



Full wwPDB EM Validation Report ⓘ

Jun 27, 2026 – 12:04 PM EDT

PDB ID : 9P9J / pdb_00009p9j
EMDB ID : EMD-71413
Title : In situ human 60S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-24
Resolution : 2.87 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

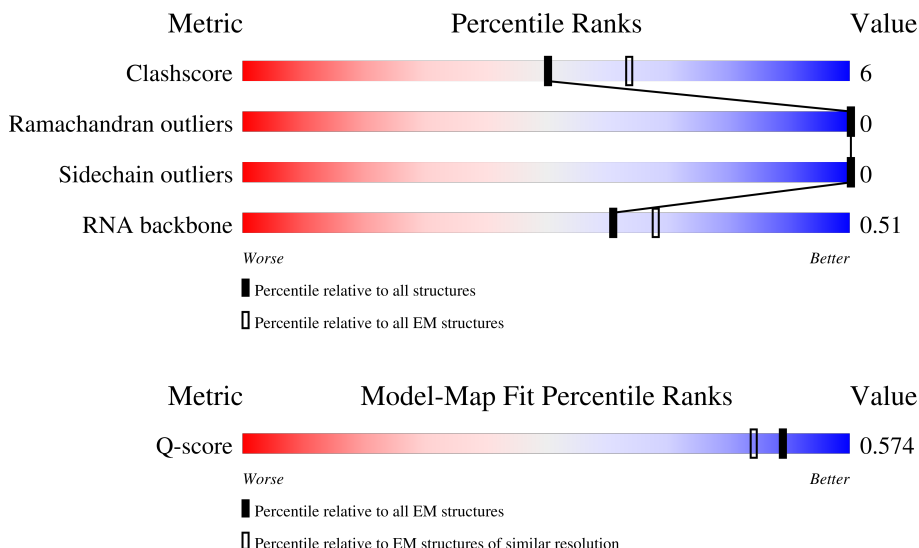
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 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.



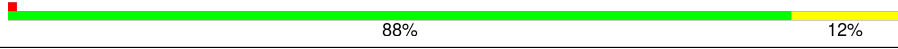
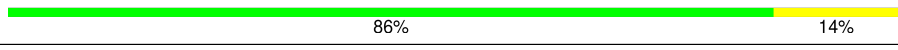
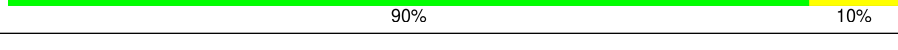
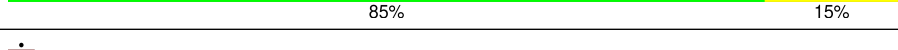
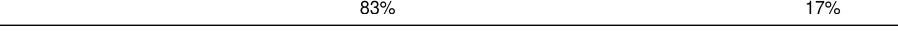
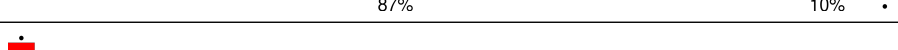
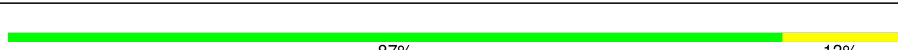
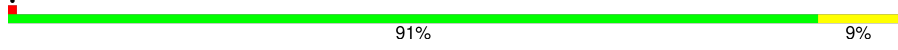
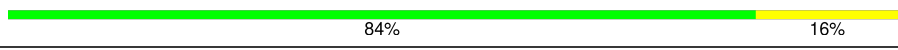
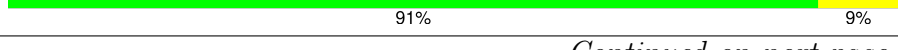
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12062 (2.37 - 3.37)

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	L5	3675	
2	L7	120	
3	L8	156	

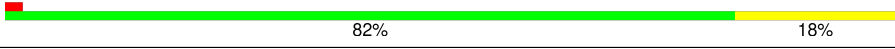
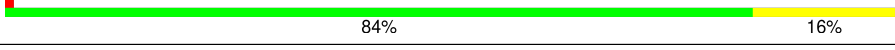
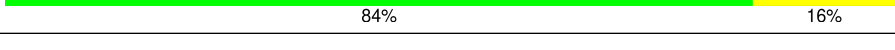
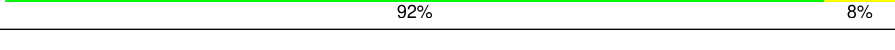
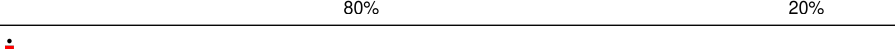
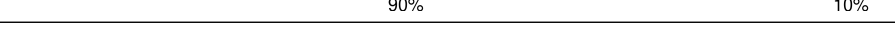
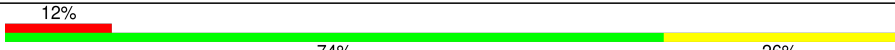
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Mol	Chain	Length	Quality of chain
4	LA	248	
5	LB	402	
6	LC	368	
7	LD	293	
8	LE	250	
9	LF	225	
10	LG	241	
11	LH	190	
12	LI	213	
13	LJ	176	
14	LL	210	
15	LM	139	
16	LN	203	
17	LO	201	
18	LP	153	
19	LQ	187	
20	LR	187	
21	LS	175	
22	LT	159	
23	LU	101	
24	LV	131	
25	LX	120	
26	LY	134	
27	LZ	135	
28	La	147	

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Mol	Chain	Length	Quality of chain
29	Lb	121	
30	Lc	98	
31	Ld	107	
32	Le	128	
33	Lf	109	
34	Lg	114	
35	Lh	122	
36	Li	102	
37	Lj	86	
38	Lk	69	
39	Ll	50	
40	Lm	52	
41	Lo	105	
42	Lp	91	
43	Lr	125	
44	CA	356	

2 Entry composition [i](#)

There are 48 unique types of molecules in this entry. The entry contains 139317 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 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L5	3655	Total	C	N	O	P	1	0
			78444	34968	14346	25475	3655		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L7	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 4 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 8 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	240	Total	C	N	O	S	0	0
			1935	1242	368	321	4		

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 11 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 12 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	213	Total	C	N	O	S	0	0
			1711	1082	329	285	15		

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 14 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 15 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 16 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 17 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 18 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 19 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	152	Total	C	N	O	S	0	0
			1273	793	275	196	9		

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 22 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 23 is a protein called Heparin-binding protein HBp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 24 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 25 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 26 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 27 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 28 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 29 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

- Molecule 30 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 31 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 32 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 33 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 34 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 35 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 36 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 37 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 38 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 39 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 40 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 41 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lo	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 42 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lp	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 43 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

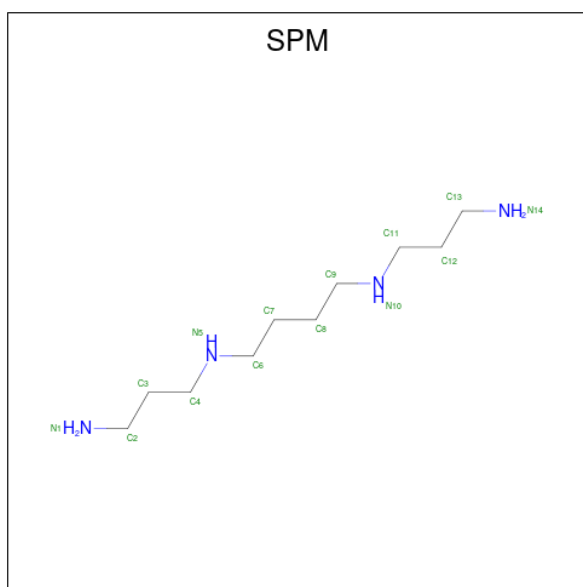
- Molecule 44 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	CA	354	Total	C	N	O	S	4	0
			2764	1744	475	528	17		

- Molecule 45 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

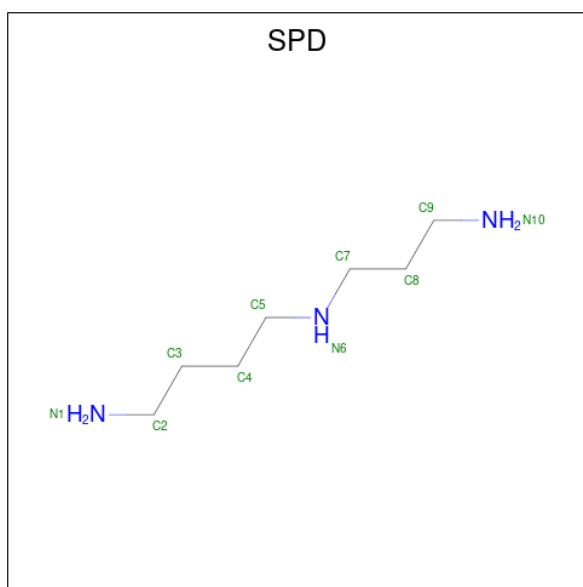
Mol	Chain	Residues	Atoms		AltConf
45	L5	178	Total	Mg	0
			178	178	
45	L7	3	Total	Mg	0
			3	3	
45	L8	5	Total	Mg	0
			5	5	
45	LA	1	Total	Mg	0
			1	1	
45	LI	1	Total	Mg	0
			1	1	
45	LP	1	Total	Mg	0
			1	1	
45	LV	1	Total	Mg	0
			1	1	
45	Le	1	Total	Mg	0
			1	1	

- Molecule 46 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
46	L5	1	Total	C	N	0
			14	10	4	
46	L5	1	Total	C	N	0
			14	10	4	
46	L5	1	Total	C	N	0
			14	10	4	
46	L5	1	Total	C	N	0
			14	10	4	
46	L5	1	Total	C	N	0
			14	10	4	
46	L5	1	Total	C	N	0
			14	10	4	

- Molecule 47 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
47	L5	1	Total	C	N	0
			10	7	3	
47	L5	1	Total	C	N	0
			10	7	3	
47	L5	1	Total	C	N	0
			10	7	3	
47	L5	1	Total	C	N	0
			10	7	3	
47	L5	1	Total	C	N	0
			10	7	3	
47	L5	1	Total	C	N	0
			10	7	3	
47	L5	1	Total	C	N	0
			10	7	3	
47	LN	1	Total	C	N	0
			10	7	3	

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
48	Lg	1	Total	Zn	0
			1	1	

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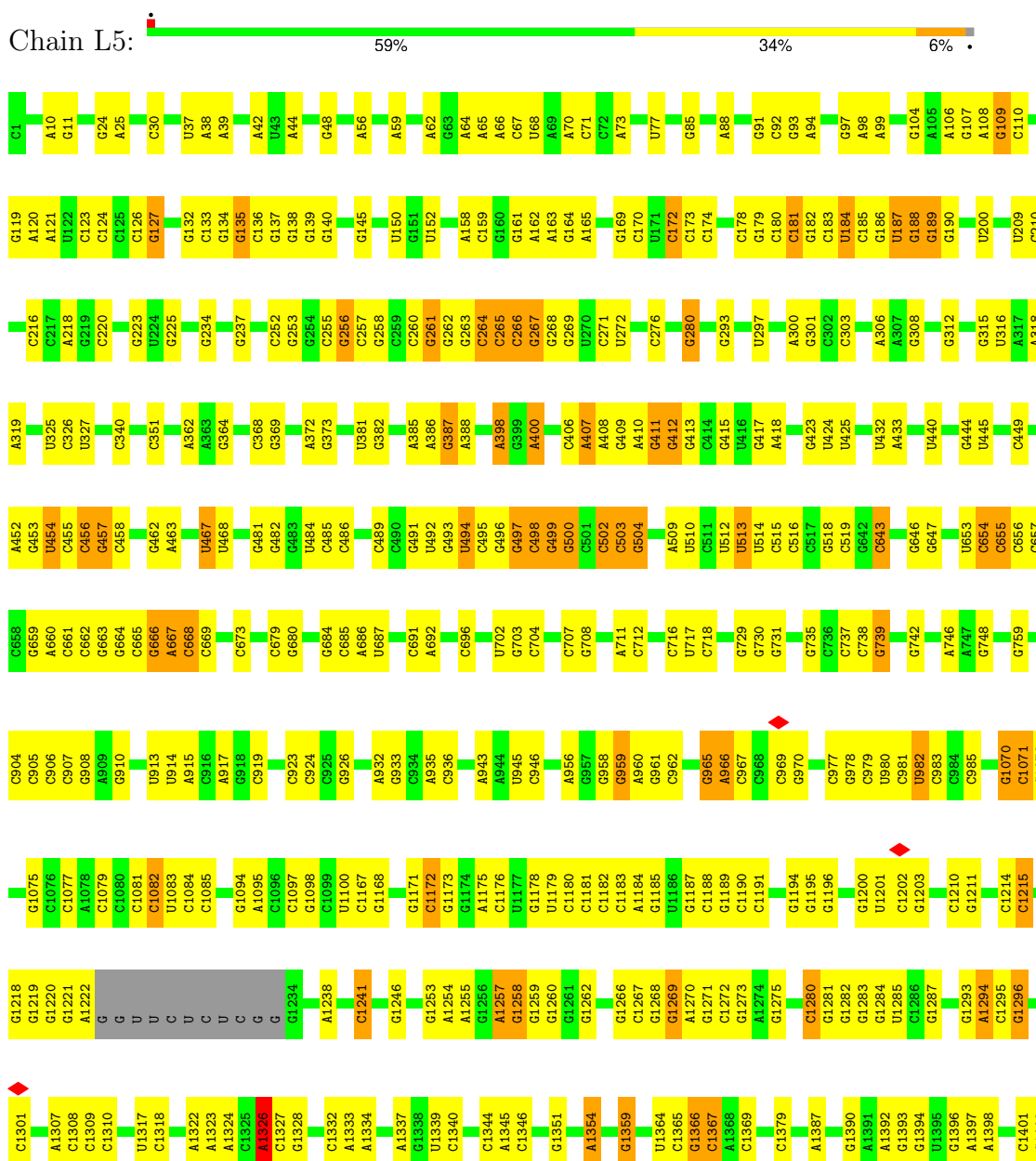
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Mol	Chain	Residues	Atoms		AltConf
48	Lj	1	Total 1	Zn 1	0
48	Lm	1	Total 1	Zn 1	0
48	Lo	1	Total 1	Zn 1	0
48	Lp	1	Total 1	Zn 1	0

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: 28S rRNA



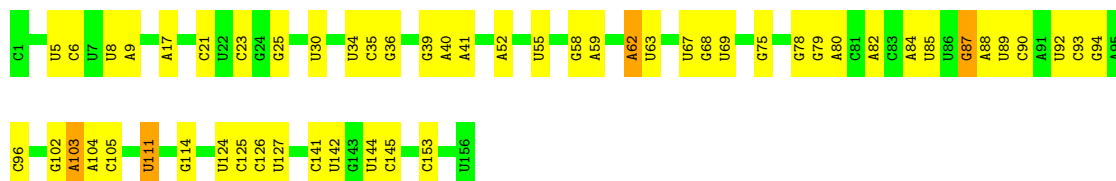




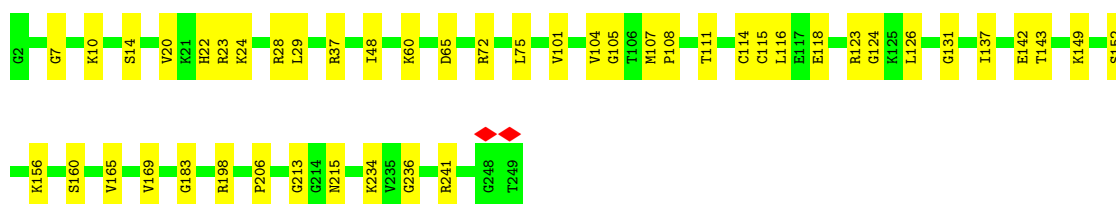
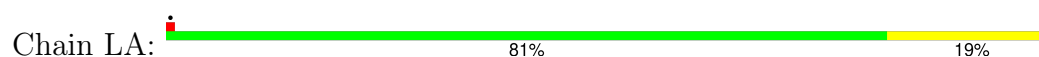
82% 17%



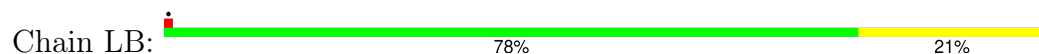
- Molecule 3: 5.8S rRNA



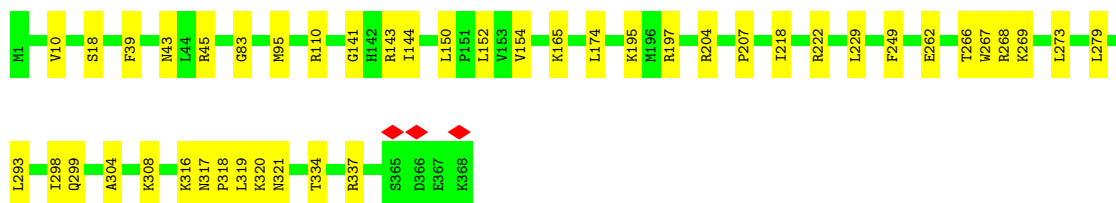
- Molecule 4: 60S ribosomal protein L8



- Molecule 5: Large ribosomal subunit protein uL3

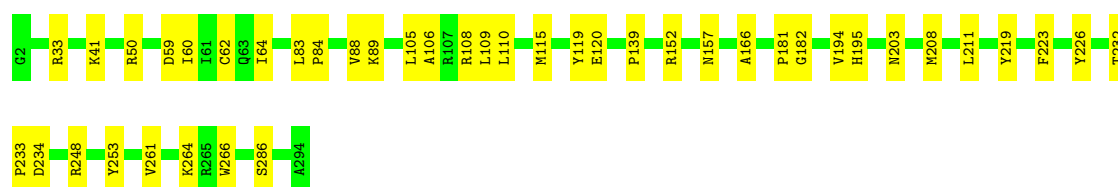


- Molecule 6: 60S ribosomal protein L4



- Molecule 7: Large ribosomal subunit protein uL18

Chain LD:  86% 14%



- Molecule 8: Large ribosomal subunit protein eL6

Chain LE:  82% 14%



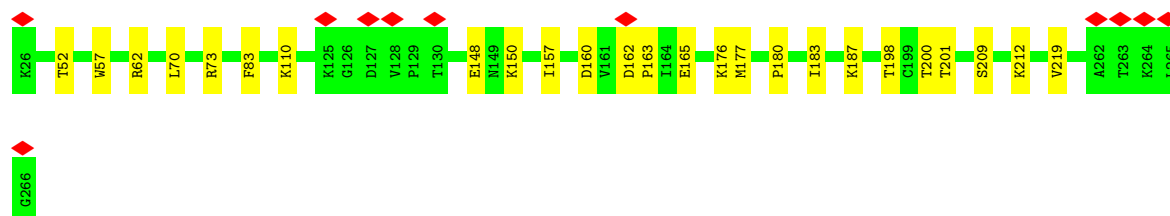
- Molecule 9: 60S ribosomal protein L7

Chain LF:  88% 12%



- Molecule 10: 60S ribosomal protein L7a

Chain LG:  5% 90% 10%



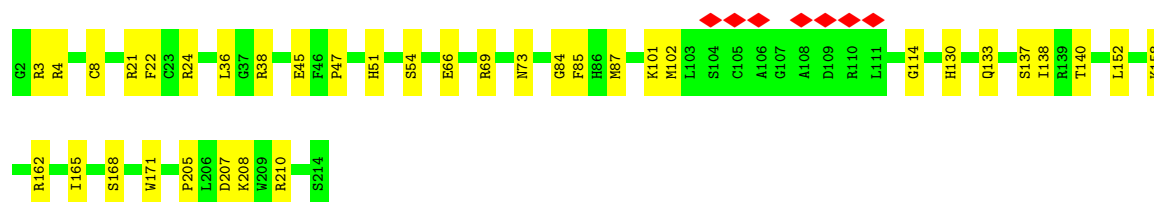
- Molecule 11: 60S ribosomal protein L9

Chain LH:  85% 15%



- Molecule 12: Ribosomal protein uL16-like

Chain LI:  83% 17%



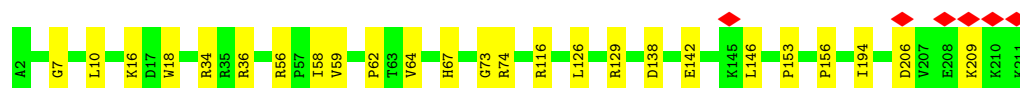
- Molecule 13: 60S ribosomal protein L11

Chain LJ: 87% 10%



- Molecule 14: Large ribosomal subunit protein eL13

Chain LL: 88% 12%



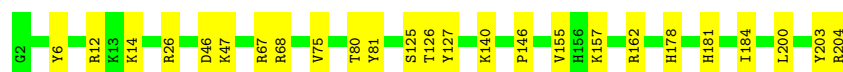
- Molecule 15: 60S ribosomal protein L14

Chain LM: 82% 18%



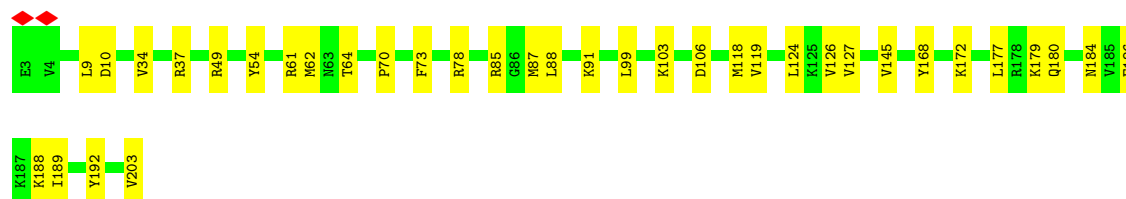
- Molecule 16: 60S ribosomal protein L15

Chain LN: 88% 12%



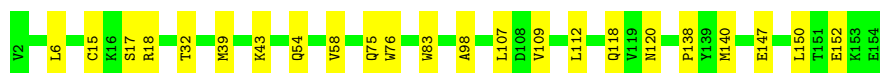
- Molecule 17: 60S ribosomal protein L13a

Chain LO: 82% 18%



- Molecule 18: 60S ribosomal protein L17

Chain LP: 85% 15%



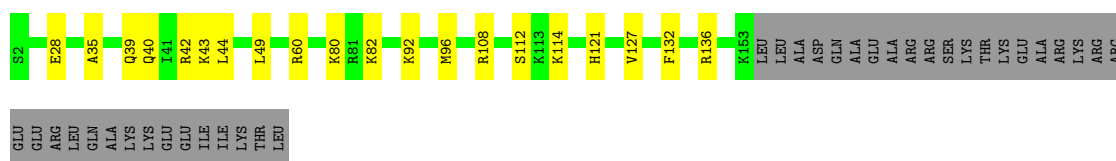
- Molecule 19: 60S ribosomal protein L18

Chain LQ: 87% 13%



- Molecule 20: 60S ribosomal protein L19

Chain LR: 71% 11% 19%



- Molecule 21: 60S ribosomal protein L18a

Chain LS: 89% 11%



- Molecule 22: 60S ribosomal protein L21

Chain LT: 84% 16%



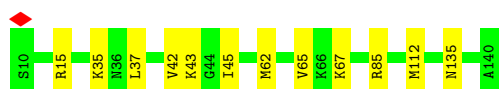
- Molecule 23: Heparin-binding protein HBp15

Chain LU: 83% 17%



- Molecule 24: 60S ribosomal protein L23

Chain LV: 91% 9%



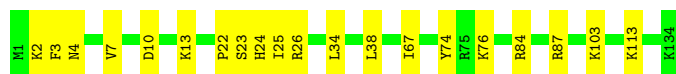
- Molecule 25: 60S ribosomal protein L23a

Chain LX:  84% 16%



- Molecule 26: 60S ribosomal protein L26

Chain LY:  85% 15%



- Molecule 27: 60S ribosomal protein L27

Chain LZ:  82% 18%



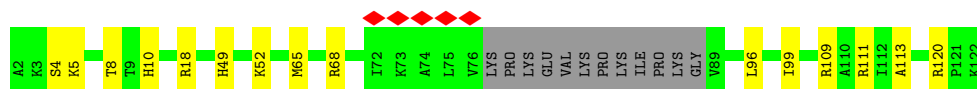
- Molecule 28: 60S ribosomal protein L27a

Chain La:  91% 9%



- Molecule 29: Large ribosomal subunit protein eL29

Chain Lb:  78% 12% 10%



- Molecule 30: 60S ribosomal protein L30

Chain Lc:  87% 13%

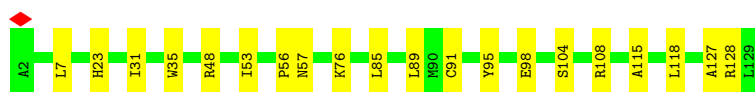
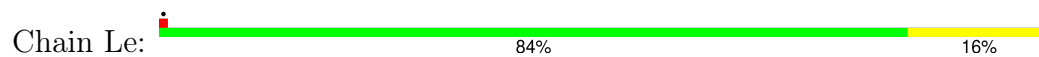


- Molecule 31: 60S ribosomal protein L31

Chain Ld:  82% 18%



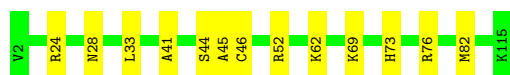
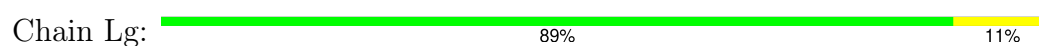
- Molecule 32: 60S ribosomal protein L32



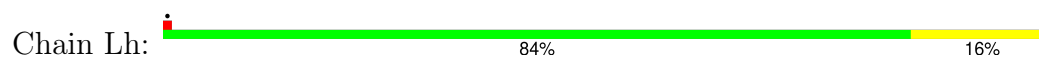
- Molecule 33: 60S ribosomal protein L35a



- Molecule 34: 60S ribosomal protein L34



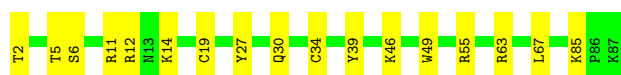
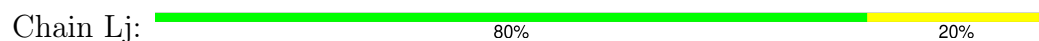
- Molecule 35: 60S ribosomal protein L35



- Molecule 36: 60S ribosomal protein L36



- Molecule 37: 60S ribosomal protein L37



- Molecule 38: 60S ribosomal protein L38



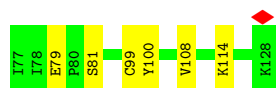
- Molecule 39: 60S ribosomal protein L39

Chain Ll:  78% 22%



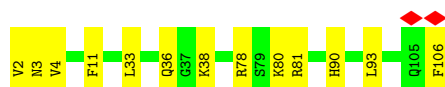
- Molecule 40: Large ribosomal subunit protein eL40

Chain Lm:  88% 12%



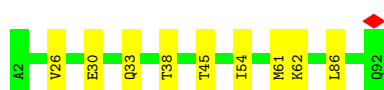
- Molecule 41: 60S ribosomal protein L36a

Chain Lo:  88% 12%



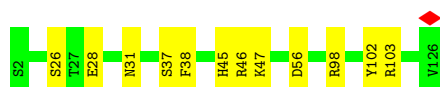
- Molecule 42: 60S ribosomal protein L37a

Chain Lp:  90% 10%



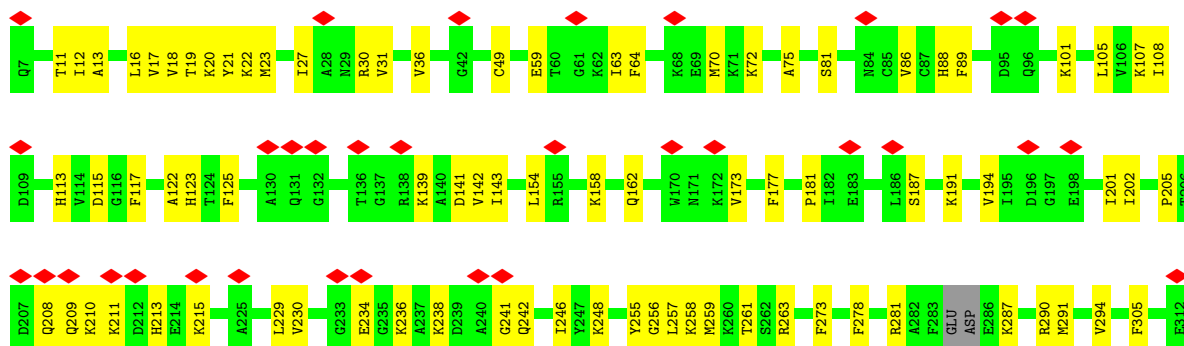
- Molecule 43: 60S ribosomal protein L28

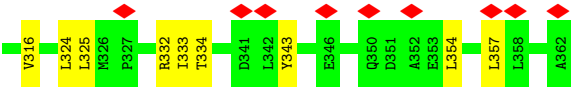
Chain Lr:  90% 10%



- Molecule 44: Proliferation-associated protein 2G4

Chain CA:  12% 74% 26%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	220618	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.298	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0134	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A2M, SPD, 6MZ, UR3, ZN, MG, OMC, 5MC, OMU, UY1, PSU, SPM, OMG, 1MA

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	L5	0.32	0/85098	0.31	0/132762
2	L7	0.30	0/2861	0.27	0/4459
3	L8	0.32	0/3631	0.29	0/5657
4	LA	0.32	0/1936	0.44	0/2596
5	LB	0.29	0/3306	0.38	0/4424
6	LC	0.30	0/2981	0.41	0/4002
7	LD	0.25	0/2428	0.34	0/3252
8	LE	0.24	0/1973	0.42	0/2645
9	LF	0.29	0/1905	0.30	0/2539
10	LG	0.25	0/1960	0.38	0/2637
11	LH	0.26	0/1537	0.35	0/2066
12	LI	0.25	0/1751	0.33	0/2340
13	LJ	0.20	0/1385	0.34	0/1852
14	LL	0.27	0/1732	0.33	0/2315
15	LM	0.28	0/1161	0.36	0/1554
16	LN	0.31	0/1746	0.35	0/2338
17	LO	0.30	0/1682	0.37	0/2250
18	LP	0.30	0/1268	0.40	0/1701
19	LQ	0.31	0/1537	0.37	0/2052
20	LR	0.26	0/1289	0.31	0/1705
21	LS	0.30	0/1493	0.35	0/2003
22	LT	0.27	0/1326	0.32	0/1770
23	LU	0.22	0/839	0.46	0/1126
24	LV	0.26	0/993	0.38	0/1332
25	LX	0.25	0/1002	0.31	0/1345
26	LY	0.28	0/1132	0.37	0/1504
27	LZ	0.25	0/1130	0.35	0/1507
28	La	0.29	0/1191	0.32	0/1591
29	Lb	0.23	0/889	0.38	0/1175
30	Lc	0.26	0/774	0.35	0/1038
31	Ld	0.27	0/903	0.35	0/1216
32	Le	0.30	0/1071	0.33	0/1429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Lf	0.31	0/895	0.38	0/1198
34	Lg	0.27	0/916	0.33	0/1220
35	Lh	0.25	0/1023	0.31	0/1351
36	Li	0.23	0/843	0.31	0/1115
37	Lj	0.31	0/720	0.41	0/952
38	Lk	0.21	0/575	0.32	0/761
39	Ll	0.28	0/454	0.31	0/599
40	Lm	0.25	0/435	0.39	1/575 (0.2%)
41	Lo	0.27	0/876	0.35	0/1156
42	Lp	0.27	0/718	0.33	0/953
43	Lr	0.28	0/1017	0.35	0/1364
44	CA	0.18	0/2810	0.40	0/3780
All	All	0.30	0/147192	0.33	1/217206 (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
5	LB	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Lm	108	VAL	N-CA-C	-5.10	107.84	112.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	LB	174	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	L5	78444	0	39717	756	0
2	L7	2561	0	1295	10	0
3	L8	3315	0	1685	31	0
4	LA	1898	0	1993	35	0
5	LB	3238	0	3376	63	0
6	LC	2927	0	3104	34	0
7	LD	2382	0	2410	28	0
8	LE	1935	0	2096	29	0
9	LF	1870	0	1996	18	0
10	LG	1927	0	2074	18	0
11	LH	1518	0	1601	19	0
12	LI	1711	0	1749	25	0
13	LJ	1362	0	1399	11	0
14	LL	1701	0	1818	20	0
15	LM	1138	0	1204	20	0
16	LN	1701	0	1749	24	0
17	LO	1650	0	1794	27	0
18	LP	1242	0	1269	18	0
19	LQ	1513	0	1628	18	0
20	LR	1273	0	1407	16	0
21	LS	1453	0	1490	12	0
22	LT	1298	0	1366	21	0
23	LU	825	0	850	11	0
24	LV	979	0	1039	8	0
25	LX	985	0	1066	49	0
26	LY	1115	0	1205	14	0
27	LZ	1107	0	1182	16	0
28	La	1162	0	1213	10	0
29	Lb	876	0	948	13	0
30	Lc	764	0	804	7	0
31	Ld	888	0	930	12	0
32	Le	1053	0	1147	14	0
33	Lf	876	0	912	8	0
34	Lg	906	0	998	12	0
35	Lh	1015	0	1148	19	0
36	Li	832	0	917	7	0
37	Lj	705	0	737	16	0
38	Lk	569	0	637	5	0
39	Ll	444	0	483	11	0
40	Lm	429	0	465	4	0
41	Lo	862	0	929	8	0
42	Lp	708	0	756	7	0
43	Lr	1002	0	1068	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	CA	2764	0	2778	113	0
45	L5	178	0	0	0	0
45	L7	3	0	0	0	0
45	L8	5	0	0	0	0
45	LA	1	0	0	0	0
45	LI	1	0	0	0	0
45	LP	1	0	0	0	0
45	LV	1	0	0	0	0
45	Le	1	0	0	0	0
46	L5	98	0	182	4	0
47	L5	90	0	171	5	0
47	LN	10	0	19	0	0
48	Lg	1	0	0	0	0
48	Lj	1	0	0	0	0
48	Lm	1	0	0	0	0
48	Lo	1	0	0	0	0
48	Lp	1	0	0	0	0
All	All	139317	0	100804	1310	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 6.

All (1310) 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)
1:L5:2709:C:O2'	44:CA:263:ARG:CD	1.96	1.12
25:LX:156:ILE:HG12	44:CA:290:ARG:HB3	1.33	1.05
25:LX:156:ILE:HD11	44:CA:291:MET:HB2	1.38	1.01
25:LX:156:ILE:HG13	44:CA:290:ARG:O	1.62	0.97
1:L5:2709:C:H2'	44:CA:263:ARG:HD3	1.47	0.95
25:LX:91:GLU:OE2	44:CA:259:MET:HB3	1.66	0.94
1:L5:1996:C:H42	1:L5:2000:G:N2	1.65	0.94
1:L5:2709:C:C2'	44:CA:263:ARG:HD3	1.99	0.92
25:LX:87:MET:HE3	44:CA:291:MET:HE3	1.51	0.92
25:LX:156:ILE:HD11	44:CA:291:MET:CB	1.99	0.91
1:L5:1996:C:H42	1:L5:2000:G:H22	1.07	0.91
25:LX:156:ILE:HG13	44:CA:290:ARG:C	1.94	0.91
25:LX:156:ILE:CD1	44:CA:291:MET:HB2	2.02	0.89
1:L5:1100:U:H3	1:L5:1194:G:H1	1.21	0.89
25:LX:156:ILE:HG12	44:CA:290:ARG:CB	2.03	0.88
14:LL:64:VAL:HA	14:LL:67:HIS:HD2	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:3946:G:H1	1:L5:4067:U:H3	0.86	0.86
1:L5:1996:C:N4	1:L5:2000:G:H22	1.74	0.84
1:L5:1095:A:H2	1:L5:1200:G:H1	1.17	0.83
25:LX:156:ILE:CG1	44:CA:290:ARG:C	2.52	0.83
25:LX:87:MET:HB2	44:CA:259:MET:HE1	1.61	0.82
25:LX:156:ILE:HD11	44:CA:291:MET:CA	2.08	0.82
1:L5:387:G:HO2'	1:L5:412:G:H1	1.28	0.81
1:L5:2007:G:H21	1:L5:2012:A:H62	1.27	0.80
25:LX:91:GLU:OE1	44:CA:261:THR:OG1	1.99	0.79
1:L5:664:G:N2	1:L5:666:G:O6	2.15	0.79
1:L5:2709:C:O2'	44:CA:263:ARG:NE	2.15	0.79
1:L5:2709:C:O2'	44:CA:263:ARG:HD3	1.77	0.78
1:L5:2709:C:O2'	44:CA:263:ARG:HD2	1.83	0.78
25:LX:156:ILE:CG1	44:CA:290:ARG:HB3	2.14	0.77
25:LX:156:ILE:HD11	44:CA:291:MET:N	2.00	0.76
4:LA:107:MET:HB3	4:LA:111:THR:HG21	1.70	0.73
1:L5:4986:G:H1'	5:LB:174:ARG:HH21	1.51	0.73
1:L5:137:G:H2'	1:L5:138:G:H8	1.54	0.73
1:L5:2557:G:H1	1:L5:2570:U:H3	1.34	0.73
25:LX:91:GLU:OE2	44:CA:259:MET:CB	2.37	0.73
1:L5:1414:C:H2'	1:L5:1415:G:H8	1.54	0.72
12:LI:205:PRO:HD2	12:LI:208:LYS:HE2	1.71	0.72
4:LA:29:LEU:O	4:LA:123:ARG:NH1	2.23	0.71
1:L5:3937:C:H1'	16:LN:125:SER:HB3	1.72	0.71
1:L5:500:G:OP1	1:L5:504:G:N2	2.23	0.71
11:LH:106:GLN:HB2	11:LH:111:LEU:HB3	1.72	0.71
1:L5:2458:C:H5''	16:LN:67:ARG:HD2	1.72	0.71
15:LM:15:VAL:HG22	15:LM:50:MET:HE1	1.71	0.71
1:L5:4242:U:H3	1:L5:4281:A:H2	1.36	0.71
1:L5:2554:U:O2	1:L5:2764:A:N7	2.24	0.71
44:CA:75:ALA:HB2	44:CA:113:HIS:HB3	1.72	0.71
1:L5:2611:A:H5'	1:L5:2688:G:H4'	1.73	0.71
1:L5:4873:G:N7	17:LO:179:LYS:NZ	2.39	0.70
1:L5:2702:C:OP1	23:LU:101:ARG:NH2	2.24	0.70
1:L5:3701:OMC:H5	1:L5:3748:A:H62	1.37	0.70
25:LX:87:MET:CE	44:CA:291:MET:HG3	2.20	0.70
1:L5:4910:G:H4'	5:LB:95:THR:HG22	1.73	0.70
1:L5:2351:OMC:HM22	6:LC:95:MET:HG3	1.74	0.70
1:L5:1702:C:H4'	6:LC:308:LYS:HD2	1.73	0.70
1:L5:2709:C:O2'	44:CA:263:ARG:CZ	2.40	0.70
44:CA:154:LEU:HD11	44:CA:332:ARG:HD2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:184:U:O2	1:L5:253:G:N2	2.18	0.70
5:LB:90:VAL:HG23	5:LB:163:ILE:HD11	1.74	0.70
44:CA:27:ILE:HD11	44:CA:59:GLU:HG3	1.74	0.70
1:L5:5016:A:H2	1:L5:5033:G:H21	1.37	0.69
1:L5:748:G:O6	21:LS:98:ARG:NH2	2.25	0.69
1:L5:2709:C:C4	44:CA:256:GLY:CA	2.47	0.69
1:L5:2484:A:H62	1:L5:2494:U:H3	1.40	0.69
1:L5:1172:C:H42	1:L5:1188:C:H42	1.40	0.69
1:L5:184:U:H3	1:L5:253:G:H1	1.41	0.69
1:L5:2601:A:N6	1:L5:2744:A:OP2	2.25	0.69
1:L5:2709:C:N3	44:CA:257:LEU:O	2.26	0.68
14:LL:64:VAL:HA	14:LL:67:HIS:CD2	2.27	0.68
31:Ld:90:ARG:HD3	31:Ld:102:LEU:HD13	1.75	0.68
1:L5:4546:A:N7	4:LA:215:ASN:ND2	2.42	0.68
1:L5:1095:A:N1	1:L5:1200:G:O6	2.27	0.67
1:L5:1669:A:OP1	29:Lb:18:ARG:NH2	2.27	0.67
46:L5:5293:SPM:H112	17:LO:91:LYS:HD3	1.75	0.67
1:L5:4910:G:N2	17:LO:106:ASP:O	2.28	0.67
25:LX:148:ASP:HB3	44:CA:287:LYS:HD2	1.76	0.67
21:LS:76:LYS:NZ	21:LS:100:LEU:O	2.28	0.66
1:L5:3954:A:H1'	1:L5:4058:U:H5'	1.76	0.66
1:L5:67:C:OP2	1:L5:312:G:N2	2.28	0.66
1:L5:1503:A:H62	19:LQ:87:THR:HG21	1.59	0.66
25:LX:156:ILE:CD1	44:CA:291:MET:CA	2.73	0.66
36:Li:2:ALA:N	36:Li:5:TYR:HH	1.93	0.66
1:L5:2092:G:O2'	1:L5:2262:G:N2	2.29	0.66
1:L5:109:G:OP2	14:LL:74:ARG:NH2	2.29	0.66
43:Lr:28:GLU:OE2	43:Lr:31:ASN:ND2	2.27	0.66
1:L5:121:A:OP1	10:LG:110:LYS:NZ	2.27	0.65
1:L5:2658:G:N2	1:L5:2676:A:OP2	2.29	0.65
1:L5:513:U:N3	1:L5:516:C:OP2	2.29	0.65
20:LR:39:GLN:OE1	20:LR:42:ARG:NH1	2.29	0.65
24:LV:35:LYS:HB2	24:LV:67:LYS:HG3	1.77	0.65
1:L5:2520:C:O2	1:L5:2640:G:N2	2.29	0.65
4:LA:104:VAL:HA	4:LA:107:MET:HE3	1.79	0.65
1:L5:1499:C:OP1	19:LQ:150:ARG:NH2	2.30	0.65
1:L5:665:C:H4'	1:L5:666:G:H5'	1.78	0.65
1:L5:3946:G:N2	1:L5:4067:U:O2	2.26	0.65
4:LA:114:CYS:HB3	4:LA:165:VAL:HB	1.78	0.65
5:LB:222:VAL:O	5:LB:343:ARG:NH1	2.29	0.65
13:LJ:146:ARG:HG2	13:LJ:147:ARG:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LO:34:VAL:HG22	17:LO:103:LYS:HB2	1.80	0.64
18:LP:39:MET:HG2	18:LP:43:LYS:HD3	1.79	0.64
1:L5:500:G:N2	1:L5:504:G:O2'	2.29	0.64
1:L5:2709:C:C4	44:CA:256:GLY:HA2	2.24	0.64
5:LB:10:ARG:NH1	5:LB:11:HIS:O	2.31	0.64
5:LB:107:ALA:HB2	5:LB:201:LEU:HD22	1.79	0.64
1:L5:1079:C:O2	1:L5:1221:G:N2	2.29	0.63
1:L5:4088:C:OP1	4:LA:37:ARG:NH1	2.31	0.63
1:L5:2708:U:H5'	44:CA:263:ARG:HG2	1.80	0.63
1:L5:2626:U:O4	23:LU:97:ARG:NH1	2.32	0.63
25:LX:87:MET:O	44:CA:291:MET:HE1	1.98	0.63
25:LX:156:ILE:HG21	44:CA:290:ARG:NE	2.14	0.63
38:Lk:26:LYS:HB2	38:Lk:69:LEU:HD12	1.81	0.63
44:CA:18:VAL:HG12	44:CA:22:LYS:HE2	1.81	0.63
1:L5:327:U:O2'	36:Li:30:ARG:NH1	2.31	0.62
1:L5:3641:U:OP2	1:L5:3646:A:N6	2.30	0.62
1:L5:4107:G:N2	1:L5:4108:G:O6	2.32	0.62
25:LX:151:ASN:HB3	44:CA:290:ARG:HH12	1.62	0.62
1:L5:3811:G:O2'	1:L5:3814:U:OP2	2.17	0.62
3:L8:62:A:OP1	35:Lh:52:LYS:NZ	2.29	0.62
1:L5:4992:G:H2'	1:L5:4993:G:C8	2.35	0.62
1:L5:2709:C:C4	44:CA:257:LEU:O	2.52	0.62
1:L5:4987:C:OP2	5:LB:116:ARG:NH2	2.32	0.62
44:CA:27:ILE:HG13	44:CA:30:ARG:HE	1.63	0.62
1:L5:4076:G:OP1	10:LG:73:ARG:NE	2.32	0.62
35:Lh:43:LYS:HD2	44:CA:241:GLY:HA3	1.81	0.62
1:L5:2007:G:N2	1:L5:2012:A:H62	1.97	0.62
4:LA:108:PRO:HB2	42:Lp:86:LEU:HD23	1.82	0.62
1:L5:1366:G:H5''	14:LL:36:ARG:HH12	1.65	0.62
1:L5:2083:C:OP2	19:LQ:14:ARG:NH2	2.31	0.62
31:Ld:64:ILE:HG23	31:Ld:68:LEU:HD23	1.80	0.62
1:L5:4302:U:H4'	22:LT:5:LYS:HD3	1.81	0.61
25:LX:156:ILE:CD1	44:CA:291:MET:CB	2.71	0.61
1:L5:3717:A:H2'	1:L5:3718:A2M:H8	1.82	0.61
26:LY:67:ILE:O	26:LY:84:ARG:NH2	2.34	0.61
44:CA:12:ILE:HG12	44:CA:324:LEU:HD11	1.82	0.61
18:LP:109:VAL:HA	18:LP:112:LEU:HD13	1.83	0.61
1:L5:1704:C:O3'	9:LF:46:ARG:NH1	2.33	0.61
1:L5:4472:G:O2'	40:Lm:100:TYR:O	2.19	0.61
13:LJ:84:GLU:OE2	13:LJ:92:TYR:OH	2.19	0.61
7:LD:120:GLU:O	7:LD:248:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LU:65:ARG:HG2	23:LU:67:LYS:H	1.65	0.61
1:L5:1408:G:O2'	1:L5:1411:C:N4	2.34	0.60
1:L5:5002:U:OP2	5:LB:385:LYS:NZ	2.35	0.60
2:L7:23:A:N3	2:L7:118:C:O2'	2.32	0.60
22:LT:43:LYS:O	22:LT:58:HIS:ND1	2.35	0.60
3:L8:21:C:OP1	6:LC:195:LYS:NZ	2.33	0.60
1:L5:1802:A:N3	22:LT:130:ARG:NH2	2.49	0.60
1:L5:2708:U:O4	44:CA:255:TYR:O	2.20	0.60
1:L5:1509:C:H5''	28:La:2:PRO:HD3	1.84	0.60
1:L5:2516:G:O2'	34:Lg:62:LYS:NZ	2.34	0.60
5:LB:165:HIS:HB3	5:LB:180:LEU:HD23	1.83	0.60
1:L5:4098:A:N1	1:L5:4112:C:N4	2.49	0.60
19:LQ:15:ARG:NH1	19:LQ:52:PHE:O	2.35	0.60
1:L5:1095:A:C2	1:L5:1200:G:N1	2.59	0.59
1:L5:2084:C:O2	19:LQ:16:LYS:NZ	2.34	0.59
1:L5:4594:U:H2'	1:L5:4595:G:H8	1.67	0.59
1:L5:4098:A:H2'	1:L5:4099:G:H4'	1.83	0.59
1:L5:4279:A:H5'	1:L5:4281:A:H1'	1.84	0.59
5:LB:10:ARG:NH2	5:LB:265:SER:O	2.34	0.59
12:LI:87:MET:HG2	12:LI:138:ILE:HG12	1.83	0.59
1:L5:1100:U:O3'	1:L5:1167:C:N4	2.35	0.59
7:LD:152:ARG:O	7:LD:157:ASN:ND2	2.35	0.59
1:L5:502:C:H3'	1:L5:503:C:H3'	1.84	0.59
3:L8:111:U:OP2	39:Ll:8:ARG:NH1	2.36	0.59
25:LX:88:LYS:CE	44:CA:259:MET:HG2	2.32	0.59
1:L5:4694:G:H4'	11:LH:71:ARG:HH12	1.67	0.59
44:CA:11:THR:HG23	44:CA:13:ALA:H	1.68	0.59
1:L5:1994:C:H2'	1:L5:1995:G:C8	2.38	0.59
1:L5:2832:A:OP1	31:Ld:47:LYS:NZ	2.29	0.59
25:LX:91:GLU:OE2	44:CA:259:MET:CG	2.50	0.59
1:L5:4431:PSU:OP2	12:LI:3:ARG:NH2	2.36	0.59
1:L5:1326:A2M:H2'	1:L5:1327:C:C6	2.37	0.58
1:L5:2093:A:N3	1:L5:2094:G:N1	2.51	0.58
1:L5:4774:C:O2'	1:L5:4775:C:O2	2.17	0.58
1:L5:121:A:H62	1:L5:152:U:H3	1.51	0.58
1:L5:4097:G:O6	1:L5:4098:A:N6	2.36	0.58
1:L5:4281:A:H2'	1:L5:4282:A:H2'	1.84	0.58
1:L5:5064:G:H21	18:LP:75:GLN:HE22	1.51	0.58
1:L5:1328:G:O2'	1:L5:2349:A:OP1	2.21	0.58
1:L5:2468:U:O2'	1:L5:2506:G:N2	2.36	0.58
5:LB:92:TYR:HB3	5:LB:99:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:5024:C:H41	1:L5:5028:G:H21	1.49	0.58
1:L5:2318:G:N2	1:L5:2321:G:OP2	2.30	0.58
1:L5:2362:U:H2'	1:L5:2363:A2M:H8	1.86	0.58
6:LC:298:ILE:HD13	19:LQ:131:PRO:HB3	1.86	0.58
44:CA:21:TYR:HE1	44:CA:117:PHE:HB3	1.68	0.58
1:L5:68:U:OP1	16:LN:178:HIS:ND1	2.33	0.58
1:L5:1703:C:O2'	1:L5:1704:C:O4'	2.20	0.58
1:L5:3688:U:OP2	4:LA:198:ARG:NH2	2.36	0.58
14:LL:126:LEU:N	14:LL:138:ASP:OD2	2.29	0.58
1:L5:62:A:N3	1:L5:77:U:O2'	2.33	0.58
1:L5:2756:G:O6	27:LZ:51:ARG:NH2	2.26	0.58
1:L5:4618:OMG:H5'	24:LV:15:ARG:HB2	1.85	0.58
1:L5:1100:U:O4	1:L5:1194:G:O6	2.22	0.57
1:L5:2758:G:O2'	1:L5:2765:A:N3	2.33	0.57
7:LD:41:LYS:NZ	22:LT:32:ARG:O	2.34	0.57
8:LE:119:GLU:HG3	32:Le:7:LEU:HD22	1.86	0.57
1:L5:3654:G:O2'	1:L5:3693:U:OP1	2.21	0.57
16:LN:146:PRO:HB2	35:Lh:104:THR:HG23	1.85	0.57
43:Lr:26:SER:OG	43:Lr:28:GLU:OE1	2.20	0.57
1:L5:1992:U:H4'	1:L5:1993:C:H5''	1.86	0.57
17:LO:54:TYR:OH	17:LO:73:PHE:O	2.22	0.57
1:L5:170:C:H42	1:L5:266:C:H42	1.51	0.57
1:L5:1982:G:N2	1:L5:2009:A:O2'	2.37	0.57
1:L5:3868:G:H22	1:L5:3900:G:H1'	1.69	0.57
1:L5:5016:A:C2	1:L5:5033:G:N2	2.63	0.57
8:LE:222:LEU:HB2	8:LE:237:LYS:HD2	1.84	0.57
1:L5:4340:U:O2	47:L5:5261:SPD:N10	2.37	0.57
5:LB:83:PRO:O	5:LB:167:GLN:NE2	2.37	0.57
1:L5:702:U:H2'	1:L5:703:G:O4'	2.05	0.57
1:L5:1175:A:H2	1:L5:1185:G:H22	1.52	0.57
8:LE:165:LEU:HD11	8:LE:176:THR:HG22	1.87	0.57
18:LP:118:GLN:OE1	18:LP:120:ASN:ND2	2.38	0.57
1:L5:3736:A:H2'	1:L5:3737:A:C8	2.40	0.56
29:Lb:5:LYS:HE2	29:Lb:8:THR:HB	1.86	0.56
38:Lk:8:ILE:HD11	38:Lk:56:LEU:HD13	1.87	0.56
43:Lr:47:LYS:HB2	43:Lr:102:TYR:CZ	2.39	0.56
1:L5:2695:A:OP1	38:Lk:35:LYS:NZ	2.29	0.56
1:L5:2709:C:C4	44:CA:257:LEU:C	2.80	0.56
1:L5:2745:A:H2'	1:L5:2746:A:C8	2.41	0.56
1:L5:5064:G:N2	18:LP:75:GLN:HE22	2.03	0.56
8:LE:223:ARG:HH22	8:LE:238:GLU:HG3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LF:105:VAL:HG13	9:LF:136:VAL:HG12	1.87	0.56
16:LN:157:LYS:O	16:LN:162:ARG:NH1	2.38	0.56
28:La:72:THR:HG22	28:La:110:LYS:HB3	1.86	0.56
1:L5:173:C:OP1	14:LL:129:ARG:NH1	2.38	0.56
1:L5:4941:G:OP2	8:LE:188:ARG:NH2	2.31	0.56
3:L8:52:A:H4'	39:Ll:19:GLN:HA	1.87	0.56
10:LG:165:GLU:OE2	16:LN:26:ARG:NH1	2.36	0.56
44:CA:333:ILE:HG13	44:CA:334:THR:HG23	1.86	0.56
4:LA:101:VAL:HG22	4:LA:165:VAL:HG22	1.87	0.56
1:L5:4251:A:H5''	13:LJ:108:GLY:HA3	1.88	0.56
41:Lo:11:PHE:O	41:Lo:81:ARG:NH2	2.38	0.56
1:L5:1281:G:N1	8:LE:128:HIS:HB2	2.20	0.56
1:L5:4897:G:OP1	15:LM:128:LYS:NZ	2.38	0.56
35:Lh:73:TYR:HB3	35:Lh:79:LYS:HG2	1.87	0.56
1:L5:2103:G:N7	1:L5:2104:G:N2	2.53	0.56
8:LE:161:ARG:NH1	8:LE:273:SER:OG	2.39	0.56
17:LO:9:LEU:HD23	17:LO:118:MET:HB2	1.88	0.56
1:L5:4260:U:H2'	1:L5:4261:C:C6	2.41	0.56
7:LD:223:PHE:HB3	7:LD:226:TYR:HB2	1.88	0.56
37:Lj:14:LYS:NZ	39:Li:51:LEU:OXT	2.36	0.56
1:L5:4363:A:H5''	41:Lo:36:GLN:HG2	1.87	0.56
44:CA:205:PRO:HB2	44:CA:210:LYS:HG3	1.87	0.56
1:L5:184:U:O2'	1:L5:189:G:O4'	2.24	0.55
1:L5:1818:G:O2'	1:L5:1820:C:OP2	2.23	0.55
1:L5:2017:A:O2'	1:L5:2018:C:O5'	2.22	0.55
5:LB:80:GLU:OE1	5:LB:323:TYR:OH	2.24	0.55
26:LY:2:LYS:HD2	26:LY:7:VAL:HG23	1.88	0.55
1:L5:1942:A:H2'	1:L5:1943:A:C8	2.41	0.55
1:L5:4525:C:OP1	5:LB:246:ARG:NH2	2.37	0.55
40:Lm:79:GLU:OE2	40:Lm:81:SER:OG	2.21	0.55
1:L5:3799:A:N3	1:L5:4506:C:O2'	2.38	0.55
1:L5:2745:A:H2'	1:L5:2746:A:H8	1.72	0.55
1:L5:4274:A:H2'	1:L5:4275:G:C8	2.42	0.55
44:CA:181:PRO:HA	44:CA:230:VAL:HA	1.88	0.55
1:L5:268:G:H2'	1:L5:269:G:H8	1.70	0.55
1:L5:2000:G:O2'	1:L5:2001:G:N7	2.39	0.55
1:L5:2018:C:H2'	1:L5:2019:C:H6	1.71	0.55
35:Lh:80:PRO:HD2	35:Lh:83:LEU:HD12	1.89	0.55
1:L5:1339:U:H2'	1:L5:1340:OMC:C6	2.41	0.55
1:L5:1480:C:O2'	1:L5:1482:G:OP2	2.25	0.55
25:LX:88:LYS:HE2	44:CA:259:MET:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1268:G:N7	29:Lb:111:ARG:NH2	2.51	0.55
1:L5:1359:G:H4'	16:LN:203:TYR:HB2	1.88	0.55
8:LE:261:ILE:HG23	8:LE:267:LEU:HD23	1.88	0.55
44:CA:142[A]:VAL:HG13	44:CA:143:ILE:HD12	1.87	0.55
1:L5:1756:U:O2'	1:L5:1758:G:OP2	2.24	0.55
1:L5:1095:A:H2	1:L5:1200:G:N1	1.98	0.55
1:L5:3717:A:OP2	1:L5:3735:G:N2	2.34	0.55
5:LB:17:LEU:O	5:LB:19:ARG:N	2.39	0.55
7:LD:64:ILE:HD13	7:LD:109:LEU:HD22	1.88	0.54
1:L5:1932:A:OP1	17:LO:49:ARG:NH2	2.29	0.54
1:L5:2709:C:O2'	44:CA:263:ARG:NH1	2.41	0.54
1:L5:3717:A:H2'	1:L5:3718:A2M:C8	2.37	0.54
33:Lf:78:HIS:HB3	33:Lf:83:MET:HB3	1.90	0.54
1:L5:267:G:OP1	35:Lh:109:ARG:NH2	2.40	0.54
1:L5:919:C:OP1	15:LM:69:HIS:ND1	2.28	0.54
12:LI:152:LEU:HB3	12:LI:165:ILE:HD12	1.89	0.54
1:L5:935:A:O2'	15:LM:44:GLN:O	2.26	0.54
1:L5:2382:A:N1	1:L5:2829:U:O2'	2.39	0.54
1:L5:2407:G:O6	39:Li:2:SER:N	2.40	0.54
5:LB:138:GLN:O	5:LB:143:LYS:NZ	2.40	0.54
5:LB:219:VAL:HG11	5:LB:337:VAL:HG13	1.90	0.54
1:L5:3661:G:N7	4:LA:152:SER:OG	2.37	0.54
1:L5:3697:U:H5''	1:L5:3698:G:H5'	1.90	0.54
1:L5:4094:G:N2	1:L5:4115:G:OP2	2.40	0.54
1:L5:4967:A:H2'	1:L5:4968:A:C8	2.42	0.54
7:LD:181:PRO:HD2	7:LD:195:HIS:CD2	2.42	0.54
16:LN:200:LEU:HB3	16:LN:204:ARG:HH21	1.71	0.54
33:Lf:43:LEU:O	33:Lf:109:ARG:NH2	2.41	0.54
1:L5:93:G:H2'	1:L5:94:A:C8	2.43	0.54
5:LB:289:GLN:HE22	5:LB:292:LEU:HD11	1.73	0.54
30:Lc:82:GLY:HA2	30:Lc:91:VAL:HG12	1.89	0.54
31:Ld:22:THR:HG23	31:Ld:122:VAL:HG13	1.88	0.54
1:L5:966:A:H5''	1:L5:2092:G:H22	1.73	0.54
1:L5:2696:A:OP1	38:Lk:26:LYS:NZ	2.38	0.54
6:LC:293:LEU:O	6:LC:299:GLN:NE2	2.37	0.54
21:LS:27:LEU:HB3	22:LT:148:PRO:HB3	1.90	0.54
1:L5:1866:U:OP1	12:LI:4:ARG:NH1	2.32	0.54
1:L5:1683:PSU:OP1	28:La:44:ASN:ND2	2.39	0.54
1:L5:1933:G:H2'	1:L5:1934:A:C8	2.43	0.54
1:L5:2017:A:O2'	1:L5:2018:C:H6	1.91	0.54
5:LB:140:GLU:OE1	5:LB:144:LYS:NZ	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LC:334:THR:HG22	6:LC:337:ARG:HH21	1.72	0.54
7:LD:62:CYS:HB3	7:LD:105:LEU:HD22	1.89	0.54
40:Lm:99:CYS:HB2	40:Lm:114:LYS:HE3	1.89	0.53
1:L5:425:U:H4'	18:LP:6:LEU:HD21	1.90	0.53
1:L5:2033:A:OP1	12:LI:162:ARG:NH2	2.35	0.53
1:L5:3946:G:O6	1:L5:4067:U:O4	2.25	0.53
9:LF:157:ARG:HE	9:LF:248:ASN:HB2	1.73	0.53
1:L5:1327:C:H2'	1:L5:1328:G:C8	2.44	0.53
1:L5:2492:C:H2'	1:L5:2493:G:H8	1.73	0.53
1:L5:2848:G:O2'	1:L5:3838:U:O4	2.23	0.53
1:L5:2899:C:OP1	20:LR:108:ARG:NH2	2.37	0.53
44:CA:141:ASP:HB2	44:CA:177:PHE:HD2	1.73	0.53
44:CA:202:ILE:HD11	44:CA:209:GLN:HB3	1.89	0.53
1:L5:679:C:H2'	1:L5:680:G:H8	1.72	0.53
1:L5:1759:G:H1	1:L5:1773:U:H3	1.57	0.53
43:Lr:38:PHE:O	43:Lr:45:HIS:NE2	2.33	0.53
1:L5:1094:G:O6	1:L5:1201:U:O2	2.27	0.53
1:L5:1857:C:H2'	1:L5:1858:A:H8	1.73	0.53
17:LO:186:GLU:N	17:LO:186:GLU:OE1	2.41	0.53
10:LG:209:SER:HA	10:LG:212:LYS:HG3	1.90	0.53
1:L5:691:C:H2'	1:L5:692:A:C8	2.44	0.53
3:L8:79:G:OP2	44:CA:238:LYS:NZ	2.40	0.53
9:LF:127:LYS:HB2	22:LT:133:ALA:HB3	1.91	0.53
18:LP:17:SER:HB2	18:LP:98:ALA:HB2	1.90	0.53
23:LU:28:PRO:HB2	23:LU:34:MET:HG3	1.90	0.53
44:CA:107:LYS:HZ2	44:CA:316:VAL:HG22	1.74	0.53
1:L5:735:G:H5''	15:LM:70:GLN:HG3	1.91	0.53
1:L5:1333:A:H2'	1:L5:1334:A:C8	2.44	0.53
3:L8:58:G:N7	37:Lj:63:ARG:NH2	2.45	0.53
13:LJ:56:THR:OG1	13:LJ:64:ARG:N	2.40	0.53
22:LT:119:ALA:HA	22:LT:122:LYS:HE3	1.91	0.53
1:L5:1411:C:H2'	1:L5:1412:G:C8	2.44	0.53
1:L5:4967:A:H2'	1:L5:4968:A:H8	1.74	0.52
5:LB:217:ILE:HD12	5:LB:347:LEU:HB3	1.92	0.52
44:CA:105:LEU:HD23	44:CA:139:LYS:HD2	1.91	0.52
1:L5:2486:G:O6	1:L5:2493:G:O6	2.27	0.52
1:L5:2846:G:OP1	24:LV:85:ARG:NH2	2.42	0.52
1:L5:4591:U:H2'	1:L5:4592:C:C6	2.44	0.52
13:LJ:141:ILE:HA	13:LJ:144:LYS:HD2	1.91	0.52
16:LN:155:VAL:O	16:LN:162:ARG:NH2	2.41	0.52
9:LF:57:TYR:OH	9:LF:189:ASP:OD1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LI:73:ASN:HB2	12:LI:87:MET:HE1	1.90	0.52
44:CA:187:SER:HB2	44:CA:201:ILE:HB	1.91	0.52
5:LB:113:GLU:OE2	5:LB:169:ARG:NH1	2.42	0.52
10:LG:162:ASP:HB3	10:LG:163:PRO:HD3	1.92	0.52
27:LZ:50:PRO:HD3	27:LZ:68:ILE:HG12	1.91	0.52
1:L5:1405:C:N3	1:L5:1413:C:N4	2.57	0.52
1:L5:2583:C:OP2	34:Lg:76:ARG:NH1	2.39	0.52
5:LB:220:ILE:HB	5:LB:346:THR:HB	1.92	0.52
25:LX:156:ILE:O	44:CA:294:VAL:HG11	2.09	0.52
7:LD:211:LEU:HB3	7:LD:219:TYR:HB2	1.91	0.52
1:L5:3611:A:H2	1:L5:5016:A:H8	1.56	0.52
1:L5:4966:A:H5''	5:LB:128:LYS:HG3	1.91	0.52
6:LC:218:ILE:HA	6:LC:229:LEU:HD22	1.91	0.52
17:LO:180:GLN:NE2	17:LO:184:ASN:OD1	2.41	0.52
1:L5:261:G:H2'	1:L5:262:G:C8	2.45	0.52
1:L5:1601:A:OP1	37:Lj:5:THR:OG1	2.19	0.52
1:L5:2049:G:HO2'	1:L5:3884:PSU:HO2'	1.48	0.52
1:L5:2724:G:O2'	1:L5:2726:G:OP2	2.28	0.52
1:L5:2566:G:H2'	1:L5:2567:G:H8	1.74	0.52
1:L5:3732:A:H2'	1:L5:3733:A:C8	2.45	0.52
1:L5:4594:U:H2'	1:L5:4595:G:C8	2.45	0.52
5:LB:161:ARG:HG2	5:LB:184:GLN:HA	1.92	0.52
15:LM:119:ARG:HG3	17:LO:189:ILE:HG23	1.91	0.52
1:L5:4225:G:OP1	12:LI:24:ARG:NH2	2.41	0.52
15:LM:24:LEU:HD11	15:LM:86:TRP:CG	2.45	0.52
25:LX:87:MET:HE3	44:CA:291:MET:HG3	1.91	0.52
3:L8:75:OMG:OP2	26:LY:74:TYR:OH	2.24	0.51
44:CA:354:LEU:HD12	44:CA:357:LEU:HD21	1.92	0.51
1:L5:3898:G:H5'	5:LB:254:ILE:HG13	1.92	0.51
1:L5:3910:C:H2'	1:L5:3911:C:C6	2.45	0.51
1:L5:4425:G:OP1	40:Lm:100:TYR:OH	2.23	0.51
3:L8:87:G:O6	26:LY:113:LYS:NZ	2.36	0.51
21:LS:161:ARG:HD2	21:LS:164:LYS:HB2	1.92	0.51
26:LY:4:ASN:HB3	26:LY:7:VAL:HG22	1.90	0.51
1:L5:1176:C:H42	1:L5:1184:A:H61	1.58	0.51
1:L5:2279:A:O2'	32:Le:48:ARG:NH2	2.44	0.51
1:L5:2111:G:N2	1:L5:2251:G:O2'	2.44	0.51
1:L5:2709:C:C2	44:CA:257:LEU:O	2.64	0.51
1:L5:4537:C:H2'	1:L5:4538:G:C8	2.44	0.51
5:LB:14:LEU:HD22	5:LB:17:LEU:HD11	1.91	0.51
1:L5:4882:U:OP1	15:LM:117:LYS:NZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LZ:68:ILE:HD12	27:LZ:119:GLU:HG2	1.93	0.51
28:La:87:ARG:HG3	28:La:120:GLN:HE22	1.76	0.51
1:L5:4537:C:H2'	1:L5:4538:G:H8	1.74	0.51
7:LD:84:PRO:HG3	7:LD:89:LYS:HA	1.92	0.51
7:LD:232:THR:OG1	7:LD:234:ASP:OD1	2.26	0.51
25:LX:64:SER:HB2	35:Lh:69:LEU:HD13	1.92	0.51
1:L5:71:C:H1'	14:LL:62:PRO:O	2.11	0.51
1:L5:654:C:H2'	1:L5:655:C:C6	2.44	0.51
1:L5:1095:A:N1	1:L5:1200:G:C6	2.79	0.51
1:L5:2714:G:H2'	1:L5:2715:G:H8	1.74	0.51
1:L5:4092:G:N7	1:L5:4114:C:N4	2.58	0.51
1:L5:4095:G:N7	1:L5:4096:C:N4	2.59	0.51
1:L5:4954:G:H2'	1:L5:4955:A:C8	2.46	0.51
1:L5:2539:C:H2'	1:L5:2540:C:C6	2.46	0.51
1:L5:2613:C:OP1	34:Lg:24:ARG:NH2	2.43	0.51
1:L5:1259:G:H2'	1:L5:1260:G:H8	1.76	0.51
1:L5:1646:A:O2'	37:Lj:49:TRP:O	2.24	0.51
1:L5:1733:G:N3	1:L5:4214:A:H2'	2.25	0.51
1:L5:3720:G:H22	1:L5:3733:A:H2	1.58	0.51
1:L5:444:G:H2'	1:L5:445:U:C6	2.46	0.51
1:L5:4612:C:C2	11:LH:120:GLU:HB2	2.46	0.51
1:L5:4742:G:H2'	1:L5:4743:G:H8	1.76	0.51
24:LV:112:MET:SD	24:LV:135:ASN:ND2	2.75	0.51
1:L5:467:U:C4	1:L5:468:U:H1'	2.46	0.50
1:L5:1824:G:H5''	22:LT:35:LYS:HE2	1.92	0.50
1:L5:2863:G:O2'	20:LR:82:LYS:O	2.27	0.50
1:L5:4115:G:O2'	1:L5:4116:C:O5'	2.28	0.50
1:L5:4940:C:O2'	8:LE:246:ARG:NH2	2.44	0.50
5:LB:57:VAL:HB	5:LB:367:PHE:HB3	1.92	0.50
6:LC:10:VAL:O	6:LC:18:SER:OG	2.27	0.50
17:LO:54:TYR:CD1	17:LO:145:VAL:HG21	2.46	0.50
25:LX:156:ILE:CD1	44:CA:291:MET:N	2.74	0.50
1:L5:97:G:OP1	14:LL:16:LYS:NZ	2.43	0.50
1:L5:1283:G:N1	1:L5:2076:G:OP1	2.32	0.50
1:L5:4601:U:H2'	1:L5:4602:A:H8	1.75	0.50
5:LB:50:LYS:NZ	5:LB:337:VAL:O	2.41	0.50
8:LE:141:ARG:NH2	33:Lf:110:ILE:O	2.44	0.50
11:LH:106:GLN:NE2	11:LH:113:GLU:OE2	2.33	0.50
1:L5:1662:C:H2'	1:L5:1663:C:C6	2.46	0.50
1:L5:2303:C:H5''	32:Le:104:SER:HB3	1.93	0.50
1:L5:3641:U:H5	1:L5:3646:A:N7	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:3664:G:H2'	1:L5:3665:G:H8	1.76	0.50
4:LA:137:ILE:HD11	4:LA:149:LYS:HB2	1.93	0.50
5:LB:167:GLN:OE1	5:LB:169:ARG:NH2	2.43	0.50
44:CA:246:ILE:HB	44:CA:305:PHE:HB2	1.93	0.50
1:L5:1238:A:O2'	9:LF:52:GLU:OE2	2.30	0.50
1:L5:2335:C:H2'	1:L5:2336:G:H8	1.75	0.50
1:L5:4095:G:H2'	1:L5:4096:C:C6	2.47	0.50
1:L5:4571:A2M:H2'	1:L5:4572:U:H6	1.76	0.50
5:LB:50:LYS:HB2	5:LB:345:LEU:HD11	1.92	0.50
17:LO:61:ARG:HA	17:LO:70:PRO:HD2	1.93	0.50
1:L5:158:A:N1	1:L5:276:C:O2'	2.42	0.50
1:L5:1308:C:H2'	1:L5:1309:C:C6	2.46	0.50
1:L5:1912:G:N2	17:LO:87:MET:HE2	2.27	0.50
1:L5:2543:A:H2	1:L5:2773:G:H22	1.60	0.50
1:L5:3732:A:H2'	1:L5:3733:A:H8	1.76	0.50
3:L8:67:U:H2'	3:L8:68:G:H8	1.77	0.50
17:LO:10:ASP:OD2	17:LO:37:ARG:NH2	2.44	0.50
1:L5:126:C:H2'	1:L5:127:G:H8	1.76	0.50
1:L5:172:C:H4'	1:L5:173:C:H5'	1.94	0.50
1:L5:2744:A:H2'	1:L5:2745:A:C8	2.47	0.50
9:LF:101:VAL:O	9:LF:106:ARG:NH1	2.44	0.50
10:LG:176:LYS:HG2	36:Li:43:MET:HE1	1.94	0.50
32:Le:108:ARG:HD2	32:Le:128:ARG:HB2	1.93	0.50
41:Lo:2:VAL:N	41:Lo:90:HIS:O	2.45	0.50
1:L5:308:G:O6	16:LN:12:ARG:NH1	2.45	0.50
1:L5:1979:A:N6	1:L5:1984:A:OP1	2.45	0.50
1:L5:1994:C:H2'	1:L5:1995:G:H8	1.77	0.50
1:L5:2491:C:O2'	1:L5:2492:C:O4'	2.25	0.50
1:L5:4935:C:H2'	1:L5:4936:G:C8	2.47	0.50
6:LC:141:GLY:O	6:LC:204:ARG:NH1	2.32	0.50
41:Lo:78:ARG:O	41:Lo:80:LYS:NZ	2.44	0.50
1:L5:1516:G:O2'	14:LL:18:TRP:NE1	2.41	0.50
4:LA:114:CYS:N	4:LA:165:VAL:O	2.45	0.50
10:LG:157:ILE:HA	10:LG:201:THR:HG22	1.94	0.50
1:L5:3911:C:H2'	1:L5:3912:U:H6	1.76	0.49
26:LY:76:LYS:HE2	39:LI:31:THR:HB	1.94	0.49
36:Li:100:ALA:HA	36:Li:103:LYS:HZ3	1.77	0.49
1:L5:491:G:H2'	1:L5:492:U:C6	2.47	0.49
1:L5:1282:G:OP2	8:LE:128:HIS:NE2	2.45	0.49
1:L5:1701:A:H5'	6:LC:304:ALA:HB3	1.93	0.49
1:L5:1785:C:OP1	12:LI:133:GLN:NE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4457:PSU:H1'	5:LB:252:ALA:HB3	1.94	0.49
14:LL:56:ARG:NH1	14:LL:74:ARG:O	2.41	0.49
29:Lb:65:MET:HG3	29:Lb:68:ARG:HH12	1.76	0.49
1:L5:717:U:H2'	1:L5:718:C:C6	2.47	0.49
1:L5:1396:G:HO2'	1:L5:1468:C:HO2'	1.56	0.49
1:L5:24:G:N7	37:Lj:46:LYS:NZ	2.61	0.49
1:L5:325:U:H2'	1:L5:326:C:C6	2.47	0.49
1:L5:711:A:H2'	1:L5:712:C:C6	2.47	0.49
1:L5:3659:G:OP1	4:LA:241:ARG:NH1	2.45	0.49
1:L5:3707:U:H2'	1:L5:3708:C:C6	2.48	0.49
5:LB:258:HIS:HA	5:LB:260:ALA:H	1.77	0.49
8:LE:190:HIS:HB3	8:LE:193:PHE:HD2	1.78	0.49
41:Lo:4:VAL:HG23	41:Lo:93:LEU:HD23	1.93	0.49
1:L5:4239:A:H2'	1:L5:4240:G:C8	2.47	0.49
18:LP:112:LEU:HD23	18:LP:150:LEU:HD13	1.94	0.49
1:L5:10:A:H2'	1:L5:11:G:C8	2.48	0.49
1:L5:654:C:O3'	6:LC:268:ARG:NH1	2.46	0.49
1:L5:1548:G:O2'	1:L5:2812:A:N3	2.41	0.49
1:L5:2764:A:H2'	1:L5:2765:A:H8	1.78	0.49
1:L5:3599:A:H2'	1:L5:3600:G:C8	2.47	0.49
1:L5:4459:U:H2'	1:L5:4460:U:C6	2.47	0.49
5:LB:258:HIS:HA	5:LB:260:ALA:N	2.26	0.49
6:LC:262:GLU:HB3	6:LC:273:LEU:HD13	1.94	0.49
30:Lc:51:ASN:HB2	30:Lc:77:ASN:HB2	1.95	0.49
1:L5:1194:G:H2'	1:L5:1195:G:H8	1.77	0.49
1:L5:1961:G:N2	1:L5:2024:G:O2'	2.43	0.49
1:L5:4636:PSU:N1	31:Ld:79:ASN:OD1	2.42	0.49
4:LA:22:HIS:O	4:LA:24:LYS:NZ	2.45	0.49
5:LB:29:VAL:HG12	5:LB:31:SER:H	1.78	0.49
9:LF:41:MET:HE2	29:Lb:113:ALA:HB2	1.94	0.49
1:L5:457:G:H2'	1:L5:458:C:C6	2.48	0.49
1:L5:1846:G:H2'	1:L5:1847:C:C6	2.47	0.49
1:L5:1867:A:H2'	1:L5:1868:A:C8	2.48	0.49
1:L5:4441:A:H5''	12:Li:114:GLY:HA2	1.94	0.49
8:LE:223:ARG:HB3	8:LE:224:LYS:HB2	1.94	0.49
20:LR:28:GLU:HG3	20:LR:49:LEU:HD22	1.94	0.49
23:LU:23:LEU:HD23	23:LU:110:TYR:HB2	1.94	0.49
44:CA:162:GLN:HB3	44:CA:215[A]:LYS:HE2	1.95	0.49
1:L5:223:G:OP2	6:LC:165:LYS:NZ	2.45	0.49
1:L5:457:G:H2'	1:L5:458:C:H6	1.78	0.49
1:L5:2300:A:N7	6:LC:143:ARG:NH1	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LB:153:MET:HB3	5:LB:194:LEU:HD11	1.95	0.49
18:LP:54:GLN:HA	18:LP:83:TRP:CD1	2.47	0.49
1:L5:3923:A:H2'	1:L5:3924:C:C6	2.48	0.49
1:L5:4093:G:H3'	1:L5:4094:G:H8	1.78	0.49
1:L5:4260:U:H2'	1:L5:4261:C:H6	1.77	0.49
1:L5:4775:C:H41	1:L5:4859:C:N4	2.11	0.49
10:LG:57:TRP:O	10:LG:62:ARG:NH1	2.46	0.49
17:LO:119:VAL:N	21:LS:168:THR:O	2.45	0.49
34:Lg:44:SER:OG	34:Lg:46:CYS:SG	2.68	0.49
1:L5:2568:C:H2'	1:L5:2569:G:H8	1.77	0.48
1:L5:4524:G:C2	5:LB:252:ALA:HB1	2.48	0.48
25:LX:148:ASP:CB	44:CA:287:LYS:HD2	2.43	0.48
33:Lf:50:VAL:HG22	33:Lf:69:VAL:HG22	1.95	0.48
7:LD:41:LYS:NZ	22:LT:30:TYR:O	2.42	0.48
10:LG:187:LYS:HB2	10:LG:198:THR:HG23	1.94	0.48
13:LJ:63:ARG:HH11	41:Lo:106:PHE:HB2	1.79	0.48
16:LN:200:LEU:HB3	16:LN:204:ARG:NH2	2.27	0.48
1:L5:1258:G:H2'	1:L5:1259:G:C8	2.47	0.48
12:LI:66:GLU:OE2	12:LI:69:ARG:NH2	2.34	0.48
27:LZ:12:LEU:HB2	27:LZ:81:MET:HB3	1.96	0.48
1:L5:178:C:N4	1:L5:179:G:O6	2.46	0.48
1:L5:1332:C:H2'	1:L5:1333:A:H8	1.78	0.48
1:L5:1403:G:N7	1:L5:1408:G:N2	2.61	0.48
1:L5:2640:G:H2'	1:L5:2641:A:C8	2.49	0.48
1:L5:4620:OMU:OP2	1:L5:4670:C:N4	2.38	0.48
3:L8:90:C:H1'	26:LY:24:HIS:HB3	1.95	0.48
5:LB:95:THR:OG1	5:LB:98:GLY:O	2.20	0.48
11:LH:51:LYS:HG3	11:LH:52:LYS:H	1.78	0.48
14:LL:59:VAL:HG21	14:LL:73:GLY:HA3	1.96	0.48
42:Lp:38:THR:HA	42:Lp:45:THR:HA	1.95	0.48
1:L5:2029:A:H2'	1:L5:2030:A:C8	2.48	0.48
1:L5:3856:A:H5''	18:LP:83:TRP:O	2.14	0.48
1:L5:4102:C:H1'	1:L5:4108:G:H1	1.79	0.48
3:L8:96:C:H5''	35:Lh:66:LYS:HG2	1.95	0.48
4:LA:28:ARG:HD2	4:LA:123:ARG:HG3	1.94	0.48
5:LB:288:GLY:HA3	5:LB:330:PHE:CE1	2.47	0.48
30:Lc:47:ILE:HD12	30:Lc:94:LEU:HD11	1.96	0.48
1:L5:88:A:N7	19:LQ:173:LYS:NZ	2.61	0.48
1:L5:1084:C:H2'	1:L5:1085:C:H6	1.79	0.48
1:L5:2326:G:H5''	32:Le:127:ALA:HB1	1.96	0.48
1:L5:3663:A:N6	1:L5:4168:G:O2'	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4584:A:H2'	1:L5:4585:U:O4'	2.14	0.48
1:L5:4974:C:H4'	5:LB:174:ARG:NH1	2.28	0.48
12:LI:207:ASP:OD1	12:LI:210:ARG:NH1	2.47	0.48
15:LM:122:ILE:HB	17:LO:189:ILE:HD11	1.96	0.48
1:L5:2411:C:H2'	1:L5:2412:A:C8	2.49	0.48
2:L7:7:G:OP1	7:LD:33:ARG:NH1	2.46	0.48
5:LB:74:GLU:OE1	5:LB:285:TYR:OH	2.27	0.48
11:LH:48:LEU:HD21	11:LH:56:ARG:HB2	1.94	0.48
14:LL:206:ASP:HA	14:LL:209:LYS:HD3	1.96	0.48
17:LO:168:TYR:CE2	17:LO:172:LYS:HD2	2.48	0.48
1:L5:1178:G:H2'	7:LD:286:SER:HB3	1.94	0.48
1:L5:3619:G:H22	1:L5:3624:A:H1'	1.78	0.48
1:L5:4413:C:O2	12:LI:158:LYS:NZ	2.47	0.48
1:L5:4456:OMC:HM21	5:LB:241:PRO:HD3	1.95	0.48
1:L5:4611:A:H2'	1:L5:4612:C:H6	1.79	0.48
12:LI:84:GLY:O	12:LI:140:THR:OG1	2.26	0.48
19:LQ:154:LYS:NZ	19:LQ:159:PRO:O	2.39	0.48
1:L5:267:G:H2'	1:L5:268:G:H8	1.78	0.48
1:L5:433:A:C2	1:L5:3867:A2M:H4'	2.48	0.48
1:L5:1324:A:O2'	1:L5:1326:A2M:OP1	2.27	0.48
1:L5:2495:U:H2'	1:L5:2496:G:C8	2.49	0.48
1:L5:3822:PSU:OP1	46:L5:5292:SPM:N5	2.34	0.48
44:CA:23:MET:HE2	44:CA:63:ILE:HG13	1.96	0.48
1:L5:351:C:OP2	6:LC:197:ARG:NH1	2.41	0.48
1:L5:386:A:O2'	26:LY:87:ARG:NH1	2.47	0.48
1:L5:1855:G:OP1	29:Lb:4:SER:HB2	2.14	0.48
1:L5:2588:C:OP1	1:L5:2768:C:O2'	2.25	0.48
1:L5:3589:G:N2	1:L5:3590:G:O6	2.47	0.48
25:LX:156:ILE:CD1	44:CA:291:MET:HA	2.44	0.48
29:Lb:99:ILE:O	29:Lb:109:ARG:NH1	2.47	0.48
1:L5:293:G:OP1	46:L5:5264:SPM:N1	2.39	0.47
1:L5:2102:G:H1'	1:L5:2103:G:C8	2.49	0.47
1:L5:2474:G:H2'	1:L5:2502:G:N2	2.29	0.47
1:L5:4088:C:H2'	1:L5:4089:G:C8	2.49	0.47
1:L5:4188:U:H2'	1:L5:4189:U:C6	2.49	0.47
14:LL:153:PRO:HG2	14:LL:156:PRO:HB3	1.96	0.47
25:LX:127:LEU:HD11	25:LX:135:LYS:HE3	1.96	0.47
32:Le:85:LEU:HD21	32:Le:115:ALA:HB2	1.95	0.47
1:L5:1857:C:H2'	1:L5:1858:A:C8	2.48	0.47
1:L5:2399:G:O2'	1:L5:2822:G:O2'	2.29	0.47
5:LB:206:PRO:HG2	5:LB:209:GLN:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LE:264:ILE:HD11	8:LE:267:LEU:HD22	1.95	0.47
11:LH:4:ILE:HG12	11:LH:61:TRP:CH2	2.49	0.47
1:L5:4113:U:H4'	1:L5:4115:G:C6	2.49	0.47
1:L5:4589:A:N1	1:L5:4621:C:O2'	2.40	0.47
1:L5:4680:G:H2'	1:L5:4681:A:C8	2.49	0.47
1:L5:5057:C:H2'	1:L5:5058:A:C8	2.49	0.47
4:LA:20:VAL:HA	4:LA:23:ARG:HG3	1.95	0.47
37:Lj:2:THR:HB	37:Lj:6:SER:HB2	1.96	0.47
44:CA:49:CYS:HB3	44:CA:281:ARG:NH2	2.29	0.47
1:L5:966:A:OP2	1:L5:2092:G:N2	2.45	0.47
1:L5:2478:C:N3	1:L5:2591:A:O2'	2.48	0.47
1:L5:2789:A:H1'	39:Ll:45:ARG:HH22	1.79	0.47
5:LB:302:ASN:HB2	5:LB:313:SER:HA	1.96	0.47
11:LH:107:GLU:N	11:LH:107:GLU:OE1	2.48	0.47
23:LU:44:GLN:HB2	23:LU:56:LEU:HD21	1.95	0.47
1:L5:1725:U:H2'	1:L5:1726:U:H6	1.80	0.47
5:LB:299:ILE:HB	5:LB:313:SER:HB3	1.97	0.47
44:CA:191:LYS:HE3	44:CA:194:VAL:HG21	1.96	0.47
1:L5:264:C:H2'	1:L5:265:C:C4	2.49	0.47
1:L5:369:G:N2	1:L5:372:A:OP2	2.41	0.47
1:L5:1241:C:O2'	29:Lb:120:ARG:O	2.33	0.47
1:L5:4076:G:H5'	10:LG:73:ARG:HG3	1.96	0.47
10:LG:52:THR:HG22	25:LX:41:ARG:HG3	1.97	0.47
21:LS:173:ASN:ND2	21:LS:175:PHE:O	2.47	0.47
35:Lh:43:LYS:CD	44:CA:241:GLY:HA3	2.44	0.47
1:L5:150:U:OP2	10:LG:200:THR:OG1	2.26	0.47
1:L5:667:A:H5''	1:L5:668:C:H5''	1.96	0.47
1:L5:737:C:C5	1:L5:739:G:H5''	2.50	0.47
1:L5:1077:C:OP1	1:L5:1215:C:O2'	2.27	0.47
1:L5:1401:C:H2'	1:L5:1402:C:C6	2.50	0.47
1:L5:2870:A:H2'	1:L5:2871:A:C8	2.50	0.47
1:L5:4536:OMC:HM22	1:L5:4537:C:O4'	2.14	0.47
1:L5:4743:G:H2'	1:L5:4744:A:C8	2.50	0.47
16:LN:46:ASP:OD1	16:LN:47:LYS:N	2.47	0.47
16:LN:140:LYS:HA	16:LN:140:LYS:HD3	1.67	0.47
22:LT:48:VAL:HG21	22:LT:94:GLU:HG2	1.95	0.47
25:LX:156:ILE:HG21	44:CA:290:ARG:CZ	2.44	0.47
1:L5:256:G:H2'	1:L5:257:C:C6	2.49	0.47
1:L5:1175:A:H2	1:L5:1185:G:H1	1.61	0.47
1:L5:1577:G:O2'	1:L5:1612:G:H4'	2.14	0.47
1:L5:2709:C:N3	44:CA:257:LEU:C	2.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LC:154:VAL:HG11	6:LC:174:LEU:HD11	1.96	0.47
11:LH:18:ILE:HG12	11:LH:27:VAL:HG22	1.97	0.47
22:LT:44:GLY:HA2	22:LT:95:HIS:HB3	1.97	0.47
32:Le:76:LYS:HD2	32:Le:98:GLU:CD	2.40	0.47
44:CA:17:VAL:HA	44:CA:20:LYS:HZ2	1.78	0.47
1:L5:257:C:H2'	1:L5:258:G:C8	2.50	0.47
1:L5:418:A:C2	3:L8:17:A:H1'	2.50	0.47
1:L5:2611:A:H2'	1:L5:2612:G:C8	2.49	0.47
1:L5:2667:C:O4'	20:LR:96:MET:HG2	2.15	0.47
1:L5:2896:G:OP1	20:LR:136:ARG:NH1	2.48	0.47
1:L5:4070:U:H2'	1:L5:4071:U:C6	2.50	0.47
11:LH:61:TRP:CZ3	15:LM:33:GLN:HG3	2.50	0.47
18:LP:107:LEU:HD13	18:LP:152:GLU:HG3	1.97	0.47
25:LX:87:MET:HE3	44:CA:291:MET:CE	2.34	0.47
39:LI:25:GLN:OE1	39:LI:28:ARG:NH2	2.47	0.47
1:L5:1097:C:H2'	1:L5:1098:G:C8	2.50	0.47
27:LZ:46:ILE:HA	27:LZ:70:SER:HA	1.97	0.47
1:L5:173:C:H2'	1:L5:174:C:C6	2.51	0.46
1:L5:1677:PSU:H4'	1:L5:1680:G:C2	2.50	0.46
1:L5:3664:G:H2'	1:L5:3665:G:C8	2.50	0.46
1:L5:4149:C:OP1	27:LZ:59:LYS:N	2.47	0.46
1:L5:4742:G:H2'	1:L5:4743:G:C8	2.50	0.46
1:L5:4883:C:N4	8:LE:181:LEU:O	2.45	0.46
7:LD:41:LYS:HD2	22:LT:93:ILE:HD13	1.97	0.46
17:LO:126:VAL:HG13	17:LO:127:VAL:HG13	1.96	0.46
35:Lh:70:ARG:HG2	35:Lh:83:LEU:HD22	1.97	0.46
1:L5:1872:G:O2'	1:L5:4219:A:N3	2.36	0.46
2:L7:26:C:O2'	13:LJ:147:ARG:NH1	2.48	0.46
2:L7:55:A:H4'	13:LJ:155:HIS:HB2	1.96	0.46
12:LI:54:SER:OG	12:LI:130:HIS:O	2.33	0.46
13:LJ:83:LEU:HD22	13:LJ:132:VAL:HG11	1.97	0.46
1:L5:1084:C:H2'	1:L5:1085:C:C6	2.50	0.46
1:L5:1188:C:H2'	1:L5:1189:G:H8	1.80	0.46
1:L5:1270:A:H8	1:L5:2106:G:H21	1.63	0.46
1:L5:1523:A:N3	1:L5:4389:C:O2'	2.46	0.46
1:L5:1645:C:H2'	1:L5:1646:A:C8	2.50	0.46
1:L5:2568:C:H2'	1:L5:2569:G:C8	2.51	0.46
1:L5:3726:A:H2'	1:L5:3727:A:C8	2.50	0.46
1:L5:4345:C:H2'	1:L5:4346:U:C6	2.50	0.46
1:L5:4345:C:H2'	1:L5:4346:U:H6	1.80	0.46
1:L5:4893:A:OP1	17:LO:188:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LO:62:MET:HE2	17:LO:64:THR:HB	1.96	0.46
44:CA:64:PHE:HB2	44:CA:72:LYS:HE3	1.97	0.46
1:L5:1494:U:H2'	1:L5:1495:G:H8	1.79	0.46
1:L5:1514:U:H2'	1:L5:1515:A:C8	2.50	0.46
35:Lh:95:LEU:HD22	35:Lh:99:GLU:HG3	1.97	0.46
1:L5:662:C:H2'	1:L5:663:G:H8	1.81	0.46
1:L5:1280:C:O2'	6:LC:321:ASN:OD1	2.22	0.46
1:L5:1538:U:H2'	1:L5:1539:G:H8	1.81	0.46
1:L5:1881:C:H5'	1:L5:2281:U:H1'	1.97	0.46
1:L5:3949:A:N1	1:L5:4064:C:N4	2.41	0.46
3:L8:141:C:H2'	3:L8:142:U:C6	2.50	0.46
8:LE:223:ARG:HA	8:LE:224:LYS:HA	1.76	0.46
12:LI:51:HIS:ND1	12:LI:137:SER:OG	2.46	0.46
28:La:84:GLU:OE1	28:La:87:ARG:NH2	2.48	0.46
1:L5:1837:A:OP2	22:LT:130:ARG:NH1	2.45	0.46
1:L5:2084:C:C4	19:LQ:14:ARG:HD2	2.50	0.46
1:L5:4543:G:H2'	1:L5:4544:A:C8	2.50	0.46
3:L8:36:G:C5	35:Lh:89:ARG:HD3	2.50	0.46
3:L8:102:G:OP2	3:L8:104:A:O2'	2.29	0.46
4:LA:118:GLU:OE2	4:LA:156:LYS:NZ	2.49	0.46
5:LB:57:VAL:HG22	5:LB:73:VAL:HG22	1.97	0.46
44:CA:209:GLN:O	44:CA:213:HIS:HB2	2.16	0.46
1:L5:1194:G:H2'	1:L5:1195:G:C8	2.51	0.46
1:L5:3660:C:OP1	4:LA:241:ARG:NH2	2.46	0.46
3:L8:67:U:H2'	3:L8:68:G:C8	2.51	0.46
4:LA:131:GLY:H	4:LA:169:VAL:HG13	1.81	0.46
1:L5:1739:G:N3	1:L5:1742:A:N6	2.64	0.46
1:L5:3595:U:H5''	1:L5:3597:G:OP2	2.15	0.46
1:L5:4153:C:H5''	25:LX:38:LYS:HD2	1.98	0.46
1:L5:4163:U:H5'	1:L5:4164:C:H5''	1.98	0.46
11:LH:92:MET:HE2	11:LH:179:ILE:HG22	1.98	0.46
19:LQ:66:MET:HE1	19:LQ:86:ILE:HD13	1.98	0.46
32:Le:91:CYS:HB3	32:Le:95:TYR:HD2	1.81	0.46
44:CA:113:HIS:HA	44:CA:117:PHE:O	2.16	0.46
1:L5:2083:C:P	19:LQ:14:ARG:HH22	2.38	0.46
1:L5:3607:U:H2'	1:L5:3608:A:C8	2.51	0.46
3:L8:5:U:H2'	3:L8:6:C:H6	1.81	0.46
6:LC:268:ARG:NH1	6:LC:269:LYS:HE2	2.31	0.46
11:LH:187:VAL:HG12	11:LH:188:GLN:HG3	1.96	0.46
1:L5:170:C:H42	1:L5:266:C:N4	2.13	0.46
1:L5:303:C:OP2	16:LN:68:ARG:NH2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1307:A:H2'	1:L5:1308:C:C6	2.50	0.46
1:L5:2580:U:O2'	27:LZ:79:HIS:ND1	2.46	0.46
1:L5:4364:G:H2'	1:L5:4365:C:H6	1.81	0.46
5:LB:36:ASP:N	5:LB:36:ASP:OD1	2.49	0.46
24:LV:43:LYS:HE2	24:LV:62:MET:HE3	1.98	0.46
44:CA:12:ILE:HD13	44:CA:21:TYR:CE2	2.50	0.46
1:L5:1195:G:H2'	1:L5:1196:G:C8	2.52	0.45
1:L5:2324:C:O2'	32:Le:98:GLU:OE1	2.30	0.45
1:L5:2709:C:H5''	20:LR:43:LYS:HD2	1.97	0.45
21:LS:93:MET:HE1	21:LS:117:HIS:CE1	2.51	0.45
25:LX:156:ILE:HG12	44:CA:290:ARG:C	2.39	0.45
1:L5:1972:G:H2'	1:L5:1973:G:C8	2.51	0.45
1:L5:4301:U:OP2	1:L5:4303:C:N4	2.49	0.45
10:LG:148:GLU:OE2	16:LN:6:TYR:OH	2.26	0.45
15:LM:36:ALA:HB3	15:LM:55:MET:HE1	1.99	0.45
15:LM:71:LYS:O	15:LM:75:GLN:HG3	2.16	0.45
31:Ld:57:MET:HG2	31:Ld:88:LEU:HD23	1.98	0.45
1:L5:454:U:H2'	1:L5:455:C:O4'	2.16	0.45
1:L5:1503:A:H4'	1:L5:1504:G:H5'	1.98	0.45
1:L5:1617:G:H1'	1:L5:2513:A:N6	2.31	0.45
1:L5:1700:G:H5''	1:L5:1704:C:H42	1.81	0.45
1:L5:1743:A:N1	1:L5:1789:C:O2'	2.47	0.45
1:L5:2579:G:N2	1:L5:2582:A:OP2	2.42	0.45
1:L5:4088:C:H2'	1:L5:4089:G:H8	1.81	0.45
7:LD:203:ASN:OD1	7:LD:203:ASN:N	2.50	0.45
11:LH:41:ILE:HG22	11:LH:43:VAL:HG13	1.98	0.45
13:LJ:22:LEU:HD22	13:LJ:128:LEU:HD12	1.99	0.45
32:Le:89:LEU:HD13	32:Le:118:LEU:HD22	1.96	0.45
41:Lo:33:LEU:HA	41:Lo:38:LYS:HG2	1.99	0.45
44:CA:27:ILE:O	44:CA:31:VAL:HG23	2.16	0.45
44:CA:86:VAL:HG13	44:CA:229:LEU:HD21	1.98	0.45
1:L5:163:A:H2'	1:L5:164:G:H8	1.81	0.45
1:L5:1751:A:H2'	1:L5:1752:G:C8	2.51	0.45
1:L5:2580:U:OP1	27:LZ:36:ARG:NH1	2.43	0.45
1:L5:4084:G:O6	4:LA:72:ARG:NH2	2.49	0.45
1:L5:4935:C:H2'	1:L5:4936:G:H8	1.81	0.45
15:LM:100:ARG:HA	15:LM:103:LYS:HG2	1.98	0.45
15:LM:130:LEU:HB3	17:LO:177:LEU:HD11	1.97	0.45
44:CA:16:LEU:O	44:CA:20:LYS:HG2	2.16	0.45
1:L5:106:A:H2'	1:L5:107:G:O4'	2.16	0.45
1:L5:268:G:H2'	1:L5:269:G:C8	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:2018:C:H2'	1:L5:2019:C:C6	2.49	0.45
1:L5:2306:G:H1'	1:L5:2332:A:N6	2.31	0.45
3:L8:30:U:OP1	14:LL:34:ARG:NH2	2.49	0.45
27:LZ:92:ASP:OD1	27:LZ:94:THR:OG1	2.30	0.45
1:L5:66:A:O2'	1:L5:326:C:O2	2.32	0.45
1:L5:519:C:H1'	1:L5:643:C:C2	2.51	0.45
1:L5:1875:C:H2'	1:L5:1876:U:C6	2.52	0.45
1:L5:3893:C:O2'	1:L5:4979:A:N1	2.47	0.45
1:L5:4524:G:N3	5:LB:252:ALA:HB1	2.32	0.45
10:LG:83:PHE:HA	10:LG:183:ILE:HD13	1.99	0.45
20:LR:80:LYS:HA	20:LR:80:LYS:HD2	1.82	0.45
26:LY:10:ASP:HB3	26:LY:13:LYS:HB2	1.99	0.45
1:L5:1410:U:H3	29:Lb:52:LYS:NZ	2.15	0.45
1:L5:1802:A:H5''	1:L5:1803:G:H5'	1.98	0.45
1:L5:1998:A:O2'	1:L5:2019:C:O2'	2.21	0.45
1:L5:2295:C:O2'	6:LC:45:ARG:NH2	2.50	0.45
1:L5:4685:U:H2'	1:L5:4686:G:C8	2.52	0.45
1:L5:5053:U:H3'	1:L5:5054:C:C6	2.52	0.45
5:LB:117:ARG:HA	5:LB:177:LYS:HD2	1.99	0.45
37:Lj:27:TYR:HA	37:Lj:34:CYS:HA	1.99	0.45
43:Lr:47:LYS:O	43:Lr:103:ARG:HD2	2.17	0.45
1:L5:729:G:H5''	9:LF:76:ARG:HD2	1.99	0.45
1:L5:1500:A:H5''	1:L5:1501:C:H5''	1.98	0.45
1:L5:2676:A:OP2	1:L5:2676:A:H8	2.00	0.45
1:L5:4460:U:H2'	1:L5:4461:C:C6	2.52	0.45
1:L5:4717:A:OP2	5:LB:30:LYS:NZ	2.33	0.45
5:LB:29:VAL:HA	5:LB:220:ILE:HD13	1.99	0.45
5:LB:35:ASP:OD2	5:LB:193:LYS:NZ	2.50	0.45
8:LE:227:HIS:HE1	8:LE:230:GLY:HA2	1.80	0.45
11:LH:24:THR:HA	11:LH:37:ASP:HA	1.99	0.45
19:LQ:43:PHE:CD2	19:LQ:133:GLY:HA3	2.52	0.45
25:LX:87:MET:O	44:CA:291:MET:CE	2.63	0.45
25:LX:151:ASN:HB3	44:CA:290:ARG:NH1	2.30	0.45
1:L5:1620:U:H5''	37:Lj:30:GLN:HE21	1.82	0.45
1:L5:1697:G:H22	1:L5:2084:C:P	2.40	0.45
1:L5:1910:G:O2'	1:L5:1917:A:N1	2.50	0.45
1:L5:2284:G:OP1	28:La:7:LYS:NZ	2.45	0.45
1:L5:4699:U:H1'	1:L5:4700:A:H5''	1.98	0.45
5:LB:173:LEU:HD22	5:LB:342:LYS:HD2	1.99	0.45
6:LC:144:ILE:O	6:LC:144:ILE:HG13	2.17	0.45
8:LE:250:GLN:NE2	8:LE:254:ASP:OD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LR:127:VAL:HG12	20:LR:132:PHE:HD2	1.81	0.45
31:Ld:59:THR:OG1	31:Ld:104:THR:OG1	2.28	0.45
44:CA:70:MET:HE2	44:CA:115:ASP:HA	1.99	0.45
1:L5:318:A:H2'	1:L5:319:A:C8	2.52	0.45
6:LC:150:LEU:O	6:LC:152:LEU:N	2.50	0.45
7:LD:208:MET:HB2	7:LD:233:PRO:HG3	1.99	0.45
16:LN:200:LEU:HD13	16:LN:204:ARG:HH21	1.82	0.45
1:L5:2739:C:OP2	42:Lp:33:GLN:NE2	2.50	0.44
1:L5:3880:G:H2'	1:L5:3881:G:C8	2.52	0.44
4:LA:206:PRO:HG3	4:LA:213:GLY:HA3	1.99	0.44
6:LC:318:PRO:O	6:LC:319:LEU:HB2	2.16	0.44
6:LC:318:PRO:C	6:LC:320:LYS:H	2.25	0.44
9:LF:37:PHE:HZ	29:Lb:113:ALA:HB1	1.82	0.44
17:LO:88:LEU:HD12	17:LO:99:LEU:HD13	1.99	0.44
44:CA:123:HIS:NE2	44:CA:125:PHE:HB3	2.32	0.44
1:L5:381:U:H4'	1:L5:415:G:H5'	1.99	0.44
1:L5:1340:OMC:HM23	1:L5:1340:OMC:H1'	1.78	0.44
1:L5:2404:A:H1'	37:Lj:12:ARG:HH21	1.82	0.44
1:L5:3928:A:H2'	1:L5:3929:G:O4'	2.16	0.44
1:L5:4322:G:N2	1:L5:4325:A:OP2	2.41	0.44
1:L5:4739:C:H2'	1:L5:4740:G:H5'	1.99	0.44
19:LQ:3:VAL:HG13	19:LQ:5:ILE:HG12	1.99	0.44
28:La:36:GLY:HA3	28:La:40:HIS:CE1	2.52	0.44
44:CA:173:VAL:HB	44:CA:354:LEU:HD21	1.98	0.44
1:L5:92:C:OP2	1:L5:4341:C:O2'	2.29	0.44
1:L5:400:A2M:H1'	1:L5:400:A2M:HM'3	1.58	0.44
1:L5:455:C:O2'	1:L5:456:C:H5'	2.17	0.44
1:L5:2262:G:OP2	43:Lr:98:ARG:NH2	2.45	0.44
1:L5:2630:U:O4	23:LU:89:LYS:NZ	2.49	0.44
1:L5:3917:A:H2'	1:L5:3918:G:H8	1.82	0.44
1:L5:5016:A:H2	1:L5:5033:G:N2	2.06	0.44
1:L5:5047:C:O2'	1:L5:5050:C:OP2	2.26	0.44
18:LP:32:THR:HG23	18:LP:58:VAL:HG11	2.00	0.44
20:LR:92:LYS:HG2	20:LR:96:MET:HE3	2.00	0.44
24:LV:42:VAL:HB	24:LV:45:ILE:HG13	2.00	0.44
27:LZ:41:ALA:HB2	27:LZ:77:TYR:HE1	1.81	0.44
1:L5:37:U:H2'	1:L5:38:A:O4'	2.17	0.44
1:L5:180:C:H2'	1:L5:181:C:H6	1.83	0.44
1:L5:500:G:H1'	1:L5:504:G:H3'	1.99	0.44
1:L5:1877:G:O6	29:Lb:10:HIS:NE2	2.50	0.44
1:L5:1976:G:C8	1:L5:2002:A:H2'	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:4508:C:N3	1:L5:4512:U:H5	2.15	0.44
1:L5:4524:G:OP1	1:L5:4559:A:N6	2.45	0.44
1:L5:4775:C:H41	1:L5:4859:C:H42	1.65	0.44
1:L5:4934:A:H2'	1:L5:4935:C:C6	2.52	0.44
3:L8:75:OMG:HM23	3:L8:75:OMG:H1'	1.73	0.44
35:Lh:89:ARG:O	35:Lh:93:ARG:HG2	2.17	0.44
39:Ll:25:GLN:NE2	39:Ll:28:ARG:HH12	2.15	0.44
44:CA:81:SER:HB2	44:CA:107:LYS:HB2	1.99	0.44
1:L5:135:G:H22	35:Lh:94:ARG:HG2	1.83	0.44
1:L5:965:G:N2	1:L5:2092:G:H1'	2.32	0.44
1:L5:2730:U:H2'	1:L5:2731:C:C6	2.53	0.44
1:L5:2811:G:N1	1:L5:2814:C:OP2	2.44	0.44
34:Lg:45:ALA:HB3	34:Lg:82:MET:HE2	1.99	0.44
1:L5:188:G:N2	1:L5:190:G:O6	2.50	0.44
1:L5:1942:A:H2'	1:L5:1943:A:H8	1.80	0.44
1:L5:2824:OMC:HM23	1:L5:2824:OMC:H1'	1.75	0.44
1:L5:3932:U:H2'	1:L5:3933:G:H8	1.83	0.44
1:L5:4504:C:H2'	1:L5:4505:C:C6	2.52	0.44
1:L5:4927:G:H5''	1:L5:4928:C:C5	2.53	0.44
1:L5:4927:G:H5''	1:L5:4928:C:H5	1.82	0.44
5:LB:27:GLY:HA2	5:LB:276:HIS:CD2	2.52	0.44
5:LB:154:LYS:HE2	5:LB:154:LYS:HB2	1.70	0.44
30:Lc:38:ILE:HD11	30:Lc:46:VAL:HG21	2.00	0.44
33:Lf:45:LYS:NZ	33:Lf:108:SER:HA	2.33	0.44
1:L5:387:G:O2'	1:L5:412:G:N1	2.33	0.44
1:L5:423:G:H21	18:LP:118:GLN:NE2	2.14	0.44
1:L5:424:U:H2'	1:L5:425:U:C6	2.53	0.44
1:L5:965:G:H21	1:L5:2092:G:H1'	1.82	0.44
1:L5:1390:G:N2	1:L5:1393:G:OP2	2.42	0.44
1:L5:1662:C:H2'	1:L5:1663:C:H6	1.83	0.44
1:L5:1870:C:H2'	1:L5:1871:A2M:H8	2.00	0.44
1:L5:1982:G:O2'	1:L5:2010:A:O2'	2.23	0.44
1:L5:3911:C:H2'	1:L5:3912:U:C6	2.52	0.44
1:L5:4069:U:H2'	1:L5:4070:U:C6	2.53	0.44
1:L5:4492:U:O2'	1:L5:4512:U:O2	2.33	0.44
5:LB:86:VAL:HG12	5:LB:201:LEU:HD23	1.99	0.44
15:LM:104:MET:HG3	15:LM:108:ASP:HB2	2.00	0.44
35:Lh:8:ASP:OD1	35:Lh:8:ASP:N	2.51	0.44
1:L5:2411:C:H2'	1:L5:2412:A:H8	1.81	0.44
5:LB:394:LYS:HA	5:LB:397:ILE:HG12	2.00	0.44
12:LI:21:ARG:O	12:LI:24:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LL:142:GLU:HA	14:LL:146:LEU:HD12	2.00	0.44
19:LQ:50:ARG:HH21	19:LQ:140:SER:HB2	1.83	0.44
26:LY:23:SER:HA	26:LY:26:ARG:HB2	2.00	0.44
37:Lj:67:LEU:HD23	37:Lj:67:LEU:HA	1.86	0.44
44:CA:248:LYS:HB2	44:CA:248:LYS:HE2	1.79	0.44
1:L5:169:G:O6	1:L5:170:C:N4	2.51	0.44
1:L5:1392:A:H2'	1:L5:1393:G:C8	2.53	0.44
1:L5:1628:C:OP1	4:LA:14:SER:OG	2.35	0.44
1:L5:2754:G:OP2	27:LZ:133:LYS:NZ	2.32	0.44
1:L5:3932:U:H2'	1:L5:3933:G:C8	2.53	0.44
1:L5:4156:G:H5''	1:L5:4157:A:H2'	2.00	0.44
7:LD:108:ARG:CZ	7:LD:253:TYR:HB2	2.48	0.44
26:LY:34:LEU:HD13	26:LY:38:LEU:HB3	1.99	0.44
33:Lf:25:THR:HB	33:Lf:87:LYS:HD3	2.00	0.44
44:CA:143:ILE:HD13	44:CA:343:TYR:OH	2.18	0.44
1:L5:907:C:H2'	1:L5:908:G:H8	1.83	0.43
1:L5:1344:C:H1'	14:LL:10:LEU:HD11	2.00	0.43
1:L5:2022:C:H2'	1:L5:2023:C:O4'	2.18	0.43
1:L5:2632:PSU:H2'	1:L5:2633:U:C6	2.52	0.43
1:L5:2666:U:O2'	1:L5:2668:G:N7	2.47	0.43
8:LE:128:HIS:O	8:LE:128:HIS:ND1	2.51	0.43
27:LZ:100:VAL:HG23	27:LZ:106:LEU:HB3	1.99	0.43
44:CA:234:GLU:HG2	44:CA:236:LYS:NZ	2.33	0.43
1:L5:979:C:OP2	8:LE:66:LYS:HD3	2.18	0.43
1:L5:2045:G:O6	1:L5:3870:C:O2'	2.34	0.43
1:L5:2275:G:H2'	1:L5:2276:A:C8	2.53	0.43
1:L5:2638:G:H22	1:L5:2719:C:P	2.40	0.43
1:L5:4111:U:H2'	1:L5:4112:C:H5	1.83	0.43
2:L7:119:U:C2	7:LD:261:VAL:HG11	2.53	0.43
6:LC:110:ARG:HA	16:LN:204:ARG:HH12	1.84	0.43
25:LX:140:LEU:HD23	25:LX:144:TYR:HB3	2.00	0.43
44:CA:19:THR:HA	44:CA:22:LYS:HE3	1.99	0.43
1:L5:327:U:HO2'	36:Li:30:ARG:HH11	1.61	0.43
1:L5:2412:A:H2'	1:L5:2413:U:C6	2.53	0.43
1:L5:2570:U:H2'	1:L5:2571:C:C6	2.53	0.43
1:L5:3944:G:H1	1:L5:4069:U:H3	1.66	0.43
1:L5:4196:OMG:HM23	1:L5:4196:OMG:H1'	1.75	0.43
3:L8:40:A:H2'	3:L8:41:A:C8	2.54	0.43
3:L8:88:A:H2'	3:L8:89:U:O4'	2.17	0.43
4:LA:105:GLY:HA3	4:LA:160:SER:HB3	1.99	0.43
6:LC:39:PHE:O	6:LC:43:ASN:ND2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LX:124:VAL:HG22	25:LX:138:VAL:HG13	2.00	0.43
1:L5:1281:G:OP1	6:LC:316:LYS:NZ	2.34	0.43
1:L5:1669:A:H4'	1:L5:1685:G:N2	2.33	0.43
1:L5:2415:U:H2'	1:L5:2416:G:C8	2.53	0.43
1:L5:3861:A:H2'	1:L5:3862:A:C8	2.53	0.43
1:L5:4744:A:H2'	1:L5:4745:G:O4'	2.19	0.43
1:L5:4872:G:C2	17:LO:203:VAL:HG23	2.53	0.43
2:L7:4:U:H2'	2:L7:5:A:H8	1.83	0.43
10:LG:70:LEU:HD23	10:LG:70:LEU:HA	1.83	0.43
10:LG:180:PRO:HG3	10:LG:219:VAL:HG13	2.00	0.43
16:LN:126:THR:HG23	16:LN:127:TYR:CD2	2.54	0.43
16:LN:178:HIS:HA	16:LN:181:HIS:NE2	2.33	0.43
36:Li:35:LYS:HE3	36:Li:35:LYS:HB3	1.81	0.43
1:L5:494:U:H2'	1:L5:495:C:C6	2.54	0.43
1:L5:1705:G:H2'	1:L5:1706:A:O4'	2.18	0.43
1:L5:3867:A2M:H2'	1:L5:3868:G:O4'	2.17	0.43
6:LC:266:THR:HG22	6:LC:267:TRP:H	1.82	0.43
7:LD:106:ALA:HB2	7:LD:166:ALA:HA	1.99	0.43
10:LG:150:LYS:NZ	10:LG:177:MET:O	2.49	0.43
11:LH:115:ARG:HD3	11:LH:123:ILE:HD12	2.01	0.43
12:LI:85:PHE:HE2	12:LI:87:MET:HE2	1.84	0.43
30:Lc:99:PRO:HG3	30:Lc:104:ILE:HB	2.01	0.43
1:L5:161:G:H2'	1:L5:162:A:H8	1.83	0.43
1:L5:660:A:H2'	1:L5:661:C:C6	2.53	0.43
1:L5:667:A:H5'	43:Lr:46:ARG:NH2	2.33	0.43
1:L5:716:C:OP1	6:LC:317:ASN:HB2	2.17	0.43
1:L5:1294:A:H1'	1:L5:1296:G:C2	2.54	0.43
1:L5:1398:A:OP1	28:La:136:LYS:NZ	2.51	0.43
1:L5:1695:U:O2'	1:L5:1719:A:N3	2.43	0.43
1:L5:1703:C:O2'	1:L5:1704:C:O5'	2.36	0.43
1:L5:1847:C:H2'	1:L5:1848:C:C6	2.53	0.43
1:L5:2267:U:OP1	43:Lr:37:SER:HB2	2.19	0.43
1:L5:2351:OMC:HM23	1:L5:2351:OMC:H1'	1.68	0.43
1:L5:2498:C:H2'	1:L5:2499:C:H6	1.84	0.43
1:L5:2664:G:OP2	20:LR:121:HIS:ND1	2.37	0.43
2:L7:111:C:H2'	2:L7:112:U:O4'	2.18	0.43
4:LA:7:GLY:HA2	4:LA:10:LYS:HG3	2.00	0.43
9:LF:213:LEU:HB3	9:LF:247:MET:HG3	2.01	0.43
12:LI:51:HIS:CD2	12:LI:168:SER:HB3	2.53	0.43
44:CA:108:ILE:O	44:CA:122:ALA:HA	2.19	0.43
1:L5:267:G:H2'	1:L5:268:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:737:C:C4	1:L5:739:G:H5''	2.53	0.43
1:L5:1431:C:H2'	1:L5:1432:G:O4'	2.18	0.43
1:L5:2864:A:H2'	1:L5:2865:U:C6	2.53	0.43
1:L5:4401:G:H2'	1:L5:4402:C:H6	1.83	0.43
2:L7:110:G:H2'	2:L7:111:C:C6	2.53	0.43
3:L8:39:G:H1'	3:L8:103:A:N6	2.34	0.43
7:LD:83:LEU:HB3	7:LD:88:VAL:HG13	2.01	0.43
1:L5:481:G:H2'	1:L5:482:G:C8	2.54	0.43
1:L5:495:C:H2'	1:L5:496:G:C8	2.53	0.43
1:L5:1537:A:H2'	1:L5:1538:U:C6	2.54	0.43
1:L5:2101:C:H2'	1:L5:2102:G:C8	2.53	0.43
1:L5:2461:G:H2'	1:L5:2462:C:C6	2.54	0.43
1:L5:2910:G:N2	1:L5:3585:G:O2'	2.52	0.43
1:L5:3610:A:H2'	1:L5:3611:A:C8	2.54	0.43
3:L8:8:U:H2'	3:L8:9:A:C8	2.53	0.43
3:L8:89:U:H2'	3:L8:90:C:C6	2.53	0.43
22:LT:50:LYS:HB3	22:LT:50:LYS:HE2	1.81	0.43
44:CA:89:PHE:HE1	44:CA:242:GLN:HE22	1.66	0.43
44:CA:354:LEU:HA	44:CA:357:LEU:HG	2.01	0.43
1:L5:300:A:H2'	1:L5:301:G:H8	1.84	0.43
1:L5:408:A:O2'	1:L5:411:G:OP2	2.25	0.43
1:L5:1545:G:H2'	1:L5:1546:C:C6	2.53	0.43
1:L5:3873:G:H2'	1:L5:3874:G:C8	2.54	0.43
5:LB:17:LEU:HA	5:LB:17:LEU:HD23	1.72	0.43
7:LD:119:TYR:OH	7:LD:139:PRO:O	2.28	0.43
10:LG:160:ASP:OD1	10:LG:160:ASP:N	2.52	0.43
30:Lc:57:LYS:HE3	30:Lc:57:LYS:HB2	1.78	0.43
1:L5:364:G:O6	37:Lj:55:ARG:NH2	2.51	0.43
1:L5:679:C:H2'	1:L5:680:G:C8	2.52	0.43
1:L5:696:C:H42	8:LE:221:LYS:HG3	1.84	0.43
1:L5:1345:A:H2'	1:L5:1346:C:C6	2.54	0.43
1:L5:3867:A2M:HM'3	1:L5:3867:A2M:H1'	1.66	0.43
6:LC:207:PRO:HB3	6:LC:249:PHE:CD2	2.54	0.43
7:LD:41:LYS:HB2	22:LT:68:THR:O	2.18	0.43
7:LD:182:GLY:HA2	7:LD:194:VAL:HG23	2.01	0.43
8:LE:104:THR:O	8:LE:105:ARG:NH1	2.51	0.43
8:LE:183:ARG:HA	8:LE:183:ARG:HD2	1.82	0.43
9:LF:214:SER:OG	9:LF:215:SER:N	2.51	0.43
16:LN:6:TYR:CZ	36:Li:40:VAL:HG22	2.54	0.43
31:Ld:114:PHE:HA	31:Ld:117:LEU:HD12	2.01	0.43
32:Le:35:TRP:CZ2	32:Le:56:PRO:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Lf:15:LYS:HB3	33:Lf:25:THR:HG23	2.00	0.43
44:CA:88:HIS:CG	44:CA:305:PHE:HB3	2.53	0.43
1:L5:162:A:H2'	1:L5:163:A:H8	1.84	0.42
1:L5:1534:A2M:N3	37:Lj:11:ARG:HB2	2.34	0.42
1:L5:2671:C:H2'	1:L5:2672:C:C6	2.54	0.42
1:L5:2864:A:H2'	1:L5:2865:U:H6	1.84	0.42
1:L5:4274:A:H2'	1:L5:4275:G:H8	1.82	0.42
7:LD:110:LEU:HB3	7:LD:115:MET:O	2.19	0.42
11:LH:44:GLU:HG3	15:LM:2:VAL:HG23	2.00	0.42
15:LM:118:MET:HG2	17:LO:192:TYR:CZ	2.54	0.42
18:LP:138:PRO:HB3	18:LP:140:MET:HE2	2.01	0.42
25:LX:151:ASN:HD22	44:CA:290:ARG:NH1	2.17	0.42
30:Lc:34:THR:HG23	30:Lc:95:ALA:HB2	2.01	0.42
1:L5:980:U:OP2	8:LE:46:ARG:NH2	2.52	0.42
1:L5:1332:C:H2'	1:L5:1333:A:C8	2.54	0.42
1:L5:1961:G:O2'	1:L5:2025:A:N6	2.52	0.42
1:L5:2347:A:C4	32:Lc:31:ILE:HD11	2.54	0.42
1:L5:2835:A:O2'	5:LB:228:TYR:O	2.31	0.42
1:L5:3712:A:C5	1:L5:3713:U:H1'	2.54	0.42
1:L5:4620:OMU:HM23	1:L5:4620:OMU:H1'	1.84	0.42
3:L8:52:A:H5'	39:Li:21:ARG:HD3	2.00	0.42
25:LX:84:GLU:O	44:CA:259:MET:HE2	2.18	0.42
25:LX:88:LYS:HE2	44:CA:259:MET:CG	2.49	0.42
1:L5:280:G:H5''	16:LN:14:LYS:HE2	2.00	0.42
1:L5:1081:C:C2'	1:L5:1082:C:H5'	2.49	0.42
1:L5:1693:U:H2'	1:L5:1694:C:O4'	2.19	0.42
1:L5:2610:G:H2'	1:L5:2611:A:C8	2.54	0.42
1:L5:4954:G:H2'	1:L5:4955:A:H8	1.83	0.42
47:L5:5284:SPD:H51	47:L5:5284:SPD:H82	1.79	0.42
37:Lj:19:CYS:SG	37:Lj:34:CYS:HB2	2.58	0.42
1:L5:162:A:H2'	1:L5:163:A:C8	2.55	0.42
1:L5:163:A:H2'	1:L5:164:G:C8	2.54	0.42
1:L5:1788:A:H2'	12:Li:22:PHE:CZ	2.53	0.42
1:L5:2438:A:O2'	1:L5:2440:U:OP2	2.37	0.42
1:L5:2634:C:H2'	1:L5:2635:U:H6	1.84	0.42
1:L5:2634:C:H2'	1:L5:2635:U:C6	2.55	0.42
1:L5:3690:U:H2'	1:L5:3691:G:O4'	2.20	0.42
1:L5:5004:C:H2'	1:L5:5005:G:O4'	2.19	0.42
3:L8:92:U:H2'	3:L8:93:C:O4'	2.19	0.42
4:LA:48:ILE:HG22	42:Lp:54:ILE:HG12	2.00	0.42
13:LJ:95:ARG:HD3	13:LJ:175:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LO:78:ARG:HD2	17:LO:78:ARG:HA	1.85	0.42
34:Lg:41:ALA:O	34:Lg:52:ARG:NH1	2.46	0.42
43:Lr:28:GLU:HG2	43:Lr:31:ASN:HB2	2.01	0.42
1:L5:99:A:H5''	16:LN:184:ILE:HD12	2.01	0.42
1:L5:179:G:H2'	1:L5:180:C:C6	2.54	0.42
1:L5:1403:G:N2	1:L5:1415:G:C4	2.88	0.42
1:L5:2008:U:N3	1:L5:2011:C:OP2	2.29	0.42
1:L5:4066:U:H2'	1:L5:4067:U:H6	1.83	0.42
1:L5:4139:G:H1'	1:L5:4146:G:N1	2.34	0.42
1:L5:4405:G:H5'	12:LI:8:CYS:SG	2.59	0.42
44:CA:36:VAL:HG12	44:CA:125:PHE:CE1	2.54	0.42
1:L5:497:G:N2	1:L5:498:C:H41	2.18	0.42
1:L5:2017:A:HO2'	1:L5:2018:C:C5'	2.32	0.42
1:L5:2763:U:H4'	1:L5:2764:A:H5''	2.00	0.42
1:L5:4451:G:N2	1:L5:4452:U:O4	2.49	0.42
6:LC:268:ARG:HH12	6:LC:269:LYS:HE2	1.85	0.42
8:LE:99:ASP:OD1	8:LE:99:ASP:N	2.49	0.42
14:LL:58:ILE:HG13	14:LL:116:ARG:HD2	2.02	0.42
24:LV:37:LEU:HD23	24:LV:65:VAL:HG12	2.01	0.42
34:Lg:82:MET:HE3	34:Lg:82:MET:HB2	1.96	0.42
1:L5:1588:U:H2'	1:L5:1589:C:C6	2.55	0.42
1:L5:2019:C:H2'	1:L5:2020:U:H6	1.84	0.42
1:L5:2465:C:H2'	1:L5:2466:G:O4'	2.20	0.42
1:L5:2538:U:H2'	1:L5:2539:C:C6	2.55	0.42
1:L5:2607:C:O5'	20:LR:96:MET:HE1	2.20	0.42
1:L5:2808:G:O3'	20:LR:60:ARG:NH1	2.53	0.42
1:L5:2844:A:O2'	1:L5:4631:G:H4'	2.20	0.42
5:LB:220:ILE:HG12	5:LB:278:THR:HG23	2.02	0.42
7:LD:264:LYS:HD3	7:LD:266:TRP:CZ2	2.55	0.42
1:L5:85:G:O2'	1:L5:97:G:O6	2.30	0.42
1:L5:1269:G:O2'	1:L5:1270:A:O4'	2.26	0.42
1:L5:1899:G:O2'	32:Le:57:ASN:OD1	2.35	0.42
1:L5:2007:G:H21	1:L5:2012:A:N6	2.06	0.42
1:L5:2765:A:H2'	1:L5:2766:A:C8	2.55	0.42
1:L5:3813:A:N3	1:L5:4538:G:O2'	2.43	0.42
1:L5:4232:U:H5'	41:Lo:3:ASN:HB3	2.01	0.42
1:L5:4489:G:H4'	47:L5:5290:SPD:H91	2.02	0.42
18:LP:18:ARG:NH2	18:LP:147:GLU:OE1	2.53	0.42
25:LX:82:THR:HG21	35:Lh:37:THR:HG22	2.00	0.42
42:Lp:26:VAL:HG22	42:Lp:30:GLU:HG3	2.02	0.42
1:L5:308:G:OP2	1:L5:308:G:N2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1613:A:H5''	4:LA:183:GLY:HA2	2.02	0.42
1:L5:2517:A:H5'	34:Lg:62:LYS:HD3	2.01	0.42
1:L5:4291:G:H5'	1:L5:4293:PSU:C6	2.55	0.42
1:L5:4460:U:H2'	1:L5:4461:C:H6	1.84	0.42
1:L5:4672:A:OP1	24:LV:15:ARG:NH2	2.36	0.42
1:L5:4723:A:H2'	1:L5:4724:A:C8	2.55	0.42
1:L5:4749:C:H2'	1:L5:4750:G:O4'	2.19	0.42
1:L5:4913:G:H4'	1:L5:4914:C:O5'	2.18	0.42
1:L5:4934:A:H2'	1:L5:4935:C:H6	1.84	0.42
35:Lh:52:LYS:HA	35:Lh:52:LYS:HD3	1.80	0.42
1:L5:497:G:H21	1:L5:498:C:H5	1.66	0.42
1:L5:707:C:O2'	1:L5:4943:A:N1	2.49	0.42
1:L5:1070:G:O2'	1:L5:1071:C:O5'	2.33	0.42
1:L5:1414:C:H2'	1:L5:1415:G:C8	2.43	0.42
1:L5:2266:C:OP1	1:L5:2271:C:O2'	2.32	0.42
1:L5:2550:G:O2'	1:L5:2587:A:N1	2.47	0.42
1:L5:2637:U:OP1	34:Lg:28:ASN:ND2	2.51	0.42
1:L5:2749:C:H2'	1:L5:2750:G:C8	2.55	0.42
1:L5:4277:G:H5''	22:LT:17:ARG:HG2	2.01	0.42
1:L5:4389:C:H2'	1:L5:4390:A:C8	2.55	0.42
1:L5:4563:U:H2'	1:L5:4564:A:H8	1.85	0.42
1:L5:4987:C:P	5:LB:116:ARG:HH22	2.42	0.42
15:LM:124:LYS:HB2	15:LM:124:LYS:HE3	1.91	0.42
17:LO:124:LEU:HD23	17:LO:124:LEU:HA	1.90	0.42
20:LR:112:SER:OG	20:LR:114:LYS:HG3	2.20	0.42
23:LU:101:ARG:HG2	23:LU:103:VAL:HG23	2.01	0.42
27:LZ:95:VAL:HG12	27:LZ:110:ALA:HA	2.02	0.42
1:L5:1309:C:H2'	1:L5:1310:C:C6	2.54	0.41
1:L5:1367:C:O2'	1:L5:1369:C:OP2	2.30	0.41
1:L5:2718:U:H5''	1:L5:2719:C:H5'	2.02	0.41
1:L5:3684:G:H2'	1:L5:3685:C:C6	2.55	0.41
1:L5:3842:C:H3'	1:L5:3843:C:H2'	2.02	0.41
1:L5:3886:G:OP1	17:LO:85:ARG:NH2	2.52	0.41
1:L5:4327:C:OP1	22:LT:70:HIS:NE2	2.53	0.41
1:L5:4920:C:H2'	1:L5:4921:C:H6	1.84	0.41
1:L5:417:G:OP1	1:L5:2329:U:O2'	2.32	0.41
1:L5:1696:C:H5'	1:L5:1719:A:H1'	2.01	0.41
1:L5:2298:U:OP1	6:LC:204:ARG:NE	2.51	0.41
1:L5:2491:C:H2'	1:L5:2492:C:C6	2.55	0.41
1:L5:3606:U:H2'	1:L5:3607:U:C6	2.55	0.41
3:L8:58:G:O6	37:Lj:63:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LN:75:VAL:HG21	16:LN:80:THR:HG22	2.02	0.41
1:L5:223:G:H4'	1:L5:225:G:N7	2.35	0.41
1:L5:260:C:H2'	1:L5:261:G:C8	2.55	0.41
1:L5:1846:G:H2'	1:L5:1847:C:H6	1.85	0.41
1:L5:2555:G:H2'	1:L5:2556:G:H8	1.85	0.41
1:L5:2803:U:H2'	1:L5:2804:OMC:H6	1.84	0.41
1:L5:4336:A:H5''	1:L5:4337:C:H5'	2.02	0.41
1:L5:4344:U:H2'	1:L5:4345:C:C6	2.56	0.41
7:LD:59:ASP:OD1	7:LD:60:ILE:N	2.54	0.41
8:LE:95:PRO:HA	8:LE:104:THR:HG22	2.03	0.41
8:LE:243:THR:HG22	8:LE:245:GLN:H	1.85	0.41
9:LF:171:ASP:OD1	9:LF:172:ASN:N	2.54	0.41
21:LS:70:LYS:HD3	21:LS:70:LYS:HA	1.85	0.41
23:LU:27:HIS:HB3	23:LU:114:TYR:HE1	1.85	0.41
26:LY:22:PRO:HD2	26:LY:25:ILE:HD11	2.02	0.41
44:CA:208:GLN:HA	44:CA:211:LYS:HE3	2.01	0.41
1:L5:252:C:H2'	1:L5:253:G:H8	1.85	0.41
1:L5:1220:G:H2'	1:L5:1221:G:C8	2.56	0.41
1:L5:2110:C:N4	1:L5:2111:G:O6	2.53	0.41
1:L5:2656:U:H5''	27:LZ:38:TYR:HB3	2.02	0.41
1:L5:3689:G:O2'	1:L5:3818:UY1:OP2	2.33	0.41
1:L5:3951:G:H1'	1:L5:4062:A:H61	1.85	0.41
1:L5:4563:U:H2'	1:L5:4564:A:C8	2.55	0.41
1:L5:4750:G:H2'	1:L5:4751:G:H8	1.86	0.41
4:LA:142:GLU:O	4:LA:143:THR:OG1	2.35	0.41
11:LH:43:VAL:HG21	11:LH:73:ILE:HD13	2.03	0.41
19:LQ:59:PRO:HG3	19:LQ:143:ARG:HA	2.00	0.41
43:Lr:56:ASP:OD1	43:Lr:56:ASP:N	2.43	0.41
44:CA:158:LYS:HA	44:CA:325:LEU:HD11	2.02	0.41
1:L5:1734:G:N2	1:L5:1735:U:O4	2.39	0.41
1:L5:2654:C:H2'	1:L5:2655:C:H6	1.85	0.41
1:L5:2683:C:H2'	1:L5:2684:C:C6	2.56	0.41
1:L5:4996:C:OP1	31:Ld:32:ARG:NH1	2.28	0.41
4:LA:75:LEU:HD12	4:LA:75:LEU:HA	1.92	0.41
9:LF:48:LYS:HE3	29:Lb:96:LEU:HD21	2.02	0.41
9:LF:241:ASN:O	9:LF:245:ARG:HG2	2.20	0.41
23:LU:39:PHE:HD1	23:LU:90:TYR:CD2	2.39	0.41
25:LX:88:LYS:HE2	44:CA:258:LYS:O	2.21	0.41
31:Ld:33:ILE:HD11	31:Ld:45:ALA:HA	2.01	0.41
34:Lg:41:ALA:O	34:Lg:52:ARG:HD3	2.21	0.41
34:Lg:69:LYS:HG3	34:Lg:73:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:135:G:N7	35:Lh:97:LYS:HE3	2.35	0.41
1:L5:398:A2M:HM'3	1:L5:398:A2M:H1'	1.70	0.41
1:L5:1333:A:H2'	1:L5:1334:A:H8	1.85	0.41
1:L5:1494:U:H2'	1:L5:1495:G:C8	2.56	0.41
1:L5:1510:G:H2'	1:L5:1511:U:C6	2.56	0.41
1:L5:3785:A2M:H2	1:L5:4551:U:O2	2.20	0.41
1:L5:3893:C:H2'	1:L5:3894:A:C8	2.55	0.41
1:L5:4390:A:H2'	1:L5:4391:G:O4'	2.21	0.41
2:L7:6:C:O2'	7:LD:50:ARG:NH2	2.53	0.41
3:L8:78:G:H5''	44:CA:238:LYS:HD2	2.01	0.41
20:LR:44:LEU:HD22	20:LR:49:LEU:HD12	2.02	0.41
25:LX:156:ILE:HG21	44:CA:290:ARG:HE	1.85	0.41
27:LZ:135:ARG:HD2	27:LZ:135:ARG:HA	1.82	0.41
42:Lp:62:LYS:HE2	42:Lp:62:LYS:HB2	1.97	0.41
1:L5:982:U:H2'	1:L5:983:C:C6	2.56	0.41
1:L5:1255:A:N7	1:L5:1257:A:H1'	2.36	0.41
1:L5:1317:U:H2'	1:L5:1318:C:C6	2.55	0.41
1:L5:2052:G:O2'	1:L5:2057:A:N1	2.49	0.41
1:L5:2409:U:H5	1:L5:2783:A:N1	2.18	0.41
1:L5:2481:G:H2'	1:L5:2482:C:C6	2.55	0.41
1:L5:4637:OMG:HM23	1:L5:4637:OMG:H1'	1.74	0.41
5:LB:46:PHE:CZ	5:LB:84:MET:HG2	2.56	0.41
11:LH:8:GLN:HG2	11:LH:74:CYS:SG	2.61	0.41
12:LI:101:LYS:NZ	12:LI:102:MET:O	2.52	0.41
38:Lk:27:LYS:O	38:Lk:70:LYS:NZ	2.51	0.41
44:CA:27:ILE:HA	44:CA:30:ARG:HG2	2.03	0.41
44:CA:202:ILE:HG12	44:CA:205:PRO:HG3	2.01	0.41
1:L5:44:A:H5''	46:L5:5264:SPM:H81	2.02	0.41
1:L5:1354:A:H5'	19:LQ:108:ARG:HH21	1.85	0.41
1:L5:1625:OMG:HM23	16:LN:81:TYR:HE2	1.86	0.41
1:L5:1802:A:H4'	22:LT:105:PHE:CE1	2.56	0.41
1:L5:3841:OMC:HM23	1:L5:3841:OMC:H1'	1.82	0.41
1:L5:3910:C:H2'	1:L5:3911:C:H6	1.83	0.41
1:L5:4625:C:O2'	1:L5:4626:A:H5'	2.21	0.41
1:L5:5003:U:H2'	1:L5:5004:C:C6	2.55	0.41
6:LC:222:ARG:HD3	26:LY:3:PHE:HZ	1.86	0.41
6:LC:279:LEU:HD23	6:LC:279:LEU:HA	1.86	0.41
21:LS:69:GLU:OE1	21:LS:102:THR:N	2.42	0.41
1:L5:92:C:C2	28:La:55:LYS:HE2	2.56	0.41
1:L5:515:C:H41	1:L5:647:G:H21	1.68	0.41
1:L5:653:U:H3'	1:L5:654:C:H5''	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L5:1364:U:OP2	14:LL:36:ARG:NH2	2.33	0.41
1:L5:1647:U:OP1	47:L5:5291:SPD:H51	2.21	0.41
1:L5:1751:A:H2'	1:L5:1752:G:H8	1.86	0.41
1:L5:2519:U:H1'	1:L5:2520:C:C6	2.55	0.41
1:L5:2638:G:N2	1:L5:2719:C:OP2	2.54	0.41
1:L5:3611:A:C2	1:L5:5016:A:H8	2.38	0.41
1:L5:3656:A:H2'	1:L5:3657:U:H6	1.85	0.41
1:L5:3867:A2M:HM'3	1:L5:3880:G:N2	2.35	0.41
1:L5:3896:C:H1'	5:LB:268:ARG:NH2	2.36	0.41
1:L5:4305:G:C6	22:LT:80:VAL:HG21	2.55	0.41
1:L5:4478:G:O2'	1:L5:4602:A:N1	2.48	0.41
1:L5:5028:G:H2'	1:L5:5029:C:C6	2.56	0.41
1:L5:5064:G:H21	18:LP:75:GLN:NE2	2.18	0.41
14:LL:7:GLY:O	28:La:49:HIS:NE2	2.41	0.41
18:LP:76:TRP:CD1	18:LP:76:TRP:H	2.38	0.41
20:LR:35:ALA:HA	20:LR:40:GLN:OE1	2.20	0.41
21:LS:83:ARG:HG3	21:LS:125:GLN:HB2	2.02	0.41
29:Lb:49:HIS:O	29:Lb:52:LYS:HG2	2.21	0.41
32:Le:23:HIS:HA	32:Le:53:ILE:HD12	2.01	0.41
33:Lf:92:LEU:HD23	33:Lf:92:LEU:HA	1.90	0.41
42:Lp:61:MET:HE3	42:Lp:61:MET:HB3	1.88	0.41
1:L5:498:C:C4	1:L5:499:G:H1'	2.56	0.41
1:L5:662:C:H2'	1:L5:663:G:C8	2.56	0.41
1:L5:1461:C:H2'	1:L5:1462:A:C8	2.55	0.41
1:L5:2610:G:H2'	1:L5:2611:A:H8	1.86	0.41
1:L5:4220:6MZ:H2'	1:L5:4222:G:H5''	2.02	0.41
1:L5:4920:C:H2'	1:L5:4921:C:C6	2.56	0.41
11:LH:41:ILE:HG21	11:LH:73:ILE:HD11	2.03	0.41
15:LM:96:GLU:O	15:LM:100:ARG:HG2	2.21	0.41
27:LZ:33:THR:C	27:LZ:35:ASP:H	2.29	0.41
44:CA:291:MET:O	44:CA:294:VAL:HG22	2.20	0.41
1:L5:10:A:H2'	1:L5:11:G:H8	1.85	0.40
1:L5:368:C:O4'	6:LC:83:GLY:HA3	2.21	0.40
1:L5:382:G:H4'	1:L5:407:A:N1	2.36	0.40
1:L5:959:G:C8	8:LE:123:ARG:HG2	2.56	0.40
1:L5:978:G:H2'	1:L5:979:C:C6	2.55	0.40
1:L5:1613:A:H5''	4:LA:183:GLY:CA	2.51	0.40
1:L5:4093:G:H3'	1:L5:4094:G:C8	2.56	0.40
1:L5:4244:A:H2'	1:L5:4245:G:O4'	2.21	0.40
1:L5:4996:C:H4'	31:Ld:26:THR:HG23	2.02	0.40
3:L8:102:G:H5''	37:Lj:39:TYR:HE1	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:LA:116:LEU:HB3	4:LA:126:LEU:HB2	2.02	0.40
12:LI:47:PRO:HB3	12:LI:171:TRP:CZ2	2.56	0.40
15:LM:33:GLN:O	15:LM:33:GLN:HG2	2.20	0.40
31:Ld:68:LEU:HD22	31:Ld:106:VAL:HG12	2.02	0.40
1:L5:252:C:H2'	1:L5:253:G:C8	2.56	0.40
1:L5:462:G:H2'	1:L5:463:A:C8	2.56	0.40
1:L5:684:G:H5''	8:LE:100:LYS:HE3	2.02	0.40
1:L5:980:U:H2'	1:L5:981:C:C6	2.56	0.40
1:L5:1327:C:H2'	1:L5:1328:G:H8	1.83	0.40
1:L5:1895:G:OP1	9:LF:96:ARG:NH2	2.50	0.40
1:L5:2630:U:OP1	23:LU:48:LYS:NZ	2.37	0.40
1:L5:3861:A:H2'	1:L5:3862:A:H8	1.87	0.40
1:L5:4458:C:H2'	1:L5:4459:U:C6	2.56	0.40
3:L8:5:U:H2'	3:L8:6:C:C6	2.55	0.40
4:LA:65:ASP:OD2	4:LA:72:ARG:NE	2.42	0.40
9:LF:209:TRP:CD1	9:LF:210:PRO:HD2	2.56	0.40
14:LL:194:ILE:HD12	14:LL:194:ILE:HA	1.88	0.40
37:Lj:85:LYS:HB3	37:Lj:85:LYS:HE3	1.74	0.40
1:L5:362:A:N6	39:LI:37:TYR:O	2.46	0.40
1:L5:1438:U:H4'	9:LF:31:LYS:HE3	2.02	0.40
1:L5:1869:G:C6	47:L5:5286:SPD:H32	2.56	0.40
1:L5:2566:G:H2'	1:L5:2567:G:C8	2.55	0.40
1:L5:3825:A2M:H2'	1:L5:3826:C:O4'	2.21	0.40
1:L5:5006:U:H4'	1:L5:5007:A:H5'	2.02	0.40
2:L7:117:G:OP1	7:LD:253:TYR:OH	2.35	0.40
4:LA:60:LYS:HE3	4:LA:60:LYS:HB2	1.80	0.40
12:LI:36:LEU:HD11	12:LI:69:ARG:HD2	2.03	0.40
19:LQ:32:TYR:HD2	19:LQ:51:LEU:HD11	1.86	0.40
25:LX:80:PRO:HA	25:LX:98:PHE:HA	2.03	0.40
44:CA:273:PHE:CG	44:CA:278:PHE:HB3	2.56	0.40
1:L5:139:G:H2'	1:L5:140:G:H8	1.86	0.40
1:L5:186:G:H4'	1:L5:187:U:O4'	2.22	0.40
1:L5:2467:U:H4'	1:L5:2468:U:H5'	2.03	0.40
1:L5:3666:C:OP1	4:LA:234:LYS:NZ	2.33	0.40
1:L5:3687:A:O2'	4:LA:236:GLY:N	2.54	0.40
1:L5:4080:C:H2'	1:L5:4081:G:H8	1.86	0.40
1:L5:4616:A:H2'	1:L5:4617:G:O4'	2.22	0.40
3:L8:144:U:H2'	3:L8:145:C:C6	2.56	0.40
4:LA:115:CYS:SG	4:LA:124:GLY:HA3	2.61	0.40
18:LP:15:CYS:SG	18:LP:150:LEU:HB2	2.61	0.40
21:LS:5:GLY:O	21:LS:111:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LT:52:MET:HG2	22:LT:95:HIS:CE1	2.57	0.40
39:LI:12:PHE:CE2	39:LI:51:LEU:HD22	2.56	0.40
44:CA:101:LYS:HE2	44:CA:101:LYS:HB2	1.97	0.40
1:L5:123:C:H2'	1:L5:124:C:H6	1.86	0.40
1:L5:271:C:H2'	1:L5:272:U:C6	2.56	0.40
1:L5:1190:C:H2'	1:L5:1191:C:C6	2.57	0.40
1:L5:1351:G:O6	19:LQ:55:ARG:NH1	2.53	0.40
1:L5:1895:G:H2'	1:L5:1896:A:O4'	2.22	0.40
1:L5:1977:C:O2'	1:L5:1978:C:OP1	2.37	0.40
1:L5:2422:OMC:HM23	1:L5:2422:OMC:H1'	1.91	0.40
1:L5:2558:C:H2'	1:L5:2559:G:H8	1.86	0.40
1:L5:3718:A2M:H2	1:L5:3934:G:O4'	2.22	0.40
1:L5:3908:A:N7	1:L5:4449:A:N6	2.69	0.40
1:L5:4064:C:H2'	1:L5:4065:G:H8	1.85	0.40
1:L5:4507:A:H2'	1:L5:4508:C:C6	2.56	0.40
1:L5:4896:G:H2'	1:L5:4897:G:C8	2.56	0.40
5:LB:214:ASP:OD2	5:LB:362:LYS:HA	2.21	0.40
12:LI:38:ARG:NH1	12:LI:45:GLU:OE1	2.43	0.40
21:LS:99:ASP:OD1	21:LS:100:LEU:N	2.53	0.40
22:LT:4:THR:OG1	22:LT:9:ARG:HD3	2.21	0.40
26:LY:103:LYS:HD3	26:LY:103:LYS:HA	1.93	0.40
34:Lg:33:LEU:HD23	34:Lg:33:LEU:HA	1.88	0.40
35:Lh:94:ARG:HE	35:Lh:94:ARG:HB3	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	246/248 (99%)	229 (93%)	17 (7%)	0	100	100
5	LB	400/402 (100%)	385 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	LC	366/368 (100%)	353 (96%)	13 (4%)	0	100	100
7	LD	291/293 (99%)	282 (97%)	9 (3%)	0	100	100
8	LE	236/250 (94%)	226 (96%)	10 (4%)	0	100	100
9	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
10	LG	239/241 (99%)	226 (95%)	13 (5%)	0	100	100
11	LH	188/190 (99%)	183 (97%)	5 (3%)	0	100	100
12	LI	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
13	LJ	168/176 (96%)	162 (96%)	6 (4%)	0	100	100
14	LL	208/210 (99%)	201 (97%)	7 (3%)	0	100	100
15	LM	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
16	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
17	LO	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
18	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
19	LQ	185/187 (99%)	182 (98%)	3 (2%)	0	100	100
20	LR	150/187 (80%)	146 (97%)	4 (3%)	0	100	100
21	LS	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
22	LT	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
23	LU	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
24	LV	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
25	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
26	LY	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
27	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
28	La	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
29	Lb	105/121 (87%)	100 (95%)	5 (5%)	0	100	100
30	Lc	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
31	Ld	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
32	Le	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
33	Lf	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
34	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
35	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
36	Li	100/102 (98%)	99 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	Lj	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
38	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
39	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
40	Lm	50/52 (96%)	50 (100%)	0	0	100	100
41	Lo	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
42	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
43	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
44	CA	350/356 (98%)	334 (95%)	16 (5%)	0	100	100
All	All	6670/6823 (98%)	6448 (97%)	222 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	LA	190/190 (100%)	190 (100%)	0	100	100
5	LB	348/348 (100%)	348 (100%)	0	100	100
6	LC	306/306 (100%)	306 (100%)	0	100	100
7	LD	246/247 (100%)	246 (100%)	0	100	100
8	LE	212/222 (96%)	212 (100%)	0	100	100
9	LF	194/194 (100%)	194 (100%)	0	100	100
10	LG	203/205 (99%)	203 (100%)	0	100	100
11	LH	169/169 (100%)	169 (100%)	0	100	100
12	LI	180/180 (100%)	180 (100%)	0	100	100
13	LJ	143/148 (97%)	143 (100%)	0	100	100
14	LL	176/176 (100%)	176 (100%)	0	100	100
15	LM	118/118 (100%)	118 (100%)	0	100	100
16	LN	171/171 (100%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	LO	173/173 (100%)	173 (100%)	0	100	100
18	LP	134/134 (100%)	134 (100%)	0	100	100
19	LQ	164/164 (100%)	164 (100%)	0	100	100
20	LR	136/166 (82%)	136 (100%)	0	100	100
21	LS	156/156 (100%)	156 (100%)	0	100	100
22	LT	139/139 (100%)	139 (100%)	0	100	100
23	LU	91/91 (100%)	91 (100%)	0	100	100
24	LV	101/101 (100%)	101 (100%)	0	100	100
25	LX	108/108 (100%)	108 (100%)	0	100	100
26	LY	124/124 (100%)	124 (100%)	0	100	100
27	LZ	117/117 (100%)	117 (100%)	0	100	100
28	La	120/120 (100%)	120 (100%)	0	100	100
29	Lb	88/101 (87%)	88 (100%)	0	100	100
30	Lc	83/83 (100%)	83 (100%)	0	100	100
31	Ld	98/98 (100%)	98 (100%)	0	100	100
32	Le	114/114 (100%)	114 (100%)	0	100	100
33	Lf	88/88 (100%)	88 (100%)	0	100	100
34	Lg	98/98 (100%)	98 (100%)	0	100	100
35	Lh	109/109 (100%)	109 (100%)	0	100	100
36	Li	86/86 (100%)	86 (100%)	0	100	100
37	Lj	73/73 (100%)	73 (100%)	0	100	100
38	Lk	64/64 (100%)	64 (100%)	0	100	100
39	Ll	47/47 (100%)	47 (100%)	0	100	100
40	Lm	48/48 (100%)	48 (100%)	0	100	100
41	Lo	93/93 (100%)	93 (100%)	0	100	100
42	Lp	74/74 (100%)	74 (100%)	0	100	100
43	Lr	109/109 (100%)	109 (100%)	0	100	100
44	CA	303/305 (99%)	303 (100%)	0	100	100
All	All	5794/5857 (99%)	5794 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43)

such sidechains are listed below:

Mol	Chain	Res	Type
4	LA	50	HIS
4	LA	97	ASN
5	LB	68	ASN
5	LB	121	ASN
5	LB	145	GLN
5	LB	203	GLN
5	LB	289	GLN
5	LB	301	ASN
6	LC	329	ASN
7	LD	131	ASN
7	LD	202	GLN
7	LD	244	HIS
9	LF	39	GLN
10	LG	112	GLN
11	LH	98	HIS
11	LH	138	GLN
12	LI	59	GLN
12	LI	73	ASN
13	LJ	71	HIS
13	LJ	110	GLN
14	LL	149	GLN
15	LM	34	ASN
15	LM	66	HIS
16	LN	37	HIS
16	LN	199	GLN
17	LO	50	ASN
18	LP	75	GLN
18	LP	137	ASN
19	LQ	21	GLN
20	LR	134	ASN
22	LT	144	ASN
23	LU	94	ASN
24	LV	77	HIS
25	LX	57	GLN
26	LY	61	HIS
28	La	34	ASN
28	La	60	HIS
28	La	120	GLN
32	Le	52	GLN
36	Li	15	HIS
37	Lj	66	HIS
43	Lr	21	ASN

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Mol	Chain	Res	Type
43	Lr	30	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3643/3675 (99%)	714 (19%)	16 (0%)
2	L7	119/120 (99%)	11 (9%)	0
3	L8	155/156 (99%)	22 (14%)	0
All	All	3917/3951 (99%)	747 (19%)	16 (0%)

All (747) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	25	A
1	L5	30	C
1	L5	39	A
1	L5	42	A
1	L5	48	G
1	L5	56	A
1	L5	59	A
1	L5	64	A
1	L5	65	A
1	L5	70	A
1	L5	73	A
1	L5	91	G
1	L5	98	A
1	L5	104	G
1	L5	108	A
1	L5	109	G
1	L5	110	C
1	L5	119	G
1	L5	120	A
1	L5	127	G
1	L5	132	G
1	L5	133	C
1	L5	134	G
1	L5	135	G
1	L5	136	C
1	L5	145	G
1	L5	159	C
1	L5	165	A

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Mol	Chain	Res	Type
1	L5	172	C
1	L5	181	C
1	L5	182	G
1	L5	183	C
1	L5	184	U
1	L5	185	C
1	L5	187	U
1	L5	188	G
1	L5	189	G
1	L5	200	U
1	L5	209	U
1	L5	210	C
1	L5	216	C
1	L5	218	A
1	L5	220	C
1	L5	234	G
1	L5	237	G
1	L5	255	C
1	L5	256	G
1	L5	261	G
1	L5	263	G
1	L5	264	C
1	L5	265	C
1	L5	266	C
1	L5	267	G
1	L5	280	G
1	L5	297	U
1	L5	306	A
1	L5	315	G
1	L5	316	U
1	L5	340	C
1	L5	373	G
1	L5	385	A
1	L5	387	G
1	L5	388	A
1	L5	407	A
1	L5	409	G
1	L5	410	A
1	L5	411	G
1	L5	412	G
1	L5	413	G
1	L5	432	U

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Mol	Chain	Res	Type
1	L5	440	U
1	L5	449	C
1	L5	452	A
1	L5	453	G
1	L5	454	U
1	L5	456	C
1	L5	457	G
1	L5	467	U
1	L5	484	U
1	L5	485	C
1	L5	486	C
1	L5	489	C
1	L5	493	G
1	L5	494	U
1	L5	497	G
1	L5	498	C
1	L5	499	G
1	L5	500	G
1	L5	502	C
1	L5	503	C
1	L5	504	G
1	L5	509	A
1	L5	510	U
1	L5	512	U
1	L5	513	U
1	L5	514	U
1	L5	518	G
1	L5	643	C
1	L5	646	G
1	L5	654	C
1	L5	655	C
1	L5	656	C
1	L5	657	C
1	L5	659	G
1	L5	666	G
1	L5	667	A
1	L5	668	C
1	L5	669	C
1	L5	673	C
1	L5	685	C
1	L5	686	A
1	L5	687	U

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Mol	Chain	Res	Type
1	L5	704	C
1	L5	708	G
1	L5	730	G
1	L5	731	G
1	L5	738	C
1	L5	739	G
1	L5	742	G
1	L5	746	A
1	L5	759	G
1	L5	904	C
1	L5	905	C
1	L5	906	C
1	L5	910	G
1	L5	913	U
1	L5	914	U
1	L5	915	A
1	L5	917	A
1	L5	923	C
1	L5	924	C
1	L5	926	G
1	L5	932	A
1	L5	933	G
1	L5	936	C
1	L5	943	A
1	L5	945	U
1	L5	946	C
1	L5	956	A
1	L5	958	G
1	L5	959	G
1	L5	960	A
1	L5	961	G
1	L5	962	C
1	L5	965	G
1	L5	966	A
1	L5	967	C
1	L5	969	C
1	L5	970	G
1	L5	977	C
1	L5	982	U
1	L5	985	C
1	L5	1070	G
1	L5	1071	C

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Mol	Chain	Res	Type
1	L5	1072	C
1	L5	1075	G
1	L5	1082	C
1	L5	1083	U
1	L5	1168	G
1	L5	1171	G
1	L5	1172	C
1	L5	1173	G
1	L5	1179	U
1	L5	1180	C
1	L5	1181	C
1	L5	1182	C
1	L5	1183	C
1	L5	1187	G
1	L5	1202	C
1	L5	1203	G
1	L5	1210	C
1	L5	1211	G
1	L5	1214	C
1	L5	1215	C
1	L5	1218	G
1	L5	1219	G
1	L5	1222	A
1	L5	1241	C
1	L5	1246	G
1	L5	1253	G
1	L5	1254	A
1	L5	1257	A
1	L5	1258	G
1	L5	1262	G
1	L5	1266	G
1	L5	1267	C
1	L5	1269	G
1	L5	1271	G
1	L5	1272	C
1	L5	1273	G
1	L5	1275	G
1	L5	1280	C
1	L5	1284	G
1	L5	1285	U
1	L5	1287	G
1	L5	1293	G

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Mol	Chain	Res	Type
1	L5	1294	A
1	L5	1295	C
1	L5	1296	G
1	L5	1301	C
1	L5	1326	A2M
1	L5	1337	A
1	L5	1354	A
1	L5	1359	G
1	L5	1365	C
1	L5	1366	G
1	L5	1367	C
1	L5	1379	C
1	L5	1387	A
1	L5	1394	G
1	L5	1397	A
1	L5	1403	G
1	L5	1404	G
1	L5	1407	C
1	L5	1409	C
1	L5	1410	U
1	L5	1411	C
1	L5	1414	C
1	L5	1417	C
1	L5	1420	A
1	L5	1425	G
1	L5	1437	C
1	L5	1439	C
1	L5	1442	C
1	L5	1443	A
1	L5	1444	G
1	L5	1446	C
1	L5	1447	C
1	L5	1482	G
1	L5	1483	C
1	L5	1497	A
1	L5	1498	G
1	L5	1502	G
1	L5	1517	G
1	L5	1534	A2M
1	L5	1537	A
1	L5	1547	A
1	L5	1566	C

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Mol	Chain	Res	Type
1	L5	1578	U
1	L5	1591	U
1	L5	1596	U
1	L5	1621	A
1	L5	1624	G
1	L5	1625	OMG
1	L5	1626	G
1	L5	1631	A
1	L5	1633	G
1	L5	1634	A
1	L5	1638	A
1	L5	1640	C
1	L5	1641	G
1	L5	1642	A
1	L5	1654	G
1	L5	1661	C
1	L5	1676	C
1	L5	1677	PSU
1	L5	1678	C
1	L5	1694	C
1	L5	1697	G
1	L5	1699	A
1	L5	1700	G
1	L5	1701	A
1	L5	1702	C
1	L5	1704	C
1	L5	1705	G
1	L5	1717	C
1	L5	1718	C
1	L5	1719	A
1	L5	1721	G
1	L5	1731	C
1	L5	1734	G
1	L5	1742	A
1	L5	1750	G
1	L5	1753	G
1	L5	1755	C
1	L5	1757	U
1	L5	1758	G
1	L5	1760	G
1	L5	1761	G
1	L5	1762	C

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Mol	Chain	Res	Type
1	L5	1763	C
1	L5	1764	G
1	L5	1765	A
1	L5	1766	A
1	L5	1767	A
1	L5	1768	C
1	L5	1770	A
1	L5	1785	C
1	L5	1787	A
1	L5	1804	A
1	L5	1806	G
1	L5	1810	G
1	L5	1821	G
1	L5	1822	U
1	L5	1834	U
1	L5	1836	G
1	L5	1837	A
1	L5	1842	G
1	L5	1855	G
1	L5	1869	G
1	L5	1882	U
1	L5	1892	A
1	L5	1897	A
1	L5	1917	A
1	L5	1918	U
1	L5	1919	G
1	L5	1920	C
1	L5	1921	C
1	L5	1922	G
1	L5	1925	G
1	L5	1931	C
1	L5	1932	A
1	L5	1936	C
1	L5	1948	G
1	L5	1951	G
1	L5	1961	G
1	L5	1962	A
1	L5	1974	U
1	L5	1975	G
1	L5	1978	C
1	L5	1980	U
1	L5	1981	G

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Mol	Chain	Res	Type
1	L5	1982	G
1	L5	1983	A
1	L5	1984	A
1	L5	1985	G
1	L5	1986	U
1	L5	1991	A
1	L5	1993	C
1	L5	1997	U
1	L5	1998	A
1	L5	1999	A
1	L5	2001	G
1	L5	2002	A
1	L5	2003	G
1	L5	2004	U
1	L5	2011	C
1	L5	2017	A
1	L5	2018	C
1	L5	2024	G
1	L5	2026	A
1	L5	2046	G
1	L5	2048	U
1	L5	2055	G
1	L5	2056	G
1	L5	2069	A
1	L5	2084	C
1	L5	2092	G
1	L5	2093	A
1	L5	2095	A
1	L5	2097	U
1	L5	2098	G
1	L5	2101	C
1	L5	2102	G
1	L5	2107	C
1	L5	2110	C
1	L5	2111	G
1	L5	2112	G
1	L5	2250	C
1	L5	2252	G
1	L5	2256	C
1	L5	2261	G
1	L5	2289	C
1	L5	2300	A

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Mol	Chain	Res	Type
1	L5	2301	G
1	L5	2313	A
1	L5	2333	G
1	L5	2348	G
1	L5	2351	OMC
1	L5	2360	A
1	L5	2364	OMG
1	L5	2383	C
1	L5	2395	A
1	L5	2397	G
1	L5	2417	A
1	L5	2425	U
1	L5	2450	G
1	L5	2453	A
1	L5	2464	C
1	L5	2465	C
1	L5	2469	C
1	L5	2471	G
1	L5	2474	G
1	L5	2475	G
1	L5	2478	C
1	L5	2479	G
1	L5	2483	G
1	L5	2484	A
1	L5	2485	U
1	L5	2486	G
1	L5	2487	G
1	L5	2488	C
1	L5	2489	C
1	L5	2490	U
1	L5	2494	U
1	L5	2504	C
1	L5	2505	C
1	L5	2506	G
1	L5	2507	A
1	L5	2513	A
1	L5	2519	U
1	L5	2520	C
1	L5	2537	A
1	L5	2544	G
1	L5	2546	G
1	L5	2547	G

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Mol	Chain	Res	Type
1	L5	2554	U
1	L5	2555	G
1	L5	2560	C
1	L5	2565	A
1	L5	2567	G
1	L5	2573	A
1	L5	2583	C
1	L5	2587	A
1	L5	2589	C
1	L5	2618	G
1	L5	2627	C
1	L5	2653	C
1	L5	2662	G
1	L5	2669	C
1	L5	2675	G
1	L5	2676	A
1	L5	2687	U
1	L5	2694	G
1	L5	2695	A
1	L5	2696	A
1	L5	2706	G
1	L5	2707	U
1	L5	2708	U
1	L5	2709	C
1	L5	2710	C
1	L5	2711	G
1	L5	2721	G
1	L5	2724	G
1	L5	2726	G
1	L5	2739	C
1	L5	2742	G
1	L5	2743	A
1	L5	2746	A
1	L5	2761	U
1	L5	2763	U
1	L5	2769	U
1	L5	2770	C
1	L5	2788	U
1	L5	2790	U
1	L5	2806	A
1	L5	2814	C
1	L5	2815	A2M

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Mol	Chain	Res	Type
1	L5	2826	U
1	L5	2827	G
1	L5	2829	U
1	L5	2838	G
1	L5	2855	G
1	L5	2867	C
1	L5	2877	G
1	L5	2892	C
1	L5	2900	U
1	L5	2902	G
1	L5	2903	G
1	L5	2904	U
1	L5	2905	C
1	L5	2907	G
1	L5	2908	U
1	L5	3588	C
1	L5	3590	G
1	L5	3591	C
1	L5	3592	G
1	L5	3594	C
1	L5	3595	U
1	L5	3596	A
1	L5	3597	G
1	L5	3604	A
1	L5	3605	C
1	L5	3616	U
1	L5	3626	G
1	L5	3630	A
1	L5	3635	A
1	L5	3644	U
1	L5	3646	A
1	L5	3648	A
1	L5	3662	A
1	L5	3664	G
1	L5	3670	C
1	L5	3673	C
1	L5	3674	G
1	L5	3701	OMC
1	L5	3710	G
1	L5	3711	A
1	L5	3713	U
1	L5	3727	A

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Mol	Chain	Res	Type
1	L5	3748	A
1	L5	3753	G
1	L5	3756	A
1	L5	3760	A
1	L5	3764	U
1	L5	3769	C
1	L5	3770	U
1	L5	3771	C
1	L5	3774	A
1	L5	3775	A
1	L5	3776	G
1	L5	3777	G
1	L5	3785	A2M
1	L5	3786	U
1	L5	3792	OMG
1	L5	3811	G
1	L5	3812	C
1	L5	3814	U
1	L5	3817	A
1	L5	3819	G
1	L5	3824	A
1	L5	3838	U
1	L5	3839	G
1	L5	3840	U
1	L5	3867	A2M
1	L5	3877	A
1	L5	3878	C
1	L5	3879	G
1	L5	3880	G
1	L5	3885	G
1	L5	3892	U
1	L5	3897	G
1	L5	3901	A
1	L5	3906	A
1	L5	3907	G
1	L5	3908	A
1	L5	3915	U
1	L5	3923	A
1	L5	3930	U
1	L5	3938	G
1	L5	3939	G
1	L5	3942	A

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Mol	Chain	Res	Type
1	L5	3947	A
1	L5	3949	A
1	L5	3950	U
1	L5	3953	G
1	L5	4057	C
1	L5	4058	U
1	L5	4059	C
1	L5	4060	U
1	L5	4061	G
1	L5	4062	A
1	L5	4064	C
1	L5	4065	G
1	L5	4068	U
1	L5	4076	G
1	L5	4084	G
1	L5	4095	G
1	L5	4097	G
1	L5	4099	G
1	L5	4101	C
1	L5	4104	G
1	L5	4108	G
1	L5	4111	U
1	L5	4114	C
1	L5	4115	G
1	L5	4116	C
1	L5	4119	C
1	L5	4122	G
1	L5	4127	A
1	L5	4141	G
1	L5	4142	C
1	L5	4143	G
1	L5	4144	C
1	L5	4146	G
1	L5	4149	C
1	L5	4162	C
1	L5	4163	U
1	L5	4170	A
1	L5	4183	G
1	L5	4184	G
1	L5	4191	G
1	L5	4203	A
1	L5	4212	A

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Mol	Chain	Res	Type
1	L5	4220	6MZ
1	L5	4222	G
1	L5	4225	G
1	L5	4229	U
1	L5	4232	U
1	L5	4233	A
1	L5	4251	A
1	L5	4254	G
1	L5	4257	A
1	L5	4258	C
1	L5	4265	U
1	L5	4268	A
1	L5	4273	A
1	L5	4281	A
1	L5	4291	G
1	L5	4304	A
1	L5	4305	G
1	L5	4314	C
1	L5	4319	C
1	L5	4329	G
1	L5	4330	G
1	L5	4332	C
1	L5	4349	C
1	L5	4354	U
1	L5	4373	G
1	L5	4376	A
1	L5	4377	G
1	L5	4378	A
1	L5	4379	A
1	L5	4387	C
1	L5	4391	G
1	L5	4394	A
1	L5	4405	G
1	L5	4421	C
1	L5	4422	A
1	L5	4438	U
1	L5	4448	G
1	L5	4449	A
1	L5	4464	A
1	L5	4466	C
1	L5	4475	G
1	L5	4488	A

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Mol	Chain	Res	Type
1	L5	4500	PSU
1	L5	4512	U
1	L5	4513	A
1	L5	4515	G
1	L5	4519	C
1	L5	4524	G
1	L5	4525	C
1	L5	4545	G
1	L5	4548	A
1	L5	4549	G
1	L5	4560	C
1	L5	4567	G
1	L5	4575	G
1	L5	4589	A
1	L5	4590	A2M
1	L5	4600	G
1	L5	4601	U
1	L5	4617	G
1	L5	4636	PSU
1	L5	4637	OMG
1	L5	4656	A
1	L5	4657	U
1	L5	4670	C
1	L5	4672	A
1	L5	4679	G
1	L5	4694	G
1	L5	4695	C
1	L5	4700	A
1	L5	4708	A
1	L5	4709	U
1	L5	4719	G
1	L5	4733	C
1	L5	4734	A
1	L5	4740	G
1	L5	4741	C
1	L5	4742	G
1	L5	4745	G
1	L5	4750	G
1	L5	4754	G
1	L5	4757	C
1	L5	4759	C
1	L5	4761	G

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Mol	Chain	Res	Type
1	L5	4764	A
1	L5	4765	G
1	L5	4771	C
1	L5	4772	C
1	L5	4775	C
1	L5	4859	C
1	L5	4870	G
1	L5	4871	C
1	L5	4875	G
1	L5	4881	U
1	L5	4882	U
1	L5	4883	C
1	L5	4889	G
1	L5	4895	C
1	L5	4896	G
1	L5	4897	G
1	L5	4899	G
1	L5	4900	C
1	L5	4901	G
1	L5	4910	G
1	L5	4912	G
1	L5	4914	C
1	L5	4922	C
1	L5	4925	U
1	L5	4926	C
1	L5	4927	G
1	L5	4928	C
1	L5	4934	A
1	L5	4940	C
1	L5	4941	G
1	L5	4943	A
1	L5	4951	G
1	L5	4955	A
1	L5	4960	G
1	L5	4975	G
1	L5	4976	U
1	L5	4985	U
1	L5	4988	U
1	L5	4989	U
1	L5	4991	U
1	L5	5007	A
1	L5	5013	C

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Mol	Chain	Res	Type
1	L5	5014	A
1	L5	5017	G
1	L5	5022	U
1	L5	5023	C
1	L5	5024	C
1	L5	5028	G
1	L5	5030	U
1	L5	5034	A
1	L5	5041	G
1	L5	5050	C
1	L5	5054	C
1	L5	5055	G
1	L5	5061	A
1	L5	5069	U
2	L7	7	G
2	L7	22	A
2	L7	33	U
2	L7	38	U
2	L7	53	U
2	L7	54	A
2	L7	64	G
2	L7	97	G
2	L7	100	A
2	L7	110	G
2	L7	120	U
3	L8	23	C
3	L8	25	G
3	L8	34	U
3	L8	35	C
3	L8	59	A
3	L8	62	A
3	L8	63	U
3	L8	80	A
3	L8	82	A
3	L8	84	A
3	L8	85	U
3	L8	87	G
3	L8	94	G
3	L8	103	A
3	L8	105	C
3	L8	111	U
3	L8	114	G

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Mol	Chain	Res	Type
3	L8	124	U
3	L8	125	C
3	L8	126	C
3	L8	127	U
3	L8	153	C

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	406	C
1	L5	493	G
1	L5	914	U
1	L5	1082	C
1	L5	1590	C
1	L5	1633	G
1	L5	1703	C
1	L5	1977	C
1	L5	2416	G
1	L5	2485	U
1	L5	2675	G
1	L5	2760	G
1	L5	3673	C
1	L5	4600	G
1	L5	4699	U
1	L5	4913	G

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

114 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	$\# Z > 2$
1	OMC	L5	2365	45,1	19,22,23	0.63	0	25,31,34	0.59	0
1	OMG	L5	1625	1	23,26,27	0.58	0	32,38,41	0.50	0
1	PSU	L5	3920	45,1	18,21,22	1.07	1 (5%)	21,30,33	1.97	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L5	4431	1	18,21,22	1.06	1 (5%)	21,30,33	1.88	4 (19%)
1	PSU	L5	4628	1	18,21,22	1.01	1 (5%)	21,30,33	1.86	4 (19%)
1	PSU	L5	4636	1	18,21,22	1.13	2 (11%)	21,30,33	2.08	6 (28%)
1	PSU	L5	3639	1	18,21,22	1.10	2 (11%)	21,30,33	1.97	5 (23%)
1	OMG	L5	4637	1	23,26,27	0.59	0	32,38,41	0.50	0
1	PSU	L5	4312	1	18,21,22	1.07	1 (5%)	21,30,33	1.91	4 (19%)
1	OMG	L5	4618	1	23,26,27	0.59	0	32,38,41	0.53	0
1	OMG	L5	4623	1	23,26,27	0.60	0	32,38,41	0.62	0
1	PSU	L5	1683	1	18,21,22	1.09	2 (11%)	21,30,33	2.06	5 (23%)
1	PSU	L5	3822	1	18,21,22	1.08	1 (5%)	21,30,33	1.99	6 (28%)
1	OMG	L5	3899	1	23,26,27	0.65	0	32,38,41	0.53	0
1	OMC	L5	4456	1	19,22,23	0.71	1 (5%)	25,31,34	0.79	0
1	PSU	L5	4500	1	18,21,22	1.13	2 (11%)	21,30,33	2.06	5 (23%)
1	OMG	L5	1522	1	23,26,27	0.60	0	32,38,41	0.69	1 (3%)
1	A2M	L5	4590	1	22,25,26	1.19	1 (4%)	30,36,39	1.51	5 (16%)
1	OMC	L5	2824	1	19,22,23	0.64	0	25,31,34	0.65	0
1	OMU	L5	4498	1	19,22,23	3.23	7 (36%)	25,31,34	1.90	5 (20%)
1	A2M	L5	1326	1	22,25,26	1.24	2 (9%)	30,36,39	1.44	8 (26%)
1	OMU	L5	3925	1	19,22,23	3.22	7 (36%)	25,31,34	1.95	5 (20%)
1	OMG	L5	1316	1	23,26,27	0.65	0	32,38,41	0.56	0
1	OMC	L5	3869	1	19,22,23	0.64	0	25,31,34	0.79	0
1	A2M	L5	2363	45,1	22,25,26	1.22	2 (9%)	30,36,39	1.55	9 (30%)
1	A2M	L5	3867	1	22,25,26	1.28	2 (9%)	30,36,39	1.48	6 (20%)
1	A2M	L5	1524	1	22,25,26	1.32	2 (9%)	30,36,39	1.51	6 (20%)
1	PSU	L5	1792	1	18,21,22	1.03	1 (5%)	21,30,33	1.92	4 (19%)
1	5MC	L5	3782	45,1	19,22,23	0.72	0	26,32,35	0.81	1 (3%)
1	PSU	L5	3853	45,1	18,21,22	1.05	1 (5%)	21,30,33	1.89	4 (19%)
1	OMC	L5	1340	1	19,22,23	0.69	0	25,31,34	0.80	0
1	OMG	L5	4370	1	23,26,27	0.57	0	32,38,41	0.53	0
1	PSU	L5	4521	45,1	18,21,22	1.09	2 (11%)	21,30,33	2.02	6 (28%)
1	OMG	L5	3627	1	23,26,27	0.57	0	32,38,41	0.58	0
1	OMG	L5	3744	1	23,26,27	0.57	0	32,38,41	0.51	0
1	PSU	L5	1677	1	18,21,22	1.06	3 (16%)	21,30,33	1.95	5 (23%)
1	OMU	L5	2837	1	19,22,23	3.25	7 (36%)	25,31,34	1.86	4 (16%)
1	A2M	L5	4523	45,1	22,25,26	1.22	3 (13%)	30,36,39	1.53	6 (20%)
3	PSU	L8	55	3	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
1	PSU	L5	4442	1	18,21,22	1.09	2 (11%)	21,30,33	2.04	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	L5	4536	1	19,22,23	0.67	0	25,31,34	0.75	0
1	OMG	L5	2876	1	23,26,27	0.58	0	32,38,41	0.52	0
1	OMU	L5	4306	1	19,22,23	3.21	7 (36%)	25,31,34	1.91	4 (16%)
1	PSU	L5	3695	1	18,21,22	1.07	2 (11%)	21,30,33	1.95	4 (19%)
3	OMG	L8	75	3	23,26,27	0.55	0	32,38,41	0.54	0
1	PSU	L5	1781	1	18,21,22	1.07	1 (5%)	21,30,33	1.79	4 (19%)
1	6MZ	L5	4220	1	22,25,26	3.96	11 (50%)	29,36,39	2.49	11 (37%)
1	OMG	L5	4196	1	23,26,27	0.55	0	32,38,41	0.46	0
1	PSU	L5	4972	1	18,21,22	1.04	1 (5%)	21,30,33	1.95	4 (19%)
1	PSU	L5	4471	1	18,21,22	1.06	1 (5%)	21,30,33	1.90	4 (19%)
1	PSU	L5	5010	1	18,21,22	1.08	1 (5%)	21,30,33	1.93	4 (19%)
1	PSU	L5	3637	1	18,21,22	1.09	1 (5%)	21,30,33	1.97	3 (14%)
1	OMC	L5	3808	45,1	19,22,23	0.69	0	25,31,34	0.85	1 (4%)
1	OMC	L5	3701	1	19,22,23	0.72	1 (5%)	25,31,34	1.82	4 (16%)
1	PSU	L5	4689	1	18,21,22	1.11	2 (11%)	21,30,33	2.07	4 (19%)
1	PSU	L5	4576	1	18,21,22	1.06	2 (11%)	21,30,33	1.86	4 (19%)
1	OMG	L5	2424	1	23,26,27	0.60	0	32,38,41	0.43	0
1	PSU	L5	4457	1	18,21,22	1.05	2 (11%)	21,30,33	1.99	5 (23%)
1	PSU	L5	4293	1	18,21,22	1.08	2 (11%)	21,30,33	2.01	4 (19%)
1	PSU	L5	4673	45,1	18,21,22	1.07	2 (11%)	21,30,33	1.90	4 (19%)
1	PSU	L5	4403	1	18,21,22	1.07	2 (11%)	21,30,33	2.06	6 (28%)
1	A2M	L5	400	1	22,25,26	1.28	3 (13%)	30,36,39	1.57	9 (30%)
1	PSU	L5	3851	1	18,21,22	1.08	1 (5%)	21,30,33	1.94	4 (19%)
1	OMC	L5	3887	1	19,22,23	0.65	0	25,31,34	0.67	0
1	PSU	L5	1536	1	18,21,22	1.05	1 (5%)	21,30,33	1.89	4 (19%)
1	OMU	L5	4227	1	19,22,23	3.26	7 (36%)	25,31,34	1.91	4 (16%)
1	OMC	L5	2861	1	19,22,23	0.63	0	25,31,34	0.82	1 (4%)
1	A2M	L5	398	1	22,25,26	1.17	1 (4%)	30,36,39	1.62	7 (23%)
1	PSU	L5	1862	1	18,21,22	1.05	1 (5%)	21,30,33	2.00	4 (19%)
1	OMC	L5	3841	1	19,22,23	0.67	0	25,31,34	0.73	0
1	PSU	L5	4353	1	18,21,22	1.09	2 (11%)	21,30,33	1.99	6 (28%)
1	A2M	L5	2787	1	22,25,26	1.16	1 (4%)	30,36,39	1.49	7 (23%)
1	A2M	L5	3785	45,1	22,25,26	1.17	2 (9%)	30,36,39	1.59	10 (33%)
1	PSU	L5	4361	1	18,21,22	1.06	2 (11%)	21,30,33	1.88	4 (19%)
1	A2M	L5	3825	1	22,25,26	1.17	2 (9%)	30,36,39	1.55	7 (23%)
1	PSU	L5	4973	1	18,21,22	1.03	1 (5%)	21,30,33	1.92	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L5	1782	1	18,21,22	1.05	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L8	69	3	18,21,22	1.06	2 (11%)	21,30,33	1.96	5 (23%)
1	OMG	L5	4499	1	23,26,27	0.53	0	32,38,41	0.48	0
1	PSU	L5	4532	1	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
1	OMG	L5	4494	1	23,26,27	0.59	0	32,38,41	0.49	0
1	PSU	L5	3844	1	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
1	PSU	L5	1744	45,1	18,21,22	1.09	1 (5%)	21,30,33	1.96	4 (19%)
1	PSU	L5	5001	1	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
1	OMG	L5	4392	1	23,26,27	0.61	0	32,38,41	0.50	0
1	OMC	L5	2804	1	19,22,23	0.66	0	25,31,34	0.91	1 (4%)
1	A2M	L5	1871	45,1	22,25,26	1.30	3 (13%)	30,36,39	1.63	7 (23%)
1	PSU	L5	4552	1	18,21,22	1.10	2 (11%)	21,30,33	2.03	4 (19%)
1	5MC	L5	4447	1	19,22,23	0.93	1 (5%)	26,32,35	0.67	0
1	A2M	L5	4571	1	22,25,26	1.24	2 (9%)	30,36,39	1.58	9 (30%)
1	PSU	L5	1582	1	18,21,22	1.08	1 (5%)	21,30,33	1.90	4 (19%)
1	A2M	L5	1534	45,1	22,25,26	1.26	3 (13%)	30,36,39	1.46	7 (23%)
1	PSU	L5	4296	1	18,21,22	1.06	1 (5%)	21,30,33	1.93	4 (19%)
1	UR3	L5	4530	1	19,22,23	2.66	6 (31%)	26,32,35	1.59	3 (11%)
1	A2M	L5	3718	1	22,25,26	1.16	1 (4%)	30,36,39	1.52	6 (20%)
1	PSU	L5	4493	1	18,21,22	1.05	1 (5%)	21,30,33	1.85	4 (19%)
1	OMG	L5	3792	1	23,26,27	0.57	0	32,38,41	0.54	0
1	PSU	L5	2632	1	18,21,22	1.06	1 (5%)	21,30,33	1.92	4 (19%)
1	A2M	L5	3830	1	22,25,26	1.19	1 (4%)	30,36,39	1.57	6 (20%)
1	OMU	L5	4620	1	19,22,23	3.16	7 (36%)	25,31,34	1.71	4 (16%)
1	PSU	L5	1860	1	18,21,22	1.07	1 (5%)	21,30,33	1.94	4 (19%)
1	A2M	L5	2815	1	22,25,26	1.21	2 (9%)	30,36,39	1.51	7 (23%)
1	1MA	L5	1322	45,1	21,25,26	0.65	0	30,37,40	0.80	2 (6%)
1	PSU	L5	4299	1	18,21,22	1.01	1 (5%)	21,30,33	1.90	4 (19%)
1	OMG	L5	2364	45,1	23,26,27	0.60	0	32,38,41	0.44	0
1	PSU	L5	4579	1	18,21,22	1.08	1 (5%)	21,30,33	1.95	4 (19%)
1	OMC	L5	2422	45,1	19,22,23	0.65	0	25,31,34	0.74	1 (4%)
1	OMG	L5	4228	1	23,26,27	0.58	0	32,38,41	0.67	0
1	PSU	L5	2839	1	18,21,22	1.02	1 (5%)	21,30,33	1.93	4 (19%)
1	OMC	L5	2351	45,1	19,22,23	0.71	1 (5%)	25,31,34	1.10	2 (8%)
1	PSU	L5	3884	1	18,21,22	1.09	2 (11%)	21,30,33	1.97	4 (19%)
1	A2M	L5	2401	1	22,25,26	1.23	1 (4%)	30,36,39	1.61	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UY1	L5	3818	1	19,22,23	4.79	9 (47%)	21,31,34	2.04	5 (23%)
1	A2M	L5	1323	1	22,25,26	1.23	2 (9%)	30,36,39	1.58	7 (23%)

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
1	OMC	L5	2365	45,1	-	0/9/27/28	0/2/2/2
1	OMG	L5	1625	1	-	2/9/27/28	0/3/3/3
1	PSU	L5	3920	45,1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4431	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4628	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4636	1	-	1/7/25/26	0/2/2/2
1	PSU	L5	3639	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	4637	1	-	3/9/27/28	0/3/3/3
1	PSU	L5	4312	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	4618	1	-	2/9/27/28	0/3/3/3
1	OMG	L5	4623	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	1683	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3822	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	3899	1	-	2/9/27/28	0/3/3/3
1	OMC	L5	4456	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	4500	1	-	3/7/25/26	0/2/2/2
1	OMG	L5	1522	1	-	0/9/27/28	0/3/3/3
1	A2M	L5	4590	1	-	3/9/27/28	0/3/3/3
1	OMC	L5	2824	1	-	1/9/27/28	0/2/2/2
1	OMU	L5	4498	1	-	0/9/27/28	0/2/2/2
1	A2M	L5	1326	1	-	3/9/27/28	0/3/3/3
1	OMU	L5	3925	1	-	0/9/27/28	0/2/2/2
1	OMG	L5	1316	1	-	0/9/27/28	0/3/3/3
1	OMC	L5	3869	1	-	1/9/27/28	0/2/2/2
1	A2M	L5	2363	45,1	-	0/9/27/28	0/3/3/3
1	A2M	L5	3867	1	-	2/9/27/28	0/3/3/3
1	A2M	L5	1524	1	-	3/9/27/28	0/3/3/3
1	PSU	L5	1792	1	-	0/7/25/26	0/2/2/2
1	5MC	L5	3782	45,1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3853	45,1	-	0/7/25/26	0/2/2/2
1	OMC	L5	1340	1	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	L5	4370	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	4521	45,1	-	0/7/25/26	0/2/2/2
1	OMG	L5	3627	1	-	1/9/27/28	0/3/3/3
1	OMG	L5	3744	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	1677	1	-	2/7/25/26	0/2/2/2
1	OMU	L5	2837	1	-	0/9/27/28	0/2/2/2
1	A2M	L5	4523	45,1	-	0/9/27/28	0/3/3/3
3	PSU	L8	55	3	-	0/7/25/26	0/2/2/2
1	PSU	L5	4442	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	4536	1	-	0/9/27/28	0/2/2/2
1	OMG	L5	2876	1	-	0/9/27/28	0/3/3/3
1	OMU	L5	4306	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	3695	1	-	0/7/25/26	0/2/2/2
3	OMG	L8	75	3	-	1/9/27/28	0/3/3/3
1	PSU	L5	1781	1	-	1/7/25/26	0/2/2/2
1	6MZ	L5	4220	1	-	2/9/27/28	0/3/3/3
1	OMG	L5	4196	1	-	1/9/27/28	0/3/3/3
1	PSU	L5	4972	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4471	1	-	1/7/25/26	0/2/2/2
1	PSU	L5	5010	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3637	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	3808	45,1	-	0/9/27/28	0/2/2/2
1	OMC	L5	3701	1	-	5/9/27/28	0/2/2/2
1	PSU	L5	4689	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4576	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	2424	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	4457	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4293	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4673	45,1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4403	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	400	1	-	1/9/27/28	0/3/3/3
1	PSU	L5	3851	1	-	1/7/25/26	0/2/2/2
1	OMC	L5	3887	1	-	1/9/27/28	0/2/2/2
1	PSU	L5	1536	1	-	2/7/25/26	0/2/2/2
1	OMU	L5	4227	1	-	0/9/27/28	0/2/2/2
1	OMC	L5	2861	1	-	0/9/27/28	0/2/2/2
1	A2M	L5	398	1	-	1/9/27/28	0/3/3/3
1	PSU	L5	1862	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	3841	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	4353	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	2787	1	-	5/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	L5	3785	45,1	-	2/9/27/28	0/3/3/3
1	PSU	L5	4361	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	3825	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	4973	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	1782	1	-	0/7/25/26	0/2/2/2
3	PSU	L8	69	3	-	0/7/25/26	0/2/2/2
1	OMG	L5	4499	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	4532	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	4494	1	-	1/9/27/28	0/3/3/3
1	PSU	L5	3844	1	-	1/7/25/26	0/2/2/2
1	PSU	L5	1744	45,1	-	0/7/25/26	0/2/2/2
1	PSU	L5	5001	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	4392	1	-	0/9/27/28	0/3/3/3
1	OMC	L5	2804	1	-	0/9/27/28	0/2/2/2
1	A2M	L5	1871	45,1	-	0/9/27/28	0/3/3/3
1	PSU	L5	4552	1	-	0/7/25/26	0/2/2/2
1	5MC	L5	4447	1	-	4/7/25/26	0/2/2/2
1	A2M	L5	4571	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	1582	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	1534	45,1	-	1/9/27/28	0/3/3/3
1	PSU	L5	4296	1	-	2/7/25/26	0/2/2/2
1	UR3	L5	4530	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	3718	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	4493	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	3792	1	-	2/9/27/28	0/3/3/3
1	PSU	L5	2632	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	3830	1	-	0/9/27/28	0/3/3/3
1	OMU	L5	4620	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	1860	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	2815	1	-	2/9/27/28	0/3/3/3
1	1MA	L5	1322	45,1	-	2/7/25/26	0/3/3/3
1	PSU	L5	4299	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	2364	45,1	-	2/9/27/28	0/3/3/3
1	PSU	L5	4579	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	2422	45,1	-	2/9/27/28	0/2/2/2
1	OMG	L5	4228	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	2839	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	2351	45,1	-	3/9/27/28	0/2/2/2
1	PSU	L5	3884	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	2401	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UY1	L5	3818	1	-	2/9/27/28	0/2/2/2
1	A2M	L5	1323	1	-	2/9/27/28	0/3/3/3

All (177) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	3818	UY1	C6-C5	12.48	1.49	1.35
1	L5	4220	6MZ	C6-N6	12.04	1.48	1.34
1	L5	3818	UY1	C2-N1	11.46	1.51	1.36
1	L5	4220	6MZ	C3'-C2'	-8.41	1.30	1.53
1	L5	4227	OMU	C2-N1	8.03	1.51	1.38
1	L5	3925	OMU	C2-N1	7.94	1.50	1.38
1	L5	2837	OMU	C2-N1	7.90	1.50	1.38
1	L5	4306	OMU	C2-N1	7.84	1.50	1.38
1	L5	4498	OMU	C2-N1	7.68	1.50	1.38
1	L5	4620	OMU	C2-N1	7.56	1.50	1.38
1	L5	3818	UY1	C2-N3	7.53	1.49	1.37
1	L5	4227	OMU	C2-N3	6.60	1.49	1.38
1	L5	2837	OMU	C2-N3	6.57	1.49	1.38
1	L5	4306	OMU	C2-N3	6.50	1.49	1.38
1	L5	4498	OMU	C2-N3	6.46	1.49	1.38
1	L5	3925	OMU	C2-N3	6.43	1.49	1.38
1	L5	4620	OMU	C2-N3	6.32	1.49	1.38
1	L5	4530	UR3	C2-N1	6.19	1.47	1.38
1	L5	4530	UR3	C6-C5	6.13	1.49	1.35
1	L5	3925	OMU	O4-C4	-5.77	1.13	1.24
1	L5	4620	OMU	O4-C4	-5.73	1.13	1.24
1	L5	4306	OMU	O4-C4	-5.73	1.13	1.24
1	L5	2837	OMU	C6-C5	5.72	1.48	1.35
1	L5	4227	OMU	O4-C4	-5.71	1.13	1.24
1	L5	4498	OMU	C6-C5	5.68	1.48	1.35
1	L5	4498	OMU	O4-C4	-5.67	1.13	1.24
1	L5	4530	UR3	C2-N3	5.65	1.50	1.39
1	L5	4227	OMU	C6-C5	5.65	1.48	1.35
1	L5	2837	OMU	O4-C4	-5.61	1.13	1.24
1	L5	4620	OMU	C6-C5	5.57	1.48	1.35
1	L5	4306	OMU	C6-C5	5.55	1.47	1.35
1	L5	3925	OMU	C6-C5	5.53	1.47	1.35
1	L5	3818	UY1	C6-N1	5.15	1.44	1.36
1	L5	4220	6MZ	O4'-C1'	-4.80	1.30	1.42
1	L5	4220	6MZ	O4'-C4'	4.67	1.55	1.45
1	L5	4220	6MZ	C5'-C4'	-4.54	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	3818	UY1	C4-N3	4.27	1.46	1.38
1	L5	4498	OMU	C4-N3	4.06	1.45	1.38
1	L5	2837	OMU	C4-N3	3.91	1.45	1.38
1	L5	4227	OMU	C4-N3	3.86	1.45	1.38
1	L5	4306	OMU	C4-N3	3.85	1.45	1.38
1	L5	3818	UY1	O4-C4	-3.80	1.16	1.23
1	L5	3925	OMU	C4-N3	3.79	1.45	1.38
1	L5	4620	OMU	C4-N3	3.77	1.45	1.38
1	L5	2401	A2M	O5'-C5'	-3.69	1.33	1.44
1	L5	3830	A2M	O5'-C5'	-3.58	1.33	1.44
1	L5	1871	A2M	O5'-C5'	-3.55	1.33	1.44
1	L5	1524	A2M	O5'-C5'	-3.55	1.33	1.44
1	L5	3785	A2M	O5'-C5'	-3.55	1.33	1.44
1	L5	400	A2M	O5'-C5'	-3.54	1.33	1.44
1	L5	3825	A2M	O5'-C5'	-3.53	1.33	1.44
1	L5	1326	A2M	O5'-C5'	-3.52	1.33	1.44
1	L5	1323	A2M	O5'-C5'	-3.52	1.33	1.44
1	L5	2787	A2M	O5'-C5'	-3.49	1.34	1.44
1	L5	3867	A2M	O5'-C5'	-3.49	1.34	1.44
1	L5	2815	A2M	O5'-C5'	-3.48	1.34	1.44
1	L5	4220	6MZ	C5-N7	-3.48	1.32	1.39
1	L5	4220	6MZ	C5-C4	-3.42	1.33	1.39
1	L5	2363	A2M	O5'-C5'	-3.41	1.34	1.44
1	L5	4571	A2M	O5'-C5'	-3.41	1.34	1.44
1	L5	1781	PSU	C6-C5	3.39	1.39	1.35
1	L5	3718	A2M	O5'-C5'	-3.39	1.34	1.44
1	L5	4500	PSU	C6-C5	3.38	1.39	1.35
1	L5	3844	PSU	C6-C5	3.36	1.39	1.35
1	L5	1744	PSU	C6-C5	3.36	1.39	1.35
1	L5	5010	PSU	C6-C5	3.36	1.39	1.35
1	L5	398	A2M	O5'-C5'	-3.35	1.34	1.44
1	L5	4552	PSU	C6-C5	3.33	1.39	1.35
1	L5	4523	A2M	O5'-C5'	-3.32	1.34	1.44
3	L8	55	PSU	C6-C5	3.31	1.39	1.35
1	L5	4590	A2M	O5'-C5'	-3.30	1.34	1.44
1	L5	4579	PSU	C6-C5	3.29	1.38	1.35
1	L5	4532	PSU	C6-C5	3.28	1.38	1.35
1	L5	2632	PSU	C6-C5	3.28	1.38	1.35
1	L5	3818	UY1	O2-C2	-3.27	1.16	1.23
1	L5	3851	PSU	C6-C5	3.26	1.38	1.35
1	L5	3695	PSU	C6-C5	3.25	1.38	1.35
1	L5	4636	PSU	C6-C5	3.24	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	1782	PSU	C6-C5	3.24	1.38	1.35
1	L5	4296	PSU	C6-C5	3.24	1.38	1.35
1	L5	1860	PSU	C6-C5	3.23	1.38	1.35
1	L5	3822	PSU	C6-C5	3.23	1.38	1.35
1	L5	3818	UY1	C1'-C5	3.22	1.57	1.50
1	L5	5001	PSU	C6-C5	3.22	1.38	1.35
1	L5	4431	PSU	C6-C5	3.22	1.38	1.35
1	L5	1534	A2M	O5'-C5'	-3.21	1.34	1.44
1	L5	4312	PSU	C6-C5	3.21	1.38	1.35
1	L5	4689	PSU	C6-C5	3.21	1.38	1.35
1	L5	1683	PSU	C6-C5	3.21	1.38	1.35
1	L5	4493	PSU	C6-C5	3.20	1.38	1.35
1	L5	4353	PSU	C6-C5	3.20	1.38	1.35
1	L5	4293	PSU	C6-C5	3.17	1.38	1.35
1	L5	1862	PSU	C6-C5	3.17	1.38	1.35
1	L5	3637	PSU	C6-C5	3.16	1.38	1.35
1	L5	1582	PSU	C6-C5	3.14	1.38	1.35
1	L5	4442	PSU	C6-C5	3.12	1.38	1.35
1	L5	4521	PSU	C6-C5	3.11	1.38	1.35
1	L5	4972	PSU	C6-C5	3.11	1.38	1.35
1	L5	1792	PSU	C6-C5	3.09	1.38	1.35
1	L5	4576	PSU	C6-C5	3.09	1.38	1.35
1	L5	3884	PSU	C6-C5	3.09	1.38	1.35
1	L5	4973	PSU	C6-C5	3.07	1.38	1.35
1	L5	3920	PSU	C6-C5	3.07	1.38	1.35
1	L5	4471	PSU	C6-C5	3.05	1.38	1.35
1	L5	3639	PSU	C6-C5	3.04	1.38	1.35
1	L5	4220	6MZ	C8-N9	-3.03	1.32	1.37
1	L5	3853	PSU	C6-C5	3.03	1.38	1.35
1	L5	4220	6MZ	C2'-C1'	3.03	1.63	1.53
3	L8	69	PSU	C6-C5	3.03	1.38	1.35
1	L5	4673	PSU	C6-C5	2.98	1.38	1.35
1	L5	4361	PSU	C6-C5	2.97	1.38	1.35
1	L5	1524	A2M	O4'-C4'	-2.95	1.38	1.45
1	L5	1534	A2M	O4'-C4'	-2.95	1.38	1.45
1	L5	1536	PSU	C6-C5	2.95	1.38	1.35
1	L5	4299	PSU	C6-C5	2.92	1.38	1.35
1	L5	2839	PSU	C6-C5	2.89	1.38	1.35
1	L5	4628	PSU	C6-C5	2.89	1.38	1.35
1	L5	4403	PSU	C6-C5	2.88	1.38	1.35
1	L5	4457	PSU	C6-C5	2.86	1.38	1.35
1	L5	2363	A2M	O4'-C4'	-2.80	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	4530	UR3	O2-C2	-2.72	1.17	1.22
1	L5	4498	OMU	C5-C4	2.68	1.49	1.43
1	L5	4220	6MZ	O3'-C3'	2.68	1.49	1.43
1	L5	1677	PSU	C6-C5	2.66	1.38	1.35
1	L5	4227	OMU	C5-C4	2.62	1.49	1.43
1	L5	1323	A2M	O4'-C4'	-2.59	1.39	1.45
1	L5	2837	OMU	C5-C4	2.57	1.49	1.43
1	L5	3925	OMU	C5-C4	2.55	1.49	1.43
1	L5	4498	OMU	C6-N1	2.54	1.44	1.38
1	L5	1871	A2M	O4'-C4'	-2.49	1.39	1.45
1	L5	4620	OMU	C6-N1	2.48	1.44	1.38
1	L5	4306	OMU	C5-C4	2.47	1.49	1.43
1	L5	4571	A2M	O4'-C4'	-2.46	1.39	1.45
1	L5	4220	6MZ	C6-N1	-2.44	1.31	1.35
1	L5	2837	OMU	C6-N1	2.44	1.43	1.38
1	L5	3925	OMU	C6-N1	2.40	1.43	1.38
1	L5	4530	UR3	C6-N1	2.40	1.43	1.38
1	L5	400	A2M	O4'-C4'	-2.38	1.39	1.45
1	L5	3867	A2M	O4'-C4'	-2.37	1.39	1.45
1	L5	4227	OMU	C6-N1	2.36	1.43	1.38
1	L5	1326	A2M	O4'-C4'	-2.35	1.39	1.45
1	L5	4620	OMU	C5-C4	2.33	1.48	1.43
1	L5	2815	A2M	O4'-C4'	-2.33	1.39	1.45
1	L5	4306	OMU	C6-N1	2.32	1.43	1.38
1	L5	3884	PSU	C4-C5	-2.21	1.38	1.44
1	L5	3818	UY1	O4'-C1'	-2.21	1.40	1.43
1	L5	4530	UR3	C5-C4	2.20	1.49	1.43
1	L5	4636	PSU	C4-C5	-2.17	1.38	1.44
1	L5	400	A2M	O3'-C3'	-2.15	1.37	1.43
1	L5	1871	A2M	O3'-C3'	-2.15	1.37	1.43
1	L5	4521	PSU	C4-C5	-2.14	1.38	1.44
1	L5	4689	PSU	C4-C5	-2.12	1.38	1.44
1	L5	4353	PSU	C4-C5	-2.10	1.38	1.44
1	L5	3825	A2M	O4'-C4'	-2.10	1.40	1.45
1	L5	4456	OMC	C4-N3	-2.10	1.30	1.34
1	L5	4442	PSU	O4'-C1'	-2.09	1.41	1.43
1	L5	4500	PSU	C4-C5	-2.08	1.38	1.44
1	L5	4673	PSU	C4-C5	-2.08	1.38	1.44
1	L5	3639	PSU	C4-C5	-2.07	1.38	1.44
1	L5	1683	PSU	C4-C5	-2.07	1.38	1.44
1	L5	4447	5MC	C4-N3	-2.07	1.30	1.34
1	L5	4523	A2M	O3'-C3'	-2.06	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	3695	PSU	C4-C5	-2.05	1.38	1.44
1	L5	4576	PSU	C4-C5	-2.05	1.38	1.44
1	L5	4552	PSU	C4-C5	-2.04	1.38	1.44
1	L5	2351	OMC	C4-N3	-2.04	1.30	1.34
1	L5	4293	PSU	C4-C5	-2.04	1.38	1.44
1	L5	3701	OMC	C4-N3	-2.04	1.30	1.34
1	L5	3785	A2M	O4'-C4'	-2.03	1.40	1.45
1	L5	4403	PSU	C4-C5	-2.03	1.38	1.44
1	L5	4361	PSU	C4-C5	-2.03	1.38	1.44
1	L5	1677	PSU	C4-C5	-2.02	1.38	1.44
3	L8	69	PSU	C4-C5	-2.01	1.38	1.44
1	L5	1534	A2M	O3'-C3'	-2.00	1.38	1.43
1	L5	1677	PSU	O4'-C1'	-2.00	1.41	1.43
1	L5	4457	PSU	C4-C5	-2.00	1.38	1.44
1	L5	4523	A2M	O4'-C4'	-2.00	1.40	1.45

All (406) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3925	OMU	C4-N3-C2	-6.15	118.98	126.61
1	L5	4227	OMU	C4-N3-C2	-6.02	119.13	126.61
1	L5	4498	OMU	C4-N3-C2	-5.91	119.28	126.61
1	L5	4306	OMU	C4-N3-C2	-5.81	119.40	126.61
1	L5	4220	6MZ	N1-C2-N3	-5.81	119.79	128.58
1	L5	4530	UR3	C4-N3-C2	-5.64	120.04	124.58
1	L5	3701	OMC	C1'-N1-C2	5.63	130.88	118.44
1	L5	2837	OMU	C4-N3-C2	-5.62	119.64	126.61
1	L5	1683	PSU	N1-C2-N3	5.40	120.86	115.17
1	L5	4689	PSU	N1-C2-N3	5.37	120.83	115.17
1	L5	4636	PSU	C4-N3-C2	-5.34	119.02	126.37
1	L5	4457	PSU	C4-N3-C2	-5.23	119.16	126.37
1	L5	4552	PSU	N1-C2-N3	5.22	120.67	115.17
1	L5	1677	PSU	C4-N3-C2	-5.21	119.19	126.37
1	L5	4403	PSU	C4-N3-C2	-5.18	119.23	126.37
1	L5	4500	PSU	N1-C2-N3	5.17	120.62	115.17
1	L5	3637	PSU	N1-C2-N3	5.17	120.62	115.17
1	L5	4293	PSU	N1-C2-N3	5.17	120.62	115.17
1	L5	4403	PSU	N1-C2-N3	5.14	120.59	115.17
1	L5	1862	PSU	N1-C2-N3	5.13	120.58	115.17
1	L5	3920	PSU	N1-C2-N3	5.11	120.56	115.17
1	L5	4636	PSU	N1-C2-N3	5.09	120.54	115.17
1	L5	3822	PSU	N1-C2-N3	5.09	120.53	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4442	PSU	N1-C2-N3	5.09	120.53	115.17
1	L5	1862	PSU	C4-N3-C2	-5.09	119.37	126.37
1	L5	4521	PSU	N1-C2-N3	5.06	120.51	115.17
1	L5	3637	PSU	C4-N3-C2	-5.05	119.41	126.37
1	L5	4442	PSU	C4-N3-C2	-5.05	119.42	126.37
1	L5	4552	PSU	C4-N3-C2	-5.04	119.43	126.37
1	L5	4293	PSU	C4-N3-C2	-5.04	119.43	126.37
1	L5	4353	PSU	N1-C2-N3	5.04	120.48	115.17
1	L5	3851	PSU	N1-C2-N3	5.01	120.46	115.17
1	L5	1744	PSU	N1-C2-N3	5.01	120.45	115.17
1	L5	3884	PSU	C4-N3-C2	-5.00	119.49	126.37
1	L5	3695	PSU	N1-C2-N3	5.00	120.44	115.17
1	L5	1792	PSU	C4-N3-C2	-5.00	119.49	126.37
1	L5	3639	PSU	N1-C2-N3	4.99	120.43	115.17
1	L5	4972	PSU	N1-C2-N3	4.99	120.43	115.17
1	L5	3818	UY1	C4-N3-C2	-4.99	119.50	126.37
1	L5	2632	PSU	N1-C2-N3	4.98	120.42	115.17
1	L5	4521	PSU	C4-N3-C2	-4.98	119.52	126.37
1	L5	4579	PSU	N1-C2-N3	4.95	120.39	115.17
1	L5	4457	PSU	N1-C2-N3	4.94	120.38	115.17
1	L5	1860	PSU	N1-C2-N3	4.94	120.38	115.17
1	L5	3884	PSU	N1-C2-N3	4.94	120.37	115.17
1	L5	3844	PSU	N1-C2-N3	4.92	120.36	115.17
1	L5	4500	PSU	C4-N3-C2	-4.92	119.60	126.37
1	L5	1860	PSU	C4-N3-C2	-4.91	119.60	126.37
1	L5	1792	PSU	N1-C2-N3	4.91	120.35	115.17
3	L8	69	PSU	N1-C2-N3	4.91	120.35	115.17
1	L5	1683	PSU	C4-N3-C2	-4.91	119.61	126.37
1	L5	3853	PSU	N1-C2-N3	4.90	120.34	115.17
1	L5	4299	PSU	C4-N3-C2	-4.90	119.63	126.37
1	L5	4689	PSU	C4-N3-C2	-4.90	119.63	126.37
1	L5	4353	PSU	C4-N3-C2	-4.89	119.64	126.37
1	L5	4973	PSU	N1-C2-N3	4.88	120.31	115.17
1	L5	5010	PSU	N1-C2-N3	4.88	120.31	115.17
1	L5	2839	PSU	C4-N3-C2	-4.87	119.66	126.37
1	L5	1582	PSU	N1-C2-N3	4.87	120.31	115.17
1	L5	4620	OMU	C4-N3-C2	-4.87	120.57	126.61
1	L5	4296	PSU	C4-N3-C2	-4.86	119.67	126.37
1	L5	4299	PSU	N1-C2-N3	4.86	120.30	115.17
1	L5	4471	PSU	N1-C2-N3	4.86	120.30	115.17
1	L5	3639	PSU	C4-N3-C2	-4.86	119.68	126.37
1	L5	1677	PSU	N1-C2-N3	4.86	120.29	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1536	PSU	N1-C2-N3	4.85	120.29	115.17
1	L5	4673	PSU	N1-C2-N3	4.85	120.29	115.17
1	L5	3695	PSU	C4-N3-C2	-4.85	119.69	126.37
1	L5	5001	PSU	C4-N3-C2	-4.85	119.69	126.37
1	L5	4493	PSU	C4-N3-C2	-4.85	119.69	126.37
1	L5	5010	PSU	C4-N3-C2	-4.84	119.71	126.37
3	L8	69	PSU	C4-N3-C2	-4.83	119.72	126.37
1	L5	1744	PSU	C4-N3-C2	-4.82	119.73	126.37
1	L5	4579	PSU	C4-N3-C2	-4.82	119.73	126.37
1	L5	1582	PSU	C4-N3-C2	-4.82	119.73	126.37
1	L5	4972	PSU	C4-N3-C2	-4.82	119.73	126.37
1	L5	4296	PSU	N1-C2-N3	4.82	120.25	115.17
1	L5	4312	PSU	N1-C2-N3	4.82	120.25	115.17
1	L5	3920	PSU	C4-N3-C2	-4.79	119.77	126.37
3	L8	55	PSU	N1-C2-N3	4.79	120.22	115.17
1	L5	4312	PSU	C4-N3-C2	-4.79	119.77	126.37
1	L5	4973	PSU	C4-N3-C2	-4.79	119.77	126.37
1	L5	4628	PSU	N1-C2-N3	4.79	120.22	115.17
1	L5	4673	PSU	C4-N3-C2	-4.78	119.78	126.37
1	L5	5001	PSU	N1-C2-N3	4.78	120.21	115.17
1	L5	3851	PSU	C4-N3-C2	-4.78	119.78	126.37
1	L5	4220	6MZ	C5-C4-N3	-4.78	120.13	126.72
1	L5	4431	PSU	N1-C2-N3	4.78	120.21	115.17
1	L5	3853	PSU	C4-N3-C2	-4.78	119.79	126.37
1	L5	4532	PSU	C4-N3-C2	-4.77	119.80	126.37
1	L5	4471	PSU	C4-N3-C2	-4.77	119.80	126.37
1	L5	4361	PSU	N1-C2-N3	4.77	120.20	115.17
1	L5	4431	PSU	C4-N3-C2	-4.76	119.81	126.37
1	L5	2632	PSU	C4-N3-C2	-4.76	119.82	126.37
1	L5	4361	PSU	C4-N3-C2	-4.76	119.82	126.37
1	L5	2839	PSU	N1-C2-N3	4.75	120.18	115.17
1	L5	1782	PSU	N1-C2-N3	4.73	120.16	115.17
1	L5	1536	PSU	C4-N3-C2	-4.72	119.86	126.37
1	L5	4628	PSU	C4-N3-C2	-4.72	119.87	126.37
1	L5	3822	PSU	C4-N3-C2	-4.71	119.88	126.37
1	L5	1782	PSU	C4-N3-C2	-4.70	119.89	126.37
1	L5	4532	PSU	N1-C2-N3	4.70	120.13	115.17
1	L5	4576	PSU	C4-N3-C2	-4.70	119.90	126.37
3	L8	55	PSU	C4-N3-C2	-4.69	119.91	126.37
1	L5	4220	6MZ	N9-C8-N7	-4.69	107.29	113.94
1	L5	4220	6MZ	C9-N6-C6	-4.67	118.52	122.85
1	L5	4493	PSU	N1-C2-N3	4.63	120.05	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3844	PSU	C4-N3-C2	-4.61	120.03	126.37
1	L5	1781	PSU	N1-C2-N3	4.57	119.99	115.17
1	L5	4576	PSU	N1-C2-N3	4.55	119.97	115.17
1	L5	1781	PSU	C4-N3-C2	-4.53	120.13	126.37
1	L5	3818	UY1	N1-C2-N3	4.51	119.92	115.17
1	L5	3830	A2M	C3'-C2'-C1'	-4.50	94.19	102.81
1	L5	3701	OMC	C1'-N1-C6	-4.44	111.29	120.78
1	L5	1871	A2M	C3'-C2'-C1'	-4.40	94.38	102.81
1	L5	3925	OMU	N3-C2-N1	4.32	120.51	114.89
1	L5	4498	OMU	N3-C2-N1	4.23	120.40	114.89
1	L5	4306	OMU	N3-C2-N1	4.12	120.25	114.89
1	L5	2837	OMU	N3-C2-N1	4.10	120.23	114.89
1	L5	4227	OMU	N3-C2-N1	4.08	120.21	114.89
1	L5	4523	A2M	C3'-C2'-C1'	-3.96	95.23	102.81
1	L5	398	A2M	C3'-C2'-C1'	-3.93	95.29	102.81
1	L5	398	A2M	O3'-C3'-C2'	3.89	122.09	111.19
1	L5	4227	OMU	C5-C4-N3	3.87	120.22	114.80
1	L5	3925	OMU	C5-C4-N3	3.86	120.21	114.80
1	L5	4620	OMU	N3-C2-N1	3.81	119.84	114.89
1	L5	4498	OMU	C5-C4-N3	3.79	120.11	114.80
1	L5	4530	UR3	C5-C4-N3	3.75	119.98	115.04
1	L5	2401	A2M	O3'-C3'-C2'	3.75	121.68	111.19
1	L5	1323	A2M	C2'-C1'-N9	3.74	119.91	113.75
1	L5	4306	OMU	C5-C4-N3	3.73	120.03	114.80
1	L5	2787	A2M	O3'-C3'-C2'	3.63	121.33	111.19
1	L5	3825	A2M	C3'-C2'-C1'	-3.60	95.91	102.81
1	L5	4590	A2M	C3'-C2'-C1'	-3.59	95.93	102.81
1	L5	3718	A2M	C3'-C2'-C1'	-3.50	96.10	102.81
1	L5	2837	OMU	C5-C4-N3	3.50	119.70	114.80
1	L5	4220	6MZ	C2-N3-C4	3.49	120.36	111.83
1	L5	4689	PSU	O2-C2-N1	-3.39	119.30	122.79
1	L5	4689	PSU	C6-N1-C2	-3.35	119.58	122.69
1	L5	1534	A2M	C3'-C2'-C1'	-3.34	96.40	102.81
1	L5	4571	A2M	O3'-C3'-C2'	3.34	120.53	111.19
1	L5	2363	A2M	C2'-C1'-N9	3.31	119.20	113.75
1	L5	4620	OMU	C5-C4-N3	3.29	119.41	114.80
1	L5	1524	A2M	O3'-C3'-C2'	3.27	120.34	111.19
1	L5	2351	OMC	C1'-N1-C2	3.26	125.65	118.44
1	L5	2839	PSU	O2-C2-N1	-3.24	119.44	122.79
1	L5	3818	UY1	C6-C5-C4	3.23	120.35	118.17
1	L5	2815	A2M	C2'-C1'-N9	3.23	119.06	113.75
1	L5	4571	A2M	C3'-C2'-C1'	-3.22	96.63	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1323	A2M	O3'-C3'-C2'	3.22	120.19	111.19
1	L5	2401	A2M	C3'-C2'-C1'	-3.21	96.66	102.81
1	L5	3718	A2M	O3'-C3'-C2'	3.19	120.11	111.19
1	L5	3830	A2M	O3'-C3'-C2'	3.16	120.04	111.19
1	L5	4220	6MZ	N3-C4-N9	3.15	132.52	127.17
1	L5	2363	A2M	C3'-C2'-C1'	-3.12	96.83	102.81
1	L5	4500	PSU	O2-C2-N1	-3.11	119.58	122.79
1	L5	4552	PSU	O2-C2-N1	-3.11	119.59	122.79
1	L5	1871	A2M	O3'-C3'-C2'	3.10	119.86	111.19
1	L5	4306	OMU	O4-C4-C5	-3.08	119.84	125.16
1	L5	3867	A2M	C2'-C1'-N9	3.07	118.81	113.75
1	L5	4296	PSU	O2-C2-N1	-3.07	119.62	122.79
1	L5	1683	PSU	O2-C2-N1	-3.07	119.63	122.79
1	L5	1860	PSU	O2-C2-N1	-3.06	119.63	122.79
1	L5	3701	OMC	O2-C2-N3	-3.06	117.51	122.33
1	L5	3818	UY1	C6-N1-C2	-3.06	119.85	122.69
1	L5	400	A2M	C3'-C2'-C1'	-3.06	96.96	102.81
1	L5	4220	6MZ	C5-N7-C8	3.05	108.25	103.45
1	L5	1871	A2M	C4-N9-C1'	-3.04	119.51	126.63
1	L5	2401	A2M	C4-N9-C1'	-3.04	119.53	126.63
1	L5	4579	PSU	O2-C2-N1	-3.04	119.66	122.79
1	L5	4523	A2M	O3'-C3'-C2'	3.03	119.68	111.19
1	L5	400	A2M	O3'-C3'-C2'	3.00	119.59	111.19
1	L5	1683	PSU	C6-N1-C2	-3.00	119.91	122.69
1	L5	1536	PSU	O2-C2-N1	-2.98	119.71	122.79
1	L5	3822	PSU	O2-C2-N1	-2.98	119.71	122.79
1	L5	3925	OMU	O4-C4-C5	-2.97	120.04	125.16
1	L5	3825	A2M	O3'-C3'-C2'	2.96	119.48	111.19
1	L5	3844	PSU	O2-C2-N1	-2.96	119.73	122.79
1	L5	4500	PSU	C6-N1-C2	-2.96	119.95	122.69
3	L8	69	PSU	O2-C2-N1	-2.95	119.75	122.79
1	L5	4498	OMU	O4-C4-C5	-2.94	120.08	125.16
1	L5	3785	A2M	O3'-C3'-C2'	2.94	119.41	111.19
1	L5	3851	PSU	O2-C2-N1	-2.94	119.76	122.79
1	L5	4220	6MZ	C4-N9-C8	2.93	108.82	105.74
1	L5	1677	PSU	O2-C2-N1	-2.92	119.77	122.79
1	L5	1862	PSU	O2-C2-N1	-2.91	119.78	122.79
1	L5	4312	PSU	O2-C2-N1	-2.90	119.80	122.79
1	L5	2363	A2M	O3'-C3'-C2'	2.88	119.25	111.19
1	L5	4576	PSU	O2-C2-N1	-2.87	119.83	122.79
1	L5	5010	PSU	O2-C2-N1	-2.87	119.83	122.79
1	L5	2837	OMU	O4-C4-C5	-2.86	120.23	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3822	PSU	C6-N1-C2	-2.86	120.04	122.69
1	L5	4521	PSU	O2-C2-N1	-2.85	119.85	122.79
1	L5	3785	A2M	C4'-O4'-C1'	-2.84	103.20	109.47
1	L5	2401	A2M	C1'-N9-C8	2.83	133.38	127.09
1	L5	3920	PSU	O2-C2-N1	-2.83	119.87	122.79
1	L5	3844	PSU	C6-N1-C2	-2.82	120.07	122.69
1	L5	4227	OMU	O4-C4-C5	-2.82	120.30	125.16
1	L5	3825	A2M	C4-N9-C1'	-2.82	120.05	126.63
1	L5	4220	6MZ	C4-C5-C6	2.81	119.12	116.78
1	L5	1871	A2M	C1'-N9-C8	2.81	133.34	127.09
1	L5	2632	PSU	O2-C2-N1	-2.80	119.90	122.79
1	L5	3884	PSU	O2-C2-N1	-2.80	119.90	122.79
1	L5	4403	PSU	O2-C2-N1	-2.80	119.90	122.79
1	L5	4293	PSU	O2-C2-N1	-2.80	119.90	122.79
1	L5	4442	PSU	O2-C2-N1	-2.79	119.91	122.79
1	L5	4972	PSU	O2-C2-N1	-2.79	119.91	122.79
1	L5	4590	A2M	O3'-C3'-C2'	2.78	118.97	111.19
1	L5	4457	PSU	O2-C2-N1	-2.77	119.93	122.79
1	L5	3853	PSU	O2-C2-N1	-2.77	119.93	122.79
1	L5	1744	PSU	O2-C2-N1	-2.77	119.93	122.79
1	L5	4532	PSU	O2-C2-N1	-2.77	119.93	122.79
1	L5	3701	OMC	O2-C2-N1	2.76	124.31	118.90
1	L5	1323	A2M	C3'-C2'-C1'	-2.75	97.54	102.81
1	L5	4552	PSU	C6-N1-C2	-2.75	120.14	122.69
1	L5	2815	A2M	O3'-C3'-C2'	2.74	118.85	111.19
1	L5	3920	PSU	C6-N1-C2	-2.74	120.15	122.69
1	L5	3639	PSU	C6-N1-C2	-2.73	120.16	122.69
1	L5	3818	UY1	O2-C2-N1	-2.72	119.98	122.79
1	L5	4972	PSU	C6-N1-C2	-2.72	120.17	122.69
1	L5	4620	OMU	O4-C4-C5	-2.70	120.50	125.16
1	L5	2632	PSU	C6-N1-C2	-2.70	120.19	122.69
1	L5	4579	PSU	C6-N1-C2	-2.70	120.19	122.69
1	L5	3695	PSU	O2-C2-N1	-2.68	120.02	122.79
1	L5	4293	PSU	C6-N1-C2	-2.67	120.21	122.69
1	L5	4353	PSU	O2-C2-N1	-2.67	120.04	122.79
1	L5	3825	A2M	C1'-N9-C8	2.66	133.00	127.09
1	L5	3639	PSU	O2-C2-N1	-2.66	120.04	122.79
1	L5	400	A2M	C2'-C1'-N9	2.65	118.12	113.75
1	L5	4590	A2M	C4-N9-C1'	-2.65	120.43	126.63
1	L5	2815	A2M	C3'-C2'-C1'	-2.64	97.75	102.81
1	L5	3695	PSU	C6-N1-C2	-2.64	120.24	122.69
1	L5	4571	A2M	C4-N9-C1'	-2.63	120.48	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4673	PSU	C6-N1-C2	-2.63	120.25	122.69
1	L5	4361	PSU	C6-N1-C2	-2.62	120.26	122.69
1	L5	4471	PSU	O2-C2-N1	-2.62	120.09	122.79
1	L5	1582	PSU	O2-C2-N1	-2.61	120.10	122.79
1	L5	1524	A2M	O4'-C1'-C2'	2.61	111.08	106.59
1	L5	1781	PSU	O2-C2-N1	-2.61	120.10	122.79
1	L5	1792	PSU	O2-C2-N1	-2.61	120.10	122.79
1	L5	400	A2M	C4-N9-C1'	-2.60	120.55	126.63
1	L5	2804	OMC	C1'-N1-C2	2.60	124.19	118.44
3	L8	55	PSU	C6-N1-C2	-2.60	120.28	122.69
1	L5	3851	PSU	C6-N1-C2	-2.60	120.28	122.69
1	L5	3785	A2M	C4-N9-C1'	-2.59	120.57	126.63
1	L5	1524	A2M	C4'-O4'-C1'	-2.59	103.75	109.47
1	L5	5010	PSU	C6-N1-C2	-2.59	120.29	122.69
1	L5	4628	PSU	O2-C2-N1	-2.58	120.13	122.79
3	L8	69	PSU	C6-N1-C2	-2.57	120.30	122.69
1	L5	4973	PSU	O2-C2-N1	-2.57	120.14	122.79
1	L5	4493	PSU	O2-C2-N1	-2.56	120.15	122.79
1	L5	2861	OMC	C1'-N1-C2	2.56	124.09	118.44
1	L5	2787	A2M	O4'-C1'-C2'	2.55	110.98	106.59
1	L5	3808	OMC	C1'-N1-C2	2.55	124.07	118.44
1	L5	1782	PSU	O2-C2-N1	-2.55	120.16	122.79
1	L5	4973	PSU	C6-N1-C2	-2.55	120.33	122.69
1	L5	4590	A2M	C1'-N9-C8	2.55	132.75	127.09
1	L5	3867	A2M	C4-N9-C1'	-2.55	120.68	126.63
1	L5	4523	A2M	C4-N9-C1'	-2.54	120.68	126.63
1	L5	398	A2M	C4-N9-C1'	-2.54	120.69	126.63
1	L5	4500	PSU	C6-C5-C4	2.54	119.89	118.17
1	L5	1744	PSU	C6-N1-C2	-2.54	120.34	122.69
1	L5	3853	PSU	C6-N1-C2	-2.52	120.35	122.69
1	L5	4312	PSU	C6-N1-C2	-2.52	120.35	122.69
1	L5	1536	PSU	C6-N1-C2	-2.51	120.36	122.69
1	L5	3830	A2M	C4-N9-C1'	-2.51	120.75	126.63
1	L5	4521	PSU	C6-N1-C2	-2.51	120.36	122.69
1	L5	4471	PSU	C6-N1-C2	-2.51	120.36	122.69
1	L5	4431	PSU	C6-N1-C2	-2.50	120.37	122.69
1	L5	2351	OMC	C1'-N1-C6	-2.50	115.45	120.78
3	L8	55	PSU	O2-C2-N1	-2.49	120.22	122.79
1	L5	1534	A2M	C2'-C1'-N9	2.49	117.86	113.75
1	L5	4353	PSU	C6-N1-C2	-2.49	120.38	122.69
1	L5	4636	PSU	O2-C2-N1	-2.49	120.22	122.79
1	L5	4220	6MZ	C5-C6-N1	2.48	120.81	118.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	1860	PSU	C6-N1-C2	-2.48	120.39	122.69
1	L5	1326	A2M	O3'-C3'-C2'	2.48	118.11	111.19
1	L5	3718	A2M	C1'-N9-C8	2.47	132.57	127.09
1	L5	3830	A2M	C1'-N9-C8	2.46	132.56	127.09
1	L5	3884	PSU	C6-N1-C2	-2.46	120.41	122.69
1	L5	4442	PSU	C6-C5-C4	2.46	119.83	118.17
1	L5	4296	PSU	C6-N1-C2	-2.46	120.41	122.69
1	L5	1582	PSU	C6-N1-C2	-2.45	120.41	122.69
1	L5	1781	PSU	C6-N1-C2	-2.45	120.41	122.69
1	L5	400	A2M	C1'-N9-C8	2.45	132.54	127.09
1	L5	3867	A2M	C1'-N9-C8	2.45	132.53	127.09
1	L5	398	A2M	C1'-N9-C8	2.45	132.53	127.09
1	L5	1326	A2M	C3'-C2'-C1'	-2.44	98.13	102.81
1	L5	4673	PSU	O2-C2-N1	-2.44	120.27	122.79
1	L5	4571	A2M	C1'-N9-C8	2.44	132.52	127.09
1	L5	1871	A2M	C6-C5-C4	-2.44	113.85	117.18
1	L5	4431	PSU	O2-C2-N1	-2.43	120.28	122.79
1	L5	1323	A2M	O4'-C1'-C2'	2.42	110.76	106.59
1	L5	4523	A2M	C1'-N9-C8	2.42	132.47	127.09
1	L5	4299	PSU	O2-C2-N1	-2.42	120.29	122.79
1	L5	4361	PSU	O2-C2-N1	-2.41	120.31	122.79
1	L5	4636	PSU	C6-C5-C4	2.40	119.79	118.17
1	L5	5001	PSU	O2-C2-N1	-2.39	120.32	122.79
1	L5	1326	A2M	C4-N9-C1'	-2.39	121.05	126.63
1	L5	5001	PSU	C6-N1-C2	-2.39	120.48	122.69
1	L5	1326	A2M	C2'-C1'-N9	2.38	117.67	113.75
1	L5	4576	PSU	C6-N1-C2	-2.38	120.48	122.69
1	L5	4403	PSU	C6-N1-C2	-2.38	120.49	122.69
1	L5	3785	A2M	C3'-C2'-C1'	-2.37	98.26	102.81
1	L5	2839	PSU	C6-N1-C2	-2.37	120.49	122.69
1	L5	4628	PSU	C6-N1-C2	-2.37	120.49	122.69
1	L5	2363	A2M	C4-N9-C1'	-2.37	121.09	126.63
1	L5	2363	A2M	C1'-N9-C8	2.37	132.35	127.09
1	L5	1326	A2M	C1'-N9-C8	2.37	132.35	127.09
1	L5	4299	PSU	C6-N1-C2	-2.37	120.50	122.69
1	L5	4498	OMU	O2-C2-N1	-2.36	119.72	122.80
1	L5	3718	A2M	C4-N9-C1'	-2.36	121.11	126.63
1	L5	1782	PSU	C6-N1-C2	-2.36	120.50	122.69
1	L5	2787	A2M	C4-N9-C1'	-2.35	121.12	126.63
1	L5	1862	PSU	C6-N1-C2	-2.35	120.51	122.69
1	L5	1522	OMG	C2'-C1'-N9	-2.34	109.80	114.24
1	L5	3867	A2M	O3'-C3'-C2'	2.34	117.72	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3785	A2M	C1'-N9-C8	2.33	132.27	127.09
1	L5	3785	A2M	C2-N1-C6	-2.33	114.91	118.73
1	L5	1524	A2M	C4-N9-C1'	-2.32	121.21	126.63
1	L5	4442	PSU	C6-N1-C2	-2.31	120.55	122.69
1	L5	4532	PSU	C6-N1-C2	-2.31	120.55	122.69
1	L5	2815	A2M	C4-N9-C1'	-2.31	121.23	126.63
1	L5	2363	A2M	O4'-C1'-C2'	2.28	110.52	106.59
1	L5	2401	A2M	C6-C5-C4	-2.28	114.06	117.18
1	L5	2815	A2M	C1'-N9-C8	2.28	132.15	127.09
1	L5	1534	A2M	C4-N9-C1'	-2.27	121.33	126.63
1	L5	1322	1MA	N1-C6-N6	2.26	125.39	119.71
1	L5	4403	PSU	O4'-C1'-C2'	2.26	108.28	105.15
1	L5	1534	A2M	C1'-N9-C8	2.26	132.11	127.09
1	L5	4521	PSU	C6-C5-C4	2.26	119.70	118.17
1	L5	3822	PSU	O4'-C1'-C2'	2.26	108.27	105.15
1	L5	2787	A2M	C1'-N9-C8	2.25	132.09	127.09
1	L5	1792	PSU	C6-N1-C2	-2.25	120.60	122.69
1	L5	4636	PSU	C6-N1-C2	-2.25	120.60	122.69
1	L5	1534	A2M	O3'-C3'-C4'	-2.25	104.63	111.08
1	L5	4442	PSU	O4'-C1'-C2'	2.24	108.26	105.15
1	L5	4403	PSU	C6-C5-C4	2.24	119.69	118.17
1	L5	1524	A2M	C1'-N9-C8	2.24	132.06	127.09
1	L5	3825	A2M	C6-C5-C4	-2.24	114.12	117.18
1	L5	4353	PSU	C6-C5-C4	2.23	119.68	118.17
1	L5	4571	A2M	O4'-C1'-C2'	2.23	110.42	106.59
1	L5	3718	A2M	C2'-C1'-N9	2.21	117.40	113.75
1	L5	400	A2M	O4'-C1'-C2'	2.21	110.39	106.59
1	L5	4590	A2M	C6-C5-C4	-2.20	114.17	117.18
1	L5	3785	A2M	C5-C6-N1	2.20	123.10	117.51
1	L5	3782	5MC	C1'-N1-C6	-2.19	117.55	121.15
1	L5	2815	A2M	O4'-C1'-C2'	2.18	110.35	106.59
1	L5	3867	A2M	C6-C5-C4	-2.17	114.21	117.18
1	L5	1677	PSU	C6-C5-C4	2.17	119.64	118.17
3	L8	69	PSU	O4'-C1'-C2'	2.16	108.14	105.15
1	L5	4571	A2M	C6-C5-C4	-2.16	114.23	117.18
1	L5	4636	PSU	O4'-C1'-C2'	2.16	108.14	105.15
1	L5	3785	A2M	O4'-C4'-C3'	2.15	109.43	105.15
1	L5	3925	OMU	O2-C2-N1	-2.15	120.00	122.80
1	L5	3637	PSU	C6-N1-C2	-2.15	120.70	122.69
1	L5	1326	A2M	O4'-C1'-C2'	2.15	110.28	106.59
1	L5	3830	A2M	C6-C5-C4	-2.15	114.25	117.18
1	L5	1534	A2M	O4'-C1'-C2'	2.14	110.27	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	4493	PSU	C6-N1-C2	-2.13	120.71	122.69
1	L5	3785	A2M	O4'-C1'-N9	2.13	112.18	108.09
1	L5	3822	PSU	C6-C5-C4	2.12	119.61	118.17
1	L5	4523	A2M	C6-C5-C4	-2.11	114.29	117.18
1	L5	3830	A2M	C4'-O4'-C1'	-2.11	104.80	109.47
1	L5	400	A2M	C6-C5-C4	-2.11	114.30	117.18
1	L5	3785	A2M	C6-C5-C4	-2.11	114.30	117.18
1	L5	1322	1MA	CM1-N1-C6	-2.10	116.89	120.15
1	L5	1683	PSU	C6-C5-C4	2.09	119.59	118.17
1	L5	2363	A2M	C2-N1-C6	-2.08	115.31	118.73
1	L5	3867	A2M	C2-N1-C6	-2.08	115.32	118.73
1	L5	1677	PSU	C6-N1-C2	-2.07	120.77	122.69
1	L5	398	A2M	C2-N1-C6	-2.07	115.33	118.73
1	L5	4457	PSU	O4'-C1'-C2'	2.07	108.01	105.15
1	L5	1326	A2M	C6-C5-C4	-2.07	114.36	117.18
1	L5	3718	A2M	C6-C5-C4	-2.07	114.36	117.18
1	L5	1323	A2M	C4-N9-C1'	-2.06	121.81	126.63
1	L5	4571	A2M	C2'-C1'-N9	2.06	117.14	113.75
1	L5	1534	A2M	C2-N1-C6	-2.05	115.36	118.73
1	L5	1871	A2M	C4'-O4'-C1'	-2.05	104.94	109.47
1	L5	398	A2M	C5-C6-N1	2.05	122.72	117.51
1	L5	4353	PSU	O4'-C1'-C2'	2.05	107.99	105.15
1	L5	2815	A2M	C6-C5-C4	-2.05	114.38	117.18
1	L5	4457	PSU	C6-N1-C2	-2.05	120.79	122.69
1	L5	3825	A2M	C5-C6-N1	2.04	122.70	117.51
1	L5	3825	A2M	C2-N1-C6	-2.04	115.37	118.73
1	L5	1323	A2M	C1'-N9-C8	2.04	131.62	127.09
1	L5	4530	UR3	C6-N1-C2	-2.04	120.13	121.80
1	L5	4523	A2M	C4'-O4'-C1'	-2.03	104.97	109.47
1	L5	1871	A2M	O4'-C1'-C2'	2.03	110.09	106.59
1	L5	1524	A2M	C2-N1-C6	-2.03	115.39	118.73
1	L5	398	A2M	C6-C5-C4	-2.03	114.40	117.18
1	L5	4571	A2M	C5-C6-N1	2.03	122.67	117.51
1	L5	1323	A2M	C2-N1-C6	-2.03	115.40	118.73
1	L5	400	A2M	C2-N1-C6	-2.03	115.40	118.73
1	L5	2787	A2M	C2-N1-C6	-2.02	115.41	118.73
1	L5	4220	6MZ	C3'-C2'-C1'	2.02	105.28	101.46
1	L5	2363	A2M	C5-C6-N1	2.02	122.63	117.51
1	L5	2422	OMC	C1'-N1-C2	2.01	122.87	118.44
1	L5	4521	PSU	O4'-C1'-C2'	2.01	107.93	105.15
1	L5	400	A2M	C5-C6-N1	2.00	122.60	117.51
1	L5	1326	A2M	C2-N1-C6	-2.00	115.44	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3639	PSU	C6-C5-C4	2.00	119.53	118.17
1	L5	2787	A2M	O4'-C4'-C3'	2.00	109.13	105.15
1	L5	4571	A2M	C2-N1-C6	-2.00	115.44	118.73
1	L5	2363	A2M	C6-C5-C4	-2.00	114.45	117.18
1	L5	2787	A2M	C6-C5-C4	-2.00	114.45	117.18

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L8	75	OMG	C1'-C2'-O2'-CM2
1	L5	400	A2M	C1'-C2'-O2'-CM'
1	L5	1326	A2M	O4'-C4'-C5'-O5'
1	L5	1340	OMC	C1'-C2'-O2'-CM2
1	L5	1625	OMG	O4'-C4'-C5'-O5'
1	L5	2351	OMC	C1'-C2'-O2'-CM2
1	L5	2787	A2M	C1'-C2'-O2'-CM'
1	L5	2815	A2M	O4'-C4'-C5'-O5'
1	L5	2824	OMC	C1'-C2'-O2'-CM2
1	L5	3701	OMC	C2'-C1'-N1-C2
1	L5	3701	OMC	O4'-C4'-C5'-O5'
1	L5	3792	OMG	O4'-C4'-C5'-O5'
1	L5	4196	OMG	C1'-C2'-O2'-CM2
1	L5	4590	A2M	O4'-C4'-C5'-O5'
1	L5	4637	OMG	O4'-C4'-C5'-O5'
1	L5	1323	A2M	O4'-C4'-C5'-O5'
1	L5	1625	OMG	C3'-C4'-C5'-O5'
1	L5	2364	OMG	O4'-C4'-C5'-O5'
1	L5	3867	A2M	C3'-C4'-C5'-O5'
1	L5	4220	6MZ	O4'-C4'-C5'-O5'
1	L5	4500	PSU	C3'-C4'-C5'-O5'
1	L5	4500	PSU	O4'-C4'-C5'-O5'
1	L5	4590	A2M	C3'-C4'-C5'-O5'
1	L5	3701	OMC	C2'-C1'-N1-C6
1	L5	1536	PSU	C3'-C4'-C5'-O5'
1	L5	1677	PSU	C3'-C4'-C5'-O5'
1	L5	3701	OMC	C3'-C4'-C5'-O5'
1	L5	3792	OMG	C3'-C4'-C5'-O5'
1	L5	4637	OMG	C3'-C4'-C5'-O5'
1	L5	1326	A2M	C3'-C4'-C5'-O5'
1	L5	2815	A2M	C3'-C4'-C5'-O5'
1	L5	4447	5MC	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
1	L5	1677	PSU	O4'-C4'-C5'-O5'
1	L5	3899	OMG	C3'-C4'-C5'-O5'
1	L5	1323	A2M	C3'-C4'-C5'-O5'
1	L5	1536	PSU	O4'-C4'-C5'-O5'
1	L5	2787	A2M	C3'-C4'-C5'-O5'
1	L5	3867	A2M	O4'-C4'-C5'-O5'
1	L5	3899	OMG	O4'-C4'-C5'-O5'
1	L5	4618	OMG	C3'-C4'-C5'-O5'
1	L5	4220	6MZ	C3'-C4'-C5'-O5'
1	L5	1524	A2M	O4'-C4'-C5'-O5'
1	L5	1524	A2M	C3'-C4'-C5'-O5'
1	L5	2364	OMG	C3'-C4'-C5'-O5'
1	L5	2787	A2M	C2'-C1'-N9-C8
1	L5	4637	OMG	C1'-C2'-O2'-CM2
1	L5	4590	A2M	C4'-C5'-O5'-P
1	L5	2422	OMC	C3'-C4'-C5'-O5'
1	L5	4447	5MC	O4'-C1'-N1-C6
1	L5	2422	OMC	O4'-C4'-C5'-O5'
1	L5	4618	OMG	O4'-C4'-C5'-O5'
1	L5	4447	5MC	C2'-C1'-N1-C2
1	L5	4447	5MC	O4'-C1'-N1-C2
1	L5	1534	A2M	C4'-C5'-O5'-P
1	L5	3818	UY1	C4'-C5'-O5'-P
1	L5	4500	PSU	C4'-C5'-O5'-P
1	L5	3818	UY1	O4'-C1'-C5-C4
1	L5	2787	A2M	C2'-C1'-N9-C4
1	L5	1781	PSU	C3'-C4'-C5'-O5'
1	L5	4296	PSU	C3'-C4'-C5'-O5'
1	L5	1524	A2M	C3'-C2'-O2'-CM'
1	L5	4494	OMG	C3'-C2'-O2'-CM2
1	L5	398	A2M	O4'-C4'-C5'-O5'
1	L5	1322	1MA	C2'-C1'-N9-C4
1	L5	3844	PSU	C4'-C5'-O5'-P
1	L5	1322	1MA	C2'-C1'-N9-C8
1	L5	3785	A2M	C1'-C2'-O2'-CM'
1	L5	3701	OMC	O4'-C1'-N1-C6
1	L5	3627	OMG	O4'-C4'-C5'-O5'
1	L5	4636	PSU	O4'-C1'-C5-C6
1	L5	3785	A2M	C3'-C2'-O2'-CM'
1	L5	3869	OMC	C3'-C2'-O2'-CM2
1	L5	3851	PSU	C3'-C4'-C5'-O5'
1	L5	4471	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	L5	2787	A2M	O4'-C1'-N9-C8
1	L5	1326	A2M	C4'-C5'-O5'-P
1	L5	4296	PSU	O4'-C4'-C5'-O5'
1	L5	2351	OMC	C2'-C1'-N1-C2
1	L5	3887	OMC	C4'-C5'-O5'-P
1	L5	2351	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

37 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	1625	OMG	1	0
1	L5	4431	PSU	1	0
1	L5	4636	PSU	1	0
1	L5	4637	OMG	1	0
1	L5	4618	OMG	1	0
1	L5	1683	PSU	1	0
1	L5	3822	PSU	1	0
1	L5	4456	OMC	1	0
1	L5	2824	OMC	1	0
1	L5	1326	A2M	2	0
1	L5	2363	A2M	1	0
1	L5	3867	A2M	4	0
1	L5	1340	OMC	2	0
1	L5	1677	PSU	1	0
1	L5	4536	OMC	1	0
3	L8	75	OMG	2	0
1	L5	4220	6MZ	1	0
1	L5	4196	OMG	1	0
1	L5	3701	OMC	1	0
1	L5	4457	PSU	1	0
1	L5	4293	PSU	1	0
1	L5	400	A2M	1	0
1	L5	398	A2M	1	0
1	L5	3841	OMC	1	0
1	L5	3785	A2M	1	0
1	L5	3825	A2M	1	0
1	L5	2804	OMC	1	0
1	L5	1871	A2M	1	0
1	L5	4571	A2M	1	0
1	L5	1534	A2M	1	0
1	L5	3718	A2M	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	2632	PSU	1	0
1	L5	4620	OMU	2	0
1	L5	2422	OMC	1	0
1	L5	2351	OMC	2	0
1	L5	3884	PSU	1	0
1	L5	3818	UY1	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 213 ligands modelled in this entry, 196 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
46	SPM	L5	5267	-	13,13,13	0.36	0	12,12,12	1.12	0
47	SPD	L5	5284	-	9,9,9	0.31	0	8,8,8	0.81	0
46	SPM	L5	5264	-	13,13,13	0.36	0	12,12,12	0.97	0
47	SPD	L5	5261	-	9,9,9	0.31	0	8,8,8	0.97	0
46	SPM	L5	5292	-	13,13,13	0.37	0	12,12,12	0.97	0
46	SPM	L5	5293	-	13,13,13	0.36	0	12,12,12	0.89	0
46	SPM	L5	5259	-	13,13,13	0.36	0	12,12,12	0.98	0
47	SPD	L5	5288	-	9,9,9	0.31	0	8,8,8	0.87	0
47	SPD	L5	5290	-	9,9,9	0.31	0	8,8,8	0.81	0
47	SPD	L5	5291	-	9,9,9	0.33	0	8,8,8	0.81	0
46	SPM	L5	5289	-	13,13,13	0.38	0	12,12,12	1.01	0
46	SPM	L5	5263	-	13,13,13	0.36	0	12,12,12	0.92	0
47	SPD	L5	5287	-	9,9,9	0.31	0	8,8,8	0.89	0
47	SPD	LN	301	-	9,9,9	0.34	0	8,8,8	0.85	0
47	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.90	0
47	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.82	0
47	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.82	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
46	SPM	L5	5267	-	-	4/11/11/11	-
47	SPD	L5	5284	-	-	3/7/7/7	-
46	SPM	L5	5264	-	-	3/11/11/11	-
47	SPD	L5	5261	-	-	0/7/7/7	-
46	SPM	L5	5292	-	-	4/11/11/11	-
46	SPM	L5	5293	-	-	4/11/11/11	-
46	SPM	L5	5259	-	-	3/11/11/11	-
47	SPD	L5	5288	-	-	1/7/7/7	-
47	SPD	L5	5290	-	-	2/7/7/7	-
47	SPD	L5	5291	-	-	3/7/7/7	-
46	SPM	L5	5289	-	-	5/11/11/11	-
46	SPM	L5	5263	-	-	7/11/11/11	-
47	SPD	L5	5287	-	-	3/7/7/7	-
47	SPD	LN	301	-	-	1/7/7/7	-
47	SPD	L5	5285	-	-	5/7/7/7	-
47	SPD	L5	5283	-	-	2/7/7/7	-
47	SPD	L5	5286	-	-	0/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	L5	5285	SPD	N6-C7-C8-C9
46	L5	5292	SPM	C7-C8-C9-N10
47	L5	5285	SPD	C3-C4-C5-N6
47	L5	5287	SPD	C3-C4-C5-N6
46	L5	5264	SPM	C2-C3-C4-N5
47	L5	5287	SPD	N6-C7-C8-C9
46	L5	5259	SPM	C3-C4-N5-C6
46	L5	5263	SPM	C7-C6-N5-C4
46	L5	5289	SPM	C8-C9-N10-C11
47	L5	5287	SPD	C2-C3-C4-C5

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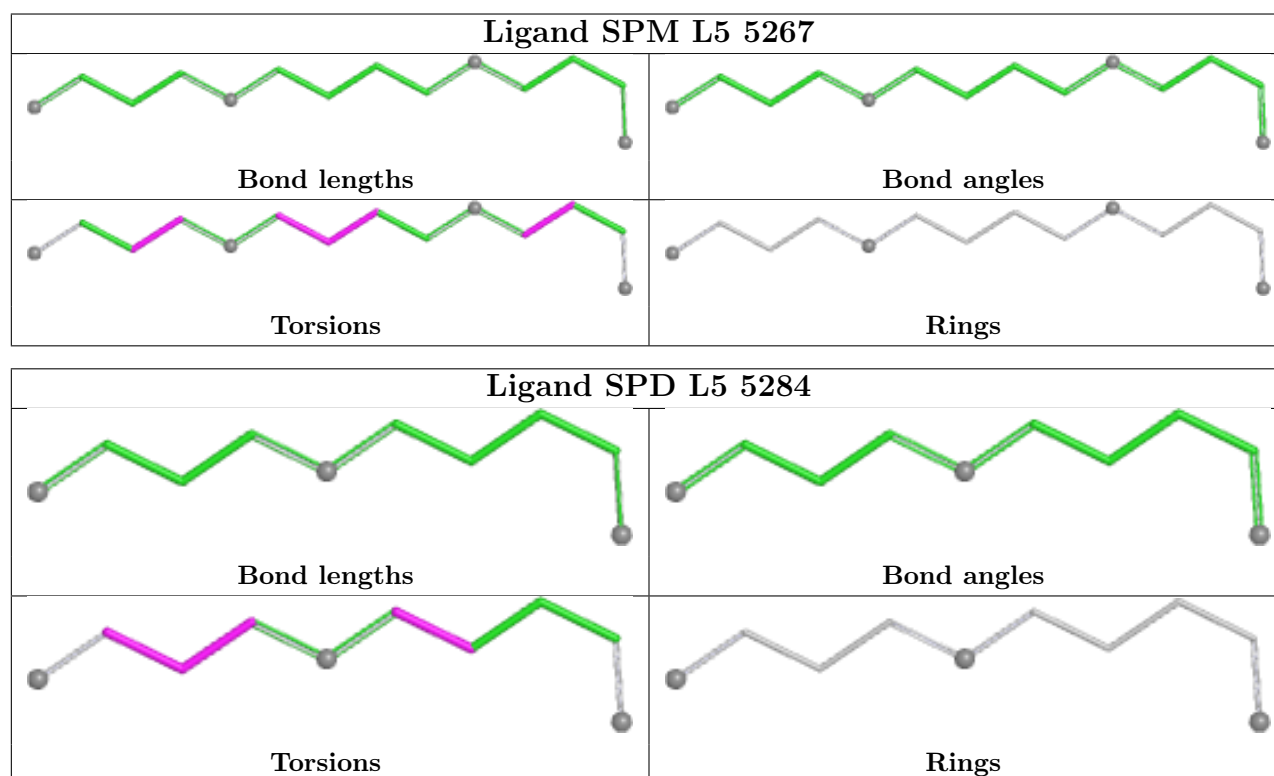
Mol	Chain	Res	Type	Atoms
46	L5	5292	SPM	N10-C11-C12-C13
46	L5	5292	SPM	N5-C6-C7-C8
46	L5	5264	SPM	N5-C6-C7-C8
46	L5	5263	SPM	C3-C4-N5-C6
47	LN	301	SPD	C4-C5-N6-C7
46	L5	5267	SPM	C7-C8-C9-N10
47	L5	5285	SPD	C2-C3-C4-C5
46	L5	5293	SPM	C6-C7-C8-C9
47	L5	5290	SPD	C2-C3-C4-C5
47	L5	5284	SPD	C3-C4-C5-N6
46	L5	5267	SPM	N10-C11-C12-C13
46	L5	5259	SPM	C6-C7-C8-C9
47	L5	5283	SPD	C3-C4-C5-N6
46	L5	5289	SPM	C12-C11-N10-C9
46	L5	5267	SPM	C6-C7-C8-C9
46	L5	5289	SPM	N1-C2-C3-C4
46	L5	5293	SPM	C8-C9-N10-C11
47	L5	5284	SPD	C7-C8-C9-N10
47	L5	5291	SPD	C4-C5-N6-C7
47	L5	5291	SPD	N1-C2-C3-C4
47	L5	5285	SPD	C4-C5-N6-C7
47	L5	5291	SPD	C8-C7-N6-C5
47	L5	5283	SPD	C2-C3-C4-C5
46	L5	5263	SPM	N10-C11-C12-C13
46	L5	5263	SPM	N1-C2-C3-C4
46	L5	5263	SPM	C11-C12-C13-N14
47	L5	5285	SPD	C7-C8-C9-N10
47	L5	5290	SPD	N6-C7-C8-C9
46	L5	5267	SPM	C2-C3-C4-N5
47	L5	5288	SPD	C8-C7-N6-C5
46	L5	5289	SPM	C2-C3-C4-N5
46	L5	5289	SPM	C7-C6-N5-C4
47	L5	5284	SPD	N6-C7-C8-C9
46	L5	5263	SPM	N5-C6-C7-C8
46	L5	5263	SPM	C6-C7-C8-C9
46	L5	5293	SPM	C7-C6-N5-C4
46	L5	5259	SPM	N10-C11-C12-C13
46	L5	5292	SPM	C6-C7-C8-C9
46	L5	5293	SPM	C11-C12-C13-N14
46	L5	5264	SPM	N10-C11-C12-C13

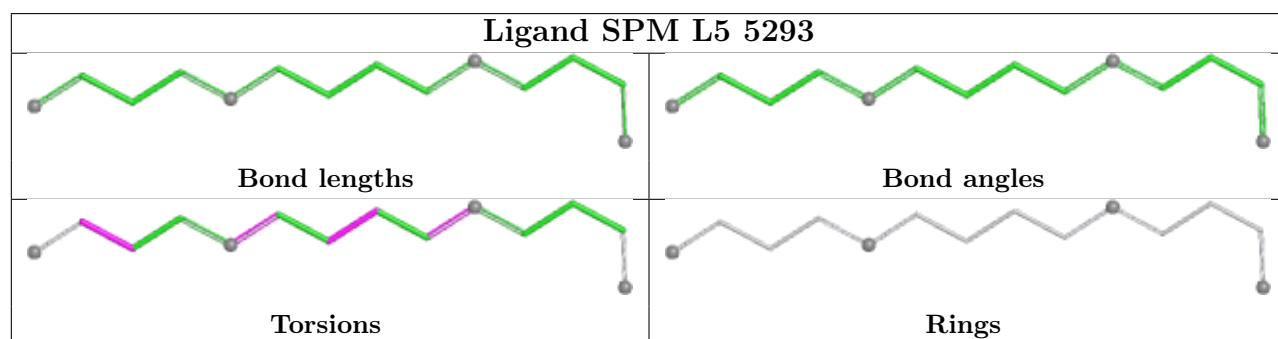
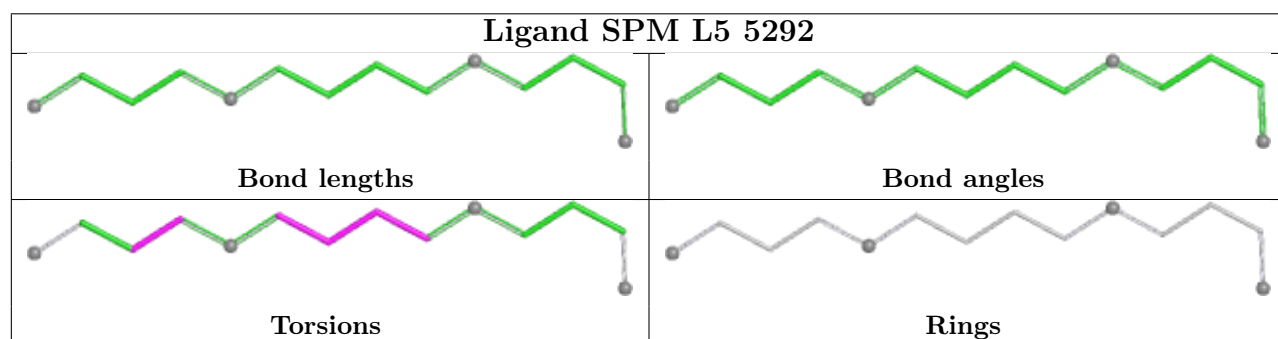
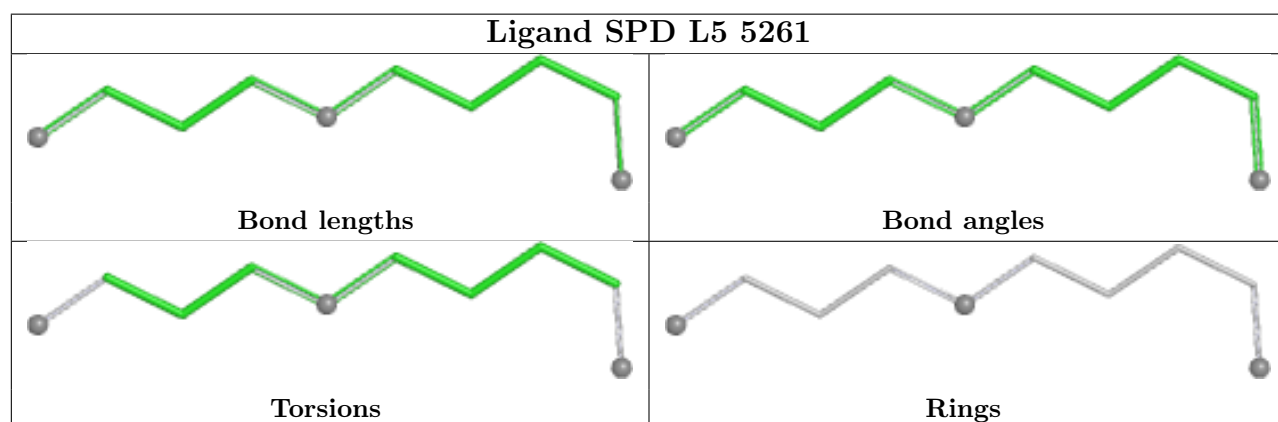
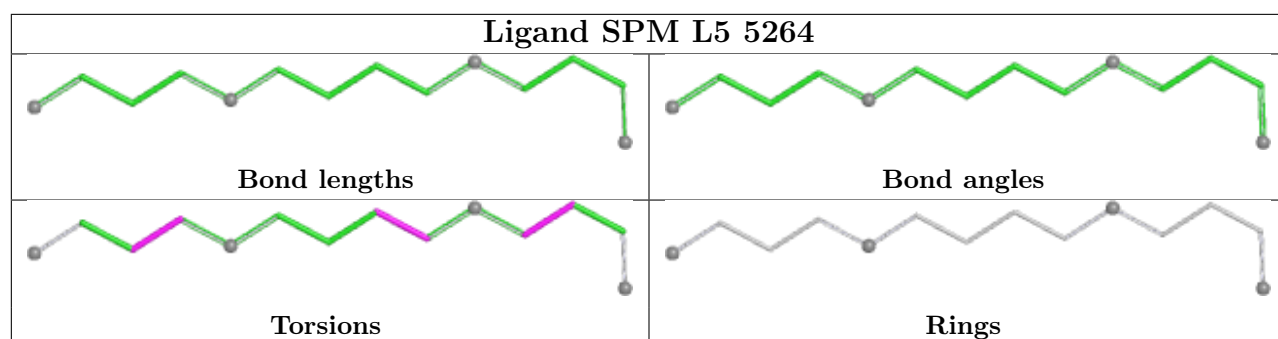
There are no ring outliers.

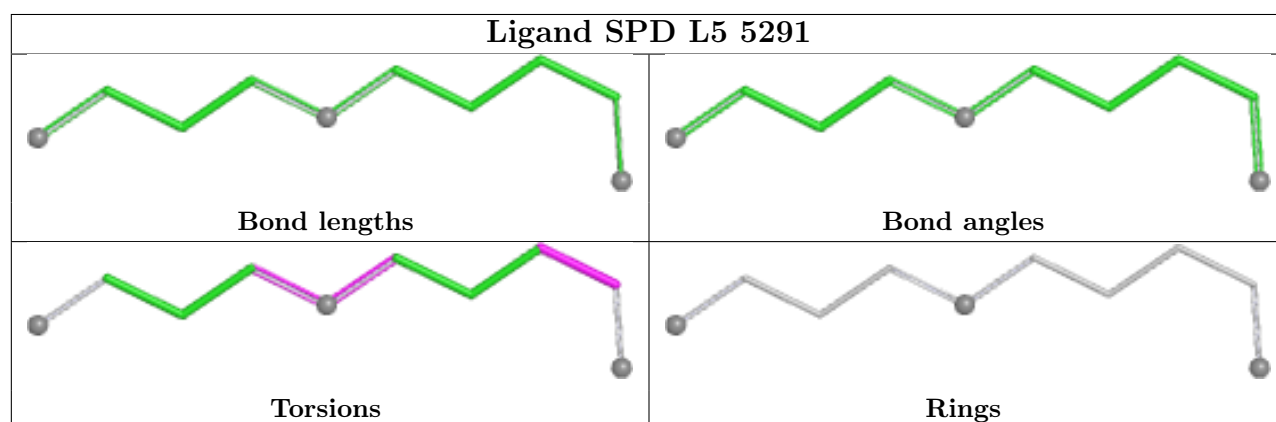
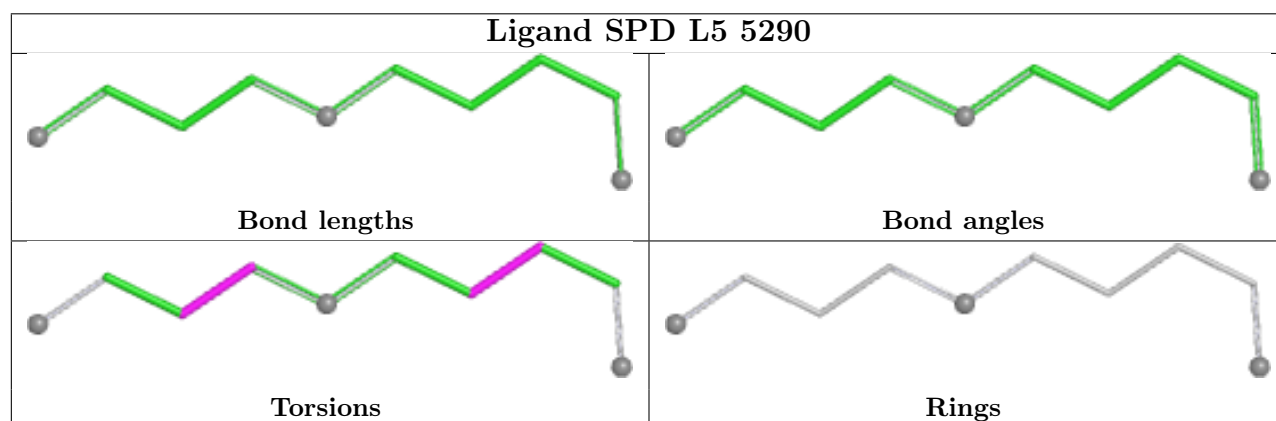
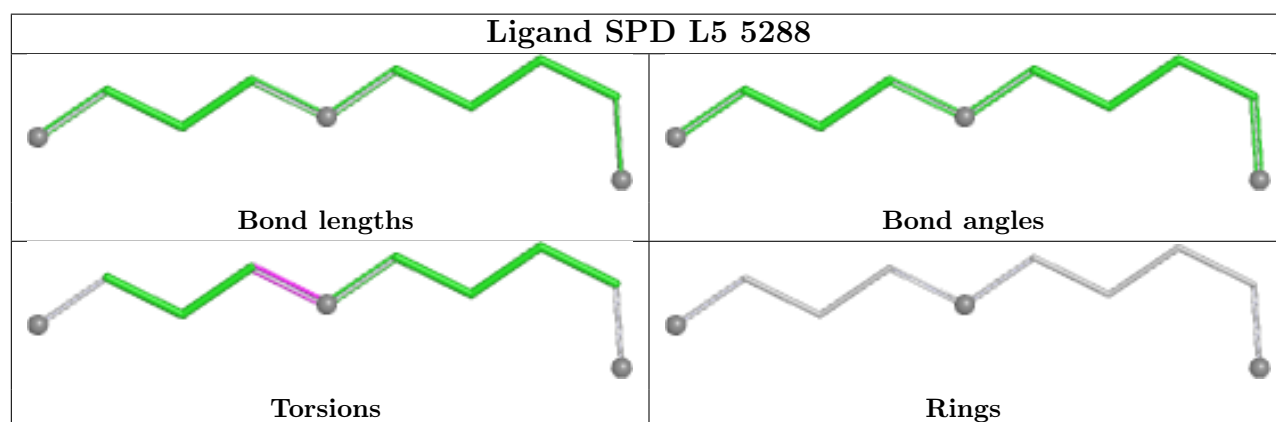
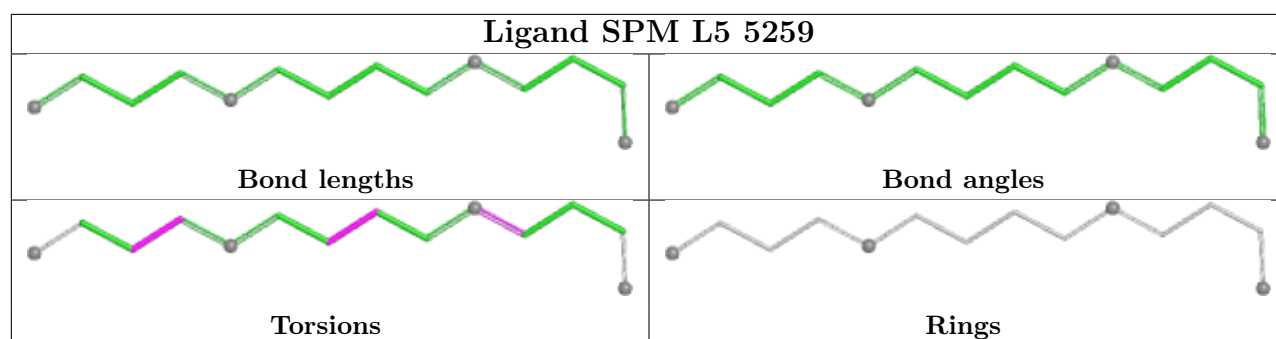
8 monomers are involved in 9 short contacts:

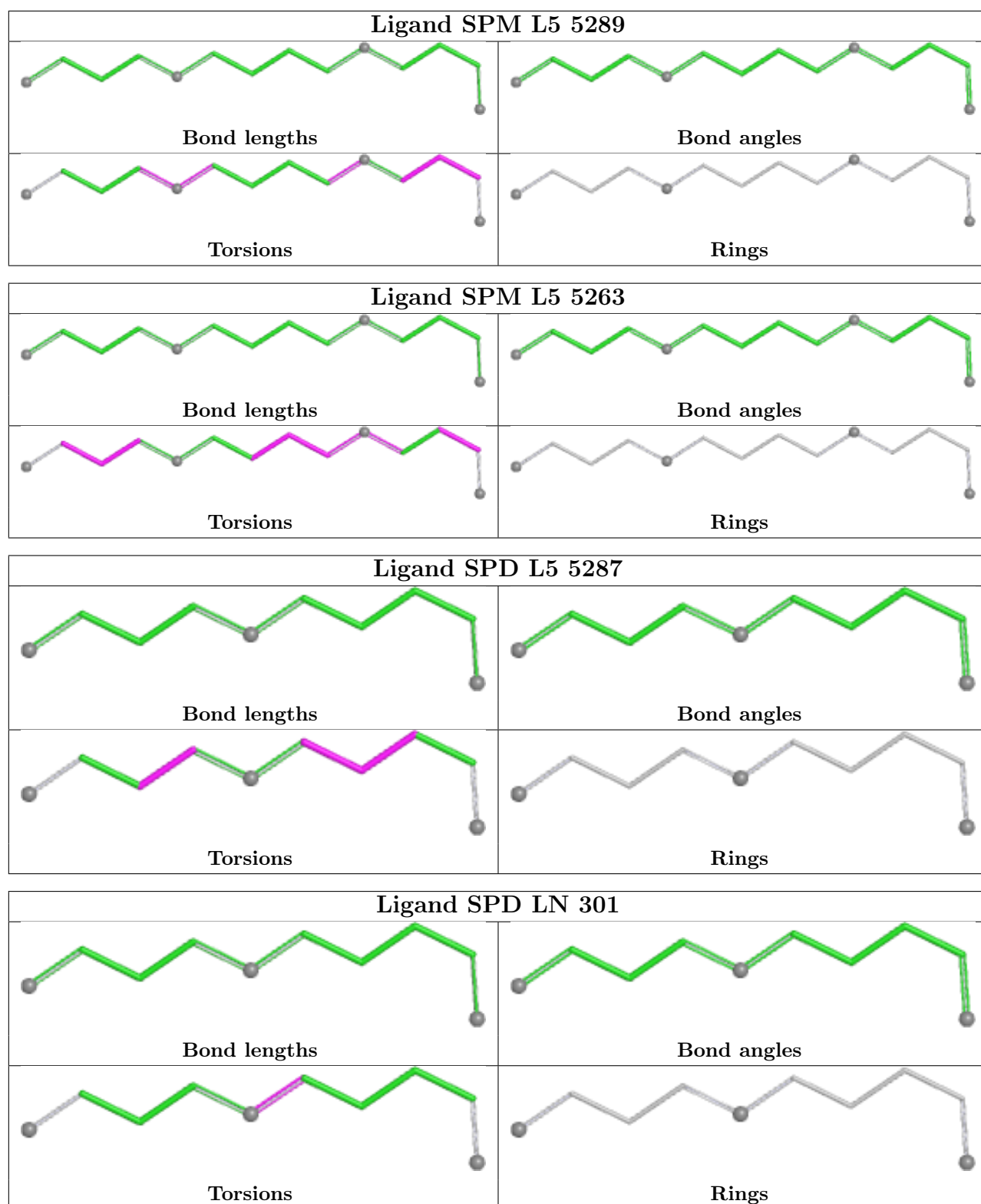
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	L5	5284	SPD	1	0
46	L5	5264	SPM	2	0
47	L5	5261	SPD	1	0
46	L5	5292	SPM	1	0
46	L5	5293	SPM	1	0
47	L5	5290	SPD	1	0
47	L5	5291	SPD	1	0
47	L5	5286	SPD	1	0

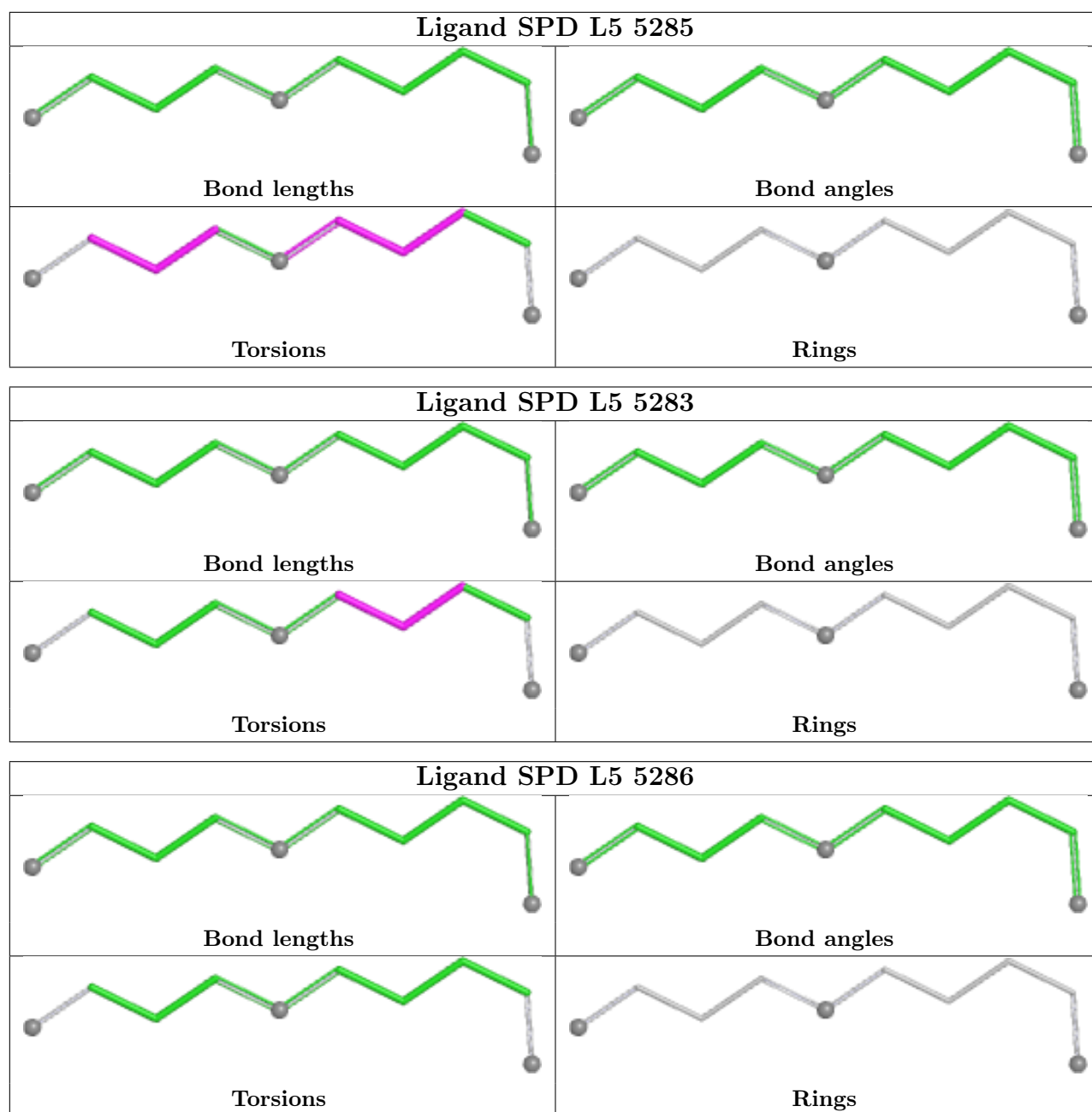
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	L5	8

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L5	2910:G	O3'	3584:C	P	21.32
1	L5	760:G	O3'	903:C	P	16.88
1	L5	519:C	O3'	642:G	P	15.66
1	L5	4776:G	O3'	4858:C	P	15.18
1	L5	2112:G	O3'	2249:C	P	14.87
1	L5	3954:A	O3'	4056:A	P	13.33
1	L5	990:C	O3'	1064:G	P	12.43
1	L5	1100:U	O3'	1167:C	P	6.88

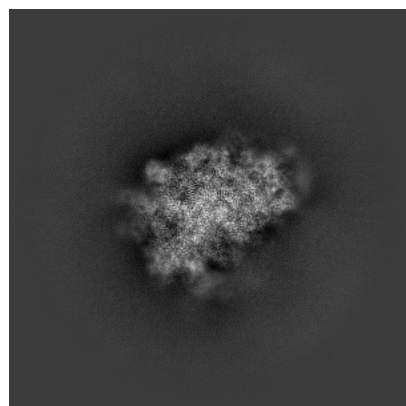
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71413. These allow visual inspection of the internal detail of the map and identification of artifacts.

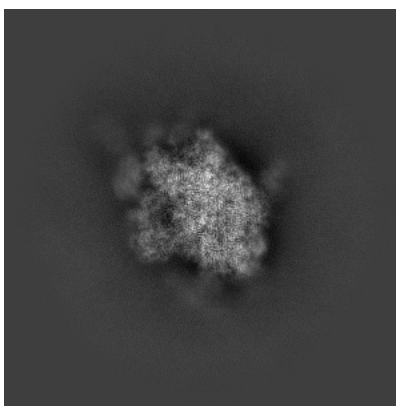
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

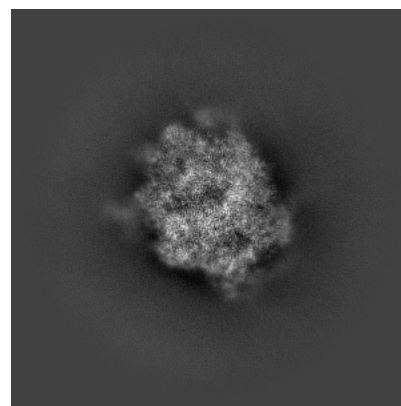
6.1.1 Primary map



X

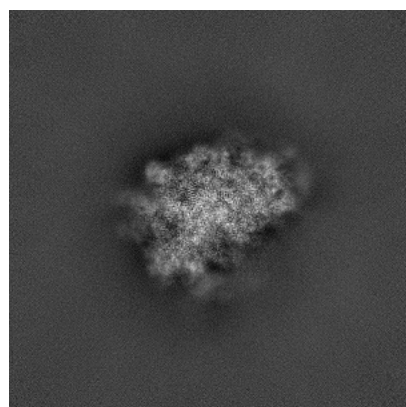


Y

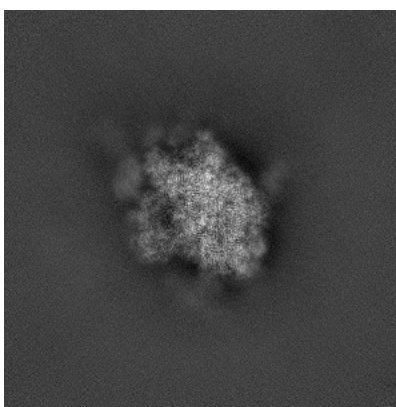


Z

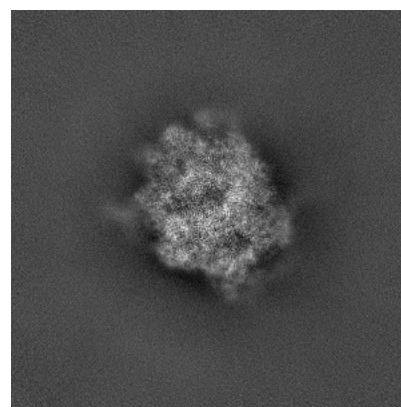
6.1.2 Raw map



X



Y

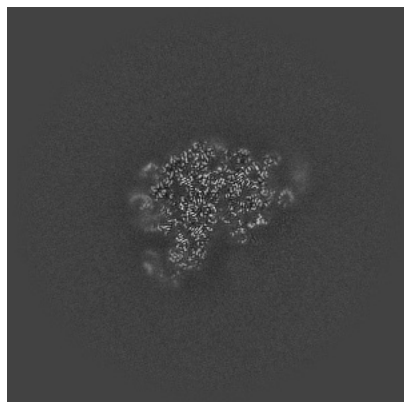


Z

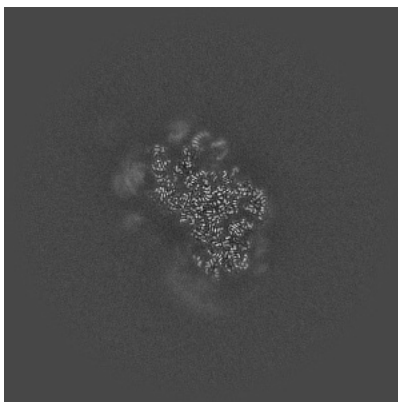
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

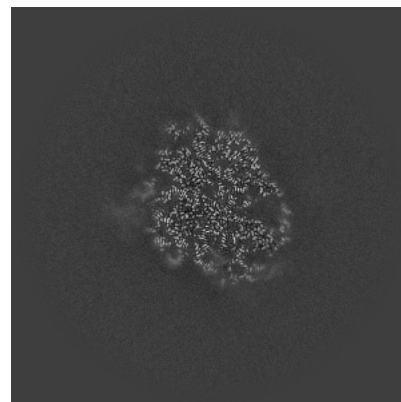
6.2.1 Primary map



X Index: 256

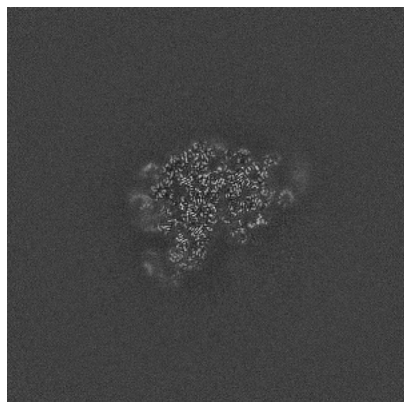


Y Index: 256

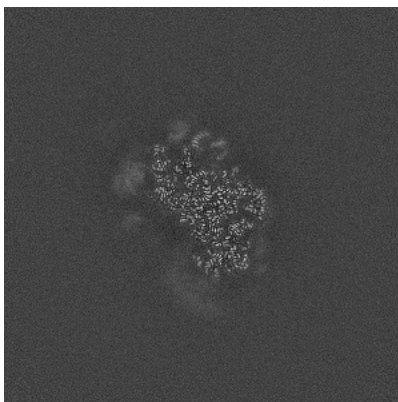


Z Index: 256

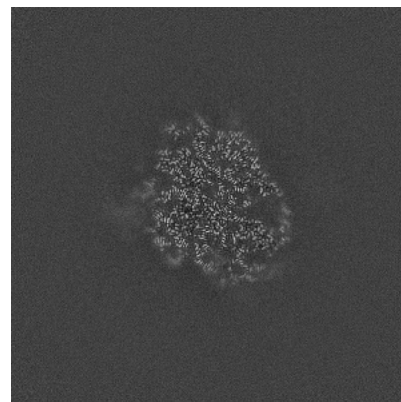
6.2.2 Raw map



X Index: 256



Y Index: 256

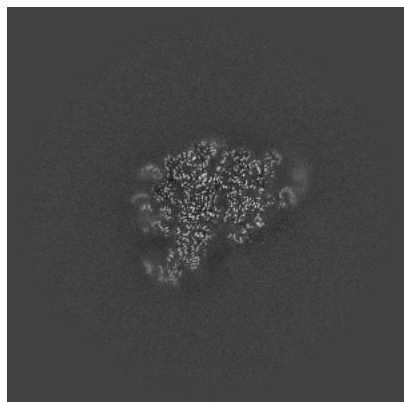


Z Index: 256

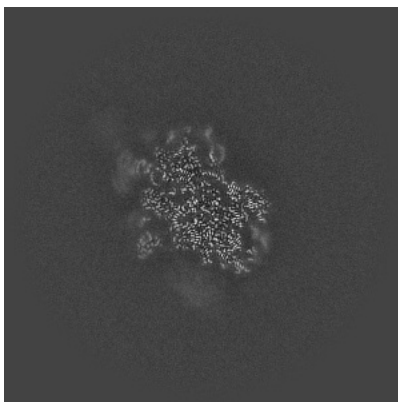
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

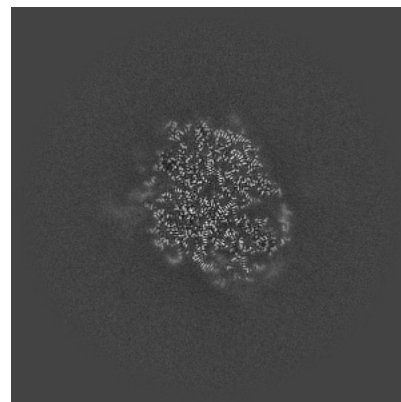
6.3.1 Primary map



X Index: 253

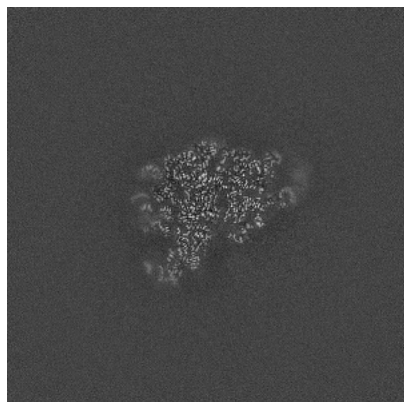


Y Index: 243

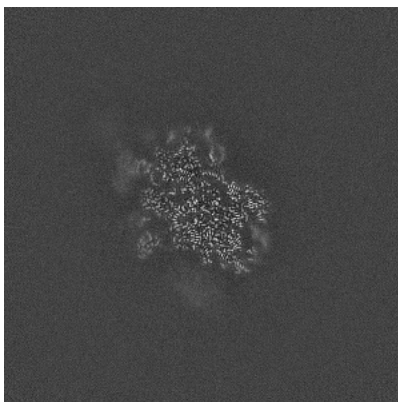


Z Index: 258

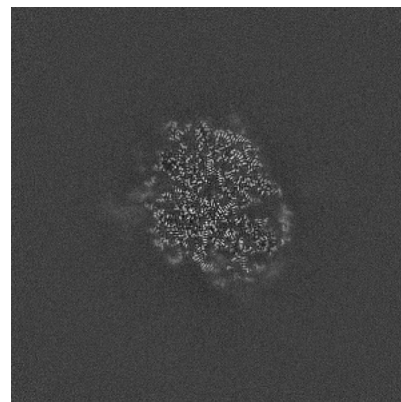
6.3.2 Raw map



X Index: 253



Y Index: 243

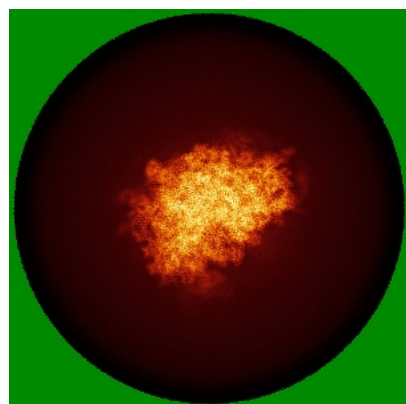


Z Index: 258

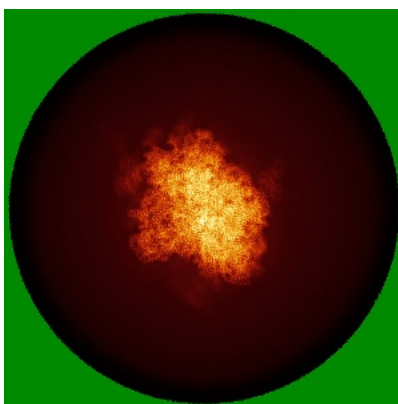
The images above show the largest variance slices of the map in three orthogonal directions.

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

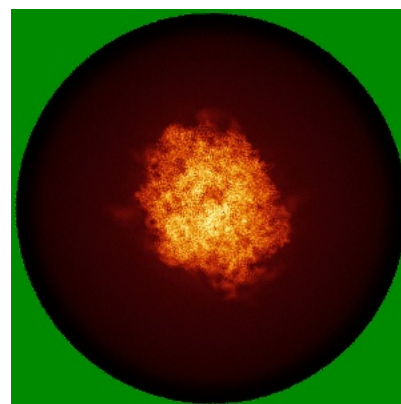
6.4.1 Primary map



X

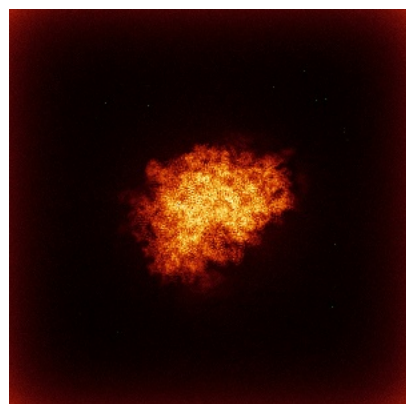


Y

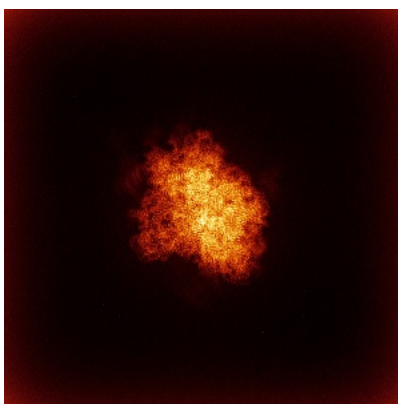


Z

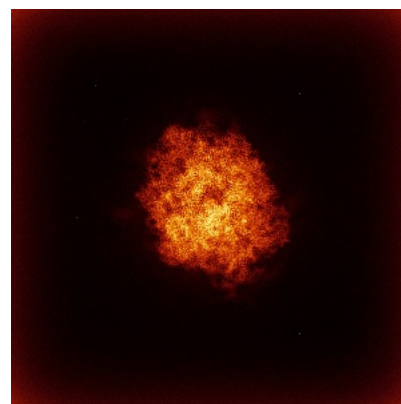
6.4.2 Raw map



X



Y

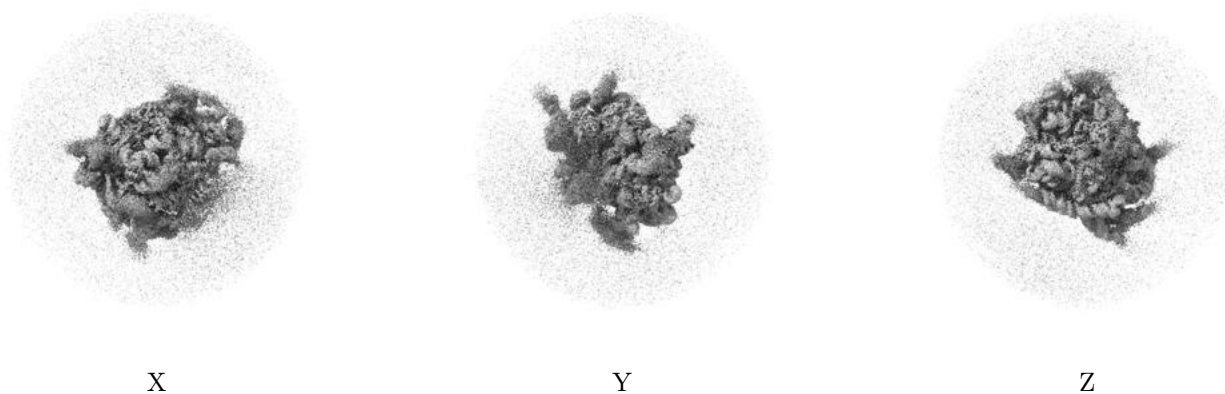


Z

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.

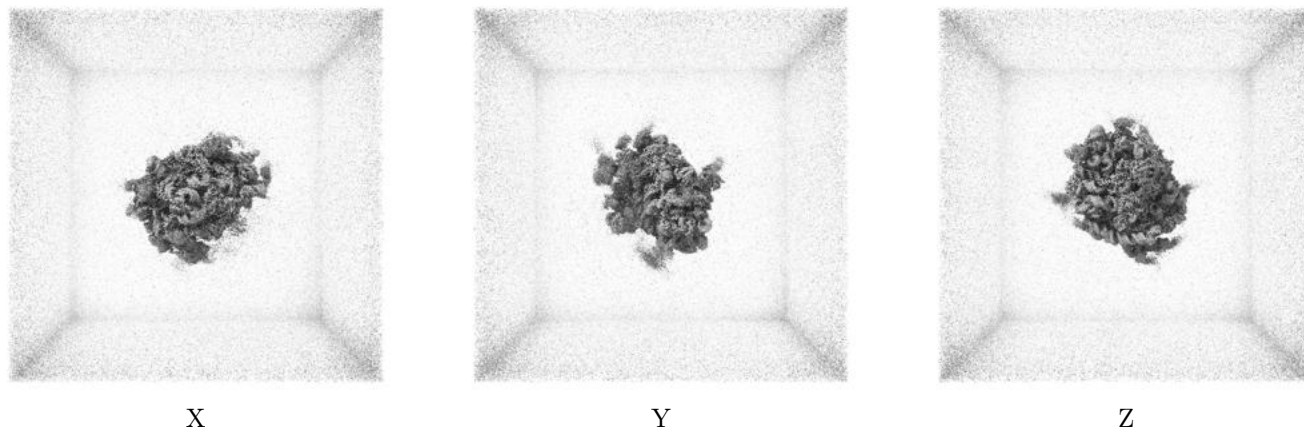
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0134. 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.

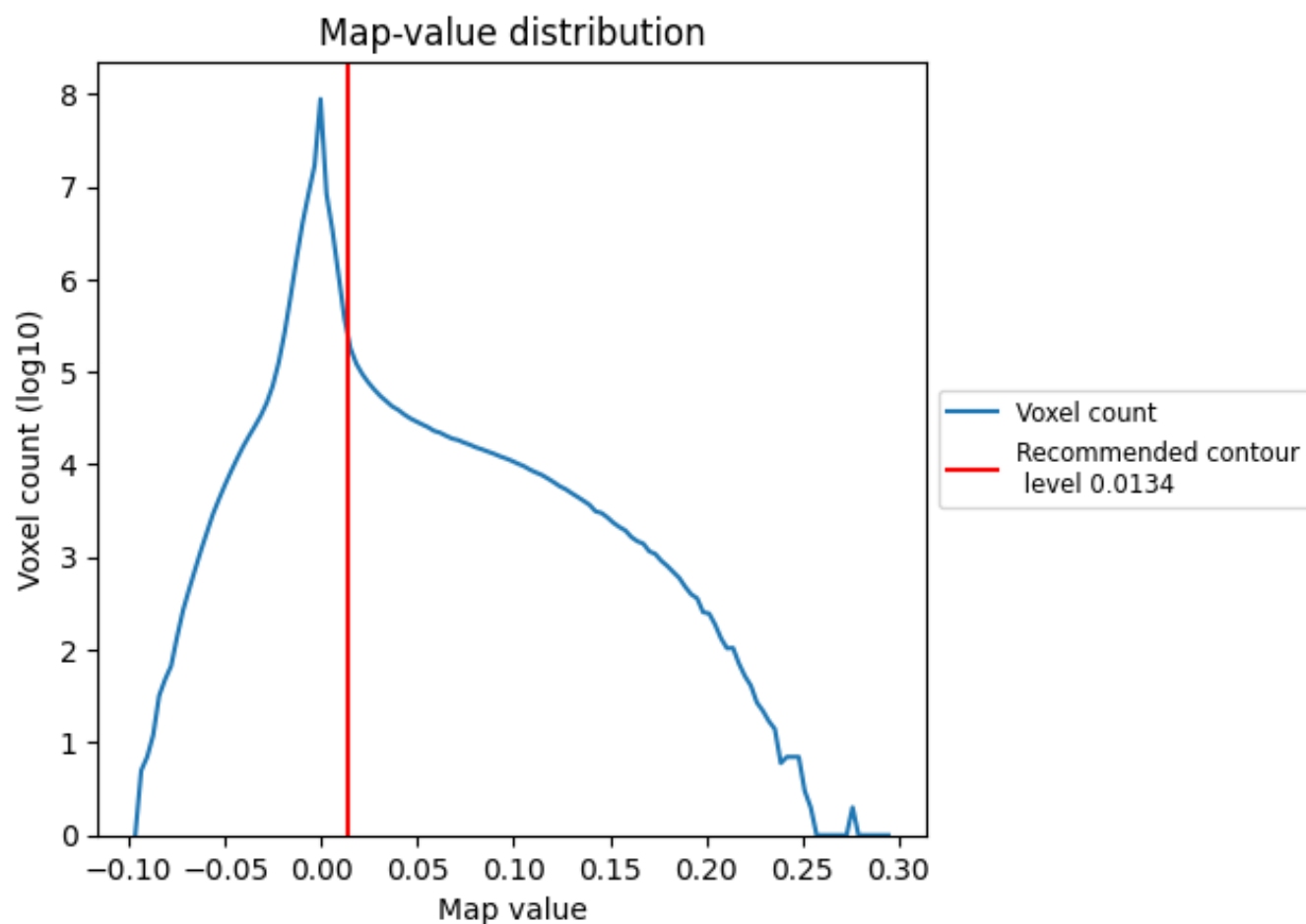
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

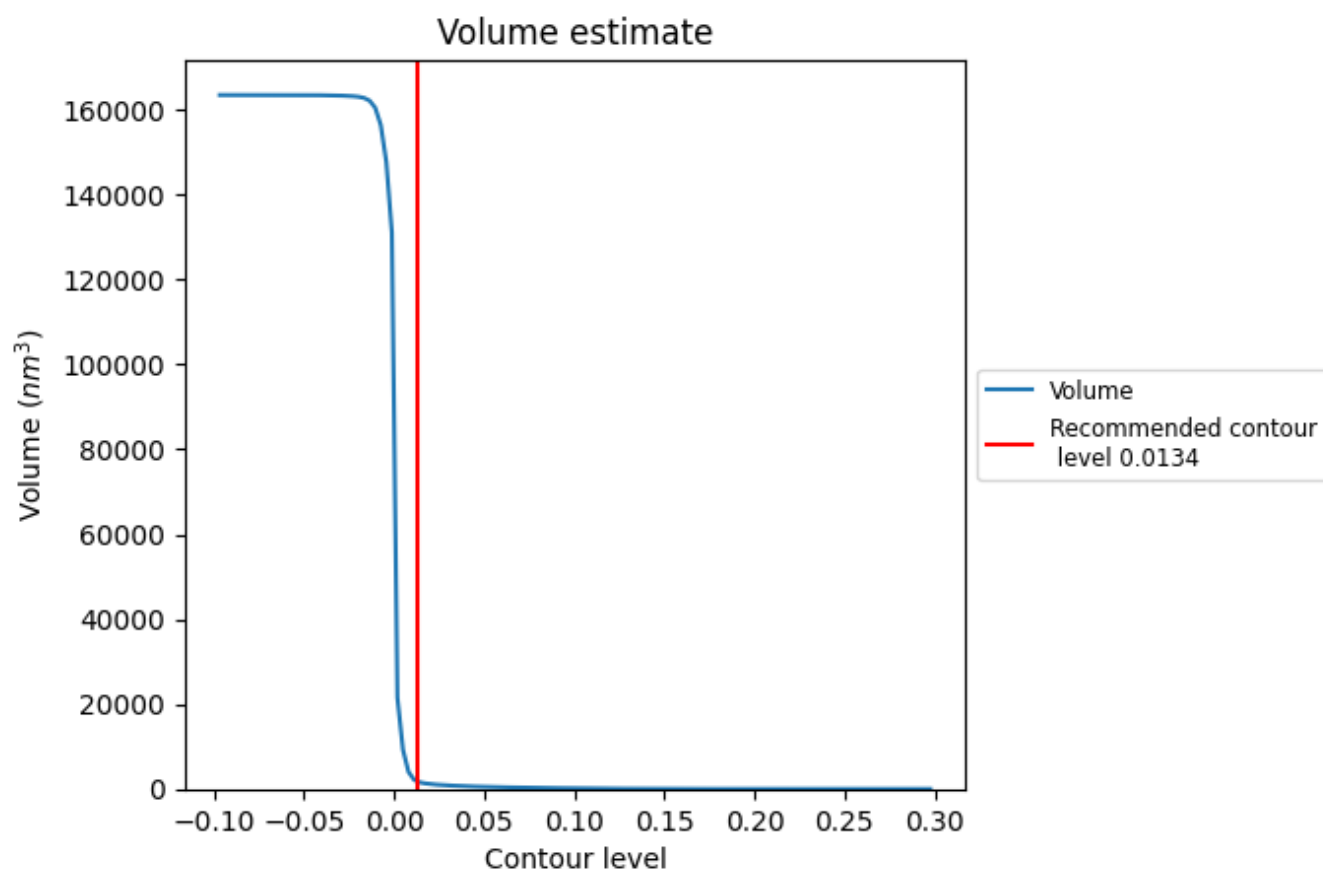
This section contains the results of statistical analysis of the map.

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.

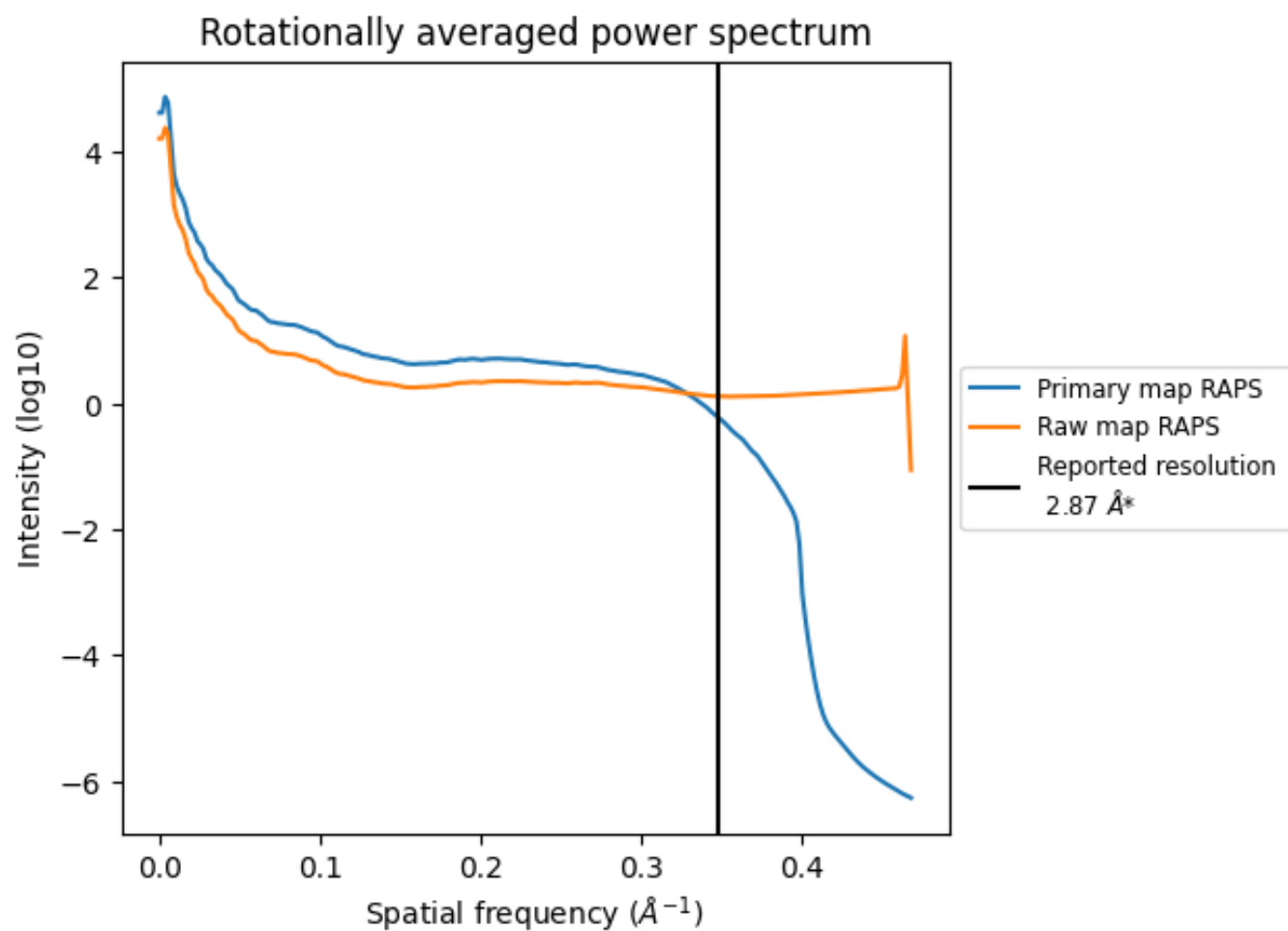
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1739 nm^3 ; this corresponds to an approximate mass of 1571 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

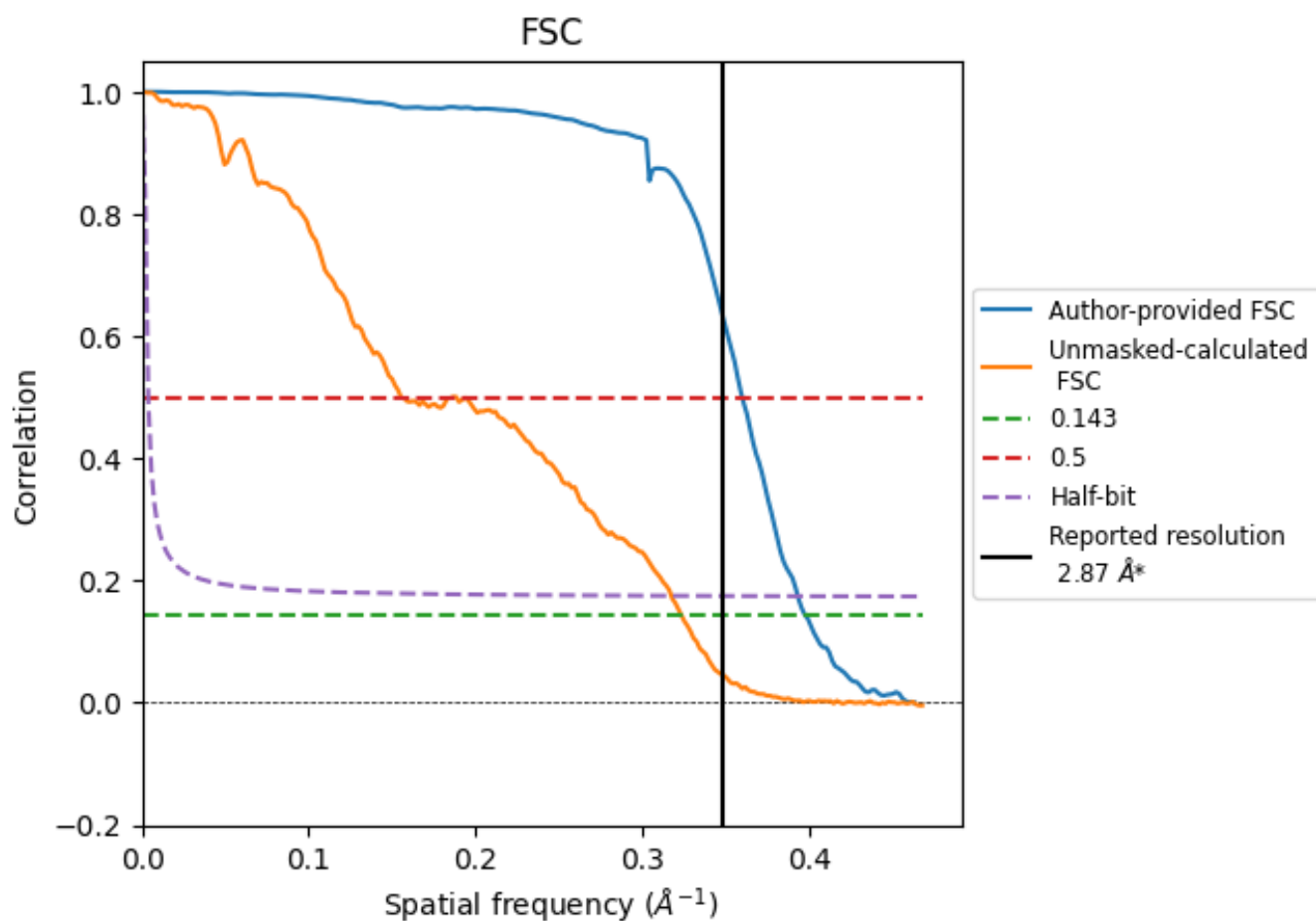


*Reported resolution corresponds to spatial frequency of 0.348 $\text{\AA}^{-1}$

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 0.348 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

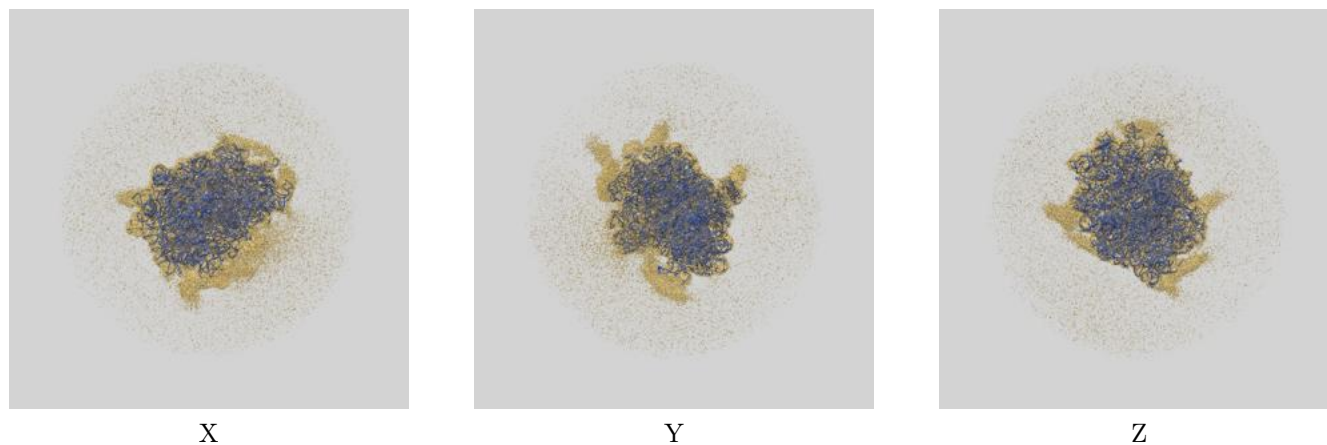
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	2.51	2.78	2.54
Unmasked-calculated*	3.09	6.44	3.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.51 differs from the reported value 2.87 by more than 10 %

9 Map-model fit [i](#)

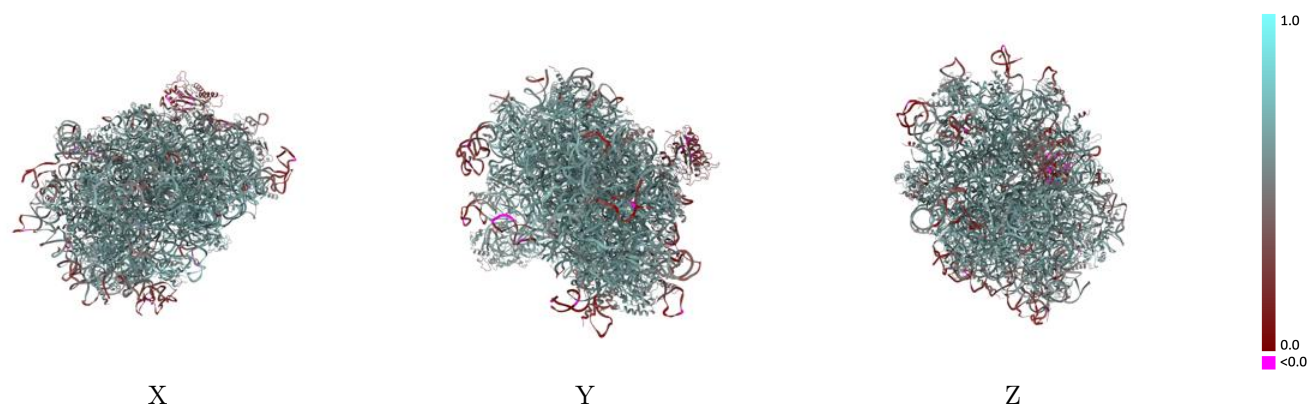
This section contains information regarding the fit between EMDB map EMD-71413 and PDB model 9P9J. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



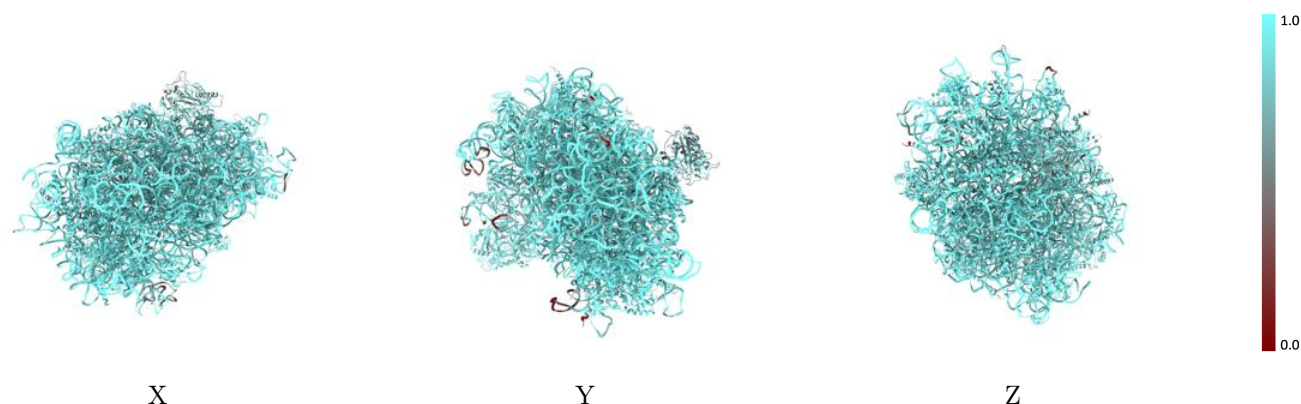
The images above show the 3D surface view of the map at the recommended contour level 0.0134 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



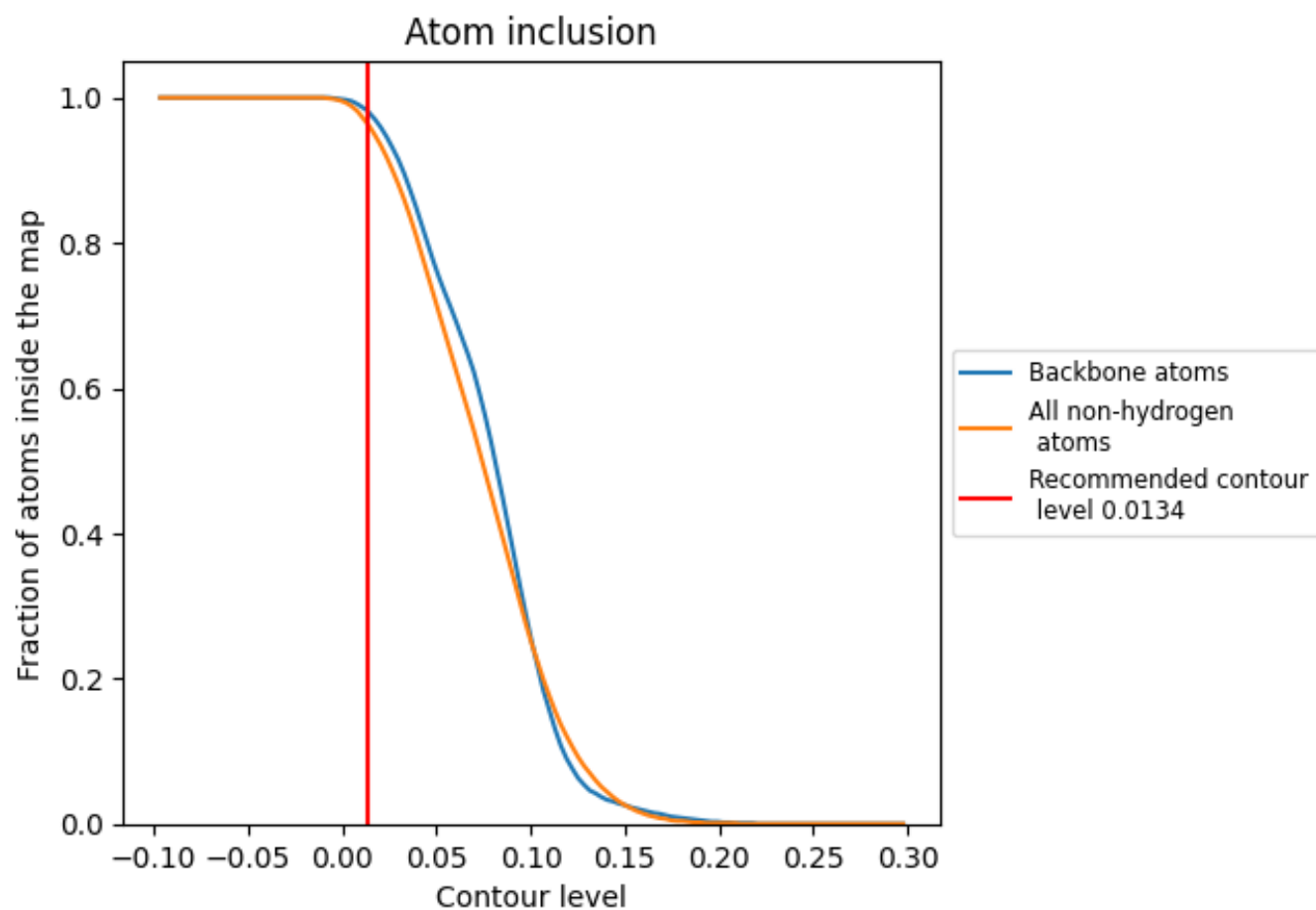
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0134).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.0134) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.5740
CA	 0.6940	 0.2890
L5	 0.9760	 0.5650
L7	 0.9980	 0.6190
L8	 0.9860	 0.5950
LA	 0.9800	 0.6280
LB	 0.9600	 0.6090
LC	 0.9600	 0.6110
LD	 0.9650	 0.5720
LE	 0.9290	 0.5480
LF	 0.9720	 0.6210
LG	 0.9210	 0.5500
LH	 0.9670	 0.6020
LI	 0.9320	 0.6010
LJ	 0.9430	 0.5260
LL	 0.9350	 0.5860
LM	 0.9680	 0.5960
LN	 0.9880	 0.6460
LO	 0.9660	 0.6150
LP	 0.9590	 0.6250
LQ	 0.9720	 0.6360
LR	 0.9680	 0.6080
LS	 0.9840	 0.6350
LT	 0.9480	 0.5960
LU	 0.9290	 0.4910
LV	 0.9680	 0.6160
LX	 0.9380	 0.5950
LY	 0.9580	 0.5980
LZ	 0.9750	 0.5840
La	 0.9780	 0.6320
Lb	 0.9000	 0.5440
Lc	 0.9470	 0.5640
Ld	 0.9480	 0.5930
Le	 0.9750	 0.6330
Lf	 0.9770	 0.6390



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Chain	Atom inclusion	Q-score
Lg	 0.9630	 0.6030
Lh	 0.9410	 0.5920
Li	 0.9500	 0.5890
Lj	 0.9760	 0.6370
Lk	 0.9050	 0.5290
Ll	 0.9620	 0.6160
Lm	 0.9450	 0.6090
Lo	 0.9400	 0.6090
Lp	 0.9610	 0.6150
Lr	 0.9740	 0.6170