



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 06:49 am BST

PDB ID : 9GUL / pdb_00009gul
EMDB ID : EMD-51611
Title : Structure of FLuc-XBP1u+ stalled human 60S ribosome nascent chain complex
Authors : Voisin, T.B.; Pellowe, G.A.; Balchin, D.
Deposited on : 2024-09-19
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

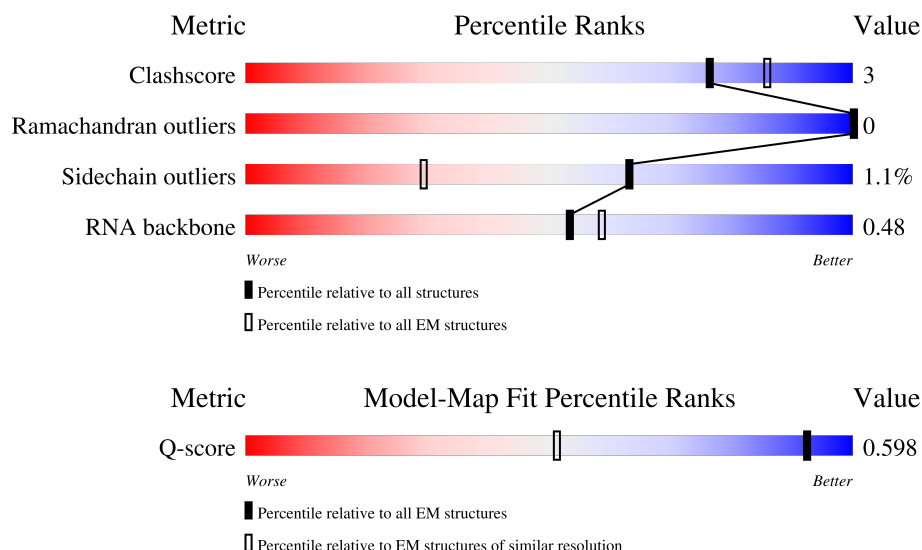
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.20 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.



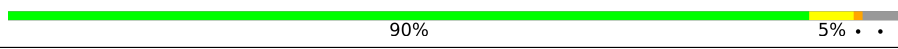
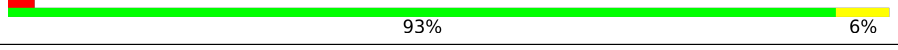
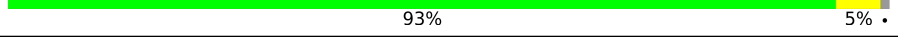
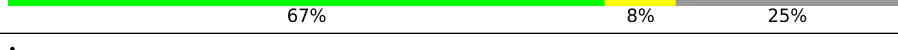
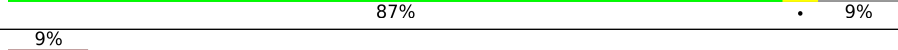
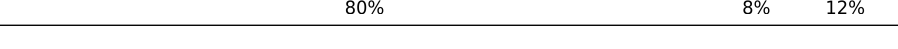
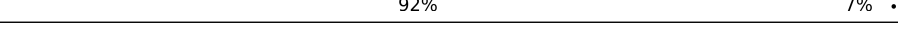
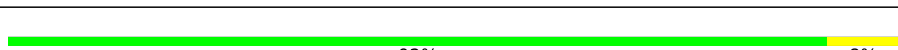
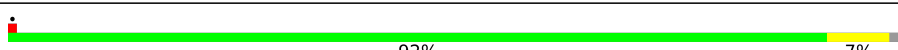
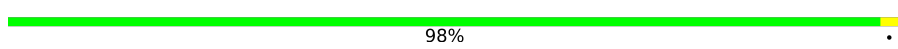
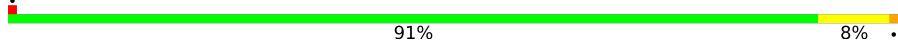
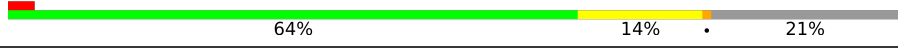
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3184 (1.71 - 2.70)

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	1	269	
2	2	3	
3	L5	5070	

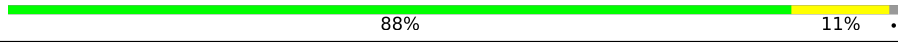
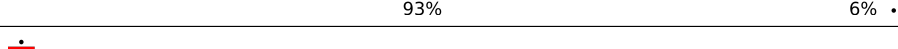
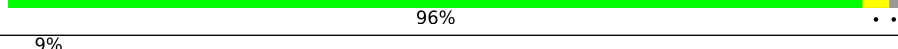
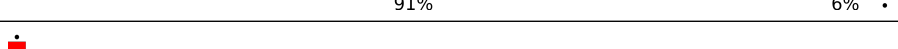
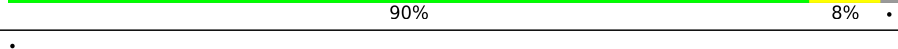
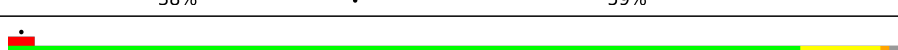
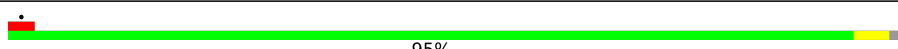
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Mol	Chain	Length	Quality of chain
4	L7	121	
5	L8	157	
6	LA	257	
7	LB	403	
8	LC	427	
9	LD	297	
10	LE	288	
11	LF	248	
12	LG	266	
13	LH	192	
14	LI	214	
15	LJ	178	
16	LL	211	
17	LM	215	
18	LN	204	
19	LO	203	
20	LP	184	
21	LQ	188	
22	LR	196	
23	LS	176	
24	LT	160	
25	LU	128	
26	LV	140	
27	LW	157	
28	LX	156	

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Mol	Chain	Length	Quality of chain
29	LY	145	
30	LZ	136	
31	La	148	
32	Lb	159	
33	Lc	115	
34	Ld	125	
35	Le	135	
36	Lf	110	
37	Lg	117	
38	Lh	123	
39	Li	105	
40	Lj	97	
41	Lk	70	
42	Ll	51	
43	Lm	128	
44	Lo	106	
45	Lp	92	
46	Lr	137	

2 Entry composition [i](#)

There are 49 unique types of molecules in this entry. The entry contains 137414 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 protein called Stalled NC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	30	Total	C	N	O	S	0	0
			229	153	40	33	3		

- Molecule 2 is a RNA chain called P-tRNA CCA tail.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3670	Total	C	N	O	P	0	0
			78733	35093	14393	25578	3669		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L8	156	Total	C	N	O	P	0	0
			3315	1480	585	1095	155		

- Molecule 6 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LA	246	Total	C	N	O	S	0	0
			1887	1183	387	311	6		

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LB	402	Total	C	N	O	S	0	0
			3239	2060	608	557	14		

- Molecule 8 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LC	368	Total	C	N	O	S	0	0
			2928	1841	583	489	15		

- Molecule 9 is a protein called 60S ribosomal protein L5.

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

- Molecule 10 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LE	217	Total	C	N	O	S	0	0
			1746	1125	331	286	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 12 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LG	234	Total	C	N	O	S	0	0
			1881	1199	362	316	4		

- Molecule 13 is a protein called 60S ribosomal protein L9.

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

- Molecule 14 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LI	203	Total	C	N	O	S	0	0
			1642	1041	316	272	13		

- Molecule 15 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LJ	176	Total	C	N	O	S	0	0
			1411	888	263	254	6		

- Molecule 16 is a protein called 60S ribosomal protein L13.

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

- Molecule 17 is a protein called 60S ribosomal protein L14.

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

- Molecule 18 is a protein called 60S ribosomal protein L15.

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

- Molecule 19 is a protein called 60S ribosomal protein L13a.

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

- Molecule 20 is a protein called 60S ribosomal protein L17.

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

- Molecule 21 is a protein called 60S ribosomal protein L18.

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

- Molecule 22 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LR	163	Total	C	N	O	S	0	0
			1358	843	293	213	9		

- Molecule 23 is a protein called 60S ribosomal protein L18a.

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

- Molecule 24 is a protein called 60S ribosomal protein L21.

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

- Molecule 25 is a protein called 60S ribosomal protein L22.

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

- Molecule 26 is a protein called 60S ribosomal protein L23.

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

- Molecule 27 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LW	65	Total	C	N	O	S	0	0
			543	345	105	90	3		

- Molecule 28 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LX	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 29 is a protein called 60S ribosomal protein L26.

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

- Molecule 30 is a protein called 60S ribosomal protein L27.

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

- Molecule 31 is a protein called 60S ribosomal protein L27a.

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

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lb	100	Total	C	N	O	S	0	0
			815	506	179	126	4		

- Molecule 33 is a protein called 60S ribosomal protein L30.

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

- Molecule 34 is a protein called 60S ribosomal protein L31.

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

- Molecule 35 is a protein called 60S ribosomal protein L32.

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

- Molecule 36 is a protein called 60S ribosomal protein L35a.

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

- Molecule 37 is a protein called 60S ribosomal protein L34.

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

- Molecule 38 is a protein called 60S ribosomal protein L35.

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

- Molecule 39 is a protein called 60S ribosomal protein L36.

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

- Molecule 40 is a protein called 60S ribosomal protein L37.

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

- Molecule 41 is a protein called 60S ribosomal protein L38.

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

- Molecule 42 is a protein called 60S ribosomal protein L39.

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

- Molecule 43 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lm	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 44 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lo	105	Total	C	N	O	S	0	0
			863	542	175	140	6		

- Molecule 45 is a protein called 60S ribosomal protein L37a.

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

- Molecule 46 is a protein called 60S ribosomal protein L28.

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

- Molecule 47 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
47	L5	265	Total	Mg	0
			265	265	
47	L7	3	Total	Mg	0
			3	3	
47	L8	5	Total	Mg	0
			5	5	
47	LA	1	Total	Mg	0
			1	1	
47	LI	1	Total	Mg	0
			1	1	
47	LN	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
47	LP	1	Total 1	Mg 1	0
47	LR	1	Total 1	Mg 1	0
47	LS	2	Total 2	Mg 2	0
47	LV	1	Total 1	Mg 1	0
47	Le	1	Total 1	Mg 1	0
47	Lf	1	Total 1	Mg 1	0
47	Lg	1	Total 1	Mg 1	0

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 49 is water.

Mol	Chain	Residues	Atoms		AltConf
49	1	2	Total 2	O 2	0
49	L5	58	Total 58	O 58	0
49	L7	1	Total 1	O 1	0
49	L8	1	Total 1	O 1	0
49	LA	1	Total 1	O 1	0
49	LB	6	Total 6	O 6	0

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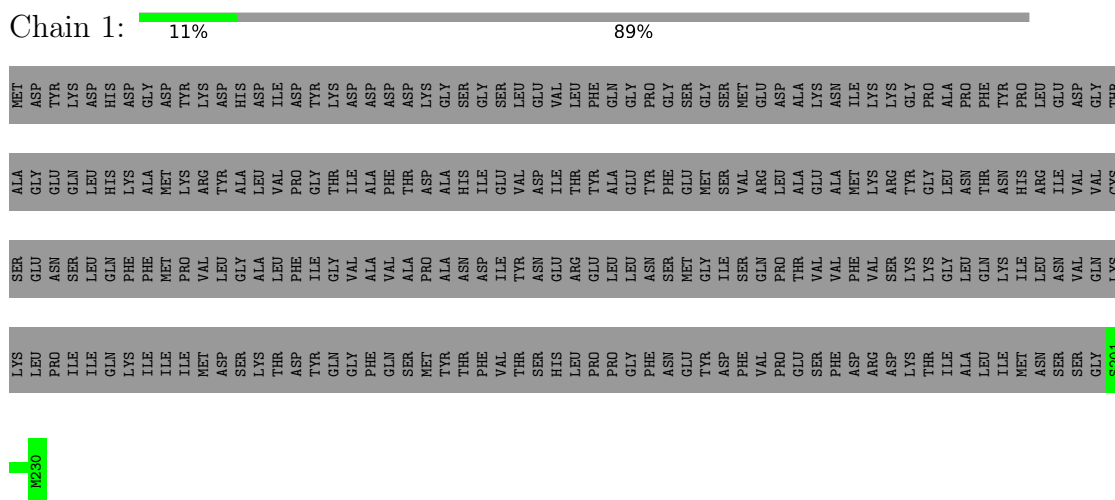
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Mol	Chain	Residues	Atoms		AltConf
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49	LF	4	Total 4	O 4	0
49	LL	2	Total 2	O 2	0
49	LP	2	Total 2	O 2	0
49	LQ	1	Total 1	O 1	0
49	LS	1	Total 1	O 1	0
49	LT	1	Total 1	O 1	0
49	LY	1	Total 1	O 1	0
49	La	1	Total 1	O 1	0
49	Le	1	Total 1	O 1	0
49	Lf	1	Total 1	O 1	0
49	Lg	1	Total 1	O 1	0
49	Ll	2	Total 2	O 2	0
49	Lo	1	Total 1	O 1	0
49	Lp	1	Total 1	O 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.

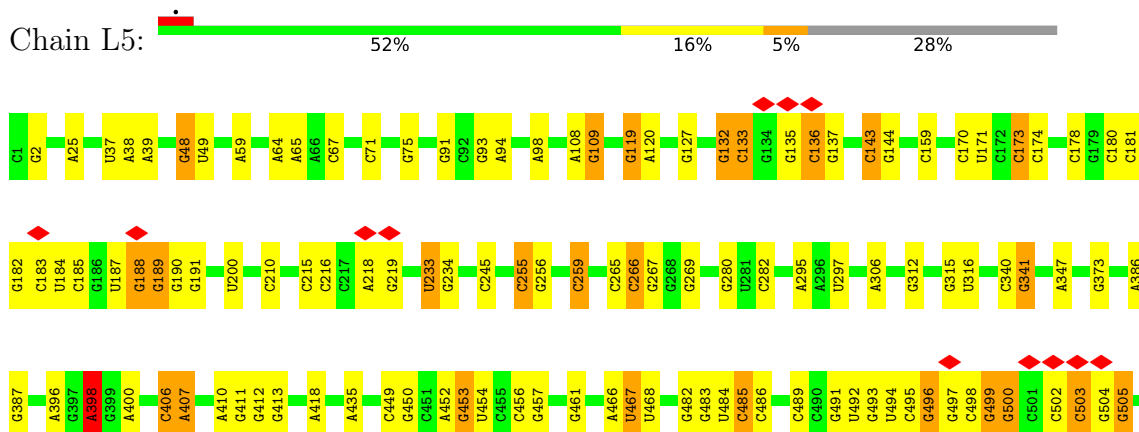
• Molecule 1: Stalled NC



• Molecule 2: P-tRNA CCA tail



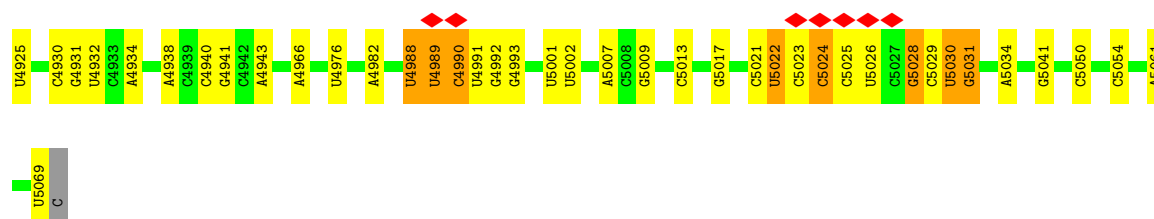
• Molecule 3: 28S rRNA



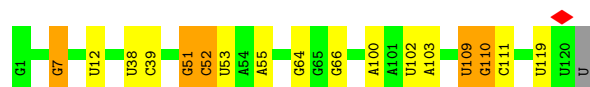
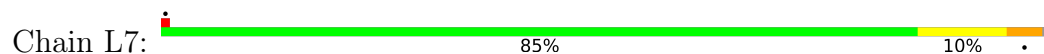




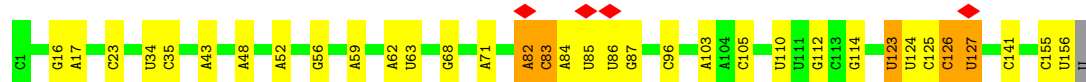
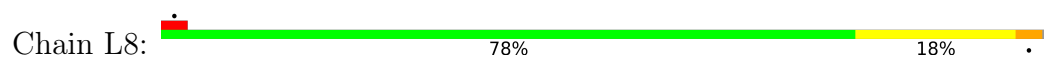




• Molecule 4: 5S rRNA



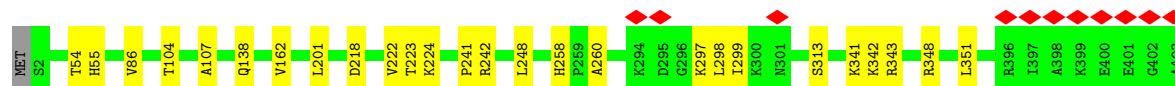
• Molecule 5: 5.8S rRNA



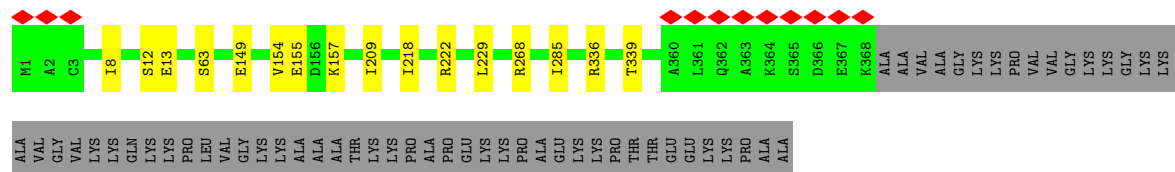
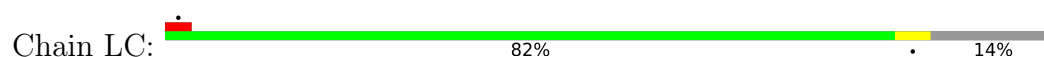
• Molecule 6: 60S ribosomal protein L8



• Molecule 7: 60S ribosomal protein L3



• Molecule 8: Large ribosomal subunit protein uL4

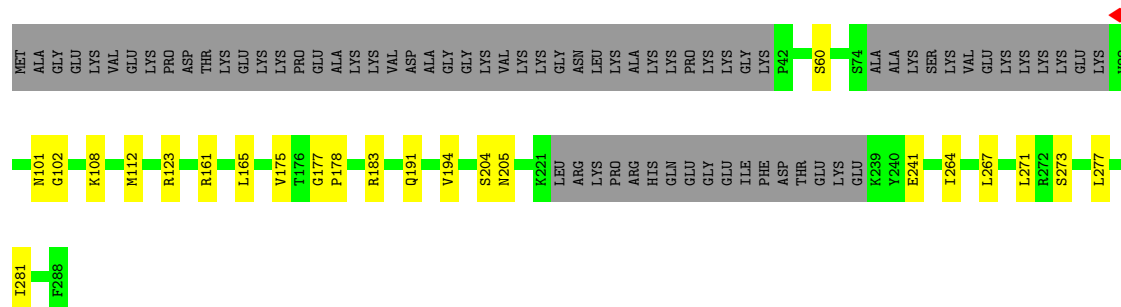


• Molecule 9: 60S ribosomal protein L5

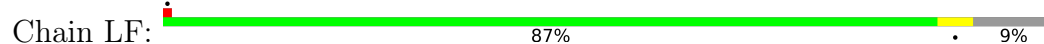




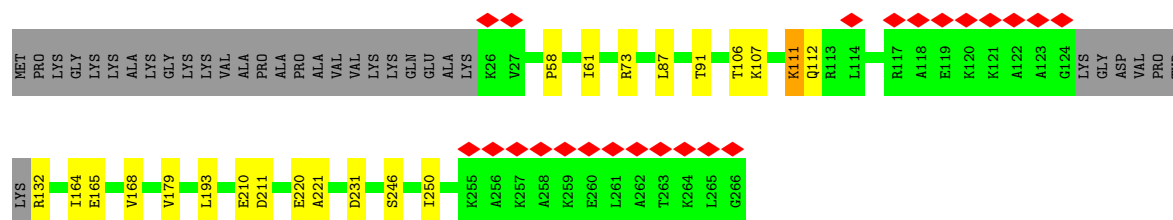
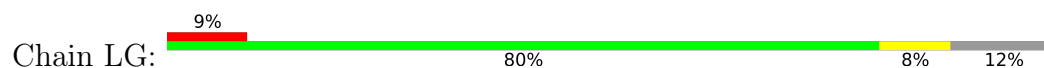
- Molecule 10: Large ribosomal subunit protein eL6



- Molecule 11: Large ribosomal subunit protein uL30



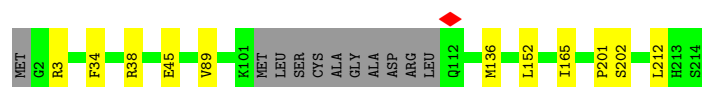
- Molecule 12: 60S ribosomal protein L7a

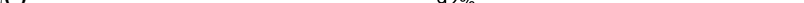


- Molecule 13: 60S ribosomal protein L9



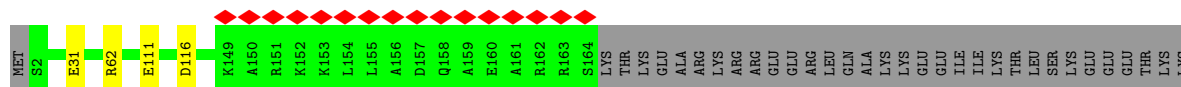
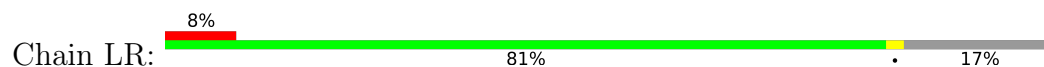
- Molecule 14: Ribosomal protein uL16-like



- Chain LQ:  92% 7%



- Molecule 22: 60S ribosomal protein L19



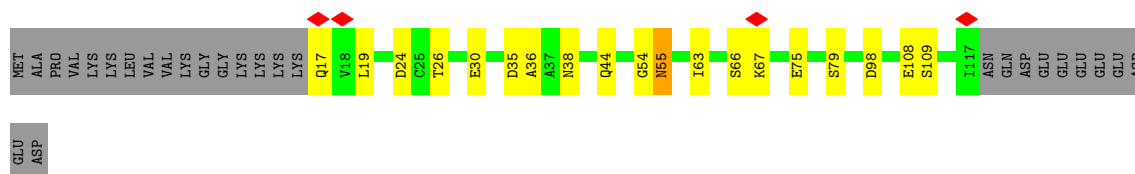
- Molecule 23: 60S ribosomal protein L18a



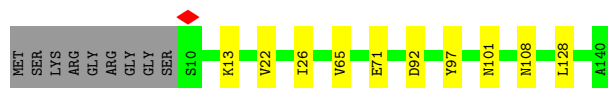
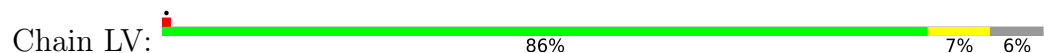
- Molecule 24: 60S ribosomal protein L21



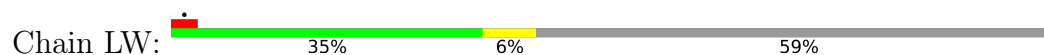
- Molecule 25: 60S ribosomal protein L22



- Molecule 26: 60S ribosomal protein L23



- Molecule 27: 60S ribosomal protein L24



Chain Ld:  80% 6% 14%

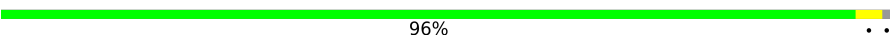


- Molecule 35: 60S ribosomal protein L32

Chain Le:  84% 11% 5%

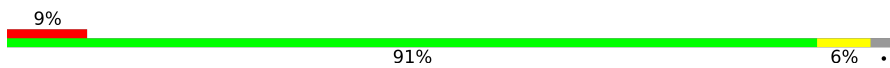


- Molecule 36: 60S ribosomal protein L35a

Chain Lf:  96% ..

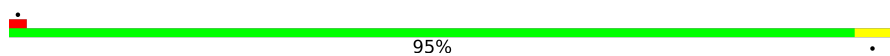


- Molecule 37: 60S ribosomal protein L34

Chain Lg:  9% 91% 6% .



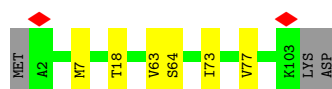
- Molecule 38: 60S ribosomal protein L35

Chain Lh:  95% ..



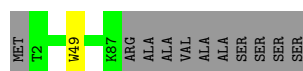
- Molecule 39: 60S ribosomal protein L36

Chain Li:  91% 6% .



- Molecule 40: 60S ribosomal protein L37

Chain Lj:  88% . 11%



- Molecule 41: 60S ribosomal protein L38

Chain Lk:  84% 13% ..



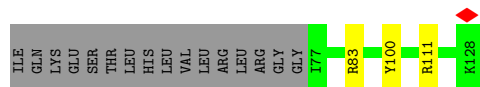
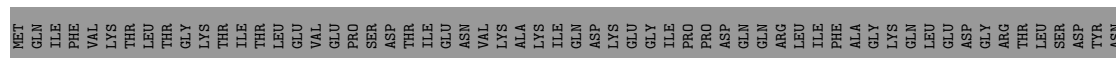
- Molecule 42: 60S ribosomal protein L39

Chain Ll:  90% 8% .



- Molecule 43: Large ribosomal subunit protein eL40

Chain Lm:  38% 59%

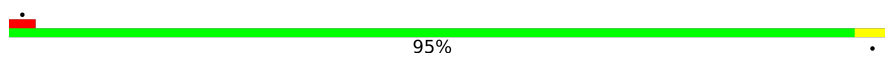


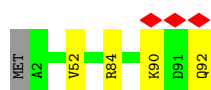
- Molecule 44: 60S ribosomal protein L36a

Chain Lo:  89% 9% ..



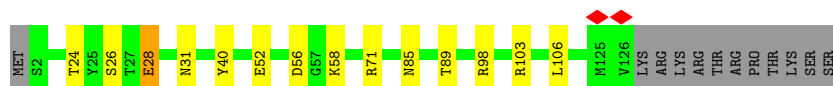
- Molecule 45: 60S ribosomal protein L37a

Chain Lp:  95% ..



- Molecule 46: 60S ribosomal protein L28

Chain Lr:  81% 9% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	788554	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0075	Depositor
Map size ($\text{\AA}$)	471.19998, 471.19998, 471.19998	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.95, 0.95, 0.95	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, JMH, UR3, MG, OMC, B8H, MLZ, 6MZ, A2M, OMG, 5MC, 5MU, PSU, B8T, ZN, A1L3O, 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	1	0.12	0/240	0.28	0/329
2	2	0.17	0/68	0.56	0/103
3	L5	0.20	7/86164 (0.0%)	0.31	0/134393
4	L7	0.18	0/2858	0.28	0/4455
5	L8	0.18	0/3678	0.29	0/5728
6	LA	0.18	0/1925	0.36	0/2581
7	LB	0.17	0/3307	0.37	0/4424
8	LC	0.18	0/2971	0.35	0/3988
9	LD	0.16	0/2428	0.34	0/3252
10	LE	0.16	0/1780	0.34	0/2388
11	LF	0.19	0/1905	0.37	0/2539
12	LG	0.16	0/1912	0.37	0/2571
13	LH	0.18	0/1537	0.39	0/2066
14	LI	0.16	0/1681	0.34	0/2245
15	LJ	0.17	0/1434	0.38	0/1915
16	LL	0.17	0/1732	0.35	0/2315
17	LM	0.18	0/1161	0.37	0/1554
18	LN	0.19	0/1746	0.39	0/2338
19	LO	0.20	0/1682	0.36	0/2250
20	LP	0.19	0/1268	0.36	0/1701
21	LQ	0.18	0/1537	0.36	0/2052
22	LR	0.16	0/1374	0.35	0/1819
23	LS	0.18	0/1493	0.39	0/2003
24	LT	0.18	0/1326	0.37	0/1770
25	LU	0.18	0/839	0.44	0/1126
26	LV	0.16	0/993	0.35	0/1332
27	LW	0.16	0/556	0.34	0/740
28	LX	0.16	0/993	0.36	0/1334
29	LY	0.17	0/1132	0.35	0/1504
30	LZ	0.16	0/1130	0.36	0/1507
31	La	0.18	0/1191	0.36	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.16	0/828	0.37	0/1092
33	Lc	0.17	0/774	0.40	0/1038
34	Ld	0.16	0/903	0.36	0/1216
35	Le	0.18	0/1071	0.35	0/1429
36	Lf	0.17	0/895	0.35	0/1198
37	Lg	0.16	0/916	0.35	0/1220
38	Lh	0.16	0/1023	0.35	0/1351
39	Li	0.14	0/843	0.33	0/1115
40	Lj	0.17	0/720	0.33	0/952
41	Lk	0.16	0/575	0.39	0/761
42	Ll	0.18	0/454	0.30	0/599
43	Lm	0.14	0/425	0.34	0/561
44	Lo	0.17	0/877	0.34	0/1156
45	Lp	0.17	0/718	0.39	0/953
46	Lr	0.17	0/1017	0.35	0/1364
All	All	0.19	7/146080 (0.0%)	0.33	0/215918

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
6	LA	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3785	A2M	O3'-P	5.39	1.61	1.56
3	L5	398	A2M	O3'-P	5.11	1.61	1.56
3	L5	1326	A2M	O3'-P	5.09	1.61	1.56
3	L5	4523	A2M	O3'-P	5.09	1.61	1.56
3	L5	3718	A2M	O3'-P	5.06	1.61	1.56
3	L5	4571	A2M	O3'-P	5.03	1.61	1.56
3	L5	1871	A2M	O3'-P	5.00	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	LA	125	LYS	Peptide

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	1	229	0	218	0	0
2	2	62	0	33	1	0
3	L5	78733	0	39782	414	0
4	L7	2558	0	1296	9	0
5	L8	3315	0	1673	13	0
6	LA	1887	0	1983	9	0
7	LB	3239	0	3376	16	0
8	LC	2928	0	3105	11	0
9	LD	2382	0	2410	11	0
10	LE	1746	0	1901	14	0
11	LF	1870	0	1996	6	0
12	LG	1881	0	2026	14	0
13	LH	1518	0	1601	10	0
14	LI	1642	0	1677	7	0
15	LJ	1411	0	1441	12	0
16	LL	1701	0	1818	12	0
17	LM	1138	0	1204	7	0
18	LN	1701	0	1749	9	0
19	LO	1650	0	1794	10	0
20	LP	1242	0	1269	4	0
21	LQ	1513	0	1628	8	0
22	LR	1358	0	1493	5	0
23	LS	1453	0	1490	2	0
24	LT	1298	0	1366	12	0
25	LU	825	0	850	13	0
26	LV	979	0	1039	8	0
27	LW	543	0	552	7	0
28	LX	976	0	1053	9	0
29	LY	1115	0	1205	8	0
30	LZ	1107	0	1182	11	0
31	La	1162	0	1213	6	0
32	Lb	815	0	881	6	0
33	Lc	764	0	804	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	Ld	888	0	930	6	0
35	Le	1053	0	1147	7	0
36	Lf	876	0	912	1	0
37	Lg	906	0	1002	4	0
38	Lh	1015	0	1148	5	0
39	Li	832	0	917	4	0
40	Lj	705	0	737	1	0
41	Lk	569	0	637	9	0
42	Ll	444	0	483	2	0
43	Lm	430	0	465	2	0
44	Lo	863	0	930	7	0
45	Lp	708	0	756	3	0
46	Lr	1002	0	1068	7	0
47	L5	265	0	0	0	0
47	L7	3	0	0	0	0
47	L8	5	0	0	0	0
47	LA	1	0	0	0	0
47	LI	1	0	0	0	0
47	LN	1	0	0	0	0
47	LP	1	0	0	0	0
47	LR	1	0	0	0	0
47	LS	2	0	0	0	0
47	LV	1	0	0	0	0
47	Le	1	0	0	0	0
47	Lf	1	0	0	0	0
47	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
49	1	2	0	0	0	0
49	L5	58	0	0	5	0
49	L7	1	0	0	0	0
49	L8	1	0	0	0	0
49	LA	1	0	0	0	0
49	LB	6	0	0	0	0
49	LC	5	0	0	1	0
49	LF	4	0	0	1	0
49	LL	2	0	0	1	0
49	LP	2	0	0	0	0
49	LQ	1	0	0	0	0
49	LS	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	LT	1	0	0	0	0
49	LY	1	0	0	0	0
49	La	1	0	0	0	0
49	Le	1	0	0	1	0
49	Lf	1	0	0	0	0
49	Lg	1	0	0	0	0
49	Ll	2	0	0	0	0
49	Lo	1	0	0	0	0
49	Lp	1	0	0	0	0
All	All	137414	0	98240	692	0

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

All (692) 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)
3:L5:4083:5MU:C5	3:L5:4083:5MU:C4	1.79	1.71
3:L5:4296:B8H:C6	3:L5:4296:B8H:N1	1.68	1.56
3:L5:1860:B8H:C6	3:L5:1860:B8H:N1	1.68	1.53
3:L5:3762:B8H:C6	3:L5:3762:B8H:N1	1.69	1.51
3:L5:3762:B8H:C4	3:L5:3762:B8H:C5	1.83	1.51
3:L5:4296:B8H:C4	3:L5:4296:B8H:C5	1.82	1.51
3:L5:1860:B8H:C5	3:L5:1860:B8H:C4	1.82	1.50
3:L5:2304:U:O2'	3:L5:2305:U:OP2	1.78	1.02
3:L5:745:G:O2'	3:L5:746:A:OP1	1.79	1.00
3:L5:915:A:N7	3:L5:918:G:N2	2.11	0.97
3:L5:3754:G:O6	3:L5:3770:U:O2	1.83	0.97
3:L5:4555:U:O2'	3:L5:4556:U:OP1	1.82	0.97
3:L5:5022:U:O2'	3:L5:5024:C:OP2	1.83	0.97
3:L5:3841:C:O2'	49:L5:5401:HOH:O	1.85	0.93
3:L5:515:C:N4	3:L5:647:G:N3	2.19	0.91
3:L5:3614:G:O2'	3:L5:3615:G:OP1	1.90	0.90
3:L5:2440:U:O2'	3:L5:2441:C:OP1	1.90	0.89
3:L5:400:A:O2'	49:L5:5402:HOH:O	1.89	0.89
3:L5:746:A:O2'	3:L5:747:A:OP1	1.91	0.89
25:LU:108:GLU:N	25:LU:108:GLU:OE1	2.06	0.88
3:L5:3709:U:O2'	3:L5:3710:G:OP2	1.92	0.88
25:LU:75:GLU:N	25:LU:75:GLU:OE1	2.08	0.87
3:L5:751:G:O6	3:L5:912:G:N2	2.06	0.87
3:L5:500:G:O2'	3:L5:505:G:OP2	1.91	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:500:G:OP2	3:L5:503:C:O2'	1.92	0.87
30:LZ:30:ASP:O	30:LZ:39:SER:OG	1.92	0.86
3:L5:1408:G:O2'	3:L5:1411:C:O2	1.93	0.85
21:LQ:94:GLU:OE2	21:LQ:94:GLU:N	2.08	0.85
3:L5:499:G:O2'	3:L5:500:G:OP1	1.95	0.85
20:LP:9:GLU:N	20:LP:9:GLU:OE2	2.10	0.85
41:Lk:6:GLU:N	41:Lk:6:GLU:OE1	2.08	0.85
6:LA:109:GLU:OE1	6:LA:109:GLU:N	2.10	0.85
3:L5:2601:A:N6	3:L5:2744:A:OP2	2.11	0.84
3:L5:1762:C:N4	3:L5:1772:C:O2	2.12	0.83
3:L5:2487:G:N2	3:L5:2493:G:N7	2.27	0.83
3:L5:2019:C:O2'	3:L5:2020:U:OP1	1.98	0.82
3:L5:453:G:N2	3:L5:1293:G:O6	2.13	0.82
3:L5:1860:B8H:N1	3:L5:1860:B8H:C5	2.36	0.82
3:L5:967:C:O2'	3:L5:969:C:OP2	1.98	0.81
3:L5:3758:U:O2	3:L5:3766:A:N6	2.13	0.81
3:L5:2894:A:O2'	3:L5:2895:A:OP1	1.97	0.80
3:L5:2760:G:O2'	3:L5:2761:U:OP2	1.98	0.80
3:L5:1974:U:O2	3:L5:2002:A:N6	2.14	0.80
33:Lc:13:SER:O	33:Lc:16:SER:OG	2.00	0.80
41:Lk:68:GLU:N	41:Lk:68:GLU:OE1	2.15	0.80
3:L5:963:G:N2	3:L5:965:G:O2'	2.12	0.80
3:L5:181:C:N4	3:L5:255:C:N3	2.31	0.79
3:L5:1697:G:N2	3:L5:2084:C:OP1	2.14	0.79
24:LT:137:GLU:OE1	24:LT:137:GLU:N	2.14	0.79
3:L5:4252:C:OP2	3:L5:4253:A:O2'	1.99	0.79
29:LY:47:MET:HE1	29:LY:118:ILE:HD11	1.64	0.79
3:L5:2112:G:O2'	3:L5:2250:C:N4	2.16	0.79
3:L5:2484:A:N6	3:L5:2495:U:O2	2.15	0.79
3:L5:3762:B8H:N1	3:L5:3762:B8H:C5	2.38	0.79
3:L5:2754:G:O2'	3:L5:2755:A:O5'	2.00	0.79
3:L5:3712:A:O2'	3:L5:3713:U:O4'	1.99	0.79
3:L5:989:U:O2'	3:L5:990:C:O4'	2.01	0.79
3:L5:496:G:N2	3:L5:658:C:O2	2.15	0.78
3:L5:4734:A:O2'	3:L5:4735:G:OP2	2.00	0.78
46:Lr:26:SER:OG	46:Lr:28:GLU:OE2	2.00	0.78
3:L5:188:G:O2'	3:L5:190:G:OP2	2.02	0.78
33:Lc:30:GLY:O	33:Lc:34:THR:HG23	1.84	0.77
3:L5:755:C:O2'	3:L5:756:G:N2	2.18	0.77
5:L8:126:C:O2'	5:L8:127:U:OP1	2.00	0.77
3:L5:282:C:O2'	49:L5:5403:HOH:O	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:755:C:O2'	3:L5:756:G:OP2	2.02	0.75
3:L5:1971:C:OP2	3:L5:2016:C:N4	2.20	0.75
5:L8:71:A:O2'	5:L8:83:C:N4	2.19	0.74
3:L5:188:G:N2	3:L5:191:G:O6	2.20	0.74
29:LY:37:GLU:OE1	29:LY:37:GLU:N	2.18	0.74
11:LF:234:GLY:O	49:LF:301:HOH:O	2.05	0.74
3:L5:182:G:N2	3:L5:255:C:O2	2.21	0.73
3:L5:1518:A:OP1	31:La:27:LYS:NZ	2.19	0.73
3:L5:915:A:O2'	3:L5:916:C:OP2	2.06	0.73
3:L5:1100:U:O3'	3:L5:1167:C:N4	2.21	0.73
27:LW:56:ARG:NH2	27:LW:61:LYS:O	2.22	0.72
3:L5:992:C:N4	3:L5:994:G:N7	2.38	0.71
3:L5:4095:G:N2	3:L5:4114:C:O4'	2.23	0.71
3:L5:2546:G:O2'	3:L5:2547:G:O5'	2.03	0.71
3:L5:1364:U:OP2	16:LL:36:ARG:NH2	2.24	0.70
3:L5:3947:A:N6	3:L5:4068:U:O2	2.24	0.70
3:L5:1360:G:OP1	49:L5:5405:HOH:O	2.09	0.70
3:L5:1860:B8H:C6	3:L5:1860:B8H:C2	2.68	0.70
3:L5:4600:G:O2'	3:L5:4601:U:OP2	2.09	0.70
3:L5:3614:G:HO2'	3:L5:3615:G:P	2.14	0.70
3:L5:2754:G:HO2'	3:L5:2755:A:P	2.15	0.69
3:L5:3951:G:N2	3:L5:4061:G:O6	2.25	0.69
3:L5:3754:G:O6	3:L5:3770:U:C2	2.46	0.69
6:LA:142:GLU:OE1	6:LA:142:GLU:N	2.23	0.69
3:L5:2562:G:N2	3:L5:2565:A:OP2	2.26	0.69
26:LV:71:GLU:N	26:LV:71:GLU:OE2	2.25	0.69
3:L5:3762:B8H:C6	3:L5:3762:B8H:C2	2.69	0.68
3:L5:1445:U:O2'	3:L5:1446:C:OP1	2.12	0.68
42:Ll:25:GLN:OE1	42:Ll:28:ARG:NH2	2.26	0.68
29:LY:88:GLU:OE2	29:LY:88:GLU:N	2.21	0.68
3:L5:4296:B8H:C6	3:L5:4296:B8H:C2	2.68	0.68
25:LU:67:LYS:HE2	25:LU:67:LYS:HA	1.76	0.68
16:LL:61:CYS:O	49:LL:301:HOH:O	2.12	0.67
16:LL:126:LEU:N	16:LL:138:ASP:OD2	2.26	0.67
8:LC:63:SER:O	49:LC:501:HOH:O	2.12	0.67
3:L5:3765:G:OP1	3:L5:3810:C:N4	2.27	0.67
3:L5:4988:U:O2'	3:L5:4989:U:OP2	2.10	0.67
3:L5:1197:C:O2'	3:L5:1198:G:OP1	2.11	0.67
3:L5:3722:G:H2'	3:L5:3723:A2M:H8	1.77	0.66
8:LC:13:GLU:OE2	8:LC:157:LYS:NZ	2.19	0.66
15:LJ:112:HIS:ND1	15:LJ:117:ILE:HD11	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LU:35:ASP:OD1	25:LU:36:ALA:N	2.28	0.66
3:L5:3717:A:OP2	3:L5:3735:G:N2	2.28	0.66
17:LM:39:ASP:OD1	17:LM:40:GLY:N	2.29	0.66
3:L5:1480:C:O2'	3:L5:1482:G:OP2	2.12	0.66
3:L5:1971:C:N4	3:L5:2001:G:O5'	2.29	0.66
3:L5:1860:B8H:C6	3:L5:1860:B8H:CN1	2.72	0.65
33:Lc:9:LYS:N	33:Lc:12:GLU:OE1	2.29	0.65
18:LN:124:ASP:OD1	18:LN:125:SER:N	2.30	0.65
46:Lr:56:ASP:OD2	46:Lr:58:LYS:NZ	2.30	0.65
7:LB:54:THR:HG22	7:LB:55:HIS:H	1.60	0.65
3:L5:5029:C:HO2'	3:L5:5030:U:H6	1.42	0.64
30:LZ:123:LYS:O	30:LZ:124:THR:OG1	2.14	0.64
3:L5:1269:G:O2'	3:L5:1440:U:O2'	2.04	0.64
15:LJ:112:HIS:CE1	15:LJ:117:ILE:HD11	2.33	0.64
33:Lc:38:ILE:HD11	33:Lc:46:VAL:HG21	1.79	0.64
3:L5:184:U:O2'	3:L5:189:G:O4'	2.16	0.64
3:L5:1273:G:H2'	3:L5:1274:A:H5'	1.77	0.64
3:L5:4894:A:H3'	3:L5:4895:C:H5'	1.78	0.64
3:L5:4296:B8H:C6	3:L5:4296:B8H:CN1	2.71	0.64
41:Lk:54:GLU:OE2	41:Lk:54:GLU:N	2.28	0.63
3:L5:744:G:O2'	3:L5:745:G:N3	2.29	0.63
3:L5:4699:U:OP2	43:Lm:111:ARG:NH1	2.31	0.63
3:L5:215:C:OP2	3:L5:219:G:N2	2.32	0.63
3:L5:2546:G:HO2'	3:L5:2547:G:P	2.20	0.63
27:LW:19:ARG:NH1	27:LW:37:GLU:OE2	2.31	0.63
3:L5:911:U:H2'	3:L5:912:G:C8	2.34	0.63
10:LE:101:ASN:OD1	10:LE:102:GLY:N	2.31	0.62
3:L5:1273:G:N7	32:Lb:117:ARG:NE	2.44	0.62
44:Lo:102:GLN:OE1	44:Lo:102:GLN:N	2.33	0.62
3:L5:4393:G:O4'	3:L5:4447:5MC:HM53	1.99	0.62
4:L7:12:U:O3'	4:L7:109:U:O2'	2.18	0.62
3:L5:3946:G:O2'	3:L5:3947:A:O5'	2.15	0.62
7:LB:218:ASP:OD2	7:LB:348:ARG:NH1	2.32	0.62
3:L5:746:A:HO2'	3:L5:747:A:P	2.17	0.62
3:L5:1700:G:H2'	3:L5:1704:C:H42	1.65	0.62
3:L5:2904:U:O4	3:L5:3592:G:N2	2.33	0.62
3:L5:3762:B8H:C6	3:L5:3762:B8H:CN1	2.72	0.61
3:L5:119:G:O4'	12:LG:132:ARG:NH2	2.34	0.61
3:L5:1703:C:O2'	3:L5:1704:C:O4'	2.14	0.60
16:LL:171:GLU:N	16:LL:171:GLU:OE1	2.33	0.60
3:L5:2755:A:OP2	30:LZ:51:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4457:U:O2'	49:L5:5404:HOH:O	2.04	0.60
4:L7:55:A:O2'	15:LJ:151:ILE:O	2.13	0.60
3:L5:2478:C:O2'	3:L5:2591:A:O2'	2.03	0.60
15:LJ:118:LYS:HE2	15:LJ:118:LYS:HA	1.84	0.60
41:Lk:23:VAL:CG1	41:Lk:66:VAL:HG22	2.31	0.60
3:L5:749:G:H3'	3:L5:750:U:H5''	1.82	0.60
3:L5:499:G:HO2'	3:L5:500:G:P	2.23	0.60
3:L5:1273:G:O6	32:Lb:117:ARG:NH2	2.33	0.60
7:LB:241:PRO:O	7:LB:248:LEU:HD22	2.02	0.59
3:L5:295:A:OP2	44:Lo:39:ARG:NH1	2.35	0.59
9:LD:92:LEU:O	9:LD:93:THR:HG22	2.02	0.59
3:L5:4597:UR3:H6	3:L5:4597:UR3:O5'	2.03	0.59
3:L5:3597:G:O2'	3:L5:3598:C:OP2	2.15	0.58
3:L5:4646:U:OP2	22:LR:62:ARG:NH2	2.36	0.58
17:LM:96:GLU:OE2	17:LM:100:ARG:NH2	2.35	0.58
3:L5:2255:C:OP1	11:LF:24:ASN:N	2.37	0.58
3:L5:3689:G:O2'	3:L5:3818:U:OP2	2.22	0.58
3:L5:1756:U:O2'	3:L5:1758:G:OP2	2.16	0.58
3:L5:3709:U:HO2'	3:L5:3710:G:P	2.23	0.57
3:L5:1976:G:OP2	3:L5:2002:A:O2'	2.22	0.57
25:LU:44:GLN:C	25:LU:44:GLN:OE1	2.46	0.57
46:Lr:85:ASN:O	46:Lr:89:THR:HG23	2.03	0.57
13:LH:57:VAL:CG2	13:LH:70:VAL:HG13	2.34	0.57
3:L5:4371:G:O2'	3:L5:4372:U:O4'	2.23	0.57
7:LB:54:THR:HG22	7:LB:55:HIS:N	2.20	0.57
24:LT:114:GLN:OE1	24:LT:115:LYS:N	2.38	0.57
41:Lk:10:ASP:N	41:Lk:10:ASP:OD1	2.35	0.57
13:LH:14:GLU:O	13:LH:14:GLU:OE2	2.23	0.57
3:L5:4895:C:O2'	3:L5:4896:G:OP1	2.22	0.56
31:La:72:THR:HG22	31:La:110:LYS:HB3	1.86	0.56
41:Lk:30:ASP:OD2	41:Lk:30:ASP:N	2.37	0.56
3:L5:1971:C:N4	3:L5:2001:G:O4'	2.36	0.56
3:L5:4600:G:O2'	3:L5:4601:U:P	2.63	0.56
3:L5:4872:2MG:HM21	19:LO:201:LEU:C	2.30	0.56
12:LG:58:PRO:HG2	12:LG:61:ILE:HD12	1.85	0.56
3:L5:3711:A:O2'	3:L5:3712:A:O5'	2.24	0.56
3:L5:132:G:N2	3:L5:133:C:O2'	2.39	0.56
3:L5:2104:G:O2'	3:L5:2105:A:O4'	2.16	0.56
3:L5:178:C:N3	3:L5:259:C:N4	2.54	0.56
16:LL:108:GLU:OE2	39:Li:18:THR:HG22	2.05	0.56
12:LG:220:GLU:OE1	12:LG:221:ALA:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4076:G:OP1	12:LG:73:ARG:NH1	2.32	0.55
3:L5:4377:G:O6	31:La:42:ARG:NH2	2.38	0.55
3:L5:966:A:OP2	3:L5:2092:G:N2	2.30	0.55
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.88	0.55
3:L5:751:G:O6	3:L5:912:G:C2	2.59	0.55
10:LE:264:ILE:HD11	10:LE:267:LEU:HD22	1.87	0.55
22:LR:111:GLU:C	22:LR:111:GLU:OE2	2.50	0.55
4:L7:51:G:O2'	4:L7:52:C:OP1	2.23	0.55
3:L5:709:C:OP1	36:Lf:89:ARG:NH2	2.39	0.55
3:L5:1633:G:H5'	3:L5:1634:A:OP1	2.06	0.55
29:LY:127:GLN:HA	29:LY:127:GLN:OE1	2.06	0.55
5:L8:126:C:HO2'	5:L8:127:U:P	2.29	0.55
3:L5:729:2MG:N2	23:LS:66:GLN:O	2.39	0.54
3:L5:1238:A:OP2	10:LE:60:SER:OG	2.23	0.54
3:L5:744:G:O2'	3:L5:745:G:H5''	2.08	0.54
3:L5:3718:A2M:H2	3:L5:3934:G:O4'	2.07	0.54
19:LO:5:GLN:OE1	19:LO:5:GLN:N	2.38	0.54
27:LW:47:ARG:CZ	27:LW:47:ARG:HB2	2.38	0.54
26:LV:92:ASP:OD2	26:LV:92:ASP:C	2.51	0.54
3:L5:1182:C:H3'	3:L5:1183:C:C5'	2.38	0.54
13:LH:17:ASP:OD1	13:LH:17:ASP:C	2.50	0.54
38:Lh:23:ASP:OD1	38:Lh:23:ASP:N	2.37	0.54
3:L5:2779:C:O2'	5:L8:112:G:OP1	2.13	0.54
30:LZ:92:ASP:O	30:LZ:96:VAL:HG22	2.07	0.54
35:Le:108:ARG:O	35:Le:112:VAL:HG13	2.08	0.54
3:L5:923:C:O2'	3:L5:924:C:OP1	2.24	0.54
3:L5:4982:A:OP1	20:LP:74:LYS:NZ	2.36	0.53
3:L5:1860:B8H:C5	3:L5:1860:B8H:C2	2.86	0.53
8:LC:285:ILE:HD12	21:LQ:125:GLN:HE22	1.74	0.53
3:L5:1974:U:O2'	3:L5:1994:C:N4	2.42	0.53
3:L5:5028:G:H2'	3:L5:5029:C:C6	2.44	0.53
3:L5:482:G:O2'	3:L5:483:G:N7	2.40	0.53
45:Lp:90:LYS:O	45:Lp:92:GLN:NE2	2.41	0.53
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.39	0.53
28:LX:118:ASP:OD1	28:LX:118:ASP:O	2.26	0.53
3:L5:233:U:H2'	3:L5:233:U:O2	2.09	0.52
5:L8:126:C:O2'	5:L8:127:U:P	2.67	0.52
7:LB:223:THR:HG22	7:LB:224:LYS:N	2.24	0.52
20:LP:115:GLU:OE2	20:LP:151:THR:OG1	2.26	0.52
30:LZ:120:GLU:C	30:LZ:120:GLU:OE1	2.51	0.52
35:Le:113:GLU:OE1	35:Le:113:GLU:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3641:U:OP2	3:L5:3646:A:N6	2.40	0.52
3:L5:749:G:C3'	3:L5:750:U:H5''	2.39	0.52
3:L5:3762:B8H:C5	3:L5:3762:B8H:C2	2.87	0.52
6:LA:137:ILE:HD11	6:LA:149:LYS:HB2	1.91	0.52
10:LE:177:GLY:O	10:LE:178:PRO:C	2.51	0.52
24:LT:118:GLU:OE1	24:LT:118:GLU:C	2.53	0.52
3:L5:2484:A:N7	3:L5:2486:G:N2	2.56	0.52
3:L5:3605:C:O2'	3:L5:3606:U:OP1	2.22	0.52
3:L5:406:C:HO2'	3:L5:407:A:P	2.31	0.52
3:L5:2258:C:O2'	3:L5:2259:G:O5'	2.28	0.52
3:L5:4296:B8H:C5	3:L5:4296:B8H:C2	2.86	0.52
6:LA:36:GLU:OE1	6:LA:163:ARG:NH1	2.42	0.52
3:L5:923:C:O2'	3:L5:924:C:P	2.68	0.51
44:Lo:24:THR:HG22	44:Lo:25:GLN:N	2.25	0.51
14:LI:38:ARG:NH2	14:LI:45:GLU:OE2	2.39	0.51
3:L5:1912:G:H21	19:LO:87:MET:HE2	1.75	0.51
3:L5:4678:G:O2'	3:L5:4679:G:OP1	2.24	0.51
3:L5:752:G:O2'	3:L5:753:C:O5'	2.25	0.51
19:LO:173:GLN:OE1	19:LO:173:GLN:O	2.28	0.51
3:L5:1553:A:N6	3:L5:1574:G:H1'	2.26	0.51
3:L5:3753:G:H22	3:L5:3772:U:H1'	1.76	0.51
3:L5:911:U:O2'	3:L5:912:G:OP1	2.27	0.51
10:LE:241:GLU:HA	10:LE:241:GLU:OE2	2.10	0.51
3:L5:173:C:H2'	3:L5:174:C:C1'	2.41	0.51
3:L5:2706:G:HO2'	3:L5:2708:U:H3	1.55	0.51
3:L5:4139:G:O2'	3:L5:4146:G:N2	2.44	0.51
8:LC:12:SER:OG	8:LC:13:GLU:OE1	2.29	0.51
3:L5:435:A:O2'	35:Le:26:ASP:OD2	2.23	0.51
3:L5:468:U:N3	3:L5:686:A:N1	2.59	0.51
3:L5:3605:C:HO2'	3:L5:3606:U:P	2.33	0.51
3:L5:2096:G:O2'	3:L5:2097:U:OP2	2.23	0.51
3:L5:4431:U:OP2	14:LI:3:ARG:NH2	2.43	0.51
3:L5:3711:A:O2'	3:L5:3712:A:P	2.69	0.50
9:LD:126:THR:HG22	9:LD:128:ASP:H	1.76	0.50
3:L5:398:A2M:O5'	3:L5:398:A2M:H8	2.11	0.50
3:L5:2304:U:HO2'	3:L5:2305:U:P	2.27	0.50
3:L5:3625:G:O2'	3:L5:3626:G:O5'	2.29	0.50
3:L5:4741:C:H4'	3:L5:4742:G:H5'	1.93	0.50
4:L7:39:C:C6	15:LJ:49:VAL:HG11	2.47	0.50
3:L5:1574:G:HO2'	3:L5:1575:A:P	2.35	0.50
3:L5:3594:C:O2'	3:L5:3595:U:OP1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3734:U:O2'	3:L5:3735:G:OP1	2.21	0.50
24:LT:80:VAL:HG23	24:LT:80:VAL:O	2.10	0.50
3:L5:1273:G:C2'	3:L5:1274:A:H5'	2.41	0.50
34:Ld:97:ASP:OD1	34:Ld:97:ASP:C	2.55	0.50
3:L5:4678:G:HO2'	3:L5:4679:G:P	2.34	0.50
3:L5:5030:U:H3'	3:L5:5031:G:H5''	1.93	0.50
4:L7:7:G:OP2	9:LD:28:THR:HG22	2.11	0.50
16:LL:81:LEU:HD22	16:LL:86:ILE:HD11	1.94	0.50
3:L5:4734:A:HO2'	3:L5:4735:G:P	2.30	0.50
34:Ld:19:GLU:HA	34:Ld:19:GLU:OE1	2.11	0.50
3:L5:1078:A:C5	3:L5:1079:C:C5	3.00	0.50
4:L7:119:U:OP2	9:LD:259:LYS:NZ	2.42	0.50
3:L5:3754:G:N7	3:L5:3771:C:N4	2.60	0.50
3:L5:5024:C:N4	3:L5:5029:C:O4'	2.38	0.50
6:LA:15:VAL:HG12	6:LA:15:VAL:O	2.12	0.50
21:LQ:83:VAL:HG12	21:LQ:83:VAL:O	2.12	0.50
3:L5:485:C:H2'	3:L5:485:C:O2	2.12	0.49
3:L5:4670:C:O2'	3:L5:4672:A:OP2	2.25	0.49
13:LH:57:VAL:HG23	13:LH:70:VAL:HG13	1.93	0.49
19:LO:190:ASP:OD2	19:LO:190:ASP:C	2.54	0.49
3:L5:406:C:O2'	3:L5:407:A:P	2.70	0.49
3:L5:911:U:O2'	3:L5:912:G:P	2.69	0.49
12:LG:165:GLU:HA	12:LG:168:VAL:HG22	1.94	0.49
33:Lc:10:SER:O	33:Lc:13:SER:OG	2.24	0.49
3:L5:4523:A2M:H5''	3:L5:4524:G:H5'	1.94	0.49
3:L5:923:C:HO2'	3:L5:924:C:P	2.35	0.49
3:L5:1912:G:N2	19:LO:87:MET:HE2	2.28	0.49
8:LC:149:GLU:OE2	46:Lr:71:ARG:NH1	2.44	0.49
14:LI:89:VAL:HG12	14:LI:136:MET:HG3	1.95	0.49
3:L5:406:C:O2'	3:L5:407:A:OP1	2.24	0.49
9:LD:83:LEU:N	9:LD:84:PRO:CD	2.76	0.49
24:LT:111:GLU:OE2	24:LT:111:GLU:N	2.46	0.49
33:Lc:36:LYS:O	33:Lc:40:GLN:HG2	2.13	0.49
42:Ll:16:LYS:HD2	42:Ll:49:LEU:HD22	1.95	0.49
3:L5:754:U:HO2'	3:L5:755:C:P	2.35	0.49
3:L5:4724:A:O2'	7:LB:104:THR:HG22	2.13	0.49
3:L5:655:C:OP2	8:LC:268:ARG:NH1	2.46	0.48
3:L5:2013:A:H2'	3:L5:2014:C:C6	2.48	0.48
3:L5:2424:OMG:HM22	3:L5:2426:U:C6	2.48	0.48
25:LU:38:ASN:OD1	25:LU:38:ASN:N	2.41	0.48
45:Lp:84:ARG:HG2	45:Lp:84:ARG:HH11	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3625:G:O2'	3:L5:3626:G:H4'	2.14	0.48
3:L5:4123:C:HO2'	3:L5:4124:G:P	2.36	0.48
3:L5:5021:C:O5'	3:L5:5022:U:OP2	2.30	0.48
17:LM:136:LEU:O	17:LM:136:LEU:HD23	2.14	0.48
3:L5:1178:G:N3	3:L5:1178:G:H2'	2.28	0.48
3:L5:2260:C:OP1	10:LE:108:LYS:NZ	2.47	0.48
9:LD:278:ASP:O	9:LD:282:GLN:HG2	2.14	0.48
3:L5:1368:A:H1'	29:LY:1:MET:HE2	1.96	0.48
3:L5:1590:C:H4'	3:L5:1591:U:OP2	2.14	0.48
3:L5:912:G:H2'	3:L5:913:U:O4'	2.13	0.48
3:L5:1772:C:O2'	3:L5:1773:U:O4'	2.30	0.48
4:L7:51:G:HO2'	4:L7:52:C:P	2.37	0.48
3:L5:4626:A:OP2	7:LB:224:LYS:NZ	2.32	0.48
3:L5:2901:G:C6	3:L5:3599:A:C6	3.02	0.48
3:L5:4633:G:O2'	3:L5:4635:A:OP2	2.30	0.48
3:L5:2546:G:HO2'	3:L5:2547:G:C5'	2.18	0.48
3:L5:2856:C:O2	7:LB:242:ARG:NH2	2.47	0.48
3:L5:2108:G:O2'	3:L5:2109:G:OP1	2.29	0.48
3:L5:4555:U:O2'	3:L5:4556:U:P	2.71	0.48
30:LZ:76:ASN:OD1	30:LZ:77:TYR:N	2.47	0.48
38:Lh:16:GLU:OE2	38:Lh:16:GLU:N	2.30	0.48
3:L5:1171:G:N2	3:L5:1190:C:N3	2.59	0.47
15:LJ:31:ASP:OD2	15:LJ:35:ARG:NE	2.47	0.47
22:LR:116:ASP:OD1	22:LR:116:ASP:C	2.56	0.47
32:Lb:94:ASP:OD1	32:Lb:94:ASP:N	2.45	0.47
39:Li:63:VAL:O	39:Li:64:SER:OG	2.21	0.47
3:L5:711:A:H2'	3:L5:712:C:C6	2.49	0.47
12:LG:164:ILE:O	12:LG:168:VAL:HG13	2.14	0.47
13:LH:120:GLU:OE1	13:LH:124:ARG:NH2	2.47	0.47
35:Le:95:TYR:O	49:Le:301:HOH:O	2.20	0.47
3:L5:916:C:O2	3:L5:916:C:C2'	2.62	0.47
28:LX:57:GLN:HG3	28:LX:57:GLN:O	2.14	0.47
3:L5:754:U:O2'	3:L5:755:C:OP1	2.31	0.47
3:L5:3771:C:H3'	3:L5:3772:U:C2	2.49	0.47
13:LH:177:ASP:N	13:LH:177:ASP:OD1	2.47	0.47
3:L5:2054:U:OP1	19:LO:18:ARG:NH1	2.47	0.47
3:L5:3948:C:O2'	3:L5:3949:A:O5'	2.29	0.47
3:L5:4620:A1L3O:OP2	3:L5:4670:C:N4	2.36	0.47
3:L5:3784:A:O2'	3:L5:3786:U:OP2	2.14	0.47
7:LB:222:VAL:O	7:LB:343:ARG:NH1	2.47	0.47
15:LJ:26:VAL:HG23	15:LJ:28:GLU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LL:62:PRO:O	16:LL:63:THR:HB	2.15	0.47
3:L5:132:G:H22	3:L5:136:C:HO2'	1.57	0.47
3:L5:418:A:C2	5:L8:17:A:H1'	2.50	0.47
3:L5:1574:G:O2'	3:L5:1575:A:P	2.73	0.47
3:L5:4600:G:HO2'	3:L5:4601:U:P	2.30	0.47
3:L5:4600:G:C2'	3:L5:4601:U:OP2	2.63	0.47
3:L5:4744:A:H2'	3:L5:4745:G:O4'	2.14	0.47
12:LG:112:GLN:CD	12:LG:112:GLN:C	2.82	0.47
12:LG:210:GLU:OE1	12:LG:210:GLU:N	2.44	0.47
24:LT:64:VAL:HG13	24:LT:72:VAL:HG22	1.96	0.47
29:LY:99:ILE:HD11	29:LY:104:VAL:CG1	2.44	0.47
3:L5:3652:A:H2'	3:L5:3653:A:C8	2.49	0.47
3:L5:5021:C:H2'	3:L5:5022:U:H4'	1.95	0.47
12:LG:106:THR:HG22	12:LG:107:LYS:N	2.30	0.47
3:L5:704:C:H5	3:L5:707:C:H41	1.63	0.47
13:LH:117:PHE:O	13:LH:120:GLU:HG3	2.15	0.47
3:L5:745:G:HO2'	3:L5:746:A:P	2.34	0.47
3:L5:2588:C:OP1	3:L5:2768:C:O2'	2.25	0.47
3:L5:4555:U:HO2'	3:L5:4556:U:P	2.23	0.47
7:LB:297:LYS:HZ3	7:LB:299:ILE:HD11	1.80	0.47
9:LD:22:ARG:HE	9:LD:28:THR:HG21	1.79	0.46
10:LE:161:ARG:NH1	10:LE:273:SER:OG	2.48	0.46
24:LT:121:GLU:C	24:LT:121:GLU:OE1	2.58	0.46
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.50	0.46
3:L5:5029:C:C4	3:L5:5030:U:C4	3.03	0.46
16:LL:60:ARG:HD2	16:LL:67:HIS:O	2.15	0.46
28:LX:145:ASP:O	28:LX:145:ASP:OD2	2.33	0.46
30:LZ:31:ASP:OD1	30:LZ:31:ASP:C	2.58	0.46
3:L5:3877:A:N3	3:L5:4401:G:O2'	2.44	0.46
17:LM:80:ALA:O	17:LM:81:ASP:OD1	2.34	0.46
3:L5:181:C:O2	3:L5:256:G:N2	2.49	0.46
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.98	0.46
3:L5:3769:C:H2'	3:L5:3770:U:O4'	2.15	0.46
15:LJ:15:LEU:HD11	15:LJ:157:ILE:HD12	1.98	0.46
24:LT:122:LYS:HD2	24:LT:122:LYS:O	2.14	0.46
3:L5:4123:C:O2'	3:L5:4124:G:P	2.74	0.46
3:L5:4913:G:H4'	3:L5:4914:C:O5'	2.15	0.46
25:LU:26:THR:O	25:LU:30:GLU:HG3	2.15	0.46
3:L5:2396:A:N7	3:L5:2814:C:O2'	2.49	0.46
3:L5:4116:C:H4'	3:L5:4117:U:OP2	2.16	0.46
3:L5:4135:G:C2	3:L5:4136:G:C8	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LD:229:ASN:O	9:LD:230:SER:OG	2.23	0.46
3:L5:741:C:C2'	3:L5:742:G:OP1	2.64	0.46
3:L5:3813:A:N3	3:L5:4538:G:O2'	2.47	0.46
3:L5:4123:C:O2'	3:L5:4124:G:OP1	2.29	0.46
28:LX:145:ASP:OD2	28:LX:145:ASP:C	2.59	0.46
3:L5:67:C:OP2	3:L5:312:G:N2	2.49	0.46
15:LJ:38:LYS:O	15:LJ:42:GLN:HG3	2.16	0.46
16:LL:108:GLU:OE1	16:LL:108:GLU:N	2.44	0.46
27:LW:45:ASN:OD1	27:LW:47:ARG:HB3	2.16	0.46
41:Lk:7:GLU:HB2	41:Lk:10:ASP:OD1	2.15	0.46
3:L5:1705:G:H2'	3:L5:1706:A:O4'	2.16	0.46
3:L5:3785:A2M:H8	3:L5:3785:A2M:H2'	1.72	0.46
4:L7:51:G:O2'	4:L7:52:C:P	2.73	0.46
16:LL:80:GLU:HG2	16:LL:110:LEU:HD12	1.98	0.46
30:LZ:22:LYS:NZ	30:LZ:132:GLN:O	2.44	0.46
3:L5:2055:G:H4'	3:L5:2056:G:OP2	2.16	0.45
3:L5:2809:G:O2'	3:L5:4644:G:OP1	2.31	0.45
3:L5:4895:C:H3'	3:L5:4896:G:H5''	1.98	0.45
32:Lb:91:ARG:HB2	32:Lb:94:ASP:OD1	2.16	0.45
3:L5:495:C:O2	3:L5:496:G:N1	2.50	0.45
3:L5:1080:C:N3	3:L5:1081:C:C5	2.85	0.45
3:L5:1355:G:OP1	21:LQ:108:ARG:NH2	2.41	0.45
3:L5:4734:A:H1'	3:L5:4735:G:C8	2.51	0.45
7:LB:298:LEU:C	7:LB:299:ILE:HD13	2.41	0.45
35:Le:92:ASN:ND2	35:Le:119:ALA:O	2.34	0.45
3:L5:187:U:C4	3:L5:245:C:C4	3.05	0.45
3:L5:2894:A:O2'	3:L5:2895:A:P	2.74	0.45
3:L5:2901:G:C6	3:L5:2902:G:C4	3.04	0.45
3:L5:5030:U:C4	3:L5:5031:G:C8	3.05	0.45
7:LB:341:LYS:O	7:LB:342:LYS:HB2	2.17	0.45
22:LR:31:GLU:OE1	22:LR:31:GLU:O	2.33	0.45
3:L5:750:U:H3'	3:L5:751:G:H21	1.82	0.45
3:L5:3718:A2M:H8	3:L5:3718:A2M:O5'	2.16	0.45
3:L5:3772:U:H2'	3:L5:3773:U:N1	2.31	0.45
26:LV:108:ASN:OD1	26:LV:108:ASN:N	2.49	0.45
31:La:88:VAL:O	31:La:92:LYS:HG3	2.16	0.45
3:L5:143:C:OP1	12:LG:111:LYS:NZ	2.43	0.45
3:L5:170:C:H42	3:L5:266:C:H42	1.65	0.45
3:L5:2638:G:O2'	3:L5:2639:U:H5'	2.17	0.45
3:L5:3946:G:HO2'	3:L5:3947:A:P	2.39	0.45
3:L5:4895:C:OP2	3:L5:4896:G:H5''	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LM:39:ASP:OD1	17:LM:41:PRO:HD3	2.17	0.45
19:LO:27:VAL:HG12	19:LO:98:ALA:HB1	1.97	0.45
26:LV:26:ILE:HG22	26:LV:101:ASN:HB2	1.99	0.45
3:L5:108:A:H4'	3:L5:109:G:OP1	2.16	0.45
3:L5:911:U:HO2'	3:L5:912:G:P	2.38	0.45
3:L5:1439:C:H2'	3:L5:1439:C:O2	2.15	0.45
3:L5:1818:G:O2'	3:L5:1820:C:OP2	2.35	0.45
8:LC:218:ILE:O	8:LC:222:ARG:HG3	2.16	0.45
25:LU:67:LYS:C	25:LU:67:LYS:HD3	2.42	0.45
33:Lc:48:LEU:HD23	33:Lc:71:VAL:HG13	1.99	0.45
34:Ld:97:ASP:OD1	34:Ld:97:ASP:O	2.34	0.45
34:Ld:22:THR:HG23	34:Ld:122:VAL:HB	1.98	0.45
3:L5:1837:A:OP2	24:LT:130:ARG:NH1	2.40	0.45
3:L5:2485:U:O2'	3:L5:2486:G:O5'	2.34	0.45
3:L5:4758:U:O2	3:L5:4758:U:O4'	2.35	0.45
17:LM:39:ASP:OD1	17:LM:39:ASP:C	2.59	0.45
2:2:75:C:H5''	2:2:76:A:OP2	2.17	0.44
3:L5:963:G:N3	3:L5:963:G:H2'	2.31	0.44
3:L5:2517:A:N3	3:L5:2539:C:O2'	2.50	0.44
3:L5:4472:G:O2'	43:Lm:100:TYR:O	2.33	0.44
3:L5:4699:U:H4'	3:L5:4700:A:OP1	2.17	0.44
37:Lg:99:GLU:O	37:Lg:103:VAL:HG13	2.16	0.44
3:L5:961:G:C6	3:L5:970:G:O4'	2.70	0.44
3:L5:1646:A:O2'	40:Lj:49:TRP:O	2.35	0.44
3:L5:1706:A:OP2	3:L5:2097:U:O4	2.35	0.44
3:L5:1816:C:H2'	3:L5:1816:C:O2	2.17	0.44
3:L5:4570:G:H2'	3:L5:4571:A2M:H8	1.99	0.44
5:L8:96:C:OP1	38:Lh:70:ARG:NH1	2.44	0.44
18:LN:75:VAL:HG22	18:LN:76:PRO:HD2	1.99	0.44
44:Lo:74:GLU:OE2	44:Lo:76:ASN:OD1	2.36	0.44
3:L5:1339:U:H2'	3:L5:1340:C:C6	2.52	0.44
3:L5:2440:U:HO2'	3:L5:2441:C:P	2.39	0.44
3:L5:3759:A:H62	3:L5:3764:PSU:HN3	1.65	0.44
23:LS:85:ASP:OD2	23:LS:85:ASP:N	2.51	0.44
32:Lb:40:LEU:HD12	32:Lb:43:MET:HE3	1.99	0.44
3:L5:25:A:C8	3:L5:341:G:C8	3.06	0.44
3:L5:1077:C:C4	3:L5:1078:A:C2	3.06	0.44
3:L5:2520:C:O2	3:L5:2640:G:N2	2.51	0.44
3:L5:2754:G:O2'	3:L5:2755:A:H8	2.00	0.44
3:L5:4992:G:H2'	3:L5:4993:G:C8	2.52	0.44
5:L8:141:C:OP1	18:LN:38:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LE:277:LEU:HA	10:LE:281:ILE:HD11	2.00	0.44
13:LH:31:ARG:NH1	13:LH:149:ASN:OD1	2.50	0.44
25:LU:24:ASP:C	25:LU:24:ASP:OD1	2.59	0.44
3:L5:2544:G:O6	5:L8:123:U:H2'	2.17	0.44
3:L5:4076:G:H4'	3:L5:4077:A:OP1	2.18	0.44
17:LM:81:ASP:CG	17:LM:81:ASP:O	2.60	0.44
3:L5:1345:A:H2'	3:L5:1346:C:C6	2.53	0.44
3:L5:4212:A:H4'	3:L5:4213:A:O5'	2.18	0.44
14:LI:89:VAL:HG12	14:LI:136:MET:CG	2.47	0.44
15:LJ:101:ASP:OD1	15:LJ:101:ASP:N	2.48	0.44
25:LU:30:GLU:C	25:LU:30:GLU:OE2	2.61	0.44
3:L5:915:A:H62	3:L5:918:G:H1	1.65	0.44
3:L5:4138:C:H2'	3:L5:4139:G:O4'	2.18	0.44
3:L5:4739:C:H2'	3:L5:4740:G:H5'	1.99	0.44
5:L8:16:G:O2'	5:L8:17:A:OP2	2.31	0.44
25:LU:17:GLN:CD	25:LU:17:GLN:N	2.75	0.44
37:Lg:94:ALA:O	37:Lg:98:GLU:HG2	2.18	0.44
3:L5:1243:C:C2	3:L5:1244:G:C8	3.06	0.44
3:L5:4137:C:H2'	3:L5:4137:C:O2	2.17	0.44
8:LC:336:ARG:O	8:LC:339:THR:HG22	2.18	0.44
16:LL:47:ALA:HB3	16:LL:48:PRO:HD3	2.00	0.44
33:Lc:11:LEU:HA	33:Lc:14:ILE:HG22	1.98	0.44
3:L5:750:U:O2	3:L5:750:U:O4'	2.36	0.43
3:L5:1755:C:H2'	3:L5:1756:U:O4'	2.17	0.43
3:L5:3909:OMC:C2	3:L5:3910:C:C6	3.06	0.43
15:LJ:119:TYR:CD1	15:LJ:119:TYR:C	2.96	0.43
3:L5:2760:G:C2'	3:L5:2761:U:OP2	2.66	0.43
3:L5:4098:A:OP2	37:Lg:115:LYS:NZ	2.41	0.43
3:L5:4882:U:O2'	3:L5:4883:C:O5'	2.32	0.43
20:LP:7:ASP:OD2	20:LP:7:ASP:N	2.52	0.43
3:L5:1081:C:O2'	3:L5:1082:C:H5'	2.17	0.43
3:L5:4254:G:N3	3:L5:4254:G:H2'	2.32	0.43
30:LZ:123:LYS:C	30:LZ:124:THR:HG23	2.43	0.43
3:L5:513:U:N3	3:L5:516:C:OP2	2.42	0.43
3:L5:1882:U:C4	3:L5:2279:A:C2	3.07	0.43
3:L5:2019:C:H2'	3:L5:2020:U:C6	2.52	0.43
13:LH:7:ASN:HB3	13:LH:58:ASP:OD1	2.17	0.43
3:L5:178:C:C2	3:L5:259:C:N4	2.87	0.43
3:L5:1701:A:C2	3:L5:1702:C:C6	3.06	0.43
12:LG:231:ASP:OD1	12:LG:231:ASP:N	2.50	0.43
3:L5:48:G:O2'	3:L5:49:U:OP2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:749:G:H3'	3:L5:750:U:C5'	2.48	0.43
3:L5:1962:A:C5	3:L5:1963:C:C5	3.07	0.43
5:L8:155:C:H2'	5:L8:156:U:O4'	2.19	0.43
7:LB:299:ILE:CG2	7:LB:313:SER:HB3	2.49	0.43
3:L5:1754:U:H2'	3:L5:1755:C:C5	2.53	0.43
3:L5:3593:C:O2'	3:L5:3595:U:O4	2.33	0.43
3:L5:683:C:H2'	3:L5:684:G:O4'	2.18	0.43
3:L5:3785:A2M:HM'1	3:L5:4537:C:H1'	2.00	0.43
6:LA:45:VAL:HG23	6:LA:84:THR:HA	2.00	0.43
8:LC:63:SER:O	8:LC:63:SER:OG	2.28	0.43
10:LE:204:SER:O	10:LE:205:ASN:CG	2.62	0.43
12:LG:193:LEU:O	12:LG:193:LEU:HD12	2.18	0.43
18:LN:98:LEU:O	18:LN:101:VAL:HG22	2.19	0.43
34:Ld:33:ILE:O	34:Ld:33:ILE:HG22	2.19	0.43
38:Lh:20:GLN:O	38:Lh:23:ASP:OD1	2.37	0.43
3:L5:180:C:H2'	3:L5:181:C:O4'	2.18	0.43
3:L5:754:U:O2'	3:L5:755:C:P	2.77	0.43
3:L5:1202:C:H3'	3:L5:1203:G:H5''	2.01	0.43
3:L5:2262:G:OP2	46:Lr:98:ARG:NH2	2.42	0.43
3:L5:5024:C:C5	3:L5:5028:G:N3	2.87	0.43
45:Lp:52:VAL:HG13	45:Lp:52:VAL:O	2.19	0.43
3:L5:508:G:O2'	3:L5:510:U:OP2	2.32	0.43
3:L5:3771:C:H2'	3:L5:3771:C:O2	2.18	0.43
5:L8:123:U:H4'	5:L8:123:U:OP1	2.19	0.43
14:LI:34:PHE:HD1	14:LI:89:VAL:HG23	1.83	0.43
15:LJ:110:GLN:H	15:LJ:110:GLN:CD	2.26	0.43
44:Lo:93:LEU:O	44:Lo:94:GLY:C	2.61	0.43
3:L5:1706:A:P	3:L5:2097:U:O4	2.77	0.42
3:L5:3910:C:H2'	3:L5:3911:C:C6	2.54	0.42
3:L5:4233:A:OP2	44:Lo:97:LYS:NZ	2.51	0.42
31:La:146:LEU:HD13	39:Li:7:MET:HE3	2.01	0.42
34:Ld:65:ASP:OD1	34:Ld:66:THR:N	2.51	0.42
38:Lh:19:LYS:O	38:Lh:23:ASP:OD1	2.36	0.42
8:LC:154:VAL:HG22	8:LC:155:GLU:N	2.35	0.42
21:LQ:66:MET:HE1	21:LQ:86:ILE:CD1	2.49	0.42
26:LV:71:GLU:H	26:LV:71:GLU:CD	2.24	0.42
46:Lr:103:ARG:HG2	46:Lr:106:LEU:HD12	2.01	0.42
3:L5:925:C:H3'	3:L5:926:G:H5''	2.01	0.42
3:L5:3709:U:O2'	3:L5:3710:G:P	2.75	0.42
3:L5:1963:C:C2	3:L5:1964:A:C8	3.08	0.42
3:L5:4938:A:OP1	10:LE:183:ARG:NE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LB:258:HIS:HA	7:LB:260:ALA:N	2.34	0.42
10:LE:205:ASN:OD1	10:LE:205:ASN:C	2.61	0.42
12:LG:246:SER:O	12:LG:250:ILE:HD13	2.19	0.42
13:LH:128:MET:HE2	13:LH:128:MET:HA	2.01	0.42
27:LW:55:TYR:CD1	27:LW:55:TYR:C	2.97	0.42
3:L5:741:C:O2	3:L5:741:C:O4'	2.37	0.42
3:L5:1249:C:H2'	3:L5:1250:C:H6	1.84	0.42
3:L5:1660:U:O2'	31:La:12:ARG:HG3	2.20	0.42
6:LA:5:ILE:HG22	6:LA:208:GLU:O	2.20	0.42
11:LF:196:THR:O	11:LF:196:THR:HG22	2.20	0.42
39:Li:73:ILE:O	39:Li:77:VAL:HG22	2.19	0.42
3:L5:741:C:H2'	3:L5:742:G:OP1	2.19	0.42
3:L5:4895:C:O2'	3:L5:4896:G:P	2.78	0.42
7:LB:107:ALA:HB2	7:LB:201:LEU:HG	2.01	0.42
3:L5:2894:A:HO2'	3:L5:2895:A:P	2.38	0.42
3:L5:3641:U:H5	3:L5:3646:A:N7	2.18	0.42
28:LX:117:TYR:O	28:LX:118:ASP:OD1	2.38	0.42
28:LX:118:ASP:OD1	28:LX:118:ASP:C	2.63	0.42
3:L5:4570:G:C2	3:L5:4571:A2M:C8	3.02	0.42
3:L5:4571:A2M:N3	3:L5:4572:U:C5	2.87	0.42
3:L5:5029:C:N3	3:L5:5030:U:C4	2.88	0.42
9:LD:22:ARG:HE	9:LD:28:THR:CG2	2.33	0.42
11:LF:184:ILE:HD11	11:LF:193:GLU:HG3	2.02	0.42
24:LT:114:GLN:OE1	24:LT:115:LYS:HG3	2.19	0.42
3:L5:75:G:O6	16:LL:103:ARG:NH1	2.53	0.42
3:L5:466:A:H2'	3:L5:467:U:C1'	2.50	0.42
3:L5:745:G:H2'	3:L5:746:A:C1'	2.50	0.42
3:L5:750:U:H5'	3:L5:751:G:N2	2.35	0.42
3:L5:2019:C:O2'	3:L5:2020:U:P	2.77	0.42
18:LN:36:LEU:C	18:LN:36:LEU:HD13	2.45	0.42
26:LV:92:ASP:OD2	26:LV:92:ASP:O	2.38	0.42
29:LY:51:LYS:O	29:LY:52:ASP:HB2	2.20	0.42
3:L5:1441:C:N4	3:L5:1442:C:H41	2.18	0.42
3:L5:1625:OMG:H4'	3:L5:1626:G:O5'	2.20	0.42
3:L5:2464:C:HO2'	3:L5:2465:C:H6	1.66	0.42
3:L5:2675:G:H1'	3:L5:2676:A:OP2	2.20	0.42
3:L5:3786:U:OP1	3:L5:4550:G:O2'	2.35	0.42
3:L5:4135:G:C6	3:L5:4150:G:C6	3.08	0.42
3:L5:4746:C:H2'	3:L5:4746:C:O2	2.19	0.42
3:L5:4989:U:O2'	3:L5:4990:C:C6	2.73	0.42
6:LA:122:ASP:C	6:LA:122:ASP:OD1	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LD:116:ASP:OD1	9:LD:117:LYS:N	2.52	0.42
10:LE:204:SER:O	10:LE:205:ASN:OD1	2.38	0.42
11:LF:203:GLU:OE1	11:LF:203:GLU:N	2.48	0.42
46:Lr:31:ASN:ND2	46:Lr:40:TYR:O	2.53	0.42
3:L5:743:G:O2'	3:L5:744:G:P	2.78	0.41
3:L5:961:G:O6	10:LE:123:ARG:NH1	2.46	0.41
3:L5:1183:C:P	3:L5:1184:A:OP2	2.78	0.41
3:L5:3597:G:N3	3:L5:3598:C:C6	2.88	0.41
3:L5:4067:U:H2'	3:L5:4068:U:C6	2.55	0.41
3:L5:4138:C:H2'	3:L5:4139:G:C5'	2.50	0.41
14:LI:201:PRO:O	14:LI:202:SER:HB3	2.20	0.41
3:L5:453:G:N3	3:L5:453:G:C2'	2.82	0.41
3:L5:754:U:H2'	3:L5:755:C:O5'	2.20	0.41
3:L5:1701:A:H2'	3:L5:1701:A:N3	2.33	0.41
3:L5:1872:G:O2'	3:L5:4219:A:N3	2.51	0.41
3:L5:2261:G:H4'	10:LE:112:MET:CE	2.50	0.41
3:L5:4137:C:C2	3:L5:4138:C:C5	3.08	0.41
29:LY:82:ILE:HG22	29:LY:83:GLU:N	2.35	0.41
3:L5:93:G:H2'	3:L5:94:A:C8	2.56	0.41
3:L5:1804:A:O4'	3:L5:1806:G:C8	2.72	0.41
3:L5:3777:G:O2'	3:L5:3815:G:O6	2.28	0.41
18:LN:159:ARG:HB2	18:LN:164:LEU:CD1	2.50	0.41
26:LV:97:TYR:OH	27:LW:37:GLU:OE1	2.22	0.41
35:Le:84:GLU:O	35:Le:87:VAL:HG22	2.21	0.41
3:L5:518:G:H22	3:L5:643:C:H3'	1.85	0.41
3:L5:754:U:C2'	3:L5:755:C:O5'	2.67	0.41
18:LN:115:VAL:HG22	18:LN:134:LEU:CD1	2.50	0.41
33:Lc:12:GLU:O	33:Lc:15:ASN:OD1	2.39	0.41
3:L5:1200:G:H2'	3:L5:1201:U:H5'	2.02	0.41
3:L5:1359:G:H4'	18:LN:203:TYR:HB2	2.02	0.41
3:L5:4220:6MZ:OP1	24:LT:2:THR:N	2.53	0.41
28:LX:73:HIS:ND1	28:LX:115:LYS:HD3	2.35	0.41
28:LX:93:ASN:O	28:LX:95:THR:HG23	2.21	0.41
3:L5:745:G:H2'	3:L5:746:A:C8	2.56	0.41
3:L5:2605:G:O2'	3:L5:2606:G:H5'	2.21	0.41
3:L5:3753:G:H1	3:L5:3772:U:H6	1.68	0.41
3:L5:4645:C:OP2	22:LR:62:ARG:NH1	2.53	0.41
18:LN:3:ALA:O	18:LN:7:ILE:HG12	2.20	0.41
35:Le:76:LYS:NZ	35:Le:98:GLU:OE1	2.51	0.41
3:L5:491:G:H2'	3:L5:492:U:C6	2.56	0.41
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:5001:U:H2'	3:L5:5002:U:O4'	2.20	0.41
11:LF:116:GLN:HB3	11:LF:119:ASN:OD1	2.21	0.41
21:LQ:39:THR:HG22	21:LQ:40:ASN:N	2.36	0.41
3:L5:755:C:O2'	3:L5:756:G:P	2.79	0.41
3:L5:2675:G:O6	33:Lc:30:GLY:HA3	2.21	0.41
7:LB:86:VAL:HG13	7:LB:162:VAL:HG13	2.02	0.41
30:LZ:106:LEU:H	30:LZ:106:LEU:HD22	1.85	0.41
3:L5:181:C:H2'	3:L5:182:G:O4'	2.20	0.41
3:L5:1253:G:O3'	3:L5:1254:A:H3'	2.21	0.41
3:L5:1700:G:O2'	3:L5:1701:A:OP1	2.33	0.41
3:L5:2693:G:H2'	3:L5:2694:G:N2	2.36	0.41
3:L5:2696:A:H62	41:Lk:35:LYS:HE2	1.86	0.41
4:L7:109:U:C2'	4:L7:110:G:OP2	2.68	0.41
5:L8:82:A:H3'	5:L8:83:C:H5''	2.03	0.41
6:LA:234:LYS:O	6:LA:234:LYS:HG3	2.21	0.41
19:LO:41:ILE:HG22	19:LO:42:ASN:N	2.36	0.41
24:LT:85:LEU:HD23	24:LT:85:LEU:H	1.86	0.41
25:LU:35:ASP:OD1	25:LU:35:ASP:C	2.63	0.41
26:LV:13:LYS:HD3	26:LV:128:LEU:HD11	2.01	0.41
27:LW:60:LYS:HZ1	27:LW:64:SER:C	2.28	0.41
28:LX:152:LYS:HE2	28:LX:152:LYS:HB3	1.95	0.41
37:Lg:73:HIS:CD2	37:Lg:73:HIS:C	2.99	0.41
44:Lo:24:THR:HG22	44:Lo:25:GLN:H	1.86	0.41
3:L5:37:U:H2'	3:L5:38:A:O4'	2.20	0.41
3:L5:965:G:H2'	3:L5:2092:G:N2	2.36	0.41
3:L5:1077:C:N3	3:L5:1078:A:C2	2.89	0.41
3:L5:2014:C:H2'	3:L5:2015:U:C5'	2.51	0.41
3:L5:2539:C:H2'	3:L5:2540:C:C6	2.55	0.41
3:L5:3648:A:H1'	3:L5:3785:A2M:N6	2.36	0.41
3:L5:4555:U:C2'	3:L5:4556:U:OP1	2.68	0.41
30:LZ:123:LYS:O	30:LZ:124:THR:CB	2.69	0.41
8:LC:209:ILE:HB	8:LC:229:LEU:HD13	2.02	0.40
9:LD:90:VAL:HG22	9:LD:91:GLY:N	2.35	0.40
12:LG:87:LEU:HG	12:LG:91:THR:HG23	2.02	0.40
14:LI:152:LEU:HB3	14:LI:165:ILE:HD12	2.03	0.40
21:LQ:3:VAL:HG23	21:LQ:5:ILE:HG12	2.03	0.40
3:L5:453:G:N3	3:L5:453:G:H2'	2.37	0.40
3:L5:923:C:C2'	3:L5:924:C:O5'	2.70	0.40
3:L5:1754:U:H2'	3:L5:1755:C:C6	2.56	0.40
3:L5:2055:G:H3'	3:L5:2056:G:C5'	2.50	0.40
21:LQ:177:ALA:O	21:LQ:184:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:704:C:H2'	3:L5:706:C:OP2	2.21	0.40
3:L5:3597:G:H1'	3:L5:3598:C:OP2	2.22	0.40
3:L5:1590:C:H5''	3:L5:1591:U:O5'	2.22	0.40
3:L5:2304:U:O2'	3:L5:2305:U:P	2.77	0.40
3:L5:3733:A:H2'	3:L5:3734:U:O4'	2.21	0.40
3:L5:4260:U:H2'	3:L5:4261:C:C6	2.56	0.40
3:L5:4739:C:H2'	3:L5:4740:G:C5'	2.52	0.40
3:L5:1174:G:N2	3:L5:1187:G:N7	2.69	0.40
19:LO:58:LEU:HD21	19:LO:74:ARG:HH22	1.87	0.40
25:LU:54:GLY:O	25:LU:55:ASN:HB3	2.21	0.40
32:Lb:116:LEU:HD23	32:Lb:116:LEU:C	2.47	0.40
41:Lk:56:LEU:O	41:Lk:56:LEU:HD12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	28/269 (10%)	28 (100%)	0	0	100	100
6	LA	244/257 (95%)	236 (97%)	8 (3%)	0	100	100
7	LB	400/403 (99%)	384 (96%)	16 (4%)	0	100	100
8	LC	365/427 (86%)	347 (95%)	18 (5%)	0	100	100
9	LD	291/297 (98%)	284 (98%)	7 (2%)	0	100	100
10	LE	211/288 (73%)	205 (97%)	6 (3%)	0	100	100
11	LF	223/248 (90%)	219 (98%)	4 (2%)	0	100	100
12	LG	230/266 (86%)	225 (98%)	5 (2%)	0	100	100
13	LH	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
14	LI	199/214 (93%)	194 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	LJ	174/178 (98%)	170 (98%)	4 (2%)	0	100	100
16	LL	208/211 (99%)	196 (94%)	12 (6%)	0	100	100
17	LM	137/215 (64%)	133 (97%)	4 (3%)	0	100	100
18	LN	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
19	LO	199/203 (98%)	195 (98%)	4 (2%)	0	100	100
20	LP	151/184 (82%)	147 (97%)	4 (3%)	0	100	100
21	LQ	185/188 (98%)	178 (96%)	7 (4%)	0	100	100
22	LR	161/196 (82%)	158 (98%)	3 (2%)	0	100	100
23	LS	173/176 (98%)	169 (98%)	4 (2%)	0	100	100
24	LT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
25	LU	99/128 (77%)	91 (92%)	8 (8%)	0	100	100
26	LV	129/140 (92%)	126 (98%)	3 (2%)	0	100	100
27	LW	63/157 (40%)	61 (97%)	2 (3%)	0	100	100
28	LX	117/156 (75%)	116 (99%)	1 (1%)	0	100	100
29	LY	132/145 (91%)	128 (97%)	4 (3%)	0	100	100
30	LZ	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
31	La	145/148 (98%)	141 (97%)	4 (3%)	0	100	100
32	Lb	96/159 (60%)	93 (97%)	3 (3%)	0	100	100
33	Lc	96/115 (84%)	92 (96%)	4 (4%)	0	100	100
34	Ld	105/125 (84%)	102 (97%)	3 (3%)	0	100	100
35	Le	126/135 (93%)	126 (100%)	0	0	100	100
36	Lf	107/110 (97%)	104 (97%)	3 (3%)	0	100	100
37	Lg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
38	Lh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
39	Li	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
40	Lj	84/97 (87%)	82 (98%)	2 (2%)	0	100	100
41	Lk	67/70 (96%)	67 (100%)	0	0	100	100
42	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
43	Lm	49/128 (38%)	49 (100%)	0	0	100	100
44	Lo	103/106 (97%)	97 (94%)	6 (6%)	0	100	100
45	Lp	89/92 (97%)	84 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	Lr	123/137 (90%)	118 (96%)	5 (4%)	0	100	100
All	All	6368/7456 (85%)	6183 (97%)	185 (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	
1	1	23/232 (10%)	23 (100%)	0	100	100
6	LA	189/199 (95%)	187 (99%)	2 (1%)	65	79
7	LB	348/349 (100%)	346 (99%)	2 (1%)	78	89
8	LC	305/347 (88%)	304 (100%)	1 (0%)	86	93
9	LD	246/250 (98%)	245 (100%)	1 (0%)	84	92
10	LE	193/252 (77%)	188 (97%)	5 (3%)	40	55
11	LF	194/215 (90%)	193 (100%)	1 (0%)	81	90
12	LG	199/223 (89%)	196 (98%)	3 (2%)	57	73
13	LH	169/171 (99%)	169 (100%)	0	100	100
14	LI	173/181 (96%)	172 (99%)	1 (1%)	78	89
15	LJ	148/149 (99%)	147 (99%)	1 (1%)	76	87
16	LL	176/177 (99%)	175 (99%)	1 (1%)	78	89
17	LM	118/161 (73%)	117 (99%)	1 (1%)	73	85
18	LN	171/172 (99%)	170 (99%)	1 (1%)	78	89
19	LO	173/174 (99%)	171 (99%)	2 (1%)	63	78
20	LP	134/163 (82%)	131 (98%)	3 (2%)	45	61
21	LQ	164/165 (99%)	162 (99%)	2 (1%)	63	78
22	LR	144/175 (82%)	144 (100%)	0	100	100
23	LS	156/157 (99%)	155 (99%)	1 (1%)	78	89
24	LT	139/140 (99%)	137 (99%)	2 (1%)	59	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	LU	91/115 (79%)	84 (92%)	7 (8%)	12	13
26	LV	101/107 (94%)	99 (98%)	2 (2%)	48	64
27	LW	57/126 (45%)	56 (98%)	1 (2%)	51	68
28	LX	107/133 (80%)	106 (99%)	1 (1%)	70	84
29	LY	124/135 (92%)	123 (99%)	1 (1%)	73	85
30	LZ	117/118 (99%)	116 (99%)	1 (1%)	70	84
31	La	120/121 (99%)	119 (99%)	1 (1%)	73	85
32	Lb	83/126 (66%)	83 (100%)	0	100	100
33	Lc	83/97 (86%)	83 (100%)	0	100	100
34	Ld	98/110 (89%)	98 (100%)	0	100	100
35	Le	114/121 (94%)	110 (96%)	4 (4%)	32	43
36	Lf	88/89 (99%)	86 (98%)	2 (2%)	44	59
37	Lg	98/100 (98%)	97 (99%)	1 (1%)	68	81
38	Lh	109/110 (99%)	109 (100%)	0	100	100
39	Li	86/89 (97%)	86 (100%)	0	100	100
40	Lj	73/80 (91%)	73 (100%)	0	100	100
41	Lk	64/65 (98%)	63 (98%)	1 (2%)	55	71
42	Ll	47/48 (98%)	47 (100%)	0	100	100
43	Lm	47/115 (41%)	46 (98%)	1 (2%)	47	63
44	Lo	93/94 (99%)	90 (97%)	3 (3%)	34	47
45	Lp	74/75 (99%)	74 (100%)	0	100	100
46	Lr	109/121 (90%)	106 (97%)	3 (3%)	38	52
All	All	5545/6347 (87%)	5486 (99%)	59 (1%)	63	79

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	LA	36	GLU
6	LA	45	VAL
7	LB	138	GLN
7	LB	351	LEU
8	LC	8	ILE
9	LD	83	LEU
10	LE	165	LEU

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Mol	Chain	Res	Type
10	LE	175	VAL
10	LE	191	GLN
10	LE	194	VAL
10	LE	271	LEU
11	LF	248	ASN
12	LG	111	LYS
12	LG	179	VAL
12	LG	211	ASP
14	LI	212	LEU
15	LJ	168	GLN
16	LL	90	VAL
17	LM	55	MET
18	LN	20	ARG
19	LO	33	VAL
19	LO	64	THR
20	LP	24	VAL
20	LP	79	THR
20	LP	119	VAL
21	LQ	147	GLU
21	LQ	188	ASN
23	LS	60	GLU
24	LT	33	ILE
24	LT	111	GLU
25	LU	19	LEU
25	LU	55	ASN
25	LU	63	ILE
25	LU	66	SER
25	LU	79	SER
25	LU	98	ASP
25	LU	109	SER
26	LV	22	VAL
26	LV	65	VAL
27	LW	7	SER
28	LX	54	LEU
29	LY	79	VAL
30	LZ	100	VAL
31	La	15	VAL
35	Le	33	ARG
35	Le	34	ASN
35	Le	86	GLU
35	Le	104	SER
36	Lf	40	GLU

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Mol	Chain	Res	Type
36	Lf	76	ARG
37	Lg	63	VAL
41	Lk	10	ASP
43	Lm	83	ARG
44	Lo	4	VAL
44	Lo	10	THR
44	Lo	102	GLN
46	Lr	24	THR
46	Lr	28	GLU
46	Lr	52	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
6	LA	86	GLN
7	LB	203	GLN
8	LC	38	ASN
8	LC	43	ASN
8	LC	89	GLN
8	LC	245	HIS
8	LC	347	HIS
9	LD	17	GLN
9	LD	202	GLN
9	LD	229	ASN
12	LG	108	GLN
14	LI	73	ASN
17	LM	75	GLN
18	LN	156	HIS
19	LO	42	ASN
19	LO	199	HIS
20	LP	80	GLN
21	LQ	7	HIS
21	LQ	125	GLN
23	LS	122	HIS
25	LU	17	GLN
27	LW	17	HIS
27	LW	50	ASN
31	La	17	HIS
31	La	25	HIS
31	La	28	HIS
31	La	60	HIS
34	Ld	100	ASN

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Mol	Chain	Res	Type
39	Li	26	HIS
41	Lk	28	ASN
44	Lo	51	GLN
46	Lr	6	GLN
46	Lr	21	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	2/3 (66%)	1 (50%)	0
3	L5	3654/5070 (72%)	713 (19%)	37 (1%)
4	L7	119/121 (98%)	11 (9%)	2 (1%)
5	L8	153/157 (97%)	25 (16%)	2 (1%)
All	All	3928/5351 (73%)	750 (19%)	41 (1%)

All (750) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	76	A
3	L5	2	G
3	L5	39	A
3	L5	48	G
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	71	C
3	L5	91	G
3	L5	98	A
3	L5	109	G
3	L5	119	G
3	L5	120	A
3	L5	127	G
3	L5	132	G
3	L5	133	C
3	L5	135	G
3	L5	136	C
3	L5	137	G
3	L5	143	C
3	L5	144	G
3	L5	159	C
3	L5	171	U

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Mol	Chain	Res	Type
3	L5	173	C
3	L5	183	C
3	L5	185	C
3	L5	188	G
3	L5	189	G
3	L5	200	U
3	L5	210	C
3	L5	216	C
3	L5	218	A
3	L5	233	U
3	L5	234	G
3	L5	255	C
3	L5	259	C
3	L5	265	C
3	L5	266	C
3	L5	267	G
3	L5	269	G
3	L5	280	G
3	L5	297	U
3	L5	306	A
3	L5	315	G
3	L5	316	U
3	L5	340	C
3	L5	341	G
3	L5	347	A
3	L5	386	A
3	L5	387	G
3	L5	396	A
3	L5	398	A2M
3	L5	407	A
3	L5	410	A
3	L5	411	G
3	L5	412	G
3	L5	413	G
3	L5	449	C
3	L5	450	G
3	L5	452	A
3	L5	453	G
3	L5	454	U
3	L5	456	C
3	L5	457	G
3	L5	461	G

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Mol	Chain	Res	Type
3	L5	467	U
3	L5	484	U
3	L5	485	C
3	L5	486	C
3	L5	489	C
3	L5	493	G
3	L5	494	U
3	L5	496	G
3	L5	497	G
3	L5	498	C
3	L5	500	G
3	L5	502	C
3	L5	503	C
3	L5	504	G
3	L5	505	G
3	L5	509	A
3	L5	510	U
3	L5	512	U
3	L5	513	U
3	L5	514	U
3	L5	515	C
3	L5	517	C
3	L5	518	G
3	L5	643	C
3	L5	644	G
3	L5	645	G
3	L5	646	G
3	L5	654	C
3	L5	657	C
3	L5	665	C
3	L5	666	G
3	L5	667	A
3	L5	668	C
3	L5	672	C
3	L5	674	G
3	L5	686	A
3	L5	703	G
3	L5	704	C
3	L5	708	G
3	L5	714	G
3	L5	731	G
3	L5	738	C

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Mol	Chain	Res	Type
3	L5	739	G
3	L5	742	G
3	L5	744	G
3	L5	746	A
3	L5	747	A
3	L5	749	G
3	L5	750	U
3	L5	753	C
3	L5	755	C
3	L5	756	G
3	L5	908	G
3	L5	912	G
3	L5	914	U
3	L5	915	A
3	L5	916	C
3	L5	918	G
3	L5	919	C
3	L5	921	C
3	L5	924	C
3	L5	925	C
3	L5	926	G
3	L5	929	A
3	L5	932	A
3	L5	933	G
3	L5	944	A
3	L5	945	U
3	L5	951	G
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	969	C
3	L5	970	G
3	L5	971	U
3	L5	976	G
3	L5	977	C
3	L5	982	U
3	L5	989	U
3	L5	990	C
3	L5	991	C
3	L5	992	C
3	L5	993	G

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Mol	Chain	Res	Type
3	L5	995	C
3	L5	1048	G
3	L5	1049	C
3	L5	1051	G
3	L5	1066	G
3	L5	1069	G
3	L5	1070	G
3	L5	1074	G
3	L5	1083	U
3	L5	1171	G
3	L5	1173	G
3	L5	1178	G
3	L5	1179	U
3	L5	1180	C
3	L5	1182	C
3	L5	1183	C
3	L5	1184	A
3	L5	1191	C
3	L5	1196	G
3	L5	1198	G
3	L5	1202	C
3	L5	1203	G
3	L5	1211	G
3	L5	1214	C
3	L5	1215	C
3	L5	1219	G
3	L5	1222	A
3	L5	1235	G
3	L5	1241	C
3	L5	1254	A
3	L5	1255	A
3	L5	1256	G
3	L5	1257	A
3	L5	1258	G
3	L5	1261	G
3	L5	1266	G
3	L5	1269	G
3	L5	1270	A
3	L5	1271	G
3	L5	1272	C
3	L5	1273	G
3	L5	1274	A

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Mol	Chain	Res	Type
3	L5	1275	G
3	L5	1280	C
3	L5	1284	G
3	L5	1287	G
3	L5	1291	G
3	L5	1293	G
3	L5	1294	A
3	L5	1295	C
3	L5	1296	G
3	L5	1301	C
3	L5	1312	A
3	L5	1326	A2M
3	L5	1337	A
3	L5	1354	A
3	L5	1358	G
3	L5	1359	G
3	L5	1365	C
3	L5	1366	G
3	L5	1367	C
3	L5	1383	G
3	L5	1387	A
3	L5	1394	G
3	L5	1397	A
3	L5	1399	G
3	L5	1402	C
3	L5	1403	G
3	L5	1405	C
3	L5	1407	C
3	L5	1409	C
3	L5	1410	U
3	L5	1420	A
3	L5	1438	U
3	L5	1439	C
3	L5	1440	U
3	L5	1443	A
3	L5	1444	G
3	L5	1446	C
3	L5	1447	C
3	L5	1483	C
3	L5	1489	G
3	L5	1494	U
3	L5	1498	G

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Mol	Chain	Res	Type
3	L5	1502	G
3	L5	1534	A2M
3	L5	1547	A
3	L5	1564	A
3	L5	1575	A
3	L5	1578	U
3	L5	1586	G
3	L5	1591	U
3	L5	1596	U
3	L5	1613	A
3	L5	1614	C
3	L5	1624	G
3	L5	1625	OMG
3	L5	1631	A
3	L5	1633	G
3	L5	1634	A
3	L5	1642	A
3	L5	1654	G
3	L5	1661	C
3	L5	1663	C
3	L5	1676	C
3	L5	1677	PSU
3	L5	1685	G
3	L5	1697	G
3	L5	1699	A
3	L5	1700	G
3	L5	1704	C
3	L5	1705	G
3	L5	1707	C
3	L5	1709	C
3	L5	1717	C
3	L5	1734	G
3	L5	1735	U
3	L5	1742	A
3	L5	1750	G
3	L5	1753	G
3	L5	1757	U
3	L5	1758	G
3	L5	1761	G
3	L5	1762	C
3	L5	1763	C
3	L5	1765	A

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Mol	Chain	Res	Type
3	L5	1766	A
3	L5	1768	C
3	L5	1769	G
3	L5	1770	A
3	L5	1787	A
3	L5	1797	G
3	L5	1804	A
3	L5	1822	U
3	L5	1834	U
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1843	A
3	L5	1855	G
3	L5	1869	G
3	L5	1882	U
3	L5	1897	A
3	L5	1918	U
3	L5	1919	G
3	L5	1920	C
3	L5	1921	C
3	L5	1922	G
3	L5	1931	C
3	L5	1932	A
3	L5	1948	G
3	L5	1949	U
3	L5	1951	G
3	L5	1959	U
3	L5	1961	G
3	L5	1962	A
3	L5	1966	C
3	L5	1967	A
3	L5	1968	G
3	L5	1971	C
3	L5	1974	U
3	L5	1975	G
3	L5	1976	G
3	L5	1977	C
3	L5	1980	U
3	L5	1981	G
3	L5	1982	G
3	L5	1983	A

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Mol	Chain	Res	Type
3	L5	1985	G
3	L5	1987	C
3	L5	1988	G
3	L5	1991	A
3	L5	1993	C
3	L5	1995	G
3	L5	1996	C
3	L5	1999	A
3	L5	2001	G
3	L5	2002	A
3	L5	2003	G
3	L5	2005	G
3	L5	2006	U
3	L5	2007	G
3	L5	2009	A
3	L5	2010	A
3	L5	2011	C
3	L5	2012	A
3	L5	2013	A
3	L5	2014	C
3	L5	2015	U
3	L5	2018	C
3	L5	2019	C
3	L5	2020	U
3	L5	2021	G
3	L5	2025	A
3	L5	2026	A
3	L5	2046	G
3	L5	2048	U
3	L5	2055	G
3	L5	2056	G
3	L5	2069	A
3	L5	2084	C
3	L5	2085	G
3	L5	2091	C
3	L5	2092	G
3	L5	2093	A
3	L5	2094	G
3	L5	2096	G
3	L5	2097	U
3	L5	2098	G
3	L5	2101	C

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Mol	Chain	Res	Type
3	L5	2102	G
3	L5	2106	G
3	L5	2109	G
3	L5	2111	G
3	L5	2112	G
3	L5	2252	G
3	L5	2253	A
3	L5	2255	C
3	L5	2256	C
3	L5	2259	G
3	L5	2277	C
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2304	U
3	L5	2305	U
3	L5	2313	A
3	L5	2314	G
3	L5	2316	G
3	L5	2333	G
3	L5	2348	G
3	L5	2351	C
3	L5	2360	A
3	L5	2364	OMG
3	L5	2397	G
3	L5	2398	U
3	L5	2404	A
3	L5	2417	A
3	L5	2421	G
3	L5	2422	OMC
3	L5	2424	OMG
3	L5	2425	U
3	L5	2441	C
3	L5	2450	G
3	L5	2465	C
3	L5	2474	G
3	L5	2475	G
3	L5	2486	G
3	L5	2488	C
3	L5	2489	C
3	L5	2490	U
3	L5	2491	C

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Mol	Chain	Res	Type
3	L5	2504	C
3	L5	2505	C
3	L5	2506	G
3	L5	2511	A
3	L5	2513	A
3	L5	2519	U
3	L5	2537	A
3	L5	2546	G
3	L5	2547	G
3	L5	2578	G
3	L5	2583	C
3	L5	2587	A
3	L5	2589	C
3	L5	2601	A
3	L5	2618	G
3	L5	2623	A
3	L5	2627	C
3	L5	2638	G
3	L5	2653	C
3	L5	2662	G
3	L5	2669	C
3	L5	2673	G
3	L5	2676	A
3	L5	2686	G
3	L5	2687	U
3	L5	2694	G
3	L5	2695	A
3	L5	2696	A
3	L5	2710	C
3	L5	2711	G
3	L5	2724	G
3	L5	2726	G
3	L5	2729	C
3	L5	2739	C
3	L5	2743	A
3	L5	2746	A
3	L5	2754	G
3	L5	2755	A
3	L5	2756	G
3	L5	2759	G
3	L5	2761	U
3	L5	2762	G

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Mol	Chain	Res	Type
3	L5	2763	U
3	L5	2764	A
3	L5	2769	U
3	L5	2770	C
3	L5	2772	C
3	L5	2788	U
3	L5	2790	U
3	L5	2796	G
3	L5	2814	C
3	L5	2820	C
3	L5	2826	U
3	L5	2827	G
3	L5	2838	G
3	L5	2855	G
3	L5	2877	G
3	L5	2895	A
3	L5	2900	U
3	L5	2903	G
3	L5	2904	U
3	L5	2906	G
3	L5	2907	G
3	L5	2908	U
3	L5	3585	G
3	L5	3587	C
3	L5	3591	C
3	L5	3593	C
3	L5	3594	C
3	L5	3595	U
3	L5	3596	A
3	L5	3597	G
3	L5	3598	C
3	L5	3605	C
3	L5	3606	U
3	L5	3615	G
3	L5	3618	C
3	L5	3625	G
3	L5	3626	G
3	L5	3635	A
3	L5	3644	U
3	L5	3646	A
3	L5	3662	A
3	L5	3673	C

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Mol	Chain	Res	Type
3	L5	3674	G
3	L5	3691	G
3	L5	3709	U
3	L5	3710	G
3	L5	3712	A
3	L5	3713	U
3	L5	3714	G
3	L5	3723	A2M
3	L5	3727	A
3	L5	3729	PSU
3	L5	3734	U
3	L5	3735	G
3	L5	3748	A
3	L5	3750	G
3	L5	3758	U
3	L5	3759	A
3	L5	3771	C
3	L5	3776	G
3	L5	3777	G
3	L5	3783	A
3	L5	3784	A
3	L5	3785	A2M
3	L5	3786	U
3	L5	3802	U
3	L5	3811	G
3	L5	3812	C
3	L5	3814	U
3	L5	3817	A
3	L5	3818	U
3	L5	3819	G
3	L5	3823	G
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3841	C
3	L5	3867	A2M
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3897	G
3	L5	3901	A
3	L5	3905	A

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Mol	Chain	Res	Type
3	L5	3906	A
3	L5	3907	G
3	L5	3908	A
3	L5	3915	U
3	L5	3930	U
3	L5	3939	G
3	L5	3947	A
3	L5	3948	C
3	L5	3949	A
3	L5	3950	U
3	L5	4056	A
3	L5	4059	C
3	L5	4062	A
3	L5	4064	C
3	L5	4065	G
3	L5	4069	U
3	L5	4076	G
3	L5	4077	A
3	L5	4084	G
3	L5	4099	G
3	L5	4101	C
3	L5	4102	C
3	L5	4104	G
3	L5	4107	G
3	L5	4111	U
3	L5	4112	C
3	L5	4113	U
3	L5	4115	G
3	L5	4116	C
3	L5	4119	C
3	L5	4122	G
3	L5	4124	G
3	L5	4127	A
3	L5	4131	G
3	L5	4133	C
3	L5	4137	C
3	L5	4139	G
3	L5	4141	G
3	L5	4142	C
3	L5	4143	G
3	L5	4144	C
3	L5	4150	G

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Mol	Chain	Res	Type
3	L5	4160	C
3	L5	4162	C
3	L5	4163	U
3	L5	4170	A
3	L5	4177	C
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4196	OMG
3	L5	4201	G
3	L5	4203	A
3	L5	4229	U
3	L5	4233	A
3	L5	4251	A
3	L5	4254	G
3	L5	4268	A
3	L5	4270	C
3	L5	4273	A
3	L5	4281	A
3	L5	4290	U
3	L5	4291	G
3	L5	4305	G
3	L5	4313	A
3	L5	4314	C
3	L5	4329	G
3	L5	4330	G
3	L5	4339	A
3	L5	4349	C
3	L5	4352	U
3	L5	4373	G
3	L5	4376	A
3	L5	4377	G
3	L5	4378	A
3	L5	4380	A
3	L5	4381	A
3	L5	4387	C
3	L5	4394	A
3	L5	4421	C
3	L5	4422	A
3	L5	4438	U
3	L5	4444	C
3	L5	4448	G

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Mol	Chain	Res	Type
3	L5	4449	A
3	L5	4452	U
3	L5	4464	A
3	L5	4466	C
3	L5	4475	G
3	L5	4500	PSU
3	L5	4512	U
3	L5	4513	A
3	L5	4519	C
3	L5	4523	A2M
3	L5	4524	G
3	L5	4530	UR3
3	L5	4545	G
3	L5	4548	A
3	L5	4549	G
3	L5	4556	U
3	L5	4560	C
3	L5	4567	G
3	L5	4570	G
3	L5	4573	G
3	L5	4575	G
3	L5	4584	A
3	L5	4590	A
3	L5	4594	U
3	L5	4600	G
3	L5	4601	U
3	L5	4618	G
3	L5	4628	PSU
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4656	A
3	L5	4670	C
3	L5	4672	A
3	L5	4679	G
3	L5	4700	A
3	L5	4708	A
3	L5	4709	U
3	L5	4732	G
3	L5	4734	A
3	L5	4741	C
3	L5	4742	G
3	L5	4745	G

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Mol	Chain	Res	Type
3	L5	4746	C
3	L5	4747	C
3	L5	4751	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4765	G
3	L5	4772	C
3	L5	4775	C
3	L5	4870	OMG
3	L5	4871	C
3	L5	4872	2MG
3	L5	4875	G
3	L5	4881	U
3	L5	4882	U
3	L5	4883	C
3	L5	4888	U
3	L5	4889	G
3	L5	4895	C
3	L5	4896	G
3	L5	4897	G
3	L5	4899	G
3	L5	4900	C
3	L5	4901	G
3	L5	4910	G
3	L5	4912	G
3	L5	4914	C
3	L5	4923	C
3	L5	4925	U
3	L5	4930	C
3	L5	4931	G
3	L5	4932	U
3	L5	4934	A
3	L5	4940	C
3	L5	4941	G
3	L5	4943	A
3	L5	4966	A
3	L5	4976	U
3	L5	4988	U
3	L5	4989	U
3	L5	4990	C

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Mol	Chain	Res	Type
3	L5	4991	U
3	L5	5007	A
3	L5	5009	G
3	L5	5013	C
3	L5	5017	G
3	L5	5022	U
3	L5	5023	C
3	L5	5024	C
3	L5	5025	C
3	L5	5026	U
3	L5	5028	G
3	L5	5030	U
3	L5	5031	G
3	L5	5034	A
3	L5	5041	G
3	L5	5050	C
3	L5	5054	C
3	L5	5061	A
3	L5	5069	U
4	L7	7	G
4	L7	38	U
4	L7	52	C
4	L7	53	U
4	L7	64	G
4	L7	66	G
4	L7	100	A
4	L7	102	U
4	L7	103	A
4	L7	110	G
4	L7	111	C
5	L8	23	C
5	L8	34	U
5	L8	35	C
5	L8	43	A
5	L8	48	A
5	L8	52	A
5	L8	56	G
5	L8	59	A
5	L8	62	A
5	L8	63	U
5	L8	68	G
5	L8	82	A

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Mol	Chain	Res	Type
5	L8	84	A
5	L8	85	U
5	L8	86	U
5	L8	87	G
5	L8	103	A
5	L8	105	C
5	L8	110	U
5	L8	114	G
5	L8	123	U
5	L8	124	U
5	L8	125	C
5	L8	126	C
5	L8	127	U

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	406	C
3	L5	499	G
3	L5	745	G
3	L5	746	A
3	L5	754	U
3	L5	907	C
3	L5	911	U
3	L5	923	C
3	L5	959	G
3	L5	1082	C
3	L5	1197	C
3	L5	1445	U
3	L5	1574	G
3	L5	1590	C
3	L5	1633	G
3	L5	2019	C
3	L5	2097	U
3	L5	2304	U
3	L5	2416	G
3	L5	2485	U
3	L5	2675	G
3	L5	2754	G
3	L5	2760	G
3	L5	2894	A
3	L5	3594	C

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Mol	Chain	Res	Type
3	L5	3597	G
3	L5	3605	C
3	L5	3614	G
3	L5	3673	C
3	L5	3734	U
3	L5	3946	G
3	L5	4123	C
3	L5	4555	U
3	L5	4600	G
3	L5	4678	G
3	L5	4699	U
3	L5	4913	G
4	L7	51	G
4	L7	109	U
5	L8	83	C
5	L8	126	C

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

77 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$
3	2MG	L5	1517	3	23,26,27	2.88	9 (39%)	32,38,41	2.26	11 (34%)
3	OMG	L5	2364	3	23,26,27	2.34	6 (26%)	33,38,41	2.23	10 (30%)
3	A2M	L5	3867	3	22,25,26	3.45	9 (40%)	31,36,39	4.10	12 (38%)
3	PSU	L5	4531	3	18,21,22	1.06	1 (5%)	22,30,33	1.80	4 (18%)
3	2MG	L5	729	3	23,26,27	2.91	8 (34%)	32,38,41	2.36	11 (34%)
3	A2M	L5	1871	47,3	22,25,26	3.47	11 (50%)	31,36,39	4.07	13 (41%)
3	A2M	L5	3723	3	22,25,26	3.45	10 (45%)	31,36,39	4.08	13 (41%)
3	OMC	L5	2804	3	19,22,23	2.94	8 (42%)	26,31,34	0.71	0
3	6MZ	L5	4220	3	22,25,26	2.84	4 (18%)	30,36,39	2.29	10 (33%)
3	PSU	L5	1582	3	18,21,22	1.04	1 (5%)	22,30,33	1.71	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	1524	3	22,25,26	3.44	11 (50%)	31,36,39	4.04	13 (41%)
3	A2M	L5	1534	47,3	22,25,26	3.41	10 (45%)	31,36,39	3.90	12 (38%)
3	OMG	L5	1522	3	23,26,27	2.33	6 (26%)	33,38,41	2.36	10 (30%)
3	OMC	L5	3869	3	19,22,23	2.94	8 (42%)	26,31,34	0.75	0
3	1MA	L5	1322	47,3	21,25,26	2.74	6 (28%)	31,37,40	2.18	8 (25%)
3	B8H	L5	1860	3	19,22,23	6.71	7 (36%)	22,32,35	2.38	5 (22%)
3	OMG	L5	2050	3	23,26,27	2.33	6 (26%)	33,38,41	2.22	9 (27%)
3	PSU	L5	4628	3	18,21,22	1.06	1 (5%)	22,30,33	1.77	4 (18%)
3	B8T	L5	4671	3	19,22,23	3.18	8 (42%)	26,31,34	0.95	1 (3%)
3	OMG	L5	1883	3	23,26,27	2.32	6 (26%)	33,38,41	2.20	9 (27%)
3	OMG	L5	4623	3	23,26,27	2.31	6 (26%)	33,38,41	2.30	10 (30%)
3	5MU	L5	4083	3	19,22,23	7.18	8 (42%)	28,32,35	3.11	10 (35%)
3	A2M	L5	2401	3	22,25,26	3.43	11 (50%)	31,36,39	4.12	13 (41%)
3	A2M	L5	3785	3	22,25,26	3.32	10 (45%)	31,36,39	3.73	15 (48%)
3	OMG	L5	1625	3	23,26,27	2.37	6 (26%)	33,38,41	2.19	9 (27%)
3	PSU	L5	4500	3	18,21,22	1.11	1 (5%)	22,30,33	1.86	5 (22%)
3	A2M	L5	2363	47,3	22,25,26	3.44	8 (36%)	31,36,39	4.13	13 (41%)
3	JMH	L5	1456	3	18,22,23	2.93	7 (38%)	21,32,35	0.82	0
8	MLZ	LC	333	8	8,9,10	0.83	0	4,9,11	0.65	0
3	PSU	L5	1677	3	18,21,22	1.10	2 (11%)	22,30,33	1.85	4 (18%)
3	OMC	L5	3887	3	19,22,23	2.95	8 (42%)	26,31,34	0.77	1 (3%)
3	OMG	L5	4870	3	23,26,27	2.35	6 (26%)	33,38,41	2.31	10 (30%)
43	MLZ	Lm	98	43	8,9,10	0.76	0	4,9,11	0.66	0
3	OMG	L5	373	3	23,26,27	2.32	6 (26%)	33,38,41	2.28	10 (30%)
3	5MC	L5	3782	47,3	18,22,23	3.66	7 (38%)	26,32,35	1.04	2 (7%)
3	A2M	L5	3718	3	22,25,26	3.45	10 (45%)	31,36,39	4.09	13 (41%)
3	OMG	L5	2424	3	23,26,27	2.34	6 (26%)	33,38,41	2.28	9 (27%)
3	B8H	L5	4296	3	19,22,23	6.70	7 (36%)	22,32,35	2.37	5 (22%)
3	PSU	L5	1683	3	18,21,22	1.02	1 (5%)	22,30,33	1.82	3 (13%)
3	UR3	L5	4597	3	19,22,23	3.04	8 (42%)	26,32,35	1.31	3 (11%)
3	OMG	L5	3792	3	23,26,27	2.37	6 (26%)	33,38,41	2.18	9 (27%)
3	A2M	L5	1326	3	22,25,26	3.44	10 (45%)	31,36,39	4.07	12 (38%)
3	PSU	L5	4293	3	18,21,22	1.06	1 (5%)	22,30,33	1.83	3 (13%)
3	OMC	L5	3909	3	19,22,23	2.96	8 (42%)	26,31,34	0.82	0
3	A2M	L5	398	3	22,25,26	3.44	10 (45%)	31,36,39	4.10	13 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UR3	L5	1866	3	19,22,23	2.97	8 (42%)	26,32,35	1.22	2 (7%)
3	OMC	L5	3701	47,3	19,22,23	2.97	8 (42%)	26,31,34	0.87	0
3	OMC	L5	2422	47,3	19,22,23	2.97	8 (42%)	26,31,34	0.77	0
3	PSU	L5	4403	3	18,21,22	1.08	1 (5%)	22,30,33	1.80	4 (18%)
3	OMG	L5	3899	47,3	23,26,27	2.34	6 (26%)	33,38,41	2.30	10 (30%)
3	B8T	L5	4483	3	19,22,23	3.13	8 (42%)	26,31,34	0.86	1 (3%)
3	OMG	L5	4637	3	23,26,27	2.34	6 (26%)	33,38,41	2.27	10 (30%)
3	5MC	L5	4335	3	18,22,23	3.63	7 (38%)	26,32,35	1.07	2 (7%)
3	PSU	L5	3729	3	18,21,22	1.08	1 (5%)	22,30,33	1.82	4 (18%)
3	PSU	L5	4450	47,3	18,21,22	1.02	1 (5%)	22,30,33	1.77	4 (18%)
3	OMC	L5	2365	47,3	19,22,23	2.96	8 (42%)	26,31,34	0.75	0
3	UR3	L5	4530	3	19,22,23	3.03	8 (42%)	26,32,35	1.29	2 (7%)
3	OMG	L5	4494	3	23,26,27	2.36	6 (26%)	33,38,41	2.25	9 (27%)
3	OMC	L5	4536	3	19,22,23	2.95	8 (42%)	26,31,34	0.78	0
3	A2M	L5	4571	3	22,25,26	3.45	9 (40%)	31,36,39	4.17	13 (41%)
3	PSU	L5	3764	3	18,21,22	1.11	1 (5%)	22,30,33	1.79	4 (18%)
3	PSU	L5	2508	3	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
3	PSU	L5	3715	3	18,21,22	1.04	1 (5%)	22,30,33	1.86	5 (22%)
3	OMG	L5	1316	47,3	23,26,27	2.33	6 (26%)	33,38,41	2.25	9 (27%)
3	1MA	L5	4415	3	21,25,26	2.82	7 (33%)	31,37,40	2.46	8 (25%)
3	A2M	L5	3825	3	22,25,26	3.45	11 (50%)	31,36,39	4.04	13 (41%)
3	2MG	L5	978	3	23,26,27	2.91	8 (34%)	32,38,41	2.31	11 (34%)
3	PSU	L5	4442	3	18,21,22	1.10	1 (5%)	22,30,33	1.80	5 (22%)
3	A2M	L5	4523	47,3	22,25,26	3.43	10 (45%)	31,36,39	4.08	13 (41%)
3	OMG	L5	4370	3	23,26,27	2.35	6 (26%)	33,38,41	2.30	10 (30%)
3	2MG	L5	4872	3	23,26,27	2.89	8 (34%)	32,38,41	2.38	11 (34%)
3	OMG	L5	4196	47,3,2	23,26,27	2.35	6 (26%)	33,38,41	2.22	9 (27%)
3	OMG	L5	2773	3	23,26,27	2.34	6 (26%)	33,38,41	2.28	10 (30%)
3	OMC	L5	2861	3	19,22,23	2.98	8 (42%)	26,31,34	0.76	0
3	PSU	L5	4636	3	18,21,22	1.04	1 (5%)	22,30,33	1.85	5 (22%)
3	B8H	L5	3762	3	19,22,23	6.66	7 (36%)	22,32,35	2.34	6 (27%)
3	5MC	L5	4447	3	18,22,23	3.63	7 (38%)	26,32,35	1.23	3 (11%)

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
3	2MG	L5	1517	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	2364	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	3867	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4531	3	-	0/7/25/26	0/2/2/2
3	2MG	L5	729	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	1871	47,3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3723	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1534	47,3	-	2/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	1MA	L5	1322	47,3	-	0/7/25/26	0/3/3/3
3	B8H	L5	1860	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2050	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	2/7/25/26	0/2/2/2
3	B8T	L5	4671	3	-	0/7/27/28	0/2/2/2
3	OMG	L5	1883	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	5MU	L5	4083	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2401	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3785	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	1625	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
3	A2M	L5	2363	47,3	-	0/9/27/28	0/3/3/3
3	JMH	L5	1456	3	-	0/7/25/26	0/2/2/2
8	MLZ	LC	333	8	-	2/7/8/10	-
3	PSU	L5	1677	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	3887	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4870	3	-	3/9/27/28	0/3/3/3
43	MLZ	Lm	98	43	-	1/7/8/10	-
3	OMG	L5	373	3	-	0/9/27/28	0/3/3/3
3	5MC	L5	3782	47,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3718	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	2424	3	-	2/9/27/28	0/3/3/3
3	B8H	L5	4296	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	UR3	L5	4597	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4293	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	3909	3	-	2/9/27/28	0/2/2/2
3	A2M	L5	398	3	-	2/9/27/28	0/3/3/3
3	UR3	L5	1866	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	3701	47,3	-	4/9/27/28	0/2/2/2
3	OMC	L5	2422	47,3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4403	3	-	3/7/25/26	0/2/2/2
3	OMG	L5	3899	47,3	-	0/9/27/28	0/3/3/3
3	B8T	L5	4483	3	-	0/7/27/28	0/2/2/2
3	OMG	L5	4637	3	-	0/9/27/28	0/3/3/3
3	5MC	L5	4335	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3729	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4450	47,3	-	4/7/25/26	0/2/2/2
3	OMC	L5	2365	47,3	-	0/9/27/28	0/2/2/2
3	UR3	L5	4530	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	4494	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3764	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	2508	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1316	47,3	-	0/9/27/28	0/3/3/3
3	1MA	L5	4415	3	-	0/7/25/26	0/3/3/3
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
3	2MG	L5	978	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	47,3	-	2/9/27/28	0/3/3/3
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
3	2MG	L5	4872	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	4196	47,3,2	-	2/9/27/28	0/3/3/3
3	OMG	L5	2773	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4636	3	-	4/7/25/26	0/2/2/2
3	B8H	L5	3762	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	3	-	2/7/25/26	0/2/2/2

All (477) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4083	5MU	C4-C5	20.86	1.79	1.44
3	L5	1860	B8H	C6-C5	-15.45	1.13	1.34
3	L5	4296	B8H	C6-C5	-15.42	1.13	1.34
3	L5	4083	5MU	C6-N1	15.22	1.64	1.38
3	L5	3762	B8H	C6-C5	-15.06	1.13	1.34
3	L5	1860	B8H	C4-N3	-13.97	1.12	1.38
3	L5	4296	B8H	C4-N3	-13.92	1.13	1.38
3	L5	3762	B8H	C4-C5	13.70	1.83	1.44
3	L5	3762	B8H	C4-N3	-13.63	1.13	1.38
3	L5	4296	B8H	C4-C5	13.52	1.82	1.44
3	L5	1860	B8H	C4-C5	13.49	1.82	1.44
3	L5	3762	B8H	C6-N1	13.26	1.69	1.36
3	L5	4296	B8H	C6-N1	13.08	1.68	1.36
3	L5	1860	B8H	C6-N1	13.08	1.68	1.36
3	L5	4220	6MZ	C6-N6	11.79	1.47	1.34
3	L5	4083	5MU	C6-C5	-11.67	1.15	1.34
3	L5	4083	5MU	C4-N3	-11.40	1.17	1.38
3	L5	4447	5MC	C6-C5	9.39	1.50	1.34
3	L5	3782	5MC	C6-C5	9.20	1.49	1.34
3	L5	4335	5MC	C6-C5	9.16	1.49	1.34
3	L5	2363	A2M	C2'-C1'	-8.65	1.30	1.53
3	L5	4571	A2M	O4'-C1'	8.62	1.62	1.42
3	L5	1871	A2M	C2'-C1'	-8.61	1.30	1.53
3	L5	3867	A2M	C2'-C1'	-8.60	1.30	1.53
3	L5	1326	A2M	C2'-C1'	-8.58	1.31	1.53
3	L5	4415	1MA	C2-N3	8.54	1.46	1.30
3	L5	3825	A2M	C2'-C1'	-8.54	1.31	1.53
3	L5	1524	A2M	C2'-C1'	-8.51	1.31	1.53
3	L5	3723	A2M	O4'-C1'	8.50	1.62	1.42
3	L5	3723	A2M	C2'-C1'	-8.49	1.31	1.53
3	L5	3718	A2M	O4'-C1'	8.48	1.62	1.42
3	L5	3718	A2M	C2'-C1'	-8.47	1.31	1.53
3	L5	4523	A2M	O4'-C1'	8.47	1.62	1.42
3	L5	398	A2M	C2'-C1'	-8.47	1.31	1.53
3	L5	2401	A2M	C2'-C1'	-8.47	1.31	1.53
3	L5	1871	A2M	O4'-C1'	8.44	1.62	1.42
3	L5	398	A2M	O4'-C1'	8.43	1.62	1.42
3	L5	2363	A2M	O4'-C1'	8.41	1.61	1.42
3	L5	1534	A2M	O4'-C1'	8.40	1.61	1.42
3	L5	1534	A2M	C2'-C1'	-8.40	1.31	1.53
3	L5	2401	A2M	O4'-C1'	8.39	1.61	1.42
3	L5	3825	A2M	O4'-C1'	8.36	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4523	A2M	C2'-C1'	-8.34	1.31	1.53
3	L5	4571	A2M	C2'-C1'	-8.32	1.31	1.53
3	L5	3867	A2M	O4'-C1'	8.26	1.61	1.42
3	L5	1524	A2M	O4'-C1'	8.25	1.61	1.42
3	L5	1326	A2M	O4'-C1'	8.24	1.61	1.42
3	L5	1322	1MA	C2-N3	8.22	1.45	1.30
3	L5	3785	A2M	C2'-C1'	-8.20	1.32	1.53
3	L5	3785	A2M	O4'-C1'	8.05	1.61	1.42
3	L5	1456	JMH	C2-N1	7.64	1.49	1.38
3	L5	4872	2MG	C2-N3	7.50	1.46	1.31
3	L5	729	2MG	C2-N3	7.41	1.46	1.31
3	L5	4597	UR3	C2-N1	7.40	1.49	1.38
3	L5	978	2MG	C2-N3	7.34	1.46	1.31
3	L5	1517	2MG	C2-N3	7.22	1.45	1.31
3	L5	4530	UR3	C2-N1	7.21	1.48	1.38
3	L5	1866	UR3	C2-N1	7.07	1.48	1.38
3	L5	4530	UR3	C6-C5	6.74	1.50	1.35
3	L5	4671	B8T	C4-N3	6.68	1.44	1.32
3	L5	4597	UR3	C6-C5	6.66	1.50	1.35
3	L5	3867	A2M	O4'-C4'	-6.65	1.30	1.45
3	L5	1866	UR3	C6-C5	6.63	1.50	1.35
3	L5	1326	A2M	O4'-C4'	-6.60	1.30	1.45
3	L5	4483	B8T	C4-N3	6.57	1.44	1.32
3	L5	1524	A2M	O4'-C4'	-6.56	1.30	1.45
3	L5	3792	OMG	C4-N3	6.50	1.49	1.34
3	L5	3825	A2M	O4'-C4'	-6.50	1.30	1.45
3	L5	1871	A2M	O4'-C4'	-6.49	1.30	1.45
3	L5	398	A2M	O4'-C4'	-6.49	1.30	1.45
3	L5	3723	A2M	O4'-C4'	-6.48	1.30	1.45
3	L5	2363	A2M	O4'-C4'	-6.47	1.30	1.45
3	L5	1534	A2M	O4'-C4'	-6.47	1.30	1.45
3	L5	1625	OMG	C4-N3	6.45	1.49	1.34
3	L5	4196	OMG	C4-N3	6.44	1.49	1.34
3	L5	3782	5MC	C2-N3	6.43	1.49	1.36
3	L5	4370	OMG	C4-N3	6.42	1.49	1.34
3	L5	4523	A2M	O4'-C4'	-6.42	1.30	1.45
3	L5	729	2MG	C2-N2	6.42	1.47	1.33
3	L5	4870	OMG	C4-N3	6.41	1.49	1.34
3	L5	978	2MG	C2-N2	6.40	1.47	1.33
3	L5	4571	A2M	O4'-C4'	-6.40	1.30	1.45
3	L5	4637	OMG	C4-N3	6.40	1.49	1.34
3	L5	2401	A2M	O4'-C4'	-6.39	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3718	A2M	O4'-C4'	-6.39	1.30	1.45
3	L5	2050	OMG	C4-N3	6.39	1.49	1.34
3	L5	4335	5MC	C2-N3	6.38	1.49	1.36
3	L5	4494	OMG	C4-N3	6.37	1.49	1.34
3	L5	1316	OMG	C4-N3	6.37	1.49	1.34
3	L5	2364	OMG	C4-N3	6.35	1.49	1.34
3	L5	2424	OMG	C4-N3	6.35	1.49	1.34
3	L5	1522	OMG	C4-N3	6.35	1.49	1.34
3	L5	373	OMG	C4-N3	6.35	1.49	1.34
3	L5	3899	OMG	C4-N3	6.35	1.49	1.34
3	L5	2773	OMG	C4-N3	6.33	1.49	1.34
3	L5	2422	OMC	C2-N3	6.33	1.49	1.36
3	L5	1883	OMG	C4-N3	6.32	1.49	1.34
3	L5	729	2MG	C4-N3	6.31	1.49	1.34
3	L5	1517	2MG	C2-N2	6.29	1.47	1.33
3	L5	2861	OMC	C2-N3	6.29	1.49	1.36
3	L5	3782	5MC	C4-N3	6.29	1.44	1.34
3	L5	4415	1MA	C4-N3	6.28	1.48	1.35
3	L5	4872	2MG	C4-N3	6.27	1.49	1.34
3	L5	4623	OMG	C4-N3	6.26	1.49	1.34
3	L5	3887	OMC	C2-N3	6.26	1.49	1.36
3	L5	3909	OMC	C2-N3	6.24	1.49	1.36
3	L5	2365	OMC	C2-N3	6.23	1.49	1.36
3	L5	4335	5MC	C4-N3	6.23	1.44	1.34
3	L5	3785	A2M	O4'-C4'	-6.22	1.31	1.45
3	L5	978	2MG	C4-N3	6.21	1.49	1.34
3	L5	4536	OMC	C2-N3	6.21	1.48	1.36
3	L5	3701	OMC	C2-N3	6.21	1.48	1.36
3	L5	1517	2MG	C4-N3	6.19	1.49	1.34
3	L5	4872	2MG	C2-N2	6.16	1.47	1.33
3	L5	2804	OMC	C2-N3	6.13	1.48	1.36
3	L5	1322	1MA	C4-N3	6.13	1.48	1.35
3	L5	4671	B8T	C2-N3	6.12	1.48	1.36
3	L5	4447	5MC	C2-N3	6.12	1.48	1.36
3	L5	3869	OMC	C2-N3	6.11	1.48	1.36
3	L5	4296	B8H	O4-C4	-6.09	1.12	1.23
3	L5	3701	OMC	C6-C5	6.06	1.49	1.35
3	L5	1860	B8H	O4-C4	-6.06	1.12	1.23
3	L5	4483	B8T	C6-C5	6.05	1.49	1.35
3	L5	4671	B8T	C6-C5	6.04	1.49	1.35
3	L5	4483	B8T	C2-N3	6.00	1.48	1.36
3	L5	2804	OMC	C6-C5	5.98	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3887	OMC	C6-C5	5.96	1.48	1.35
3	L5	3909	OMC	C6-C5	5.96	1.48	1.35
3	L5	4536	OMC	C6-C5	5.95	1.48	1.35
3	L5	2365	OMC	C6-C5	5.94	1.48	1.35
3	L5	2861	OMC	C6-C5	5.93	1.48	1.35
3	L5	3869	OMC	C6-C5	5.93	1.48	1.35
3	L5	2422	OMC	C6-C5	5.91	1.48	1.35
3	L5	3762	B8H	O4-C4	-5.89	1.12	1.23
3	L5	4447	5MC	C4-N3	5.82	1.44	1.34
3	L5	1625	OMG	C2-N3	5.81	1.47	1.33
3	L5	4196	OMG	C2-N3	5.80	1.47	1.33
3	L5	4637	OMG	C2-N3	5.80	1.47	1.33
3	L5	3792	OMG	C2-N3	5.78	1.47	1.33
3	L5	4494	OMG	C2-N3	5.76	1.47	1.33
3	L5	2050	OMG	C2-N3	5.73	1.47	1.33
3	L5	2424	OMG	C2-N3	5.71	1.47	1.33
3	L5	4370	OMG	C2-N3	5.70	1.46	1.33
3	L5	3899	OMG	C2-N3	5.69	1.46	1.33
3	L5	1316	OMG	C2-N3	5.68	1.46	1.33
3	L5	2773	OMG	C2-N3	5.67	1.46	1.33
3	L5	4597	UR3	C2-N3	5.67	1.50	1.39
3	L5	2364	OMG	C2-N3	5.67	1.46	1.33
3	L5	373	OMG	C2-N3	5.64	1.46	1.33
3	L5	4870	OMG	C2-N3	5.63	1.46	1.33
3	L5	1883	OMG	C2-N3	5.63	1.46	1.33
3	L5	4623	OMG	C2-N3	5.56	1.46	1.33
3	L5	1522	OMG	C2-N3	5.56	1.46	1.33
3	L5	4530	UR3	C2-N3	5.55	1.49	1.39
3	L5	1866	UR3	C2-N3	5.40	1.49	1.39
3	L5	1456	JMH	C6-C5	5.32	1.47	1.35
3	L5	2365	OMC	C4-N3	5.05	1.44	1.34
3	L5	4536	OMC	C4-N3	5.02	1.44	1.34
3	L5	2422	OMC	C4-N3	5.00	1.44	1.34
3	L5	978	2MG	C2-N1	4.99	1.44	1.36
3	L5	2861	OMC	C4-N3	4.99	1.44	1.34
3	L5	3887	OMC	C4-N3	4.97	1.44	1.34
3	L5	3869	OMC	C4-N3	4.95	1.44	1.34
3	L5	3909	OMC	C4-N3	4.93	1.44	1.34
3	L5	3701	OMC	C4-N3	4.93	1.44	1.34
3	L5	2804	OMC	C4-N3	4.92	1.44	1.34
3	L5	3701	OMC	C4-N4	4.84	1.45	1.33
3	L5	729	2MG	C2-N1	4.83	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2861	OMC	C4-N4	4.83	1.45	1.33
3	L5	2422	OMC	C4-N4	4.82	1.45	1.33
3	L5	3887	OMC	C4-N4	4.82	1.45	1.33
3	L5	1517	2MG	C2-N1	4.82	1.44	1.36
3	L5	4536	OMC	C4-N4	4.81	1.45	1.33
3	L5	2365	OMC	C4-N4	4.79	1.45	1.33
3	L5	3909	OMC	C4-N4	4.78	1.45	1.33
3	L5	3869	OMC	C4-N4	4.78	1.45	1.33
3	L5	3782	5MC	C4-N4	4.78	1.46	1.34
3	L5	4447	5MC	C6-N1	4.78	1.46	1.38
3	L5	2804	OMC	C4-N4	4.77	1.45	1.33
3	L5	4335	5MC	C4-N4	4.76	1.46	1.34
3	L5	4872	2MG	C2-N1	4.71	1.44	1.36
3	L5	4447	5MC	C4-N4	4.71	1.46	1.34
3	L5	3782	5MC	C6-N1	4.68	1.46	1.38
3	L5	4335	5MC	C6-N1	4.63	1.45	1.38
3	L5	4671	B8T	C4-N4	4.62	1.45	1.35
3	L5	4483	B8T	C4-N4	4.60	1.45	1.35
3	L5	4571	A2M	C6-N6	4.52	1.45	1.34
3	L5	3825	A2M	C6-N6	4.51	1.45	1.34
3	L5	3723	A2M	C6-N6	4.51	1.45	1.34
3	L5	3867	A2M	C6-N6	4.50	1.45	1.34
3	L5	1524	A2M	C6-N6	4.48	1.45	1.34
3	L5	1534	A2M	C6-N6	4.46	1.45	1.34
3	L5	1871	A2M	C6-N6	4.46	1.45	1.34
3	L5	3718	A2M	C6-N6	4.45	1.45	1.34
3	L5	4523	A2M	C6-N6	4.44	1.45	1.34
3	L5	2401	A2M	C6-N6	4.43	1.45	1.34
3	L5	4415	1MA	C2-N1	4.43	1.44	1.35
3	L5	398	A2M	C6-N6	4.43	1.45	1.34
3	L5	3762	B8H	C2-N3	4.42	1.45	1.38
3	L5	1326	A2M	C6-N6	4.42	1.45	1.34
3	L5	2363	A2M	C6-N6	4.41	1.45	1.34
3	L5	1456	JMH	O2-C2	-4.41	1.14	1.22
3	L5	3785	A2M	C6-N6	4.39	1.45	1.34
3	L5	4671	B8T	C2-N1	4.38	1.49	1.40
3	L5	2422	OMC	C2-N1	4.36	1.49	1.40
3	L5	2861	OMC	C2-N1	4.36	1.49	1.40
3	L5	3701	OMC	C2-N1	4.36	1.49	1.40
3	L5	3782	5MC	C2-N1	4.35	1.49	1.40
3	L5	3909	OMC	C2-N1	4.34	1.49	1.40
3	L5	3869	OMC	C2-N1	4.32	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4335	5MC	C2-N1	4.32	1.49	1.40
3	L5	4447	5MC	C2-N1	4.30	1.49	1.40
3	L5	2365	OMC	C2-N1	4.30	1.49	1.40
3	L5	4536	OMC	C2-N1	4.29	1.49	1.40
3	L5	2804	OMC	C2-N1	4.24	1.49	1.40
3	L5	3887	OMC	C2-N1	4.24	1.49	1.40
3	L5	1322	1MA	C2-N1	4.19	1.43	1.35
3	L5	4483	B8T	C2-N1	4.12	1.48	1.40
3	L5	4296	B8H	C2-N3	4.11	1.45	1.38
3	L5	1860	B8H	C2-N3	4.04	1.45	1.38
3	L5	4083	5MU	C2-N3	3.98	1.45	1.38
3	L5	1625	OMG	C2-N2	3.87	1.43	1.34
3	L5	2773	OMG	C2-N2	3.86	1.43	1.34
3	L5	2364	OMG	C2-N2	3.84	1.43	1.34
3	L5	4870	OMG	C2-N2	3.84	1.43	1.34
3	L5	3792	OMG	C2-N2	3.83	1.43	1.34
3	L5	4370	OMG	C2-N2	3.83	1.43	1.34
3	L5	4494	OMG	C2-N2	3.80	1.43	1.34
3	L5	4623	OMG	C2-N2	3.80	1.43	1.34
3	L5	2424	OMG	C2-N2	3.80	1.43	1.34
3	L5	1456	JMH	C6-N1	3.79	1.47	1.38
3	L5	1522	OMG	C2-N2	3.78	1.43	1.34
3	L5	4196	OMG	C2-N2	3.77	1.43	1.34
3	L5	1316	OMG	C2-N2	3.76	1.43	1.34
3	L5	4637	OMG	C2-N2	3.76	1.43	1.34
3	L5	3899	OMG	C2-N2	3.73	1.43	1.34
3	L5	2050	OMG	C2-N2	3.72	1.43	1.34
3	L5	373	OMG	C2-N2	3.69	1.43	1.34
3	L5	1883	OMG	C2-N2	3.68	1.42	1.34
3	L5	4671	B8T	C5-C4	3.67	1.48	1.40
3	L5	3764	PSU	C6-C5	3.66	1.39	1.35
3	L5	4083	5MU	C2-N1	3.62	1.44	1.38
3	L5	1456	JMH	C5-C4	3.61	1.51	1.42
3	L5	4483	B8T	C5-C4	3.60	1.48	1.40
3	L5	4220	6MZ	C5-C4	-3.53	1.32	1.39
3	L5	1866	UR3	O2-C2	-3.52	1.16	1.22
3	L5	4597	UR3	O2-C2	-3.47	1.16	1.22
3	L5	1322	1MA	C5-C6	3.44	1.52	1.43
3	L5	4500	PSU	C6-C5	3.43	1.39	1.35
3	L5	4530	UR3	O2-C2	-3.43	1.16	1.22
3	L5	4530	UR3	C6-N1	3.41	1.46	1.38
3	L5	4415	1MA	C5-C6	3.40	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1456	JMH	C2-N3	3.40	1.45	1.39
3	L5	4531	PSU	C6-C5	3.39	1.39	1.35
3	L5	2773	OMG	C2-N1	3.39	1.46	1.37
3	L5	4442	PSU	C6-C5	3.39	1.39	1.35
3	L5	1866	UR3	C6-N1	3.38	1.46	1.38
3	L5	3792	OMG	C2-N1	3.37	1.46	1.37
3	L5	4870	OMG	C2-N1	3.37	1.46	1.37
3	L5	4597	UR3	C6-N1	3.37	1.46	1.38
3	L5	1883	OMG	C5-N7	-3.36	1.32	1.39
3	L5	4370	OMG	C2-N1	3.36	1.46	1.37
3	L5	4403	PSU	C6-C5	3.35	1.39	1.35
3	L5	2424	OMG	C2-N1	3.35	1.46	1.37
3	L5	4494	OMG	C2-N1	3.34	1.45	1.37
3	L5	3899	OMG	C2-N1	3.33	1.45	1.37
3	L5	3729	PSU	C6-C5	3.31	1.39	1.35
3	L5	1625	OMG	C5-N7	-3.31	1.32	1.39
3	L5	4494	OMG	C5-N7	-3.31	1.32	1.39
3	L5	2364	OMG	C2-N1	3.30	1.45	1.37
3	L5	1316	OMG	C5-N7	-3.30	1.32	1.39
3	L5	4293	PSU	C6-C5	3.30	1.39	1.35
3	L5	4196	OMG	C5-N7	-3.30	1.32	1.39
3	L5	1625	OMG	C2-N1	3.30	1.45	1.37
3	L5	4623	OMG	C2-N1	3.29	1.45	1.37
3	L5	1522	OMG	C2-N1	3.28	1.45	1.37
3	L5	1883	OMG	C2-N1	3.28	1.45	1.37
3	L5	3792	OMG	C5-N7	-3.28	1.32	1.39
3	L5	2050	OMG	C2-N1	3.27	1.45	1.37
3	L5	4196	OMG	C2-N1	3.27	1.45	1.37
3	L5	2364	OMG	C5-N7	-3.27	1.32	1.39
3	L5	2050	OMG	C5-N7	-3.27	1.32	1.39
3	L5	4628	PSU	C6-C5	3.26	1.39	1.35
3	L5	4636	PSU	C6-C5	3.25	1.39	1.35
3	L5	4637	OMG	C2-N1	3.24	1.45	1.37
3	L5	1582	PSU	C6-C5	3.23	1.39	1.35
3	L5	4450	PSU	C6-C5	3.23	1.39	1.35
3	L5	1316	OMG	C2-N1	3.22	1.45	1.37
3	L5	373	OMG	C5-N7	-3.22	1.32	1.39
3	L5	4637	OMG	C5-N7	-3.22	1.32	1.39
3	L5	373	OMG	C2-N1	3.21	1.45	1.37
3	L5	3715	PSU	C6-C5	3.21	1.39	1.35
3	L5	2508	PSU	C6-C5	3.20	1.39	1.35
3	L5	3701	OMC	C6-N1	3.19	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1522	OMG	C5-N7	-3.19	1.32	1.39
3	L5	3899	OMG	C5-N7	-3.18	1.32	1.39
3	L5	2424	OMG	C5-N7	-3.18	1.32	1.39
3	L5	4370	OMG	C5-N7	-3.15	1.33	1.39
3	L5	4623	OMG	C5-N7	-3.15	1.33	1.39
3	L5	4870	OMG	C5-N7	-3.15	1.33	1.39
3	L5	2804	OMC	C6-N1	3.15	1.45	1.38
3	L5	2773	OMG	C5-N7	-3.14	1.33	1.39
3	L5	3869	OMC	C6-N1	3.13	1.45	1.38
3	L5	1683	PSU	C6-C5	3.13	1.39	1.35
3	L5	2422	OMC	C6-N1	3.12	1.45	1.38
3	L5	2861	OMC	C6-N1	3.11	1.45	1.38
3	L5	4447	5MC	O2-C2	-3.10	1.18	1.23
3	L5	2401	A2M	C5-C4	-3.10	1.33	1.39
3	L5	1871	A2M	O3'-C3'	-3.09	1.35	1.43
3	L5	4671	B8T	C6-N1	3.09	1.45	1.38
3	L5	2365	OMC	C6-N1	3.08	1.45	1.38
3	L5	1677	PSU	C6-C5	3.07	1.38	1.35
3	L5	1524	A2M	O3'-C3'	-3.07	1.35	1.43
3	L5	1871	A2M	C5-C4	-3.07	1.33	1.39
3	L5	4483	B8T	C6-N1	3.06	1.45	1.38
3	L5	1860	B8H	O2-C2	-3.06	1.17	1.23
3	L5	4872	2MG	C5-N7	-3.05	1.33	1.39
3	L5	3825	A2M	O3'-C3'	-3.05	1.35	1.43
3	L5	3887	OMC	C6-N1	3.05	1.45	1.38
3	L5	4536	OMC	C6-N1	3.04	1.45	1.38
3	L5	3785	A2M	C5-C4	-3.04	1.33	1.39
3	L5	1524	A2M	C5-C4	-3.04	1.33	1.39
3	L5	3909	OMC	C6-N1	3.04	1.45	1.38
3	L5	2861	OMC	O2-C2	-3.04	1.18	1.23
3	L5	3909	OMC	O2-C2	-3.03	1.18	1.23
3	L5	1534	A2M	C5-C4	-3.03	1.33	1.39
3	L5	2363	A2M	C5-C4	-3.02	1.33	1.39
3	L5	3825	A2M	C5-C4	-3.01	1.33	1.39
3	L5	3867	A2M	O3'-C3'	-3.01	1.35	1.43
3	L5	398	A2M	O3'-C3'	-3.01	1.35	1.43
3	L5	4571	A2M	O3'-C3'	-3.00	1.35	1.43
3	L5	1326	A2M	C5-C4	-3.00	1.33	1.39
3	L5	3718	A2M	O3'-C3'	-3.00	1.35	1.43
3	L5	1322	1MA	C5-N7	-2.99	1.33	1.39
3	L5	4523	A2M	C5-C4	-2.99	1.33	1.39
3	L5	4523	A2M	O3'-C3'	-2.99	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2363	A2M	O3'-C3'	-2.98	1.35	1.43
3	L5	1517	2MG	C5-N7	-2.98	1.33	1.39
3	L5	3718	A2M	C8-N9	-2.98	1.32	1.37
3	L5	2401	A2M	O3'-C3'	-2.96	1.36	1.43
3	L5	3723	A2M	O3'-C3'	-2.96	1.36	1.43
3	L5	729	2MG	C5-N7	-2.96	1.33	1.39
3	L5	398	A2M	C5-C4	-2.96	1.33	1.39
3	L5	3867	A2M	C5-C4	-2.95	1.33	1.39
3	L5	978	2MG	C5-N7	-2.95	1.33	1.39
3	L5	3825	A2M	O2'-C2'	2.95	1.50	1.42
3	L5	2422	OMC	O2-C2	-2.94	1.18	1.23
3	L5	398	A2M	O2'-C2'	2.94	1.50	1.42
3	L5	1326	A2M	O3'-C3'	-2.94	1.36	1.43
3	L5	4296	B8H	O2-C2	-2.93	1.17	1.23
3	L5	4415	1MA	C5-N7	-2.93	1.33	1.39
3	L5	3867	A2M	O2'-C2'	2.92	1.50	1.42
3	L5	4335	5MC	O2-C2	-2.92	1.18	1.23
3	L5	4571	A2M	C8-N9	-2.91	1.32	1.37
3	L5	2804	OMC	O2-C2	-2.91	1.18	1.23
3	L5	1326	A2M	O2'-C2'	2.91	1.50	1.42
3	L5	3723	A2M	C5-C4	-2.91	1.33	1.39
3	L5	3782	5MC	O2-C2	-2.89	1.18	1.23
3	L5	3723	A2M	O2'-C2'	2.89	1.50	1.42
3	L5	3718	A2M	C5-C4	-2.89	1.33	1.39
3	L5	4483	B8T	O2-C2	-2.88	1.18	1.23
3	L5	2401	A2M	O2'-C2'	2.88	1.50	1.42
3	L5	3718	A2M	O2'-C2'	2.87	1.50	1.42
3	L5	4571	A2M	C5-C4	-2.87	1.33	1.39
3	L5	2365	OMC	O2-C2	-2.87	1.18	1.23
3	L5	4523	A2M	O2'-C2'	2.86	1.50	1.42
3	L5	4571	A2M	O2'-C2'	2.86	1.49	1.42
3	L5	4220	6MZ	C8-N9	-2.85	1.32	1.37
3	L5	3887	OMC	O2-C2	-2.85	1.18	1.23
3	L5	1524	A2M	O2'-C2'	2.85	1.49	1.42
3	L5	4536	OMC	O2-C2	-2.84	1.18	1.23
3	L5	2363	A2M	O2'-C2'	2.84	1.49	1.42
3	L5	4083	5MU	O4-C4	-2.84	1.18	1.23
3	L5	3869	OMC	O2-C2	-2.83	1.18	1.23
3	L5	3701	OMC	O2-C2	-2.83	1.18	1.23
3	L5	4671	B8T	O2-C2	-2.82	1.18	1.23
3	L5	1871	A2M	O2'-C2'	2.82	1.49	1.42
3	L5	1322	1MA	C4-N9	-2.82	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4870	OMG	C5-C6	2.81	1.54	1.44
3	L5	1534	A2M	O3'-C3'	-2.80	1.36	1.43
3	L5	3792	OMG	C5-C6	2.79	1.54	1.44
3	L5	4637	OMG	C5-C6	2.78	1.54	1.44
3	L5	3762	B8H	O2-C2	-2.78	1.18	1.23
3	L5	3899	OMG	C5-C6	2.77	1.54	1.44
3	L5	2773	OMG	C5-C6	2.77	1.54	1.44
3	L5	4196	OMG	C5-C6	2.77	1.54	1.44
3	L5	1871	A2M	C8-N9	-2.77	1.32	1.37
3	L5	4623	OMG	C5-C6	2.76	1.54	1.44
3	L5	1522	OMG	C5-C6	2.76	1.54	1.44
3	L5	4370	OMG	C5-C6	2.76	1.54	1.44
3	L5	2050	OMG	C5-C6	2.75	1.54	1.44
3	L5	2364	OMG	C5-C6	2.74	1.54	1.44
3	L5	4494	OMG	C5-C6	2.74	1.54	1.44
3	L5	1524	A2M	C8-N9	-2.72	1.32	1.37
3	L5	1625	OMG	C5-C6	2.72	1.54	1.44
3	L5	2424	OMG	C5-C6	2.72	1.54	1.44
3	L5	3785	A2M	O2'-C2'	2.72	1.49	1.42
3	L5	1316	OMG	C5-C6	2.71	1.54	1.44
3	L5	3825	A2M	C8-N9	-2.69	1.32	1.37
3	L5	373	OMG	C5-C6	2.68	1.54	1.44
3	L5	2401	A2M	C8-N9	-2.68	1.32	1.37
3	L5	4415	1MA	C4-N9	-2.68	1.31	1.38
3	L5	3723	A2M	C8-N9	-2.68	1.32	1.37
3	L5	1326	A2M	C8-N9	-2.67	1.32	1.37
3	L5	4083	5MU	O2-C2	-2.65	1.18	1.23
3	L5	1456	JMH	C31-N3	2.65	1.51	1.47
3	L5	1534	A2M	O2'-C2'	2.64	1.49	1.42
3	L5	1883	OMG	C5-C6	2.64	1.54	1.44
3	L5	2363	A2M	C8-N9	-2.63	1.32	1.37
3	L5	3867	A2M	C8-N9	-2.61	1.32	1.37
3	L5	4530	UR3	C4-N3	2.61	1.46	1.40
3	L5	4872	2MG	C5-C6	2.60	1.54	1.44
3	L5	729	2MG	C5-C6	2.59	1.54	1.44
3	L5	4597	UR3	C4-N3	2.57	1.46	1.40
3	L5	978	2MG	C5-C6	2.57	1.54	1.44
3	L5	4530	UR3	C5-C4	2.56	1.50	1.43
3	L5	4523	A2M	C8-N9	-2.54	1.33	1.37
3	L5	1517	2MG	C5-C6	2.54	1.53	1.44
3	L5	1866	UR3	C5-C4	2.52	1.50	1.43
3	L5	398	A2M	C8-N9	-2.51	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1866	UR3	C4-N3	2.49	1.46	1.40
3	L5	978	2MG	C6-N1	2.49	1.43	1.38
3	L5	4597	UR3	C5-C4	2.48	1.50	1.43
3	L5	1677	PSU	O4'-C1'	-2.46	1.40	1.43
3	L5	1534	A2M	C8-N9	-2.45	1.33	1.37
3	L5	3785	A2M	O3'-C3'	-2.44	1.37	1.43
3	L5	1866	UR3	O4-C4	-2.44	1.18	1.23
3	L5	1517	2MG	O6-C6	-2.43	1.19	1.23
3	L5	2861	OMC	C5-C4	2.43	1.48	1.42
3	L5	3701	OMC	C5-C4	2.42	1.48	1.42
3	L5	3785	A2M	C8-N9	-2.42	1.33	1.37
3	L5	3887	OMC	C5-C4	2.41	1.48	1.42
3	L5	4530	UR3	O4-C4	-2.41	1.18	1.23
3	L5	1517	2MG	C6-N1	2.40	1.43	1.38
3	L5	4597	UR3	O4-C4	-2.40	1.18	1.23
3	L5	3909	OMC	C5-C4	2.39	1.48	1.42
3	L5	2804	OMC	C5-C4	2.38	1.48	1.42
3	L5	4536	OMC	C5-C4	2.38	1.48	1.42
3	L5	729	2MG	O6-C6	-2.37	1.19	1.23
3	L5	2365	OMC	C5-C4	2.35	1.48	1.42
3	L5	3869	OMC	C5-C4	2.35	1.48	1.42
3	L5	729	2MG	C6-N1	2.34	1.43	1.38
3	L5	4872	2MG	C6-N1	2.33	1.43	1.38
3	L5	2422	OMC	C5-C4	2.32	1.48	1.42
3	L5	978	2MG	O6-C6	-2.30	1.19	1.23
3	L5	4872	2MG	O6-C6	-2.29	1.19	1.23
3	L5	4220	6MZ	C5-N7	-2.26	1.34	1.39
3	L5	3718	A2M	C5-N7	-2.23	1.34	1.39
3	L5	1871	A2M	C4-N9	-2.22	1.32	1.37
3	L5	4523	A2M	O5'-C5'	-2.21	1.39	1.44
3	L5	4571	A2M	C5-N7	-2.20	1.34	1.39
3	L5	4415	1MA	CM1-N1	2.18	1.51	1.46
3	L5	1326	A2M	C4-N9	-2.14	1.32	1.37
3	L5	1524	A2M	C4-N9	-2.14	1.32	1.37
3	L5	3785	A2M	C5-N7	-2.13	1.35	1.39
3	L5	3825	A2M	C4-N9	-2.12	1.33	1.37
3	L5	1534	A2M	C4-N9	-2.12	1.33	1.37
3	L5	1534	A2M	C5-N7	-2.11	1.35	1.39
3	L5	2401	A2M	C5-N7	-2.10	1.35	1.39
3	L5	4523	A2M	C5-N7	-2.09	1.35	1.39
3	L5	3867	A2M	C4-N9	-2.09	1.33	1.37
3	L5	1517	2MG	C4-N9	-2.09	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3785	A2M	O5'-C5'	-2.08	1.39	1.44
3	L5	3723	A2M	C4-N9	-2.07	1.33	1.37
3	L5	1524	A2M	O5'-C5'	-2.07	1.39	1.44
3	L5	2401	A2M	C4-N9	-2.07	1.33	1.37
3	L5	3825	A2M	O5'-C5'	-2.06	1.39	1.44
3	L5	398	A2M	C5-N7	-2.05	1.35	1.39
3	L5	1326	A2M	C5-N7	-2.04	1.35	1.39
3	L5	1871	A2M	C5-N7	-2.03	1.35	1.39
3	L5	2401	A2M	O5'-C5'	-2.03	1.39	1.44
3	L5	3825	A2M	C5-N7	-2.02	1.35	1.39
3	L5	3718	A2M	C4-N9	-2.01	1.33	1.37
3	L5	398	A2M	C4-N9	-2.01	1.33	1.37
3	L5	3723	A2M	C5-N7	-2.00	1.35	1.39
3	L5	1871	A2M	O5'-C5'	-2.00	1.39	1.44
3	L5	1524	A2M	C5-N7	-2.00	1.35	1.39

All (517) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4571	A2M	C1'-N9-C8	-11.25	101.73	127.14
3	L5	3718	A2M	C1'-N9-C8	-10.90	102.53	127.14
3	L5	3723	A2M	C1'-N9-C8	-10.55	103.31	127.14
3	L5	3867	A2M	C1'-N9-C8	-10.54	103.33	127.14
3	L5	2363	A2M	C1'-N9-C8	-10.47	103.50	127.14
3	L5	1326	A2M	C1'-N9-C8	-10.37	103.72	127.14
3	L5	2401	A2M	C1'-N9-C8	-10.36	103.75	127.14
3	L5	398	A2M	C1'-N9-C8	-10.35	103.78	127.14
3	L5	1871	A2M	C1'-N9-C8	-10.23	104.04	127.14
3	L5	4523	A2M	C1'-N9-C8	-10.17	104.18	127.14
3	L5	3825	A2M	C1'-N9-C8	-10.08	104.38	127.14
3	L5	1524	A2M	C1'-N9-C8	-9.92	104.73	127.14
3	L5	4083	5MU	C5-C4-N3	9.47	123.39	115.31
3	L5	1534	A2M	C1'-N9-C8	-9.37	105.97	127.14
3	L5	2363	A2M	N6-C6-N1	-9.20	98.20	118.35
3	L5	1326	A2M	N6-C6-N1	-9.04	98.55	118.35
3	L5	3825	A2M	N6-C6-N1	-8.97	98.70	118.35
3	L5	2401	A2M	N6-C6-N1	-8.94	98.76	118.35
3	L5	3867	A2M	N6-C6-N1	-8.93	98.78	118.35
3	L5	398	A2M	N6-C6-N1	-8.92	98.82	118.35
3	L5	1524	A2M	N6-C6-N1	-8.92	98.82	118.35
3	L5	3785	A2M	N6-C6-N1	-8.89	98.87	118.35
3	L5	1871	A2M	N6-C6-N1	-8.89	98.88	118.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3718	A2M	N6-C6-N1	-8.87	98.93	118.35
3	L5	1534	A2M	N6-C6-N1	-8.85	98.98	118.35
3	L5	4523	A2M	N6-C6-N1	-8.79	99.10	118.35
3	L5	4571	A2M	N6-C6-N1	-8.77	99.15	118.35
3	L5	3723	A2M	N6-C6-N1	-8.75	99.18	118.35
3	L5	3785	A2M	C1'-N9-C8	-7.97	109.14	127.14
3	L5	1524	A2M	C4-N9-C8	7.77	114.15	105.73
3	L5	3867	A2M	C4-N9-C8	7.69	114.06	105.73
3	L5	2401	A2M	C4-N9-C8	7.66	114.03	105.73
3	L5	1524	A2M	N9-C8-N7	-7.65	103.45	113.91
3	L5	4571	A2M	C4-N9-C1'	7.62	144.75	126.59
3	L5	1871	A2M	C4-N9-C8	7.60	113.97	105.73
3	L5	2401	A2M	N9-C8-N7	-7.58	103.54	113.91
3	L5	4415	1MA	C1'-N9-C8	-7.56	105.17	126.70
3	L5	2363	A2M	C4-N9-C8	7.50	113.86	105.73
3	L5	1326	A2M	C4-N9-C8	7.50	113.86	105.73
3	L5	3825	A2M	C4-N9-C8	7.49	113.85	105.73
3	L5	3723	A2M	C4-N9-C8	7.48	113.83	105.73
3	L5	3867	A2M	N9-C8-N7	-7.47	103.69	113.91
3	L5	398	A2M	C4-N9-C8	7.47	113.83	105.73
3	L5	398	A2M	N9-C8-N7	-7.47	103.70	113.91
3	L5	1326	A2M	N9-C8-N7	-7.44	103.73	113.91
3	L5	1871	A2M	N9-C8-N7	-7.43	103.75	113.91
3	L5	2363	A2M	N9-C8-N7	-7.43	103.75	113.91
3	L5	3825	A2M	N9-C8-N7	-7.43	103.75	113.91
3	L5	3718	A2M	C4-N9-C1'	7.34	144.08	126.59
3	L5	4083	5MU	C5-C6-N1	-7.33	115.80	123.34
3	L5	4523	A2M	N9-C8-N7	-7.28	103.96	113.91
3	L5	1534	A2M	N9-C8-N7	-7.27	103.97	113.91
3	L5	3723	A2M	N9-C8-N7	-7.26	103.98	113.91
3	L5	4523	A2M	C4-N9-C8	7.21	113.55	105.73
3	L5	4571	A2M	C4-N9-C8	7.15	113.48	105.73
3	L5	1534	A2M	C4-N9-C8	7.13	113.45	105.73
3	L5	4571	A2M	N9-C8-N7	-7.08	104.23	113.91
3	L5	3718	A2M	C4-N9-C8	7.03	113.35	105.73
3	L5	4296	B8H	C4-N3-C2	-6.92	118.39	127.35
3	L5	1860	B8H	C4-N3-C2	-6.91	118.40	127.35
3	L5	3723	A2M	C4-N9-C1'	6.83	142.86	126.59
3	L5	3718	A2M	N9-C8-N7	-6.82	104.58	113.91
3	L5	3762	B8H	C4-N3-C2	-6.77	118.58	127.35
3	L5	1326	A2M	C5-C6-N6	6.77	138.16	123.43
3	L5	3785	A2M	N9-C8-N7	-6.75	104.68	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2363	A2M	C4-N9-C1'	6.73	142.63	126.59
3	L5	2363	A2M	C5-C6-N6	6.72	138.06	123.43
3	L5	3867	A2M	C4-N9-C1'	6.72	142.60	126.59
3	L5	2401	A2M	C5-C6-N6	6.71	138.03	123.43
3	L5	1871	A2M	C5-C6-N6	6.69	137.98	123.43
3	L5	3825	A2M	C5-C6-N6	6.68	137.98	123.43
3	L5	1524	A2M	C5-C6-N6	6.65	137.89	123.43
3	L5	1326	A2M	C4-N9-C1'	6.64	142.42	126.59
3	L5	398	A2M	C4-N9-C1'	6.62	142.37	126.59
3	L5	3867	A2M	C5-C6-N6	6.61	137.81	123.43
3	L5	398	A2M	C5-C6-N6	6.61	137.81	123.43
3	L5	3718	A2M	C5-C6-N6	6.59	137.78	123.43
3	L5	978	2MG	C2-N3-C4	6.57	120.19	112.04
3	L5	3723	A2M	C5-C6-N6	6.56	137.71	123.43
3	L5	1534	A2M	C5-C6-N6	6.56	137.70	123.43
3	L5	729	2MG	C2-N3-C4	6.55	120.16	112.04
3	L5	4523	A2M	C4-N9-C1'	6.55	142.20	126.59
3	L5	2401	A2M	C4-N9-C1'	6.53	142.15	126.59
3	L5	4571	A2M	C5-C6-N6	6.52	137.61	123.43
3	L5	4415	1MA	C1'-N9-C4	6.47	145.73	126.50
3	L5	3785	A2M	C5-C6-N6	6.47	137.50	123.43
3	L5	4523	A2M	C5-C6-N6	6.46	137.49	123.43
3	L5	1871	A2M	C4-N9-C1'	6.45	141.95	126.59
3	L5	1517	2MG	C2-N3-C4	6.44	120.02	112.04
3	L5	3785	A2M	C4-N9-C8	6.41	112.68	105.73
3	L5	4872	2MG	C2-N3-C4	6.37	119.93	112.04
3	L5	3825	A2M	C4-N9-C1'	6.36	141.76	126.59
3	L5	4083	5MU	C4-N3-C2	-6.18	119.34	127.35
3	L5	4637	OMG	C5-C4-N3	-6.13	118.51	128.46
3	L5	3792	OMG	C5-C4-N3	-6.11	118.55	128.46
3	L5	1883	OMG	C5-C4-N3	-6.10	118.56	128.46
3	L5	1524	A2M	C4-N9-C1'	6.09	141.09	126.59
3	L5	4196	OMG	C5-C4-N3	-6.05	118.65	128.46
3	L5	1625	OMG	C5-C4-N3	-6.02	118.70	128.46
3	L5	1522	OMG	C1'-N9-C4	-5.97	108.77	126.50
3	L5	2050	OMG	C5-C4-N3	-5.94	118.82	128.46
3	L5	4494	OMG	C5-C4-N3	-5.89	118.91	128.46
3	L5	1860	B8H	N3-C2-N1	5.88	121.50	115.14
3	L5	1534	A2M	C4-N9-C1'	5.86	140.55	126.59
3	L5	1316	OMG	C5-C4-N3	-5.86	118.96	128.46
3	L5	1522	OMG	C1'-N9-C8	5.79	143.18	126.70
3	L5	4296	B8H	N3-C2-N1	5.78	121.39	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3762	B8H	N3-C2-N1	5.77	121.37	115.14
3	L5	2364	OMG	C5-C4-N3	-5.74	119.14	128.46
3	L5	2424	OMG	C5-C4-N3	-5.70	119.21	128.46
3	L5	3899	OMG	C5-C4-N3	-5.67	119.27	128.46
3	L5	4870	OMG	C5-C4-N3	-5.66	119.27	128.46
3	L5	373	OMG	C5-C4-N3	-5.66	119.28	128.46
3	L5	2773	OMG	C5-C4-N3	-5.64	119.31	128.46
3	L5	1326	A2M	N3-C2-N1	-5.61	119.83	128.60
3	L5	4370	OMG	C1'-N9-C4	-5.60	109.86	126.50
3	L5	3785	A2M	N3-C2-N1	-5.59	119.86	128.60
3	L5	4870	OMG	C1'-N9-C4	-5.59	109.91	126.50
3	L5	4370	OMG	C5-C4-N3	-5.58	119.40	128.46
3	L5	2401	A2M	N3-C2-N1	-5.57	119.88	128.60
3	L5	1322	1MA	C1'-N9-C8	-5.57	110.84	126.70
3	L5	4623	OMG	C1'-N9-C4	-5.56	109.98	126.50
3	L5	1871	A2M	N3-C2-N1	-5.56	119.91	128.60
3	L5	3723	A2M	N3-C2-N1	-5.56	119.91	128.60
3	L5	398	A2M	N3-C2-N1	-5.54	119.93	128.60
3	L5	3825	A2M	N3-C2-N1	-5.54	119.93	128.60
3	L5	4523	A2M	N3-C2-N1	-5.54	119.93	128.60
3	L5	1534	A2M	N3-C2-N1	-5.53	119.95	128.60
3	L5	4623	OMG	C5-C4-N3	-5.53	119.50	128.46
3	L5	4220	6MZ	N1-C2-N3	-5.51	119.98	128.60
3	L5	2363	A2M	N3-C2-N1	-5.47	120.05	128.60
3	L5	1524	A2M	N3-C2-N1	-5.46	120.06	128.60
3	L5	3899	OMG	C1'-N9-C4	-5.46	110.29	126.50
3	L5	1522	OMG	C5-C4-N3	-5.42	119.66	128.46
3	L5	2773	OMG	C1'-N9-C4	-5.42	110.41	126.50
3	L5	4870	OMG	C1'-N9-C8	5.41	142.11	126.70
3	L5	2424	OMG	C1'-N9-C4	-5.40	110.47	126.50
3	L5	4623	OMG	C1'-N9-C8	5.39	142.03	126.70
3	L5	4571	A2M	N3-C2-N1	-5.38	120.19	128.60
3	L5	4370	OMG	C1'-N9-C8	5.37	141.99	126.70
3	L5	3867	A2M	N3-C2-N1	-5.35	120.23	128.60
3	L5	373	OMG	C1'-N9-C4	-5.33	110.66	126.50
3	L5	3718	A2M	N3-C2-N1	-5.29	120.33	128.60
3	L5	2773	OMG	C1'-N9-C8	5.28	141.72	126.70
3	L5	3899	OMG	C1'-N9-C8	5.25	141.65	126.70
3	L5	2424	OMG	C1'-N9-C8	5.25	141.64	126.70
3	L5	2364	OMG	C1'-N9-C4	-5.18	111.11	126.50
3	L5	4571	A2M	N3-C4-N9	5.09	135.47	127.08
3	L5	4494	OMG	C1'-N9-C4	-5.05	111.50	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4872	2MG	C5-C4-N3	-5.05	120.27	128.46
3	L5	373	OMG	C1'-N9-C8	5.04	141.04	126.70
3	L5	1316	OMG	C1'-N9-C4	-5.03	111.55	126.50
3	L5	2364	OMG	C1'-N9-C8	5.02	140.99	126.70
3	L5	3718	A2M	N3-C4-N9	5.02	135.35	127.08
3	L5	1322	1MA	N1-C2-N3	-4.99	120.07	126.00
3	L5	4494	OMG	C1'-N9-C8	4.96	140.82	126.70
3	L5	4636	PSU	C4-N3-C2	-4.95	119.20	126.34
3	L5	4220	6MZ	C5-C4-N3	-4.95	120.29	126.75
3	L5	4637	OMG	C1'-N9-C4	-4.93	111.87	126.50
3	L5	398	A2M	N3-C4-N9	4.92	135.19	127.08
3	L5	4571	A2M	C5-C4-N3	-4.92	120.33	126.75
3	L5	4523	A2M	N3-C4-N9	4.91	135.18	127.08
3	L5	1316	OMG	C1'-N9-C8	4.89	140.61	126.70
3	L5	3785	A2M	C4-N9-C1'	4.86	138.16	126.59
3	L5	3867	A2M	N3-C4-N9	4.85	135.08	127.08
3	L5	1683	PSU	C4-N3-C2	-4.85	119.35	126.34
3	L5	4530	UR3	C4-N3-C2	-4.84	120.00	124.56
3	L5	2363	A2M	N3-C4-N9	4.84	135.06	127.08
3	L5	4293	PSU	C4-N3-C2	-4.84	119.36	126.34
3	L5	2050	OMG	C1'-N9-C4	-4.84	112.14	126.50
3	L5	3723	A2M	N3-C4-N9	4.82	135.02	127.08
3	L5	4450	PSU	C4-N3-C2	-4.81	119.40	126.34
3	L5	4637	OMG	C1'-N9-C8	4.80	140.35	126.70
3	L5	3718	A2M	C5-C4-N3	-4.79	120.50	126.75
3	L5	1677	PSU	C4-N3-C2	-4.79	119.43	126.34
3	L5	1322	1MA	C1'-N9-C4	4.79	140.72	126.50
3	L5	3715	PSU	C4-N3-C2	-4.79	119.44	126.34
3	L5	4403	PSU	C4-N3-C2	-4.79	119.44	126.34
3	L5	4872	2MG	C1'-N9-C8	-4.78	113.09	126.70
3	L5	729	2MG	C5-C4-N3	-4.77	120.72	128.46
3	L5	729	2MG	C1'-N9-C8	-4.77	113.12	126.70
3	L5	2508	PSU	C4-N3-C2	-4.75	119.49	126.34
3	L5	4523	A2M	C5-C4-N3	-4.75	120.56	126.75
3	L5	2401	A2M	N3-C4-N9	4.72	134.86	127.08
3	L5	3729	PSU	C4-N3-C2	-4.72	119.53	126.34
3	L5	4628	PSU	C4-N3-C2	-4.72	119.54	126.34
3	L5	4531	PSU	C4-N3-C2	-4.71	119.55	126.34
3	L5	4442	PSU	C4-N3-C2	-4.70	119.57	126.34
3	L5	1582	PSU	C4-N3-C2	-4.70	119.57	126.34
3	L5	4415	1MA	N1-C2-N3	-4.69	120.42	126.00
3	L5	3792	OMG	C2-N3-C4	4.69	120.66	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4500	PSU	C4-N3-C2	-4.69	119.59	126.34
3	L5	4196	OMG	C1'-N9-C4	-4.68	112.59	126.50
3	L5	2050	OMG	C1'-N9-C8	4.68	140.03	126.70
3	L5	978	2MG	C5-C4-N3	-4.68	120.87	128.46
3	L5	398	A2M	C5-C4-N3	-4.67	120.66	126.75
3	L5	3785	A2M	C5-C4-N3	-4.65	120.68	126.75
3	L5	3764	PSU	C4-N3-C2	-4.65	119.64	126.34
3	L5	4636	PSU	N1-C2-N3	4.65	120.39	115.13
3	L5	3715	PSU	N1-C2-N3	4.64	120.39	115.13
3	L5	4220	6MZ	N9-C8-N7	-4.62	107.59	113.91
3	L5	4500	PSU	N1-C2-N3	4.62	120.37	115.13
3	L5	4637	OMG	C2-N3-C4	4.62	120.53	112.30
3	L5	1524	A2M	N3-C4-N9	4.62	134.69	127.08
3	L5	1883	OMG	C2-N3-C4	4.62	120.52	112.30
3	L5	1534	A2M	N3-C4-N9	4.62	134.69	127.08
3	L5	4531	PSU	N1-C2-N3	4.60	120.35	115.13
3	L5	4870	OMG	C2-N3-C4	4.60	120.49	112.30
3	L5	2363	A2M	C5-C4-N3	-4.60	120.75	126.75
3	L5	4450	PSU	N1-C2-N3	4.60	120.34	115.13
3	L5	4293	PSU	N1-C2-N3	4.59	120.33	115.13
3	L5	3825	A2M	N3-C4-N9	4.59	134.65	127.08
3	L5	1683	PSU	N1-C2-N3	4.58	120.32	115.13
3	L5	4083	5MU	C5M-C5-C6	-4.58	116.73	122.85
3	L5	4597	UR3	C4-N3-C2	-4.58	120.25	124.56
3	L5	4403	PSU	N1-C2-N3	4.57	120.31	115.13
3	L5	4196	OMG	C2-N3-C4	4.57	120.44	112.30
3	L5	3764	PSU	N1-C2-N3	4.56	120.30	115.13
3	L5	1326	A2M	N3-C4-N9	4.56	134.59	127.08
3	L5	1871	A2M	N3-C4-N9	4.55	134.59	127.08
3	L5	1316	OMG	C2-N3-C4	4.55	120.41	112.30
3	L5	4623	OMG	C2-N3-C4	4.55	120.41	112.30
3	L5	4494	OMG	C2-N3-C4	4.54	120.39	112.30
3	L5	2773	OMG	C2-N3-C4	4.54	120.39	112.30
3	L5	3899	OMG	C2-N3-C4	4.53	120.37	112.30
3	L5	4442	PSU	N1-C2-N3	4.53	120.26	115.13
3	L5	1517	2MG	C5-C4-N3	-4.53	121.12	128.46
3	L5	4196	OMG	C1'-N9-C8	4.53	139.58	126.70
3	L5	4628	PSU	N1-C2-N3	4.53	120.26	115.13
3	L5	3785	A2M	N3-C4-N9	4.52	134.53	127.08
3	L5	4872	2MG	C2-N1-C6	-4.51	119.30	124.48
3	L5	2424	OMG	C2-N3-C4	4.50	120.33	112.30
3	L5	3729	PSU	N1-C2-N3	4.50	120.23	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1534	A2M	C5-C4-N3	-4.50	120.88	126.75
3	L5	1522	OMG	C2-N3-C4	4.49	120.30	112.30
3	L5	2050	OMG	C2-N3-C4	4.49	120.29	112.30
3	L5	3723	A2M	C5-C4-N3	-4.48	120.91	126.75
3	L5	1625	OMG	C2-N3-C4	4.48	120.28	112.30
3	L5	2508	PSU	N1-C2-N3	4.47	120.20	115.13
3	L5	3867	A2M	C5-C4-N3	-4.47	120.92	126.75
3	L5	1677	PSU	N1-C2-N3	4.47	120.20	115.13
3	L5	4415	1MA	C5-C4-N3	-4.47	120.59	127.26
3	L5	1625	OMG	C1'-N9-C4	-4.46	113.25	126.50
3	L5	373	OMG	C2-N3-C4	4.45	120.23	112.30
3	L5	2364	OMG	C2-N3-C4	4.43	120.19	112.30
3	L5	4370	OMG	C2-N3-C4	4.42	120.18	112.30
3	L5	3825	A2M	C5-C4-N3	-4.39	121.02	126.75
3	L5	1883	OMG	C1'-N9-C4	-4.36	113.56	126.50
3	L5	4083	5MU	N3-C2-N1	4.35	120.67	114.89
3	L5	2401	A2M	C5-C4-N3	-4.35	121.07	126.75
3	L5	1866	UR3	C4-N3-C2	-4.33	120.48	124.56
3	L5	1326	A2M	C5-C4-N3	-4.33	121.11	126.75
3	L5	1524	A2M	C5-C4-N3	-4.32	121.12	126.75
3	L5	1582	PSU	N1-C2-N3	4.30	120.00	115.13
3	L5	1625	OMG	C1'-N9-C8	4.28	138.89	126.70
3	L5	1322	1MA	C5-C4-N3	-4.26	120.90	127.26
3	L5	3792	OMG	C1'-N9-C4	-4.26	113.85	126.50
3	L5	1871	A2M	C5-C4-N3	-4.25	121.21	126.75
3	L5	978	2MG	C2-N1-C6	-4.25	119.59	124.48
3	L5	1883	OMG	C1'-N9-C8	4.24	138.77	126.70
3	L5	3792	OMG	C1'-N9-C8	4.18	138.59	126.70
3	L5	978	2MG	C1'-N9-C8	-4.18	114.81	126.70
3	L5	1517	2MG	C2-N1-C6	-4.16	119.70	124.48
3	L5	729	2MG	C2-N1-C6	-4.09	119.78	124.48
3	L5	1524	A2M	C5-N7-C8	4.08	109.30	103.51
3	L5	4872	2MG	C1'-N9-C4	4.06	138.56	126.50
3	L5	2401	A2M	C5-N7-C8	4.04	109.25	103.51
3	L5	398	A2M	C5-N7-C8	4.04	109.25	103.51
3	L5	1883	OMG	N9-C4-N3	4.04	134.05	125.94
3	L5	1517	2MG	C1'-N9-C8	-4.01	115.27	126.70
3	L5	2363	A2M	C5-N7-C8	4.00	109.19	103.51
3	L5	1625	OMG	N9-C4-N3	3.99	133.95	125.94
3	L5	1326	A2M	C5-N7-C8	3.98	109.16	103.51
3	L5	3792	OMG	N9-C4-N3	3.97	133.92	125.94
3	L5	729	2MG	C1'-N9-C4	3.97	138.30	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3825	A2M	C5-N7-C8	3.95	109.13	103.51
3	L5	4523	A2M	C5-N7-C8	3.94	109.11	103.51
3	L5	3867	A2M	C5-N7-C8	3.93	109.09	103.51
3	L5	4083	5MU	C5M-C5-C4	3.92	123.09	118.77
3	L5	4196	OMG	N9-C4-N3	3.92	133.82	125.94
3	L5	1534	A2M	C5-N7-C8	3.91	109.07	103.51
3	L5	1871	A2M	C5-N7-C8	3.91	109.06	103.51
3	L5	1322	1MA	C2-N3-C4	3.91	120.09	112.41
3	L5	4571	A2M	C5-N7-C8	3.90	109.06	103.51
3	L5	4220	6MZ	C4-C5-C6	3.90	119.83	116.81
3	L5	4637	OMG	N9-C4-N3	3.90	133.77	125.94
3	L5	2050	OMG	N9-C4-N3	3.86	133.68	125.94
3	L5	3723	A2M	C5-N7-C8	3.82	108.94	103.51
3	L5	1316	OMG	N9-C4-N3	3.79	133.54	125.94
3	L5	4415	1MA	C2-N3-C4	3.75	119.77	112.41
3	L5	4523	A2M	C2-N3-C4	3.71	120.51	111.75
3	L5	4494	OMG	N9-C4-N3	3.70	133.37	125.94
3	L5	2401	A2M	C2'-C1'-N9	-3.70	107.31	113.53
3	L5	3785	A2M	C2-N3-C4	3.70	120.48	111.75
3	L5	2363	A2M	C2-N3-C4	3.66	120.40	111.75
3	L5	398	A2M	C2-N3-C4	3.66	120.40	111.75
3	L5	3785	A2M	C5-N7-C8	3.66	108.70	103.51
3	L5	3718	A2M	C5-N7-C8	3.63	108.67	103.51
3	L5	4571	A2M	C2-N3-C4	3.63	120.32	111.75
3	L5	1534	A2M	C2-N3-C4	3.61	120.29	111.75
3	L5	4296	B8H	C5-C4-N3	3.60	124.73	116.58
3	L5	4220	6MZ	C9-N6-C6	-3.59	119.78	122.87
3	L5	373	OMG	N9-C4-N3	3.59	133.16	125.94
3	L5	4523	A2M	C2'-C1'-N9	-3.59	107.48	113.53
3	L5	1326	A2M	C2-N3-C4	3.59	120.23	111.75
3	L5	4335	5MC	C5-C6-N1	-3.58	119.65	123.34
3	L5	4447	5MC	C5-C6-N1	-3.58	119.65	123.34
3	L5	1860	B8H	C5-C4-N3	3.57	124.66	116.58
3	L5	3825	A2M	C2-N3-C4	3.57	120.18	111.75
3	L5	3718	A2M	C2-N3-C4	3.56	120.17	111.75
3	L5	3723	A2M	C2-N3-C4	3.56	120.15	111.75
3	L5	2364	OMG	N9-C4-N3	3.55	133.07	125.94
3	L5	2401	A2M	C2-N3-C4	3.55	120.14	111.75
3	L5	2424	OMG	N9-C4-N3	3.54	133.05	125.94
3	L5	3867	A2M	C2-N3-C4	3.52	120.06	111.75
3	L5	1524	A2M	C2-N3-C4	3.51	120.05	111.75
3	L5	4370	OMG	N9-C4-N3	3.51	132.99	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3762	B8H	C5-C4-N3	3.51	124.52	116.58
3	L5	1871	A2M	C2-N3-C4	3.51	120.04	111.75
3	L5	3782	5MC	C5-C6-N1	-3.50	119.73	123.34
3	L5	3899	OMG	N9-C4-N3	3.49	132.94	125.94
3	L5	978	2MG	C1'-N9-C4	3.48	136.85	126.50
3	L5	4870	OMG	N9-C4-N3	3.48	132.92	125.94
3	L5	2773	OMG	N9-C4-N3	3.46	132.88	125.94
3	L5	1871	A2M	C2'-C1'-N9	-3.44	107.74	113.53
3	L5	1883	OMG	C2-N1-C6	-3.44	118.83	125.10
3	L5	4083	5MU	O4-C4-C5	-3.43	120.92	124.90
3	L5	4220	6MZ	C2-N3-C4	3.42	119.82	111.75
3	L5	4637	OMG	C2-N1-C6	-3.41	118.89	125.10
3	L5	4196	OMG	C2-N1-C6	-3.34	119.01	125.10
3	L5	4623	OMG	N9-C4-N3	3.32	132.61	125.94
3	L5	2424	OMG	C2-N1-C6	-3.28	119.11	125.10
3	L5	1517	2MG	C1'-N9-C4	3.27	136.22	126.50
3	L5	2050	OMG	C2-N1-C6	-3.26	119.15	125.10
3	L5	1517	2MG	N9-C8-N7	-3.26	107.26	113.39
3	L5	3792	OMG	C2-N1-C6	-3.26	119.16	125.10
3	L5	4415	1MA	N9-C8-N7	-3.25	107.26	113.39
3	L5	373	OMG	C2-N1-C6	-3.24	119.19	125.10
3	L5	1625	OMG	C2-N1-C6	-3.24	119.19	125.10
3	L5	1522	OMG	N9-C4-N3	3.23	132.43	125.94
3	L5	2773	OMG	C2-N1-C6	-3.21	119.25	125.10
3	L5	1316	OMG	C2-N1-C6	-3.20	119.27	125.10
3	L5	3899	OMG	C2-N1-C6	-3.19	119.28	125.10
3	L5	4870	OMG	C2-N1-C6	-3.19	119.28	125.10
3	L5	978	2MG	N9-C8-N7	-3.18	107.39	113.39
3	L5	4494	OMG	C2-N1-C6	-3.17	119.31	125.10
3	L5	2364	OMG	C2-N1-C6	-3.16	119.33	125.10
3	L5	4370	OMG	C2-N1-C6	-3.16	119.34	125.10
3	L5	729	2MG	N9-C8-N7	-3.15	107.45	113.39
3	L5	1860	B8H	O2-C2-N1	-3.15	119.32	122.87
3	L5	1322	1MA	N9-C8-N7	-3.13	107.49	113.39
3	L5	4623	OMG	C2-N1-C6	-3.13	119.39	125.10
3	L5	1522	OMG	C2-N1-C6	-3.10	119.45	125.10
3	L5	4220	6MZ	C5-N7-C8	3.09	107.90	103.51
3	L5	4872	2MG	N9-C8-N7	-3.08	107.60	113.39
3	L5	3762	B8H	O2-C2-N1	-3.07	119.41	122.87
3	L5	398	A2M	C2'-C1'-N9	-3.03	108.42	113.53
3	L5	4220	6MZ	N3-C4-N9	3.03	132.07	127.08
3	L5	4671	B8T	C6-C5-C4	2.99	120.62	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2363	A2M	C5-C6-N1	2.96	123.75	117.39
3	L5	3785	A2M	C5-C6-N1	2.91	123.63	117.39
3	L5	373	OMG	N9-C8-N7	-2.90	107.94	113.39
3	L5	4220	6MZ	C4-N9-C8	2.84	108.81	105.73
3	L5	3899	OMG	N9-C8-N7	-2.82	108.07	113.39
3	L5	1522	OMG	N9-C8-N7	-2.82	108.08	113.39
3	L5	4870	OMG	N9-C8-N7	-2.81	108.09	113.39
3	L5	4296	B8H	O2-C2-N1	-2.81	119.71	122.87
3	L5	4523	A2M	C5-C6-N1	2.81	123.41	117.39
3	L5	4872	2MG	N9-C4-N3	2.80	131.57	125.94
3	L5	4623	OMG	N9-C8-N7	-2.80	108.11	113.39
3	L5	3867	A2M	C5-C6-N1	2.80	123.40	117.39
3	L5	4370	OMG	N9-C8-N7	-2.79	108.13	113.39
3	L5	2424	OMG	C5-C6-N1	2.79	120.28	113.19
3	L5	1883	OMG	C5-C6-N1	2.79	120.28	113.19
3	L5	1683	PSU	O2-C2-N1	-2.79	119.72	122.79
3	L5	398	A2M	C5-C6-N1	2.79	123.37	117.39
3	L5	4500	PSU	O2-C2-N1	-2.78	119.72	122.79
3	L5	373	OMG	C5-C6-N1	2.78	120.25	113.19
3	L5	4637	OMG	C5-C6-N1	2.78	120.25	113.19
3	L5	1522	OMG	C5-C6-N1	2.78	120.25	113.19
3	L5	4531	PSU	O2-C2-N1	-2.78	119.73	122.79
3	L5	4196	OMG	C5-C6-N1	2.76	120.21	113.19
3	L5	1534	A2M	C5-C6-N1	2.76	123.32	117.39
3	L5	3825	A2M	C5-C6-N1	2.76	123.32	117.39
3	L5	3899	OMG	C5-C6-N1	2.75	120.19	113.19
3	L5	1524	A2M	C5-C6-N1	2.75	123.29	117.39
3	L5	3718	A2M	C5-C6-N1	2.75	123.28	117.39
3	L5	1326	A2M	C5-C6-N1	2.75	123.28	117.39
3	L5	4483	B8T	C6-C5-C4	2.74	120.32	116.96
3	L5	4623	OMG	C5-C6-N1	2.74	120.15	113.19
3	L5	2773	OMG	C5-C6-N1	2.74	120.14	113.19
3	L5	3792	OMG	C5-C6-N1	2.74	120.14	113.19
3	L5	1316	OMG	C5-C6-N1	2.73	120.13	113.19
3	L5	4870	OMG	C5-C6-N1	2.73	120.13	113.19
3	L5	978	2MG	C5-C6-N1	2.73	120.12	113.19
3	L5	729	2MG	C5-C6-N1	2.73	120.12	113.19
3	L5	4370	OMG	C5-C6-N1	2.73	120.12	113.19
3	L5	4571	A2M	C5-C6-N1	2.72	123.24	117.39
3	L5	729	2MG	N1-C2-N3	-2.72	119.75	123.95
3	L5	1517	2MG	C5-C6-N1	2.72	120.09	113.19
3	L5	4296	B8H	O4-C4-N3	-2.72	114.91	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2401	A2M	C5-C6-N1	2.71	123.21	117.39
3	L5	2773	OMG	N9-C8-N7	-2.70	108.30	113.39
3	L5	978	2MG	N1-C2-N3	-2.70	119.77	123.95
3	L5	1517	2MG	N1-C2-N3	-2.70	119.78	123.95
3	L5	3718	A2M	C2'-C1'-N9	-2.69	109.00	113.53
3	L5	2050	OMG	C5-C6-N1	2.69	120.02	113.19
3	L5	2424	OMG	N9-C8-N7	-2.68	108.34	113.39
3	L5	1871	A2M	C5-C6-N1	2.68	123.14	117.39
3	L5	4872	2MG	C5-C6-N1	2.67	119.97	113.19
3	L5	3715	PSU	O2-C2-N1	-2.67	119.85	122.79
3	L5	2364	OMG	N9-C8-N7	-2.67	108.37	113.39
3	L5	4500	PSU	C6-C5-C4	2.67	120.06	118.20
3	L5	3723	A2M	C5-C6-N1	2.66	123.11	117.39
3	L5	1625	OMG	C5-C6-N1	2.66	119.95	113.19
3	L5	4293	PSU	O2-C2-N1	-2.66	119.86	122.79
3	L5	729	2MG	N9-C4-N3	2.66	131.28	125.94
3	L5	4494	OMG	C5-C6-N1	2.65	119.92	113.19
3	L5	2364	OMG	C5-C6-N1	2.63	119.88	113.19
3	L5	3729	PSU	O2-C2-N1	-2.63	119.89	122.79
3	L5	1883	OMG	O6-C6-C5	-2.62	119.66	126.60
3	L5	3762	B8H	O4-C4-N3	-2.61	115.11	120.12
3	L5	1860	B8H	O4-C4-N3	-2.61	115.12	120.12
3	L5	1677	PSU	O2-C2-N1	-2.60	119.93	122.79
3	L5	3764	PSU	O2-C2-N1	-2.59	119.93	122.79
3	L5	4597	UR3	C1'-N1-C2	2.59	121.36	116.99
3	L5	1316	OMG	N9-C8-N7	-2.59	108.52	113.39
3	L5	1625	OMG	N9-C8-N7	-2.59	108.52	113.39
3	L5	3825	A2M	C2'-C1'-N9	-2.58	109.18	113.53
3	L5	2050	OMG	N9-C8-N7	-2.58	108.53	113.39
3	L5	4083	5MU	C6-C5-C4	2.58	120.19	118.03
3	L5	4637	OMG	N9-C8-N7	-2.57	108.54	113.39
3	L5	4196	OMG	N9-C8-N7	-2.56	108.57	113.39
3	L5	978	2MG	O6-C6-C5	-2.56	119.82	126.60
3	L5	2424	OMG	O6-C6-C5	-2.55	119.83	126.60
3	L5	4494	OMG	N9-C8-N7	-2.55	108.59	113.39
3	L5	3792	OMG	O6-C6-C5	-2.54	119.86	126.60
3	L5	1625	OMG	O6-C6-C5	-2.53	119.89	126.60
3	L5	4628	PSU	O2-C2-N1	-2.51	120.02	122.79
3	L5	4531	PSU	C6-C5-C4	2.50	119.94	118.20
3	L5	4196	OMG	O6-C6-C5	-2.49	119.98	126.60
3	L5	1517	2MG	O6-C6-C5	-2.49	119.99	126.60
3	L5	4370	OMG	O6-C6-C5	-2.49	119.99	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2050	OMG	O6-C6-C5	-2.48	120.01	126.60
3	L5	3785	A2M	O4'-C1'-N9	2.48	112.94	108.06
3	L5	2773	OMG	O6-C6-C5	-2.48	120.03	126.60
3	L5	373	OMG	O6-C6-C5	-2.47	120.03	126.60
3	L5	4450	PSU	O2-C2-N1	-2.46	120.09	122.79
3	L5	4494	OMG	O6-C6-C5	-2.45	120.09	126.60
3	L5	3792	OMG	N9-C8-N7	-2.45	108.77	113.39
3	L5	4623	OMG	O6-C6-C5	-2.45	120.11	126.60
3	L5	1524	A2M	C2'-C1'-N9	-2.44	109.42	113.53
3	L5	2508	PSU	O2-C2-N1	-2.44	120.10	122.79
3	L5	3729	PSU	C6-C5-C4	2.44	119.90	118.20
3	L5	1316	OMG	O6-C6-C5	-2.44	120.14	126.60
3	L5	3715	PSU	C6-C5-C4	2.44	119.90	118.20
3	L5	4637	OMG	O6-C6-C5	-2.43	120.14	126.60
3	L5	1522	OMG	O6-C6-C5	-2.42	120.17	126.60
3	L5	4870	OMG	O6-C6-C5	-2.42	120.19	126.60
3	L5	1883	OMG	N9-C8-N7	-2.42	108.84	113.39
3	L5	3899	OMG	O6-C6-C5	-2.41	120.20	126.60
3	L5	3723	A2M	C2'-C1'-N9	-2.41	109.48	113.53
3	L5	2363	A2M	C2'-C1'-N9	-2.39	109.50	113.53
3	L5	729	2MG	O6-C6-C5	-2.38	120.28	126.60
3	L5	4872	2MG	O6-C6-C5	-2.37	120.31	126.60
3	L5	2364	OMG	O6-C6-C5	-2.37	120.31	126.60
3	L5	978	2MG	N9-C4-N3	2.36	130.68	125.94
3	L5	3782	5MC	CM5-C5-C6	-2.33	119.73	122.85
3	L5	4083	5MU	O4-C4-N3	-2.31	115.68	120.12
3	L5	4636	PSU	O2-C2-N1	-2.30	120.26	122.79
3	L5	4442	PSU	O2-C2-N1	-2.30	120.26	122.79
3	L5	1517	2MG	N9-C4-N3	2.28	130.53	125.94
3	L5	4872	2MG	N1-C2-N3	-2.28	120.43	123.95
3	L5	4571	A2M	C2'-C1'-N9	-2.27	109.71	113.53
3	L5	2508	PSU	C6-C5-C4	2.24	119.76	118.20
3	L5	4415	1MA	C8-N7-C5	2.24	108.29	104.24
3	L5	978	2MG	C8-N7-C5	2.21	108.25	104.24
3	L5	4872	2MG	C8-N7-C5	2.20	108.23	104.24
3	L5	1517	2MG	C8-N7-C5	2.20	108.23	104.24
3	L5	4447	5MC	C1'-N1-C6	2.19	124.78	121.12
3	L5	1322	1MA	C8-N7-C5	2.19	108.21	104.24
3	L5	729	2MG	C8-N7-C5	2.19	108.21	104.24
3	L5	3785	A2M	C2'-C1'-N9	2.18	117.20	113.53
3	L5	4636	PSU	C6-C5-C4	2.18	119.72	118.20
3	L5	4597	UR3	C6-N1-C2	-2.17	119.84	121.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4415	1MA	N9-C4-N3	2.17	132.00	126.94
3	L5	1677	PSU	O4'-C1'-C2'	2.16	108.19	105.14
3	L5	4403	PSU	O2-C2-N1	-2.15	120.42	122.79
3	L5	4530	UR3	C6-N1-C2	-2.14	119.87	121.79
3	L5	3899	OMG	C8-N7-C5	2.13	108.10	104.24
3	L5	4442	PSU	O4'-C1'-C2'	2.12	108.14	105.14
3	L5	1582	PSU	O2-C2-N1	-2.12	120.46	122.79
3	L5	3762	B8H	O4'-C1'-C2'	2.12	108.13	105.14
3	L5	4447	5MC	O2-C2-N3	-2.12	118.89	122.33
3	L5	4870	OMG	C8-N7-C5	2.12	108.07	104.24
3	L5	4450	PSU	C6-C5-C4	2.11	119.67	118.20
3	L5	4220	6MZ	C4-C5-N7	-2.10	108.06	110.62
3	L5	4083	5MU	O2-C2-N1	-2.09	120.01	122.79
3	L5	4442	PSU	C6-C5-C4	2.09	119.66	118.20
3	L5	373	OMG	C8-N7-C5	2.09	108.02	104.24
3	L5	4623	OMG	C8-N7-C5	2.08	108.01	104.24
3	L5	3764	PSU	C6-N1-C2	-2.08	120.56	122.68
3	L5	1522	OMG	C8-N7-C5	2.06	107.97	104.24
3	L5	4637	OMG	C8-N7-C5	2.06	107.97	104.24
3	L5	4500	PSU	C6-N1-C2	-2.05	120.58	122.68
3	L5	2364	OMG	C8-N7-C5	2.05	107.95	104.24
3	L5	3785	A2M	C4'-O4'-C1'	-2.05	104.96	109.47
3	L5	3887	OMC	C2'-C1'-N1	-2.04	110.26	114.22
3	L5	4335	5MC	CM5-C5-C6	-2.04	120.12	122.85
3	L5	4370	OMG	C8-N7-C5	2.04	107.93	104.24
3	L5	4403	PSU	O4'-C1'-C2'	2.04	108.02	105.14
3	L5	3715	PSU	C6-N1-C2	-2.03	120.61	122.68
3	L5	1866	UR3	C1'-N1-C2	2.02	120.41	116.99
3	L5	1322	1MA	C4-C5-N7	-2.02	107.52	110.72
3	L5	2773	OMG	C8-N7-C5	2.02	107.89	104.24
3	L5	4628	PSU	C6-N1-C2	-2.01	120.62	122.68
3	L5	4636	PSU	O4'-C1'-C2'	2.01	107.98	105.14

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	Lm	98	MLZ	C-CA-CB-CG
3	L5	398	A2M	O4'-C4'-C5'-O5'
3	L5	2424	OMG	O4'-C4'-C5'-O5'
3	L5	3701	OMC	C2'-C1'-N1-C6
3	L5	3723	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	L5	3729	PSU	O4'-C4'-C5'-O5'
3	L5	3867	A2M	O4'-C4'-C5'-O5'
3	L5	3867	A2M	C3'-C4'-C5'-O5'
3	L5	4403	PSU	C2'-C1'-C5-C4
3	L5	4403	PSU	O4'-C1'-C5-C4
3	L5	4403	PSU	O4'-C1'-C5-C6
3	L5	4450	PSU	C2'-C1'-C5-C4
3	L5	4450	PSU	C2'-C1'-C5-C6
3	L5	4500	PSU	C3'-C4'-C5'-O5'
3	L5	4523	A2M	O4'-C4'-C5'-O5'
3	L5	4523	A2M	C3'-C4'-C5'-O5'
3	L5	4530	UR3	O4'-C4'-C5'-O5'
3	L5	4530	UR3	C3'-C4'-C5'-O5'
3	L5	4636	PSU	C2'-C1'-C5-C6
3	L5	4636	PSU	C3'-C4'-C5'-O5'
3	L5	4636	PSU	O4'-C4'-C5'-O5'
3	L5	4870	OMG	C3'-C4'-C5'-O5'
3	L5	4872	2MG	O4'-C4'-C5'-O5'
3	L5	3701	OMC	C2'-C1'-N1-C2
3	L5	2364	OMG	O4'-C4'-C5'-O5'
3	L5	2424	OMG	C3'-C4'-C5'-O5'
3	L5	3723	A2M	C3'-C4'-C5'-O5'
3	L5	3729	PSU	C3'-C4'-C5'-O5'
3	L5	3785	A2M	O4'-C4'-C5'-O5'
3	L5	3785	A2M	C3'-C4'-C5'-O5'
3	L5	4500	PSU	O4'-C4'-C5'-O5'
3	L5	4870	OMG	O4'-C4'-C5'-O5'
3	L5	4872	2MG	C3'-C4'-C5'-O5'
3	L5	398	A2M	C3'-C4'-C5'-O5'
3	L5	2364	OMG	C3'-C4'-C5'-O5'
3	L5	3718	A2M	O4'-C4'-C5'-O5'
3	L5	4196	OMG	O4'-C4'-C5'-O5'
3	L5	729	2MG	O4'-C4'-C5'-O5'
3	L5	4196	OMG	C3'-C4'-C5'-O5'
3	L5	4628	PSU	O4'-C4'-C5'-O5'
3	L5	4500	PSU	C4'-C5'-O5'-P
3	L5	3701	OMC	O4'-C1'-N1-C2
3	L5	4494	OMG	C3'-C2'-O2'-CM2
8	LC	333	MLZ	N-CA-CB-CG
3	L5	3701	OMC	O4'-C1'-N1-C6
8	LC	333	MLZ	C-CA-CB-CG
3	L5	1866	UR3	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	L5	1883	OMG	C3'-C4'-C5'-O5'
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	729	2MG	C3'-C4'-C5'-O5'
3	L5	1326	A2M	C4'-C5'-O5'-P
3	L5	4870	OMG	C4'-C5'-O5'-P
3	L5	4293	PSU	O4'-C4'-C5'-O5'
3	L5	3909	OMC	C2'-C1'-N1-C6
3	L5	1677	PSU	O4'-C1'-C5-C4
3	L5	4450	PSU	O4'-C1'-C5-C4
3	L5	4447	5MC	O4'-C1'-N1-C6
3	L5	4447	5MC	C2'-C1'-N1-C6
3	L5	1883	OMG	O4'-C4'-C5'-O5'
3	L5	2508	PSU	O4'-C4'-C5'-O5'
3	L5	4628	PSU	C3'-C4'-C5'-O5'
3	L5	4450	PSU	O4'-C1'-C5-C6
3	L5	4636	PSU	O4'-C1'-C5-C6
3	L5	3909	OMC	C2'-C1'-N1-C2
3	L5	1534	A2M	O4'-C4'-C5'-O5'
3	L5	3764	PSU	C3'-C4'-C5'-O5'
3	L5	2422	OMC	O4'-C4'-C5'-O5'
3	L5	3718	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

20 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	729	2MG	1	0
3	L5	1871	A2M	1	0
3	L5	3723	A2M	1	0
3	L5	4220	6MZ	1	0
3	L5	1860	B8H	6	0
3	L5	4083	5MU	1	0
3	L5	3785	A2M	3	0
3	L5	1625	OMG	1	0
3	L5	3718	A2M	4	0
3	L5	2424	OMG	1	0
3	L5	4296	B8H	5	0
3	L5	4597	UR3	1	0
3	L5	3909	OMC	1	0
3	L5	398	A2M	1	0
3	L5	4571	A2M	3	0
3	L5	3764	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4523	A2M	1	0
3	L5	4872	2MG	1	0
3	L5	3762	B8H	6	0
3	L5	4447	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 288 ligands modelled in this entry, 288 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

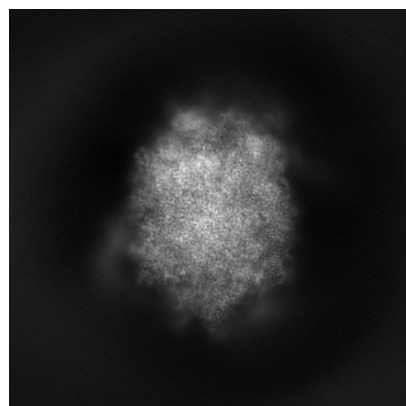
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51611. These allow visual inspection of the internal detail of the map and identification of artifacts.

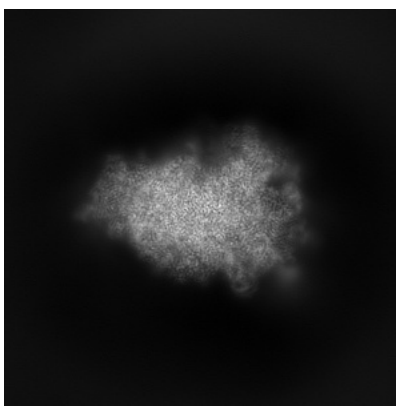
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

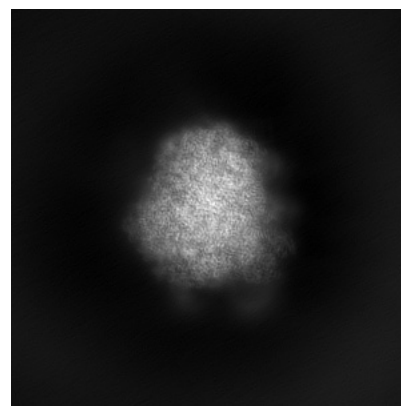
6.1.1 Primary map



X

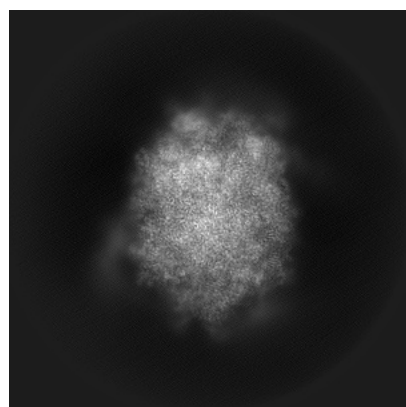


Y

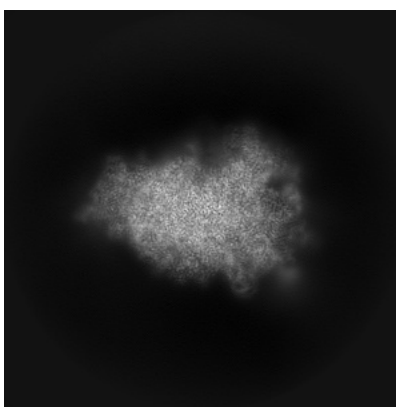


Z

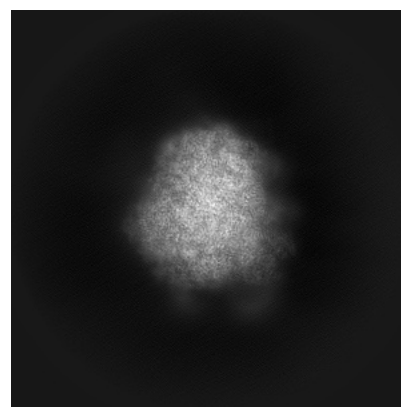
6.1.2 Raw map



X



Y

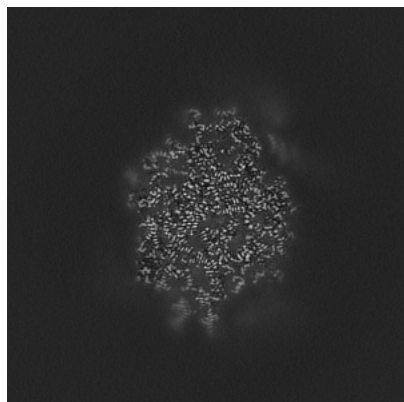


Z

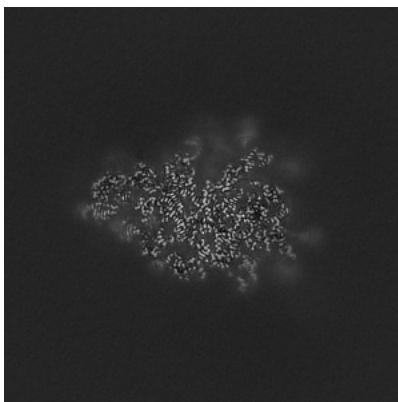
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

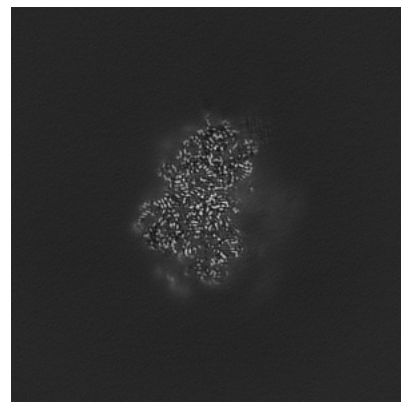
6.2.1 Primary map



X Index: 248

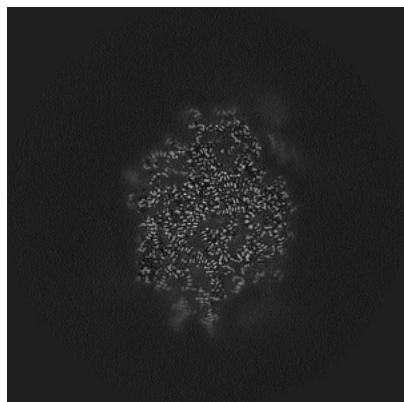


Y Index: 248

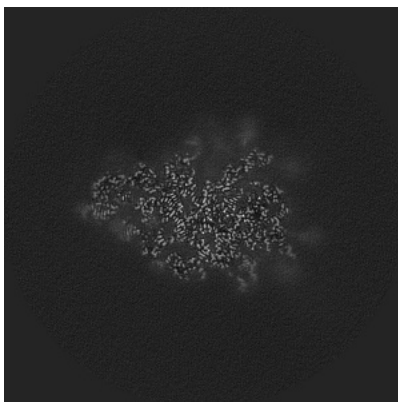


Z Index: 248

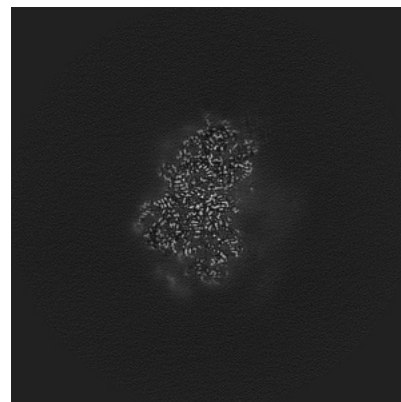
6.2.2 Raw map



X Index: 248



Y Index: 248

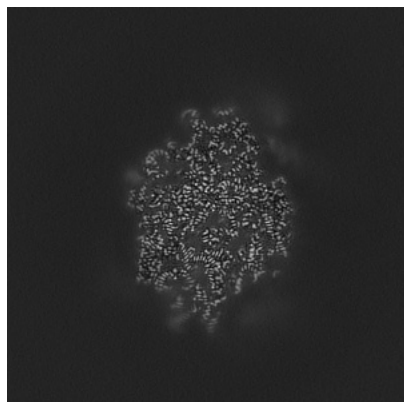


Z Index: 248

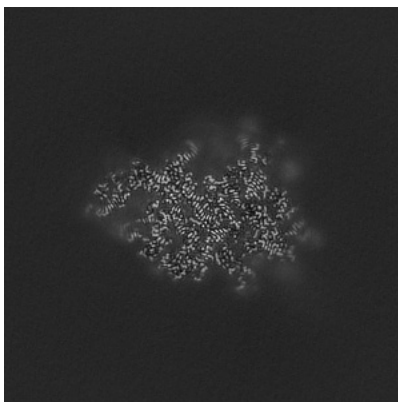
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

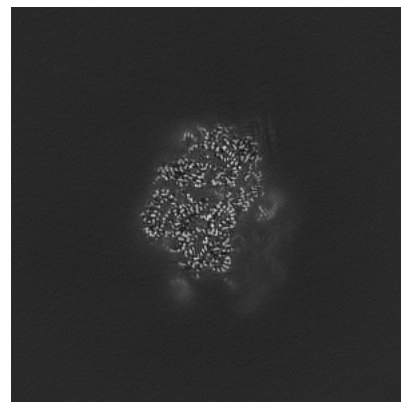
6.3.1 Primary map



X Index: 251

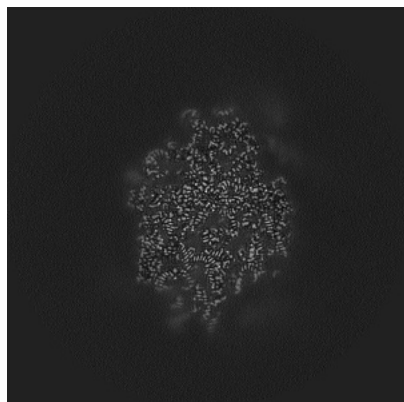


Y Index: 241

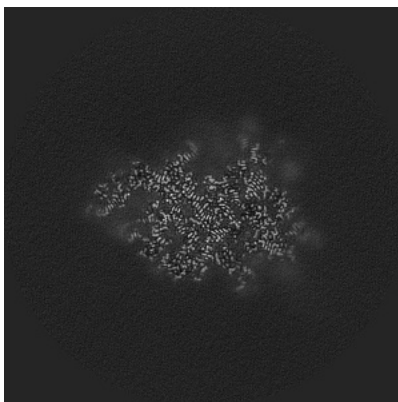


Z Index: 234

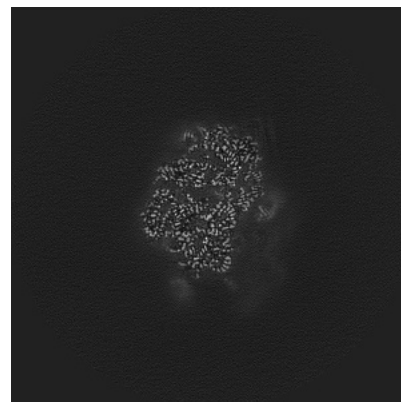
6.3.2 Raw map



X Index: 251



Y Index: 241

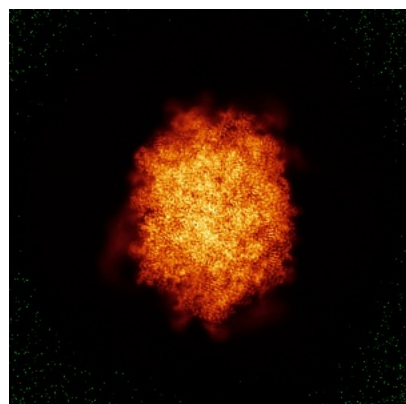


Z Index: 234

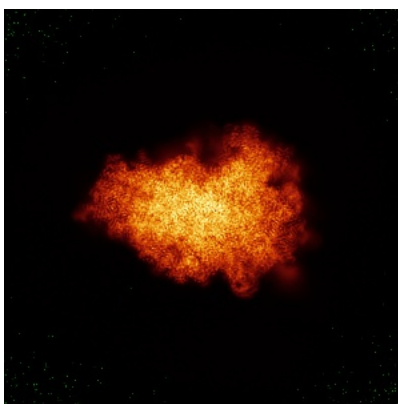
The images above show the largest variance slices of the map in three orthogonal directions.

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

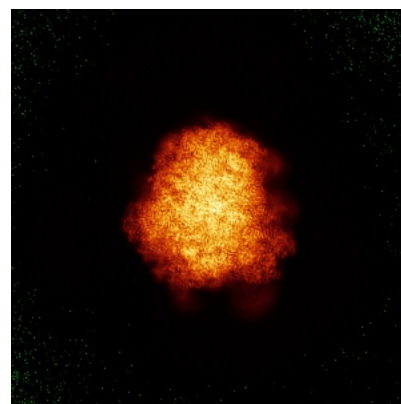
6.4.1 Primary map



X

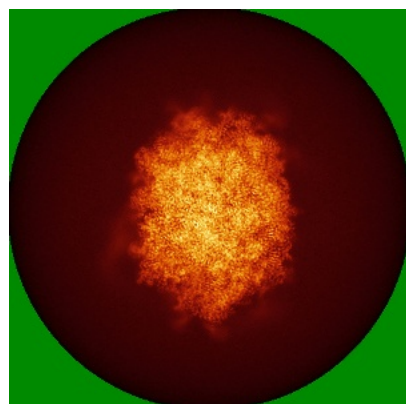


Y

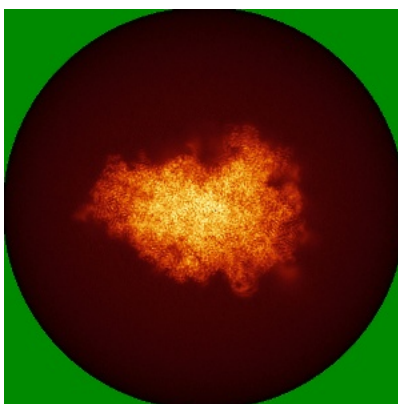


Z

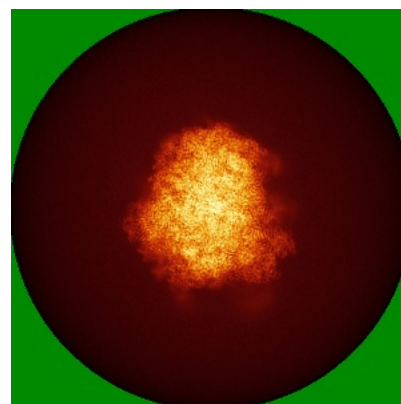
6.4.2 Raw map



X



Y

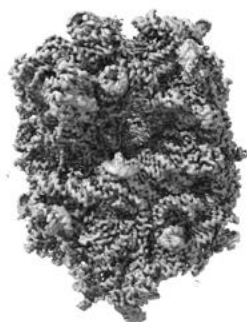


Z

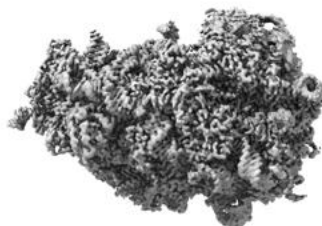
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

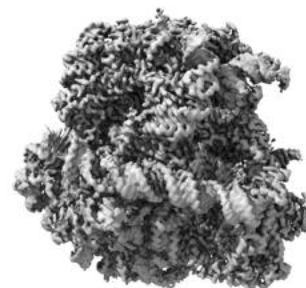
6.5.1 Primary map



X



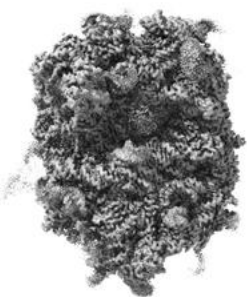
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

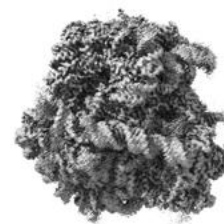
6.5.2 Raw map



X



Y



Z

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

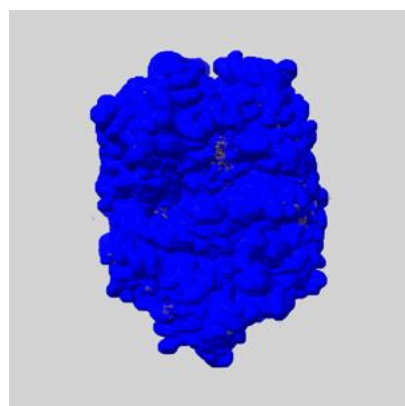
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

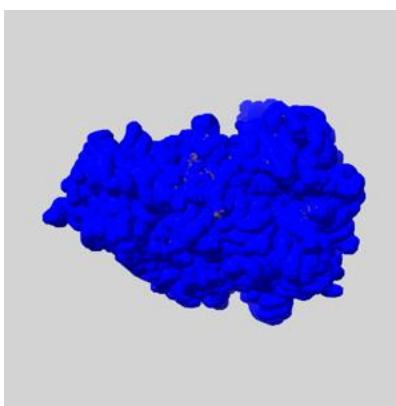
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

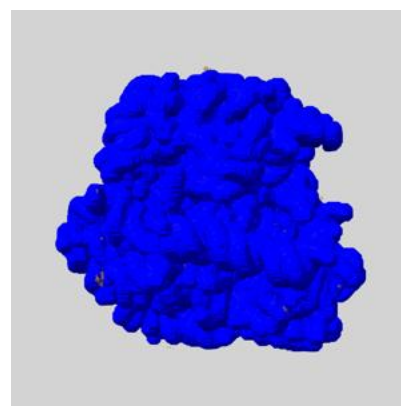
6.6.1 emd_51611_msk_1.map [i](#)



X



Y

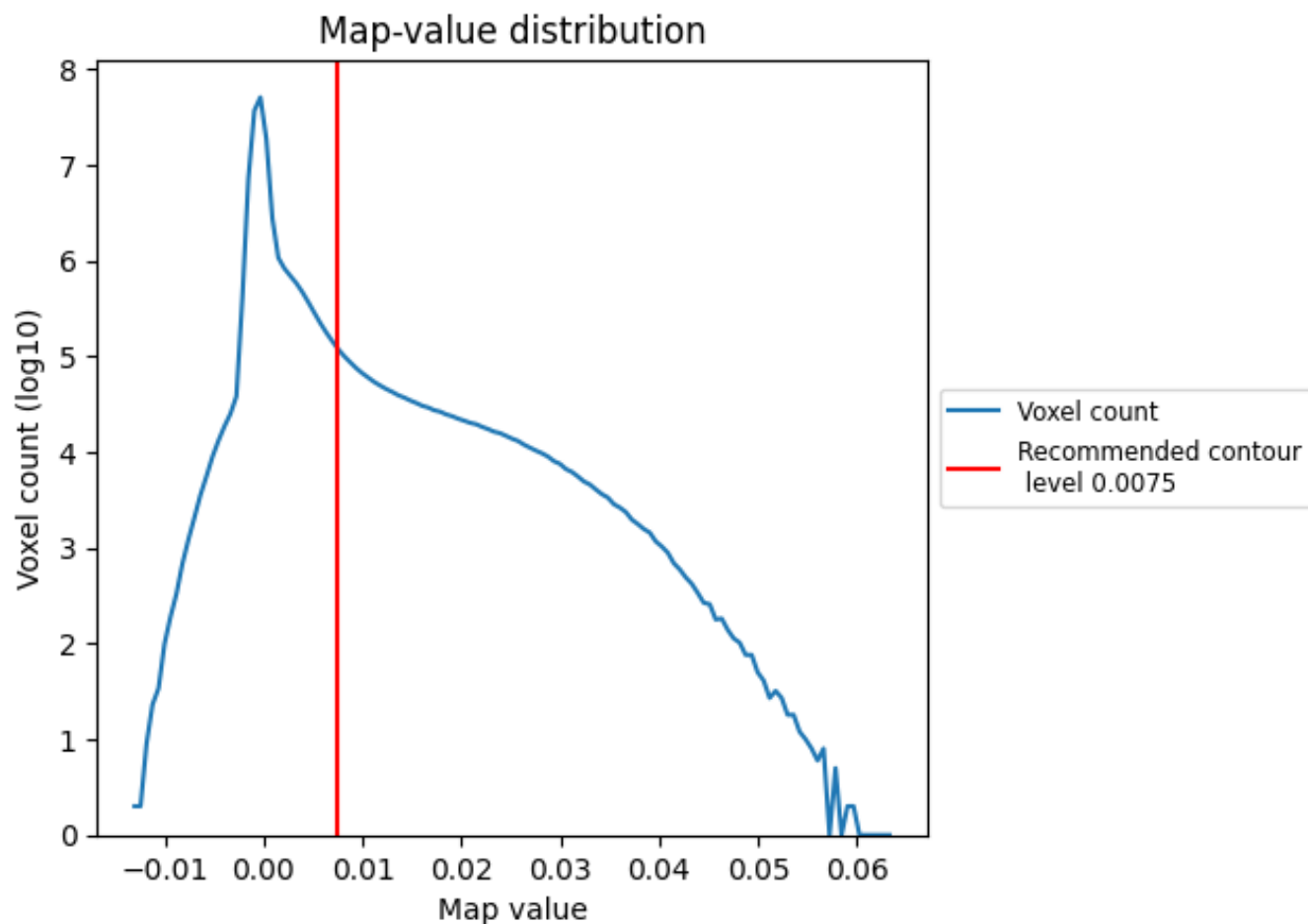


Z

7 Map analysis [i](#)

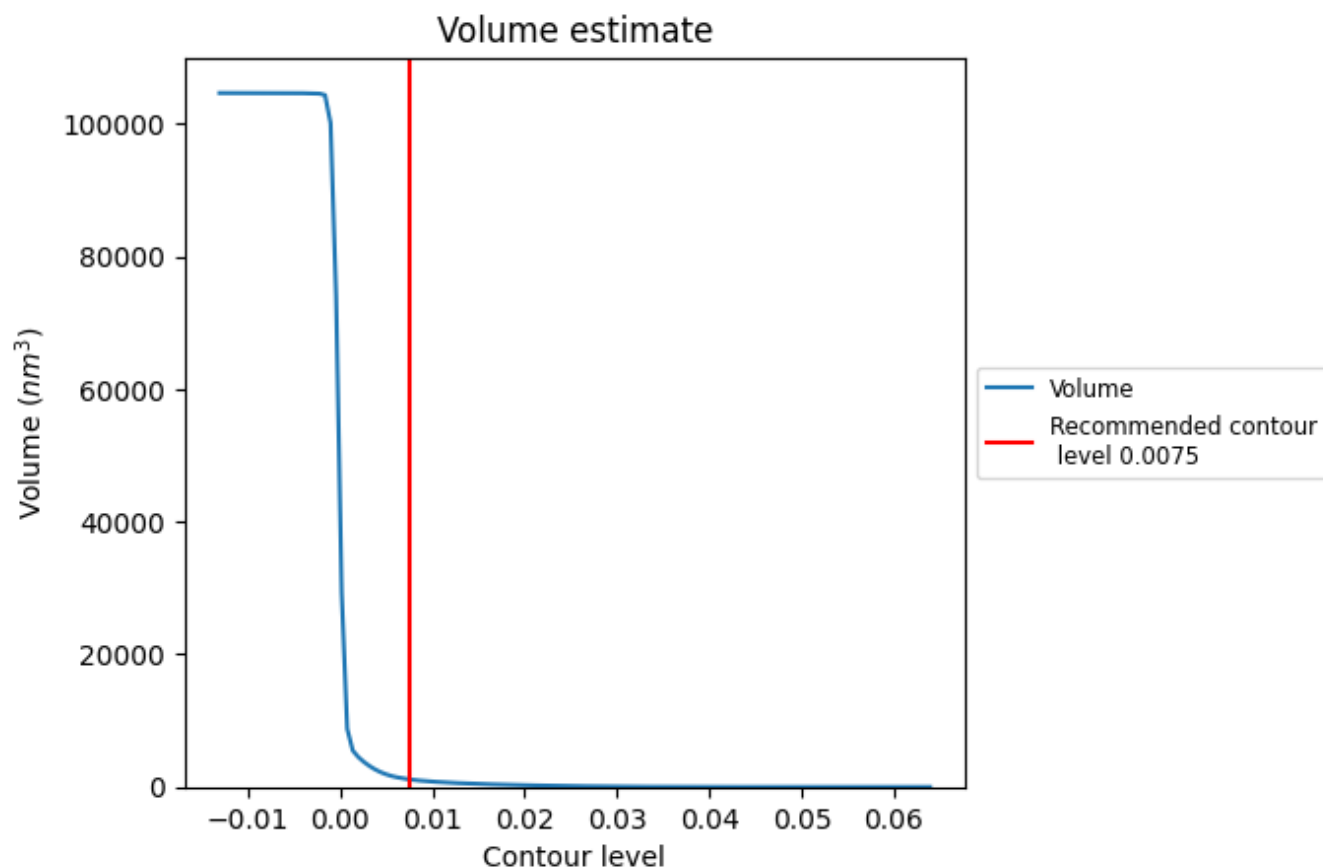
This section contains the results of statistical analysis of the map.

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.

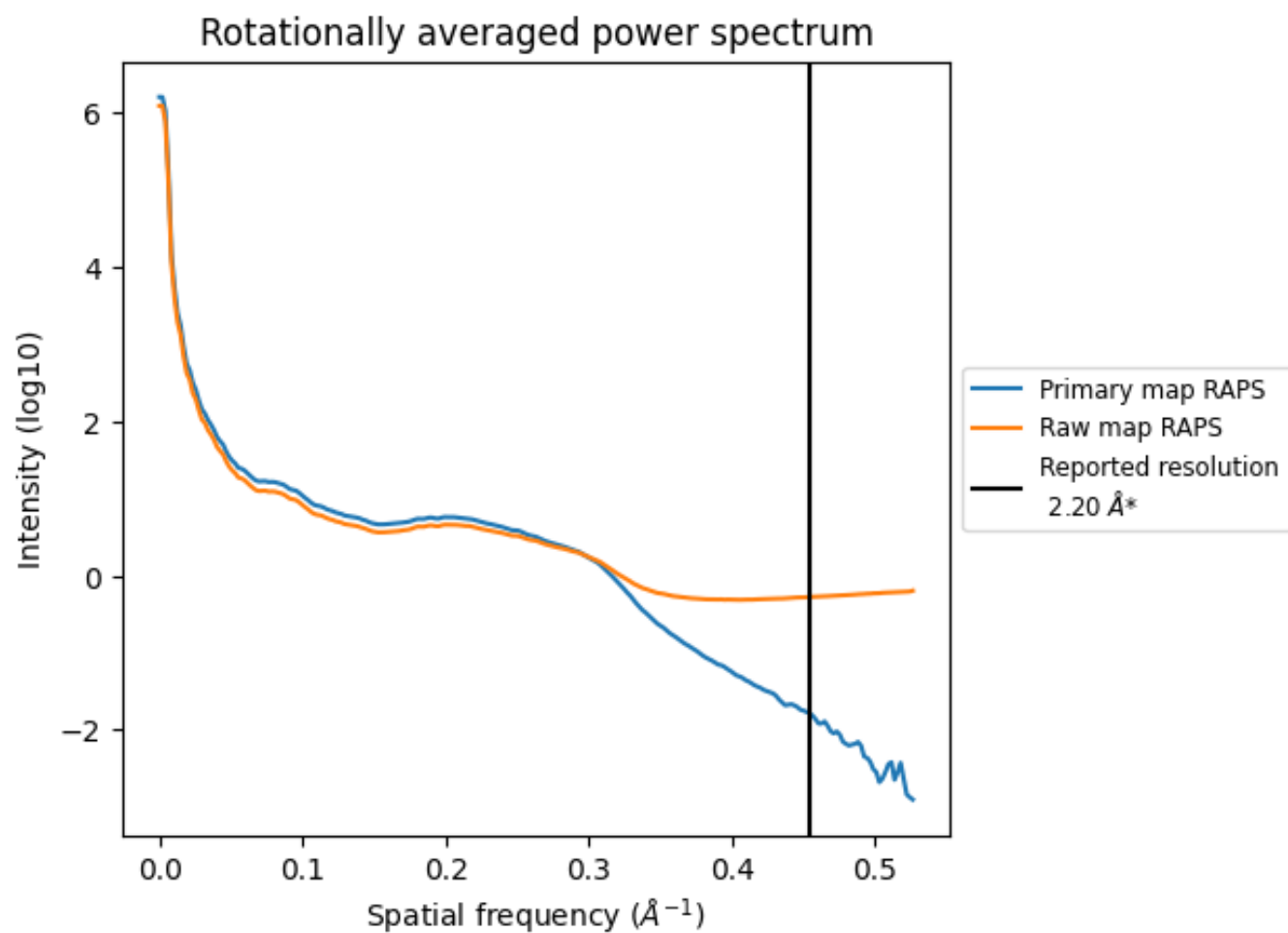
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1142 nm^3 ; this corresponds to an approximate mass of 1032 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 ⓘ

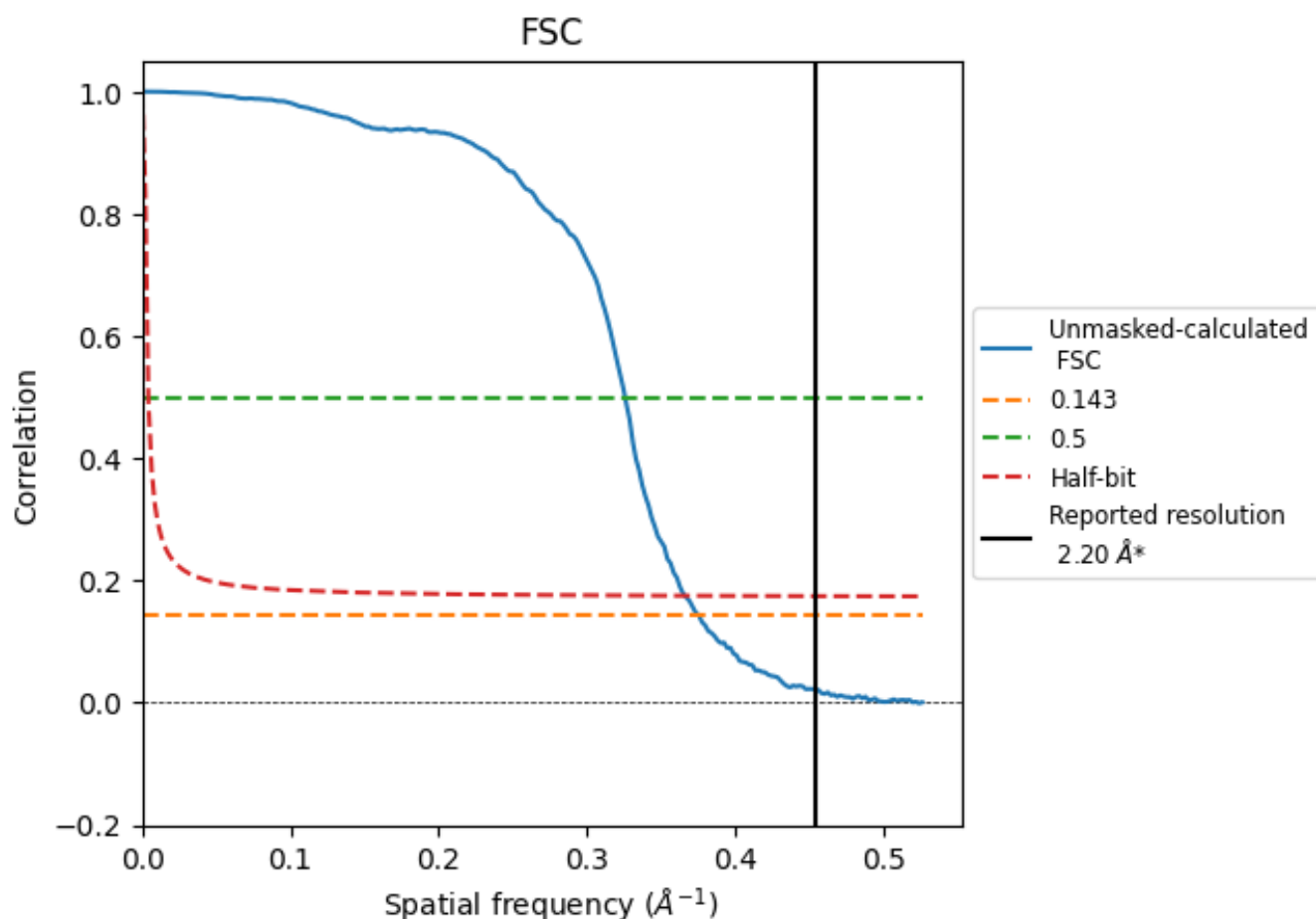


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

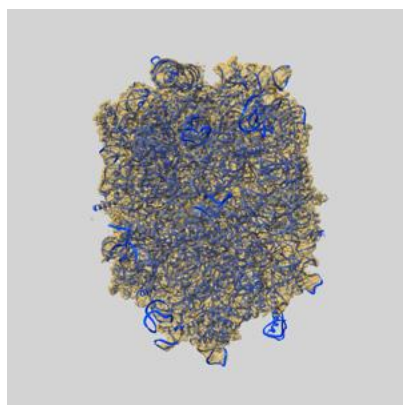
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.66	3.07	2.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.66 differs from the reported value 2.2 by more than 10 %

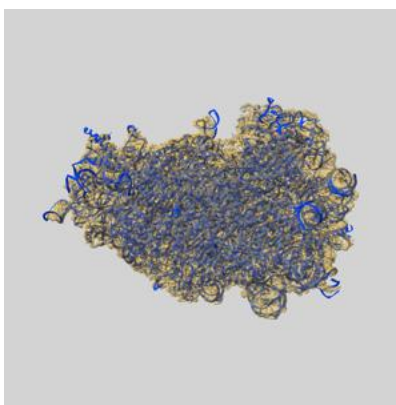
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51611 and PDB model 9GUL. Per-residue inclusion information can be found in section 3 on page 14.

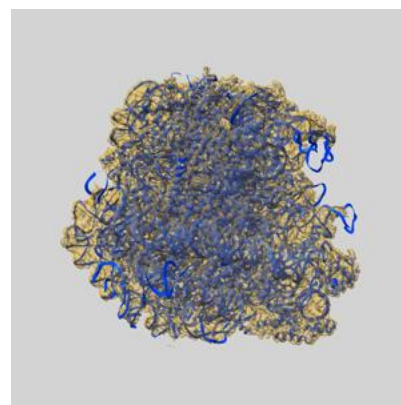
9.1 Map-model overlay [i](#)



X



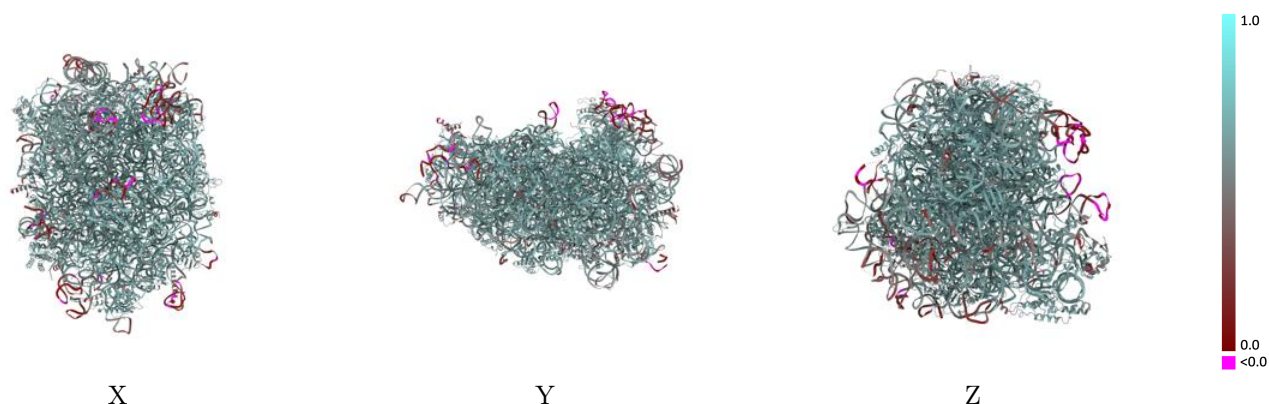
Y



Z

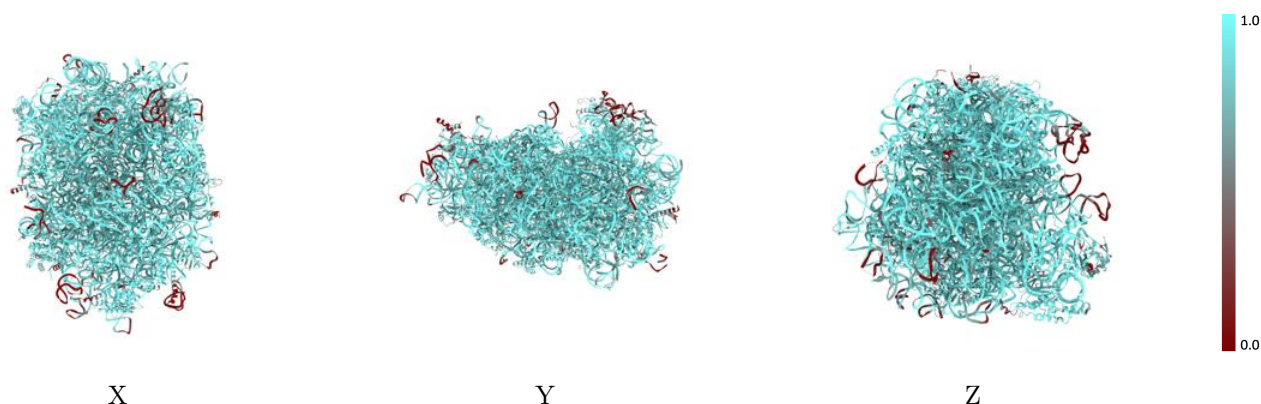
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



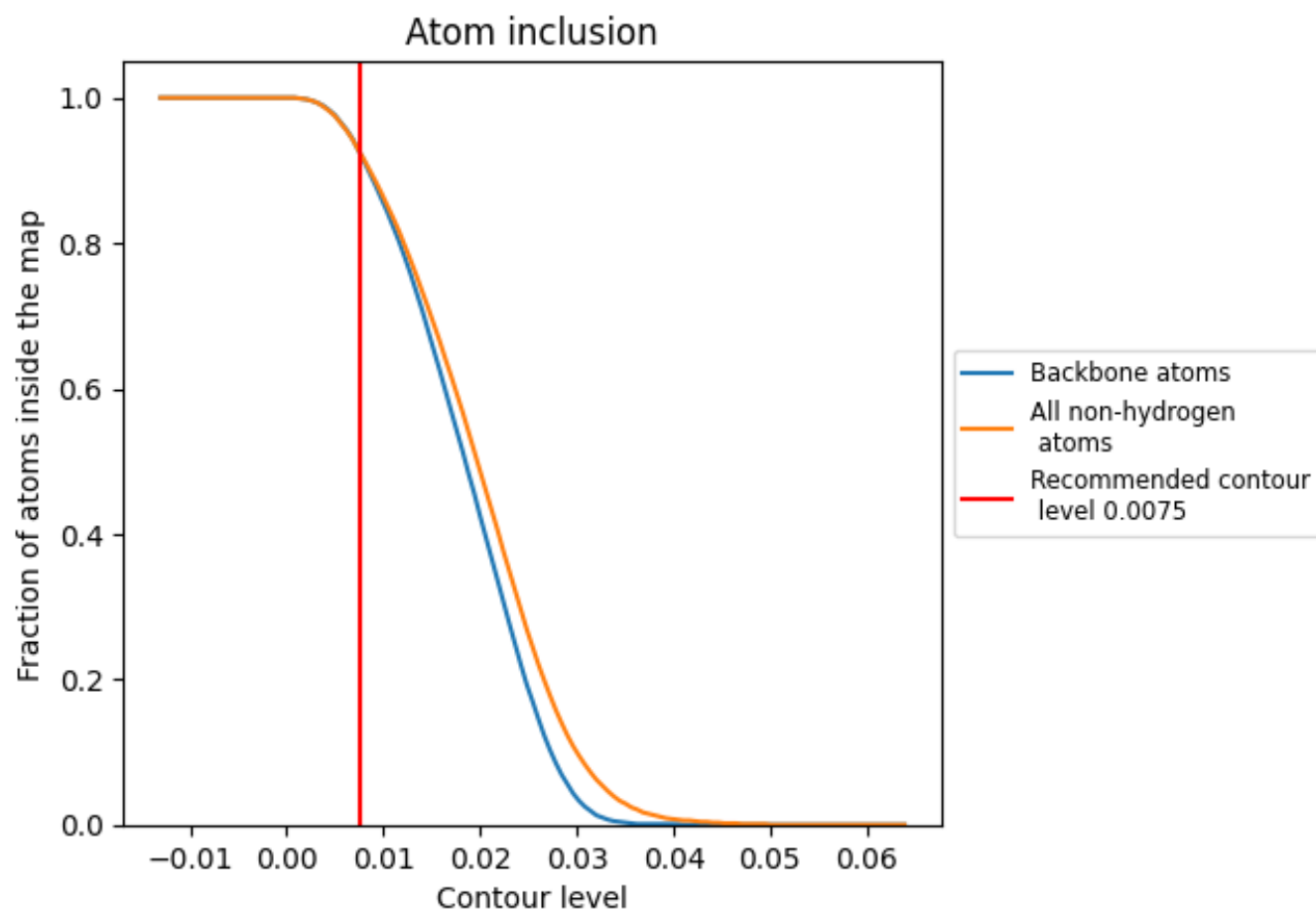
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% 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 (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9260	 0.5980
1	 0.9730	 0.6090
2	 0.9680	 0.5380
L5	 0.9190	 0.5800
L7	 0.9930	 0.6340
L8	 0.9640	 0.6150
LA	 0.9890	 0.6600
LB	 0.9340	 0.6320
LC	 0.9440	 0.6360
LD	 0.9190	 0.6040
LE	 0.9350	 0.6150
LF	 0.9590	 0.6390
LG	 0.8600	 0.5840
LH	 0.9450	 0.6280
LI	 0.9540	 0.6280
LJ	 0.7930	 0.5340
LL	 0.8990	 0.5990
LM	 0.9380	 0.6290
LN	 0.9980	 0.6660
LO	 0.9620	 0.6390
LP	 0.9660	 0.6470
LQ	 0.9840	 0.6510
LR	 0.8780	 0.5910
LS	 0.9820	 0.6550
LT	 0.9460	 0.6230
LU	 0.8340	 0.5400
LV	 0.9520	 0.6400
LW	 0.8170	 0.5850
LX	 0.9470	 0.6290
LY	 0.9280	 0.6270
LZ	 0.9350	 0.6190
La	 0.9730	 0.6560
Lb	 0.8980	 0.5800
Lc	 0.8740	 0.5910
Ld	 0.9260	 0.6140



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Chain	Atom inclusion	Q-score
Le	 0.9870	 0.6550
Lf	 0.9820	 0.6660
Lg	 0.8940	 0.6110
Lh	 0.9190	 0.6200
Li	 0.9250	 0.5990
Lj	 0.9910	 0.6610
Lk	 0.8190	 0.5690
Ll	 0.9810	 0.6360
Lm	 0.9450	 0.6320
Lo	 0.9240	 0.6170
Lp	 0.9270	 0.6300
Lr	 0.9600	 0.6340