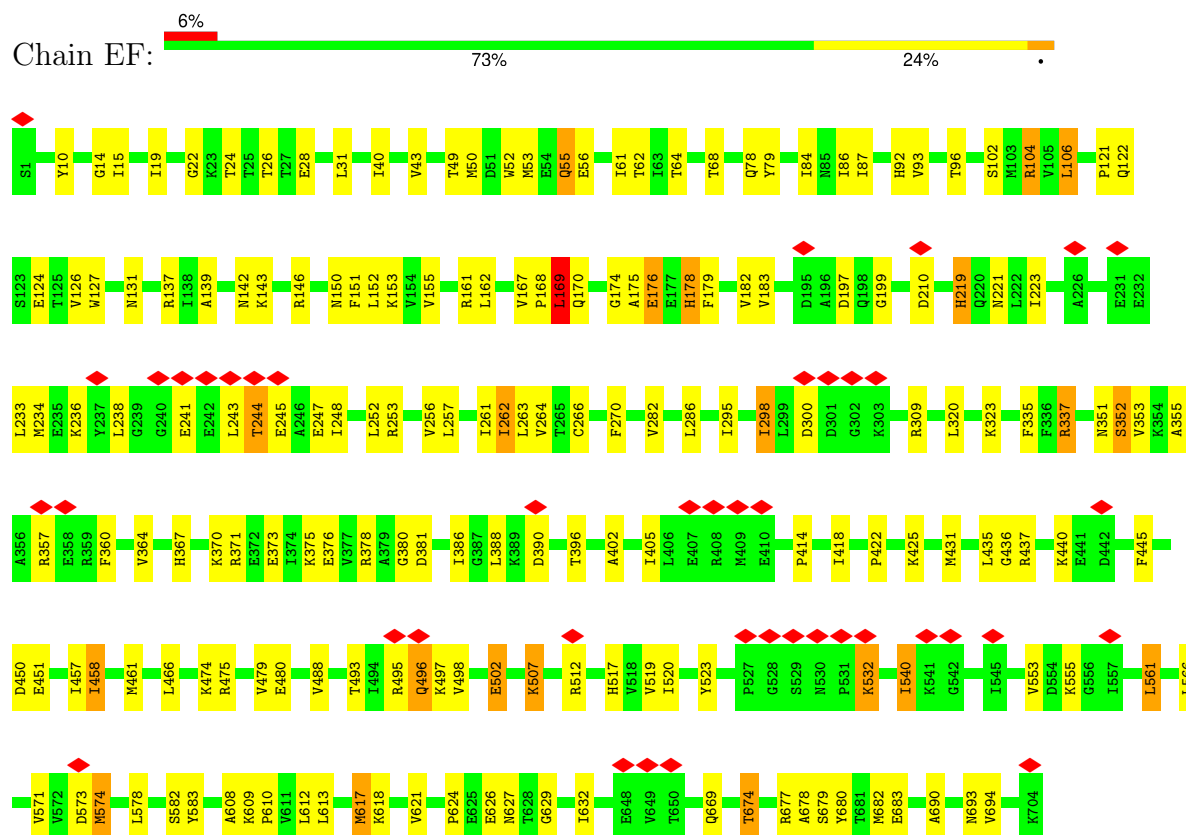
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



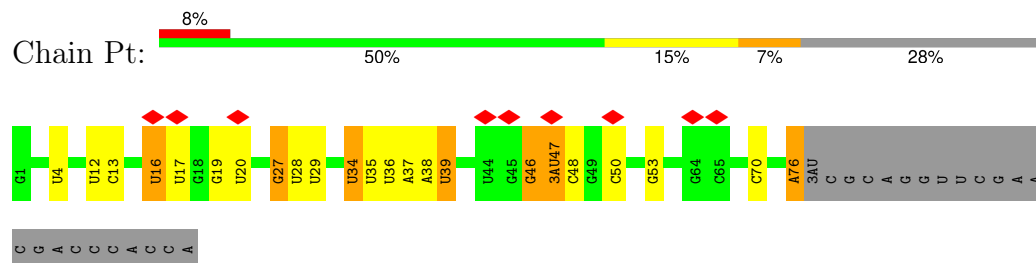
- Molecule 56: Elongation factor G



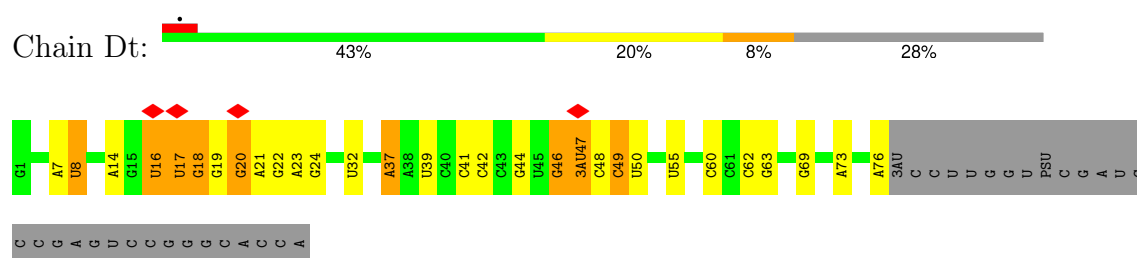
- Molecule 57: Nascent peptide



- Molecule 58: tRNA



- Molecule 59: tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33688	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	0.103	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	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: 4OC, GTP, PSU, UR3, 2MG, MA6, 3AU, 7MG, 5MC, MG, 5MU, MIA, OMC, OMG, 6MZ, SCM, SPD, 4D4, ZN, H2U, ATP, U8U, PUT, 1MG, D2T, OMU, 2MA, 3TD, 4SU, T6A

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	0.34	0/36619	0.38	8/57122 (0.0%)
2	SB	0.44	0/1784	0.74	0/2403
3	SC	0.41	2/1680 (0.1%)	0.62	0/2263
4	SD	0.33	0/1665	0.52	0/2227
5	SE	0.37	0/1157	0.57	0/1557
6	SF	0.40	0/881	0.66	0/1189
7	SG	0.59	0/1195	1.08	4/1602 (0.2%)
8	SH	0.33	0/989	0.41	0/1326
9	SI	0.75	1/1034 (0.1%)	0.99	0/1375
10	SJ	0.46	0/805	0.78	1/1089 (0.1%)
11	SK	0.44	0/911	0.68	0/1229
12	SL	0.32	0/960	0.45	0/1286
13	SM	0.58	0/892	1.03	3/1193 (0.3%)
14	SN	0.53	0/817	1.15	4/1088 (0.4%)
15	SO	0.33	0/722	0.49	0/964
16	SP	0.36	0/659	0.51	0/884
17	SQ	0.39	0/657	0.64	0/881
18	SR	0.33	0/564	0.51	0/756
19	SS	0.66	0/685	0.97	2/922 (0.2%)
20	ST	0.33	0/670	0.54	0/888
21	SU	0.67	0/597	1.00	0/792
22	mR	0.30	0/283	0.39	0/438
23	23	0.40	0/69284	0.40	12/108082 (0.0%)
24	5	0.35	0/2873	0.36	1/4478 (0.0%)
25	LB	0.38	0/2121	0.48	0/2852
26	LC	0.38	0/1586	0.52	0/2134
27	LD	0.35	0/1571	0.46	0/2113
28	LE	0.61	1/1434 (0.1%)	0.90	3/1926 (0.2%)
29	LF	0.32	0/1343	0.54	0/1816
30	LI	0.35	0/1112	1.01	5/1503 (0.3%)
31	LJ	0.55	0/1006	0.85	2/1358 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LK	0.77	0/993	1.02	1/1341 (0.1%)
33	LM	0.37	0/1152	0.44	0/1551
34	LN	0.40	0/947	0.53	0/1268
35	LO	0.40	0/1062	0.56	0/1413
36	LP	0.37	0/1081	0.49	0/1443
37	LQ	0.34	0/973	0.40	0/1301
38	LR	0.40	1/902 (0.1%)	0.58	0/1209
39	LS	0.35	0/929	0.45	0/1242
40	LT	0.36	0/960	0.38	0/1278
41	LU	0.42	0/829	0.60	0/1107
42	LV	0.41	0/864	0.50	0/1156
43	LW	0.34	0/744	0.51	0/994
44	LX	0.42	0/787	0.61	0/1051
45	LY	0.32	0/766	0.47	0/1025
46	La	0.35	0/589	0.44	0/779
47	Lb	0.38	0/635	0.59	1/848 (0.1%)
48	Lc	0.54	0/502	0.81	0/667
49	Ld	0.47	0/453	0.63	0/605
50	Le	0.57	0/543	0.97	0/726
51	Lf	0.37	0/450	0.47	0/599
52	Lg	0.40	0/434	0.57	0/576
53	Lh	0.40	0/380	0.43	0/498
54	Li	0.36	0/513	0.50	0/676
55	Lj	0.35	0/303	0.46	0/397
56	EF	0.51	0/5490	0.74	2/7437 (0.0%)
57	Pp	0.58	0/28	1.61	0/34
58	Pt	0.38	2/1684 (0.1%)	0.44	0/2615
59	Dt	0.33	0/1654	0.46	0/2572
All	All	0.40	7/165203 (0.0%)	0.49	49/246144 (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	2
4	SD	0	3
5	SE	0	1
9	SI	0	3
10	SJ	0	2
12	SL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	SM	0	4
14	SN	0	2
17	SQ	0	3
19	SS	0	1
21	SU	0	1
25	LB	0	3
27	LD	0	1
28	LE	0	3
30	LI	0	2
34	LN	0	2
36	LP	0	2
37	LQ	0	2
38	LR	0	1
41	LU	0	1
44	LX	0	1
45	LY	0	1
46	La	0	1
49	Ld	0	1
51	Lf	0	2
55	Lj	0	1
56	EF	0	3
All	All	0	50

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	LE	93	GLY	C-N	-15.39	1.14	1.33
9	SI	41	ARG	C-O	7.29	1.32	1.24
38	LR	88	LYS	C-N	6.71	1.43	1.33
58	Pt	16	U	C1'-N1	6.67	1.58	1.48
3	SC	182	ILE	C-N	-5.92	1.25	1.33
58	Pt	20	U	C1'-N1	5.76	1.56	1.47
3	SC	35	SER	C-N	5.05	1.41	1.34

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	SN	24	ARG	N-CA-C	19.09	131.78	110.97
30	LI	75	LEU	N-CA-C	18.30	131.34	111.03
14	SN	25	ALA	N-CA-CB	-14.51	88.78	110.12
1	16	1490	U	OP1-P-OP2	-13.48	79.15	119.60
13	SM	114	LYS	CB-CA-C	-13.02	88.58	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	LE	93	GLY	CA-C-N	12.88	137.18	120.44
28	LE	93	GLY	C-N-CA	12.88	137.18	120.44
1	16	1490	U	O5'-P-OP1	-11.01	74.96	108.00
1	16	1489	G	OP2-P-O3'	-10.69	75.92	108.00
23	23	1060	U	C2'-C3'-O3'	10.18	124.77	109.50
1	16	1489	G	OP1-P-O3'	9.31	135.93	108.00
30	LI	75	LEU	CB-CA-C	-9.31	96.53	110.95
23	23	43	G	C2'-C3'-O3'	8.41	126.31	113.70
1	16	1490	U	O5'-P-OP2	7.78	131.33	108.00
32	LK	22	PRO	N-CA-C	7.47	119.81	110.70
23	23	2858	C	C2'-C3'-O3'	7.17	124.45	113.70
13	SM	47	GLU	CA-CB-CG	6.92	127.94	114.10
23	23	827	U	C1'-C2'-O2'	-6.64	101.84	111.80
23	23	704	G	C2'-C3'-O3'	-6.50	103.95	113.70
23	23	1486	U	C2'-C3'-O3'	6.45	123.38	113.70
23	23	404	A	C4'-C3'-O3'	6.35	118.93	109.40
30	LI	32	PRO	CB-CA-C	-6.35	102.47	113.20
23	23	1416	G	C4'-C3'-O3'	6.31	118.86	109.40
7	SG	2	PRO	CA-N-CD	-6.28	103.20	112.00
19	SS	28	LYS	N-CA-C	-6.24	105.69	113.55
7	SG	97	ASN	CB-CA-C	-6.18	101.44	110.96
1	16	1053	G	O3'-P-O5'	-6.13	94.81	104.00
31	LJ	84	TYR	CB-CA-C	-6.01	100.05	110.45
23	23	277	G	C4'-C3'-O3'	5.84	118.16	109.40
1	16	1489	G	O3'-P-O5'	-5.76	95.37	104.00
23	23	13	A	C2'-C3'-O3'	5.76	118.14	109.50
23	23	158	U	P-O3'-C3'	5.71	128.76	120.20
23	23	1508	A	C4'-C3'-O3'	5.70	117.95	109.40
7	SG	55	GLY	CA-C-O	-5.62	118.27	122.37
30	LI	32	PRO	N-CA-C	5.61	122.87	113.78
31	LJ	124	ASP	N-CA-C	-5.45	106.33	112.87
1	16	1015	G	C2'-C3'-O3'	-5.36	105.66	113.70
28	LE	93	GLY	O-C-N	-5.32	115.78	122.70
47	Lb	44	LYS	CA-CB-CG	5.31	124.72	114.10
24	5	40	U	C4'-C3'-O3'	5.30	117.35	109.40
19	SS	47	LEU	CA-CB-CG	5.29	134.80	116.30
14	SN	27	LEU	N-CA-C	5.28	116.72	110.97
14	SN	36	ALA	N-CA-C	-5.18	105.63	111.28
10	SJ	57	VAL	N-CA-C	5.17	120.09	109.34
56	EF	169	LEU	N-CA-C	-5.14	106.69	113.17
13	SM	31	LYS	CA-CB-CG	5.10	124.29	114.10
7	SG	146	GLU	N-CA-C	-5.09	107.45	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	EF	573	ASP	CB-CA-C	5.06	119.07	111.89
30	LI	147	VAL	CA-C-O	-5.04	116.70	121.64

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
56	EF	104	ARG	Sidechain
56	EF	378	ARG	Sidechain
56	EF	475	ARG	Sidechain
25	LB	221	ARG	Sidechain
25	LB	258	ARG	Sidechain
25	LB	269	ARG	Sidechain
27	LD	69	ARG	Sidechain
28	LE	167	ARG	Sidechain
28	LE	30	ARG	Sidechain
28	LE	71	ARG	Sidechain
30	LI	104	THR	Peptide
30	LI	108	VAL	Peptide
34	LN	31	ARG	Sidechain
34	LN	70	ARG	Sidechain
36	LP	18	ARG	Sidechain
36	LP	59	ARG	Sidechain
37	LQ	118	ARG	Sidechain
37	LQ	2	ARG	Sidechain
38	LR	102	ARG	Sidechain
41	LU	51	VAL	Peptide
44	LX	7	ARG	Sidechain
45	LY	21	ARG	Sidechain
46	La	41	ARG	Sidechain
49	Ld	16	ARG	Sidechain
51	Lf	10	ARG	Sidechain
51	Lf	17	ARG	Sidechain
55	Lj	24	ARG	Sidechain
3	SC	40	ARG	Sidechain
3	SC	88	ARG	Sidechain
4	SD	26	ARG	Sidechain
4	SD	44	ARG	Sidechain
4	SD	56	ARG	Sidechain
5	SE	112	ARG	Sidechain
9	SI	11	ARG	Sidechain
9	SI	123	ARG	Sidechain

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Mol	Chain	Res	Type	Group
9	SI	40	GLY	Mainchain
10	SJ	16	ARG	Sidechain
10	SJ	48	ARG	Sidechain
12	SL	86	ARG	Sidechain
13	SM	113	ARG	Sidechain
13	SM	114	LYS	Peptide
13	SM	70	ARG	Sidechain
13	SM	87	ARG	Sidechain
14	SN	75	ARG	Sidechain
14	SN	85	ARG	Sidechain
17	SQ	40	ARG	Sidechain
17	SQ	6	ARG	Sidechain
17	SQ	65	ARG	Sidechain
19	SS	3	ARG	Sidechain
21	SU	7	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	32929	0	16590	158	0
2	SB	1753	0	1780	36	0
3	SC	1653	0	1727	35	0
4	SD	1643	0	1707	27	0
5	SE	1144	0	1185	18	0
6	SF	862	0	864	16	0
7	SG	1181	0	1238	53	0
8	SH	979	0	1031	17	0
9	SI	1022	0	1070	29	0
10	SJ	795	0	836	40	0
11	SK	895	0	909	19	0
12	SL	957	0	1017	17	0
13	SM	883	0	941	25	0
14	SN	805	0	844	19	0
15	SO	714	0	734	5	0
16	SP	649	0	666	8	0
17	SQ	648	0	691	10	0
18	SR	555	0	578	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	SS	668	0	693	24	0
20	ST	664	0	714	9	0
21	SU	589	0	629	9	0
22	mR	254	0	129	2	0
23	23	62355	0	31382	238	0
24	5	2570	0	1301	7	0
25	LB	2082	0	2154	31	0
26	LC	1565	0	1616	13	0
27	LD	1552	0	1619	15	0
28	LE	1410	0	1443	46	0
29	LF	1323	0	1371	32	0
30	LI	1101	0	1141	34	0
31	LJ	992	0	1022	23	0
32	LK	979	0	1028	28	0
33	LM	1129	0	1162	7	0
34	LN	938	0	1012	12	0
35	LO	1053	0	1129	18	0
36	LP	1075	0	1155	22	0
37	LQ	960	0	1000	16	0
38	LR	892	0	923	11	0
39	LS	917	0	962	9	0
40	LT	947	0	1019	8	0
41	LU	816	0	839	10	0
42	LV	857	0	922	11	0
43	LW	738	0	807	8	0
44	LX	779	0	830	5	0
45	LY	753	0	780	14	0
46	La	582	0	599	6	0
47	Lb	625	0	652	12	0
48	Lc	501	0	531	10	0
49	Ld	449	0	488	5	0
50	Le	533	0	529	23	0
51	Lf	444	0	458	3	0
52	Lg	427	0	464	3	0
53	Lh	377	0	418	5	0
54	Li	504	0	572	10	0
55	Lj	302	0	340	7	0
56	EF	5388	0	5318	130	0
57	Pp	28	0	33	3	0
58	Pt	1636	0	836	9	0
59	Dt	1641	0	844	8	0
60	16	46	0	48	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	23	23	0	24	1	0
61	16	18	0	36	2	0
61	23	78	0	156	3	0
61	LC	6	0	10	1	0
62	16	63	0	0	0	0
62	23	264	0	0	0	0
62	5	6	0	0	0	0
62	EF	1	0	0	0	0
62	LB	1	0	0	0	0
62	LC	1	0	0	0	0
62	LD	1	0	0	0	0
62	LO	1	0	0	0	0
62	LQ	1	0	0	0	0
62	Lf	1	0	0	0	0
62	Pt	1	0	0	0	0
62	SK	1	0	0	0	0
62	SN	1	0	0	0	0
62	SR	1	0	0	0	0
63	Le	1	0	0	0	0
63	Lj	1	0	0	0	0
63	SB	1	0	0	0	0
64	23	62	0	24	0	0
65	23	20	0	38	6	0
66	EF	32	0	11	7	0
67	16	1	0	0	0	0
67	23	22	0	0	0	0
67	EF	1	0	0	0	0
67	LB	1	0	0	0	0
67	SB	1	0	0	0	0
All	All	154120	0	105619	1312	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 5.

All (1312) 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)
7:SG:62:PHE:CZ	7:SG:124:LEU:HD22	1.09	1.59
7:SG:62:PHE:CZ	7:SG:124:LEU:CD2	1.90	1.49
57:Pp:3:LYS:C	58:Pt:76:A:O3'	1.67	1.35
7:SG:62:PHE:CE1	7:SG:124:LEU:HD22	1.73	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SG:62:PHE:HZ	7:SG:124:LEU:CD2	1.31	1.18
15:SO:89:ARG:OXT	15:SO:89:ARG:HG3	1.42	1.17
7:SG:62:PHE:HZ	7:SG:124:LEU:HD23	1.24	1.00
56:EF:31:LEU:HD11	56:EF:50:MET:HE3	1.47	0.97
23:23:2744:G:H21	29:LF:143:GLN:HE22	1.14	0.94
19:SS:3:ARG:HE	19:SS:7:LYS:HB2	1.34	0.93
50:Le:37:CYS:H	50:Le:40:CYS:HB2	1.32	0.91
7:SG:62:PHE:HE1	7:SG:124:LEU:CB	1.83	0.90
10:SJ:35:GLN:HE22	10:SJ:78:GLU:HB2	1.40	0.86
7:SG:62:PHE:HE1	7:SG:124:LEU:HB3	1.38	0.86
56:EF:104:ARG:HH21	56:EF:320:LEU:CD2	1.89	0.83
30:LI:9:VAL:HG11	30:LI:12:LEU:HD23	1.61	0.83
49:Ld:24:LEU:HD11	49:Ld:54:MET:HE1	1.60	0.83
23:23:476:G:H22	23:23:479:A:H5''	1.43	0.83
14:SN:34:VAL:HG13	14:SN:37:SER:H	1.44	0.82
57:Pp:3:LYS:C	58:Pt:76:A:C3'	2.51	0.82
9:SI:24:GLY:HA2	9:SI:61:LEU:HA	1.62	0.82
7:SG:62:PHE:CE1	7:SG:124:LEU:CB	2.62	0.81
19:SS:3:ARG:NH1	19:SS:10:PHE:HB2	1.98	0.79
9:SI:15:SER:HA	9:SI:69:GLY:HA3	1.66	0.77
23:23:448:U:P	65:23:3017:SPD:H21	2.23	0.77
29:LF:19:ILE:HD12	29:LF:24:ILE:HD12	1.66	0.77
10:SJ:40:ILE:HB	10:SJ:73:LEU:HB3	1.67	0.77
36:LP:50:ARG:HA	36:LP:53:MET:HE2	1.67	0.76
31:LJ:67:THR:HG22	31:LJ:68:PRO:HD2	1.67	0.76
56:EF:507:LYS:HA	56:EF:507:LYS:HE2	1.67	0.75
9:SI:6:TYR:HB2	9:SI:21:ILE:HB	1.69	0.74
1:16:458:U:H3	1:16:474:G:H1	1.36	0.74
27:LD:1:MET:HG2	27:LD:16:GLU:HG3	1.70	0.73
7:SG:62:PHE:CE1	7:SG:124:LEU:CD2	2.47	0.73
26:LC:123:LYS:HG2	26:LC:165:MET:HE1	1.71	0.73
28:LE:111:ILE:HD12	28:LE:111:ILE:H	1.53	0.73
19:SS:3:ARG:HH12	19:SS:10:PHE:HB2	1.53	0.73
28:LE:140:GLU:HG3	50:Le:28:VAL:HG13	1.70	0.73
56:EF:674:THR:HG21	56:EF:678:ALA:HB2	1.70	0.73
9:SI:51:PRO:HG3	9:SI:80:ARG:HG2	1.71	0.72
42:LV:48:LYS:O	42:LV:52:GLU:HG3	1.90	0.72
7:SG:71:PRO:HG3	7:SG:103:TRP:HZ3	1.54	0.71
26:LC:148:GLN:HB2	26:LC:152:PRO:HG3	1.71	0.71
36:LP:5:LYS:HD2	58:Pt:53:G:H4'	1.72	0.71
20:ST:76:LYS:O	20:ST:80:THR:HG23	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LI:132:PHE:HB2	30:LI:140:ALA:HB3	1.71	0.71
1:16:76:G:H1	1:16:93:U:H3	1.38	0.71
13:SM:69:LEU:HA	13:SM:72:GLU:HG3	1.72	0.71
36:LP:20:LEU:HD13	45:LY:81:PRO:HG3	1.72	0.71
9:SI:57:MET:HE3	9:SI:57:MET:HA	1.73	0.71
10:SJ:8:ILE:HD12	10:SJ:100:ILE:HD13	1.73	0.70
56:EF:143:LYS:HB3	56:EF:146:ARG:HG3	1.73	0.70
28:LE:110:ARG:HG2	28:LE:137:ILE:HA	1.74	0.70
50:Le:14:ALA:HB1	50:Le:34:LEU:HD11	1.73	0.70
7:SG:62:PHE:CZ	7:SG:124:LEU:HD23	2.06	0.70
54:Li:16:LYS:HE3	54:Li:20:GLY:HA2	1.74	0.70
1:16:1106:G:H5''	3:SC:172:ARG:HG2	1.72	0.70
7:SG:50:LEU:HD22	7:SG:124:LEU:HD13	1.73	0.69
29:LF:35:ARG:HB2	29:LF:75:MET:HE1	1.72	0.69
15:SO:89:ARG:OXT	15:SO:89:ARG:CG	2.30	0.69
3:SC:47:LEU:HD23	3:SC:76:VAL:HG12	1.74	0.69
8:SH:96:MET:HE3	8:SH:130:ALA:HB1	1.73	0.69
13:SM:106:ALA:HB3	13:SM:110:LYS:HE3	1.75	0.69
29:LF:18:LYS:HE2	29:LF:20:ASN:HD21	1.58	0.68
36:LP:35:ALA:HB2	36:LP:102:LEU:HD21	1.75	0.68
1:16:1238:A:H5'	1:16:1336:C:H41	1.58	0.68
1:16:664:G:H22	1:16:741:G:H1	1.40	0.68
23:23:2117:A:H61	23:23:2170:A:H61	1.39	0.68
56:EF:50:MET:HE1	56:EF:68:THR:HG21	1.76	0.68
56:EF:298:ILE:HG22	56:EF:300:ASP:H	1.58	0.68
56:EF:370:LYS:H	56:EF:370:LYS:HD2	1.57	0.68
19:SS:45:ILE:HD11	19:SS:64:ASP:HA	1.75	0.67
56:EF:609:LYS:HE2	56:EF:609:LYS:HA	1.74	0.67
31:LJ:61:ARG:HH12	31:LJ:76:PHE:HB2	1.59	0.67
1:16:718:A:H5'	11:SK:119:ASN:HB2	1.76	0.67
8:SH:87:LYS:CG	8:SH:125:ILE:HD11	2.23	0.67
12:SL:114:ARG:HB3	12:SL:119:VAL:HB	1.77	0.67
29:LF:137:ASP:HB3	29:LF:140:VAL:HG22	1.77	0.67
28:LE:135:GLN:HG3	28:LE:141:ILE:HG21	1.75	0.67
27:LD:97:ASN:HB2	27:LD:100:MET:HG3	1.75	0.67
4:SD:28:ILE:HG12	4:SD:34:ILE:HD11	1.77	0.67
28:LE:30:ARG:H	28:LE:159:THR:HG1	1.43	0.67
56:EF:517:HIS:HB3	56:EF:582:SER:HB3	1.75	0.67
8:SH:87:LYS:HB3	8:SH:91:GLU:HG3	1.77	0.67
21:SU:4:ILE:HG13	21:SU:19:PHE:HA	1.77	0.67
66:EF:901:GTP:H8	66:EF:901:GTP:H5''	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SI:61:LEU:HD13	9:SI:61:LEU:O	1.96	0.66
35:LO:75:ALA:HB2	35:LO:105:ILE:HD12	1.77	0.66
28:LE:34:ILE:HG12	28:LE:96:MET:HG3	1.78	0.66
1:16:1218:C:H2'	1:16:1219:A:C8	2.30	0.66
28:LE:63:GLN:HA	50:Le:6:HIS:HD2	1.61	0.66
30:LI:59:ALA:HA	30:LI:62:LEU:HG	1.78	0.66
32:LK:31:GLN:HB3	32:LK:61:VAL:HG21	1.75	0.66
17:SQ:15:ASP:HA	17:SQ:21:ILE:HG22	1.78	0.65
27:LD:108:ILE:HG23	35:LO:1:MET:HE1	1.78	0.65
30:LI:100:ALA:HA	30:LI:103:VAL:HG22	1.78	0.65
13:SM:23:TYR:HE1	13:SM:69:LEU:HD22	1.61	0.65
23:23:1077:A:H4'	32:LK:94:ASN:HD21	1.61	0.65
7:SG:62:PHE:CE1	7:SG:124:LEU:HB3	2.26	0.65
29:LF:24:ILE:HG12	29:LF:37:LEU:HD13	1.77	0.65
56:EF:566:LEU:C	56:EF:566:LEU:HD23	2.22	0.65
11:SK:31:ILE:HG23	11:SK:46:THR:HG22	1.78	0.65
23:23:1105:U:H2'	23:23:1106:G:H8	1.60	0.65
23:23:2744:G:N2	29:LF:143:GLN:HE22	1.90	0.65
3:SC:157:LEU:HD23	3:SC:164:ARG:HB2	1.78	0.64
1:16:1516:2MG:N7	61:16:1603:PUT:H22	2.13	0.64
19:SS:40:ILE:HG12	19:SS:62:VAL:HG21	1.79	0.64
36:LP:53:MET:HG3	36:LP:120:ALA:HB2	1.80	0.64
56:EF:43:VAL:HG11	66:EF:901:GTP:H5'	1.80	0.63
2:SB:161:LEU:HD12	2:SB:176:ALA:HB2	1.80	0.63
10:SJ:9:ARG:HB2	10:SJ:99:GLN:HB3	1.80	0.63
25:LB:175:ARG:HH11	25:LB:175:ARG:HG2	1.63	0.63
23:23:1176:U:H4'	23:23:1177:G:H8	1.64	0.63
53:Lh:10:LEU:HD21	53:Lh:14:ARG:HH21	1.64	0.63
4:SD:150:LYS:HG2	4:SD:178:MET:HE3	1.81	0.63
18:SR:14:THR:HG21	18:SR:48:ARG:HE	1.64	0.63
56:EF:627:ASN:OD1	56:EF:674:THR:HG23	1.99	0.62
3:SC:40:ARG:O	3:SC:44:THR:HG22	1.99	0.62
36:LP:71:LYS:HD2	36:LP:95:LEU:HD21	1.81	0.62
1:16:1123:U:H4'	10:SJ:38:GLY:HA3	1.80	0.62
3:SC:130:PHE:O	3:SC:134:MET:HG3	1.99	0.62
9:SI:22:LYS:HB2	9:SI:62:ASP:HB3	1.81	0.62
13:SM:48:LEU:HD21	13:SM:53:ILE:HG23	1.80	0.62
16:SP:52:LEU:HD23	16:SP:78:VAL:HG21	1.81	0.62
30:LI:8:LYS:HA	30:LI:14:SER:HB3	1.81	0.62
7:SG:71:PRO:HG3	7:SG:103:TRP:CZ3	2.33	0.62
23:23:1057:A:C8	23:23:1057:A:H5''	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Lb:31:PRO:HB2	47:Lb:33:LEU:HD13	1.80	0.62
56:EF:253:ARG:O	56:EF:257:LEU:HD12	1.99	0.62
17:SQ:21:ILE:HG13	17:SQ:48:ASP:HB2	1.82	0.62
16:SP:4:ILE:HG12	16:SP:21:VAL:HG22	1.82	0.62
56:EF:31:LEU:HD11	56:EF:50:MET:CE	2.28	0.62
23:23:284:U:H3	23:23:356:G:H1	1.48	0.61
23:23:448:U:OP2	65:23:3017:SPD:H21	1.99	0.61
27:LD:106:LYS:HG2	27:LD:200:LEU:HD13	1.82	0.61
1:16:1086:U:H3	1:16:1099:G:H22	1.47	0.61
56:EF:502:GLU:HB3	56:EF:519:VAL:HG22	1.82	0.61
30:LI:8:LYS:HD3	30:LI:14:SER:HB3	1.81	0.61
37:LQ:35:LYS:HD3	37:LQ:110:MET:HE3	1.81	0.61
30:LI:72:ILE:HD11	30:LI:140:ALA:HB1	1.81	0.61
33:LM:13:ARG:HD3	33:LM:51:GLY:O	2.00	0.61
2:SB:76:ALA:O	2:SB:80:VAL:HG12	2.01	0.61
26:LC:116:LYS:HD2	37:LQ:1:MET:HE1	1.82	0.61
28:LE:140:GLU:HG3	50:Le:28:VAL:CG1	2.29	0.61
1:16:1314:C:OP2	19:SS:4:SER:HB3	2.01	0.61
1:16:1356:G:H2'	1:16:1357:A:C8	2.35	0.61
2:SB:43:LEU:HA	2:SB:46:THR:HG22	1.83	0.61
7:SG:58:GLU:HA	7:SG:61:ALA:HB3	1.83	0.60
26:LC:99:GLU:HG2	26:LC:182:ALA:HB2	1.83	0.60
30:LI:46:PHE:CE1	30:LI:50:ARG:HD2	2.35	0.60
45:LY:20:LEU:HD22	45:LY:25:LYS:HB2	1.82	0.60
9:SI:63:LEU:O	9:SI:63:LEU:HD12	2.01	0.60
11:SK:69:ARG:HH11	11:SK:69:ARG:HB2	1.65	0.60
23:23:1068:G:H21	23:23:1096:A:H5'	1.66	0.60
35:LO:108:ALA:HB3	35:LO:125:LEU:HD22	1.83	0.60
7:SG:62:PHE:CE1	7:SG:124:LEU:HB2	2.35	0.60
23:23:1820:U:C2	25:LB:201:MET:HG2	2.37	0.60
1:16:1218:C:H2'	1:16:1219:A:H8	1.67	0.60
23:23:372:G:H2'	47:Lb:58:VAL:HG12	1.82	0.60
25:LB:240:PHE:O	25:LB:242:LYS:HE3	2.01	0.60
56:EF:87:ILE:HD12	56:EF:106:LEU:HD21	1.84	0.60
45:LY:4:ILE:HG12	45:LY:50:MET:HE1	1.84	0.60
45:LY:75:GLN:HB2	45:LY:92:VAL:HG13	1.82	0.60
23:23:1172:C:C4	23:23:1173:U:H1'	2.37	0.60
56:EF:124:GLU:HA	56:EF:162:LEU:HD21	1.83	0.60
10:SJ:11:LYS:HD3	10:SJ:69:THR:HG21	1.84	0.59
50:Le:62:LYS:HE3	50:Le:62:LYS:HA	1.84	0.59
23:23:1089:A:H5'	23:23:1089:A:H8	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LE:29:PRO:HB2	28:LE:169:LEU:HD13	1.83	0.59
31:LJ:25:ALA:HB3	31:LJ:112:ALA:HB3	1.83	0.59
42:LV:73:LYS:HB2	42:LV:106:VAL:HB	1.83	0.59
7:SG:133:THR:HA	7:SG:136:LYS:HB2	1.83	0.59
6:SF:10:VAL:HG22	6:SF:58:HIS:HB3	1.84	0.59
28:LE:128:TYR:HB3	28:LE:156:ILE:HB	1.84	0.59
56:EF:422:PRO:HG3	56:EF:431:MET:HE3	1.84	0.59
56:EF:553:VAL:HG21	56:EF:578:LEU:HD22	1.85	0.59
6:SF:47:LEU:HD13	6:SF:55:HIS:HA	1.85	0.59
18:SR:11:CYS:HB2	18:SR:47:THR:HA	1.83	0.59
58:Pt:34:U8U:H2'	58:Pt:35:U:C6	2.37	0.59
23:23:1485:U:H2'	23:23:1486:U:O4'	2.03	0.59
30:LI:104:THR:HA	30:LI:107:GLY:H	1.67	0.59
32:LK:76:ALA:O	32:LK:80:LEU:HD23	2.03	0.59
24:5:48:U:H4'	38:LR:100:HIS:HD2	1.67	0.59
23:23:2153:C:H2'	23:23:2154:A:C8	2.38	0.58
23:23:2114:A:N6	23:23:2119:A:N7	2.50	0.58
1:16:1516:2MG:C8	61:16:1603:PUT:H22	2.39	0.58
56:EF:219:HIS:CE1	56:EF:223:ILE:HD11	2.37	0.58
3:SC:162:ILE:HG13	22:mR:48:C:H5'	1.85	0.58
9:SI:25:ASN:HB3	9:SI:62:ASP:HB2	1.85	0.58
42:LV:17:VAL:HG12	42:LV:76:VAL:HG21	1.83	0.58
56:EF:131:ASN:HA	56:EF:137:ARG:HH22	1.69	0.58
1:16:108:G:H5'	1:16:109:A:H5''	1.85	0.58
10:SJ:21:ALA:HB1	10:SJ:92:LEU:HD23	1.86	0.58
11:SK:89:PRO:HB3	21:SU:32:VAL:HG21	1.86	0.58
41:LU:38:VAL:HG22	41:LU:59:ILE:HD12	1.86	0.58
51:Lf:54:VAL:HG23	51:Lf:55:ILE:HG12	1.86	0.58
28:LE:122:PHE:CZ	28:LE:170:LEU:HD12	2.39	0.58
29:LF:23:VAL:C	29:LF:24:ILE:HD13	2.29	0.58
56:EF:497:LYS:HG2	56:EF:523:TYR:HB3	1.86	0.58
23:23:1054:A:H2'	23:23:1055:G:H8	1.69	0.57
2:SB:54:LEU:HD12	2:SB:220:THR:HG21	1.86	0.57
14:SN:47:LYS:HB3	19:SS:13:LEU:HD12	1.86	0.57
23:23:1329:U:H5''	23:23:1330:C:H5	1.69	0.57
7:SG:62:PHE:HE1	7:SG:124:LEU:HB2	1.69	0.57
8:SH:7:ILE:HD12	8:SH:36:ILE:HD12	1.86	0.57
13:SM:33:ILE:HD11	13:SM:63:PHE:HD2	1.69	0.57
29:LF:4:VAL:O	29:LF:69:ARG:HD2	2.04	0.57
30:LI:96:THR:O	30:LI:99:ILE:HG22	2.04	0.57
59:Dt:18:G:H4'	59:Dt:60:C:C2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:651:G:H5'	54:Li:19:LYS:HG3	1.87	0.57
56:EF:375:LYS:HG3	56:EF:376:GLU:HG2	1.86	0.57
56:EF:169:LEU:HD23	56:EF:170:GLN:HG3	1.86	0.57
32:LK:56:PRO:HD3	32:LK:75:PRO:HD3	1.85	0.57
2:SB:199:VAL:O	2:SB:200:ILE:HD13	2.05	0.57
6:SF:18:VAL:HG23	6:SF:19:PRO:HD3	1.87	0.57
10:SJ:14:ASP:HB3	10:SJ:17:LEU:HB3	1.86	0.57
42:LV:28:LYS:HB2	42:LV:31:GLN:HG2	1.87	0.57
56:EF:234:MET:O	56:EF:238:LEU:HD12	2.04	0.57
1:16:1346:A:N1	1:16:1374:A:H5''	2.20	0.57
56:EF:298:ILE:HB	56:EF:405:ILE:HB	1.86	0.57
8:SH:87:LYS:HG2	8:SH:125:ILE:HD11	1.85	0.57
23:23:1057:A:H5''	23:23:1057:A:H8	1.69	0.57
23:23:726:G:H5''	23:23:1432:G:O2'	2.05	0.57
23:23:1357:C:H2'	23:23:1358:G:O4'	2.04	0.57
31:LJ:5:LEU:O	31:LJ:9:GLN:HG2	2.05	0.57
6:SF:11:HIS:NE2	6:SF:54:LEU:HD21	2.21	0.56
23:23:2328:A:H2'	23:23:2329:U:C6	2.40	0.56
2:SB:199:VAL:C	2:SB:200:ILE:HD13	2.30	0.56
7:SG:116:MET:HA	7:SG:119:ARG:HB2	1.87	0.56
15:SO:49:ASP:OD1	15:SO:52:SER:HB2	2.06	0.56
23:23:181:A:H1'	23:23:435:C:H5'	1.87	0.56
30:LI:125:THR:HA	30:LI:146:VAL:HG21	1.87	0.56
56:EF:176:GLU:H	56:EF:176:GLU:CD	2.12	0.56
12:SL:44:LYS:HB3	12:SL:45:PRO:HD3	1.87	0.56
45:LY:30:ILE:HD11	45:LY:63:ILE:HD12	1.86	0.56
2:SB:49:MET:HA	2:SB:52:GLU:OE1	2.06	0.56
41:LU:68:ARG:HD3	41:LU:92:TRP:CE2	2.41	0.56
23:23:1105:U:H2'	23:23:1106:G:C8	2.40	0.56
1:16:108:G:C8	1:16:108:G:H5''	2.41	0.56
1:16:1398:A:H8	1:16:1398:A:H5''	1.71	0.56
23:23:2010:G:H5''	42:LV:42:LYS:HB2	1.88	0.56
23:23:2680:U:H5'	26:LC:194:PRO:HA	1.87	0.56
48:Lc:5:GLU:HG3	48:Lc:6:LEU:HD22	1.88	0.56
23:23:979:A:H2'	23:23:982:C:H42	1.71	0.56
28:LE:122:PHE:HZ	28:LE:170:LEU:HD12	1.70	0.56
41:LU:30:GLY:O	41:LU:31:GLU:HG2	2.05	0.56
66:EF:901:GTP:H5''	66:EF:901:GTP:C8	2.39	0.56
4:SD:44:ARG:O	4:SD:46:PRO:HD3	2.06	0.55
23:23:1172:C:H2'	23:23:1173:U:H4'	1.88	0.55
28:LE:40:VAL:HG11	28:LE:50:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:SR:10:PHE:HD1	18:SR:10:PHE:H	1.52	0.55
23:23:1089:A:H5'	23:23:1089:A:C8	2.42	0.55
45:LY:40:ILE:HD12	45:LY:42:LEU:HD21	1.88	0.55
7:SG:138:ARG:NH2	7:SG:139:GLU:HB2	2.20	0.55
23:23:2478:A:H5'	55:Lj:32:LYS:HD3	1.88	0.55
52:Lg:35:GLU:OE2	52:Lg:50:LYS:HG3	2.06	0.55
3:SC:83:ASP:HA	3:SC:86:LYS:HG2	1.89	0.55
5:SE:15:LEU:HD23	5:SE:37:THR:HG22	1.88	0.55
5:SE:152:MET:O	5:SE:156:LYS:HG3	2.06	0.55
11:SK:25:ALA:O	11:SK:88:GLY:HA3	2.06	0.55
23:23:1534:U:H3	23:23:1537:G:H22	1.53	0.55
2:SB:72:THR:HG22	2:SB:72:THR:O	2.06	0.55
4:SD:102:VAL:HG13	4:SD:107:PHE:HB2	1.88	0.55
19:SS:3:ARG:NE	19:SS:7:LYS:HB2	2.12	0.55
8:SH:29:SER:HB2	8:SH:59:LEU:HB2	1.89	0.55
19:SS:3:ARG:HD2	19:SS:4:SER:H	1.71	0.55
35:LO:96:LYS:HD3	35:LO:103:ILE:HA	1.88	0.55
5:SE:115:LEU:HD13	5:SE:123:VAL:HG21	1.89	0.55
6:SF:67:PRO:HG2	6:SF:70:VAL:HG12	1.89	0.55
2:SB:46:THR:HB	2:SB:201:PRO:HG2	1.88	0.55
38:LR:83:LEU:HD11	38:LR:114:GLY:HA3	1.89	0.55
56:EF:104:ARG:HH21	56:EF:320:LEU:HD22	1.71	0.55
13:SM:14:HIS:H	13:SM:44:LYS:HG2	1.72	0.54
34:LN:63:VAL:HG12	34:LN:107:LEU:HD11	1.90	0.54
56:EF:169:LEU:HG	56:EF:169:LEU:O	2.05	0.54
1:16:922:G:H1'	5:SE:24:THR:HG22	1.88	0.54
37:LQ:97:ILE:HG12	37:LQ:113:ILE:HG13	1.89	0.54
56:EF:674:THR:O	56:EF:677:ARG:HG2	2.08	0.54
3:SC:152:GLU:HG3	3:SC:167:TRP:HB3	1.90	0.54
38:LR:62:LEU:HD11	38:LR:70:ALA:HA	1.89	0.54
44:LX:88:GLU:HG2	44:LX:93:VAL:HG21	1.90	0.54
56:EF:431:MET:HB2	56:EF:479:VAL:HG11	1.88	0.54
1:16:946:A:H2'	1:16:947:G:C8	2.42	0.54
2:SB:27:MET:O	2:SB:31:ILE:HG13	2.08	0.54
14:SN:73:PHE:O	14:SN:74:LEU:HD23	2.07	0.54
42:LV:4:ILE:HD12	42:LV:6:LYS:HD2	1.90	0.54
1:16:1530:G:H2'	1:16:1531:A:C8	2.42	0.54
46:La:70:GLU:HG3	46:La:72:LYS:HD3	1.90	0.54
56:EF:323:LYS:HB3	56:EF:335:PHE:HB2	1.89	0.54
56:EF:436:GLY:O	56:EF:440:LYS:HG3	2.08	0.54
1:16:1241:G:H2'	1:16:1242:G:H8	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:740:C:H5'	23:23:1784:A:H3'	1.90	0.54
23:23:1057:A:H1'	31:LJ:35:VAL:HG11	1.89	0.54
40:LT:87:SER:HB2	41:LU:51:VAL:HG23	1.88	0.54
56:EF:22:GLY:HA3	56:EF:142:ASN:HD22	1.70	0.54
23:23:2182:U:H2'	23:23:2183:A:C8	2.43	0.54
28:LE:34:ILE:HD12	28:LE:156:ILE:HG12	1.90	0.54
31:LJ:55:VAL:HG23	31:LJ:60:LEU:HG	1.88	0.54
36:LP:95:LEU:C	36:LP:96:ILE:HD13	2.33	0.54
13:SM:22:ILE:HD12	13:SM:22:ILE:N	2.22	0.53
17:SQ:21:ILE:CD1	17:SQ:46:VAL:HB	2.38	0.53
56:EF:127:TRP:CD1	56:EF:162:LEU:HD22	2.43	0.53
41:LU:26:ASP:C	41:LU:27:ILE:HD13	2.33	0.53
54:Li:32:ILE:O	54:Li:32:ILE:HG22	2.08	0.53
7:SG:50:LEU:HD12	7:SG:54:SER:HB2	1.91	0.53
23:23:1872:A:C5	23:23:1873:G:H1'	2.44	0.53
23:23:2002:G:H5''	37:LQ:9:GLN:NE2	2.23	0.53
45:LY:9:ARG:HG3	45:LY:41:GLU:HB3	1.89	0.53
47:Lb:7:VAL:HG23	47:Lb:8:THR:HG23	1.90	0.53
10:SJ:11:LYS:HG2	10:SJ:69:THR:CG2	2.39	0.53
16:SP:6:LEU:HB3	16:SP:17:TYR:HB3	1.89	0.53
29:LF:12:PRO:HD2	29:LF:15:VAL:HG21	1.90	0.53
5:SE:74:VAL:HG11	5:SE:144:LEU:HB3	1.91	0.53
3:SC:130:PHE:CE2	3:SC:157:LEU:HB3	2.44	0.53
23:23:1872:A:C6	23:23:1873:G:H1'	2.44	0.53
56:EF:53:MET:O	56:EF:56:GLU:HB2	2.09	0.53
56:EF:104:ARG:HH21	56:EF:320:LEU:HD23	1.70	0.53
56:EF:396:THR:HG21	56:EF:405:ILE:HA	1.90	0.53
5:SE:111:MET:HE1	5:SE:125:ALA:HB1	1.91	0.53
23:23:833:A:H2'	23:23:834:G:C8	2.44	0.53
46:La:50:ASN:HB2	46:La:82:ILE:HB	1.91	0.53
2:SB:15:HIS:HB3	2:SB:43:LEU:HD11	1.90	0.52
23:23:1090:A:C2	23:23:1102:C:H1'	2.44	0.52
50:Le:18:CYS:HB3	50:Le:40:CYS:SG	2.49	0.52
10:SJ:32:THR:HG21	10:SJ:83:THR:HG23	1.91	0.52
13:SM:45:ILE:O	13:SM:48:LEU:HB3	2.09	0.52
13:SM:92:ARG:HG3	13:SM:92:ARG:HH11	1.74	0.52
24:5:30:C:H1'	24:5:57:A:H61	1.74	0.52
28:LE:99:PHE:HD1	28:LE:102:ARG:HH21	1.55	0.52
30:LI:117:LEU:HD23	30:LI:130:VAL:HG13	1.91	0.52
2:SB:61:ALA:HB2	2:SB:221:VAL:HG23	1.90	0.52
23:23:639:U:H2'	23:23:640:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Le:64:PHE:HB3	50:Le:66:ILE:HD11	1.90	0.52
1:16:465:A:H2'	1:16:466:A:C8	2.44	0.52
1:16:677:U:H3	1:16:713:G:H22	1.56	0.52
25:LB:53:HIS:HA	25:LB:217:ARG:HB2	1.92	0.52
37:LQ:107:ASN:OD1	42:LV:40:ASN:HB3	2.09	0.52
3:SC:155:GLY:HA2	3:SC:163:ALA:HB1	1.92	0.52
29:LF:27:LYS:HG3	29:LF:32:GLU:HG2	1.90	0.52
29:LF:164:TYR:HB2	29:LF:167:GLU:HB2	1.91	0.52
17:SQ:14:SER:HB3	17:SQ:22:VAL:HB	1.92	0.52
29:LF:137:ASP:O	29:LF:141:ILE:HG22	2.09	0.52
37:LQ:66:ALA:O	37:LQ:70:THR:HG23	2.09	0.52
45:LY:77:VAL:HG22	45:LY:89:ILE:HD13	1.92	0.52
23:23:570:G:H2'	23:23:2030:6MZ:N7	2.25	0.52
23:23:1077:A:N1	23:23:1088:A:H2'	2.25	0.52
29:LF:121:ILE:HD11	29:LF:140:VAL:HG23	1.92	0.52
39:LS:6:LYS:HD2	39:LS:6:LYS:O	2.10	0.52
45:LY:21:ARG:HE	45:LY:87:GLN:HA	1.75	0.52
56:EF:437:ARG:HG2	56:EF:437:ARG:HH11	1.74	0.52
1:16:1430:A:H2'	1:16:1431:A:C8	2.45	0.52
14:SN:48:LEU:O	14:SN:48:LEU:HD12	2.10	0.52
28:LE:74:VAL:H	28:LE:79:ILE:HD12	1.74	0.52
23:23:1094:U:H1'	23:23:1097:U:H5	1.74	0.52
28:LE:4:LEU:HA	28:LE:7:TYR:HB3	1.91	0.52
28:LE:106:ILE:HG12	50:Le:34:LEU:HD21	1.91	0.52
39:LS:114:LEU:O	39:LS:114:LEU:HD23	2.10	0.52
44:LX:49:VAL:HG13	44:LX:52:LEU:O	2.10	0.52
56:EF:22:GLY:O	56:EF:26:THR:HG23	2.10	0.52
56:EF:496:GLN:O	56:EF:496:GLN:HG3	2.10	0.52
43:LW:36:LYS:HA	43:LW:81:LYS:HE2	1.91	0.51
23:23:830:G:H2'	61:23:3007:PUT:H22	1.91	0.51
23:23:1478:G:H1	23:23:1513:U:H3	1.58	0.51
25:LB:53:HIS:CD2	25:LB:219:THR:HA	2.45	0.51
54:Li:31:HIS:O	54:Li:32:ILE:HD13	2.11	0.51
56:EF:24:THR:HG23	56:EF:50:MET:HB2	1.93	0.51
1:16:942:G:H21	9:SI:126:GLN:HE21	1.58	0.51
23:23:1079:C:H5''	32:LK:134:ARG:NH2	2.26	0.51
23:23:2052:A:H4'	26:LC:148:GLN:O	2.11	0.51
1:16:1130:A:H2'	1:16:1131:G:C8	2.46	0.51
18:SR:41:PRO:HB2	18:SR:43:ARG:HG3	1.92	0.51
30:LI:137:GLU:CD	30:LI:137:GLU:H	2.19	0.51
55:Lj:18:LYS:HG3	55:Lj:23:ILE:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:675:A:H1'	11:SK:118:HIS:CD2	2.46	0.51
1:16:1308:U:H2'	1:16:1309:G:C8	2.45	0.51
7:SG:137:LYS:O	7:SG:141:VAL:HG12	2.10	0.51
1:16:206:C:H3'	1:16:207:C:H6	1.76	0.51
3:SC:24:ALA:HB1	3:SC:28:GLU:HG3	1.93	0.51
23:23:547:A:H2	23:23:548:G:H1'	1.74	0.51
23:23:2634:A:N1	23:23:2784:U:H5	2.09	0.51
23:23:2660:A:H4'	56:EF:121:PRO:HG2	1.93	0.51
24:5:13:G:H4'	24:5:15:A:H2'	1.93	0.51
31:LJ:41:LEU:HD21	31:LJ:99:PHE:CG	2.45	0.51
56:EF:414:PRO:HA	56:EF:461:MET:SD	2.50	0.51
19:SS:47:LEU:HD13	19:SS:48:THR:H	1.76	0.51
1:16:1004:A:H2'	1:16:1005:A:O4'	2.10	0.51
1:16:1064:G:H1'	1:16:1190:G:H21	1.76	0.51
2:SB:163:VAL:HG11	2:SB:173:ILE:HD11	1.93	0.51
9:SI:55:VAL:HG12	9:SI:55:VAL:O	2.10	0.51
10:SJ:11:LYS:HG3	10:SJ:71:LEU:HB3	1.93	0.51
6:SF:45:ARG:HB3	6:SF:59:TYR:HD2	1.76	0.51
23:23:668:A:H2'	23:23:670:A:H62	1.76	0.51
28:LE:44:ILE:HG21	28:LE:79:ILE:HG22	1.92	0.51
29:LF:2:SER:HG	29:LF:62:TRP:CG	2.29	0.51
31:LJ:72:LEU:HD13	31:LJ:117:LEU:HD12	1.93	0.51
56:EF:252:LEU:O	56:EF:256:VAL:HG23	2.11	0.51
56:EF:540:ILE:HG12	56:EF:578:LEU:HG	1.91	0.51
6:SF:22:ILE:CD1	6:SF:39:LEU:HD21	2.41	0.51
47:Lb:13:VAL:HG23	47:Lb:29:PHE:HB2	1.93	0.51
56:EF:418:ILE:HG12	56:EF:466:LEU:HD13	1.93	0.51
1:16:21:G:H2'	1:16:22:G:C8	2.45	0.50
7:SG:92:ARG:HD3	7:SG:94:VAL:HG22	1.94	0.50
19:SS:11:ILE:HD12	19:SS:16:LEU:HB2	1.92	0.50
23:23:945:A:H1'	65:23:3018:SPD:H91	1.93	0.50
31:LJ:27:VAL:HA	31:LJ:82:ILE:HA	1.93	0.50
23:23:1820:U:C4	25:LB:159:GLY:HA3	2.46	0.50
31:LJ:94:ARG:HG2	31:LJ:127:ALA:HA	1.93	0.50
16:SP:61:VAL:HG22	16:SP:67:ILE:HD11	1.94	0.50
29:LF:35:ARG:HD2	29:LF:75:MET:HE3	1.93	0.50
6:SF:45:ARG:HB3	6:SF:59:TYR:CD2	2.45	0.50
8:SH:87:LYS:HG3	8:SH:125:ILE:HD11	1.93	0.50
25:LB:60:GLN:HG2	25:LB:85:PRO:HB2	1.94	0.50
29:LF:101:ASN:HA	29:LF:117:LEU:HD12	1.92	0.50
19:SS:47:LEU:HD13	19:SS:48:THR:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1432:G:H2'	23:23:1433:A:C8	2.46	0.50
27:LD:194:LYS:O	27:LD:198:GLU:HG2	2.11	0.50
41:LU:2:TYR:HE1	41:LU:40:MET:HE2	1.76	0.50
56:EF:31:LEU:CD1	56:EF:50:MET:HE3	2.33	0.50
1:16:515:G:H2'	1:16:516:PSU:H6	1.76	0.50
1:16:1492:A:H2'	23:23:1913:A:C2	2.46	0.50
1:16:1493:A:H2'	23:23:1913:A:C2	2.47	0.50
7:SG:106:GLU:O	7:SG:110:LYS:HD2	2.12	0.50
23:23:191:A:H2'	23:23:192:C:C6	2.46	0.50
28:LE:74:VAL:HB	28:LE:79:ILE:HD11	1.94	0.50
50:Le:39:LYS:HD2	50:Le:39:LYS:N	2.26	0.50
7:SG:20:SER:HB3	7:SG:23:LEU:HG	1.93	0.50
10:SJ:11:LYS:CG	10:SJ:69:THR:HG22	2.42	0.50
30:LI:36:ALA:O	30:LI:37:VAL:HG23	2.11	0.50
1:16:1175:G:H2'	1:16:1176:A:H8	1.75	0.50
1:16:1431:A:H2	1:16:1469:C:H42	1.60	0.50
6:SF:10:VAL:HA	6:SF:84:VAL:HA	1.94	0.50
23:23:373:U:H2'	23:23:374:A:H8	1.77	0.50
23:23:764:A:H5''	25:LB:209:GLY:HA3	1.94	0.50
31:LJ:123:ILE:C	31:LJ:125:ARG:N	2.67	0.50
52:Lg:8:LYS:HB3	52:Lg:54:ILE:HD12	1.93	0.50
4:SD:62:ARG:NH1	4:SD:69:GLU:HG2	2.26	0.50
13:SM:69:LEU:O	13:SM:73:ILE:HG23	2.12	0.50
23:23:1809:A:H2'	23:23:1810:A:C8	2.47	0.50
32:LK:127:ARG:O	32:LK:130:GLU:HG3	2.11	0.50
56:EF:122:GLN:O	56:EF:126:VAL:HG22	2.12	0.50
10:SJ:7:ARG:C	10:SJ:8:ILE:HD13	2.37	0.49
23:23:2178:C:H2'	23:23:2179:C:H6	1.77	0.49
42:LV:4:ILE:HG22	42:LV:106:VAL:HG22	1.93	0.49
56:EF:152:LEU:HA	56:EF:155:VAL:HG22	1.93	0.49
4:SD:105:MET:HG3	4:SD:171:LEU:HD22	1.94	0.49
6:SF:29:ILE:HD12	6:SF:64:VAL:HG11	1.94	0.49
8:SH:40:LEU:HD21	8:SH:129:VAL:HG21	1.94	0.49
23:23:1386:C:H2'	23:23:1387:A:C8	2.47	0.49
30:LI:80:ILE:HG21	30:LI:94:ILE:HG12	1.93	0.49
40:LT:89:GLU:OE1	41:LU:52:PRO:HB3	2.12	0.49
3:SC:62:LYS:HG3	3:SC:97:VAL:HG12	1.93	0.49
23:23:1796:U:H2'	23:23:1797:G:C8	2.47	0.49
36:LP:26:VAL:HG13	36:LP:104:GLU:HG2	1.94	0.49
56:EF:357:ARG:HH11	56:EF:357:ARG:HG2	1.77	0.49
7:SG:138:ARG:HH22	7:SG:139:GLU:HB2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:SS:41:PHE:HB2	19:SS:44:MET:HG2	1.94	0.49
8:SH:43:GLU:HG3	8:SH:101:ILE:HD13	1.94	0.49
23:23:1900:A:H1'	23:23:1970:A:H2'	1.93	0.49
37:LQ:72:ASP:O	37:LQ:76:VAL:HG12	2.12	0.49
3:SC:117:ALA:O	3:SC:121:THR:HG23	2.13	0.49
12:SL:3:THR:OG1	12:SL:6:GLN:HG3	2.12	0.49
43:LW:14:PRO:HD3	48:Lc:30:MET:HE1	1.94	0.49
56:EF:139:ALA:HB3	56:EF:264:VAL:HA	1.93	0.49
2:SB:72:THR:O	2:SB:72:THR:CG2	2.60	0.49
11:SK:34:ILE:HG22	11:SK:42:LEU:HD23	1.95	0.49
23:23:2898:U:H2'	23:23:2899:A:C8	2.48	0.49
1:16:1013:G:N2	1:16:1015:G:H3'	2.28	0.49
2:SB:50:PHE:O	2:SB:54:LEU:HD22	2.13	0.49
10:SJ:11:LYS:HD3	10:SJ:69:THR:CG2	2.42	0.49
25:LB:247:PRO:HG2	25:LB:248:TRP:CZ3	2.47	0.49
30:LI:26:ALA:O	30:LI:31:VAL:HG23	2.13	0.49
30:LI:46:PHE:O	30:LI:50:ARG:HG2	2.13	0.49
31:LJ:98:GLU:HA	31:LJ:101:LYS:HE3	1.95	0.49
34:LN:18:ARG:HG2	34:LN:18:ARG:HH11	1.76	0.49
7:SG:26:PHE:CD1	7:SG:30:LEU:HD23	2.47	0.49
23:23:2180:U:H2'	23:23:2181:U:C6	2.48	0.49
56:EF:693:ASN:ND2	56:EF:694:VAL:HG13	2.28	0.49
23:23:1054:A:H2'	23:23:1055:G:C8	2.48	0.49
30:LI:97:ARG:O	30:LI:101:ASP:N	2.44	0.49
33:LM:9:GLU:CD	33:LM:9:GLU:H	2.20	0.49
56:EF:15:ILE:HD11	56:EF:86:ILE:HD11	1.95	0.49
56:EF:121:PRO:HA	56:EF:677:ARG:HH21	1.78	0.49
1:16:1220:G:P	14:SN:53:ARG:HH12	2.35	0.48
3:SC:153:VAL:HG12	3:SC:198:VAL:HG22	1.95	0.48
1:16:1126:U:P	10:SJ:7:ARG:HH22	2.36	0.48
1:16:1138:G:C5	1:16:1140:C:H1'	2.48	0.48
4:SD:170:TRP:CD2	4:SD:186:PRO:HB3	2.48	0.48
23:23:1028:A:N6	23:23:1125:G:H2'	2.28	0.48
38:LR:56:LYS:HD2	38:LR:59:ALA:HB3	1.95	0.48
39:LS:89:ARG:HE	39:LS:113:ARG:HH22	1.62	0.48
8:SH:96:MET:CE	8:SH:130:ALA:HB1	2.43	0.48
10:SJ:11:LYS:HG2	10:SJ:69:THR:HG22	1.96	0.48
23:23:1664:A:H2	34:LN:1:MET:HE1	1.78	0.48
25:LB:227:PRO:HA	25:LB:233:GLY:HA2	1.94	0.48
30:LI:2:GLN:OE1	30:LI:18:GLN:HG3	2.13	0.48
36:LP:82:MET:HE2	36:LP:82:MET:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:LQ:103:ARG:HD3	37:LQ:110:MET:HE2	1.95	0.48
3:SC:76:VAL:HG23	3:SC:77:ILE:HG13	1.95	0.48
4:SD:128:ARG:HA	4:SD:128:ARG:HH11	1.79	0.48
10:SJ:80:THR:O	10:SJ:84:VAL:HG23	2.14	0.48
29:LF:124:GLU:OE2	29:LF:126:PRO:HD3	2.14	0.48
30:LI:110:VAL:HG11	30:LI:132:PHE:CE2	2.47	0.48
49:Ld:3:LYS:HE2	49:Ld:3:LYS:HA	1.94	0.48
56:EF:680:TYR:HE2	56:EF:682:MET:HG3	1.79	0.48
1:16:8:A:C6	4:SD:206:LYS:HB3	2.48	0.48
1:16:1206:G:H2'	1:16:1207:G:O4'	2.13	0.48
23:23:1086:A:H2'	23:23:1086:A:N3	2.28	0.48
36:LP:110:GLU:O	36:LP:114:ARG:HG3	2.14	0.48
58:Pt:12:U:H2'	58:Pt:13:C:O4'	2.13	0.48
1:16:202:G:HO2'	1:16:468:A:H8	1.58	0.48
1:16:714:G:H2'	1:16:715:A:C8	2.48	0.48
5:SE:36:LEU:HD22	5:SE:134:ILE:HG13	1.94	0.48
7:SG:31:MET:HE2	7:SG:36:LYS:HE3	1.94	0.48
11:SK:85:MET:HE3	11:SK:113:VAL:HG11	1.96	0.48
14:SN:85:ARG:HG2	14:SN:85:ARG:HH11	1.77	0.48
23:23:1405:U:H2'	23:23:1406:U:C6	2.48	0.48
23:23:2246:G:H2'	23:23:2247:A:C8	2.48	0.48
35:LO:79:LEU:HD11	35:LO:112:LEU:HD12	1.94	0.48
56:EF:512:ARG:HH11	56:EF:512:ARG:HG2	1.79	0.48
2:SB:23:TRP:CZ3	2:SB:25:PRO:HA	2.49	0.48
4:SD:157:ALA:O	4:SD:161:LEU:HD13	2.13	0.48
14:SN:28:LYS:HE2	14:SN:48:LEU:HG	1.95	0.48
23:23:833:A:H2'	23:23:834:G:H8	1.78	0.48
34:LN:70:ARG:HG2	34:LN:76:VAL:HG22	1.95	0.48
56:EF:282:VAL:HG13	56:EF:286:LEU:HD12	1.95	0.48
56:EF:337:ARG:NH1	56:EF:380:GLY:HA2	2.28	0.48
7:SG:62:PHE:CE1	7:SG:124:LEU:CG	2.97	0.48
14:SN:8:ALA:O	14:SN:11:VAL:HG12	2.14	0.48
23:23:2113:U:H2'	23:23:2114:A:H8	1.79	0.48
40:LT:49:ASP:HA	40:LT:52:GLN:HB2	1.96	0.48
41:LU:28:ALA:HB3	41:LU:31:GLU:HG3	1.95	0.48
56:EF:219:HIS:HE1	56:EF:223:ILE:HD11	1.79	0.48
30:LI:66:ASN:O	30:LI:70:GLU:HG2	2.14	0.48
1:16:269:C:H2'	1:16:270:A:C8	2.49	0.48
12:SL:107:VAL:CG2	12:SL:110:ARG:HG3	2.44	0.48
19:SS:9:PRO:HD3	50:Le:64:PHE:CD2	2.49	0.48
23:23:2176:A:H2'	23:23:2177:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LD:124:PHE:HE2	27:LD:141:MET:HE1	1.79	0.48
28:LE:40:VAL:CG1	28:LE:43:ALA:HB2	2.44	0.48
12:SL:64:THR:OG1	12:SL:93:VAL:HG12	2.14	0.47
23:23:764:A:H2	25:LB:218:PRO:HG3	1.79	0.47
1:16:49:U:O4	1:16:365:U:H5	1.97	0.47
3:SC:64:ILE:HG22	3:SC:97:VAL:HG23	1.96	0.47
14:SN:45:VAL:HA	14:SN:48:LEU:HB3	1.95	0.47
27:LD:46:GLN:HB3	27:LD:83:VAL:HG21	1.95	0.47
27:LD:83:VAL:HB	27:LD:86:ALA:HB2	1.97	0.47
36:LP:34:LYS:HD2	36:LP:131:VAL:HG11	1.96	0.47
56:EF:19:ILE:HD11	56:EF:92:HIS:HA	1.94	0.47
2:SB:81:LYS:O	2:SB:85:LEU:HD23	2.14	0.47
11:SK:94:GLU:OE2	21:SU:16:LEU:HD11	2.14	0.47
13:SM:12:HIS:HA	13:SM:45:ILE:HD11	1.96	0.47
19:SS:45:ILE:CD1	19:SS:64:ASP:HA	2.43	0.47
30:LI:121:VAL:O	30:LI:122:LEU:HG	2.13	0.47
44:LX:48:PRO:HB3	44:LX:56:GLY:N	2.29	0.47
46:La:37:ILE:HG21	46:La:80:ILE:HG21	1.96	0.47
1:16:222:C:H2'	1:16:223:A:H8	1.80	0.47
1:16:515:G:H2'	1:16:516:PSU:C6	2.49	0.47
19:SS:42:PRO:O	19:SS:45:ILE:HB	2.14	0.47
25:LB:165:VAL:HG21	25:LB:181:MET:HE3	1.96	0.47
30:LI:68:ARG:O	30:LI:72:ILE:HG23	2.14	0.47
1:16:1356:G:H2'	1:16:1357:A:H8	1.77	0.47
1:16:1492:A:H2'	23:23:1913:A:H2	1.78	0.47
11:SK:20:VAL:HG22	11:SK:83:GLU:CG	2.44	0.47
23:23:1716:U:H2'	23:23:1717:A:H8	1.79	0.47
23:23:2394:C:H5''	35:LO:63:LYS:HD3	1.95	0.47
32:LK:12:GLN:HA	32:LK:56:PRO:HA	1.96	0.47
2:SB:19:GLN:HA	2:SB:38:VAL:HA	1.95	0.47
3:SC:35:SER:O	3:SC:39:VAL:HG13	2.14	0.47
11:SK:87:LYS:HG3	11:SK:115:PRO:HD3	1.97	0.47
19:SS:18:LYS:HB3	19:SS:18:LYS:HE3	1.75	0.47
29:LF:120:GLY:O	29:LF:121:ILE:HD13	2.15	0.47
32:LK:73:THR:HG21	32:LK:113:LYS:HA	1.95	0.47
44:LX:26:LYS:HD2	44:LX:37:GLU:HG3	1.97	0.47
59:Dt:49:C:H2'	59:Dt:50:U:C6	2.49	0.47
1:16:964:A:H1'	10:SJ:57:VAL:HG11	1.97	0.47
1:16:1151:A:H5'	10:SJ:43:PRO:HA	1.96	0.47
1:16:1402:4OC:O5'	1:16:1402:4OC:H6	2.15	0.47
5:SE:38:VAL:HG11	5:SE:114:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SJ:8:ILE:HB	10:SJ:74:VAL:HG23	1.97	0.47
10:SJ:21:ALA:O	10:SJ:25:ILE:HG22	2.14	0.47
10:SJ:81:GLU:H	10:SJ:81:GLU:HG3	1.47	0.47
14:SN:90:ARG:HB2	14:SN:92:GLU:HG3	1.95	0.47
17:SQ:21:ILE:HD12	17:SQ:46:VAL:HB	1.95	0.47
23:23:593:U:H2'	23:23:594:U:C6	2.49	0.47
23:23:1637:A:H5'	23:23:1760:C:O2'	2.15	0.47
23:23:2123:G:H2'	23:23:2124:G:C8	2.49	0.47
48:Lc:12:GLU:CD	48:Lc:13:GLU:H	2.22	0.47
56:EF:561:LEU:HD22	56:EF:571:VAL:HB	1.96	0.47
1:16:559:A:H4'	1:16:560:A:H3'	1.97	0.47
13:SM:73:ILE:O	13:SM:77:ILE:HG13	2.15	0.47
26:LC:148:GLN:HB2	26:LC:152:PRO:CG	2.44	0.47
34:LN:105:ARG:HG3	34:LN:122:VAL:HG12	1.96	0.47
37:LQ:54:LEU:HD23	37:LQ:66:ALA:HB2	1.97	0.47
39:LS:51:ARG:CZ	39:LS:53:ARG:HG3	2.45	0.47
56:EF:170:GLN:HB3	56:EF:182:VAL:HG11	1.97	0.47
56:EF:458:ILE:CG2	56:EF:466:LEU:HD22	2.45	0.47
1:16:382:A:H2'	1:16:383:A:C8	2.49	0.47
1:16:1227:A:OP2	13:SM:110:LYS:HD3	2.15	0.47
2:SB:53:ALA:HB2	2:SB:200:ILE:HD11	1.96	0.47
9:SI:30:ILE:HG21	9:SI:38:TYR:CG	2.50	0.47
12:SL:54:ARG:HD2	12:SL:64:THR:HG22	1.97	0.47
25:LB:78:VAL:HA	25:LB:94:VAL:HG12	1.95	0.47
23:23:358:U:H3'	23:23:359:G:H5''	1.96	0.47
23:23:1141:U:H4'	23:23:1142:A:O4'	2.15	0.47
23:23:1783:A:H5'	23:23:2608:G:H4'	1.96	0.47
56:EF:28:GLU:OE1	56:EF:49:THR:HG22	2.15	0.47
1:16:1430:A:H2'	1:16:1431:A:H8	1.80	0.46
23:23:729:G:C6	25:LB:207:LYS:HB2	2.50	0.46
23:23:1084:A:H2'	23:23:1085:A:C8	2.50	0.46
38:LR:43:ASN:HD21	38:LR:46:GLU:HG2	1.80	0.46
56:EF:270:PHE:HB2	66:EF:901:GTP:C5	2.50	0.46
56:EF:629:GLY:HA2	56:EF:632:ILE:HD12	1.96	0.46
4:SD:27:ALA:HB3	4:SD:30:THR:HG23	1.96	0.46
23:23:554:U:H2'	23:23:555:G:O4'	2.15	0.46
23:23:597:G:O2'	35:LO:11:GLY:O	2.26	0.46
23:23:1665:A:H1'	34:LN:1:MET:HE2	1.97	0.46
23:23:2074:U:H2'	23:23:2075:U:C6	2.51	0.46
23:23:2359:C:O2'	54:Li:54:ASP:OD2	2.28	0.46
23:23:2528:U:O2'	23:23:2530:A:OP1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:LO:57:LEU:HD22	54:Li:54:ASP:HB3	1.97	0.46
40:LT:72:ASN:HB3	40:LT:110:VAL:HG11	1.98	0.46
1:16:460:A:H2'	1:16:461:A:H8	1.79	0.46
3:SC:23:PHE:HZ	10:SJ:11:LYS:HD2	1.79	0.46
3:SC:25:ASN:O	3:SC:29:PHE:HB2	2.16	0.46
11:SK:108:THR:O	21:SU:6:VAL:HG23	2.16	0.46
23:23:473:G:OP2	65:23:3017:SPD:N1	2.48	0.46
23:23:1539:U:H2'	23:23:1540:G:C8	2.50	0.46
32:LK:28:LEU:HD13	32:LK:28:LEU:N	2.30	0.46
55:Lj:2:LYS:HE2	55:Lj:32:LYS:O	2.15	0.46
55:Lj:18:LYS:HE2	55:Lj:21:GLY:HA2	1.97	0.46
2:SB:81:LYS:HE2	2:SB:81:LYS:HB3	1.82	0.46
5:SE:14:LYS:HD2	5:SE:113:ALA:HB1	1.97	0.46
23:23:447:A:O3'	65:23:3017:SPD:H21	2.15	0.46
29:LF:52:PHE:HE1	29:LF:72:LEU:HD22	1.80	0.46
48:Lc:14:LEU:HD22	48:Lc:53:VAL:HG23	1.98	0.46
56:EF:245:GLU:HA	56:EF:248:ILE:CD1	2.44	0.46
1:16:460:A:H2'	1:16:461:A:C8	2.50	0.46
19:SS:43:ASN:HD22	19:SS:44:MET:HE2	1.80	0.46
23:23:1479:G:HO2'	23:23:1560:G:HO2'	1.62	0.46
25:LB:144:VAL:HB	25:LB:154:LEU:HB2	1.98	0.46
31:LJ:69:PHE:O	31:LJ:72:LEU:HD23	2.16	0.46
42:LV:29:VAL:HB	42:LV:55:ILE:HD11	1.98	0.46
56:EF:102:SER:O	56:EF:106:LEU:HG	2.15	0.46
56:EF:261:ILE:O	56:EF:262:ILE:HD13	2.15	0.46
13:SM:25:VAL:HG23	13:SM:29:ARG:HB2	1.98	0.46
23:23:1539:U:H2'	23:23:1540:G:H8	1.81	0.46
36:LP:30:SER:OG	36:LP:106:ASP:OD1	2.24	0.46
56:EF:175:ALA:O	56:EF:179:PHE:HB2	2.15	0.46
1:16:1053:G:N7	1:16:1200:C:H5'	2.31	0.46
1:16:1150:A:O2'	10:SJ:41:PRO:O	2.32	0.46
3:SC:73:PRO:HA	3:SC:76:VAL:HG22	1.98	0.46
4:SD:60:LYS:O	4:SD:64:ILE:HG13	2.16	0.46
7:SG:21:GLU:H	7:SG:21:GLU:HG2	1.44	0.46
20:ST:72:ALA:O	20:ST:76:LYS:HG3	2.15	0.46
21:SU:21:ARG:O	21:SU:25:LYS:HG2	2.15	0.46
23:23:1179:G:H3'	23:23:1180:U:H5''	1.98	0.46
26:LC:104:VAL:HG23	26:LC:177:VAL:HG21	1.98	0.46
38:LR:39:VAL:HG12	38:LR:48:LEU:HD23	1.96	0.46
56:EF:56:GLU:HG2	56:EF:61:ILE:O	2.16	0.46
56:EF:495:ARG:HB2	56:EF:609:LYS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Dt:19:G:H4'	59:Dt:20:G:O5'	2.14	0.46
1:16:337:G:H2'	1:16:338:A:C8	2.51	0.46
7:SG:17:LYS:HG2	9:SI:46:MET:SD	2.55	0.46
7:SG:93:PRO:HA	7:SG:96:ARG:HB3	1.98	0.46
9:SI:71:GLY:O	9:SI:75:GLN:HB2	2.16	0.46
30:LI:110:VAL:HG11	30:LI:132:PHE:HE2	1.80	0.46
32:LK:90:SER:HB2	32:LK:136:MET:O	2.16	0.46
56:EF:608:ALA:O	56:EF:610:PRO:HD3	2.16	0.46
1:16:1033:G:H2'	1:16:1034:G:H8	1.81	0.46
1:16:1405:G:H2'	1:16:1406:U:C6	2.50	0.46
10:SJ:7:ARG:O	10:SJ:8:ILE:HD13	2.16	0.46
12:SL:108:LYS:HE2	12:SL:108:LYS:HA	1.97	0.46
18:SR:56:ALA:O	18:SR:60:LYS:HD2	2.16	0.46
23:23:360:U:H3'	23:23:361:G:C8	2.50	0.46
23:23:876:C:H2'	23:23:877:A:O4'	2.16	0.46
23:23:1254:A:H5''	23:23:1255:U:H5''	1.98	0.46
23:23:2233:U:H2'	23:23:2234:G:C8	2.51	0.46
25:LB:158:ALA:HB1	25:LB:197:ASN:O	2.16	0.46
30:LI:55:GLU:HA	30:LI:58:LEU:HG	1.97	0.46
39:LS:25:THR:HB	39:LS:88:ARG:HB3	1.98	0.46
56:EF:174:GLY:HA3	56:EF:178:HIS:O	2.16	0.46
1:16:652:U:O4	1:16:752:G:O2'	2.34	0.46
10:SJ:19:ASP:O	10:SJ:22:THR:HG22	2.16	0.46
28:LE:44:ILE:H	28:LE:44:ILE:HG13	1.64	0.46
29:LF:94:TYR:HA	29:LF:106:SER:O	2.15	0.46
30:LI:64:ALA:O	30:LI:68:ARG:HG2	2.16	0.46
32:LK:81:LYS:HE3	32:LK:81:LYS:HB3	1.59	0.46
41:LU:63:VAL:HA	41:LU:96:VAL:HG12	1.97	0.46
47:Lb:55:GLY:O	47:Lb:59:ILE:HG13	2.16	0.46
50:Le:8:LYS:HB2	50:Le:8:LYS:HE2	1.70	0.46
56:EF:295:ILE:HD12	56:EF:295:ILE:O	2.15	0.46
1:16:71:A:H61	1:16:99:C:H1'	1.80	0.45
7:SG:135:VAL:HG13	7:SG:138:ARG:HH21	1.80	0.45
23:23:1013:C:H2'	23:23:1014:A:H8	1.81	0.45
23:23:1026:G:H2'	23:23:1027:A:H8	1.82	0.45
23:23:2188:U:H2'	23:23:2189:U:O4'	2.16	0.45
48:Lc:6:LEU:HD13	48:Lc:9:LYS:HE3	1.98	0.45
56:EF:360:PHE:CD1	56:EF:388:LEU:HD21	2.51	0.45
58:Pt:38:A:H2'	58:Pt:39:PSU:O4'	2.16	0.45
1:16:202:G:O2'	1:16:468:A:H8	1.99	0.45
1:16:1203:C:H4'	14:SN:67:THR:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:SS:21:LYS:O	19:SS:24:GLU:HG3	2.16	0.45
23:23:447:A:O2'	65:23:3017:SPD:H22	2.16	0.45
23:23:2345:G:N3	23:23:2381:A:H2'	2.30	0.45
32:LK:141:GLU:H	32:LK:141:GLU:HG2	1.44	0.45
36:LP:21:ALA:HB2	36:LP:97:GLN:HB2	1.97	0.45
56:EF:261:ILE:C	56:EF:262:ILE:HD13	2.41	0.45
1:16:17:U:H2'	1:16:18:C:C6	2.52	0.45
9:SI:58:VAL:HG12	9:SI:58:VAL:O	2.17	0.45
13:SM:40:ALA:O	13:SM:43:VAL:HG12	2.17	0.45
15:SO:49:ASP:OD1	15:SO:52:SER:CB	2.65	0.45
17:SQ:12:VAL:HG22	17:SQ:23:VAL:HG12	1.98	0.45
23:23:848:C:H2'	23:23:849:A:H8	1.81	0.45
26:LC:11:MET:HE2	26:LC:11:MET:HB3	1.86	0.45
30:LI:132:PHE:CB	30:LI:140:ALA:HB3	2.41	0.45
32:LK:76:ALA:O	32:LK:80:LEU:N	2.49	0.45
48:Lc:49:ASP:O	48:Lc:53:VAL:HG12	2.16	0.45
56:EF:43:VAL:HG13	66:EF:901:GTP:H3'	1.98	0.45
56:EF:84:ILE:N	56:EF:84:ILE:HD12	2.32	0.45
56:EF:233:LEU:HD11	56:EF:247:GLU:HG3	1.98	0.45
1:16:613:C:H2'	1:16:614:C:C6	2.51	0.45
2:SB:117:LEU:HA	2:SB:120:GLN:HG2	1.99	0.45
3:SC:121:THR:HB	3:SC:189:ALA:HB2	1.98	0.45
13:SM:83:LEU:HD23	13:SM:83:LEU:HA	1.73	0.45
23:23:1469:A:H2'	23:23:1470:A:C8	2.51	0.45
27:LD:21:ARG:CD	27:LD:106:LYS:HB3	2.47	0.45
31:LJ:4:ASN:O	31:LJ:8:LYS:HG3	2.17	0.45
31:LJ:123:ILE:C	31:LJ:125:ARG:H	2.24	0.45
53:Lh:3:ARG:HA	53:Lh:3:ARG:HD3	1.66	0.45
56:EF:574:MET:HE3	56:EF:574:MET:HB2	1.77	0.45
1:16:410:G:H2'	1:16:429:U:C4	2.51	0.45
1:16:1287:A:H2'	1:16:1288:A:C8	2.51	0.45
13:SM:33:ILE:HD11	13:SM:63:PHE:CD2	2.50	0.45
23:23:45:G:H5'	23:23:46:G:OP1	2.17	0.45
23:23:373:U:H2'	23:23:374:A:C8	2.52	0.45
23:23:704:G:H2'	23:23:726:G:H22	1.80	0.45
1:16:1125:U:C2	1:16:1127:G:C8	3.05	0.45
17:SQ:68:SER:OG	17:SQ:71:LYS:HB2	2.16	0.45
19:SS:29:LYS:HA	19:SS:29:LYS:HD3	1.80	0.45
23:23:589:U:H2'	23:23:590:A:C8	2.52	0.45
23:23:611:C:H2'	23:23:612:G:O4'	2.16	0.45
23:23:1720:U:H2'	23:23:1721:G:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LD:129:PRO:HD3	27:LD:156:ASN:ND2	2.31	0.45
39:LS:100:LEU:HD11	39:LS:110:ILE:HD11	1.98	0.45
49:Ld:3:LYS:HE2	49:Ld:3:LYS:CA	2.46	0.45
1:16:109:A:C6	1:16:326:G:C6	3.05	0.45
1:16:244:U:O4	1:16:906:A:H1'	2.17	0.45
4:SD:9:LEU:HD23	4:SD:9:LEU:HA	1.82	0.45
23:23:677:A:OP1	61:23:3012:PUT:H11	2.17	0.45
60:23:3001:SCM:C4	60:23:3001:SCM:H12	2.46	0.45
56:EF:10:TYR:HE2	56:EF:381:ASP:HB3	1.80	0.45
56:EF:151:PHE:CE1	56:EF:266:CYS:HB3	2.50	0.45
11:SK:87:LYS:HB2	11:SK:113:VAL:HG23	1.98	0.45
21:SU:20:LYS:HE3	21:SU:20:LYS:HB2	1.54	0.45
23:23:581:C:H2'	23:23:582:A:C8	2.52	0.45
23:23:1083:U:H2'	23:23:1085:A:OP2	2.17	0.45
28:LE:65:PRO:HB3	28:LE:89:VAL:HG23	1.98	0.45
28:LE:122:PHE:HB3	28:LE:163:ASP:OD1	2.17	0.45
56:EF:352:SER:HB2	56:EF:405:ILE:HG12	1.99	0.45
1:16:231:U:H2'	1:16:232:G:H8	1.81	0.45
1:16:1251:A:H2'	1:16:1252:A:C8	2.52	0.45
1:16:1391:U:H2'	1:16:1392:G:C8	2.52	0.45
7:SG:16:PRO:HG2	9:SI:46:MET:HE3	1.99	0.45
9:SI:61:LEU:HD13	9:SI:61:LEU:C	2.41	0.45
10:SJ:11:LYS:CD	10:SJ:69:THR:CG2	2.95	0.45
10:SJ:62:ARG:HE	10:SJ:62:ARG:HB3	1.49	0.45
11:SK:14:LYS:HG3	11:SK:15:GLN:N	2.32	0.45
23:23:594:U:H2'	23:23:595:C:C6	2.51	0.45
23:23:620:G:N3	23:23:620:G:H5'	2.32	0.45
23:23:884:U:H3	23:23:892:A:H2	1.64	0.45
27:LD:58:LYS:HG3	27:LD:71:GLY:HA2	1.98	0.45
32:LK:35:ILE:CG2	32:LK:36:MET:N	2.79	0.45
38:LR:27:VAL:HG11	38:LR:40:ILE:HD11	1.99	0.45
45:LY:55:GLU:O	45:LY:59:GLU:HG3	2.17	0.45
50:Le:4:ASP:N	50:Le:4:ASP:OD1	2.49	0.45
58:Pt:35:U:H2'	58:Pt:36:U:C6	2.52	0.45
59:Dt:41:C:H2'	59:Dt:42:C:C6	2.52	0.45
3:SC:116:VAL:HG23	3:SC:200:VAL:HG21	1.98	0.45
13:SM:34:LEU:O	13:SM:34:LEU:HD23	2.17	0.45
14:SN:81:ARG:HG2	14:SN:82:ILE:N	2.32	0.45
23:23:1012:U:OP2	40:LT:70:ARG:NH2	2.50	0.45
23:23:1078:U:H4'	23:23:1079:C:H5'	1.99	0.45
32:LK:30:GLN:H	32:LK:30:GLN:HG2	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:LO:92:LEU:HD23	35:LO:92:LEU:HA	1.77	0.45
45:LY:29:ILE:HD12	45:LY:38:LEU:O	2.17	0.45
56:EF:445:PHE:CZ	56:EF:458:ILE:HG13	2.52	0.45
1:16:501:C:H2'	1:16:502:A:C8	2.53	0.44
1:16:1015:G:H2'	1:16:1016:A:O4'	2.17	0.44
8:SH:29:SER:HB3	8:SH:57:PRO:HB2	2.00	0.44
23:23:1199:U:H1'	40:LT:4:VAL:HG22	1.98	0.44
52:Lg:28:ARG:HB2	52:Lg:28:ARG:HH11	1.82	0.44
55:Lj:2:LYS:HB2	55:Lj:35:GLN:HG2	1.98	0.44
4:SD:48:LEU:HD22	4:SD:52:GLY:HA3	1.98	0.44
7:SG:111:ARG:HA	7:SG:111:ARG:HD3	1.67	0.44
7:SG:114:LYS:HB3	7:SG:118:LEU:HD13	1.98	0.44
23:23:910:A:H2'	23:23:911:A:C8	2.52	0.44
23:23:1078:U:H1'	23:23:1088:A:H5''	1.99	0.44
23:23:1085:A:C6	23:23:1086:A:N6	2.86	0.44
29:LF:26:ILE:N	29:LF:26:ILE:HD12	2.32	0.44
36:LP:46:ILE:HD12	36:LP:69:PRO:HG3	1.99	0.44
37:LQ:28:LEU:HD23	37:LQ:48:VAL:HG21	2.00	0.44
56:EF:621:VAL:HG12	56:EF:680:TYR:HB2	1.99	0.44
1:16:1250:A:H2'	1:16:1251:A:C8	2.52	0.44
2:SB:114:LEU:HD13	2:SB:144:LEU:HB3	2.00	0.44
12:SL:107:VAL:HG21	12:SL:110:ARG:HG3	1.99	0.44
23:23:570:G:H2'	23:23:2030:6MZ:C8	2.47	0.44
23:23:833:A:OP1	35:LO:39:LYS:HE3	2.17	0.44
23:23:1090:A:N1	23:23:1101:U:H5	2.14	0.44
23:23:1361:G:H2'	23:23:1362:C:C6	2.53	0.44
23:23:2615:U:C2	51:Lf:4:GLN:HA	2.52	0.44
25:LB:16:VAL:HG22	25:LB:206:GLY:HA3	2.00	0.44
36:LP:1:MET:HB2	36:LP:43:ALA:HB1	2.00	0.44
36:LP:24:THR:O	36:LP:34:LYS:HE3	2.17	0.44
51:Lf:36:GLU:OE1	51:Lf:44:THR:HB	2.17	0.44
1:16:522:C:H41	12:SL:50:ARG:NH2	2.15	0.44
1:16:599:C:H2'	1:16:600:A:H8	1.83	0.44
1:16:713:G:H2'	1:16:714:G:C8	2.53	0.44
1:16:1387:G:H5''	60:16:1601:SCM:H8M3	1.98	0.44
1:16:1513:A:H2'	1:16:1514:G:C8	2.52	0.44
2:SB:68:LEU:HD11	2:SB:92:VAL:HG23	2.00	0.44
3:SC:42:TYR:CZ	3:SC:90:VAL:HG11	2.53	0.44
13:SM:85:CYS:O	13:SM:89:LEU:HD22	2.17	0.44
23:23:1087:G:H2'	23:23:1089:A:H5''	1.99	0.44
23:23:1453:A:N6	37:LQ:74:GLU:HG2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:2140:G:H2'	23:23:2141:G:O4'	2.18	0.44
31:LJ:72:LEU:HD11	31:LJ:112:ALA:HB2	2.00	0.44
56:EF:507:LYS:HA	56:EF:507:LYS:CE	2.41	0.44
56:EF:617:MET:HE3	56:EF:617:MET:HB3	1.84	0.44
1:16:1377:A:C4	7:SG:7:ILE:HG13	2.52	0.44
4:SD:147:GLU:OE1	4:SD:150:LYS:HD2	2.17	0.44
7:SG:27:VAL:HG22	7:SG:43:VAL:HG11	1.99	0.44
7:SG:140:ASP:O	7:SG:143:ARG:HG2	2.18	0.44
11:SK:35:THR:HA	11:SK:42:LEU:HD22	1.98	0.44
23:23:126:A:O5'	53:Lh:19:ARG:HG3	2.16	0.44
23:23:1790:C:H2'	23:23:1791:A:C5	2.53	0.44
48:Lc:51:ALA:O	48:Lc:55:THR:OG1	2.35	0.44
49:Ld:5:ILE:HG22	49:Ld:59:GLU:HB3	1.99	0.44
3:SC:7:PRO:HA	3:SC:10:ILE:HG22	1.99	0.44
4:SD:45:LYS:O	4:SD:45:LYS:HG2	2.18	0.44
5:SE:111:MET:HE2	5:SE:111:MET:HB3	1.86	0.44
11:SK:123:PRO:HG2	21:SU:38:TYR:HA	2.00	0.44
12:SL:123:LYS:HD2	12:SL:123:LYS:HA	1.75	0.44
23:23:2291:U:H2'	23:23:2292:U:C6	2.52	0.44
36:LP:38:ARG:HB2	36:LP:98:PRO:HD3	1.98	0.44
56:EF:127:TRP:CG	56:EF:162:LEU:HD22	2.52	0.44
56:EF:167:VAL:HA	56:EF:168:PRO:HD3	1.88	0.44
1:16:1004:A:N6	1:16:1026:G:H1'	2.32	0.44
1:16:1323:G:H2'	1:16:1324:A:C8	2.53	0.44
2:SB:171:ILE:O	2:SB:175:GLU:HG3	2.18	0.44
6:SF:71:ILE:O	6:SF:75:GLU:HG3	2.18	0.44
7:SG:100:ALA:O	7:SG:104:ILE:HG12	2.17	0.44
10:SJ:8:ILE:CD1	10:SJ:100:ILE:HD13	2.45	0.44
10:SJ:52:LEU:HD12	10:SJ:52:LEU:HA	1.78	0.44
14:SN:73:PHE:CZ	14:SN:78:GLY:HA2	2.53	0.44
14:SN:83:LYS:HD3	14:SN:83:LYS:HA	1.85	0.44
23:23:1080:A:H2'	23:23:1081:U:H5'	2.00	0.44
27:LD:18:THR:HA	27:LD:106:LYS:HD2	2.00	0.44
48:Lc:12:GLU:C	48:Lc:14:LEU:H	2.26	0.44
50:Le:1:MET:HE3	50:Le:1:MET:HB3	1.74	0.44
56:EF:386:ILE:N	56:EF:386:ILE:HD12	2.32	0.44
23:23:2547:A:H4'	34:LN:29:HIS:CE1	2.53	0.44
23:23:2627:G:O2'	23:23:2781:A:N1	2.42	0.44
26:LC:49:GLN:OE1	26:LC:79:LEU:HD13	2.18	0.44
28:LE:170:LEU:O	28:LE:175:PHE:HB2	2.17	0.44
29:LF:91:GLY:HA3	29:LF:94:TYR:CG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:LJ:113:PHE:CD1	31:LJ:114:GLU:HG2	2.53	0.44
56:EF:50:MET:HE1	56:EF:68:THR:CG2	2.45	0.44
56:EF:244:THR:O	56:EF:248:ILE:HD12	2.17	0.44
1:16:171:A:H2'	1:16:172:A:C8	2.53	0.44
1:16:269:C:H2'	1:16:270:A:H8	1.83	0.44
1:16:522:C:OP2	12:SL:66:TYR:OH	2.32	0.44
7:SG:50:LEU:CD1	7:SG:54:SER:HB2	2.47	0.44
17:SQ:5:ILE:O	17:SQ:5:ILE:HG13	2.18	0.44
23:23:742:A:H2'	23:23:743:A:C8	2.53	0.44
23:23:2151:U:H2'	23:23:2152:G:H8	1.83	0.44
34:LN:4:GLU:C	34:LN:5:GLN:HG2	2.43	0.44
39:LS:4:ILE:HD12	39:LS:4:ILE:H	1.83	0.44
40:LT:61:TRP:CZ2	40:LT:93:LYS:HG3	2.53	0.44
9:SI:84:THR:HG21	9:SI:103:PHE:CB	2.48	0.43
20:ST:39:ILE:HD13	20:ST:39:ILE:N	2.33	0.43
23:23:372:G:H5''	47:Lb:61:LYS:HD3	2.00	0.43
23:23:2135:A:H4'	23:23:2160:C:H4'	1.99	0.43
28:LE:143:TYR:CD1	28:LE:143:TYR:C	2.96	0.43
29:LF:154:PRO:HD3	29:LF:162:VAL:O	2.18	0.43
56:EF:364:VAL:HB	56:EF:371:ARG:HB3	2.00	0.43
1:16:1100:C:OP2	2:SB:95:ARG:HD2	2.18	0.43
1:16:1145:A:H2	1:16:1147:C:H41	1.65	0.43
4:SD:9:LEU:HD13	4:SD:32:CYS:HB3	2.00	0.43
23:23:494:G:H4'	42:LV:6:LYS:HB2	1.99	0.43
23:23:1338:G:O2'	23:23:1393:A:N1	2.50	0.43
28:LE:122:PHE:C	28:LE:124:GLY:H	2.26	0.43
36:LP:31:PHE:CE1	36:LP:110:GLU:HG3	2.52	0.43
38:LR:27:VAL:HA	38:LR:93:ASP:HB3	1.99	0.43
56:EF:52:TRP:CZ2	56:EF:64:THR:HG21	2.53	0.43
56:EF:309:ARG:HH21	56:EF:402:ALA:HB1	1.82	0.43
1:16:147:G:H2'	1:16:148:G:C8	2.53	0.43
1:16:206:C:H41	1:16:214:C:H1'	1.84	0.43
4:SD:160:GLU:O	4:SD:163:GLU:HG3	2.17	0.43
8:SH:66:PHE:CE2	8:SH:67:GLN:HG3	2.53	0.43
23:23:1013:C:H2'	23:23:1014:A:C8	2.53	0.43
24:5:115:A:H2'	24:5:116:G:C8	2.53	0.43
28:LE:4:LEU:HD13	28:LE:100:PHE:HD2	1.82	0.43
28:LE:79:ILE:HD12	28:LE:79:ILE:O	2.18	0.43
40:LT:61:TRP:O	40:LT:65:ILE:HG13	2.18	0.43
43:LW:67:VAL:O	43:LW:68:LYS:HD3	2.19	0.43
47:Lb:7:VAL:HG22	47:Lb:51:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Ld:4:THR:HG23	49:Ld:4:THR:O	2.18	0.43
8:SH:96:MET:HB3	8:SH:99:LEU:HB2	2.00	0.43
20:ST:85:LYS:HA	20:ST:85:LYS:HD3	1.83	0.43
30:LI:130:VAL:HG12	30:LI:131:SER:H	1.84	0.43
31:LJ:94:ARG:O	31:LJ:97:LYS:HG3	2.18	0.43
33:LM:69:ARG:O	33:LM:90:GLU:HG3	2.18	0.43
53:Lh:25:LYS:HE3	53:Lh:25:LYS:HB3	1.66	0.43
56:EF:690:ALA:HB1	56:EF:694:VAL:HG23	1.99	0.43
7:SG:56:LYS:HD2	7:SG:56:LYS:HA	1.71	0.43
23:23:1669:A:C8	34:LN:5:GLN:HG3	2.54	0.43
23:23:1796:U:H2'	23:23:1797:G:H8	1.83	0.43
35:LO:76:GLU:C	35:LO:77:ILE:HD12	2.43	0.43
35:LO:89:VAL:HA	35:LO:121:THR:HG23	1.99	0.43
1:16:523:A:C2	12:SL:88:LYS:HB3	2.53	0.43
1:16:1119:C:H2'	1:16:1120:C:H6	1.84	0.43
1:16:1241:G:H2'	1:16:1242:G:C8	2.51	0.43
3:SC:150:LYS:HB2	3:SC:173:VAL:HG21	2.01	0.43
7:SG:113:ASP:HB2	7:SG:119:ARG:HG3	2.00	0.43
10:SJ:56:HIS:CE1	10:SJ:57:VAL:HG13	2.54	0.43
11:SK:72:ASP:O	11:SK:75:LYS:HG3	2.19	0.43
13:SM:109:ARG:HD2	13:SM:109:ARG:HA	1.83	0.43
15:SO:3:LEU:HG	15:SO:35:GLN:HG2	2.00	0.43
19:SS:44:MET:N	19:SS:44:MET:SD	2.91	0.43
23:23:2316:G:H2'	23:23:2317:A:H8	1.84	0.43
25:LB:2:ALA:N	25:LB:20:VAL:O	2.52	0.43
28:LE:117:LEU:H	28:LE:117:LEU:HG	1.66	0.43
35:LO:62:PRO:HG2	54:Li:25:LYS:HD3	2.00	0.43
56:EF:422:PRO:HB2	56:EF:425:LYS:HA	2.00	0.43
1:16:618:C:H5'	1:16:619:U:H5''	2.00	0.43
10:SJ:11:LYS:CG	10:SJ:69:THR:CG2	2.96	0.43
23:23:848:C:H2'	23:23:849:A:C8	2.54	0.43
23:23:1175:A:H4'	23:23:1176:U:C2	2.53	0.43
23:23:2251:OMG:H1'	23:23:2251:OMG:HM23	1.72	0.43
39:LS:106:LYS:O	39:LS:109:ARG:HG2	2.18	0.43
43:LW:26:LYS:HA	43:LW:26:LYS:HD2	1.76	0.43
56:EF:435:LEU:HD22	56:EF:458:ILE:HD11	2.00	0.43
1:16:265:G:N2	1:16:267:C:H5'	2.33	0.43
2:SB:165:ASP:HA	2:SB:204:ASP:OD2	2.18	0.43
4:SD:105:MET:HG3	4:SD:171:LEU:CD2	2.48	0.43
5:SE:66:LYS:HE3	5:SE:66:LYS:HB2	1.75	0.43
5:SE:109:GLY:HA2	5:SE:112:ARG:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:2751:G:H5'	23:23:2752:C:C5	2.54	0.43
29:LF:156:PRO:HB2	29:LF:172:LYS:HB2	2.01	0.43
33:LM:32:LEU:HD22	33:LM:54:ILE:HG21	1.99	0.43
43:LW:10:VAL:HG12	43:LW:11:LEU:HD23	2.00	0.43
47:Lb:10:LYS:HE3	47:Lb:54:LYS:HD3	2.00	0.43
56:EF:261:ILE:HD12	56:EF:263:LEU:HD23	2.00	0.43
1:16:1226:C:H4'	19:SS:80:TYR:CZ	2.54	0.43
4:SD:105:MET:HE2	4:SD:180:GLY:HA3	2.01	0.43
20:ST:10:ARG:HD2	20:ST:10:ARG:HA	1.78	0.43
23:23:405:U:H6	23:23:405:U:H2'	1.71	0.43
23:23:1792:G:H5'	25:LB:204:VAL:HG13	2.00	0.43
23:23:2467:C:O2	36:LP:123:LYS:HE3	2.19	0.43
37:LQ:118:ARG:HB3	37:LQ:120:GLU:OE1	2.17	0.43
38:LR:30:ARG:HG3	38:LR:35:ILE:HD12	2.01	0.43
56:EF:143:LYS:HG2	66:EF:901:GTP:C6	2.54	0.43
1:16:539:A:H2'	1:16:540:G:C8	2.54	0.43
1:16:1010:U:H2'	1:16:1011:C:C6	2.54	0.43
3:SC:150:LYS:HD3	3:SC:201:TRP:CE3	2.54	0.43
6:SF:37:HIS:O	6:SF:97:THR:HG23	2.19	0.43
10:SJ:10:LEU:HD22	10:SJ:98:VAL:HG12	2.00	0.43
23:23:2095:A:H2'	23:23:2096:C:O4'	2.19	0.43
32:LK:122:ILE:O	32:LK:126:THR:HG23	2.18	0.43
4:SD:188:ARG:HD2	4:SD:191:LEU:HD21	2.00	0.42
7:SG:76:LYS:HD3	7:SG:89:VAL:HG21	2.01	0.42
10:SJ:17:LEU:HD12	10:SJ:17:LEU:O	2.19	0.42
23:23:639:U:H2'	23:23:640:C:H6	1.83	0.42
35:LO:77:ILE:N	35:LO:109:LYS:O	2.50	0.42
1:16:673:A:H2'	1:16:674:G:C8	2.54	0.42
1:16:712:A:H5'	25:LB:138:GLY:HA3	2.01	0.42
13:SM:12:HIS:HA	13:SM:45:ILE:HG12	2.00	0.42
14:SN:3:LYS:H	14:SN:3:LYS:HG3	1.70	0.42
23:23:84:A:N1	23:23:98:G:O2'	2.46	0.42
23:23:481:G:O2'	23:23:507:A:N1	2.52	0.42
25:LB:175:ARG:HB2	25:LB:181:MET:HE1	2.00	0.42
29:LF:32:GLU:O	29:LF:33:LEU:HD23	2.19	0.42
31:LJ:25:ALA:O	31:LJ:112:ALA:N	2.52	0.42
32:LK:79:LEU:HD22	32:LK:79:LEU:HA	1.75	0.42
32:LK:117:MET:HE3	32:LK:129:ILE:HD11	2.00	0.42
56:EF:624:PRO:HG3	56:EF:677:ARG:HG3	2.01	0.42
6:SF:90:MET:HB3	6:SF:90:MET:HE2	1.60	0.42
23:23:320:A:H4'	23:23:322:A:N7	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:1088:A:H61	32:LK:132:THR:HA	1.85	0.42
23:23:1424:G:H2'	23:23:1425:G:O4'	2.19	0.42
23:23:1682:G:H2'	23:23:1683:U:C6	2.55	0.42
23:23:1870:C:C5	23:23:1871:A:C4	3.07	0.42
28:LE:40:VAL:CG1	28:LE:50:LEU:HD13	2.50	0.42
29:LF:120:GLY:C	29:LF:121:ILE:HD13	2.44	0.42
56:EF:14:GLY:HA3	56:EF:106:LEU:HD11	2.01	0.42
56:EF:197:ASP:C	56:EF:199:GLY:H	2.27	0.42
3:SC:134:MET:O	3:SC:138:VAL:HG23	2.20	0.42
6:SF:19:PRO:O	6:SF:23:GLU:HG3	2.19	0.42
16:SP:63:GLN:HA	16:SP:63:GLN:OE1	2.19	0.42
23:23:2364:C:OP1	46:La:55:ARG:HD3	2.20	0.42
26:LC:129:THR:HG22	61:LC:301:PUT:HN11	1.84	0.42
31:LJ:126:LEU:N	31:LJ:126:LEU:HD23	2.34	0.42
32:LK:82:LYS:HE2	32:LK:82:LYS:HB3	1.79	0.42
50:Le:47:LYS:HE3	50:Le:47:LYS:HB3	1.90	0.42
50:Le:49:ARG:HH11	50:Le:51:VAL:HG23	1.85	0.42
56:EF:93:VAL:O	56:EF:96:THR:HG23	2.19	0.42
1:16:662:U:H2'	1:16:663:A:C8	2.55	0.42
2:SB:104:TRP:HA	2:SB:107:VAL:HG22	2.02	0.42
10:SJ:42:LEU:HB2	10:SJ:71:LEU:HD11	2.00	0.42
23:23:684:G:H5'	53:Lh:16:HIS:HE1	1.83	0.42
23:23:723:C:H2'	23:23:724:U:O4'	2.19	0.42
24:5:66:A:N6	24:5:107:G:H2'	2.35	0.42
28:LE:18:THR:HG22	28:LE:18:THR:O	2.20	0.42
28:LE:64:LYS:HE3	50:Le:5:ILE:HG13	2.01	0.42
28:LE:164:GLU:N	28:LE:164:GLU:CD	2.77	0.42
32:LK:100:LYS:HG2	32:LK:139:VAL:HG23	2.00	0.42
43:LW:53:VAL:HG11	43:LW:93:LEU:HB2	2.02	0.42
46:La:53:CYS:SG	46:La:57:HIS:HA	2.59	0.42
47:Lb:3:ARG:O	47:Lb:12:PRO:HD3	2.19	0.42
59:Dt:62:C:H2'	59:Dt:63:G:H8	1.85	0.42
1:16:719:C:C2	18:SR:39:ILE:HD12	2.54	0.42
1:16:1036:A:H2'	1:16:1037:C:C6	2.55	0.42
1:16:1398:A:H5''	1:16:1398:A:C8	2.53	0.42
2:SB:135:LEU:O	2:SB:139:ARG:HG3	2.20	0.42
18:SR:28:THR:H	18:SR:28:THR:HG1	1.58	0.42
23:23:414:C:H2'	23:23:415:A:C8	2.55	0.42
23:23:1198:U:H2'	23:23:1199:U:C6	2.55	0.42
23:23:1548:A:H2'	23:23:1549:A:C8	2.55	0.42
23:23:2834:G:H2'	23:23:2879:A:H61	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LE:134:GLU:CD	28:LE:134:GLU:H	2.26	0.42
29:LF:81:GLU:HG2	29:LF:82:GLY:H	1.84	0.42
37:LQ:28:LEU:HD13	37:LQ:34:ILE:HG12	2.02	0.42
39:LS:91:ALA:HB3	39:LS:111:LYS:HG3	2.01	0.42
42:LV:11:ARG:HD2	42:LV:11:ARG:HA	1.87	0.42
47:Lb:56:MET:HE2	47:Lb:56:MET:HB3	1.96	0.42
58:Pt:27:G:N3	58:Pt:27:G:H2'	2.34	0.42
3:SC:112:ASP:HB3	3:SC:115:LEU:CD2	2.49	0.42
8:SH:36:ILE:HD11	8:SH:126:ILE:HG21	2.01	0.42
12:SL:30:LYS:HD3	12:SL:30:LYS:HA	1.86	0.42
13:SM:52:GLN:O	13:SM:55:THR:OG1	2.35	0.42
16:SP:34:GLU:OE2	16:SP:56:ARG:HD3	2.20	0.42
21:SU:36:GLU:HG2	21:SU:37:PHE:CD2	2.55	0.42
23:23:2504:PSU:H6	23:23:2504:PSU:O5'	2.02	0.42
29:LF:171:THR:HG22	29:LF:172:LYS:H	1.85	0.42
33:LM:32:LEU:O	33:LM:36:LEU:HG	2.20	0.42
41:LU:71:LYS:HD3	41:LU:90:ARG:HG3	2.00	0.42
56:EF:502:GLU:HB2	56:EF:517:HIS:HE1	1.85	0.42
1:16:131:A:H2'	1:16:132:C:C6	2.55	0.42
1:16:1028:C:H2'	1:16:1029:U:H4'	2.00	0.42
1:16:1033:G:H2'	1:16:1034:G:C8	2.55	0.42
2:SB:6:MET:HE1	2:SB:44:GLU:HG3	2.02	0.42
5:SE:47:GLY:HA3	5:SE:71:MET:HG2	2.01	0.42
5:SE:83:HIS:CG	8:SH:96:MET:HG2	2.55	0.42
8:SH:10:MET:HG3	8:SH:27:MET:SD	2.59	0.42
19:SS:3:ARG:HD2	19:SS:4:SER:N	2.34	0.42
20:ST:79:LEU:O	20:ST:83:ILE:HG12	2.19	0.42
23:23:500:G:N1	23:23:503:A:OP2	2.52	0.42
23:23:1387:A:H5'	23:23:1469:A:H1'	2.02	0.42
23:23:1857:G:H1'	23:23:1885:A:N6	2.34	0.42
23:23:2081:U:H2'	23:23:2082:A:H8	1.85	0.42
23:23:2377:A:H8	23:23:2377:A:OP2	2.02	0.42
23:23:2419:U:H2'	23:23:2420:C:C6	2.55	0.42
23:23:2661:G:H4'	56:EF:19:ILE:HD13	2.01	0.42
38:LR:24:THR:HG23	38:LR:90:VAL:HA	2.02	0.42
56:EF:261:ILE:HD12	56:EF:263:LEU:CD2	2.49	0.42
56:EF:520:ILE:HG22	56:EF:578:LEU:HA	2.01	0.42
56:EF:566:LEU:HD21	56:EF:612:LEU:HD21	2.02	0.42
1:16:509:A:H5'	4:SD:52:GLY:HA2	2.02	0.42
1:16:1338:G:H2'	1:16:1339:A:C8	2.54	0.42
2:SB:35:ARG:O	2:SB:38:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SD:85:ASN:HB3	4:SD:88:GLU:HB2	2.02	0.42
7:SG:27:VAL:O	7:SG:31:MET:HB2	2.19	0.42
9:SI:83:ILE:O	9:SI:87:LEU:HG	2.20	0.42
9:SI:118:LEU:HA	9:SI:125:PRO:HD3	2.02	0.42
12:SL:87:VAL:HG11	12:SL:90:LEU:HD12	2.02	0.42
32:LK:22:PRO:HG2	32:LK:23:PRO:HD3	2.01	0.42
32:LK:56:PRO:HG2	32:LK:72:LYS:HB2	2.01	0.42
35:LO:62:PRO:HG2	54:Li:25:LYS:HB3	2.02	0.42
45:LY:68:LYS:HE2	45:LY:68:LYS:HB2	1.88	0.42
54:Li:15:LYS:HB2	54:Li:23:LYS:HE2	2.02	0.42
56:EF:55:GLN:HE21	56:EF:55:GLN:HB2	1.58	0.42
1:16:51:A:H61	1:16:314:C:H1'	1.85	0.42
1:16:106:C:H2'	1:16:107:G:O4'	2.20	0.42
2:SB:100:MET:HE3	2:SB:100:MET:HB2	1.93	0.42
4:SD:188:ARG:HE	4:SD:197:GLU:CD	2.27	0.42
7:SG:18:PHE:CE2	7:SG:47:LEU:HD21	2.55	0.42
7:SG:43:VAL:HG13	7:SG:44:TYR:HD1	1.84	0.42
9:SI:25:ASN:H	9:SI:61:LEU:HA	1.85	0.42
10:SJ:51:VAL:HG22	14:SN:81:ARG:HB2	2.02	0.42
11:SK:123:PRO:O	21:SU:38:TYR:HB2	2.20	0.42
23:23:459:U:H2'	23:23:460:A:H8	1.85	0.42
23:23:903:C:H2'	23:23:904:G:H8	1.84	0.42
23:23:2895:G:H2'	23:23:2896:C:C6	2.55	0.42
27:LD:111:GLU:HG2	35:LO:1:MET:HG2	2.01	0.42
28:LE:40:VAL:HG13	28:LE:43:ALA:HB2	2.01	0.42
33:LM:45:THR:HB	33:LM:48:VAL:HB	2.00	0.42
43:LW:23:ALA:HB1	43:LW:29:THR:CG2	2.50	0.42
45:LY:10:LYS:H	45:LY:10:LYS:HG2	1.66	0.42
45:LY:21:ARG:HA	45:LY:25:LYS:O	2.20	0.42
47:Lb:38:PHE:HE2	47:Lb:49:LEU:HB2	1.84	0.42
1:16:6:G:C4	5:SE:124:LEU:HD11	2.55	0.41
3:SC:130:PHE:CD2	3:SC:157:LEU:HB3	2.55	0.41
6:SF:12:PRO:HB3	6:SF:56:LYS:O	2.20	0.41
9:SI:55:VAL:HG13	9:SI:94:LEU:HD13	2.02	0.41
23:23:1754:A:N1	23:23:2716:C:O2'	2.47	0.41
23:23:2064:C:H2'	23:23:2065:C:C6	2.55	0.41
25:LB:74:ILE:HD13	25:LB:98:ASP:OD2	2.20	0.41
25:LB:160:THR:O	25:LB:195:VAL:HG23	2.20	0.41
37:LQ:82:GLU:O	37:LQ:86:ARG:HB2	2.20	0.41
56:EF:150:ASN:HB3	56:EF:153:LYS:HB3	2.02	0.41
56:EF:351:ASN:O	56:EF:355:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Dt:23:A:H2'	59:Dt:24:G:H8	1.84	0.41
1:16:2:A:H1'	1:16:613:C:O2'	2.20	0.41
1:16:1071:C:H2'	1:16:1072:G:C8	2.56	0.41
3:SC:23:PHE:CZ	10:SJ:11:LYS:HD2	2.55	0.41
4:SD:191:LEU:H	4:SD:191:LEU:HD23	1.85	0.41
9:SI:53:GLU:CD	9:SI:53:GLU:C	2.87	0.41
23:23:155:A:H2'	23:23:156:A:C8	2.55	0.41
23:23:1664:A:C2	34:LN:1:MET:HE1	2.56	0.41
23:23:1935:G:H21	23:23:1964:G:H5'	1.84	0.41
23:23:2796:U:H3	23:23:2799:A:H61	1.66	0.41
26:LC:56:LYS:HG3	26:LC:59:ARG:HB2	2.01	0.41
36:LP:112:LEU:HD12	36:LP:112:LEU:O	2.21	0.41
38:LR:40:ILE:HA	38:LR:47:VAL:HA	2.02	0.41
1:16:695:A:H2'	1:16:696:A:C8	2.55	0.41
1:16:737:C:H2'	1:16:738:C:C6	2.55	0.41
1:16:985:C:H2'	1:16:986:U:C6	2.55	0.41
1:16:1167:A:N6	1:16:1169:A:N1	2.69	0.41
1:16:1299:A:O2'	1:16:1300:G:H4'	2.20	0.41
13:SM:46:SER:O	13:SM:47:GLU:CD	2.63	0.41
18:SR:11:CYS:SG	18:SR:14:THR:HB	2.60	0.41
23:23:548:G:H4'	23:23:549:G:C2	2.56	0.41
23:23:882:G:N2	23:23:894:U:H2'	2.35	0.41
23:23:1027:A:C6	23:23:1126:A:C4	3.08	0.41
23:23:1569:A:H2'	23:23:1570:A:C8	2.55	0.41
23:23:1653:G:C6	37:LQ:9:GLN:HB3	2.55	0.41
23:23:2031:A:C6	23:23:2498:OMC:H1'	2.55	0.41
30:LI:53:GLU:H	30:LI:53:GLU:HG3	1.73	0.41
33:LM:95:ARG:HE	33:LM:95:ARG:HB3	1.56	0.41
36:LP:75:GLU:HB2	36:LP:90:GLU:HG3	2.01	0.41
46:La:55:ARG:HG3	46:La:55:ARG:HH11	1.85	0.41
56:EF:223:ILE:HD13	56:EF:223:ILE:N	2.34	0.41
56:EF:566:LEU:C	56:EF:566:LEU:CD2	2.92	0.41
1:16:451:A:H61	1:16:481:G:H5'	1.85	0.41
1:16:1034:G:H2'	1:16:1035:A:H8	1.86	0.41
1:16:1363:A:O2'	1:16:1365:G:N7	2.51	0.41
3:SC:40:ARG:HE	3:SC:57:ILE:HD12	1.85	0.41
7:SG:18:PHE:HB2	7:SG:23:LEU:HD21	2.03	0.41
8:SH:66:PHE:CD2	8:SH:67:GLN:HG3	2.55	0.41
20:ST:2:ALA:N	20:ST:8:LYS:HE2	2.35	0.41
25:LB:142:HIS:CD2	25:LB:195:VAL:HG22	2.55	0.41
26:LC:38:LYS:O	26:LC:46:ARG:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LE:134:GLU:CD	28:LE:134:GLU:N	2.78	0.41
2:SB:161:LEU:HD23	2:SB:161:LEU:HA	1.80	0.41
3:SC:110:GLU:CD	3:SC:144:LEU:HG	2.45	0.41
9:SI:19:VAL:HB	9:SI:65:ILE:HG22	2.02	0.41
14:SN:10:GLU:HG3	14:SN:11:VAL:N	2.35	0.41
23:23:987:C:O2'	23:23:1000:A:N3	2.51	0.41
23:23:2114:A:N6	23:23:2119:A:H62	2.18	0.41
50:Le:66:ILE:N	50:Le:66:ILE:HD13	2.35	0.41
56:EF:451:GLU:CD	56:EF:451:GLU:H	2.28	0.41
1:16:181:A:O2'	1:16:194:C:N4	2.53	0.41
1:16:222:C:H2'	1:16:223:A:C8	2.56	0.41
1:16:815:A:N7	1:16:1509:C:O2'	2.44	0.41
1:16:1071:C:H2'	1:16:1072:G:H8	1.84	0.41
2:SB:47:VAL:HG23	2:SB:48:PRO:CD	2.49	0.41
12:SL:46:ASN:ND2	12:SL:89:D2T:SB	2.94	0.41
23:23:396:G:H1'	47:Lb:29:PHE:HB3	2.02	0.41
27:LD:29:HIS:CE1	35:LO:8:PRO:HG3	2.56	0.41
28:LE:62:GLY:C	28:LE:95:ARG:HH12	2.27	0.41
56:EF:170:GLN:HB3	56:EF:182:VAL:CG1	2.51	0.41
56:EF:618:LYS:N	56:EF:683:GLU:O	2.53	0.41
1:16:7:A:H5'	1:16:298:A:O4'	2.21	0.41
17:SQ:16:LYS:HE3	17:SQ:16:LYS:HB3	1.88	0.41
23:23:483:A:H5''	44:LX:47:LYS:HD3	2.02	0.41
23:23:2705:A:O2'	23:23:2852:G:OP1	2.36	0.41
25:LB:41:GLY:O	25:LB:43:ARG:NH1	2.53	0.41
29:LF:48:ASN:HD22	29:LF:48:ASN:HA	1.69	0.41
32:LK:54:PRO:HD2	32:LK:78:VAL:HG11	2.03	0.41
55:Lj:8:LYS:HB3	55:Lj:8:LYS:HE3	1.86	0.41
56:EF:493:THR:HG22	56:EF:613:LEU:HD21	2.02	0.41
58:Pt:34:U8U:H2'	58:Pt:35:U:H6	1.85	0.41
59:Dt:16:U:H5''	59:Dt:17:U:OP1	2.20	0.41
1:16:1350:A:OP2	9:SI:120:LYS:HE2	2.21	0.41
2:SB:47:VAL:HG23	2:SB:48:PRO:HD3	2.03	0.41
3:SC:65:ARG:HA	3:SC:100:GLN:O	2.21	0.41
7:SG:132:GLY:O	7:SG:136:LYS:HE3	2.20	0.41
9:SI:21:ILE:HG23	9:SI:61:LEU:HD23	2.02	0.41
12:SL:66:TYR:HE1	12:SL:68:GLY:HA2	1.86	0.41
13:SM:23:TYR:CE1	13:SM:69:LEU:HD22	2.48	0.41
23:23:247:G:H4'	23:23:386:G:C5	2.55	0.41
23:23:1287:A:N7	37:LQ:105:GLY:HA3	2.35	0.41
23:23:2182:U:H2'	23:23:2183:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:2514:U:H2'	23:23:2515:C:C6	2.55	0.41
23:23:2903:U:H2'	23:23:2904:U:H2'	2.03	0.41
24:5:43:C:OP1	50:Le:6:HIS:HE1	2.04	0.41
25:LB:76:ALA:HB2	25:LB:96:TYR:CD2	2.55	0.41
27:LD:1:MET:HE2	27:LD:1:MET:HB3	1.89	0.41
28:LE:40:VAL:HG12	28:LE:85:ILE:O	2.21	0.41
34:LN:12:ASP:HB3	34:LN:99:ILE:HD13	2.02	0.41
56:EF:62:THR:N	66:EF:901:GTP:O2G	2.54	0.41
59:Dt:23:A:H2'	59:Dt:24:G:C8	2.55	0.41
1:16:235:C:H2'	1:16:236:A:C8	2.56	0.41
1:16:404:G:N7	4:SD:2:ALA:HB3	2.36	0.41
1:16:530:G:C6	22:mR:46:G:H4'	2.55	0.41
1:16:563:A:H2'	1:16:567:G:C8	2.56	0.41
1:16:769:G:H4'	1:16:1513:A:H4'	2.01	0.41
1:16:1081:A:H5'	5:SE:23:LYS:HG3	2.02	0.41
1:16:1255:G:O2'	1:16:1258:G:N3	2.50	0.41
2:SB:162:PHE:CZ	2:SB:217:VAL:HG21	2.56	0.41
7:SG:15:ASP:O	7:SG:19:GLY:N	2.54	0.41
10:SJ:10:LEU:O	10:SJ:71:LEU:HA	2.21	0.41
12:SL:42:PRO:HB2	12:SL:89:D2T:H5	2.03	0.41
13:SM:12:HIS:HA	13:SM:45:ILE:CD1	2.51	0.41
20:ST:2:ALA:O	20:ST:8:LYS:HE2	2.21	0.41
23:23:908:C:OP1	61:23:3015:PUT:H32	2.20	0.41
23:23:1746:A:H2'	23:23:1747:U:C6	2.56	0.41
23:23:2038:G:H2'	23:23:2039:U:O4'	2.20	0.41
23:23:2552:OMU:H6	23:23:2552:OMU:O5'	2.21	0.41
23:23:2747:G:O6	23:23:2755:C:H5''	2.20	0.41
25:LB:123:ALA:O	25:LB:128:ASN:ND2	2.54	0.41
28:LE:102:ARG:NH1	50:Le:25:ARG:O	2.54	0.41
29:LF:23:VAL:O	29:LF:24:ILE:HD13	2.20	0.41
32:LK:138:LEU:HD13	32:LK:138:LEU:HA	1.85	0.41
35:LO:77:ILE:HD12	35:LO:77:ILE:N	2.35	0.41
36:LP:53:MET:HE1	36:LP:103:TYR:CD1	2.56	0.41
54:Li:29:LEU:HD12	54:Li:29:LEU:HA	1.84	0.41
56:EF:555:LYS:HA	56:EF:555:LYS:HD3	1.86	0.41
56:EF:578:LEU:HG	56:EF:578:LEU:O	2.21	0.41
1:16:73:C:O2'	1:16:74:A:H8	2.03	0.41
1:16:649:A:H2'	1:16:650:G:O4'	2.21	0.41
1:16:780:A:OP1	11:SK:125:LYS:HG2	2.20	0.41
1:16:1029:U:C4	1:16:1031:C:C2	3.09	0.41
1:16:1166:G:N1	1:16:1169:A:OP2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:1414:U:H2'	1:16:1415:G:H8	1.86	0.41
10:SJ:11:LYS:CD	10:SJ:69:THR:HG21	2.49	0.41
23:23:976:G:O2'	23:23:1155:A:O2'	2.38	0.41
23:23:2061:G:N2	57:Pp:2:PHE:O	2.54	0.41
24:5:43:C:OP1	50:Le:6:HIS:CE1	2.73	0.41
28:LE:139:PRO:HB2	50:Le:32:LEU:HD22	2.02	0.41
29:LF:134:LYS:HE3	29:LF:134:LYS:HB2	1.90	0.41
30:LI:100:ALA:HA	30:LI:103:VAL:CG2	2.49	0.41
55:Lj:15:LYS:HB2	55:Lj:15:LYS:HE2	1.89	0.41
56:EF:367:HIS:ND1	56:EF:370:LYS:HD3	2.36	0.41
56:EF:512:ARG:HG2	56:EF:512:ARG:NH1	2.36	0.41
4:SD:156:LYS:HB3	4:SD:156:LYS:HE2	1.82	0.40
6:SF:32:ALA:C	6:SF:33:GLU:OE1	2.64	0.40
7:SG:101:MET:HB3	7:SG:101:MET:HE2	1.88	0.40
23:23:1786:A:H1'	23:23:1938:A:N6	2.36	0.40
23:23:1918:A:O2'	23:23:1919:A:N7	2.45	0.40
23:23:2153:C:H2'	23:23:2154:A:H8	1.85	0.40
25:LB:245:VAL:HA	25:LB:251:GLN:HA	2.03	0.40
28:LE:34:ILE:CD1	28:LE:156:ILE:HG12	2.51	0.40
31:LJ:41:LEU:HD11	31:LJ:99:PHE:CD2	2.57	0.40
31:LJ:113:PHE:CE1	31:LJ:114:GLU:HG2	2.56	0.40
56:EF:233:LEU:HA	56:EF:236:LYS:HB2	2.02	0.40
56:EF:474:LYS:HG3	56:EF:480:GLU:HG3	2.02	0.40
1:16:1040:U:H2'	1:16:1041:G:H8	1.85	0.40
1:16:1053:G:H5''	1:16:1054:C:H3'	2.03	0.40
1:16:1081:A:OP2	5:SE:52:LYS:NZ	2.52	0.40
1:16:1397:C:P	5:SE:29:ARG:HH22	2.44	0.40
3:SC:110:GLU:CD	3:SC:110:GLU:H	2.29	0.40
7:SG:12:ILE:HG23	7:SG:12:ILE:O	2.20	0.40
7:SG:140:ASP:HA	7:SG:143:ARG:HD3	2.02	0.40
9:SI:61:LEU:H	9:SI:61:LEU:CD1	2.34	0.40
9:SI:67:VAL:O	9:SI:67:VAL:HG13	2.22	0.40
20:ST:2:ALA:HB3	20:ST:8:LYS:HG3	2.04	0.40
23:23:1172:C:N3	23:23:1173:U:H1'	2.37	0.40
23:23:1820:U:O2	25:LB:201:MET:HG2	2.21	0.40
23:23:2061:G:H2'	23:23:2501:C:O2'	2.21	0.40
34:LN:121:GLU:HB3	34:LN:122:VAL:H	1.68	0.40
48:Lc:14:LEU:HD23	48:Lc:14:LEU:HA	1.90	0.40
1:16:310:G:H5''	16:SP:31:ARG:HB2	2.04	0.40
1:16:1042:A:H2'	1:16:1043:G:C1'	2.51	0.40
1:16:1222:G:H5''	19:SS:78:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:23:249:C:OP2	23:23:2394:C:O2'	2.36	0.40
23:23:783:A:H4'	23:23:2588:G:H4'	2.02	0.40
23:23:832:U:H2'	23:23:833:A:C8	2.56	0.40
23:23:1438:U:H2'	23:23:1439:A:C8	2.57	0.40
23:23:1818:U:O2'	25:LB:153:GLN:O	2.28	0.40
23:23:2376:A:H2'	23:23:2377:A:O4'	2.21	0.40
30:LI:69:ALA:O	30:LI:72:ILE:HG12	2.21	0.40
56:EF:263:LEU:HA	56:EF:263:LEU:HD22	1.85	0.40
1:16:1412:C:H2'	1:16:1413:A:C8	2.56	0.40
2:SB:135:LEU:HG	2:SB:139:ARG:HE	1.87	0.40
3:SC:179:ARG:HD2	3:SC:206:GLU:HB3	2.04	0.40
10:SJ:41:PRO:HA	10:SJ:72:ARG:HD3	2.03	0.40
14:SN:12:LYS:HE2	14:SN:12:LYS:HB2	1.89	0.40
14:SN:31:ILE:O	14:SN:34:VAL:HG12	2.22	0.40
17:SQ:20:SER:HA	17:SQ:48:ASP:H	1.86	0.40
23:23:632:A:H2'	23:23:633:A:C8	2.56	0.40
23:23:1818:U:H2'	25:LB:156:ARG:HG3	2.02	0.40
23:23:1856:U:H2'	23:23:1857:G:O4'	2.21	0.40
23:23:2522:U:O2'	23:23:2647:U:OP1	2.39	0.40
23:23:2554:U:H2'	23:23:2555:U:C6	2.56	0.40
28:LE:103:LEU:HA	28:LE:107:ALA:HB3	2.03	0.40
28:LE:109:PRO:HB3	50:Le:44:PHE:HE2	1.87	0.40
28:LE:130:MET:SD	28:LE:154:ILE:HB	2.62	0.40
30:LI:75:LEU:O	30:LI:77:THR:N	2.55	0.40
31:LJ:69:PHE:C	31:LJ:72:LEU:HD23	2.47	0.40
32:LK:28:LEU:HA	32:LK:31:GLN:HG2	2.04	0.40
32:LK:123:GLU:O	32:LK:127:ARG:HG3	2.21	0.40
56:EF:532:LYS:O	56:EF:532:LYS:HD2	2.22	0.40
1:16:451:A:H5'	16:SP:70:ARG:NH2	2.37	0.40
9:SI:61:LEU:C	9:SI:61:LEU:HD22	2.47	0.40
23:23:1882:U:H2'	23:23:1883:U:H6	1.87	0.40
23:23:2898:U:H2'	23:23:2899:A:H8	1.86	0.40
28:LE:98:GLU:O	28:LE:101:GLU:HG2	2.22	0.40
30:LI:71:LYS:O	30:LI:75:LEU:HG	2.22	0.40
30:LI:122:LEU:O	30:LI:122:LEU:HD12	2.22	0.40
32:LK:33:VAL:HG22	32:LK:67:PHE:CD2	2.57	0.40
43:LW:14:PRO:HD3	48:Lc:30:MET:CE	2.51	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	222/241 (92%)	210 (95%)	12 (5%)	0	100	100
3	SC	209/233 (90%)	200 (96%)	9 (4%)	0	100	100
4	SD	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
5	SE	153/167 (92%)	150 (98%)	3 (2%)	0	100	100
6	SF	104/135 (77%)	101 (97%)	3 (3%)	0	100	100
7	SG	149/179 (83%)	141 (95%)	8 (5%)	0	100	100
8	SH	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
9	SI	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
10	SJ	97/103 (94%)	91 (94%)	6 (6%)	0	100	100
11	SK	117/129 (91%)	111 (95%)	6 (5%)	0	100	100
12	SL	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
13	SM	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
14	SN	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
15	SO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	SP	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
17	SQ	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
18	SR	65/75 (87%)	60 (92%)	5 (8%)	0	100	100
19	SS	82/92 (89%)	75 (92%)	7 (8%)	0	100	100
20	ST	83/87 (95%)	83 (100%)	0	0	100	100
21	SU	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
25	LB	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
26	LC	207/209 (99%)	198 (96%)	8 (4%)	1 (0%)	24	34
27	LD	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
28	LE	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
29	LF	174/177 (98%)	169 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	LI	146/149 (98%)	129 (88%)	17 (12%)	0	100	100
31	LJ	129/165 (78%)	121 (94%)	8 (6%)	0	100	100
32	LK	132/142 (93%)	121 (92%)	11 (8%)	0	100	100
33	LM	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
34	LN	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
35	LO	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
36	LP	133/136 (98%)	133 (100%)	0	0	100	100
37	LQ	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
38	LR	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
39	LS	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
40	LT	115/118 (98%)	115 (100%)	0	0	100	100
41	LU	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
42	LV	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
43	LW	91/100 (91%)	87 (96%)	4 (4%)	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	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
47	Lb	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
48	Lc	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
49	Ld	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	Le	66/70 (94%)	58 (88%)	8 (12%)	0	100	100
51	Lf	54/57 (95%)	54 (100%)	0	0	100	100
52	Lg	50/55 (91%)	49 (98%)	1 (2%)	0	100	100
53	Lh	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	Li	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
55	Lj	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
56	EF	702/704 (100%)	664 (95%)	38 (5%)	0	100	100
57	Pp	1/3 (33%)	1 (100%)	0	0	100	100
All	All	6575/6927 (95%)	6304 (96%)	270 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	LC	149	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SB	186/199 (94%)	181 (97%)	5 (3%)	39	58
3	SC	172/190 (90%)	162 (94%)	10 (6%)	18	27
4	SD	172/173 (99%)	165 (96%)	7 (4%)	27	41
5	SE	118/126 (94%)	115 (98%)	3 (2%)	42	60
6	SF	92/116 (79%)	86 (94%)	6 (6%)	15	22
7	SG	124/147 (84%)	100 (81%)	24 (19%)	1	1
8	SH	104/105 (99%)	100 (96%)	4 (4%)	29	44
9	SI	105/107 (98%)	95 (90%)	10 (10%)	8	9
10	SJ	87/90 (97%)	75 (86%)	12 (14%)	3	3
11	SK	92/99 (93%)	88 (96%)	4 (4%)	26	39
12	SL	102/103 (99%)	96 (94%)	6 (6%)	18	27
13	SM	92/96 (96%)	78 (85%)	14 (15%)	3	2
14	SN	83/84 (99%)	74 (89%)	9 (11%)	6	7
15	SO	76/77 (99%)	70 (92%)	6 (8%)	11	16
16	SP	65/65 (100%)	63 (97%)	2 (3%)	35	53
17	SQ	74/78 (95%)	69 (93%)	5 (7%)	14	20
18	SR	58/65 (89%)	54 (93%)	4 (7%)	14	20
19	SS	72/79 (91%)	56 (78%)	16 (22%)	1	1
20	ST	65/66 (98%)	59 (91%)	6 (9%)	8	10
21	SU	60/61 (98%)	57 (95%)	3 (5%)	22	33
25	LB	216/218 (99%)	208 (96%)	8 (4%)	30	45
26	LC	164/164 (100%)	161 (98%)	3 (2%)	51	70
27	LD	165/165 (100%)	161 (98%)	4 (2%)	43	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	LE	148/150 (99%)	133 (90%)	15 (10%)	7	8
29	LF	137/138 (99%)	132 (96%)	5 (4%)	31	46
30	LI	113/114 (99%)	104 (92%)	9 (8%)	11	15
31	LJ	100/123 (81%)	86 (86%)	14 (14%)	3	3
32	LK	104/110 (94%)	85 (82%)	19 (18%)	2	1
33	LM	116/116 (100%)	114 (98%)	2 (2%)	53	72
34	LN	103/104 (99%)	99 (96%)	4 (4%)	28	43
35	LO	103/103 (100%)	96 (93%)	7 (7%)	14	20
36	LP	108/108 (100%)	103 (95%)	5 (5%)	24	36
37	LQ	100/103 (97%)	98 (98%)	2 (2%)	48	67
38	LR	86/87 (99%)	78 (91%)	8 (9%)	8	10
39	LS	99/100 (99%)	96 (97%)	3 (3%)	36	53
40	LT	89/90 (99%)	88 (99%)	1 (1%)	65	79
41	LU	84/84 (100%)	81 (96%)	3 (4%)	31	46
42	LV	93/93 (100%)	89 (96%)	4 (4%)	26	39
43	LW	80/84 (95%)	78 (98%)	2 (2%)	42	60
44	LX	83/85 (98%)	78 (94%)	5 (6%)	17	26
45	LY	78/78 (100%)	77 (99%)	1 (1%)	61	76
46	La	58/63 (92%)	54 (93%)	4 (7%)	14	20
47	Lb	67/68 (98%)	66 (98%)	1 (2%)	57	74
48	Lc	54/55 (98%)	53 (98%)	1 (2%)	50	69
49	Ld	48/49 (98%)	44 (92%)	4 (8%)	10	14
50	Le	60/62 (97%)	50 (83%)	10 (17%)	2	2
51	Lf	47/48 (98%)	46 (98%)	1 (2%)	47	66
52	Lg	47/49 (96%)	42 (89%)	5 (11%)	6	7
53	Lh	38/38 (100%)	36 (95%)	2 (5%)	20	31
54	Li	51/52 (98%)	51 (100%)	0	100	100
55	Lj	34/34 (100%)	32 (94%)	2 (6%)	18	27
56	EF	561/578 (97%)	520 (93%)	41 (7%)	13	18
57	Pp	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	5436/5642 (96%)	5084 (94%)	352 (6%)	17	22

All (352) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	105	LYS
2	SB	108	ARG
2	SB	123	ASP
2	SB	138	THR
2	SB	161	LEU
3	SC	20	SER
3	SC	43	LEU
3	SC	63	SER
3	SC	115	LEU
3	SC	118	ASP
3	SC	127	ARG
3	SC	135	LYS
3	SC	162	ILE
3	SC	192	THR
3	SC	211	MET
4	SD	45	LYS
4	SD	69	GLU
4	SD	73	ARG
4	SD	78	GLU
4	SD	124	MET
4	SD	152	GLN
4	SD	167	LYS
5	SE	19	ASN
5	SE	161	VAL
5	SE	164	ILE
6	SF	1	MET
6	SF	2	ARG
6	SF	41	ASP
6	SF	53	LYS
6	SF	68	GLN
6	SF	97	THR
7	SG	4	ARG
7	SG	15	ASP
7	SG	21	GLU
7	SG	22	LEU
7	SG	53	ARG
7	SG	56	LYS
7	SG	58	GLU
7	SG	60	GLU
7	SG	62	PHE
7	SG	63	GLU
7	SG	75	VAL

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Mol	Chain	Res	Type
7	SG	84	THR
7	SG	85	TYR
7	SG	89	VAL
7	SG	90	GLU
7	SG	92	ARG
7	SG	99	LEU
7	SG	110	LYS
7	SG	111	ARG
7	SG	113	ASP
7	SG	114	LYS
7	SG	119	ARG
7	SG	146	GLU
7	SG	149	LYS
8	SH	54	ASP
8	SH	60	GLU
8	SH	114	ARG
8	SH	118	GLN
9	SI	9	THR
9	SI	19	VAL
9	SI	46	MET
9	SI	47	VAL
9	SI	57	MET
9	SI	61	LEU
9	SI	65	ILE
9	SI	85	ARG
9	SI	98	LEU
9	SI	107	ASP
10	SJ	15	HIS
10	SJ	18	ILE
10	SJ	22	THR
10	SJ	30	LYS
10	SJ	51	VAL
10	SJ	52	LEU
10	SJ	62	ARG
10	SJ	78	GLU
10	SJ	80	THR
10	SJ	81	GLU
10	SJ	88	MET
10	SJ	90	LEU
11	SK	13	ARG
11	SK	42	LEU
11	SK	57	LYS

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Mol	Chain	Res	Type
11	SK	59	THR
12	SL	6	GLN
12	SL	19	SER
12	SL	21	VAL
12	SL	40	THR
12	SL	76	GLU
12	SL	123	LYS
13	SM	7	ILE
13	SM	8	ASN
13	SM	9	ILE
13	SM	16	VAL
13	SM	41	GLU
13	SM	69	LEU
13	SM	73	ILE
13	SM	74	SER
13	SM	79	ARG
13	SM	83	LEU
13	SM	97	VAL
13	SM	98	ARG
13	SM	113	ARG
13	SM	114	LYS
14	SN	10	GLU
14	SN	19	LYS
14	SN	23	LYS
14	SN	38	ASP
14	SN	48	LEU
14	SN	51	LEU
14	SN	81	ARG
14	SN	86	GLU
14	SN	89	MET
15	SO	11	ILE
15	SO	18	ASP
15	SO	40	GLN
15	SO	84	ARG
15	SO	88	ARG
15	SO	89	ARG
16	SP	50	THR
16	SP	76	LYS
17	SQ	7	THR
17	SQ	75	LEU
17	SQ	77	ARG
17	SQ	81	LYS

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Mol	Chain	Res	Type
17	SQ	83	VAL
18	SR	10	PHE
18	SR	14	THR
18	SR	43	ARG
18	SR	74	HIS
19	SS	3	ARG
19	SS	11	ILE
19	SS	16	LEU
19	SS	21	LYS
19	SS	23	VAL
19	SS	29	LYS
19	SS	36	ARG
19	SS	40	ILE
19	SS	43	ASN
19	SS	45	ILE
19	SS	60	VAL
19	SS	62	VAL
19	SS	65	GLU
19	SS	67	VAL
19	SS	81	ARG
19	SS	83	HIS
20	ST	4	ILE
20	ST	10	ARG
20	ST	43	ASP
20	ST	52	ASN
20	ST	74	ARG
20	ST	84	ASN
21	SU	5	LYS
21	SU	20	LYS
21	SU	62	ARG
25	LB	34	LEU
25	LB	37	ASN
25	LB	98	ASP
25	LB	133	ARG
25	LB	252	THR
25	LB	259	SER
25	LB	264	ASP
25	LB	268	VAL
26	LC	2	ILE
26	LC	175	LEU
26	LC	197	THR
27	LD	16	GLU

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Mol	Chain	Res	Type
27	LD	49	ARG
27	LD	69	ARG
27	LD	194	LYS
28	LE	4	LEU
28	LE	17	MET
28	LE	44	ILE
28	LE	50	LEU
28	LE	79	ILE
28	LE	98	GLU
28	LE	111	ILE
28	LE	115	ARG
28	LE	117	LEU
28	LE	120	LYS
28	LE	123	ASP
28	LE	153	ASP
28	LE	154	ILE
28	LE	167	ARG
28	LE	175	PHE
29	LF	16	ASP
29	LF	32	GLU
29	LF	56	ASP
29	LF	60	ASP
29	LF	134	LYS
30	LI	4	ILE
30	LI	12	LEU
30	LI	15	LEU
30	LI	40	THR
30	LI	42	LYS
30	LI	44	ILE
30	LI	61	VAL
30	LI	82	SER
30	LI	147	VAL
31	LJ	36	ASP
31	LJ	43	LYS
31	LJ	54	VAL
31	LJ	65	GLU
31	LJ	67	THR
31	LJ	71	CYS
31	LJ	85	SER
31	LJ	87	GLU
31	LJ	95	LEU
31	LJ	98	GLU

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Mol	Chain	Res	Type
31	LJ	116	GLU
31	LJ	117	LEU
31	LJ	122	GLN
31	LJ	126	LEU
32	LK	28	LEU
32	LK	33	VAL
32	LK	35	ILE
32	LK	59	ILE
32	LK	61	VAL
32	LK	79	LEU
32	LK	81	LYS
32	LK	87	LYS
32	LK	90	SER
32	LK	97	LYS
32	LK	98	VAL
32	LK	100	LYS
32	LK	102	SER
32	LK	103	ARG
32	LK	113	LYS
32	LK	121	ASP
32	LK	132	THR
32	LK	139	VAL
32	LK	141	GLU
33	LM	10	THR
33	LM	60	ASP
34	LN	17	ARG
34	LN	86	LEU
34	LN	110	GLU
34	LN	121	GLU
35	LO	42	SER
35	LO	67	THR
35	LO	70	LYS
35	LO	73	ILE
35	LO	89	VAL
35	LO	121	THR
35	LO	143	GLU
36	LP	1	MET
36	LP	6	ARG
36	LP	95	LEU
36	LP	102	LEU
36	LP	123	LYS
37	LQ	57	THR

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Mol	Chain	Res	Type
37	LQ	89	SER
38	LR	33	ARG
38	LR	47	VAL
38	LR	48	LEU
38	LR	63	LYS
38	LR	65	THR
38	LR	87	ILE
38	LR	89	ASP
38	LR	94	ARG
39	LS	2	SER
39	LS	12	GLN
39	LS	37	LYS
40	LT	75	SER
41	LU	51	VAL
41	LU	58	VAL
41	LU	79	ARG
42	LV	65	ASP
42	LV	66	ILE
42	LV	70	LYS
42	LV	101	SER
43	LW	37	ASP
43	LW	48	GLN
44	LX	7	ARG
44	LX	49	VAL
44	LX	68	SER
44	LX	81	ASP
44	LX	98	SER
45	LY	24	ASN
46	La	10	THR
46	La	58	THR
46	La	68	LYS
46	La	81	SER
47	Lb	41	GLU
48	Lc	24	GLU
49	Ld	5	ILE
49	Ld	7	ILE
49	Ld	11	ARG
49	Ld	38	ARG
50	Le	5	ILE
50	Le	25	ARG
50	Le	35	ASP
50	Le	49	ARG

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Mol	Chain	Res	Type
50	Le	50	ASP
50	Le	51	VAL
50	Le	57	VAL
50	Le	58	ASP
50	Le	59	ARG
50	Le	64	PHE
51	Lf	10	ARG
52	Lg	7	GLU
52	Lg	9	ILE
52	Lg	25	LYS
52	Lg	30	LYS
52	Lg	35	GLU
53	Lh	8	SER
53	Lh	14	ARG
55	Lj	26	ILE
55	Lj	34	LYS
56	EF	40	ILE
56	EF	55	GLN
56	EF	78	GLN
56	EF	79	TYR
56	EF	106	LEU
56	EF	161	ARG
56	EF	169	LEU
56	EF	176	GLU
56	EF	178	HIS
56	EF	183	VAL
56	EF	210	ASP
56	EF	219	HIS
56	EF	221	ASN
56	EF	241	GLU
56	EF	243	LEU
56	EF	244	THR
56	EF	262	ILE
56	EF	298	ILE
56	EF	337	ARG
56	EF	352	SER
56	EF	353	VAL
56	EF	373	GLU
56	EF	390	ASP
56	EF	450	ASP
56	EF	457	ILE
56	EF	458	ILE

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Mol	Chain	Res	Type
56	EF	488	VAL
56	EF	496	GLN
56	EF	498	VAL
56	EF	502	GLU
56	EF	507	LYS
56	EF	532	LYS
56	EF	540	ILE
56	EF	561	LEU
56	EF	574	MET
56	EF	583	TYR
56	EF	617	MET
56	EF	626	GLU
56	EF	669	GLN
56	EF	674	THR
56	EF	679	SER
57	Pp	3	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
2	SB	177	ASN
4	SD	85	ASN
4	SD	136	GLN
6	SF	63	ASN
6	SF	68	GLN
7	SG	9	GLN
7	SG	122	ASN
7	SG	148	ASN
9	SI	50	GLN
9	SI	110	GLN
9	SI	126	GLN
10	SJ	20	GLN
11	SK	22	HIS
11	SK	118	HIS
13	SM	14	HIS
14	SN	35	ASN
19	SS	43	ASN
20	ST	68	HIS
20	ST	78	ASN
25	LB	21	ASN
25	LB	25	HIS
25	LB	115	GLN

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Mol	Chain	Res	Type
25	LB	260	ASN
26	LC	150	GLN
26	LC	173	GLN
27	LD	9	GLN
27	LD	92	HIS
27	LD	136	GLN
27	LD	163	ASN
28	LE	63	GLN
29	LF	48	ASN
29	LF	143	GLN
30	LI	18	GLN
30	LI	33	GLN
30	LI	73	ASN
31	LJ	4	ASN
31	LJ	88	HIS
31	LJ	103	ASN
31	LJ	122	GLN
32	LK	31	GLN
32	LK	94	ASN
33	LM	80	HIS
34	LN	3	GLN
34	LN	29	HIS
34	LN	88	ASN
34	LN	93	GLN
36	LP	3	GLN
36	LP	13	HIS
37	LQ	62	ASN
41	LU	12	HIS
42	LV	15	GLN
45	LY	51	GLN
47	Lb	6	GLN
48	Lc	27	ASN
48	Lc	36	GLN
48	Lc	39	GLN
50	Le	6	HIS
50	Le	61	ASN
55	Lj	13	ASN
56	EF	55	GLN
56	EF	78	GLN
56	EF	122	GLN
56	EF	156	ASN
56	EF	259	ASN

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Mol	Chain	Res	Type
56	EF	272	ASN
56	EF	344	ASN
56	EF	454	ASN
56	EF	487	GLN
56	EF	517	HIS
56	EF	530	ASN
56	EF	558	GLN
56	EF	560	GLN
56	EF	645	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1533/1534 (99%)	236 (15%)	10 (0%)
22	mR	11/60 (18%)	2 (18%)	0
23	23	2903/2904 (99%)	524 (18%)	28 (0%)
24	5	119/120 (99%)	16 (13%)	1 (0%)
58	Pt	75/106 (70%)	13 (17%)	0
59	Dt	75/106 (70%)	18 (24%)	0
All	All	4716/4830 (97%)	809 (17%)	39 (0%)

All (809) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	2	A
1	16	4	U
1	16	7	A
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
1	16	51	A
1	16	70	U
1	16	71	A
1	16	72	A
1	16	74	A
1	16	77	A
1	16	78	A

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Mol	Chain	Res	Type
1	16	80	A
1	16	81	A
1	16	83	C
1	16	84	U
1	16	85	U
1	16	86	G
1	16	87	C
1	16	88	U
1	16	89	U
1	16	90	C
1	16	91	U
1	16	97	G
1	16	108	G
1	16	121	U
1	16	130	A
1	16	131	A
1	16	141	G
1	16	143	A
1	16	144	G
1	16	159	G
1	16	163	C
1	16	177	G
1	16	182	A
1	16	183	C
1	16	188	C
1	16	189	A
1	16	197	A
1	16	204	G
1	16	205	A
1	16	206	C
1	16	207	C
1	16	210	C
1	16	215	C
1	16	226	G
1	16	240	G
1	16	247	G
1	16	251	G
1	16	266	G
1	16	267	C
1	16	281	G
1	16	282	A
1	16	289	G

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Mol	Chain	Res	Type
1	16	306	A
1	16	321	A
1	16	328	C
1	16	329	A
1	16	330	C
1	16	332	G
1	16	352	C
1	16	354	G
1	16	356	A
1	16	367	U
1	16	372	C
1	16	376	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	422	C
1	16	423	G
1	16	424	G
1	16	429	U
1	16	439	U
1	16	456	A
1	16	457	G
1	16	458	U
1	16	465	A
1	16	466	A
1	16	467	U
1	16	468	A
1	16	481	G
1	16	484	G
1	16	486	U
1	16	491	G
1	16	495	A
1	16	496	A
1	16	497	G
1	16	509	A
1	16	510	A
1	16	511	C
1	16	518	C
1	16	521	G

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Mol	Chain	Res	Type
1	16	527	7MG
1	16	530	G
1	16	531	U
1	16	533	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	596	A
1	16	632	U
1	16	642	A
1	16	650	G
1	16	653	U
1	16	654	G
1	16	665	A
1	16	666	G
1	16	686	U
1	16	703	G
1	16	721	G
1	16	723	U
1	16	734	G
1	16	755	G
1	16	777	A
1	16	790	A
1	16	793	U
1	16	794	A
1	16	814	A
1	16	815	A
1	16	817	C
1	16	821	G
1	16	828	U
1	16	829	G
1	16	832	G
1	16	836	G
1	16	841	C
1	16	842	U
1	16	843	U
1	16	844	G

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Mol	Chain	Res	Type
1	16	845	A
1	16	846	G
1	16	848	C
1	16	876	C
1	16	902	G
1	16	914	A
1	16	926	G
1	16	927	G
1	16	934	C
1	16	935	A
1	16	958	A
1	16	960	U
1	16	969	A
1	16	971	G
1	16	975	A
1	16	976	G
1	16	977	A
1	16	982	U
1	16	987	G
1	16	992	U
1	16	993	G
1	16	1004	A
1	16	1015	G
1	16	1020	G
1	16	1021	A
1	16	1027	C
1	16	1029	U
1	16	1030	U
1	16	1031	C
1	16	1043	G
1	16	1044	A
1	16	1055	A
1	16	1064	G
1	16	1065	U
1	16	1070	U
1	16	1085	U
1	16	1091	U
1	16	1092	A
1	16	1094	G
1	16	1095	U
1	16	1101	A
1	16	1108	G

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Mol	Chain	Res	Type
1	16	1136	C
1	16	1139	G
1	16	1152	A
1	16	1154	G
1	16	1157	A
1	16	1158	C
1	16	1159	U
1	16	1167	A
1	16	1168	U
1	16	1184	G
1	16	1196	A
1	16	1197	A
1	16	1200	C
1	16	1213	A
1	16	1214	C
1	16	1225	A
1	16	1226	C
1	16	1227	A
1	16	1236	A
1	16	1238	A
1	16	1241	G
1	16	1257	A
1	16	1258	G
1	16	1260	G
1	16	1280	A
1	16	1281	C
1	16	1285	A
1	16	1286	U
1	16	1287	A
1	16	1298	U
1	16	1299	A
1	16	1302	C
1	16	1305	G
1	16	1320	C
1	16	1363	A
1	16	1364	U
1	16	1379	G
1	16	1381	U
1	16	1383	C
1	16	1397	C
1	16	1398	A
1	16	1441	A

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Mol	Chain	Res	Type
1	16	1446	A
1	16	1449	C
1	16	1499	A
1	16	1503	A
1	16	1506	U
1	16	1517	G
1	16	1519	MA6
1	16	1529	G
1	16	1530	G
22	mR	39	G
22	mR	48	C
23	23	3	U
23	23	6	A
23	23	10	A
23	23	14	A
23	23	15	G
23	23	27	G
23	23	44	A
23	23	46	G
23	23	51	G
23	23	55	G
23	23	71	A
23	23	74	A
23	23	75	G
23	23	84	A
23	23	96	C
23	23	101	A
23	23	102	U
23	23	103	A
23	23	110	G
23	23	112	U
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	140	C
23	23	141	G
23	23	142	A
23	23	159	G
23	23	163	C

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Mol	Chain	Res	Type
23	23	174	U
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	222	A
23	23	248	G
23	23	252	G
23	23	265	A
23	23	266	G
23	23	267	C
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	281	C
23	23	282	A
23	23	283	G
23	23	284	U
23	23	285	G
23	23	286	U
23	23	291	G
23	23	311	A
23	23	330	A
23	23	345	A
23	23	353	C
23	23	359	G
23	23	360	U
23	23	361	G
23	23	369	U
23	23	370	G
23	23	371	A
23	23	372	G
23	23	386	G
23	23	387	U
23	23	388	G
23	23	395	U
23	23	396	G

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Mol	Chain	Res	Type
23	23	401	A
23	23	404	A
23	23	405	U
23	23	406	G
23	23	412	A
23	23	455	C
23	23	456	C
23	23	457	A
23	23	459	U
23	23	467	G
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	529	A
23	23	530	G
23	23	531	C
23	23	532	A
23	23	546	U
23	23	547	A
23	23	548	G
23	23	549	G
23	23	550	C
23	23	563	A
23	23	573	U
23	23	575	A
23	23	603	A
23	23	614	A
23	23	615	U
23	23	637	A
23	23	645	C
23	23	646	U
23	23	647	G
23	23	654	A
23	23	655	A
23	23	684	G
23	23	686	U

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Mol	Chain	Res	Type
23	23	704	G
23	23	719	C
23	23	724	U
23	23	725	G
23	23	726	G
23	23	727	A
23	23	730	A
23	23	740	C
23	23	747	5MU
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	811	U
23	23	812	C
23	23	819	A
23	23	827	U
23	23	830	G
23	23	845	A
23	23	846	U
23	23	859	G
23	23	869	G
23	23	888	C
23	23	889	C
23	23	890	C
23	23	895	U
23	23	896	A
23	23	897	C
23	23	907	G
23	23	910	A
23	23	917	A
23	23	931	U
23	23	932	U
23	23	934	U
23	23	941	A
23	23	946	C
23	23	953	G
23	23	961	C

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Mol	Chain	Res	Type
23	23	973	A
23	23	974	G
23	23	980	A
23	23	983	A
23	23	989	G
23	23	996	A
23	23	999	U
23	23	1009	A
23	23	1012	U
23	23	1013	C
23	23	1026	G
23	23	1033	U
23	23	1041	G
23	23	1046	A
23	23	1047	G
23	23	1057	A
23	23	1058	U
23	23	1060	U
23	23	1061	U
23	23	1062	G
23	23	1070	A
23	23	1077	A
23	23	1079	C
23	23	1080	A
23	23	1084	A
23	23	1085	A
23	23	1087	G
23	23	1088	A
23	23	1089	A
23	23	1090	A
23	23	1110	G
23	23	1112	G
23	23	1114	C
23	23	1116	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	1170	C

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Mol	Chain	Res	Type
23	23	1171	G
23	23	1173	U
23	23	1174	U
23	23	1175	A
23	23	1178	C
23	23	1179	G
23	23	1180	U
23	23	1206	G
23	23	1212	G
23	23	1236	G
23	23	1238	G
23	23	1247	A
23	23	1249	U
23	23	1253	A
23	23	1256	G
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	1314	C
23	23	1321	A
23	23	1329	U
23	23	1352	U
23	23	1365	A
23	23	1368	G
23	23	1378	A
23	23	1379	U
23	23	1382	G
23	23	1383	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	1437	C
23	23	1451	C
23	23	1452	G

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Mol	Chain	Res	Type
23	23	1453	A
23	23	1458	U
23	23	1460	U
23	23	1461	C
23	23	1482	G
23	23	1486	U
23	23	1493	C
23	23	1494	A
23	23	1497	U
23	23	1502	A
23	23	1503	A
23	23	1509	A
23	23	1524	G
23	23	1529	G
23	23	1534	U
23	23	1535	A
23	23	1537	G
23	23	1538	G
23	23	1558	C
23	23	1566	A
23	23	1569	A
23	23	1570	A
23	23	1571	A
23	23	1578	U
23	23	1579	A
23	23	1580	A
23	23	1581	G
23	23	1583	A
23	23	1584	U
23	23	1585	C
23	23	1603	A
23	23	1608	A
23	23	1610	A
23	23	1618	6MZ
23	23	1619	G
23	23	1646	C
23	23	1647	U
23	23	1648	U
23	23	1649	G
23	23	1674	G
23	23	1690	A
23	23	1715	G

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Mol	Chain	Res	Type
23	23	1724	G
23	23	1725	U
23	23	1727	C
23	23	1729	U
23	23	1730	C
23	23	1731	G
23	23	1732	C
23	23	1737	G
23	23	1738	G
23	23	1745	A
23	23	1757	A
23	23	1764	C
23	23	1773	A
23	23	1776	G
23	23	1782	U
23	23	1784	A
23	23	1799	G
23	23	1800	C
23	23	1801	A
23	23	1807	G
23	23	1808	A
23	23	1816	C
23	23	1829	A
23	23	1833	C
23	23	1841	U
23	23	1842	G
23	23	1847	A
23	23	1848	A
23	23	1858	A
23	23	1864	U
23	23	1866	A
23	23	1867	G
23	23	1868	C
23	23	1870	C
23	23	1872	A
23	23	1873	G
23	23	1874	C
23	23	1875	G
23	23	1876	A
23	23	1877	A
23	23	1901	A
23	23	1906	G

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Mol	Chain	Res	Type
23	23	1912	A
23	23	1913	A
23	23	1914	C
23	23	1919	A
23	23	1925	C
23	23	1927	A
23	23	1930	G
23	23	1931	U
23	23	1938	A
23	23	1940	U
23	23	1941	C
23	23	1954	G
23	23	1955	U
23	23	1960	A
23	23	1964	G
23	23	1967	C
23	23	1970	A
23	23	1971	U
23	23	1972	G
23	23	1975	G
23	23	1980	G
23	23	1981	A
23	23	1982	U
23	23	1991	U
23	23	1992	G
23	23	1993	U
23	23	1997	C
23	23	2002	G
23	23	2020	A
23	23	2022	U
23	23	2023	C
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	7MG
23	23	2093	G

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Mol	Chain	Res	Type
23	23	2113	U
23	23	2116	G
23	23	2117	A
23	23	2118	U
23	23	2126	A
23	23	2131	U
23	23	2132	U
23	23	2133	G
23	23	2136	G
23	23	2141	G
23	23	2145	C
23	23	2146	C
23	23	2161	C
23	23	2162	G
23	23	2163	A
23	23	2164	C
23	23	2165	C
23	23	2170	A
23	23	2171	A
23	23	2172	U
23	23	2173	A
23	23	2174	C
23	23	2198	A
23	23	2204	G
23	23	2211	A
23	23	2220	U
23	23	2225	A
23	23	2238	G
23	23	2239	G
23	23	2243	U
23	23	2251	OMG
23	23	2278	A
23	23	2283	C
23	23	2287	A
23	23	2288	A
23	23	2303	G
23	23	2304	G
23	23	2305	U
23	23	2306	C
23	23	2307	G
23	23	2308	G
23	23	2309	A

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Mol	Chain	Res	Type
23	23	2311	A
23	23	2312	U
23	23	2319	G
23	23	2320	U
23	23	2321	U
23	23	2322	A
23	23	2325	G
23	23	2333	A
23	23	2334	U
23	23	2336	A
23	23	2347	C
23	23	2350	C
23	23	2354	C
23	23	2357	G
23	23	2361	G
23	23	2372	U
23	23	2376	A
23	23	2379	G
23	23	2380	C
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	2407	A
23	23	2410	G
23	23	2423	U
23	23	2425	A
23	23	2427	C
23	23	2428	G
23	23	2429	G
23	23	2430	A
23	23	2441	U
23	23	2448	A
23	23	2474	U
23	23	2475	C
23	23	2476	A
23	23	2480	C
23	23	2484	G
23	23	2491	U
23	23	2492	U

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Mol	Chain	Res	Type
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
23	23	2566	A
23	23	2567	G
23	23	2572	A
23	23	2573	C
23	23	2576	G
23	23	2602	A
23	23	2606	C
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	2636	C
23	23	2639	A
23	23	2646	C
23	23	2663	G
23	23	2689	U
23	23	2690	U
23	23	2714	G
23	23	2718	G
23	23	2726	A
23	23	2732	G
23	23	2733	A
23	23	2739	U
23	23	2744	G
23	23	2748	A
23	23	2752	C
23	23	2762	C
23	23	2765	A

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Mol	Chain	Res	Type
23	23	2777	G
23	23	2778	A
23	23	2779	U
23	23	2790	U
23	23	2791	G
23	23	2797	U
23	23	2798	U
23	23	2799	A
23	23	2818	U
23	23	2820	A
23	23	2823	A
23	23	2832	U
23	23	2833	U
23	23	2835	A
23	23	2849	U
23	23	2850	A
23	23	2858	C
23	23	2859	G
23	23	2861	U
23	23	2872	A
23	23	2873	A
23	23	2879	A
23	23	2880	C
23	23	2883	A
23	23	2884	U
23	23	2885	G
23	23	2886	A
23	23	2891	U
23	23	2900	A
23	23	2901	C
23	23	2904	U
24	5	13	G
24	5	15	A
24	5	16	G
24	5	24	G
24	5	31	C
24	5	35	C
24	5	36	C
24	5	41	G
24	5	51	G
24	5	67	G
24	5	87	U

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Mol	Chain	Res	Type
24	5	88	C
24	5	89	U
24	5	90	C
24	5	99	A
24	5	109	A
58	Pt	4	U
58	Pt	16	U
58	Pt	17	U
58	Pt	19	G
58	Pt	27	G
58	Pt	28	U
58	Pt	29	U
58	Pt	46	7MG
58	Pt	47	3AU
58	Pt	48	C
58	Pt	50	C
58	Pt	70	C
58	Pt	76	A
59	Dt	7	A
59	Dt	8	4SU
59	Dt	14	A
59	Dt	16	U
59	Dt	17	U
59	Dt	18	G
59	Dt	20	G
59	Dt	21	A
59	Dt	22	G
59	Dt	37	MIA
59	Dt	44	G
59	Dt	46	7MG
59	Dt	47	3AU
59	Dt	48	C
59	Dt	49	C
59	Dt	69	G
59	Dt	73	A
59	Dt	76	A

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	16	250	A
1	16	251	G

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Mol	Chain	Res	Type
1	16	281	G
1	16	496	A
1	16	532	A
1	16	653	U
1	16	845	A
1	16	1157	A
1	16	1183	U
1	16	1397	C
23	23	43	G
23	23	134	G
23	23	158	U
23	23	277	G
23	23	352	A
23	23	369	U
23	23	395	U
23	23	404	A
23	23	405	U
23	23	784	G
23	23	1057	A
23	23	1060	U
23	23	1088	A
23	23	1089	A
23	23	1266	G
23	23	1416	G
23	23	1452	G
23	23	1486	U
23	23	1508	A
23	23	1570	A
23	23	1876	A
23	23	1980	G
23	23	2145	C
23	23	2311	A
23	23	2468	A
23	23	2536	G
23	23	2585	U
23	23	2858	C
24	5	15	A

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

47 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$
36	4D4	LP	81	36	9,11,12	2.57	3 (33%)	7,13,15	0.93	0
23	PSU	23	2457	23	18,21,22	4.17	8 (44%)	21,30,33	2.33	5 (23%)
23	OMG	23	2251	23,58	23,26,27	2.29	9 (39%)	32,38,41	1.94	8 (25%)
23	PSU	23	2604	23	18,21,22	4.13	7 (38%)	21,30,33	2.10	5 (23%)
59	4SU	Dt	8	59	18,21,22	4.29	8 (44%)	25,30,33	2.40	5 (20%)
23	PSU	23	746	62,23	18,21,22	4.21	7 (38%)	21,30,33	1.84	5 (23%)
58	T6A	Pt	37	58	31,34,35	1.76	7 (22%)	43,49,52	2.28	12 (27%)
23	5MU	23	747	23	19,22,23	4.78	7 (36%)	27,32,35	3.72	10 (37%)
1	7MG	16	527	1	23,26,27	1.37	3 (13%)	27,39,42	2.65	7 (25%)
23	6MZ	23	1618	23	22,25,26	2.40	5 (22%)	29,36,39	3.19	11 (37%)
59	3AU	Dt	47	59	24,28,29	1.06	1 (4%)	30,40,43	1.58	3 (10%)
23	6MZ	23	2030	23	22,25,26	2.58	6 (27%)	29,36,39	3.25	12 (41%)
23	2MG	23	2445	23	23,26,27	2.72	8 (34%)	33,38,41	2.33	11 (33%)
59	PSU	Dt	39	59	18,21,22	4.27	7 (38%)	21,30,33	2.06	5 (23%)
1	2MG	16	1516	1	23,26,27	2.80	9 (39%)	33,38,41	2.30	13 (39%)
58	U8U	Pt	34	22,58	20,24,25	1.63	4 (20%)	22,34,37	1.12	4 (18%)
59	PSU	Dt	32	59	18,21,22	4.29	7 (38%)	21,30,33	2.07	5 (23%)
23	3TD	23	1915	23	19,22,23	4.34	6 (31%)	23,32,35	1.87	3 (13%)
23	5MC	23	1962	23	19,22,23	3.64	8 (42%)	26,32,35	0.97	1 (3%)
58	7MG	Pt	46	58	23,26,27	3.53	10 (43%)	27,39,42	2.25	9 (33%)
23	OMU	23	2552	23	19,22,23	2.88	8 (42%)	25,31,34	2.02	5 (20%)
23	OMC	23	2498	62,23	19,22,23	2.84	8 (42%)	25,31,34	0.79	0
12	D2T	SL	89	12	8,9,10	2.40	1 (12%)	6,11,13	2.29	2 (33%)
1	5MC	16	967	1	19,22,23	3.66	8 (42%)	26,32,35	1.01	1 (3%)
23	H2U	23	2449	23	18,21,22	2.93	5 (27%)	19,30,33	1.53	4 (21%)
23	1MG	23	745	23	23,26,27	3.13	8 (34%)	33,39,42	2.32	8 (24%)
59	7MG	Dt	46	59	23,26,27	3.43	10 (43%)	27,39,42	2.14	9 (33%)
1	MA6	16	1519	1	23,26,27	1.66	4 (17%)	33,38,41	2.47	12 (36%)
23	PSU	23	1911	23	18,21,22	4.21	8 (44%)	21,30,33	1.89	4 (19%)

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	4.17	7 (38%)	21,30,33	2.00	5 (23%)
59	PSU	Dt	55	59	18,21,22	4.43	7 (38%)	21,30,33	2.09	5 (23%)
1	MA6	16	1518	1	23,26,27	1.48	4 (17%)	33,38,41	3.20	11 (33%)
1	UR3	16	1498	1	19,22,23	2.75	7 (36%)	26,32,35	1.61	3 (11%)
23	PSU	23	2605	23	18,21,22	4.20	8 (44%)	21,30,33	2.05	5 (23%)
1	5MC	16	1407	1	19,22,23	3.66	8 (42%)	26,32,35	1.03	2 (7%)
58	3AU	Pt	47	58	24,28,29	1.02	1 (4%)	30,40,43	1.51	4 (13%)
1	2MG	16	966	1	23,26,27	2.78	9 (39%)	33,38,41	2.21	10 (30%)
23	5MU	23	1939	23	19,22,23	4.78	7 (36%)	27,32,35	3.81	9 (33%)
23	2MA	23	2503	62,23	22,25,26	3.79	11 (50%)	32,37,40	2.63	10 (31%)
23	PSU	23	2580	23	18,21,22	4.19	8 (44%)	21,30,33	2.11	6 (28%)
58	PSU	Pt	39	58	18,21,22	4.32	7 (38%)	21,30,33	2.09	5 (23%)
1	4OC	16	1402	62,1	20,23,24	3.01	8 (40%)	25,32,35	0.93	1 (4%)
23	PSU	23	955	23	18,21,22	4.16	7 (38%)	21,30,33	2.19	5 (23%)
23	7MG	23	2069	23	23,26,27	1.38	3 (13%)	27,39,42	2.67	6 (22%)
23	2MG	23	1835	23	23,26,27	2.74	8 (34%)	33,38,41	2.35	11 (33%)
1	PSU	16	516	1	18,21,22	4.23	7 (38%)	21,30,33	1.92	5 (23%)
59	MIA	Dt	37	59	28,31,32	2.35	6 (21%)	38,44,47	2.92	15 (39%)

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
36	4D4	LP	81	36	-	1/11/12/14	-
23	PSU	23	2457	23	-	0/7/25/26	0/2/2/2
23	OMG	23	2251	23,58	-	3/9/27/28	0/3/3/3
23	PSU	23	2604	23	-	0/7/25/26	0/2/2/2
59	4SU	Dt	8	59	-	0/7/25/26	0/2/2/2
23	PSU	23	746	62,23	-	2/7/25/26	0/2/2/2
58	T6A	Pt	37	58	-	10/23/41/42	0/3/3/3
23	5MU	23	747	23	-	1/7/25/26	0/2/2/2
1	7MG	16	527	1	-	3/7/37/38	0/3/3/3
23	6MZ	23	1618	23	-	4/9/27/28	0/3/3/3
59	3AU	Dt	47	59	-	9/16/34/35	0/2/2/2
23	6MZ	23	2030	23	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	2MG	23	2445	23	-	0/9/27/28	0/3/3/3
59	PSU	Dt	39	59	-	0/7/25/26	0/2/2/2
1	2MG	16	1516	1	-	0/9/27/28	0/3/3/3
58	U8U	Pt	34	22,58	-	2/10/28/29	0/2/2/2
59	PSU	Dt	32	59	-	0/7/25/26	0/2/2/2
23	3TD	23	1915	23	-	2/7/25/26	0/2/2/2
23	5MC	23	1962	23	-	2/7/25/26	0/2/2/2
58	7MG	Pt	46	58	-	4/7/37/38	0/3/3/3
23	OMU	23	2552	23	-	0/9/27/28	0/2/2/2
23	OMC	23	2498	62,23	-	2/9/27/28	0/2/2/2
12	D2T	SL	89	12	-	1/7/12/14	-
1	5MC	16	967	1	-	0/7/25/26	0/2/2/2
23	H2U	23	2449	23	-	1/7/38/39	0/2/2/2
23	1MG	23	745	23	-	0/7/25/26	0/3/3/3
59	7MG	Dt	46	59	-	2/7/37/38	0/3/3/3
1	MA6	16	1519	1	-	6/11/29/30	0/3/3/3
23	PSU	23	1911	23	-	2/7/25/26	0/2/2/2
23	PSU	23	2504	23	-	0/7/25/26	0/2/2/2
59	PSU	Dt	55	59	-	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	-	2/7/25/26	0/2/2/2
23	PSU	23	2605	23	-	0/7/25/26	0/2/2/2
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
58	3AU	Pt	47	58	-	10/16/34/35	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	2MA	23	2503	62,23	-	2/7/25/26	0/3/3/3
23	PSU	23	2580	23	-	1/7/25/26	0/2/2/2
58	PSU	Pt	39	58	-	0/7/25/26	0/2/2/2
1	4OC	16	1402	62,1	-	1/9/29/30	0/2/2/2
23	PSU	23	955	23	-	0/7/25/26	0/2/2/2
23	7MG	23	2069	23	-	0/7/37/38	0/3/3/3
23	2MG	23	1835	23	-	2/9/27/28	0/3/3/3
1	PSU	16	516	1	-	0/7/25/26	0/2/2/2
59	MIA	Dt	37	59	-	6/15/33/34	0/3/3/3

All (313) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	1915	3TD	C6-C5	13.19	1.49	1.35
59	Dt	55	PSU	C6-C5	11.60	1.48	1.35
58	Pt	39	PSU	C6-C5	11.39	1.47	1.35
23	23	2503	2MA	C4-N3	11.38	1.49	1.34
59	Dt	39	PSU	C6-C5	11.24	1.47	1.35
59	Dt	32	PSU	C6-C5	11.24	1.47	1.35
23	23	2504	PSU	C6-C5	11.14	1.47	1.35
23	23	1911	PSU	C6-C5	11.12	1.47	1.35
23	23	2605	PSU	C6-C5	11.07	1.47	1.35
1	16	516	PSU	C6-C5	11.06	1.47	1.35
23	23	2457	PSU	C6-C5	11.04	1.47	1.35
23	23	2580	PSU	C6-C5	11.04	1.47	1.35
23	23	746	PSU	C6-C5	10.87	1.47	1.35
23	23	955	PSU	C6-C5	10.84	1.47	1.35
23	23	2604	PSU	C6-C5	10.74	1.47	1.35
23	23	747	5MU	C2-N1	10.72	1.55	1.38
23	23	1939	5MU	C2-N1	10.67	1.55	1.38
23	23	747	5MU	C6-N1	10.45	1.55	1.38
23	23	1939	5MU	C6-N1	10.38	1.55	1.38
23	23	1915	3TD	C2-N1	10.34	1.49	1.37
59	Dt	55	PSU	C2-N1	10.07	1.49	1.36
59	Dt	32	PSU	C2-N1	9.74	1.49	1.36
23	23	747	5MU	C4-C5	9.70	1.60	1.44
58	Pt	39	PSU	C2-N1	9.68	1.49	1.36
23	23	1939	5MU	C4-C5	9.63	1.60	1.44
23	23	2030	6MZ	C6-N6	9.57	1.45	1.34
23	23	746	PSU	C2-N1	9.54	1.49	1.36
59	Dt	39	PSU	C2-N1	9.52	1.49	1.36
23	23	955	PSU	C2-N1	9.50	1.49	1.36
23	23	2605	PSU	C2-N1	9.37	1.48	1.36
23	23	1911	PSU	C2-N1	9.36	1.48	1.36
1	16	516	PSU	C2-N1	9.36	1.48	1.36
23	23	2604	PSU	C2-N1	9.31	1.48	1.36
23	23	2457	PSU	C2-N1	9.28	1.48	1.36
23	23	1618	6MZ	C6-N6	9.26	1.44	1.34
23	23	2580	PSU	C2-N1	9.23	1.48	1.36
23	23	2504	PSU	C2-N1	9.08	1.48	1.36
59	Dt	8	4SU	C2-N1	9.04	1.52	1.38
1	16	1407	5MC	C6-C5	8.86	1.49	1.34
1	16	967	5MC	C6-C5	8.85	1.49	1.34
23	23	2449	H2U	C2-N1	8.79	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	1962	5MC	C6-C5	8.77	1.48	1.34
23	23	745	1MG	C2-N2	8.64	1.49	1.34
58	Pt	46	7MG	C8-N9	8.48	1.51	1.45
59	Dt	8	4SU	C4-N3	8.39	1.46	1.37
59	Dt	46	7MG	C8-N9	7.86	1.51	1.45
23	23	1939	5MU	C4-N3	-7.73	1.24	1.38
59	Dt	55	PSU	C2-N3	7.66	1.50	1.37
23	23	747	5MU	C4-N3	-7.63	1.24	1.38
1	16	516	PSU	C2-N3	7.51	1.49	1.37
59	Dt	37	MIA	C2-S10	-7.47	1.69	1.75
59	Dt	39	PSU	C2-N3	7.43	1.49	1.37
58	Pt	39	PSU	C2-N3	7.42	1.49	1.37
59	Dt	8	4SU	C5-C4	7.26	1.51	1.42
1	16	966	2MG	C2-N3	7.26	1.45	1.32
23	23	746	PSU	C2-N3	7.25	1.49	1.37
59	Dt	32	PSU	C2-N3	7.24	1.49	1.37
23	23	2504	PSU	C2-N3	7.17	1.49	1.37
1	16	1516	2MG	C2-N3	7.17	1.45	1.32
23	23	1835	2MG	C2-N3	7.13	1.45	1.32
23	23	2580	PSU	C2-N3	7.12	1.49	1.37
23	23	2604	PSU	C2-N3	7.10	1.49	1.37
23	23	2605	PSU	C2-N3	7.07	1.49	1.37
23	23	2457	PSU	C2-N3	7.03	1.49	1.37
23	23	955	PSU	C2-N3	7.02	1.49	1.37
23	23	1911	PSU	C2-N3	6.95	1.48	1.37
23	23	2445	2MG	C2-N3	6.89	1.45	1.32
59	Dt	46	7MG	C5-N7	6.85	1.44	1.35
23	23	2503	2MA	C2-N3	6.78	1.45	1.34
59	Dt	37	MIA	C13-C14	6.76	1.52	1.32
59	Dt	8	4SU	C2-N3	6.68	1.49	1.38
58	Pt	46	7MG	C5-N7	6.67	1.44	1.35
1	16	1402	4OC	C4-N3	6.63	1.43	1.32
1	16	1498	UR3	C2-N1	6.55	1.47	1.38
23	23	2503	2MA	C6-N1	6.55	1.43	1.35
1	16	967	5MC	C4-N3	6.52	1.44	1.34
1	16	1498	UR3	C6-C5	6.51	1.50	1.35
23	23	2552	OMU	C2-N1	6.48	1.48	1.38
1	16	1407	5MC	C4-N3	6.48	1.44	1.34
23	23	1962	5MC	C4-N3	6.47	1.44	1.34
23	23	2552	OMU	C2-N3	6.36	1.49	1.38
59	Dt	8	4SU	C6-C5	6.32	1.49	1.35
1	16	1516	2MG	C4-N3	6.30	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	966	2MG	C4-N3	6.29	1.48	1.34
23	23	745	1MG	C2-N3	6.25	1.43	1.33
23	23	1835	2MG	C4-N3	6.19	1.48	1.34
23	23	1939	5MU	C6-C5	6.18	1.44	1.34
12	SL	89	D2T	CB-CA	-6.16	1.52	1.54
23	23	747	5MU	C6-C5	6.15	1.44	1.34
23	23	1962	5MC	C5-C4	6.14	1.48	1.44
1	16	1402	4OC	C6-C5	6.08	1.49	1.35
1	16	967	5MC	C5-C4	6.07	1.48	1.44
23	23	2445	2MG	C4-N3	6.06	1.48	1.34
23	23	2251	OMG	C4-N3	6.02	1.48	1.34
23	23	2498	OMC	C2-N3	6.01	1.48	1.36
23	23	745	1MG	C4-N3	6.00	1.48	1.34
1	16	1407	5MC	C2-N3	5.98	1.48	1.36
1	16	967	5MC	C2-N3	5.95	1.48	1.36
23	23	2449	H2U	C2-N3	5.95	1.48	1.38
58	Pt	46	7MG	C2-N3	5.94	1.47	1.33
1	16	1407	5MC	C5-C4	5.91	1.48	1.44
36	LP	81	4D4	CZ-NE	5.86	1.44	1.33
23	23	1962	5MC	C2-N3	5.83	1.47	1.36
1	16	1402	4OC	C2-N3	5.80	1.47	1.36
23	23	2503	2MA	C2-N1	5.76	1.43	1.34
59	Dt	46	7MG	C2-N3	5.74	1.47	1.33
58	Pt	46	7MG	C4-N3	5.73	1.47	1.34
23	23	2498	OMC	C6-C5	5.65	1.48	1.35
23	23	1915	3TD	C6-N1	5.58	1.45	1.36
59	Dt	46	7MG	C4-N3	5.56	1.47	1.34
1	16	1516	2MG	C2-N2	5.54	1.45	1.33
1	16	966	2MG	C2-N2	5.46	1.44	1.33
23	23	2552	OMU	C6-C5	5.39	1.47	1.35
59	Dt	55	PSU	C6-N1	5.22	1.44	1.36
23	23	1835	2MG	C2-N2	5.22	1.44	1.33
1	16	1498	UR3	C2-N3	5.21	1.49	1.39
23	23	2445	2MG	C2-N2	5.19	1.44	1.33
59	Dt	8	4SU	C4-S4	-5.14	1.59	1.68
58	Pt	34	U8U	C2-S2	-5.12	1.59	1.67
23	23	2251	OMG	C2-N3	5.10	1.45	1.33
58	Pt	46	7MG	C4-N9	5.08	1.44	1.37
58	Pt	39	PSU	C6-N1	5.04	1.44	1.36
59	Dt	32	PSU	C6-N1	5.03	1.44	1.36
1	16	1519	MA6	C5-C4	5.01	1.48	1.39
23	23	746	PSU	C6-N1	4.98	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	Pt	46	7MG	C2-N2	4.96	1.45	1.34
58	Pt	37	T6A	C10-N6	4.93	1.48	1.37
1	16	516	PSU	C6-N1	4.92	1.44	1.36
59	Dt	46	7MG	C2-N2	4.91	1.45	1.34
59	Dt	39	PSU	C6-N1	4.90	1.44	1.36
23	23	1911	PSU	C6-N1	4.88	1.44	1.36
23	23	955	PSU	C6-N1	4.82	1.44	1.36
23	23	2580	PSU	C6-N1	4.82	1.44	1.36
23	23	2498	OMC	C4-N3	4.80	1.44	1.34
23	23	2504	PSU	C6-N1	4.77	1.44	1.36
23	23	2604	PSU	C6-N1	4.77	1.44	1.36
23	23	2457	PSU	C6-N1	4.75	1.44	1.36
58	Pt	37	T6A	C10-N11	4.75	1.48	1.35
23	23	2605	PSU	C6-N1	4.70	1.44	1.36
23	23	745	1MG	C2-N1	4.66	1.45	1.37
23	23	1915	3TD	C2-N3	4.63	1.48	1.38
59	Dt	46	7MG	C4-N9	4.58	1.43	1.37
23	23	2449	H2U	C4-N3	4.55	1.45	1.37
1	16	1402	4OC	C4-N4	4.54	1.45	1.36
1	16	1516	2MG	C2-N1	4.51	1.43	1.36
23	23	2498	OMC	C4-N4	4.50	1.44	1.33
1	16	966	2MG	C2-N1	4.49	1.43	1.36
23	23	2503	2MA	C5-C6	4.32	1.53	1.41
59	Dt	37	MIA	C5-C4	4.32	1.46	1.39
1	16	967	5MC	C4-N4	4.31	1.45	1.34
23	23	2445	2MG	C2-N1	4.27	1.43	1.36
23	23	1835	2MG	C2-N1	4.26	1.43	1.36
1	16	1407	5MC	C4-N4	4.24	1.44	1.34
23	23	1962	5MC	C4-N4	4.23	1.44	1.34
1	16	1407	5MC	C6-N1	4.23	1.45	1.38
1	16	967	5MC	C6-N1	4.22	1.45	1.38
23	23	1962	5MC	C6-N1	4.20	1.45	1.38
23	23	745	1MG	O6-C6	-4.16	1.14	1.23
23	23	2498	OMC	C2-N1	4.15	1.48	1.40
1	16	1407	5MC	C2-N1	4.05	1.48	1.40
23	23	2552	OMU	C4-N3	3.90	1.45	1.38
59	Dt	46	7MG	C2-N1	3.86	1.47	1.37
23	23	745	1MG	C5-N7	-3.84	1.31	1.39
58	Pt	46	7MG	C2-N1	3.81	1.46	1.37
1	16	1402	4OC	C2-N1	3.80	1.48	1.40
59	Dt	55	PSU	C4-N3	3.80	1.46	1.38
23	23	2251	OMG	C2-N2	3.79	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	2030	6MZ	C5-N7	-3.78	1.32	1.39
1	16	967	5MC	C2-N1	3.73	1.47	1.40
23	23	1962	5MC	C2-N1	3.68	1.47	1.40
1	16	1518	MA6	C6-N6	3.68	1.47	1.36
1	16	516	PSU	C4-N3	3.67	1.45	1.38
36	LP	81	4D4	CZ-NH2	3.63	1.45	1.32
58	Pt	39	PSU	C4-N3	3.62	1.45	1.38
23	23	2503	2MA	C6-N6	-3.62	1.25	1.34
59	Dt	39	PSU	C4-N3	3.55	1.45	1.38
58	Pt	46	7MG	C5-C6	3.54	1.52	1.43
59	Dt	46	7MG	C5-C6	3.51	1.52	1.43
59	Dt	32	PSU	C4-N3	3.51	1.45	1.38
23	23	746	PSU	C4-N3	3.49	1.45	1.38
23	23	2030	6MZ	C5-C4	-3.49	1.32	1.39
1	16	1402	4OC	C5-C4	3.42	1.48	1.41
23	23	2504	PSU	C4-N3	3.40	1.45	1.38
23	23	1618	6MZ	C5-N7	-3.39	1.32	1.39
23	23	2030	6MZ	C8-N9	-3.38	1.31	1.37
23	23	1911	PSU	C4-N3	3.38	1.45	1.38
1	16	1518	MA6	C5-C4	-3.38	1.33	1.39
23	23	2069	7MG	C4-N9	-3.37	1.33	1.37
1	16	1519	MA6	C5-C6	3.33	1.49	1.41
23	23	2445	2MG	C5-N7	-3.33	1.32	1.39
23	23	2604	PSU	C4-N3	3.31	1.45	1.38
23	23	1835	2MG	C5-N7	-3.27	1.32	1.39
23	23	1939	5MU	O4-C4	-3.24	1.17	1.23
1	16	527	7MG	C5-C4	3.22	1.47	1.37
23	23	2605	PSU	C4-N3	3.21	1.44	1.38
23	23	2580	PSU	C4-N3	3.17	1.44	1.38
58	Pt	46	7MG	C6-N1	3.14	1.44	1.38
23	23	955	PSU	C4-N3	3.13	1.44	1.38
23	23	1962	5MC	O2-C2	-3.12	1.17	1.23
23	23	2552	OMU	O4-C4	-3.12	1.18	1.24
23	23	2069	7MG	C5-C4	3.11	1.47	1.37
23	23	2449	H2U	O2-C2	-3.11	1.17	1.23
23	23	2251	OMG	O6-C6	-3.10	1.17	1.23
1	16	1516	2MG	C5-N7	-3.09	1.32	1.39
59	Dt	46	7MG	C6-N1	3.09	1.44	1.38
23	23	2457	PSU	C4-N3	3.09	1.44	1.38
1	16	527	7MG	C4-N9	-3.08	1.34	1.37
23	23	1618	6MZ	C5-C4	-3.08	1.33	1.39
23	23	1939	5MU	O2-C2	-3.06	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	967	5MC	O2-C2	-3.06	1.18	1.23
1	16	1402	4OC	O2-C2	-3.06	1.18	1.23
1	16	1498	UR3	C6-N1	3.05	1.45	1.38
1	16	966	2MG	C5-N7	-3.05	1.33	1.39
1	16	1407	5MC	O2-C2	-3.02	1.18	1.23
23	23	2251	OMG	C5-N7	-3.01	1.33	1.39
23	23	747	5MU	O4-C4	-2.98	1.17	1.23
23	23	955	PSU	O4-C4	-2.97	1.17	1.23
23	23	2445	2MG	O6-C6	-2.95	1.18	1.23
23	23	745	1MG	C5-C6	2.93	1.53	1.45
1	16	1402	4OC	C6-N1	2.93	1.45	1.38
23	23	2605	PSU	O4-C4	-2.93	1.18	1.23
23	23	2457	PSU	O4-C4	-2.92	1.18	1.23
23	23	2498	OMC	O2-C2	-2.91	1.18	1.23
23	23	2552	OMU	O2-C2	-2.91	1.17	1.23
23	23	2503	2MA	C5-N7	-2.89	1.33	1.39
58	Pt	37	T6A	C5-N7	-2.89	1.33	1.39
23	23	1835	2MG	O6-C6	-2.89	1.18	1.23
23	23	747	5MU	O2-C2	-2.88	1.18	1.23
23	23	2504	PSU	O4-C4	-2.88	1.18	1.23
23	23	1911	PSU	O4-C4	-2.88	1.18	1.23
23	23	2580	PSU	O4-C4	-2.88	1.18	1.23
23	23	2498	OMC	C6-N1	2.87	1.44	1.38
23	23	1915	3TD	C4-N3	2.87	1.46	1.40
23	23	2604	PSU	O4-C4	-2.86	1.18	1.23
59	Dt	8	4SU	O2-C2	-2.79	1.18	1.23
58	Pt	34	U8U	C4-N3	-2.78	1.33	1.38
23	23	746	PSU	O4-C4	-2.77	1.18	1.23
59	Dt	32	PSU	O4-C4	-2.73	1.18	1.23
1	16	1516	2MG	O6-C6	-2.70	1.18	1.23
1	16	966	2MG	O6-C6	-2.70	1.18	1.23
23	23	2503	2MA	C4-N9	-2.68	1.32	1.37
59	Dt	39	PSU	O4-C4	-2.67	1.18	1.23
1	16	516	PSU	O4-C4	-2.66	1.18	1.23
58	Pt	39	PSU	O4-C4	-2.65	1.18	1.23
59	Dt	46	7MG	O6-C6	-2.62	1.18	1.23
1	16	1518	MA6	C8-N9	-2.60	1.33	1.37
1	16	1518	MA6	C5-N7	-2.56	1.34	1.39
23	23	2457	PSU	O2-C2	-2.54	1.18	1.23
23	23	955	PSU	O2-C2	-2.53	1.18	1.23
23	23	1618	6MZ	C8-N9	-2.51	1.33	1.37
58	Pt	46	7MG	O6-C6	-2.51	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	23	1915	3TD	O2-C2	-2.50	1.18	1.23
23	23	2580	PSU	O2-C2	-2.50	1.18	1.23
23	23	2069	7MG	C6-N1	-2.49	1.34	1.38
36	LP	81	4D4	CZ-NH1	-2.49	1.25	1.34
59	Dt	37	MIA	C5-C6	2.49	1.47	1.41
23	23	745	1MG	C4-N9	-2.49	1.31	1.38
59	Dt	55	PSU	O4-C4	-2.47	1.18	1.23
1	16	527	7MG	C6-N1	-2.47	1.34	1.38
59	Dt	8	4SU	C6-N1	2.46	1.43	1.38
59	Dt	37	MIA	C5-N7	-2.45	1.34	1.39
23	23	2445	2MG	C4-N9	-2.43	1.31	1.38
23	23	2605	PSU	O2-C2	-2.43	1.18	1.23
23	23	2604	PSU	O2-C2	-2.43	1.18	1.23
58	Pt	34	U8U	C6-N1	-2.42	1.33	1.38
23	23	2580	PSU	O4'-C1'	-2.41	1.40	1.43
58	Pt	37	T6A	C5-C4	-2.41	1.34	1.39
23	23	2552	OMU	C6-N1	2.40	1.43	1.38
59	Dt	32	PSU	O2-C2	-2.40	1.18	1.23
59	Dt	39	PSU	O2-C2	-2.38	1.18	1.23
1	16	1516	2MG	C4-N9	-2.38	1.32	1.38
23	23	2504	PSU	O2-C2	-2.38	1.18	1.23
1	16	1516	2MG	C5-C6	2.38	1.53	1.44
58	Pt	37	T6A	ODA-C13	2.37	1.29	1.22
23	23	1618	6MZ	C6-N1	-2.32	1.31	1.35
23	23	1911	PSU	O2-C2	-2.32	1.18	1.23
58	Pt	39	PSU	O2-C2	-2.31	1.18	1.23
1	16	966	2MG	C5-C6	2.30	1.53	1.44
23	23	2030	6MZ	C5-C6	-2.29	1.36	1.41
23	23	2030	6MZ	C6-N1	-2.29	1.31	1.35
23	23	2251	OMG	C4-N9	-2.27	1.32	1.38
1	16	966	2MG	C4-N9	-2.25	1.32	1.38
23	23	2251	OMG	C2-N1	2.24	1.43	1.37
23	23	2449	H2U	O4-C4	-2.20	1.18	1.23
23	23	1835	2MG	C4-N9	-2.20	1.32	1.38
59	Dt	37	MIA	C8-N7	2.20	1.35	1.31
23	23	1835	2MG	C5-C6	2.19	1.52	1.44
23	23	2445	2MG	C5-C6	2.19	1.52	1.44
1	16	1516	2MG	C6-N1	2.19	1.43	1.38
23	23	2251	OMG	C6-N1	2.19	1.42	1.38
1	16	516	PSU	O2-C2	-2.19	1.18	1.23
23	23	2498	OMC	C5-C4	2.18	1.48	1.42
23	23	2552	OMU	C5-C4	2.17	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	Dt	47	3AU	C2-N1	2.17	1.41	1.38
23	23	746	PSU	O2-C2	-2.17	1.18	1.23
23	23	1911	PSU	O4'-C1'	-2.17	1.40	1.43
1	16	1498	UR3	O2-C2	-2.16	1.18	1.22
23	23	2251	OMG	C5-C6	2.16	1.52	1.44
23	23	2457	PSU	O4'-C1'	-2.15	1.40	1.43
1	16	1519	MA6	C5-N7	-2.15	1.35	1.39
1	16	1498	UR3	C4-N3	2.15	1.44	1.40
58	Pt	47	3AU	C2-N1	2.13	1.41	1.38
59	Dt	55	PSU	O2-C2	-2.13	1.18	1.23
1	16	1519	MA6	C8-N7	2.12	1.35	1.31
23	23	2503	2MA	C8-N7	2.11	1.35	1.31
58	Pt	37	T6A	O10-C10	-2.10	1.18	1.23
23	23	2605	PSU	O4'-C1'	-2.08	1.41	1.43
1	16	966	2MG	C6-N1	2.08	1.42	1.38
58	Pt	34	U8U	C-N	-2.07	1.43	1.46
23	23	2503	2MA	C5-C4	-2.06	1.35	1.39
23	23	2503	2MA	C8-N9	-2.05	1.34	1.37
1	16	1498	UR3	C5-C4	2.05	1.49	1.43
58	Pt	37	T6A	C2-N1	2.03	1.37	1.33

All (297) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	1939	5MU	C5-C4-N3	12.60	126.27	115.32
23	23	747	5MU	C5-C4-N3	12.05	125.80	115.32
1	16	1518	MA6	N1-C6-N6	-11.49	102.86	116.86
23	23	1939	5MU	C5-C6-N1	-10.26	112.17	123.31
23	23	747	5MU	C5-C6-N1	-10.12	112.31	123.31
1	16	527	7MG	N9-C4-N3	8.86	138.44	125.46
59	Dt	37	MIA	C12-C13-C14	-8.82	111.18	127.01
23	23	2030	6MZ	C4-N9-C1'	-8.81	106.03	126.63
23	23	2069	7MG	N9-C4-N3	8.50	137.92	125.46
23	23	2030	6MZ	C1'-N9-C8	8.49	145.94	127.09
59	Dt	37	MIA	C5-C4-N3	-8.37	118.36	127.18
59	Dt	8	4SU	C4-N3-C2	-8.32	119.34	127.31
1	16	1518	MA6	C5-C6-N6	7.50	137.20	125.33
23	23	1618	6MZ	C1'-N9-C8	7.41	143.55	127.09
23	23	1618	6MZ	C4-N9-C1'	-7.13	109.96	126.63
23	23	1618	6MZ	C5-C4-N3	-6.92	117.18	126.72
23	23	2503	2MA	C1'-N9-C8	-6.92	111.74	127.09
59	Dt	37	MIA	N3-C4-N9	6.85	135.68	126.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	745	1MG	C1'-N9-C4	-6.81	106.37	126.49
23	23	1835	2MG	C2-N3-C4	6.61	120.27	112.00
58	Pt	37	T6A	N6-C10-N11	6.47	122.67	113.77
23	23	2552	OMU	C4-N3-C2	-6.42	118.64	126.61
1	16	1516	2MG	C2-N3-C4	6.41	120.02	112.00
23	23	2445	2MG	C2-N3-C4	6.34	119.93	112.00
23	23	745	1MG	C1'-N9-C8	6.26	144.53	126.73
1	16	966	2MG	C2-N3-C4	6.22	119.78	112.00
23	23	2503	2MA	N9-C8-N7	-5.94	105.51	113.94
59	Dt	8	4SU	C5-C4-N3	5.93	120.27	114.75
23	23	1915	3TD	N1-C2-N3	5.73	120.30	116.13
1	16	1518	MA6	N1-C2-N3	-5.73	119.91	128.58
58	Pt	37	T6A	N3-C2-N1	-5.69	119.96	128.58
23	23	2030	6MZ	C5-C4-N3	-5.67	118.90	126.72
1	16	1519	MA6	C5-C4-N3	-5.63	118.97	126.72
23	23	1618	6MZ	N1-C2-N3	-5.53	120.21	128.58
23	23	2030	6MZ	C4-C5-C6	5.50	121.36	116.78
23	23	1835	2MG	C5-C4-N3	-5.50	119.64	128.39
1	16	527	7MG	C5-C4-N3	-5.45	117.89	128.13
1	16	1498	UR3	C4-N3-C2	-5.44	120.20	124.58
23	23	2457	PSU	C4-N3-C2	-5.44	118.88	126.37
23	23	2457	PSU	N1-C2-N3	5.40	120.86	115.17
23	23	1939	5MU	C4-N3-C2	-5.37	120.29	127.34
23	23	2069	7MG	N9-C8-N7	-5.34	95.82	103.37
23	23	2503	2MA	C5-C4-N3	-5.31	121.58	127.18
23	23	2069	7MG	C5-C4-N3	-5.29	118.21	128.13
23	23	955	PSU	C4-N3-C2	-5.28	119.09	126.37
1	16	527	7MG	N9-C8-N7	-5.27	95.92	103.37
58	Pt	37	T6A	C5-C4-N3	-5.26	119.48	126.72
23	23	2445	2MG	C5-C4-N3	-5.23	120.07	128.39
59	Dt	32	PSU	C4-N3-C2	-5.20	119.21	126.37
23	23	2604	PSU	C4-N3-C2	-5.16	119.27	126.37
58	Pt	46	7MG	C5-C6-N1	5.15	120.00	110.94
23	23	1939	5MU	O4-C4-C5	-5.14	119.04	124.92
58	Pt	39	PSU	C4-N3-C2	-5.09	119.37	126.37
1	16	966	2MG	C5-C4-N3	-5.08	120.30	128.39
23	23	747	5MU	O4-C4-C5	-5.08	119.10	124.92
23	23	745	1MG	C5-C4-N3	-5.08	120.30	128.39
23	23	2605	PSU	C4-N3-C2	-5.05	119.41	126.37
23	23	2251	OMG	C5-C4-N3	-5.04	120.37	128.39
23	23	955	PSU	N1-C2-N3	5.02	120.46	115.17
23	23	1618	6MZ	C4-C5-C6	4.99	120.93	116.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	747	5MU	C4-N3-C2	-4.98	120.81	127.34
59	Dt	55	PSU	C4-N3-C2	-4.97	119.53	126.37
1	16	1516	2MG	C5-C4-N3	-4.96	120.50	128.39
59	Dt	46	7MG	C5-C6-N1	4.95	119.66	110.94
23	23	1911	PSU	C4-N3-C2	-4.94	119.57	126.37
23	23	2580	PSU	C4-N3-C2	-4.92	119.59	126.37
1	16	1519	MA6	C4-C5-N7	-4.92	104.96	110.58
23	23	746	PSU	C4-N3-C2	-4.91	119.60	126.37
23	23	2503	2MA	C4-N9-C8	4.91	110.89	105.74
59	Dt	47	3AU	C4-N3-C2	-4.89	118.92	124.66
23	23	2445	2MG	C2-N1-C6	-4.81	118.74	124.55
23	23	2504	PSU	C4-N3-C2	-4.80	119.75	126.37
59	Dt	39	PSU	C4-N3-C2	-4.80	119.75	126.37
23	23	2580	PSU	N1-C2-N3	4.79	120.22	115.17
58	Pt	47	3AU	C4-N3-C2	-4.78	119.05	124.66
1	16	1518	MA6	C5-C4-N3	-4.74	120.19	126.72
23	23	2605	PSU	N1-C2-N3	4.73	120.16	115.17
23	23	2604	PSU	N1-C2-N3	4.72	120.14	115.17
58	Pt	39	PSU	N1-C2-N3	4.69	120.12	115.17
23	23	1618	6MZ	N3-C4-N9	4.69	135.14	127.17
1	16	1519	MA6	C10-N6-C6	-4.67	108.63	120.52
59	Dt	39	PSU	N1-C2-N3	4.67	120.09	115.17
23	23	2030	6MZ	N1-C2-N3	-4.67	121.52	128.58
58	Pt	46	7MG	C2-N3-C4	4.67	120.34	112.30
1	16	516	PSU	C4-N3-C2	-4.65	119.97	126.37
23	23	1939	5MU	N3-C2-N1	4.65	120.94	114.89
23	23	1835	2MG	C2-N1-C6	-4.63	118.95	124.55
23	23	2069	7MG	C2-N3-C4	4.62	120.26	112.30
23	23	2504	PSU	N1-C2-N3	4.62	120.04	115.17
23	23	2251	OMG	C2-N3-C4	4.59	120.20	112.30
59	Dt	32	PSU	N1-C2-N3	4.59	120.01	115.17
23	23	2503	2MA	C4-N9-C1'	4.59	137.36	126.63
59	Dt	55	PSU	N1-C2-N3	4.56	119.98	115.17
1	16	1519	MA6	C2-N1-C6	4.51	122.85	111.83
1	16	527	7MG	C2-N3-C4	4.48	120.01	112.30
23	23	1911	PSU	N1-C2-N3	4.45	119.87	115.17
1	16	966	2MG	C2-N1-C6	-4.44	119.19	124.55
1	16	1518	MA6	N9-C8-N7	-4.42	107.66	113.94
23	23	747	5MU	N3-C2-N1	4.42	120.64	114.89
58	Pt	46	7MG	C5-C4-N3	-4.41	119.85	128.13
59	Dt	46	7MG	C2-N3-C4	4.39	119.85	112.30
23	23	2445	2MG	N1-C2-N2	4.33	120.98	116.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	2552	OMU	N3-C2-N1	4.28	120.47	114.89
58	Pt	37	T6A	C4-C5-C6	4.28	120.34	116.78
1	16	516	PSU	N1-C2-N3	4.24	119.64	115.17
23	23	2457	PSU	C6-C5-C4	4.23	121.03	118.17
1	16	1516	2MG	C2-N1-C6	-4.22	119.45	124.55
1	16	1516	2MG	N1-C2-N2	4.15	120.80	116.56
23	23	1835	2MG	N1-C2-N2	4.10	120.75	116.56
23	23	1618	6MZ	C2-N3-C4	4.10	121.84	111.83
58	Pt	37	T6A	N9-C8-N7	-4.08	108.14	113.94
23	23	746	PSU	N1-C2-N3	4.06	119.45	115.17
59	Dt	37	MIA	C15-C14-C13	-4.05	110.50	122.66
23	23	1915	3TD	C1'-C5-C4	4.04	123.73	117.61
59	Dt	46	7MG	C5-C4-N3	-4.02	120.59	128.13
58	Pt	46	7MG	C4-C5-N7	3.98	110.08	105.38
23	23	747	5MU	C5M-C5-C6	-3.98	117.47	122.85
23	23	2030	6MZ	N3-C4-N9	3.96	133.91	127.17
59	Dt	55	PSU	C6-C5-C4	3.95	120.84	118.17
1	16	1498	UR3	C5-C4-N3	3.92	120.21	115.04
1	16	1518	MA6	C4-C5-C6	3.92	119.97	115.91
23	23	2552	OMU	C5-C4-N3	3.91	120.27	114.80
23	23	1915	3TD	C4-N3-C2	-3.89	120.50	124.61
12	SL	89	D2T	CB1-SB-CB	3.89	109.35	102.36
23	23	2030	6MZ	N9-C8-N7	-3.86	108.46	113.94
59	Dt	8	4SU	N3-C2-N1	3.82	119.86	114.89
23	23	747	5MU	C5M-C5-C4	3.77	122.80	118.78
59	Dt	8	4SU	C5-C4-S4	-3.74	120.03	124.31
59	Dt	46	7MG	C4-C5-N7	3.72	109.77	105.38
59	Dt	37	MIA	C11-S10-C2	-3.69	99.48	102.25
1	16	1519	MA6	N3-C4-N9	3.69	133.44	127.17
59	Dt	37	MIA	C16-C14-C13	-3.67	111.63	122.66
1	16	1519	MA6	C2-N3-C4	3.66	120.77	111.83
23	23	2504	PSU	C6-N1-C2	-3.65	119.30	122.69
23	23	1939	5MU	C5M-C5-C6	-3.65	117.90	122.85
1	16	967	5MC	C5-C6-N1	-3.64	119.36	123.31
1	16	966	2MG	N1-C2-N2	3.61	120.24	116.56
23	23	2503	2MA	N3-C4-N9	3.58	131.53	126.99
23	23	2580	PSU	C6-N1-C2	-3.57	119.38	122.69
1	16	516	PSU	C6-N1-C2	-3.57	119.38	122.69
23	23	955	PSU	C6-C5-C4	3.57	120.58	118.17
58	Pt	39	PSU	C6-C5-C4	3.52	120.55	118.17
59	Dt	37	MIA	C2-N3-C4	3.49	121.43	112.29
23	23	1939	5MU	C5M-C5-C4	3.48	122.50	118.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Pt	37	T6A	C2-N3-C4	3.47	120.30	111.83
23	23	2503	2MA	C5-N7-C8	3.45	108.88	103.45
23	23	955	PSU	C6-N1-C2	-3.44	119.50	122.69
23	23	745	1MG	N9-C8-N7	-3.43	107.03	113.40
23	23	745	1MG	C2-N3-C4	3.43	119.70	111.98
23	23	2251	OMG	N9-C8-N7	-3.42	107.06	113.40
59	Dt	39	PSU	C6-C5-C4	3.41	120.48	118.17
1	16	1518	MA6	C2-N1-C6	3.40	120.12	111.83
59	Dt	39	PSU	C6-N1-C2	-3.39	119.54	122.69
23	23	1962	5MC	C5-C6-N1	-3.39	119.63	123.31
23	23	2605	PSU	C6-N1-C2	-3.39	119.55	122.69
23	23	2449	H2U	C5-C4-N3	3.39	120.29	116.69
23	23	2457	PSU	C6-N1-C2	-3.39	119.55	122.69
23	23	2604	PSU	C6-C5-C4	3.36	120.44	118.17
23	23	2503	2MA	N3-C2-N1	-3.35	119.86	125.77
59	Dt	32	PSU	C6-C5-C4	3.33	120.42	118.17
23	23	2449	H2U	N3-C2-N1	3.32	119.99	116.65
23	23	745	1MG	N9-C4-N3	3.31	132.58	125.95
1	16	1518	MA6	C2-N3-C4	3.29	119.86	111.83
23	23	2251	OMG	C2-N1-C6	-3.27	119.18	125.11
23	23	2580	PSU	C6-C5-C4	3.25	120.37	118.17
23	23	2604	PSU	C6-N1-C2	-3.22	119.70	122.69
23	23	1835	2MG	N9-C4-N3	3.20	132.34	125.95
1	16	1519	MA6	C5-N7-C8	3.17	108.43	103.45
59	Dt	46	7MG	C5-C4-N9	3.16	110.38	106.33
59	Dt	37	MIA	C4-C5-N7	-3.16	106.97	110.58
58	Pt	37	T6A	N3-C4-N9	3.16	132.53	127.17
23	23	2445	2MG	CM2-N2-C2	-3.15	116.87	123.65
1	16	1518	MA6	N3-C4-N9	3.15	132.52	127.17
23	23	2251	OMG	N9-C4-N3	3.12	132.19	125.95
23	23	2030	6MZ	C2-N3-C4	3.11	119.43	111.83
1	16	1519	MA6	N1-C2-N3	-3.10	123.88	128.58
1	16	1516	2MG	N9-C8-N7	-3.10	107.66	113.40
1	16	1516	2MG	C1'-N9-C4	-3.06	117.44	126.49
23	23	1835	2MG	CM2-N2-C2	-3.06	117.08	123.65
58	Pt	46	7MG	N9-C4-N3	3.05	129.93	125.46
59	Dt	39	PSU	O2-C2-N1	-3.04	119.65	122.79
58	Pt	46	7MG	C2-N1-C6	-3.04	119.60	125.11
58	Pt	46	7MG	C5-C4-N9	3.03	110.22	106.33
58	Pt	39	PSU	C6-N1-C2	-3.03	119.88	122.69
1	16	966	2MG	N9-C4-N3	3.02	131.99	125.95
23	23	2445	2MG	N9-C4-N3	3.01	131.97	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	Dt	55	PSU	C6-N1-C2	-3.00	119.91	122.69
1	16	966	2MG	N9-C8-N7	-2.98	107.87	113.40
23	23	1911	PSU	C6-N1-C2	-2.97	119.93	122.69
1	16	1519	MA6	C6-C5-N7	2.97	138.18	133.43
23	23	1939	5MU	O2-C2-N1	-2.96	118.94	122.80
23	23	2445	2MG	N9-C8-N7	-2.96	107.91	113.40
1	16	1518	MA6	C4-N9-C8	2.94	108.83	105.74
1	16	1407	5MC	C5-C6-N1	-2.94	120.12	123.31
23	23	1835	2MG	N9-C8-N7	-2.93	107.96	113.40
1	16	516	PSU	O2-C2-N1	-2.93	119.77	122.79
23	23	1618	6MZ	C5-C6-N1	2.91	121.27	118.15
12	SL	89	D2T	OD2-CG-CB	2.90	119.42	113.15
59	Dt	37	MIA	C4-N9-C8	2.89	108.78	105.74
23	23	1939	5MU	O4-C4-N3	-2.88	114.69	120.11
58	Pt	37	T6A	C5-N7-C8	2.88	107.98	103.45
58	Pt	46	7MG	O6-C6-C5	-2.88	120.56	127.62
59	Dt	46	7MG	C2-N1-C6	-2.87	119.90	125.11
23	23	2552	OMU	O4-C4-C5	-2.87	120.21	125.16
23	23	2457	PSU	O2-C2-N1	-2.87	119.83	122.79
23	23	1618	6MZ	N9-C8-N7	-2.85	109.89	113.94
58	Pt	39	PSU	O2-C2-N1	-2.85	119.85	122.79
23	23	2069	7MG	C5-C6-N1	2.85	115.96	110.94
23	23	2605	PSU	C6-C5-C4	2.85	120.10	118.17
59	Dt	32	PSU	C6-N1-C2	-2.85	120.05	122.69
23	23	1618	6MZ	C9-N6-C6	-2.84	120.22	122.85
23	23	2449	H2U	C5-C6-N1	2.81	120.02	111.52
59	Dt	46	7MG	O6-C6-C5	-2.79	120.77	127.62
23	23	2251	OMG	C5-C6-N1	2.78	120.34	113.25
23	23	747	5MU	O2-C2-N1	-2.78	119.18	122.80
23	23	746	PSU	C6-N1-C2	-2.78	120.11	122.69
58	Pt	37	T6A	O10-C10-N6	-2.77	118.72	123.64
23	23	2445	2MG	C5-C6-N1	2.77	120.30	113.25
59	Dt	55	PSU	O2-C2-N1	-2.77	119.94	122.79
23	23	745	1MG	C5-C6-N1	2.76	120.13	115.02
1	16	1518	MA6	C5-N7-C8	2.76	107.79	103.45
59	Dt	37	MIA	C6-C5-N7	2.76	135.43	132.43
23	23	1835	2MG	C5-C6-N1	2.75	120.25	113.25
23	23	2030	6MZ	C5-N7-C8	2.74	107.76	103.45
1	16	527	7MG	C5-C6-N1	2.74	115.76	110.94
59	Dt	47	3AU	C5-C4-N3	2.74	119.42	115.64
23	23	2605	PSU	O2-C2-N1	-2.74	119.97	122.79
23	23	955	PSU	O2-C2-N1	-2.74	119.97	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	23	2504	PSU	O2-C2-N1	-2.73	119.97	122.79
1	16	966	2MG	C5-C6-N1	2.71	120.16	113.25
58	Pt	37	T6A	C12-N11-C10	-2.71	117.47	121.99
1	16	1519	MA6	C10-N6-C9	-2.69	107.54	116.18
58	Pt	47	3AU	C5-C4-N3	2.68	119.35	115.64
23	23	2552	OMU	O2-C2-N1	-2.67	119.32	122.80
1	16	1516	2MG	C5-C6-N1	2.67	120.06	113.25
1	16	1516	2MG	C1'-N9-C8	2.67	134.32	126.73
23	23	747	5MU	O4-C4-N3	-2.67	115.10	120.11
59	Dt	37	MIA	N6-C6-N1	2.65	121.89	118.33
1	16	1516	2MG	N9-C4-N3	2.62	131.19	125.95
59	Dt	37	MIA	C2'-C1'-N9	-2.61	106.83	113.30
1	16	966	2MG	O6-C6-C5	-2.61	119.65	126.53
23	23	2445	2MG	O6-C6-C5	-2.57	119.75	126.53
23	23	2449	H2U	O2-C2-N1	-2.56	120.03	123.10
58	Pt	34	U8U	O4-C4-C5	-2.55	120.42	124.71
23	23	2251	OMG	O6-C6-C5	-2.54	119.83	126.53
23	23	746	PSU	O2-C2-N1	-2.54	120.17	122.79
59	Dt	32	PSU	O2-C2-N1	-2.52	120.19	122.79
23	23	2604	PSU	O2-C2-N1	-2.52	120.19	122.79
23	23	746	PSU	C6-C5-C4	2.50	119.86	118.17
23	23	2503	2MA	CM2-C2-N1	2.49	120.86	117.13
59	Dt	37	MIA	C5-N7-C8	2.49	107.36	103.45
23	23	2580	PSU	O2-C2-N1	-2.48	120.23	122.79
23	23	1835	2MG	O6-C6-C5	-2.48	119.98	126.53
23	23	2069	7MG	O4'-C1'-N9	2.45	112.64	109.30
59	Dt	46	7MG	N9-C4-N3	2.43	129.02	125.46
58	Pt	47	3AU	C3'-C2'-C1'	2.41	106.02	101.46
58	Pt	46	7MG	N9-C8-N7	2.41	106.78	103.37
1	16	1516	2MG	O6-C6-C5	-2.40	120.19	126.53
23	23	2503	2MA	C4-C5-N7	-2.40	107.84	110.58
1	16	1519	MA6	O3'-C3'-C4'	2.40	117.97	111.08
23	23	1911	PSU	O2-C2-N1	-2.39	120.32	122.79
1	16	966	2MG	CM2-N2-C2	-2.39	118.52	123.65
1	16	1402	4OC	C6-C5-C4	2.38	119.87	117.00
23	23	1618	6MZ	C5-N7-C8	2.37	107.18	103.45
23	23	2504	PSU	C6-C5-C4	2.33	119.75	118.17
1	16	1516	2MG	CM2-N2-C2	-2.31	118.69	123.65
23	23	2251	OMG	C8-N7-C5	2.27	108.30	104.26
58	Pt	34	U8U	C5-C4-N3	2.25	118.65	115.21
23	23	745	1MG	C8-N7-C5	2.25	108.26	104.26
59	Dt	37	MIA	N3-C2-N1	-2.23	122.93	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	Dt	46	7MG	N9-C8-N7	2.22	106.52	103.37
1	16	527	7MG	O4'-C1'-N9	2.22	112.32	109.30
1	16	966	2MG	C1'-N9-C4	-2.21	119.95	126.49
23	23	1835	2MG	C1'-N9-C4	-2.20	119.98	126.49
1	16	1519	MA6	C2'-C3'-C4'	2.20	106.86	102.61
23	23	2580	PSU	O4'-C1'-C2'	2.19	108.18	105.15
23	23	2030	6MZ	C4-N9-C8	2.19	108.04	105.74
1	16	1516	2MG	C8-N7-C5	2.16	108.10	104.26
23	23	2030	6MZ	C6-C5-N7	-2.15	130.09	132.43
23	23	2445	2MG	C1'-N9-C4	-2.14	120.16	126.49
59	Dt	47	3AU	C1'-N1-C2	2.13	120.53	117.04
59	Dt	8	4SU	O2-C2-N1	-2.12	120.04	122.80
59	Dt	37	MIA	N9-C8-N7	-2.11	110.94	113.94
23	23	1835	2MG	C8-N7-C5	2.11	108.01	104.26
58	Pt	34	U8U	C5-C6-N1	-2.11	120.11	122.94
1	16	1516	2MG	N1-C2-N3	-2.08	120.17	123.68
1	16	527	7MG	C5-C4-N9	-2.08	103.67	106.33
58	Pt	37	T6A	C4-C5-N7	-2.08	108.20	110.58
58	Pt	34	U8U	C3'-C2'-C1'	2.07	105.38	101.46
23	23	747	5MU	C6-C5-C4	2.07	119.72	118.02
58	Pt	37	T6A	N6-C6-N1	2.07	122.89	117.54
1	16	1498	UR3	C6-N1-C2	-2.06	120.11	121.80
1	16	1407	5MC	CM5-C5-C6	-2.06	120.06	122.85
23	23	2030	6MZ	C5-C6-N1	2.06	120.36	118.15
23	23	2445	2MG	C8-N7-C5	2.04	107.90	104.26
1	16	516	PSU	C6-C5-C4	2.02	119.54	118.17
58	Pt	47	3AU	C10-N3-C2	2.01	120.61	117.64

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16	1519	MA6	O4'-C4'-C5'-O5'
1	16	1519	MA6	C3'-C4'-C5'-O5'
1	16	1519	MA6	C5-C6-N6-C10
23	23	1618	6MZ	C5-C6-N6-C9
23	23	1618	6MZ	N1-C6-N6-C9
23	23	1911	PSU	O4'-C1'-C5-C4
23	23	1911	PSU	O4'-C1'-C5-C6
23	23	1915	3TD	O4'-C1'-C5-C4
23	23	1915	3TD	O4'-C1'-C5-C6
23	23	2251	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
23	23	2251	OMG	C1'-C2'-O2'-CM2
58	Pt	37	T6A	N11-C12-C14-O14
58	Pt	37	T6A	N11-C12-C14-C15
58	Pt	37	T6A	C13-C12-C14-O14
58	Pt	37	T6A	C13-C12-C14-C15
58	Pt	47	3AU	N3-C10-C11-C12
59	Dt	37	MIA	O4'-C4'-C5'-O5'
59	Dt	37	MIA	C3'-C4'-C5'-O5'
59	Dt	37	MIA	C12-C13-C14-C15
59	Dt	37	MIA	C12-C13-C14-C16
59	Dt	47	3AU	N3-C10-C11-C12
59	Dt	47	3AU	C10-C11-C12-N40
59	Dt	47	3AU	N40-C12-C13-O30
59	Dt	47	3AU	O4'-C4'-C5'-O5'
1	16	527	7MG	C3'-C4'-C5'-O5'
23	23	2251	OMG	C3'-C4'-C5'-O5'
23	23	2498	OMC	C3'-C4'-C5'-O5'
23	23	2503	2MA	O4'-C4'-C5'-O5'
58	Pt	37	T6A	O4'-C4'-C5'-O5'
58	Pt	37	T6A	C3'-C4'-C5'-O5'
59	Dt	47	3AU	C3'-C4'-C5'-O5'
58	Pt	47	3AU	N40-C12-C13-O31
23	23	2498	OMC	O4'-C4'-C5'-O5'
23	23	2503	2MA	C3'-C4'-C5'-O5'
1	16	1519	MA6	N1-C6-N6-C10
59	Dt	47	3AU	N40-C12-C13-O31
1	16	527	7MG	O4'-C4'-C5'-O5'
58	Pt	37	T6A	C14-C12-C13-ODA
58	Pt	37	T6A	C14-C12-C13-ODB
23	23	1618	6MZ	C3'-C4'-C5'-O5'
23	23	2030	6MZ	O4'-C4'-C5'-O5'
23	23	2030	6MZ	C3'-C4'-C5'-O5'
58	Pt	47	3AU	C3'-C4'-C5'-O5'
58	Pt	47	3AU	C11-C10-N3-C4
58	Pt	37	T6A	N11-C12-C13-ODA
23	23	1835	2MG	O4'-C4'-C5'-O5'
58	Pt	34	U8U	O4'-C4'-C5'-O5'
58	Pt	46	7MG	O4'-C4'-C5'-O5'
58	Pt	47	3AU	O4'-C4'-C5'-O5'
58	Pt	47	3AU	C11-C10-N3-C2
23	23	1618	6MZ	O4'-C4'-C5'-O5'
23	23	1835	2MG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
59	Dt	37	MIA	C5-C6-N6-C12
59	Dt	37	MIA	N1-C6-N6-C12
58	Pt	34	U8U	C3'-C4'-C5'-O5'
58	Pt	46	7MG	C3'-C4'-C5'-O5'
58	Pt	47	3AU	C4'-C5'-O5'-P
59	Dt	47	3AU	C4'-C5'-O5'-P
58	Pt	47	3AU	N40-C12-C13-O30
58	Pt	37	T6A	N11-C12-C13-ODB
58	Pt	46	7MG	C2'-C1'-N9-C8
59	Dt	46	7MG	C2'-C1'-N9-C8
12	SL	89	D2T	CG-CB-SB-CB1
59	Dt	47	3AU	C11-C12-C13-O31
23	23	747	5MU	C3'-C4'-C5'-O5'
1	16	1402	4OC	O4'-C4'-C5'-O5'
1	16	1498	UR3	O4'-C4'-C5'-O5'
1	16	1519	MA6	C4'-C5'-O5'-P
59	Dt	47	3AU	C11-C12-C13-O30
1	16	1519	MA6	C5-C6-N6-C9
23	23	2449	H2U	C4'-C5'-O5'-P
1	16	527	7MG	C4'-C5'-O5'-P
58	Pt	46	7MG	O4'-C1'-N9-C8
23	23	746	PSU	O4'-C1'-C5-C6
23	23	1962	5MC	C2'-C1'-N1-C6
23	23	1962	5MC	O4'-C1'-N1-C6
23	23	2580	PSU	O4'-C4'-C5'-O5'
59	Dt	46	7MG	O4'-C1'-N9-C8
23	23	746	PSU	C2'-C1'-C5-C6
58	Pt	47	3AU	C11-C12-C13-O30
58	Pt	47	3AU	C11-C12-C13-O31
36	LP	81	4D4	O-C-CA-CB
1	16	1498	UR3	C3'-C4'-C5'-O5'

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	23	2251	OMG	1	0
23	23	2030	6MZ	2	0
1	16	1516	2MG	2	0
58	Pt	34	U8U	2	0
23	23	2552	OMU	1	0
23	23	2498	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	SL	89	D2T	2	0
23	23	2504	PSU	1	0
58	Pt	39	PSU	1	0
1	16	1402	4OC	1	0
1	16	516	PSU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 372 ligands modelled in this entry, 347 are monoatomic - leaving 25 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
66	GTP	EF	901	62	33,34,34	3.63	18 (54%)	50,54,54	1.79	12 (24%)
61	PUT	16	1603	-	5,5,5	0.23	0	4,4,4	0.47	0
60	SCM	16	1601	-	23,25,25	1.35	3 (13%)	27,39,39	1.50	3 (11%)
64	ATP	23	3003	-	32,33,33	0.54	0	48,52,52	0.55	0
61	PUT	23	3011	-	5,5,5	0.23	0	4,4,4	0.44	0
61	PUT	23	3016	-	5,5,5	0.22	0	4,4,4	0.47	0
61	PUT	16	1605	-	5,5,5	0.15	0	4,4,4	0.23	0
61	PUT	23	3012	-	5,5,5	0.22	0	4,4,4	0.47	0
61	PUT	23	3006	-	5,5,5	0.21	0	4,4,4	0.48	0
61	PUT	23	3004	-	5,5,5	0.18	0	4,4,4	0.54	0
61	PUT	23	3015	-	5,5,5	0.23	0	4,4,4	0.41	0
61	PUT	23	3010	-	5,5,5	0.20	0	4,4,4	0.54	0
64	ATP	23	3002	-	32,33,33	0.56	0	48,52,52	0.57	0
61	PUT	23	3007	-	5,5,5	0.14	0	4,4,4	0.22	0
60	SCM	16	1602	-	23,25,25	1.37	3 (13%)	27,39,39	1.43	3 (11%)
65	SPD	23	3017	-	9,9,9	0.31	0	8,8,8	0.91	0
61	PUT	23	3008	-	5,5,5	0.22	0	4,4,4	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	PUT	16	1604	-	5,5,5	0.16	0	4,4,4	0.22	0
60	SCM	23	3001	-	23,25,25	1.38	4 (17%)	27,39,39	1.65	5 (18%)
65	SPD	23	3018	-	9,9,9	0.31	0	8,8,8	0.95	0
61	PUT	23	3013	-	5,5,5	0.15	0	4,4,4	0.60	0
61	PUT	23	3009	-	5,5,5	0.22	0	4,4,4	0.48	0
61	PUT	23	3014	-	5,5,5	0.20	0	4,4,4	0.41	0
61	PUT	23	3005	-	5,5,5	0.23	0	4,4,4	0.42	0
61	PUT	LC	301	-	5,5,5	0.22	0	4,4,4	0.76	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
66	GTP	EF	901	62	-	2/22/38/38	0/3/3/3
61	PUT	16	1603	-	-	0/3/3/3	-
64	ATP	23	3003	-	1/1/7/7	7/22/38/38	0/3/3/3
60	SCM	16	1601	-	-	2/4/57/57	0/3/3/3
61	PUT	23	3011	-	-	1/3/3/3	-
61	PUT	23	3016	-	-	1/3/3/3	-
61	PUT	16	1605	-	-	3/3/3/3	-
61	PUT	23	3012	-	-	2/3/3/3	-
61	PUT	23	3006	-	-	1/3/3/3	-
61	PUT	23	3004	-	-	2/3/3/3	-
61	PUT	23	3015	-	-	2/3/3/3	-
61	PUT	23	3010	-	-	1/3/3/3	-
64	ATP	23	3002	-	-	3/22/38/38	0/3/3/3
61	PUT	23	3007	-	-	2/3/3/3	-
60	SCM	16	1602	-	-	0/4/57/57	0/3/3/3
65	SPD	23	3017	-	-	4/7/7/7	-
61	PUT	23	3008	-	-	0/3/3/3	-
61	PUT	16	1604	-	-	0/3/3/3	-
60	SCM	23	3001	-	-	0/4/57/57	0/3/3/3
65	SPD	23	3018	-	-	0/7/7/7	-
61	PUT	23	3013	-	-	2/3/3/3	-
61	PUT	23	3009	-	-	1/3/3/3	-
61	PUT	23	3014	-	-	1/3/3/3	-
61	PUT	23	3005	-	-	0/3/3/3	-
61	PUT	LC	301	-	-	1/3/3/3	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
66	EF	901	GTP	O4'-C1'	8.31	1.61	1.42
66	EF	901	GTP	C2'-C1'	-8.03	1.28	1.53
66	EF	901	GTP	PB-O3B	7.21	1.67	1.59
66	EF	901	GTP	O4'-C4'	-6.51	1.30	1.45
66	EF	901	GTP	C4-N3	6.34	1.48	1.34
66	EF	901	GTP	C2-N3	6.20	1.48	1.33
66	EF	901	GTP	PA-O3A	5.26	1.65	1.59
66	EF	901	GTP	C2-N2	4.47	1.44	1.34
66	EF	901	GTP	C5-N7	-3.17	1.32	1.39
66	EF	901	GTP	O6-C6	-2.97	1.17	1.23
66	EF	901	GTP	O3'-C3'	-2.92	1.35	1.43
66	EF	901	GTP	PB-O3A	2.77	1.62	1.59
60	16	1601	SCM	C10-N10	-2.58	1.43	1.47
66	EF	901	GTP	C2-N1	2.56	1.43	1.37
66	EF	901	GTP	C6-N1	2.53	1.43	1.38
66	EF	901	GTP	O5'-C5'	-2.49	1.35	1.44
66	EF	901	GTP	C5-C6	2.49	1.53	1.44
60	23	3001	SCM	C10-N10	-2.38	1.43	1.47
60	16	1602	SCM	C10-N10	-2.33	1.43	1.47
66	EF	901	GTP	O2'-C2'	2.28	1.48	1.43
60	23	3001	SCM	C11-C10	2.26	1.57	1.53
60	23	3001	SCM	C3-C4	-2.18	1.47	1.50
66	EF	901	GTP	C4-N9	-2.16	1.32	1.38
60	23	3001	SCM	C9-C8	2.06	1.56	1.53
60	16	1601	SCM	C3-C4	-2.04	1.47	1.50
60	16	1602	SCM	C3-C4	-2.03	1.47	1.50
60	16	1602	SCM	C12-C7	2.02	1.56	1.52
60	16	1601	SCM	C8-N8	-2.01	1.44	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	EF	901	GTP	C5-C4-N3	-5.27	120.00	128.39
60	16	1601	SCM	C8M-N8-C8	-4.74	108.11	114.23
66	EF	901	GTP	C2-N3-C4	4.45	119.97	112.30
60	23	3001	SCM	C1M-N10-C10	-3.79	109.34	114.23
60	16	1601	SCM	C1M-N10-C10	-3.70	109.46	114.23
60	16	1602	SCM	C8M-N8-C8	-3.57	109.61	114.23
60	16	1602	SCM	C1M-N10-C10	-3.54	109.67	114.23
66	EF	901	GTP	C2-N1-C6	-3.49	118.79	125.11
60	23	3001	SCM	C8M-N8-C8	-3.38	109.86	114.23
60	23	3001	SCM	O1B-C7-C12	3.29	114.71	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	EF	901	GTP	N9-C8-N7	-3.28	107.32	113.40
66	EF	901	GTP	N9-C4-N3	3.11	132.18	125.95
66	EF	901	GTP	C5-C6-N1	2.97	120.83	113.25
66	EF	901	GTP	C5'-C4'-C3'	-2.95	104.60	115.21
60	23	3001	SCM	C2M-C2-C3	-2.61	108.57	113.27
60	16	1602	SCM	C2M-C2-C3	-2.59	108.62	113.27
66	EF	901	GTP	C2'-C1'-N9	-2.47	106.38	113.25
66	EF	901	GTP	O6-C6-C5	-2.43	120.12	126.53
60	16	1601	SCM	C2M-C2-C3	-2.37	109.01	113.27
60	23	3001	SCM	O2B-C12-C7	2.37	113.19	108.23
66	EF	901	GTP	O3A-PB-O1B	-2.25	103.93	110.70
66	EF	901	GTP	C8-N7-C5	2.21	108.19	104.26
66	EF	901	GTP	C2'-C3'-C4'	-2.06	98.63	102.61

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
64	23	3003	ATP	C4'

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
64	23	3002	ATP	PB-O3B-PG-O3G
64	23	3002	ATP	O4'-C4'-C5'-O5'
64	23	3003	ATP	C5'-O5'-PA-O1A
64	23	3003	ATP	C5'-O5'-PA-O3A
66	EF	901	GTP	C5'-O5'-PA-O3A
61	23	3015	PUT	C1-C2-C3-C4
64	23	3003	ATP	O4'-C4'-C5'-O5'
65	23	3017	SPD	C3-C4-C5-N6
64	23	3003	ATP	C3'-C4'-C5'-O5'
64	23	3002	ATP	C3'-C4'-C5'-O5'
61	23	3016	PUT	C1-C2-C3-C4
61	23	3013	PUT	C1-C2-C3-C4
60	16	1601	SCM	C9-C10-N10-C1M
60	16	1601	SCM	C11-C10-N10-C1M
61	16	1605	PUT	N1-C1-C2-C3
65	23	3017	SPD	C8-C7-N6-C5
61	23	3007	PUT	C1-C2-C3-C4
61	LC	301	PUT	C1-C2-C3-C4
61	23	3006	PUT	C1-C2-C3-C4
61	23	3011	PUT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
61	16	1605	PUT	C1-C2-C3-C4
61	23	3007	PUT	N1-C1-C2-C3
61	23	3014	PUT	N1-C1-C2-C3
65	23	3017	SPD	C7-C8-C9-N10
61	23	3004	PUT	C1-C2-C3-C4
61	23	3012	PUT	C1-C2-C3-C4
66	EF	901	GTP	C5'-O5'-PA-O1A
65	23	3017	SPD	N1-C2-C3-C4
64	23	3003	ATP	C4'-C5'-O5'-PA
61	23	3013	PUT	C2-C3-C4-N2
61	23	3010	PUT	C2-C3-C4-N2
61	23	3015	PUT	C2-C3-C4-N2
64	23	3003	ATP	PB-O3B-PG-O3G
61	23	3012	PUT	N1-C1-C2-C3
61	23	3009	PUT	C1-C2-C3-C4
61	16	1605	PUT	C2-C3-C4-N2
61	23	3004	PUT	N1-C1-C2-C3
64	23	3003	ATP	O4'-C1'-N9-C8

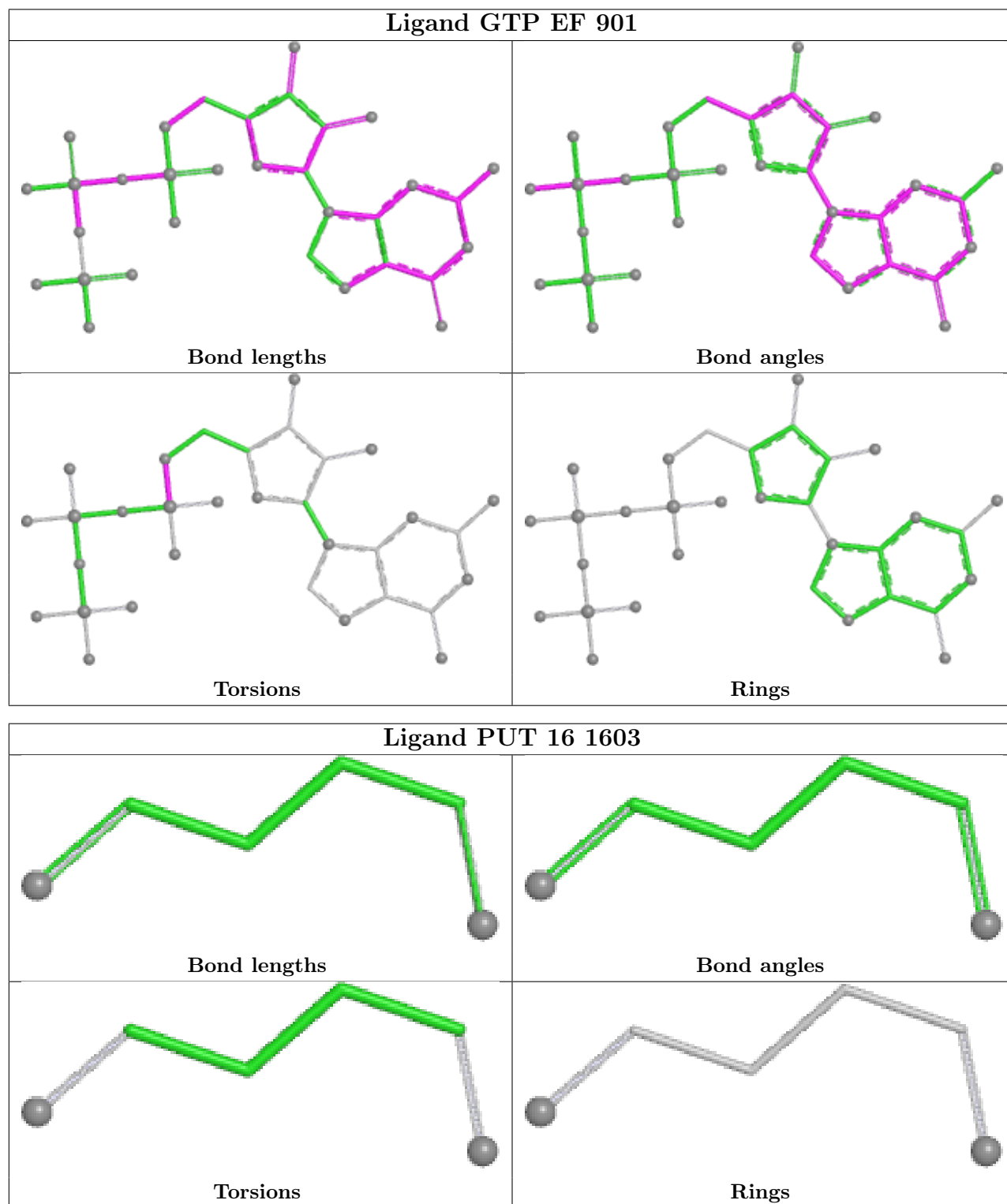
There are no ring outliers.

10 monomers are involved in 21 short contacts:

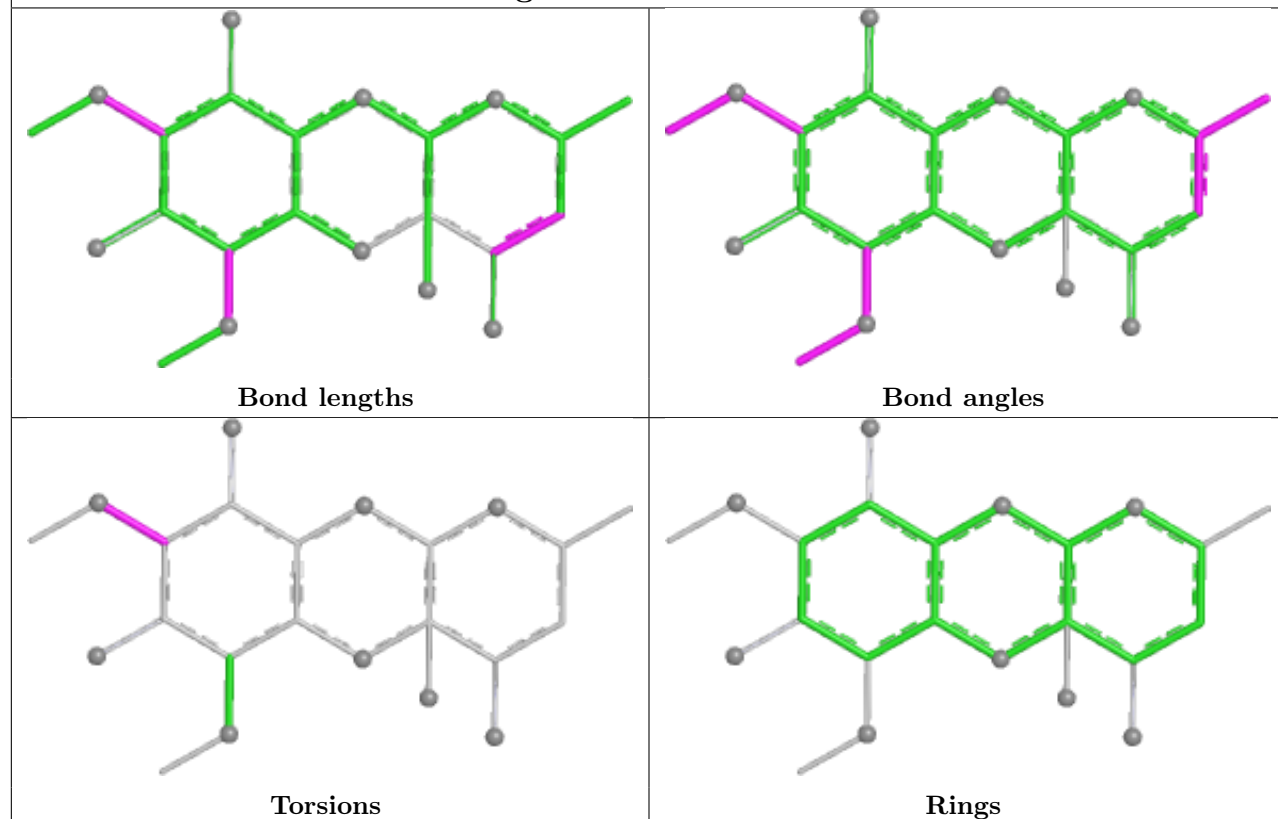
Mol	Chain	Res	Type	Clashes	Symm-Clashes
66	EF	901	GTP	7	0
61	16	1603	PUT	2	0
60	16	1601	SCM	1	0
61	23	3012	PUT	1	0
61	23	3015	PUT	1	0
61	23	3007	PUT	1	0
65	23	3017	SPD	5	0
60	23	3001	SCM	1	0
65	23	3018	SPD	1	0
61	LC	301	PUT	1	0

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

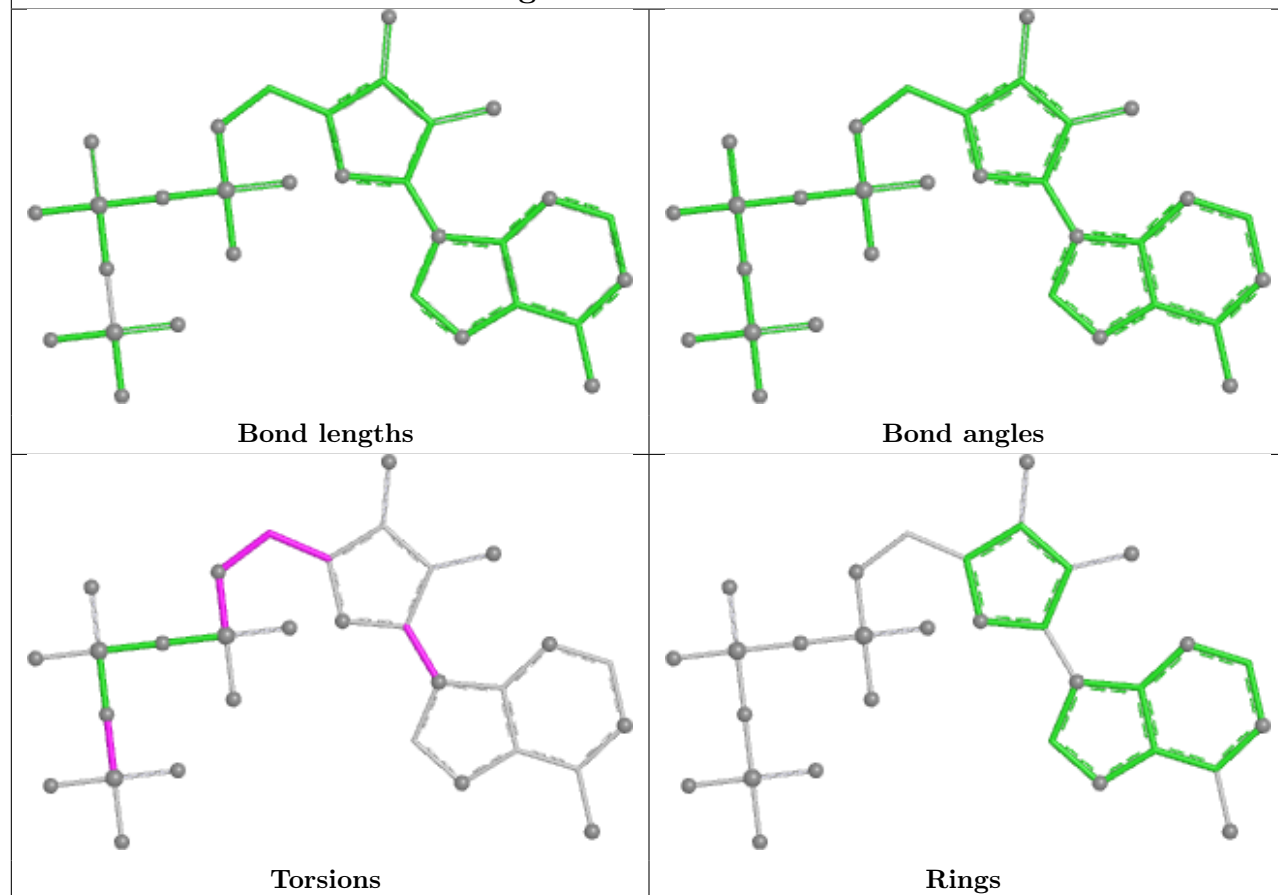
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

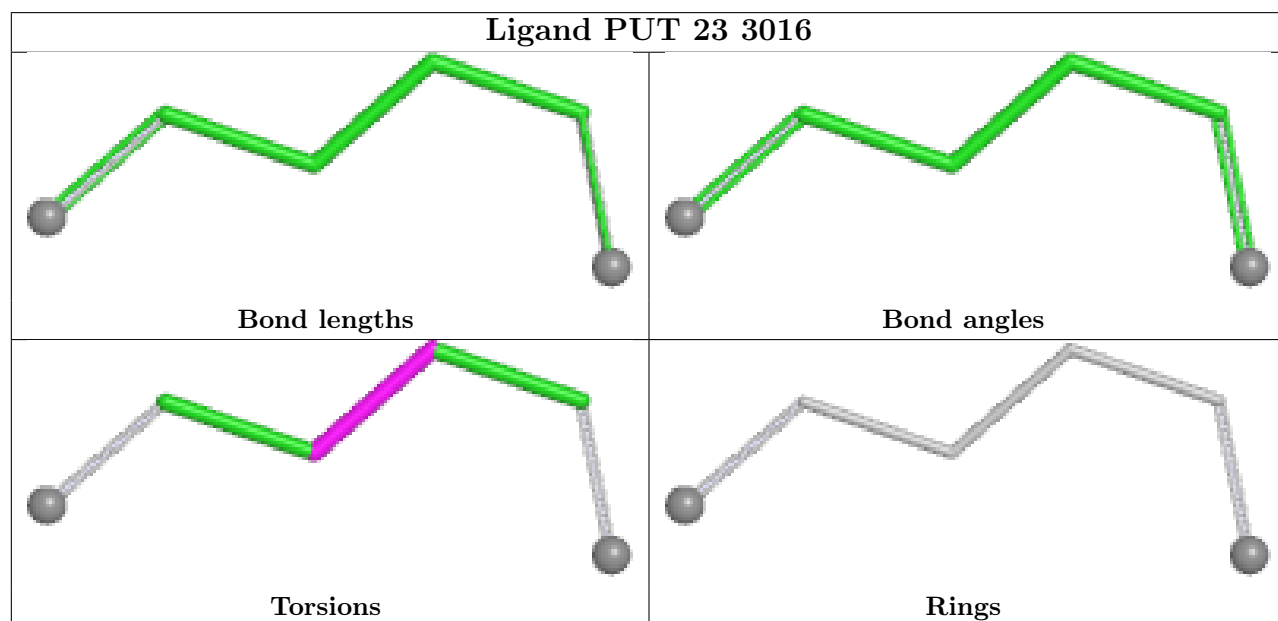
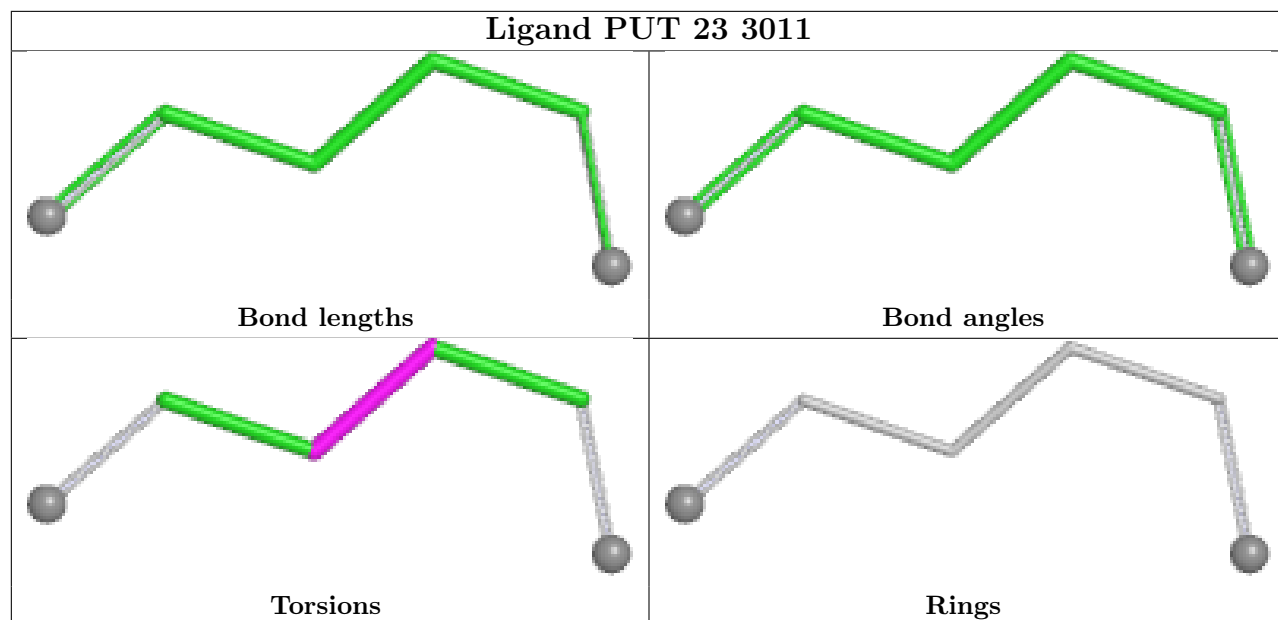


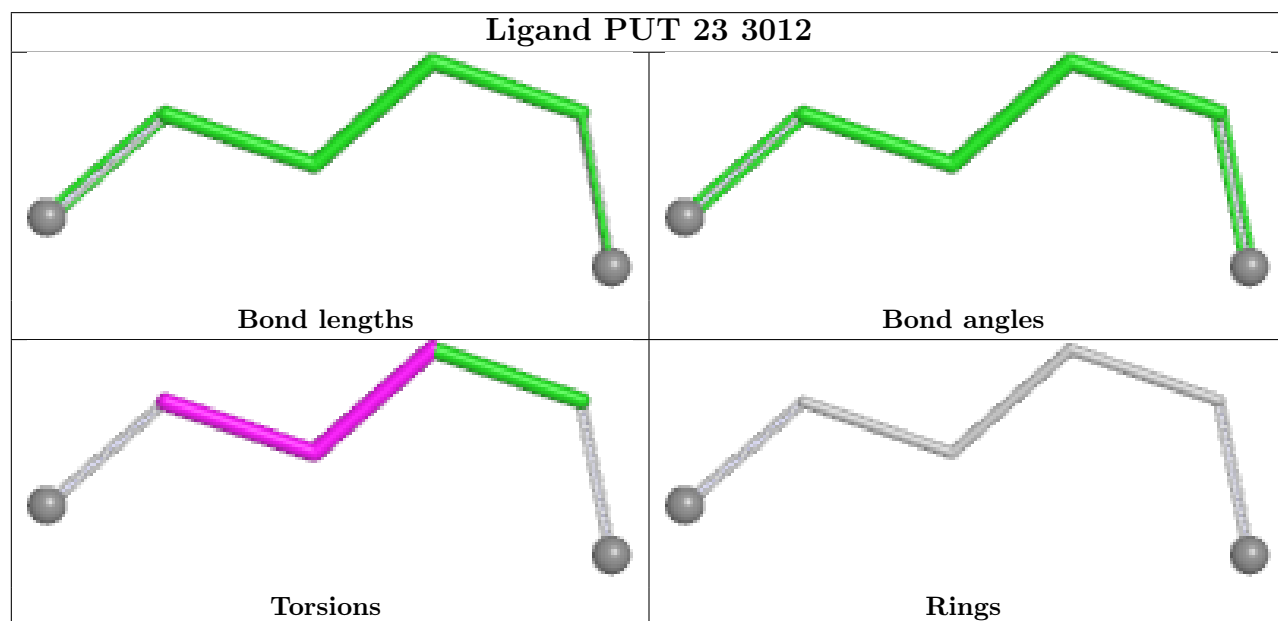
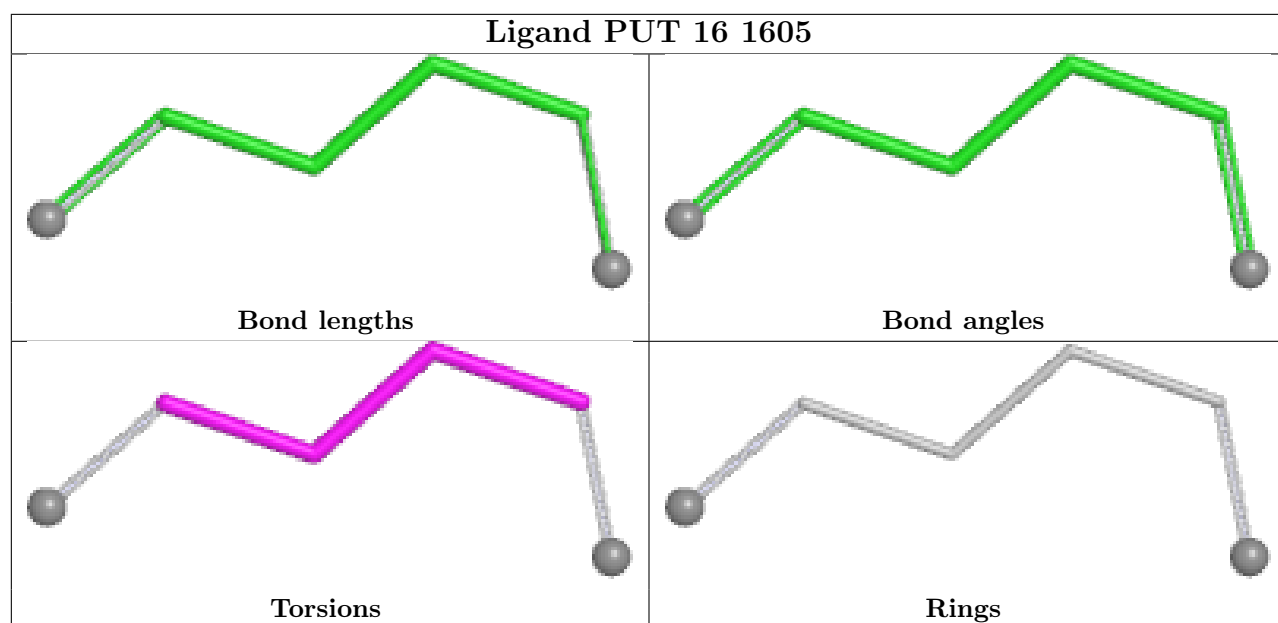
Ligand SCM 16 1601

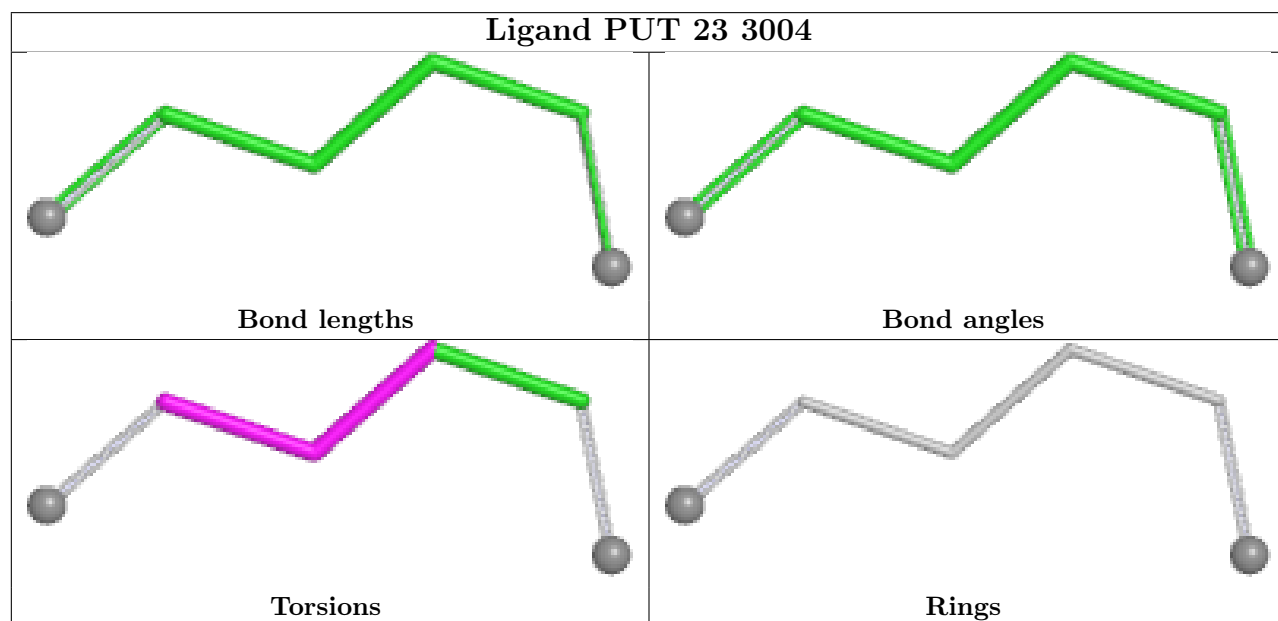
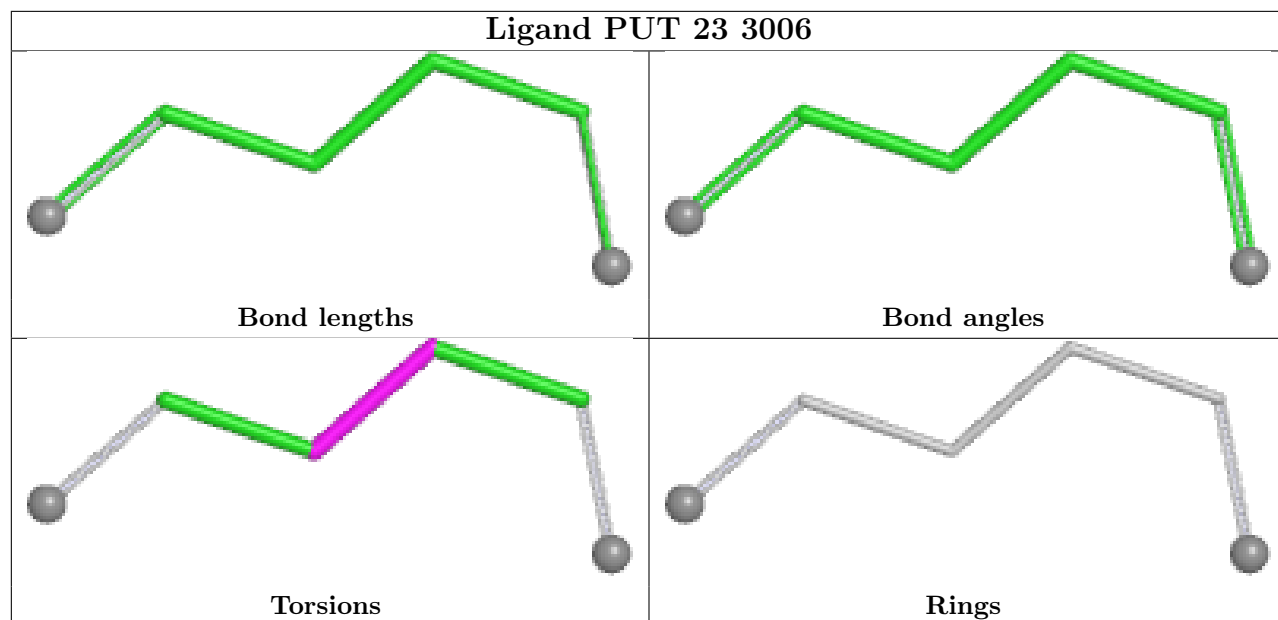


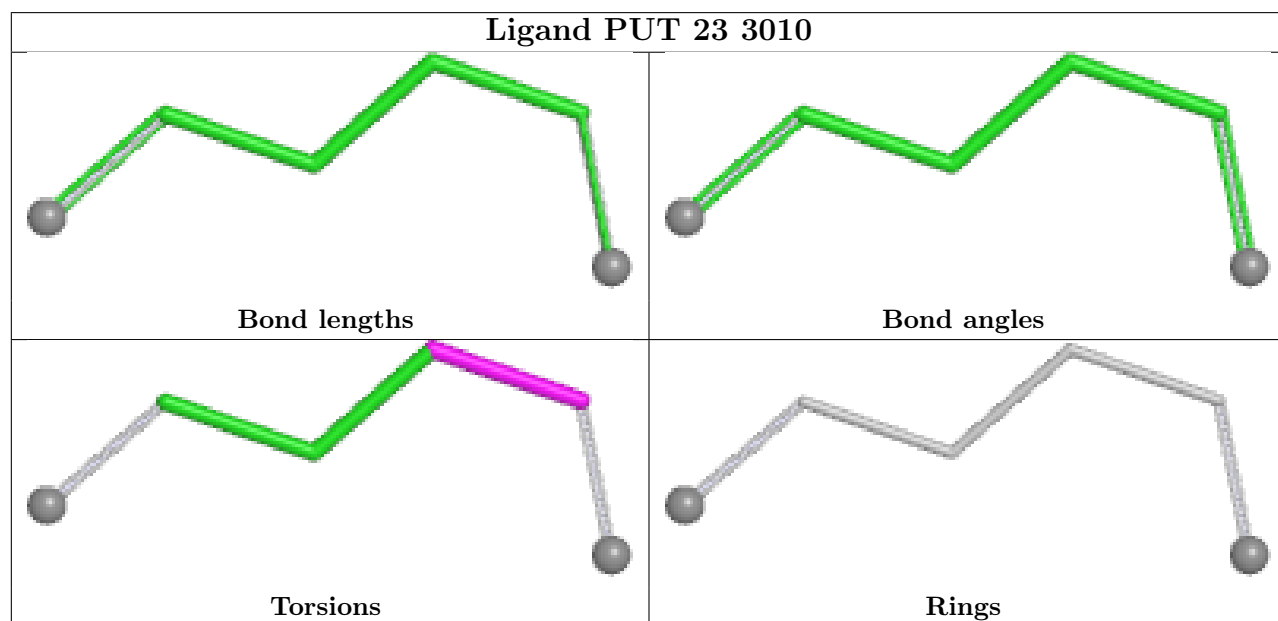
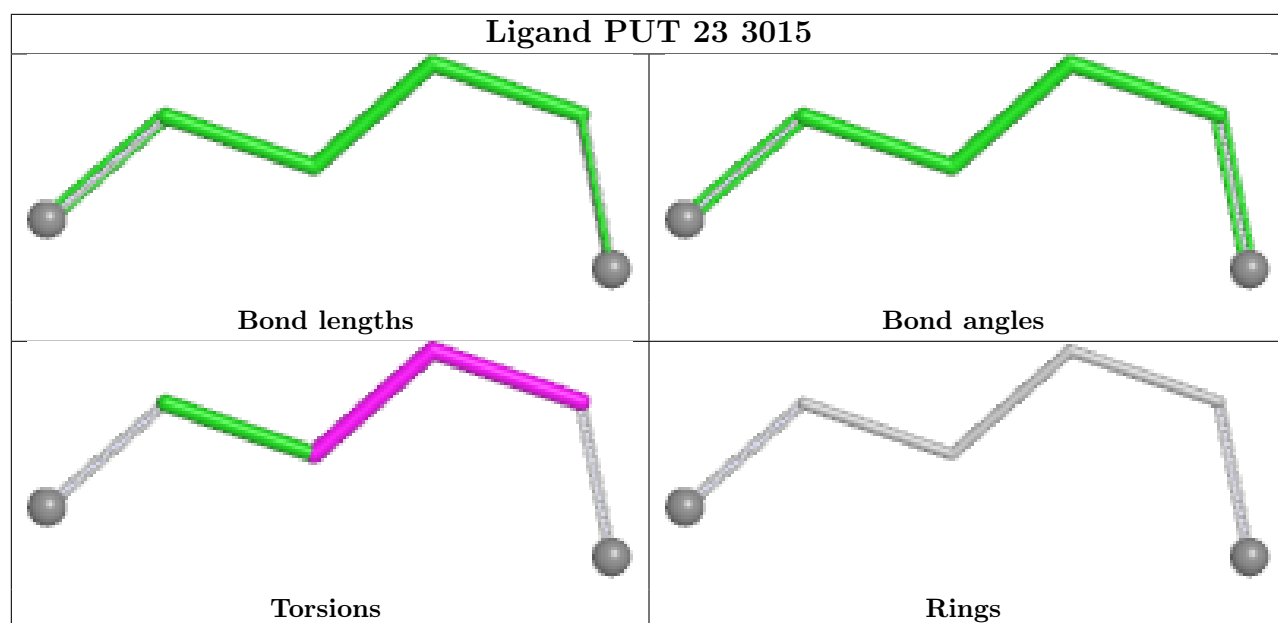
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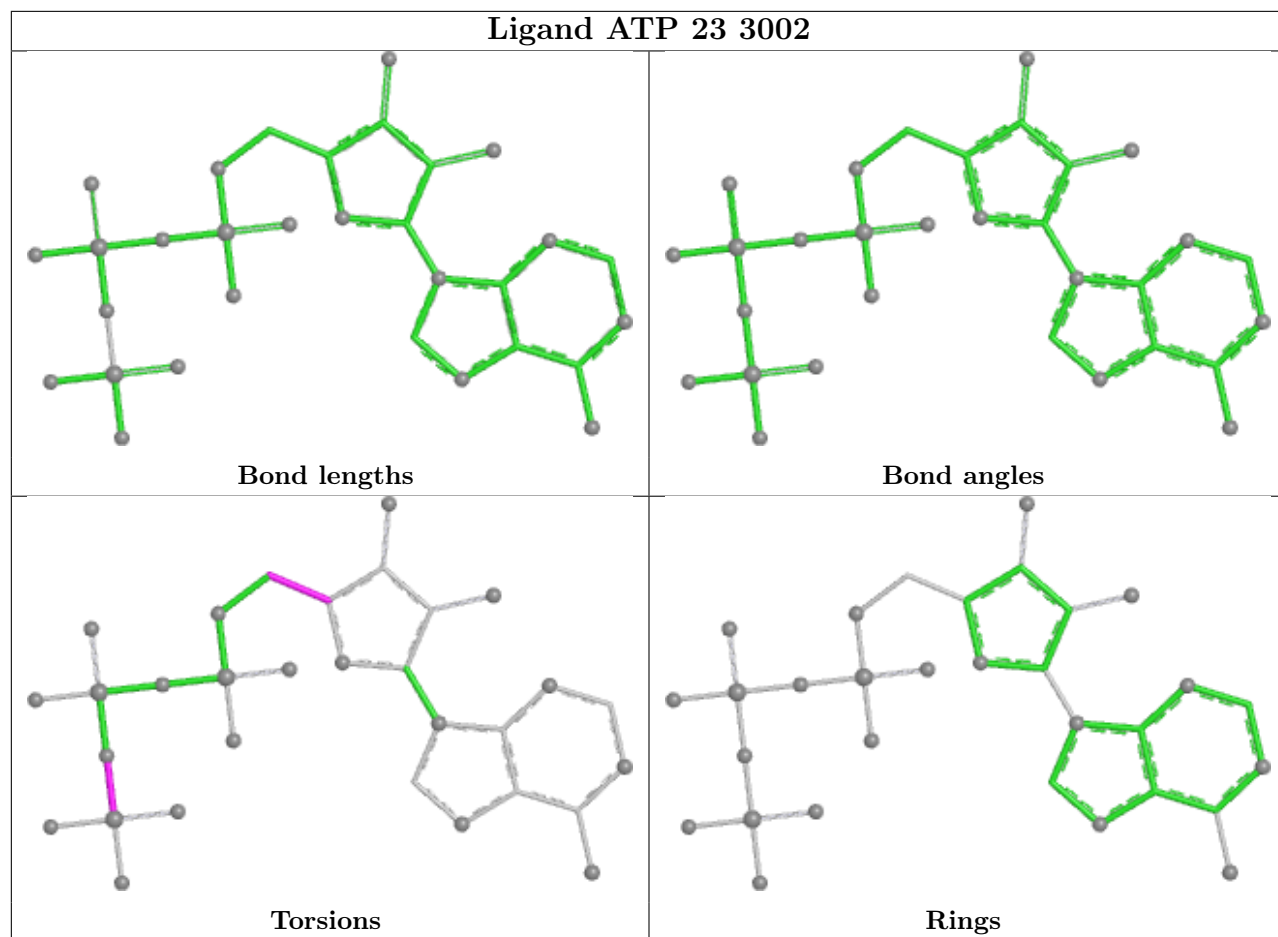




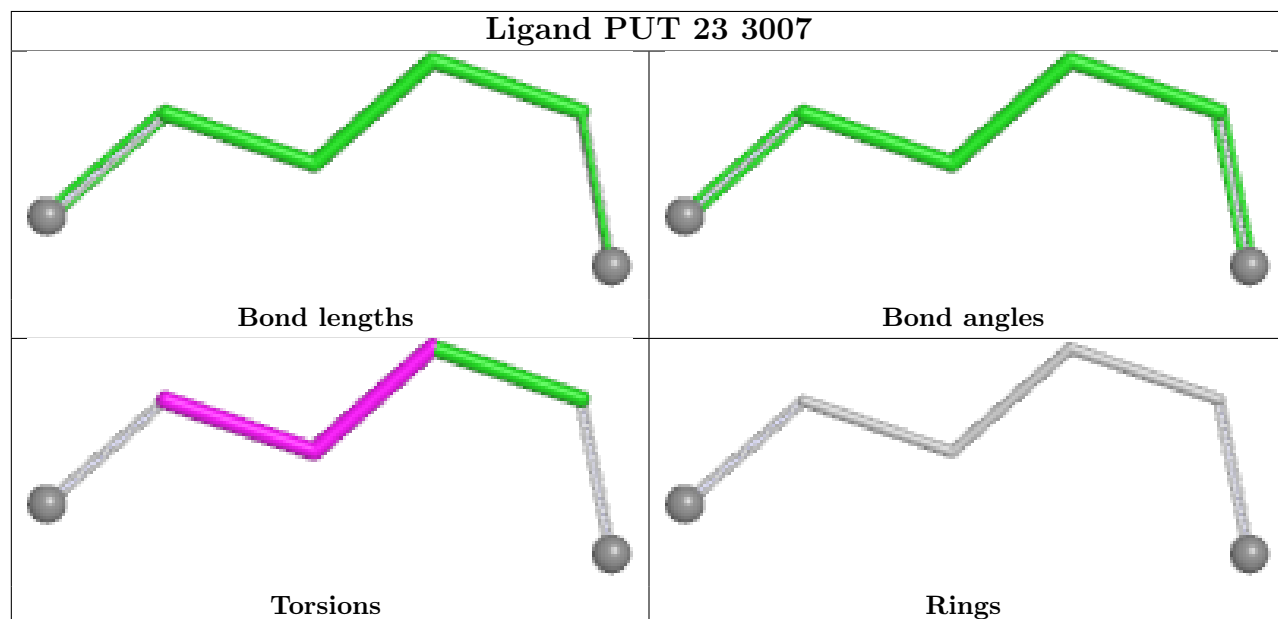




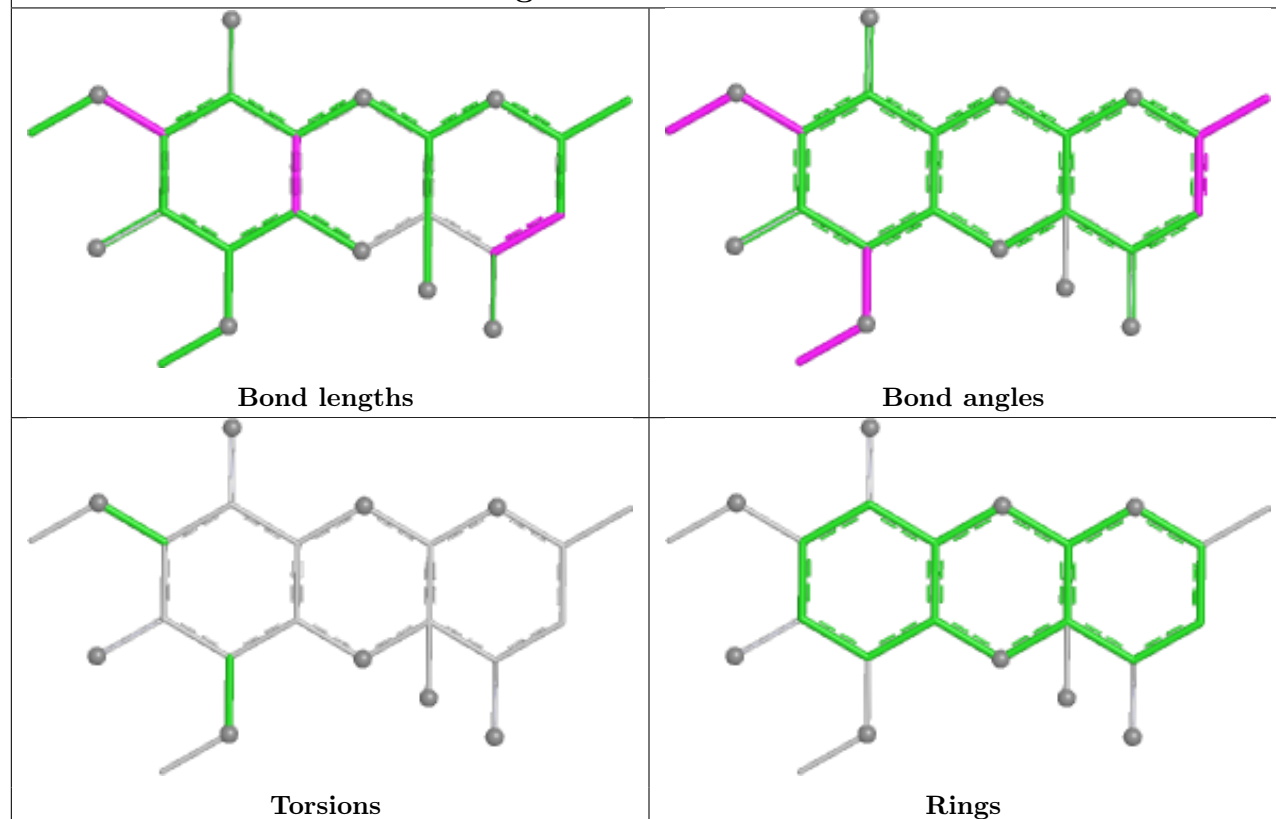
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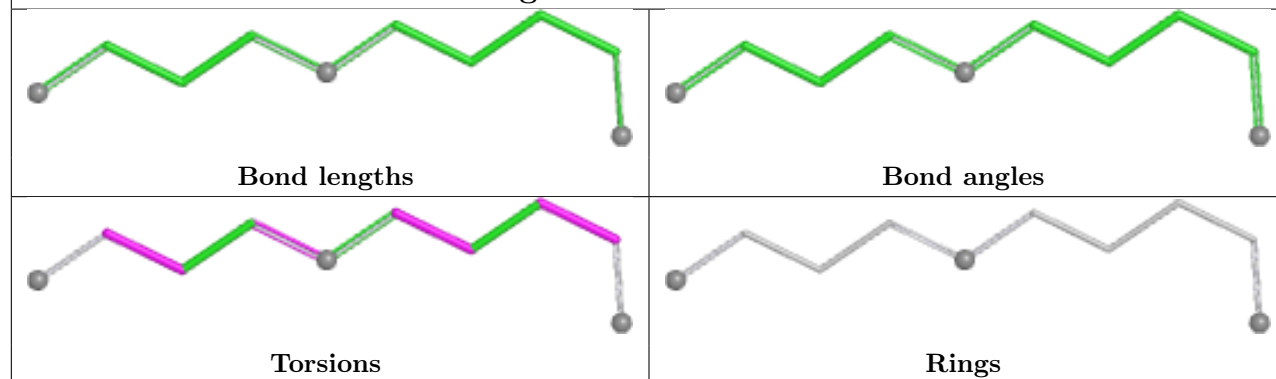
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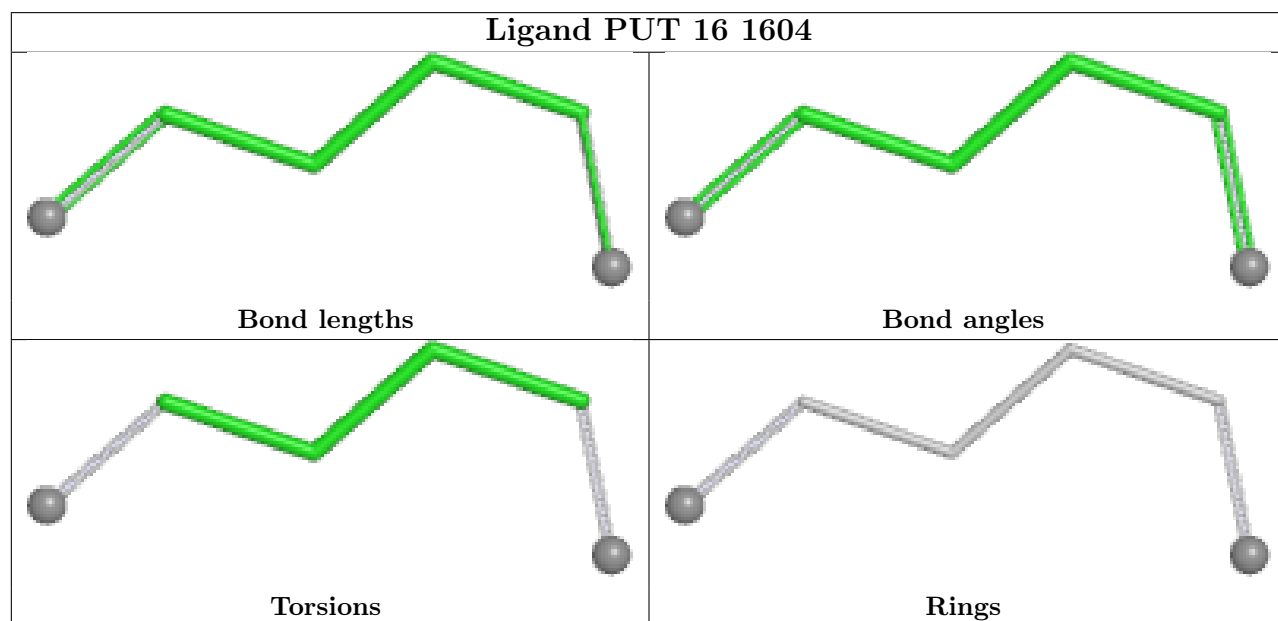
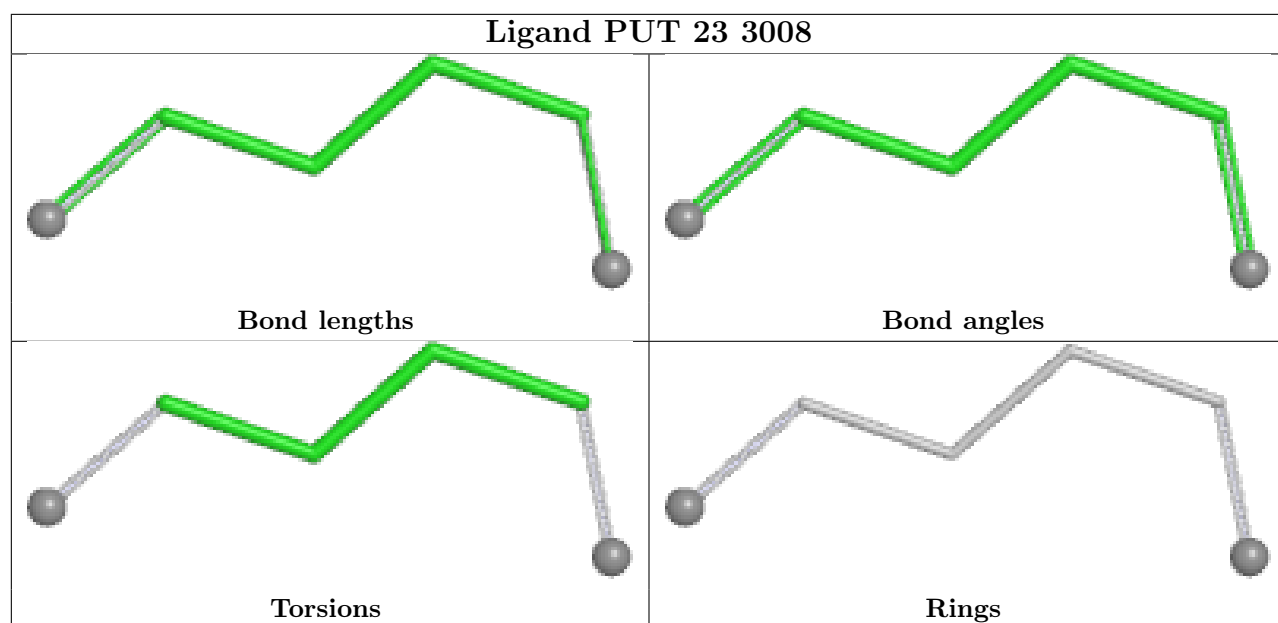


Ligand SCM 16 1602

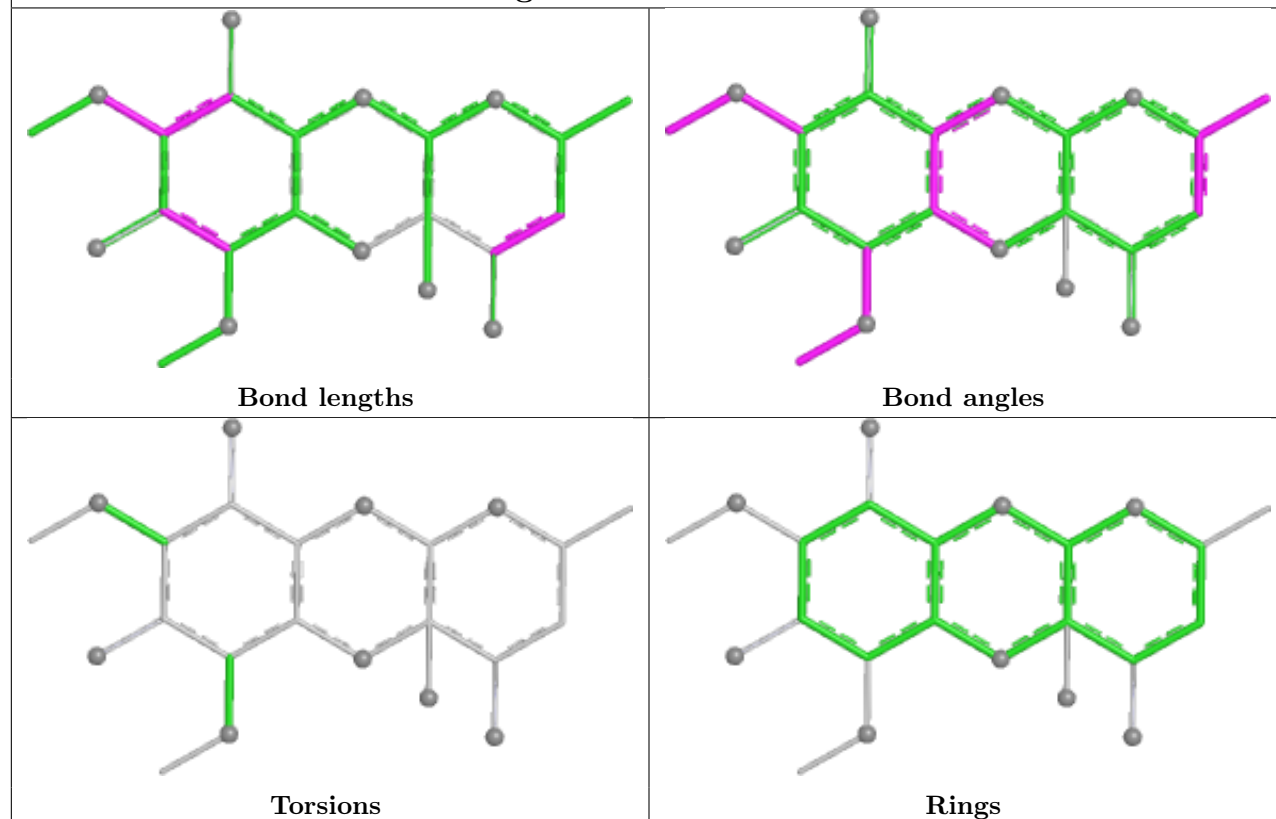


Ligand SPD 23 3017

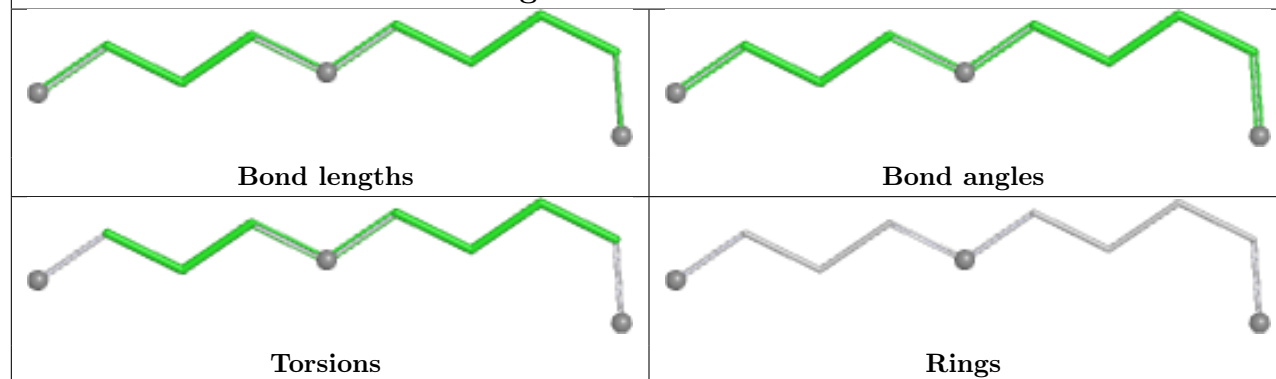


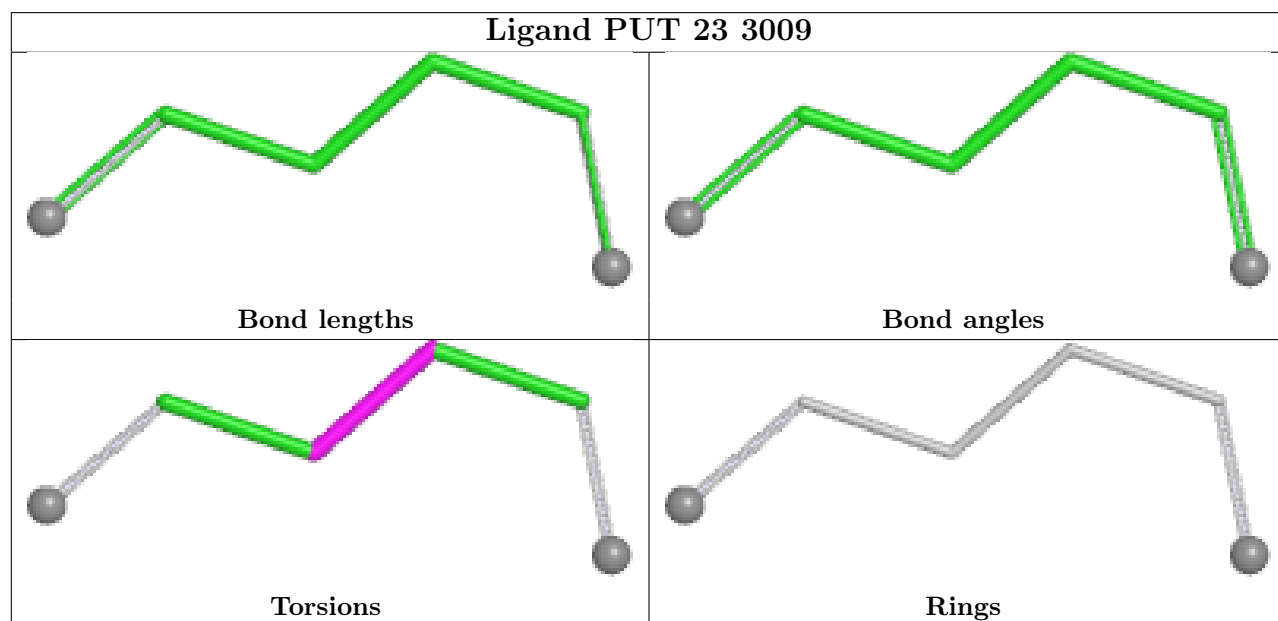
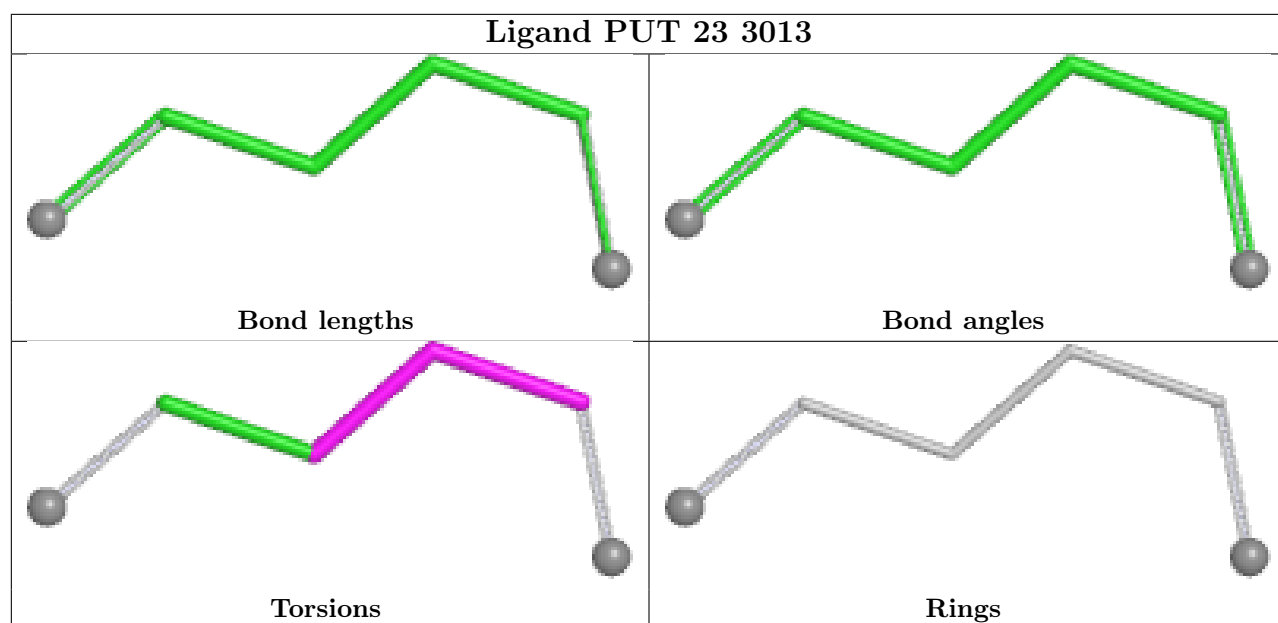


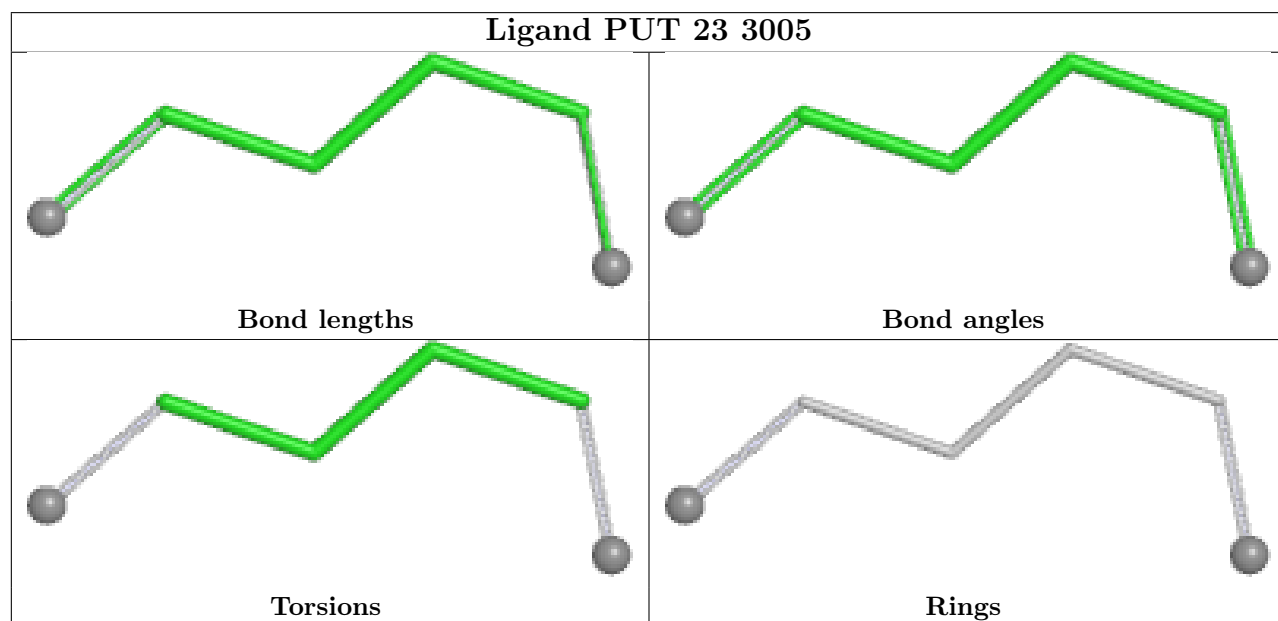
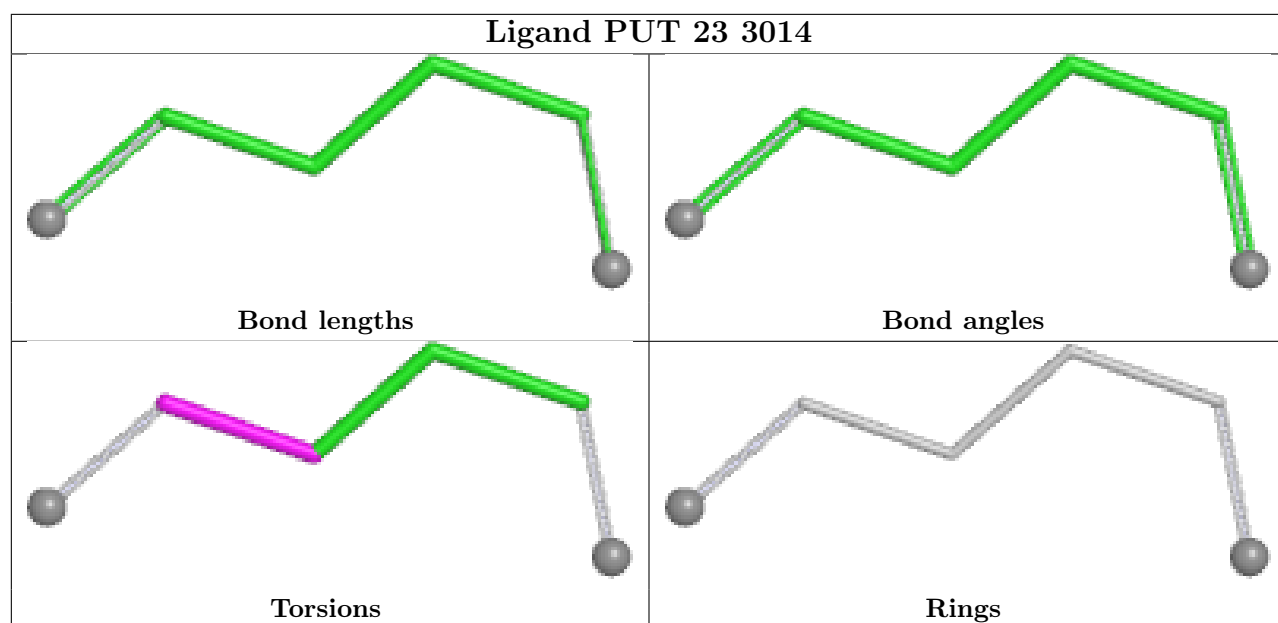
Ligand SCM 23 3001

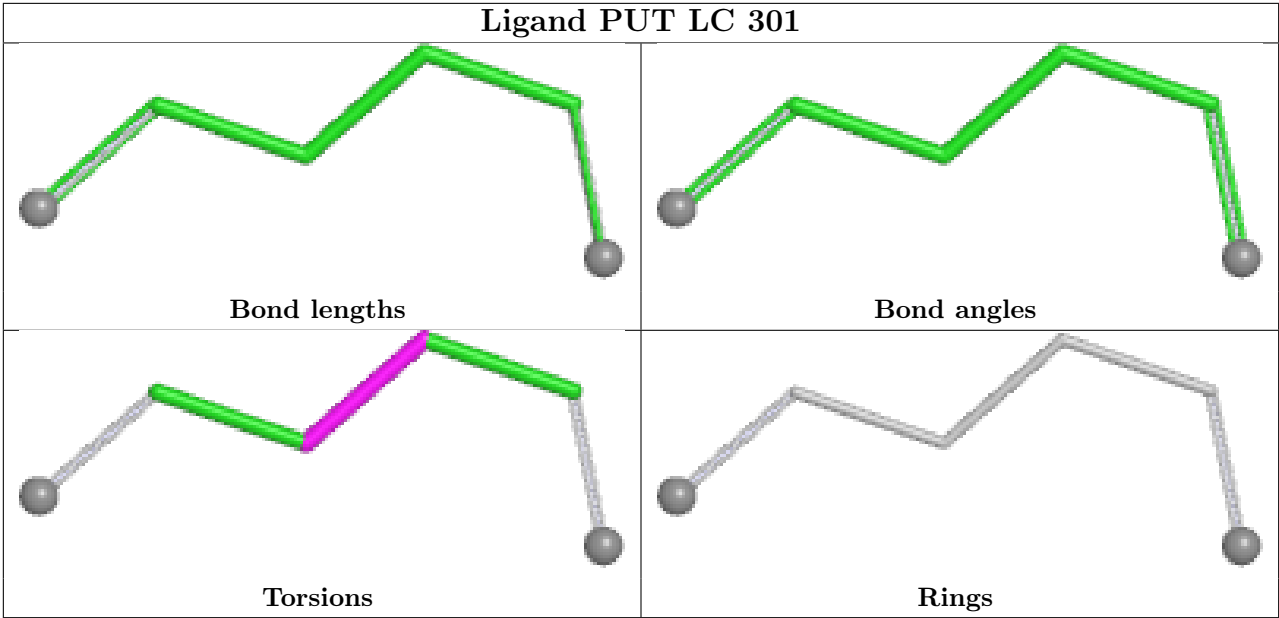


Ligand SPD 23 3018









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
28	LE	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	LE	93:GLY	C	94:GLU	N	1.14

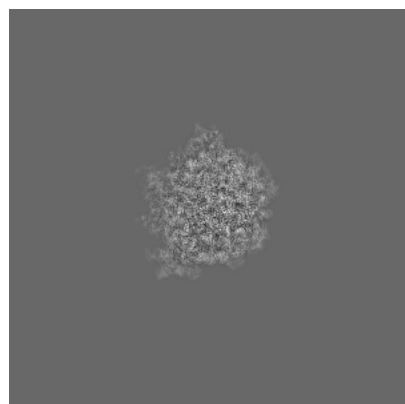
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24134. These allow visual inspection of the internal detail of the map and identification of artifacts.

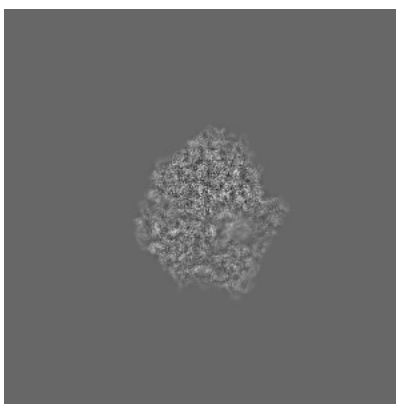
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

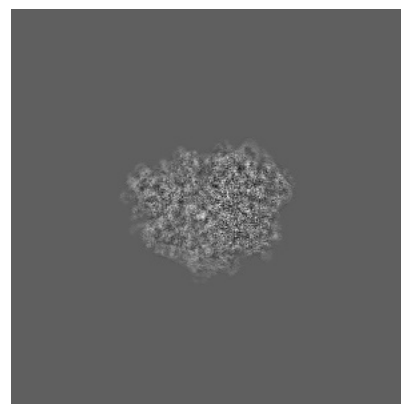
6.1.1 Primary map



X

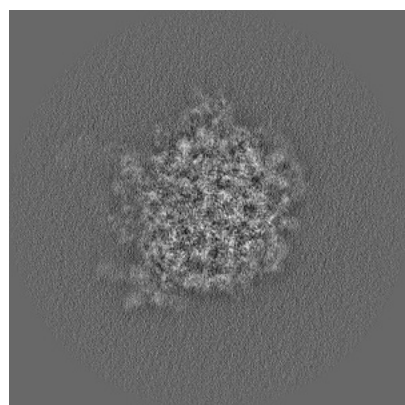


Y

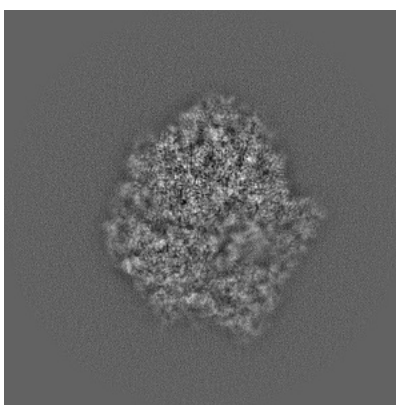


Z

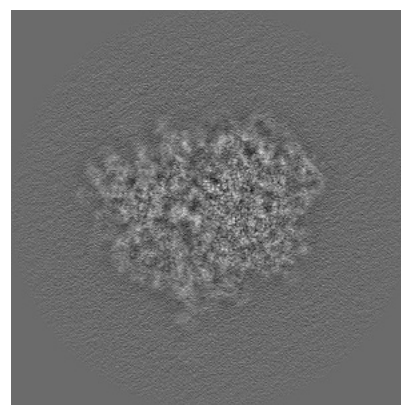
6.1.2 Raw map



X



Y

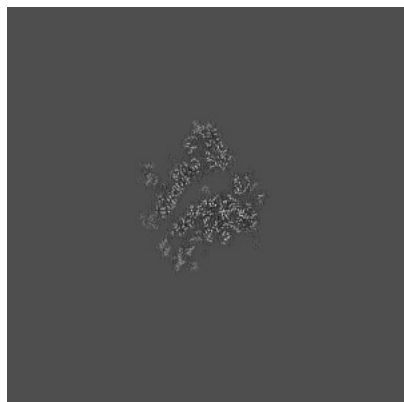


Z

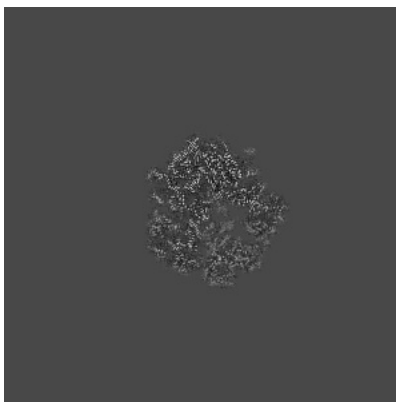
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

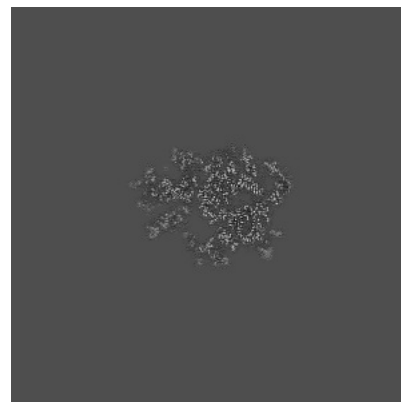
6.2.1 Primary map



X Index: 288

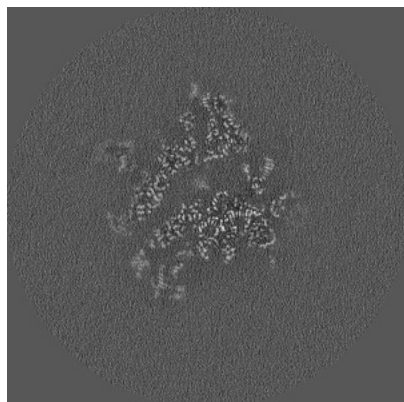


Y Index: 288

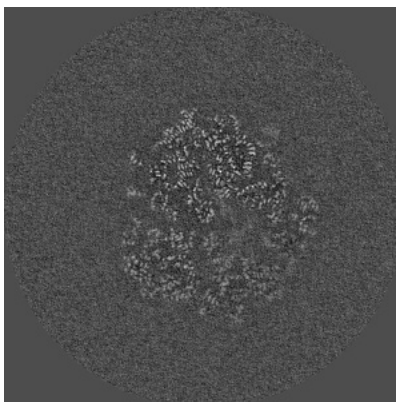


Z Index: 288

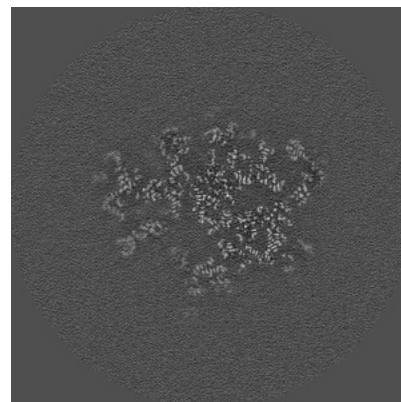
6.2.2 Raw map



X Index: 256



Y Index: 256

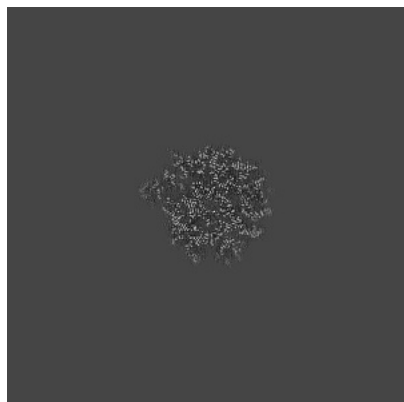


Z Index: 256

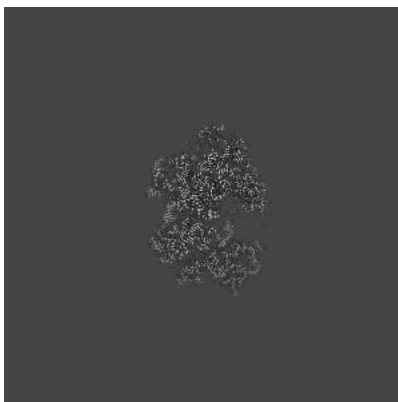
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

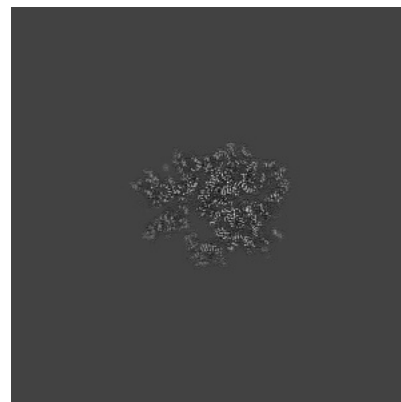
6.3.1 Primary map



X Index: 316

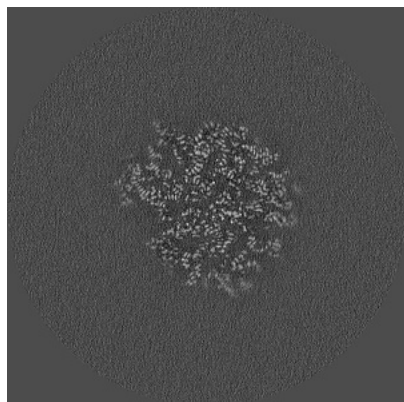


Y Index: 313

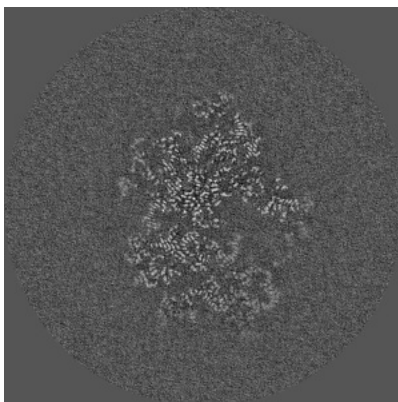


Z Index: 283

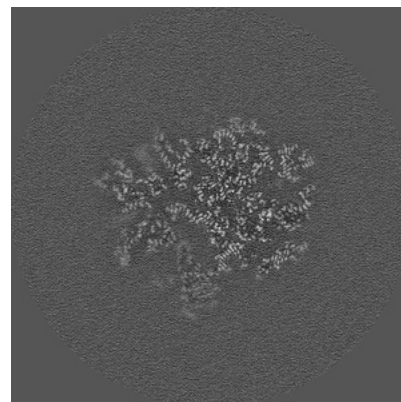
6.3.2 Raw map



X Index: 284



Y Index: 283

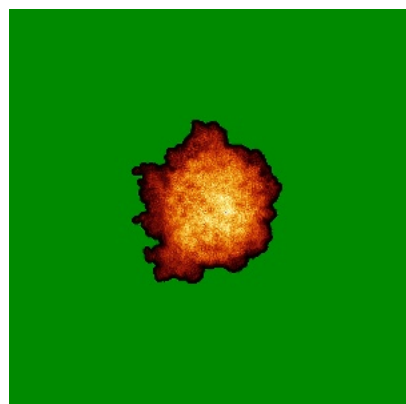


Z Index: 241

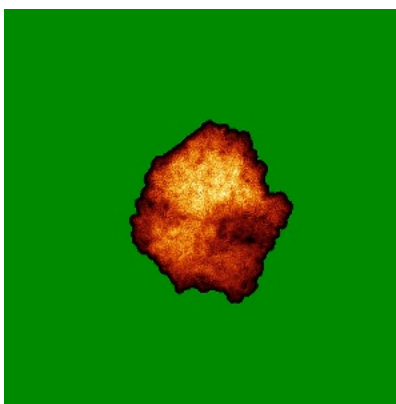
The images above show the largest variance slices of the map in three orthogonal directions.

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

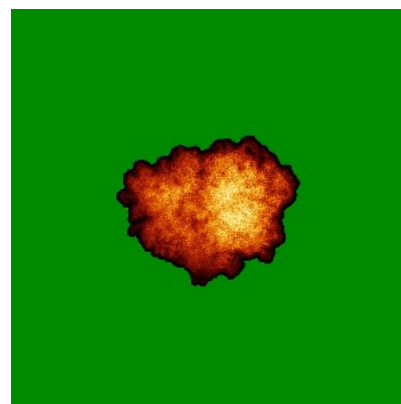
6.4.1 Primary map



X

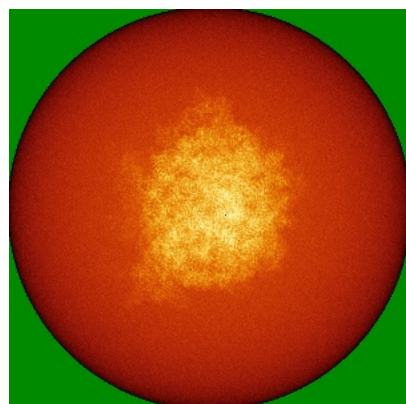


Y

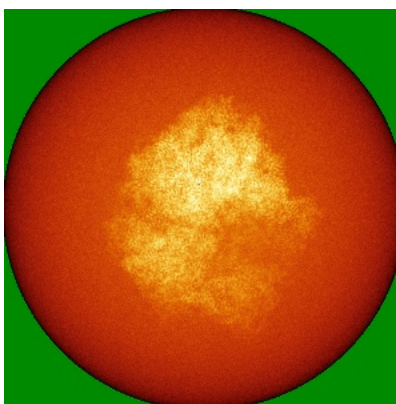


Z

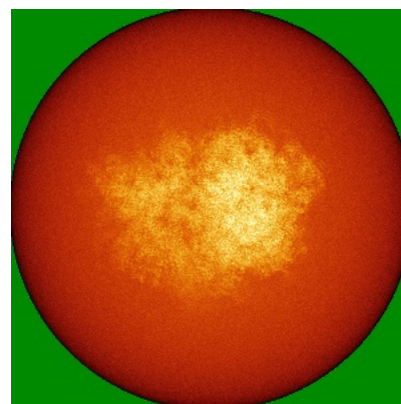
6.4.2 Raw map



X



Y

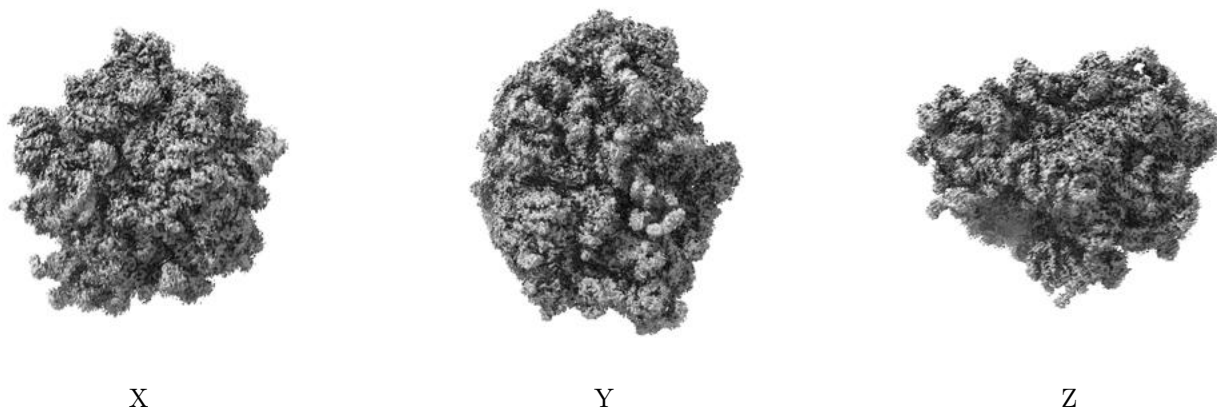


Z

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.

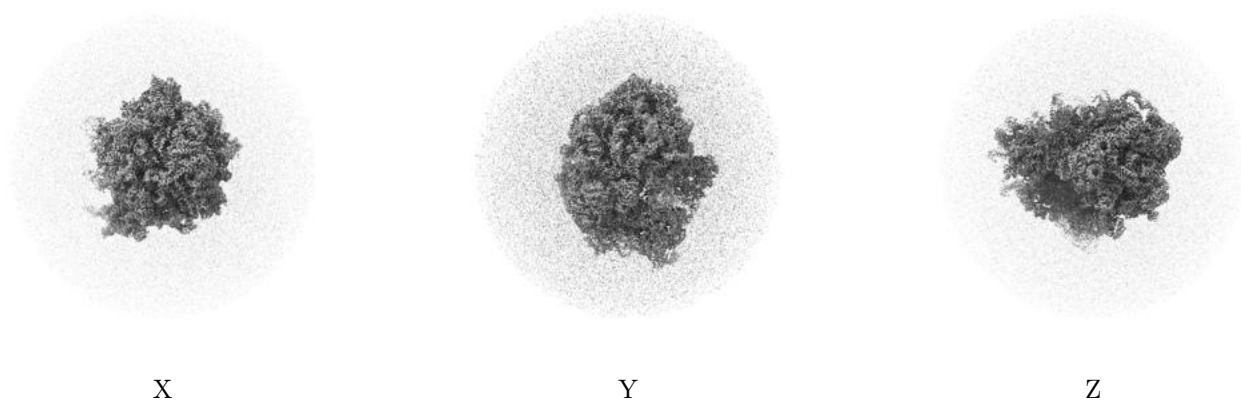
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

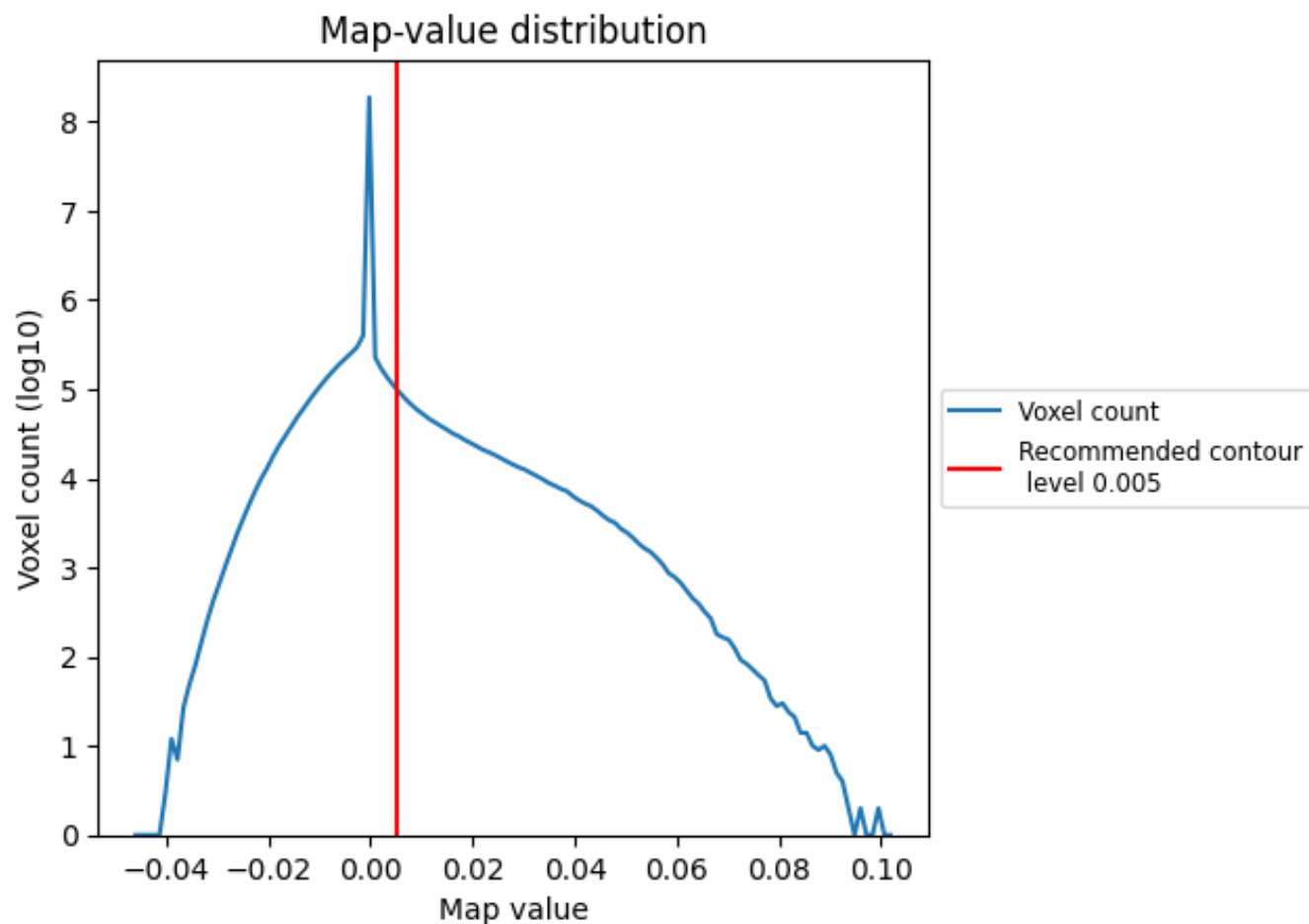
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

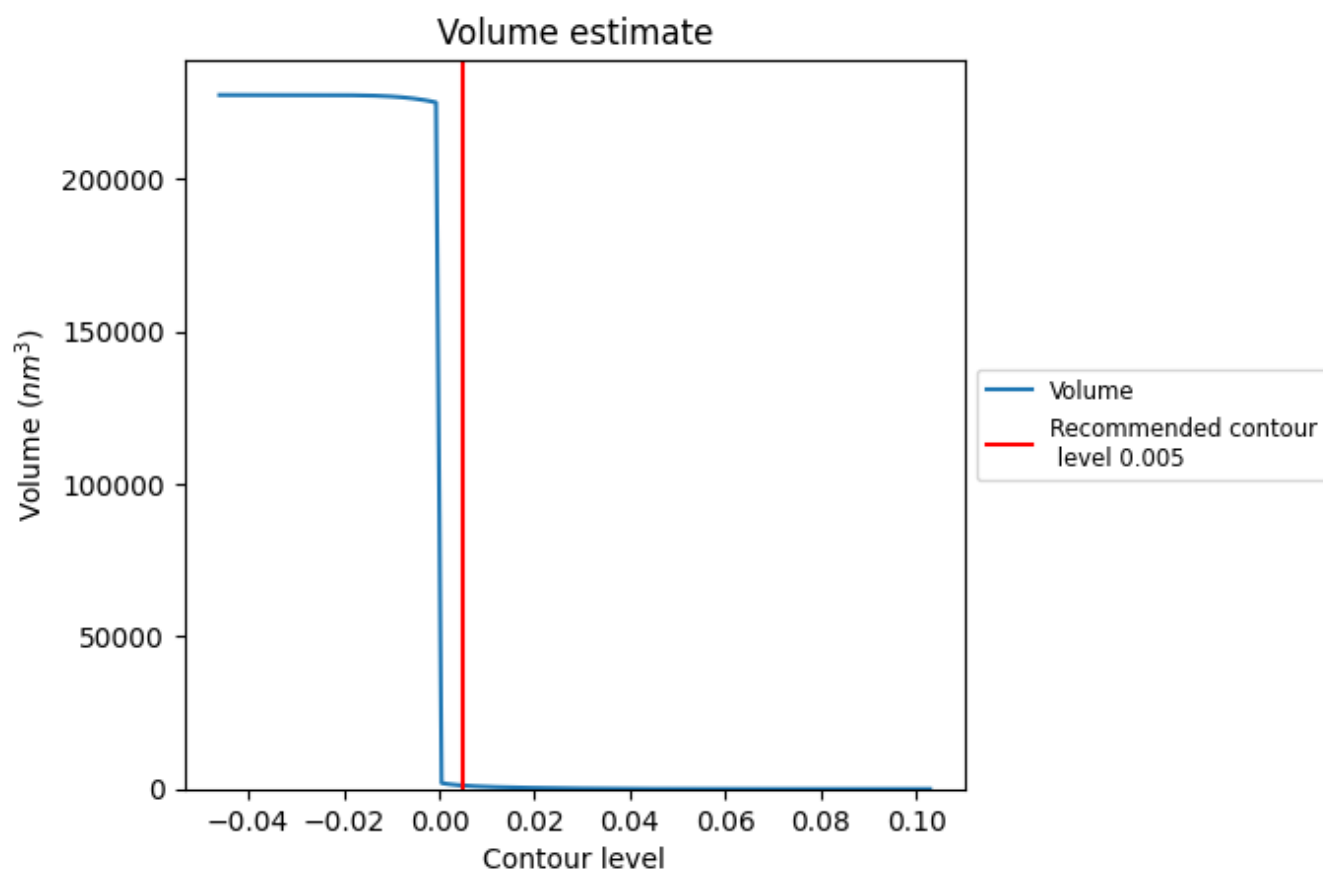
This section contains the results of statistical analysis of the map.

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.

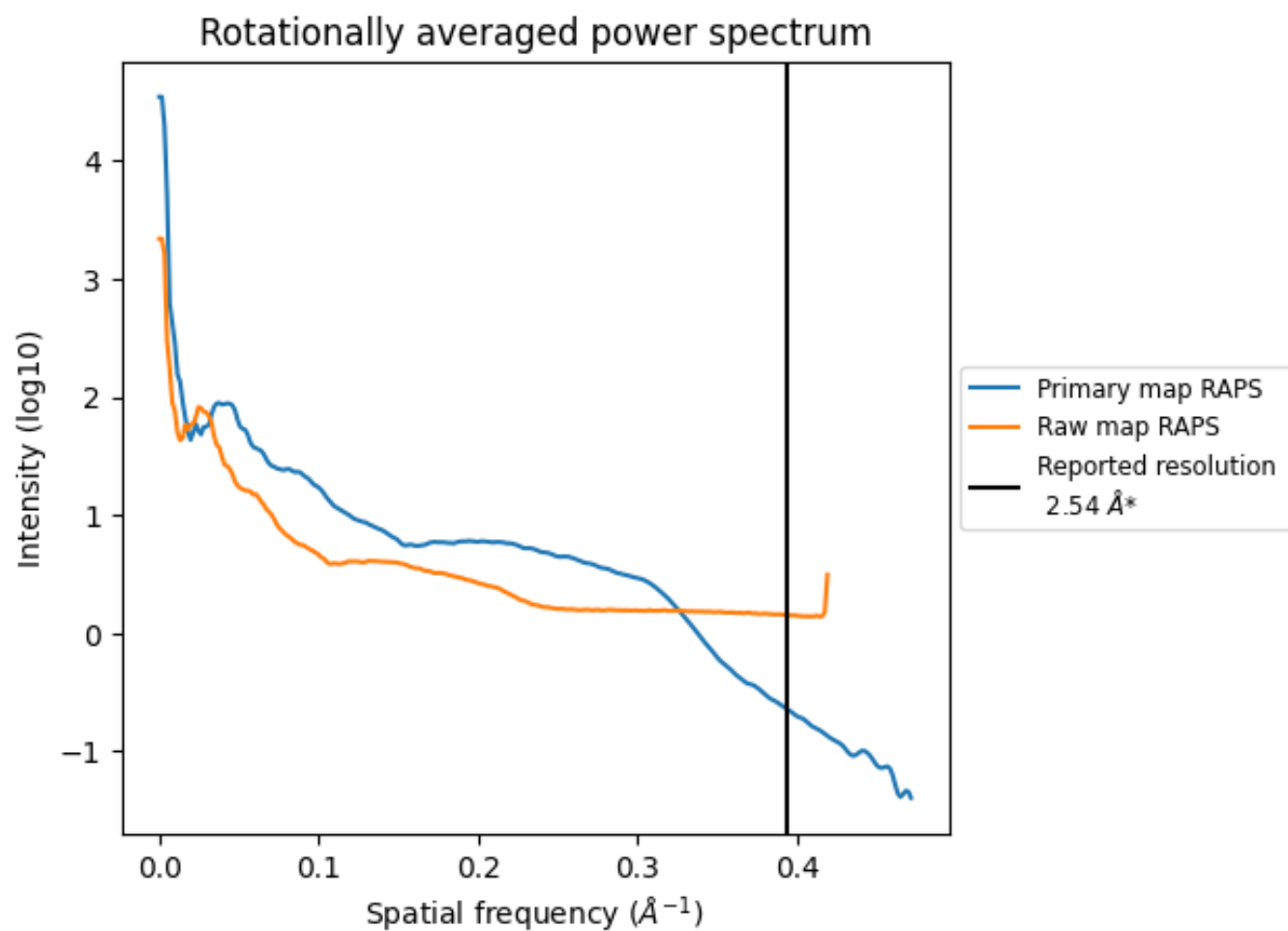
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1138 nm^3 ; this corresponds to an approximate mass of 1028 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

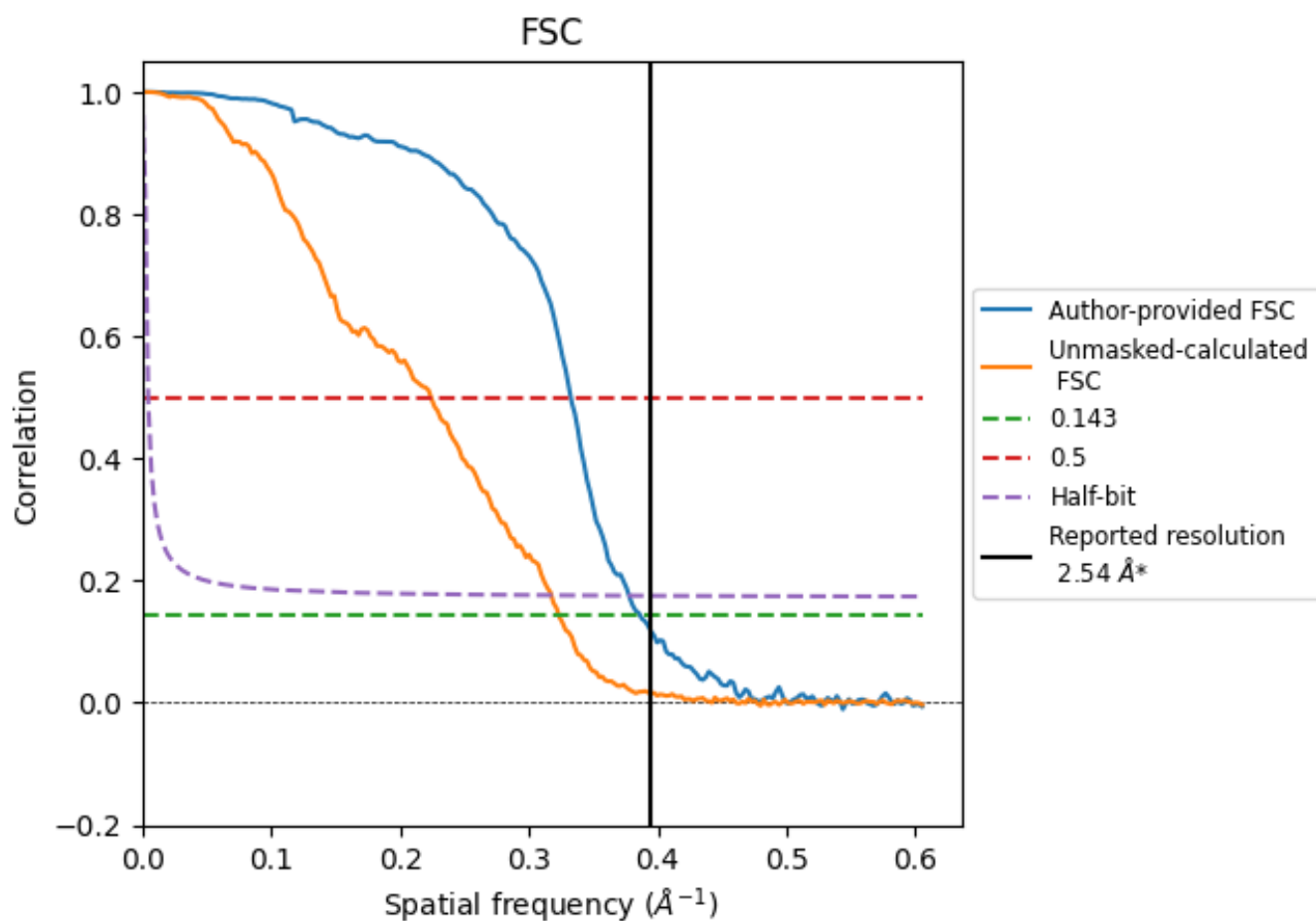


*Reported resolution corresponds to spatial frequency of 0.394 $\text{\AA}^{-1}$

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 $0.394 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

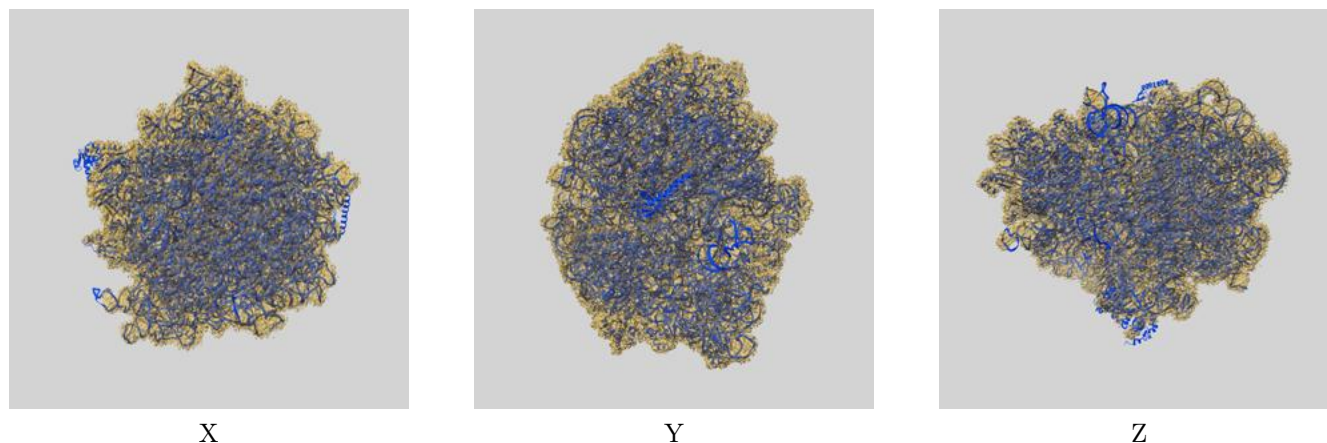
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.59	3.01	2.65
Unmasked-calculated*	3.09	4.46	3.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.09 differs from the reported value 2.54 by more than 10 %

9 Map-model fit [i](#)

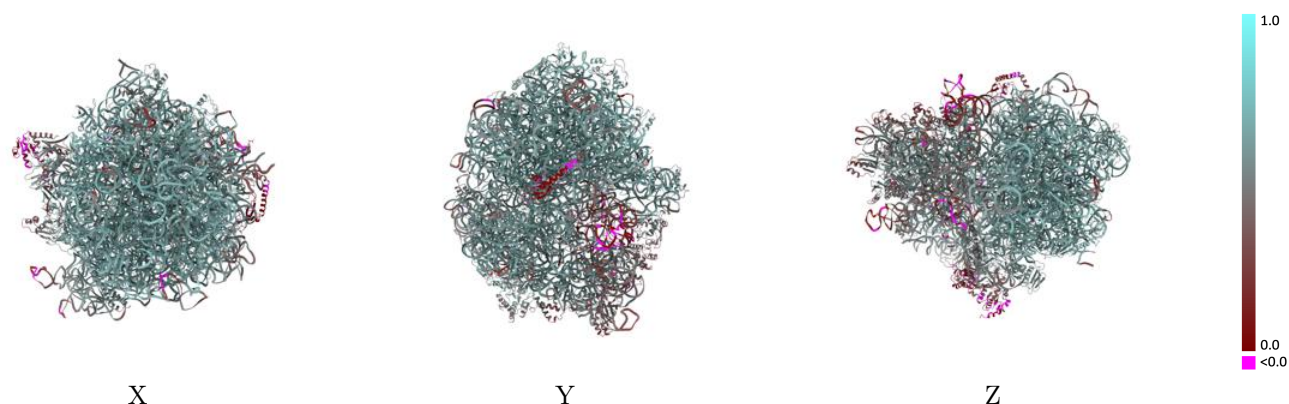
This section contains information regarding the fit between EMDB map EMD-24134 and PDB model 7N2V. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



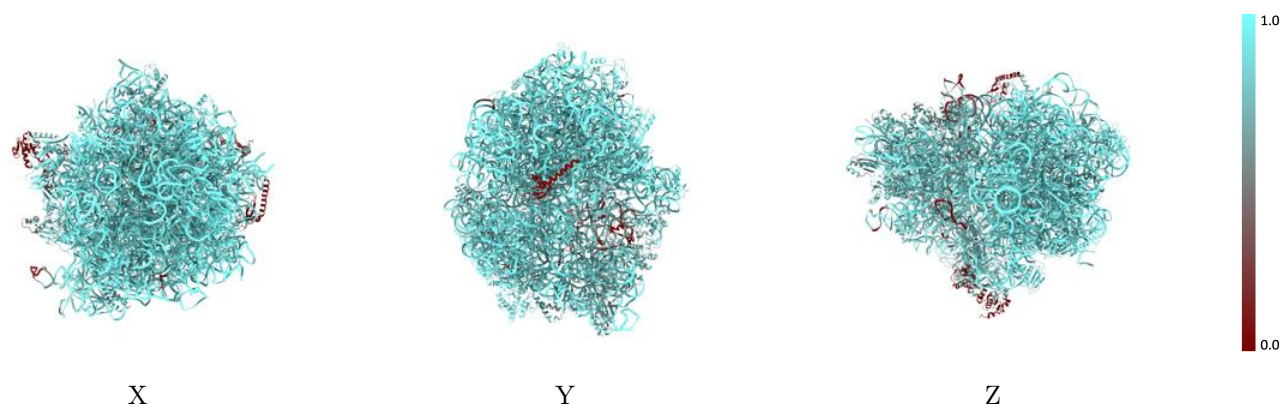
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



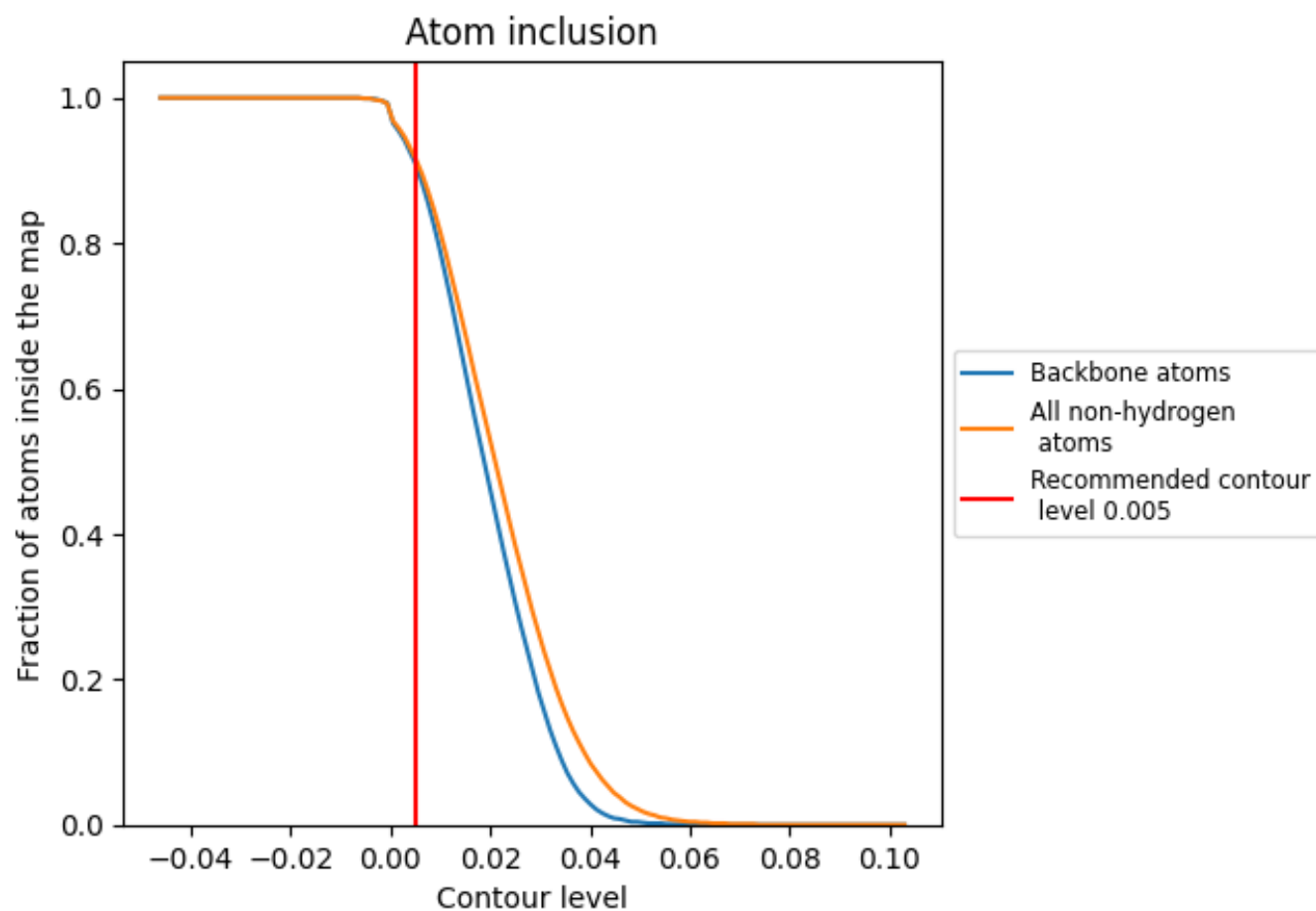
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 92% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9170	 0.5720
16	 0.9590	 0.5690
23	 0.9640	 0.6090
5	 0.9780	 0.6000
Dt	 0.8910	 0.4920
EF	 0.7830	 0.4930
LB	 0.9650	 0.6490
LC	 0.9550	 0.6400
LD	 0.9450	 0.6130
LE	 0.8080	 0.4680
LF	 0.9030	 0.5430
LI	 0.3000	 0.1740
LJ	 0.2670	 0.1690
LK	 0.2660	 0.1600
LM	 0.9600	 0.6430
LN	 0.9610	 0.6400
LO	 0.9560	 0.6290
LP	 0.9590	 0.6400
LQ	 0.9600	 0.6440
LR	 0.9110	 0.5740
LS	 0.9320	 0.6190
LT	 0.9710	 0.6620
LU	 0.9460	 0.6210
LV	 0.9450	 0.6390
LW	 0.9090	 0.5920
LX	 0.9260	 0.5800
LY	 0.9360	 0.5950
La	 0.9400	 0.6330
Lb	 0.9380	 0.6210
Lc	 0.8900	 0.5650
Ld	 0.9380	 0.6210
Le	 0.7840	 0.4100
Lf	 0.9390	 0.6280
Lg	 0.9040	 0.5960
Lh	 0.9470	 0.6590



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Chain	Atom inclusion	Q-score
Li	 0.9590	 0.6550
Lj	 0.9210	 0.6330
Pp	 0.7860	 0.5470
Pt	 0.6950	 0.3690
SB	 0.8530	 0.5020
SC	 0.8540	 0.5200
SD	 0.8650	 0.5320
SE	 0.9390	 0.6010
SF	 0.8910	 0.5170
SG	 0.6150	 0.3520
SH	 0.9460	 0.6090
SI	 0.7730	 0.4500
SJ	 0.7540	 0.4310
SK	 0.9130	 0.5740
SL	 0.9090	 0.5920
SM	 0.7760	 0.3940
SN	 0.8250	 0.4890
SO	 0.9190	 0.5860
SP	 0.8990	 0.5700
SQ	 0.8640	 0.5580
SR	 0.8740	 0.5590
SS	 0.7390	 0.4270
ST	 0.8780	 0.5560
SU	 0.8280	 0.5010
mR	 0.8780	 0.5250