



Full wwPDB EM Validation Report ⓘ

Jun 27, 2026 – 01:28 PM EDT

PDB ID : 9P7D / pdb_00009p7d
EMDB ID : EMD-71338
Title : In situ human Hibernating class4 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 2.57 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

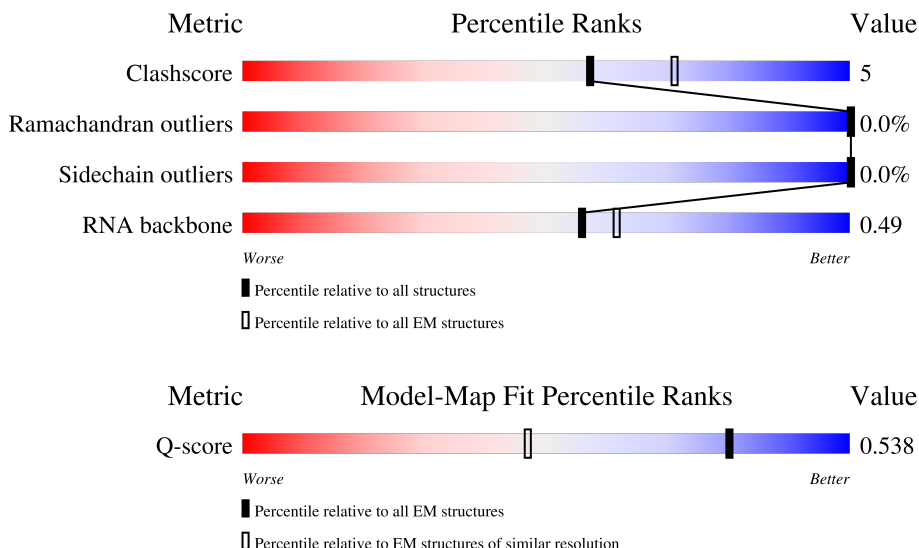
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.57 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.



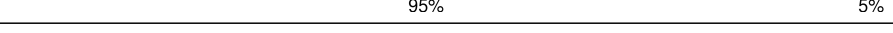
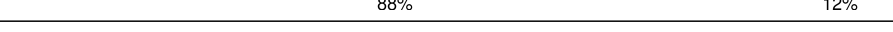
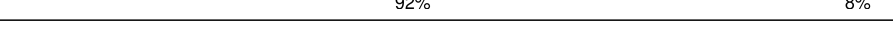
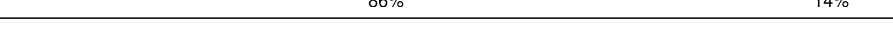
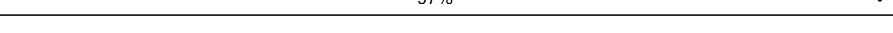
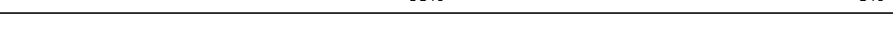
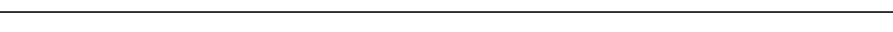
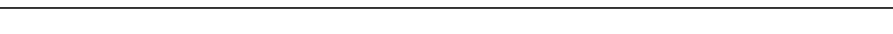
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7615 (2.07 - 3.07)

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	CD	408	
2	CI	31	
3	L5	5070	

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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	156	
6	LA	248	
7	LB	402	
8	LC	368	
9	LD	293	
10	LE	250	
11	LF	225	
12	LG	241	
13	LH	190	
14	LI	213	
15	LJ	176	
16	LL	210	
17	LM	139	
18	LN	203	
19	LO	201	
20	LP	153	
21	LQ	187	
22	LR	187	
23	LS	175	
24	LT	159	
25	LU	101	
26	LV	131	
27	LW	124	
28	LX	120	

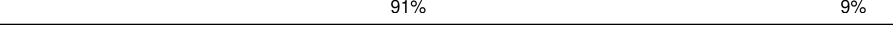
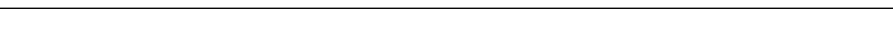
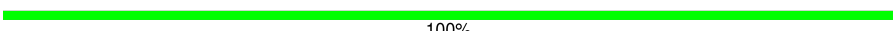
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Mol	Chain	Length	Quality of chain
29	LY	134	
30	LZ	135	
31	La	147	
32	Lb	121	
33	Lc	98	
34	Ld	107	
35	Le	128	
36	Lf	109	
37	Lg	114	
38	Lh	122	
39	Li	102	
40	Lj	86	
41	Lk	69	
42	Ll	50	
43	Lm	52	
44	Ln	24	
45	Lo	105	
46	Lp	91	
47	Lr	125	
48	Ls	196	
49	Lt	157	
50	SA	221	
51	SB	214	
52	SC	222	
53	SE	262	

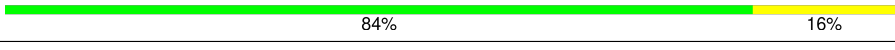
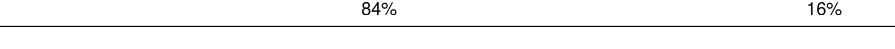
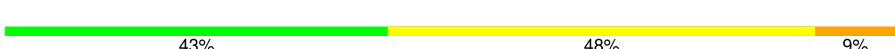
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Mol	Chain	Length	Quality of chain
54	SG	237	
55	SH	189	
56	SI	206	
57	SJ	185	
58	SL	153	
59	SN	150	
60	SO	140	
61	SV	83	
62	SW	129	
63	SX	141	
64	SY	131	
65	Sa	102	
66	Sb	83	
67	Se	58	
68	S2	1740	
69	SR	135	
70	SD	227	
71	SF	189	
72	SK	98	
73	SM	122	
74	SP	121	
75	SQ	144	
76	SS	145	
77	ST	143	
78	SU	104	

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Mol	Chain	Length	Quality of chain
79	SZ	75	 80% 20%
80	Sc	64	 84% 16%
81	Sd	55	 84% 16%
82	Sf	67	 79% 21%
83	Sg	313	 81% 19%
84	Et	75	 43% 48% 9%
85	CB	856	 77% 21%
86	CA	356	 7% 80% 20%

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 228149 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 SERPINE1 mRNA-binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	CD	55	Total	C	N	O	0	0
			440	263	87	90		

- Molecule 2 is a protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CI	31	Total	C	N	O	S	0	0
			247	153	55	38	1		

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

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

- 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
			2561	1141	456	844	120		

- 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	1481	585	1094	155		

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

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 8 is a protein called 60S ribosomal protein L4.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL18.

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	240	Total	C	N	O	S	0	0
			1935	1242	368	321	4		

- Molecule 11 is a protein called 60S ribosomal protein L7.

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	241	Total	C	N	O	S	0	0
			1927	1228	371	324	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	205	Total	C	N	O	S	0	0
			1658	1052	318	274	14		

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

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

- Molecule 16 is a protein called Large ribosomal subunit protein eL13.

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	187	Total	C	N	O	S	0	0
			1566	971	336	250	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 Heparin-binding protein HBp15.

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 Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LW	116	Total	C	N	O	S	0	0
			945	592	193	156	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	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 Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	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
			429	266	90	67	6		

- Molecule 44 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 45 is a protein called 60S ribosomal protein L36a.

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

- Molecule 46 is a protein called 60S ribosomal protein L37a.

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

- Molecule 47 is a protein called 60S ribosomal protein L28.

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

- Molecule 48 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Ls	196	Total	C	N	O	S	0	0
			1496	952	259	276	9		

- Molecule 49 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lt	134	Total	C	N	O	S	0	0
			998	626	180	189	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SA	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 51 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 52 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SC	220	Total	C	N	O	S	0	0
			1707	1104	293	300	10		

- Molecule 53 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 54 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 55 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 56 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 57 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 58 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 59 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 60 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SO	137	Total	C	N	O	S	0	0
			1024	627	200	191	6		

- Molecule 61 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 62 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 63 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 64 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 65 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 66 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 67 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 68 is a RNA chain called 18S rRNA [homo sapiens].

Mol	Chain	Residues	Atoms					AltConf	Trace
68	S2	1740	Total	C	N	O	P	0	0
			36952	16508	6600	12105	1739		

- Molecule 69 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 70 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 71 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 72 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 73 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 74 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SP	121	Total	C	N	O	S	0	0
			985	623	185	170	7		

- Molecule 75 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 76 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 77 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 78 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 79 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 80 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 81 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 82 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 83 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 84 is a RNA chain called E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Et	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 85 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	CB	846	Total	C	N	O	S	0	0
			6605	4193	1136	1232	44		

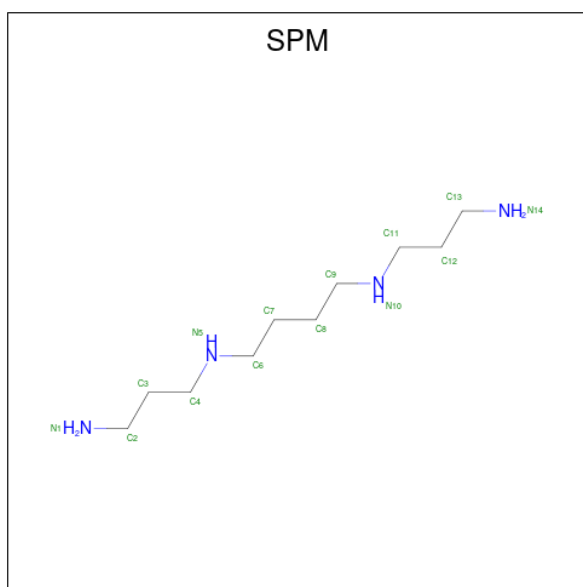
- Molecule 86 is a protein called Proliferation-associated protein 2G4.

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

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

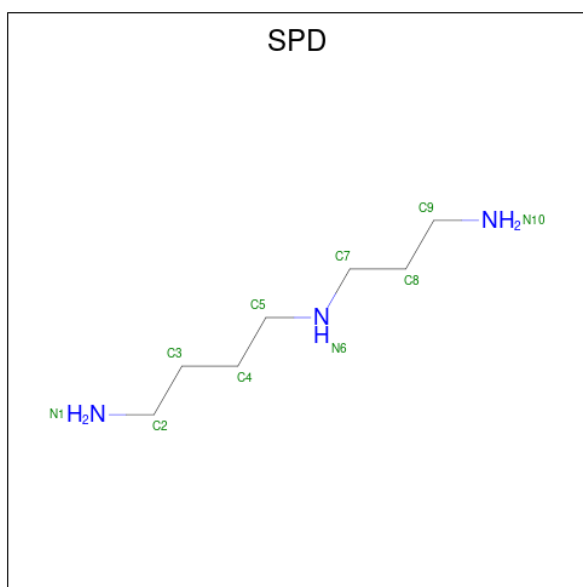
Mol	Chain	Residues	Atoms		AltConf
87	L5	179	Total	Mg	0
			179	179	
87	L7	3	Total	Mg	0
			3	3	
87	L8	5	Total	Mg	0
			5	5	
87	LA	1	Total	Mg	0
			1	1	
87	LP	1	Total	Mg	0
			1	1	
87	LV	1	Total	Mg	0
			1	1	
87	Le	1	Total	Mg	0
			1	1	
87	S2	27	Total	Mg	0
			27	27	

- Molecule 88 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 89 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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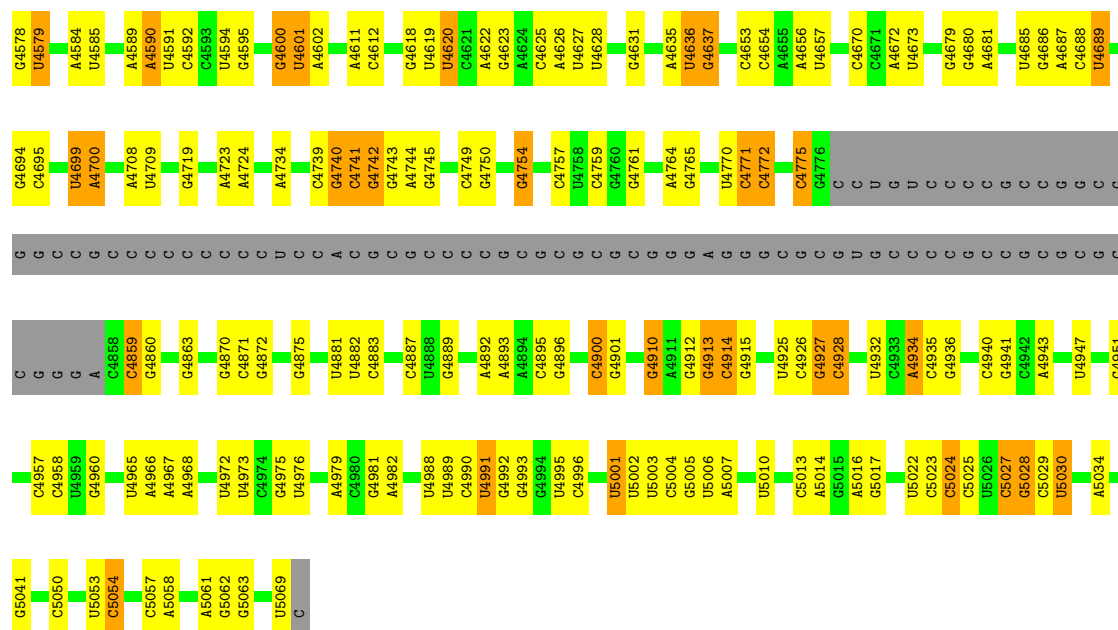
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Mol	Chain	Residues	Atoms		AltConf
90	Lj	1	Total 1	Zn 1	0
90	Lm	1	Total 1	Zn 1	0
90	Lo	1	Total 1	Zn 1	0
90	Lp	1	Total 1	Zn 1	0
90	Sa	1	Total 1	Zn 1	0



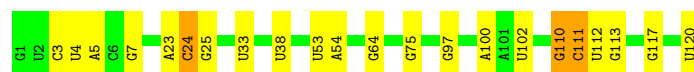


U4481	C4365	G4143	G	C	U3920	U3838	A3717	A3610	G	U	C	G
U4482	G4371	C4144	A	C	U3921	G3839	A3718	A3611	G	C	U	G
G4488	U4372	C4145	A	C	G3922	G3840	A3719	U3611	U	G	G	G
G4489	G4373	G4146	A	C	A3923	C3841	A3720	G3615	C	C	G	G
U4493	A4273	G4150	C	C	U3925	U3844	U3721	U3616	C	C	A	C
U4498	A4274	C4162	C	G	A3928	U3848	G3722	G3619	C	C	G	A
G4499	G4275	U4163	C	U	G3929	U3849	A3726	A3624	C	G	G	G
U4500	G4276	C4164	C	G	U3930	C3850	A3727	G3625	C	G	A	U
C4504	C4277	G4170	U	U	C3931	U3851	A3732	G3626	C	C	C	C
C4505	C4278	A4183	C	C	U3932	A3852	A3733	A3630	G	C	C	C
C4508	A4279	G4184	C	C	G3933	U3853	A3734	A3635	G	C	C	C
U4512	A4280	U4188	C	C	C3937	A3856	A3736	A3636	G	G	G	G
A4513	A4281	G4189	C	C	G3938	A3861	A3737	C3636	G	C	G	G
G4514	A4282	U4190	C	A	A3942	A3862	A3748	U3637	C	C	C	C
G4515	G4291	U4191	G	G	G3944	A3867	G3754	U3639	C	G	G	C
C4519	U4295	G4196	G	G	A3945	G3868	G3755	U3640	G	A	G	G
G4520	U4296	U4201	G	G	A3946	C3869	A3756	U3641	U	C	C	G
U4521	U4299	G4202	C	C	C3948	C3870	U3764	U3644	C	C	C	G
A4522	U4302	A4203	C	C	A3949	A3871	A3774	A3645	C	A	G	G
G4523	C4303	A4214	G	G	U3950	A3872	A3775	A3646	G	C	G	G
G4524	A4304	G4220	G	G	G3951	G3873	U3770	A3647	C	G	U	C
G4525	G4305	C4221	C	G	A3952	G3874	U3772	A3648	C	C	C	C
U4530	U4306	G4222	C	C	G3953	A3877	U3773	A3652	C	G	G	C
U4531	U4312	G4225	G	G	A3954	C3878	A3774	A3653	G	C	U	G
U4532	A4313	G4226	G	G	G	C3879	A3775	G3661	C	G	C	G
C4434	C4314	U4227	G	G	U3880	G3880	A3776	A3662	C	A	C	A
A4441	C4319	G4228	U	C	G3881	A3884	G3777	A3663	C	C	C	C
U4442	G4328	U4229	C	A	U3885	G3885	C3782	G3664	C	U	C	C
G4443	G4329	C4101	C	A	G3886	C3887	A3785	G3665	U	C	C	C
G4444	G4330	C4102	C	A	C3887	A3889	U3786	C3670	C	C	G	G
C4447	G4331	U4103	C	U	A3890	A3891	G3792	G3673	C	C	U	G
A4448	C4332	G4104	C	A	U3892	U3892	C3808	G3674	U	C	C	C
G4449	G4338	A4105	G	G	G3897	G3898	G3811	U3690	G	G	C	C
U4452	U4344	G4108	C	C	G3899	G3899	U3814	G3691	G	C	G	C
C4456	C4345	U4111	C	G	G3900	G3900	U3817	U3695	C	C	G	G
U4457	G4346	U4112	G	U	A3901	A3901	U3818	C3696	C	U	C	C
U4458	U4347	U4113	C	G	A3906	G3907	G3819	U3697	C	U	C	C
U4459	A4348	G4115	G	C	G3908	C3909	U3822	A3595	C	C	U	C
U4460	C4349	C4116	G	C	C3910	A3824	U3825	C3597	C	C	C	C
U4464	C4350	C4119	C	C	C3911	A3826	G3828	C3598	C	U	C	C
A4464	U4353	U4122	C	C	U3912	G3827	A3830	C3599	C	C	C	C
U4465	U4354	A4127	C	C	U3915	A3830	A3830	C3600	C	C	C	C
G4466	U4361	G4141	G	G	U3915	A3830	A3830	C3605	C	C	C	C
U4471	A4362	C4142	U	U	U3915	A3830	A3830	U3606	C	C	C	C
U4574	G4364							U3607	C			
G4575												
U4576												
U4577												



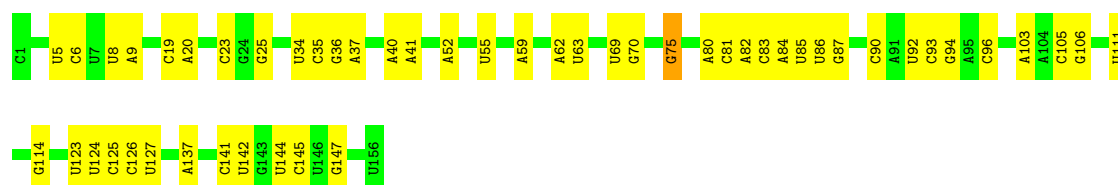
- Molecule 4: 5S rRNA

Chain L7: 82% 16%



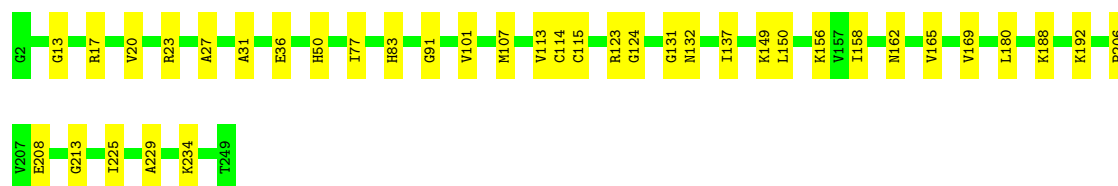
- Molecule 5: 5.8S rRNA

Chain L8: 67% 32%



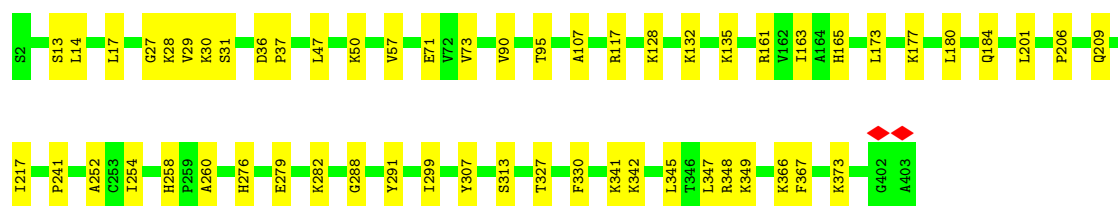
- Molecule 6: 60S ribosomal protein L8

Chain LA: 85% 15%



- Molecule 7: Large ribosomal subunit protein uL3

Chain LB: 86% 14%



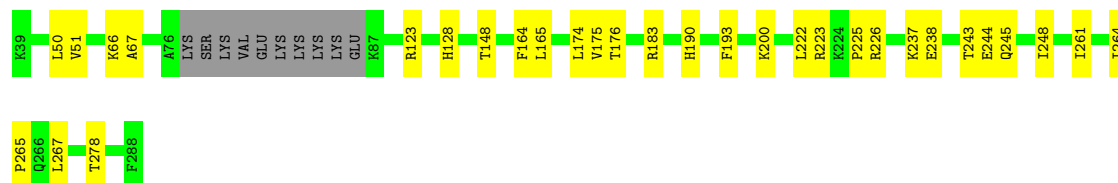
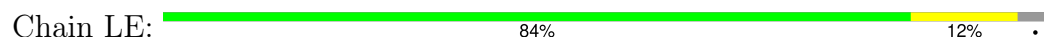
- Molecule 8: 60S ribosomal protein L4



- Molecule 9: Large ribosomal subunit protein uL18



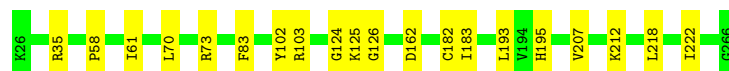
- Molecule 10: Large ribosomal subunit protein eL6



- Molecule 11: 60S ribosomal protein L7



- Molecule 12: 60S ribosomal protein L7a



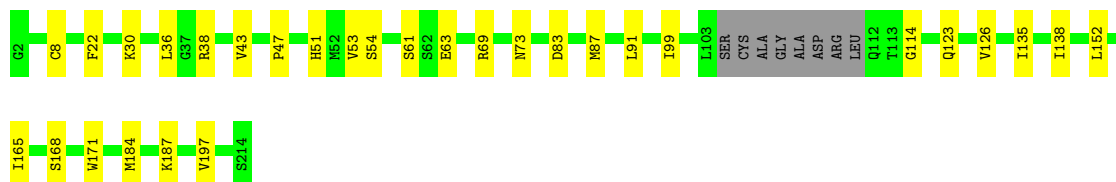
- Molecule 13: 60S ribosomal protein L9





- Molecule 14: Ribosomal protein uL16-like

Chain LI: 82% 14%



- Molecule 15: 60S ribosomal protein L11

Chain LJ: 88% 9%



- Molecule 16: Large ribosomal subunit protein eL13

Chain LL: 95% 5%



- Molecule 17: 60S ribosomal protein L14

Chain LM: 88% 12%



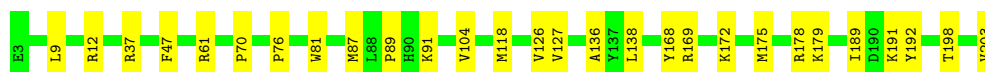
- Molecule 18: 60S ribosomal protein L15

Chain LN: 92% 8%



- Molecule 19: 60S ribosomal protein L13a

Chain LO: 86% 14%

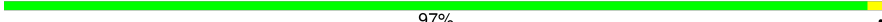


- Molecule 20: 60S ribosomal protein L17

Chain LP:  86% 14%

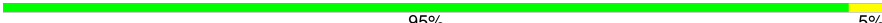


- Molecule 21: 60S ribosomal protein L18

Chain LQ:  97% .



- Molecule 22: 60S ribosomal protein L19

Chain LR:  95% 5%



- Molecule 23: 60S ribosomal protein L18a

Chain LS:  91% 9%



- Molecule 24: 60S ribosomal protein L21

Chain LT:  91% 9%



- Molecule 25: Heparin-binding protein HBp15

Chain LU:  79% 21%



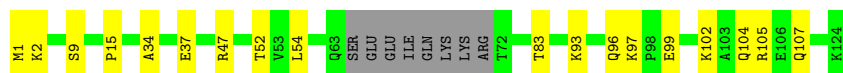
- Molecule 26: 60S ribosomal protein L23

Chain LV:  92% 8%



- Molecule 27: Ribosomal protein L24

Chain LW:  79% 15% 6%

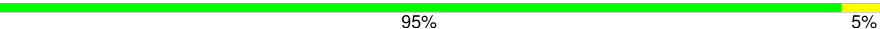


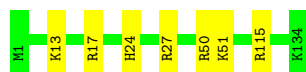
- Molecule 28: 60S ribosomal protein L23a

Chain LX:  90% 10%



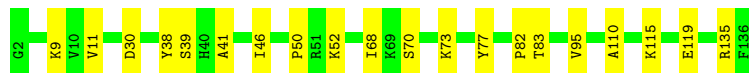
- Molecule 29: 60S ribosomal protein L26

Chain LY:  95% 5%



- Molecule 30: 60S ribosomal protein L27

Chain LZ:  85% 15%



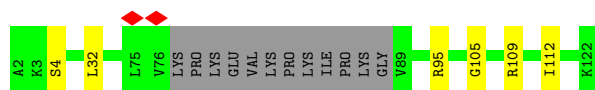
- Molecule 31: 60S ribosomal protein L27a

Chain La:  89% 11%



- Molecule 32: Large ribosomal subunit protein eL29

Chain Lb:  85% 5% 10%



- Molecule 33: 60S ribosomal protein L30

Chain Lc:  88% 12%



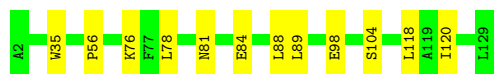
- Molecule 34: 60S ribosomal protein L31

Chain Ld:  90% 10%



- Molecule 35: 60S ribosomal protein L32

Chain Le:  91% 9%

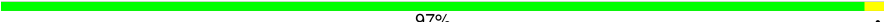


- Molecule 36: 60S ribosomal protein L35a

Chain Lf:  92% 8%



- Molecule 37: 60S ribosomal protein L34

Chain Lg:  97%

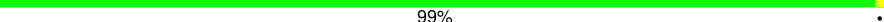


- Molecule 38: 60S ribosomal protein L35

Chain Lh:  84% 16%



- Molecule 39: 60S ribosomal protein L36

Chain Li:  99%



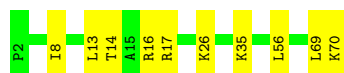
- Molecule 40: 60S ribosomal protein L37

Chain Lj:  93% 7%



- Molecule 41: 60S ribosomal protein L38

Chain Lk:  86% 14%



- Molecule 42: 60S ribosomal protein L39

Chain Ll:  86% 14%

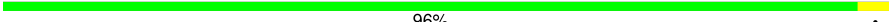


- Molecule 43: Large ribosomal subunit protein eL40

Chain Lm:  87% 13%



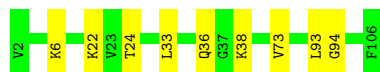
- Molecule 44: 60S ribosomal protein L41

Chain Ln:  96%



- Molecule 45: 60S ribosomal protein L36a

Chain Lo:  91% 9%



- Molecule 46: 60S ribosomal protein L37a

Chain Lp:  93% 7%



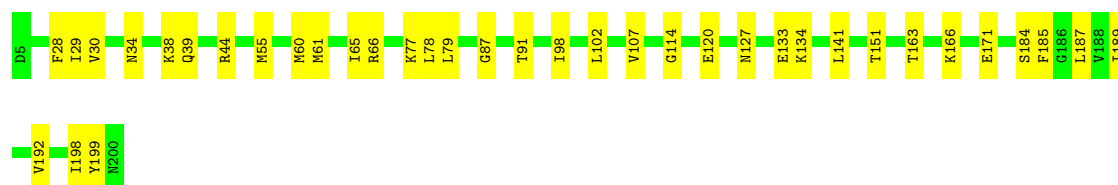
- Molecule 47: 60S ribosomal protein L28

Chain Lr:  94% 6%



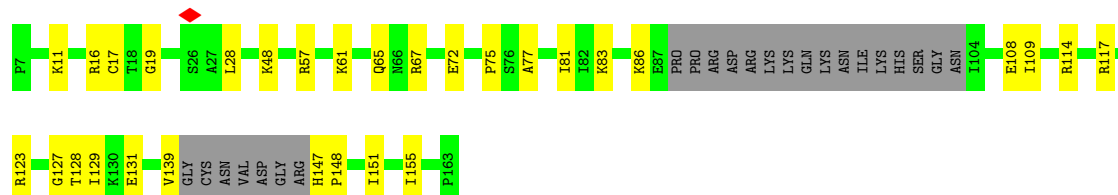
- Molecule 48: 60S acidic ribosomal protein P0

Chain Ls:  81% 19%



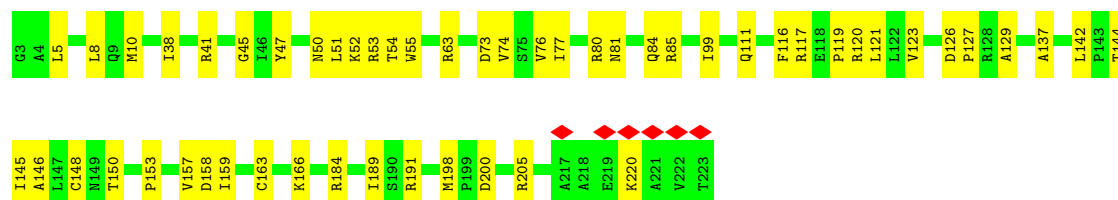
- Molecule 49: Large ribosomal subunit protein uL11

Chain Lt:  66% 19% 15%



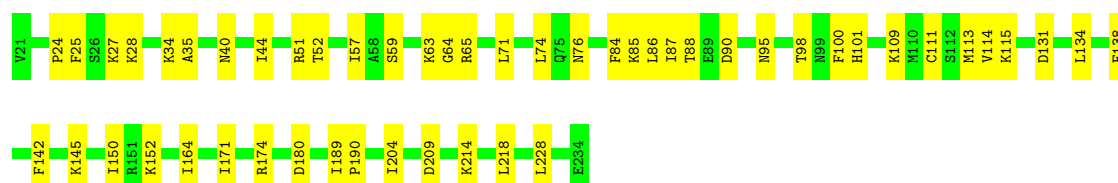
- Molecule 50: 40S ribosomal protein SA

Chain SA:  76% 24%



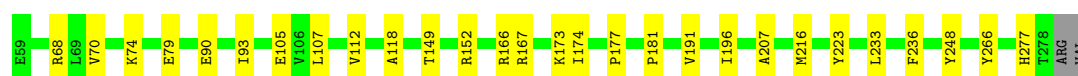
- Molecule 51: 40S ribosomal protein S3a

Chain SB:  76% 24%



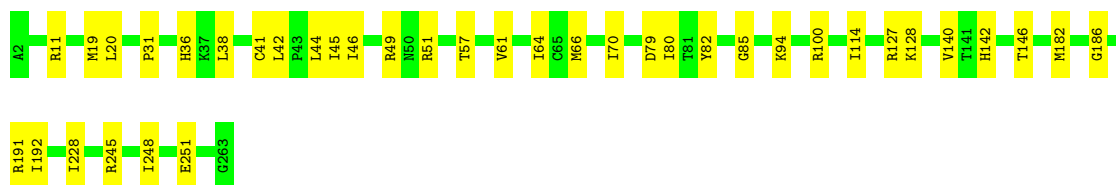
- Molecule 52: 40S ribosomal protein S2

Chain SC:  86% 13%



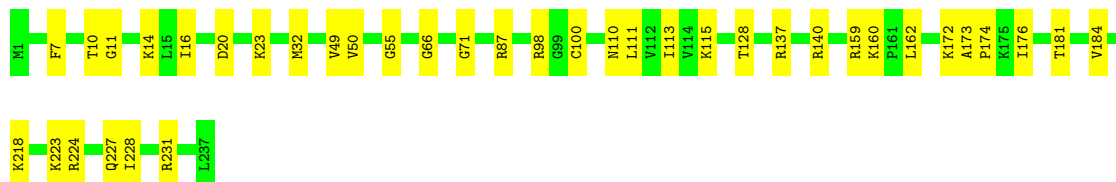
- Molecule 53: Small ribosomal subunit protein eS4, X isoform

Chain SE:  85% 15%



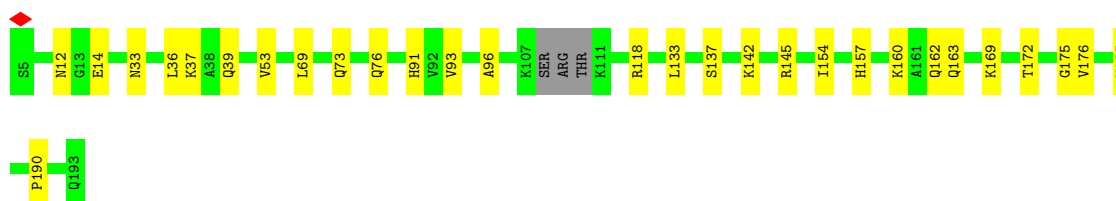
- Molecule 54: 40S ribosomal protein S6

Chain SG: 84% 16%



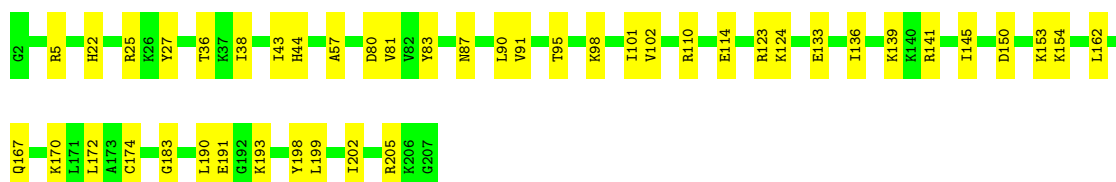
- Molecule 55: Small ribosomal subunit protein eS7

Chain SH: 83% 15%



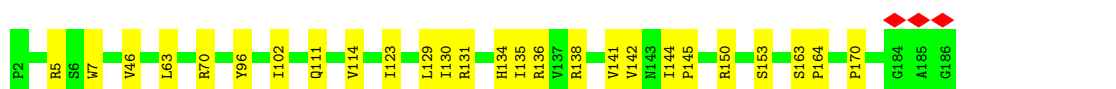
- Molecule 56: 40S ribosomal protein S8

Chain SI: 79% 21%



- Molecule 57: 40S ribosomal protein S9

Chain SJ: 86% 14%



- Molecule 58: 40S ribosomal protein S11

Chain SL: 88% 12%



- Molecule 59: 40S ribosomal protein S13

Chain SN: 91% 9%



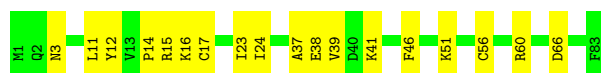
- Molecule 60: Small ribosomal subunit protein uS11

Chain SO: 79% 19%



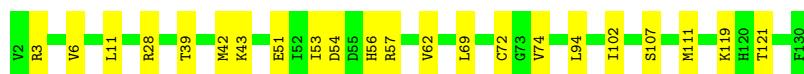
- Molecule 61: Small ribosomal subunit protein eS21

Chain SV: 78% 22%



- Molecule 62: 40S ribosomal protein S15a

Chain SW: 83% 17%



- Molecule 63: 40S ribosomal protein S23

Chain SX: 87% 13%



- Molecule 64: 40S ribosomal protein S24

Chain SY: 83% 17%

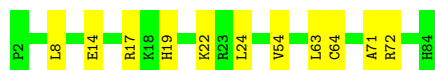


- Molecule 65: 40S ribosomal protein S26

Chain Sa: 84% 16%



- Molecule 66: Small ribosomal subunit protein eS27

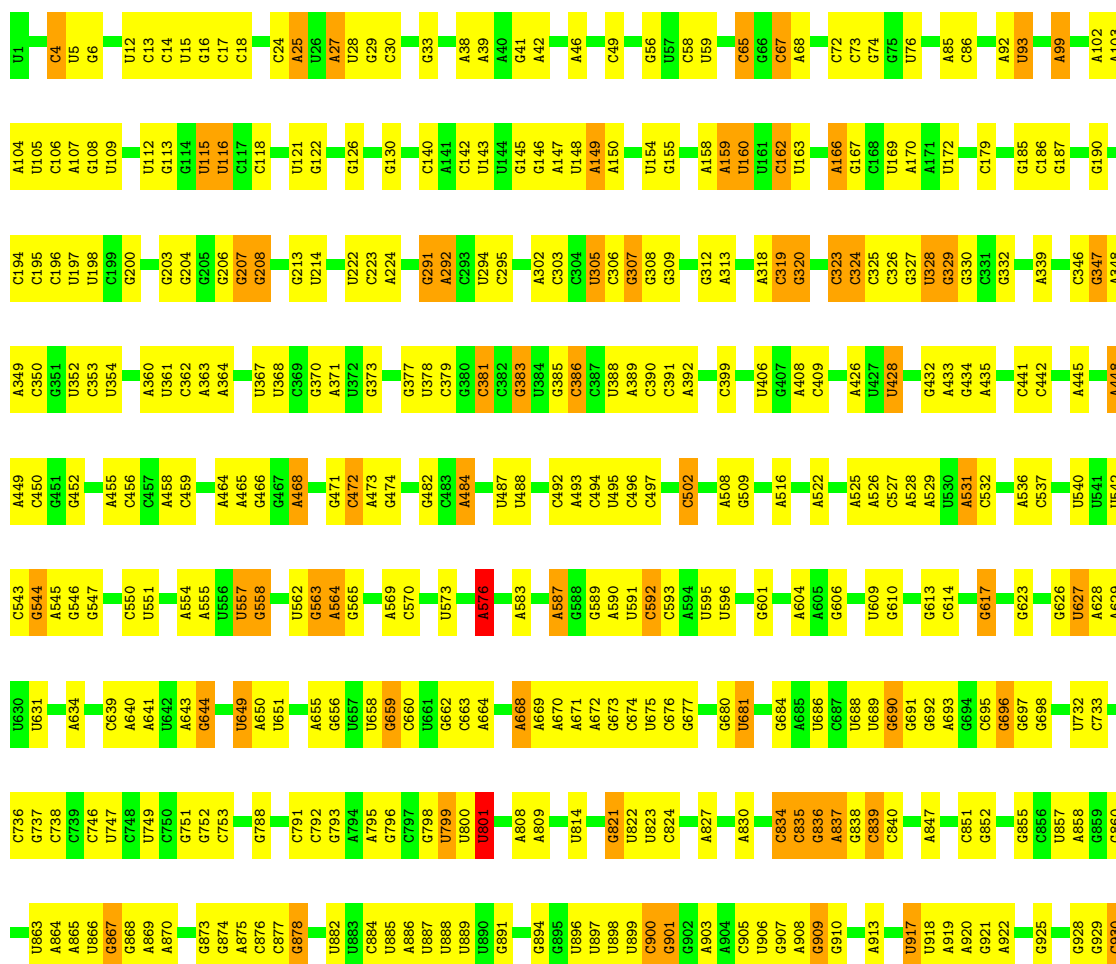


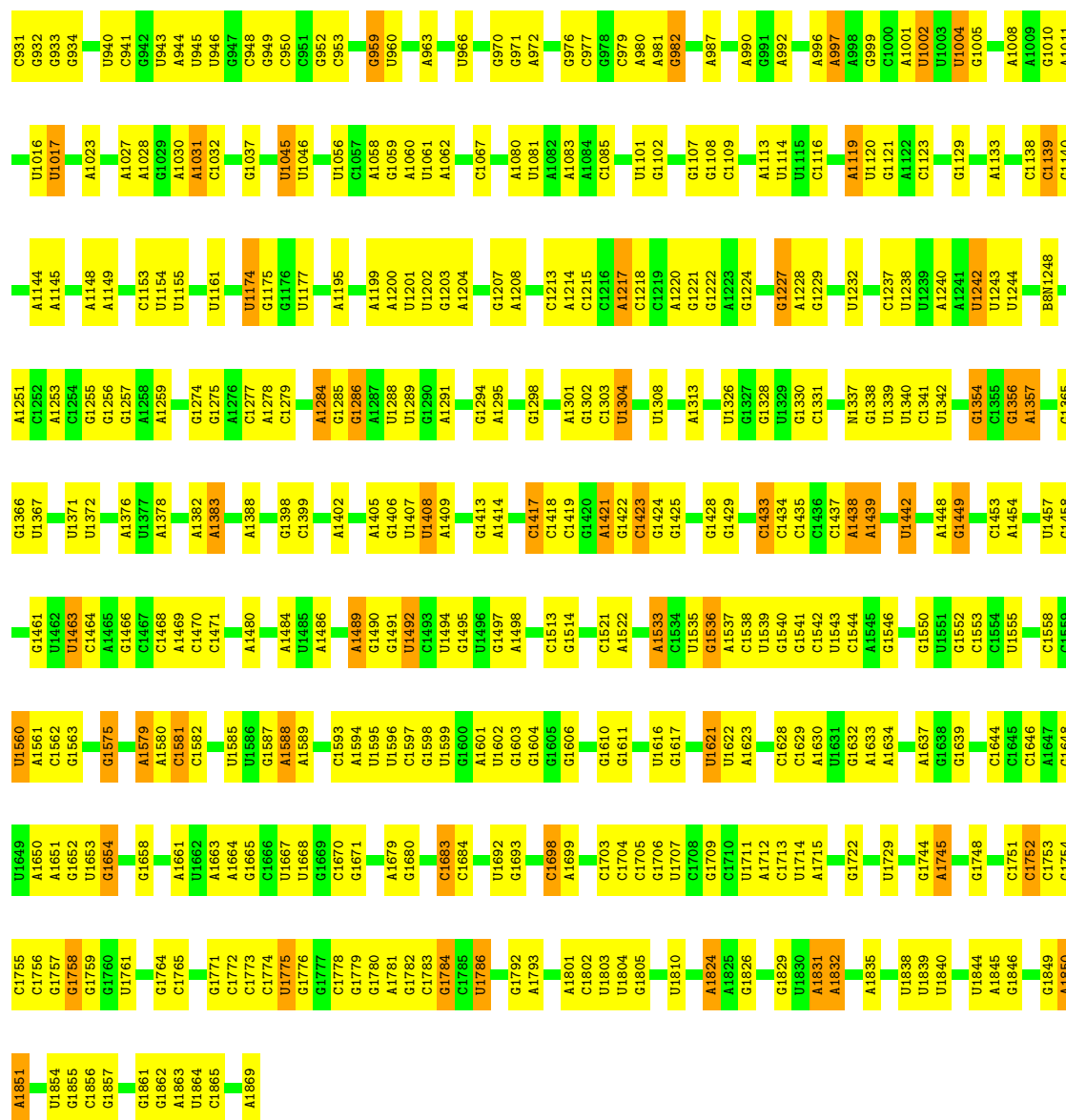
- Molecule 67: Small ribosomal subunit protein eS30



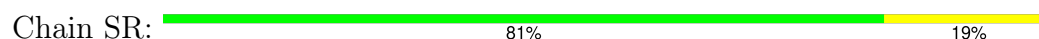
There are no outlier residues recorded for this chain.

- Molecule 68: 18S rRNA [homo sapiens]





- Molecule 69: Small ribosomal subunit protein eS17

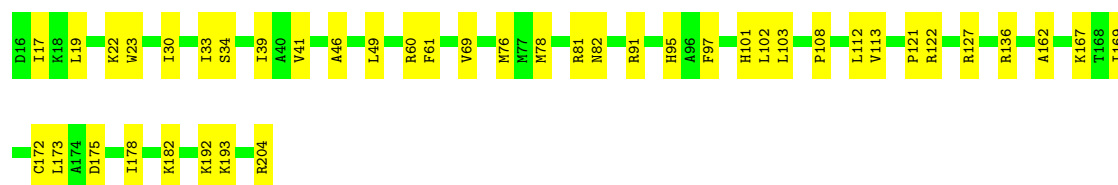


- Molecule 70: Small ribosomal subunit protein uS3



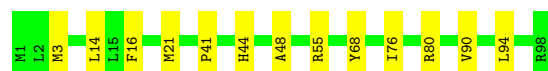
- Molecule 71: 40S ribosomal protein S5

Chain SF:  78% 22%



- Molecule 72: 40S ribosomal protein S10

Chain SK:  87% 13%



- Molecule 73: Small ribosomal subunit protein eS12

Chain SM:  84% 16%



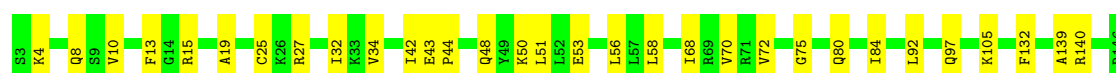
- Molecule 74: Small ribosomal subunit protein uS19

Chain SP:  79% 21%



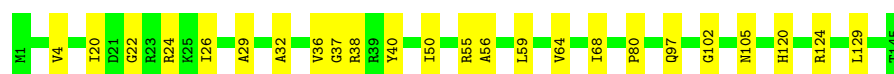
- Molecule 75: Small ribosomal subunit protein uS9

Chain SQ:  78% 22%



- Molecule 76: 40S ribosomal protein S18

Chain SS:  83% 17%

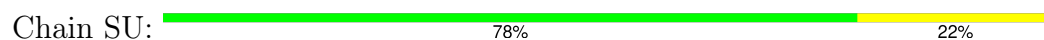


- Molecule 77: 40S ribosomal protein S19

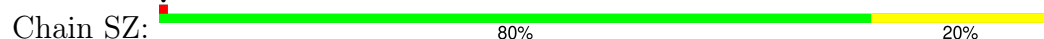
Chain ST:  85% 15%



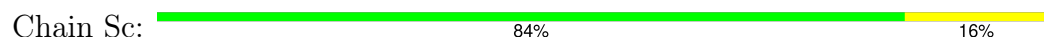
- Molecule 78: 40S ribosomal protein S20



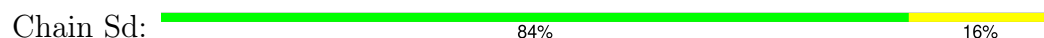
- Molecule 79: Small ribosomal subunit protein eS25



- Molecule 80: 40S ribosomal protein S28



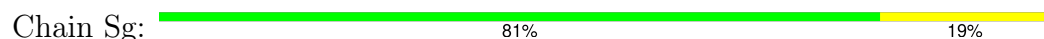
- Molecule 81: 40S ribosomal protein S29



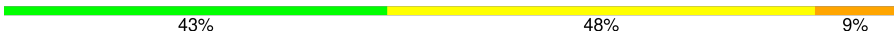
- Molecule 82: Ubiquitin-40S ribosomal protein S27a

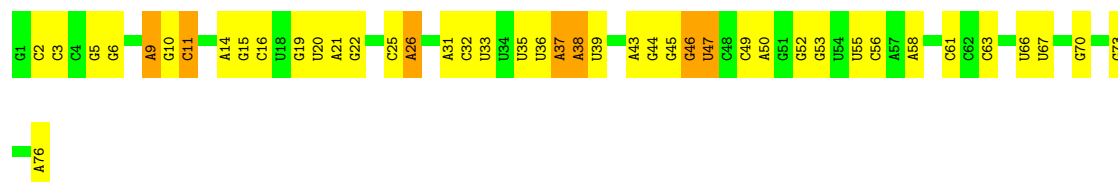


- Molecule 83: Receptor of activated protein C kinase 1



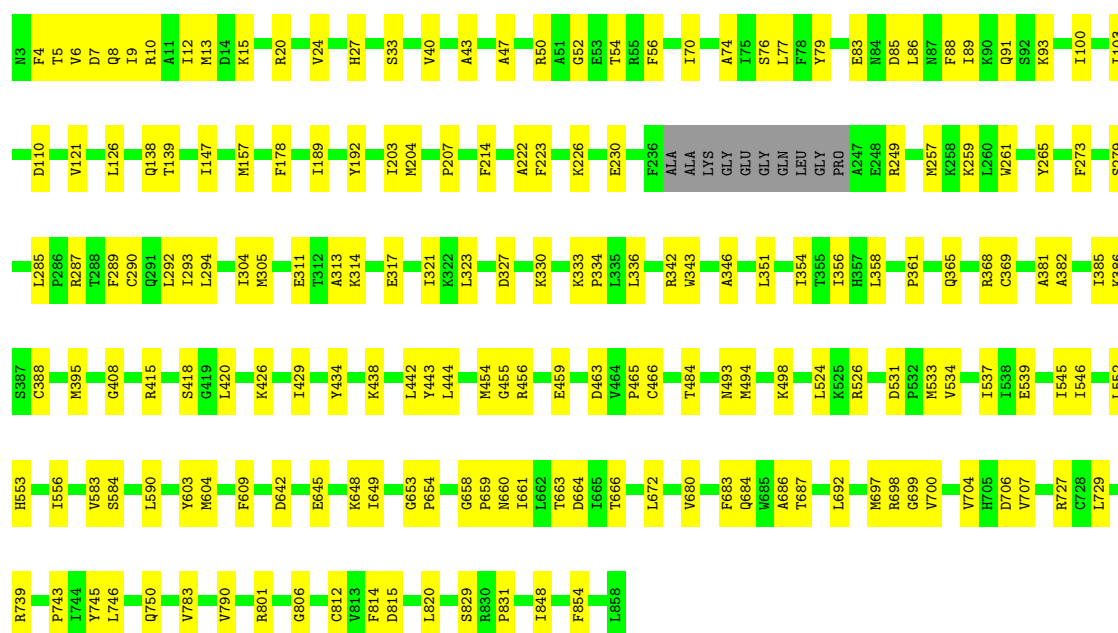
- Molecule 84: E site tRNA

Chain Et: 



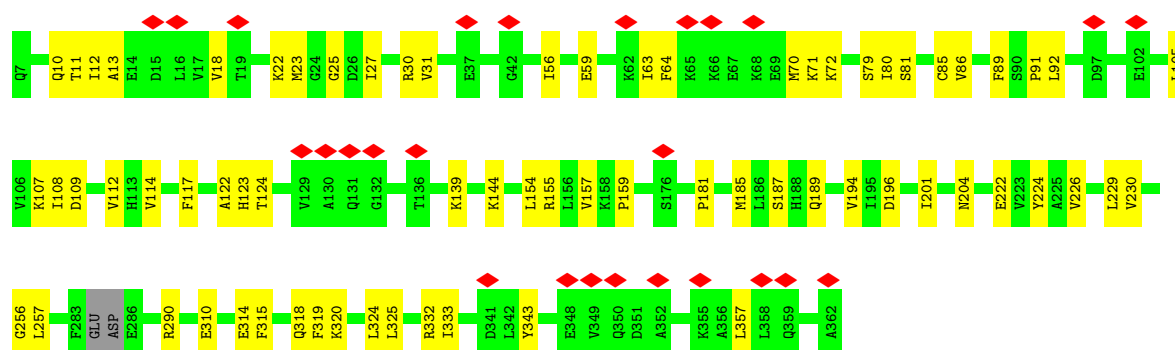
- Molecule 85: Elongation factor 2

Chain CB: 



- Molecule 86: Proliferation-associated protein 2G4

Chain CA: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219754	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.299	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0145	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, MG, OMC, OMU, ZN, A2M, 5MC, OMG, 6MZ, 1MA, MA6, UY1, UR3, SPM, B8N, 4AC, PSU, SPD

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	CD	0.17	0/447	0.31	0/592
2	CI	0.16	0/247	0.32	0/323
3	L5	0.36	0/85098	0.33	0/132762
4	L7	0.34	0/2861	0.28	0/4459
5	L8	0.36	0/3631	0.30	0/5657
6	LA	0.35	0/1936	0.40	0/2596
7	LB	0.32	0/3306	0.39	0/4424
8	LC	0.34	0/2981	0.40	0/4002
9	LD	0.27	0/2428	0.35	0/3252
10	LE	0.26	0/1973	0.41	0/2645
11	LF	0.33	0/1905	0.34	0/2539
12	LG	0.28	0/1960	0.37	0/2637
13	LH	0.30	0/1537	0.37	0/2066
14	LI	0.29	0/1697	0.33	0/2266
15	LJ	0.24	0/1385	0.36	0/1852
16	LL	0.30	0/1732	0.35	0/2315
17	LM	0.30	0/1161	0.38	0/1554
18	LN	0.36	0/1746	0.34	0/2338
19	LO	0.34	0/1682	0.37	0/2250
20	LP	0.34	0/1268	0.41	0/1701
21	LQ	0.34	0/1537	0.37	0/2052
22	LR	0.27	0/1582	0.31	0/2091
23	LS	0.33	0/1493	0.34	0/2003
24	LT	0.31	0/1326	0.32	0/1770
25	LU	0.23	0/839	0.34	0/1126
26	LV	0.32	0/993	0.39	0/1332
27	LW	0.23	0/959	0.32	0/1270
28	LX	0.30	0/1002	0.32	0/1345
29	LY	0.30	0/1132	0.35	0/1504
30	LZ	0.28	0/1130	0.34	0/1507
31	La	0.34	0/1191	0.34	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.27	0/889	0.38	0/1175
33	Lc	0.28	0/774	0.37	0/1038
34	Ld	0.30	0/903	0.37	0/1216
35	Le	0.34	0/1071	0.35	0/1429
36	Lf	0.36	0/895	0.39	0/1198
37	Lg	0.30	0/916	0.33	0/1220
38	Lh	0.28	0/1023	0.34	0/1351
39	Li	0.25	0/843	0.32	0/1115
40	Lj	0.37	0/720	0.42	0/952
41	Lk	0.25	0/575	0.32	0/761
42	Ll	0.31	0/454	0.31	0/599
43	Lm	0.30	0/435	0.34	0/575
44	Ln	0.23	0/231	0.27	0/294
45	Lo	0.30	0/876	0.35	0/1156
46	Lp	0.32	0/718	0.33	0/953
47	Lr	0.32	0/1017	0.34	0/1364
48	Ls	0.17	0/1519	0.34	0/2052
49	Lt	0.17	0/1009	0.46	0/1363
50	SA	0.20	0/1778	0.36	0/2416
51	SB	0.18	0/1765	0.37	0/2362
52	SC	0.21	0/1744	0.33	0/2357
53	SE	0.19	0/2118	0.35	0/2849
54	SG	0.14	0/1946	0.33	0/2590
55	SH	0.17	0/1519	0.41	0/2033
56	SI	0.18	0/1715	0.37	0/2287
57	SJ	0.18	0/1550	0.31	0/2069
58	SL	0.20	0/1268	0.30	0/1696
59	SN	0.18	0/1232	0.30	0/1656
60	SO	0.19	0/1037	0.36	0/1391
61	SV	0.19	0/643	0.33	0/860
62	SW	0.22	0/1051	0.35	0/1406
63	SX	0.23	0/1116	0.39	0/1490
64	SY	0.15	0/1083	0.32	0/1438
65	Sa	0.22	0/836	0.36	0/1121
66	Sb	0.19	0/665	0.36	0/891
67	Se	0.17	0/465	0.34	0/612
68	S2	0.24	0/39756	0.29	0/61939
69	SR	0.17	0/1105	0.43	0/1484
70	SD	0.18	0/1793	0.32	0/2414
71	SF	0.15	0/1516	0.33	0/2037
72	SK	0.18	0/851	0.36	0/1147
73	SM	0.13	0/950	0.35	0/1275
74	SP	0.18	0/1003	0.34	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SQ	0.19	0/1160	0.40	0/1553
76	SS	0.17	0/1216	0.37	0/1628
77	ST	0.17	0/1131	0.33	0/1515
78	SU	0.20	0/831	0.36	0/1115
79	SZ	0.19	0/604	0.39	0/810
80	Sc	0.17	0/508	0.35	0/680
81	Sd	0.23	0/470	0.45	0/623
82	Sf	0.16	0/560	0.49	0/745
83	Sg	0.15	0/2493	0.36	0/3394
84	Et	0.19	0/1778	0.39	0/2767
85	CB	0.19	0/6734	0.34	0/9094
86	CA	0.15	0/2810	0.39	0/3780
All	All	0.29	0/239833	0.34	0/350498

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	CD	440	0	402	5	0
2	CI	247	0	283	1	0
3	L5	78444	0	39720	520	0
4	L7	2561	0	1295	12	0
5	L8	3315	0	1685	17	0
6	LA	1898	0	1993	23	0
7	LB	3238	0	3376	41	0
8	LC	2927	0	3104	20	0
9	LD	2382	0	2410	17	0
10	LE	1935	0	2096	22	0
11	LF	1870	0	1996	13	0
12	LG	1927	0	2074	15	0
13	LH	1518	0	1601	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	LI	1658	0	1697	19	0
15	LJ	1362	0	1399	10	0
16	LL	1701	0	1818	10	0
17	LM	1138	0	1204	13	0
18	LN	1701	0	1749	12	0
19	LO	1650	0	1794	19	0
20	LP	1242	0	1269	14	0
21	LQ	1513	0	1628	6	0
22	LR	1566	0	1729	7	0
23	LS	1453	0	1490	9	0
24	LT	1298	0	1366	10	0
25	LU	825	0	850	12	0
26	LV	979	0	1039	7	0
27	LW	945	0	1003	13	0
28	LX	985	0	1066	8	0
29	LY	1115	0	1205	5	0
30	LZ	1107	0	1182	14	0
31	La	1162	0	1213	11	0
32	Lb	876	0	948	5	0
33	Lc	764	0	804	8	0
34	Ld	888	0	930	8	0
35	Le	1053	0	1147	7	0
36	Lf	876	0	912	6	0
37	Lg	906	0	998	2	0
38	Lh	1015	0	1148	17	0
39	Li	832	0	917	1	0
40	Lj	705	0	737	5	0
41	Lk	569	0	637	7	0
42	Ll	444	0	483	5	0
43	Lm	429	0	465	4	0
44	Ln	230	0	276	1	0
45	Lo	862	0	929	6	0
46	Lp	708	0	756	5	0
47	Lr	1002	0	1068	4	0
48	Ls	1496	0	1540	25	0
49	Lt	998	0	1032	20	0
50	SA	1741	0	1744	38	0
51	SB	1738	0	1809	32	0
52	SC	1707	0	1791	19	0
53	SE	2076	0	2177	26	0
54	SG	1923	0	2089	27	0
55	SH	1497	0	1590	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	SI	1686	0	1772	31	0
57	SJ	1525	0	1640	18	0
58	SL	1247	0	1323	12	0
59	SN	1208	0	1294	10	0
60	SO	1024	0	1050	16	0
61	SV	636	0	637	14	0
62	SW	1034	0	1080	18	0
63	SX	1098	0	1167	15	0
64	SY	1065	0	1142	16	0
65	Sa	821	0	870	10	0
66	Sb	651	0	669	10	0
67	Se	459	0	503	0	0
68	S2	36952	0	18677	367	0
69	SR	1090	0	1149	18	0
70	SD	1765	0	1865	19	0
71	SF	1495	0	1549	33	0
72	SK	827	0	854	8	0
73	SM	940	0	965	12	0
74	SP	985	0	1031	18	0
75	SQ	1142	0	1213	22	0
76	SS	1198	0	1261	18	0
77	ST	1112	0	1146	14	0
78	SU	821	0	883	17	0
79	SZ	598	0	656	15	0
80	Sc	506	0	536	13	0
81	Sd	459	0	449	8	0
82	Sf	548	0	551	11	0
83	Sg	2436	0	2391	39	0
84	Et	1593	0	810	17	0
85	CB	6605	0	6679	106	0
86	CA	2764	0	2779	45	0
87	L5	179	0	0	0	0
87	L7	3	0	0	0	0
87	L8	5	0	0	0	0
87	LA	1	0	0	0	0
87	LP	1	0	0	0	0
87	LV	1	0	0	0	0
87	Le	1	0	0	0	0
87	S2	27	0	0	0	0
88	L5	98	0	182	3	0
89	L5	100	0	190	2	0
90	Lg	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	Lj	1	0	0	0	0
90	Lm	1	0	0	0	0
90	Lo	1	0	0	0	0
90	Lp	1	0	0	0	0
90	Sa	1	0	0	0	0
All	All	228149	0	172626	1917	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1917) 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)
68:S2:1417:C:H42	68:S2:1422:G:H22	1.12	0.95
3:L5:3944:G:H1	3:L5:4069:U:H3	0.92	0.92
83:Sg:8:ARG:HD2	83:Sg:311:GLN:HG2	1.53	0.90
84:Et:26:A:H62	84:Et:44:G:H21	1.22	0.86
68:S2:1748:G:H1	68:S2:1786:U:H3	1.30	0.80
3:L5:1404:G:N7	3:L5:1408:G:N2	2.31	0.79
13:LH:106:GLN:HB2	13:LH:111:LEU:HB3	1.66	0.78
10:LE:223:ARG:HH22	10:LE:238:GLU:HG2	1.48	0.77
51:SB:189:ILE:HG13	51:SB:190:PRO:HD3	1.68	0.76
3:L5:1414:C:H2'	3:L5:1415:G:H8	1.51	0.75
57:SJ:7:TRP:HE1	68:S2:39:A:H5'	1.51	0.75
3:L5:4618:OMG:H5'	26:LV:15:ARG:HB2	1.67	0.74
3:L5:3701:OMC:H5	3:L5:3748:A:H62	1.33	0.74
86:CA:181:PRO:HA	86:CA:230:VAL:HA	1.69	0.74
86:CA:122:ALA:HB3	86:CA:320:LYS:HG2	1.71	0.73
86:CA:154:LEU:HD11	86:CA:332:ARG:HD2	1.70	0.73
3:L5:4775:C:H41	3:L5:4859:C:H42	1.35	0.73
7:LB:90:VAL:HG23	7:LB:163:ILE:HD11	1.70	0.73
68:S2:1417:C:N4	68:S2:1422:G:H22	1.87	0.73
3:L5:2351:OMC:HM22	8:LC:95:MET:HG3	1.70	0.73
3:L5:1177:U:H3	3:L5:1183:C:H42	1.36	0.72
81:Sd:39:CYS:HB2	81:Sd:42:CYS:H	1.54	0.72
26:LV:13:LYS:HD2	26:LV:128:LEU:HD11	1.70	0.72
3:L5:1270:A:H8	3:L5:2106:G:H21	1.37	0.71
3:L5:2554:U:O2	3:L5:2764:A:N7	2.24	0.71
31:La:87:ARG:HH12	31:La:118:PRO:HG3	1.56	0.71
54:SG:20:ASP:HB3	54:SG:23:LYS:HG2	1.73	0.71
13:LH:93:ARG:HD2	13:LH:143:GLU:HG3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Sg:247:TRP:HB3	83:Sg:258:ILE:HD11	1.72	0.71
85:CB:745:TYR:HE2	85:CB:812:CYS:HB3	1.56	0.70
64:SY:9:THR:H	68:S2:837:A:H61	1.39	0.69
73:SM:79:VAL:HG11	73:SM:85:LEU:HD23	1.72	0.69
3:L5:150:U:H3	12:LG:162:ASP:HB2	1.57	0.69
3:L5:2611:A:H5'	3:L5:2688:G:H4'	1.73	0.69
68:S2:943:U:H2'	68:S2:944:A:H8	1.57	0.69
7:LB:367:PHE:HB2	27:LW:1:MET:HB2	1.75	0.69
74:SP:100:LYS:HG3	74:SP:101:THR:HG23	1.74	0.69
6:LA:31:ALA:HB2	6:LA:123:ARG:HH21	1.58	0.69
69:SR:66:VAL:HG23	69:SR:68:GLY:H	1.58	0.69
78:SU:66:ARG:HH12	78:SU:75:LYS:HA	1.58	0.69
85:CB:745:TYR:HB2	85:CB:814:PHE:HA	1.75	0.69
71:SF:127:ARG:HA	71:SF:136:ARG:HD3	1.74	0.68
68:S2:1417:C:H42	68:S2:1422:G:N2	1.89	0.68
83:Sg:87:LEU:HB2	83:Sg:101:PHE:HB2	1.75	0.68
85:CB:330:LYS:HD3	85:CB:334:PRO:HB2	1.75	0.68
86:CA:229:LEU:HD13	86:CA:318:GLN:HB3	1.75	0.68
86:CA:23:MET:HE2	86:CA:63:ILE:HD11	1.73	0.68
3:L5:4571:A2M:H2'	3:L5:4572:U:H6	1.59	0.68
74:SP:34:MET:HB3	74:SP:42:ARG:HG3	1.76	0.68
86:CA:122:ALA:HB1	86:CA:318:GLN:HE22	1.59	0.67
3:L5:2458:C:H5''	18:LN:67:ARG:HD2	1.77	0.67
3:L5:2557:G:H1	3:L5:2570:U:H3	1.40	0.67
55:SH:93:VAL:HG21	55:SH:133:LEU:HD12	1.74	0.67
63:SX:140:ARG:HD3	63:SX:141:PRO:HD2	1.76	0.67
8:LC:5:ARG:HH22	8:LC:266:THR:HG23	1.59	0.67
10:LE:165:LEU:HD11	10:LE:176:THR:HG22	1.77	0.67
68:S2:116:OMU:HN3	68:S2:347:G:H1	1.42	0.67
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.76	0.67
71:SF:34:SER:HA	80:Sc:55:VAL:HG13	1.77	0.67
14:LI:30:LYS:HD3	14:LI:63:GLU:HG3	1.76	0.67
85:CB:6:VAL:HG11	85:CB:459:GLU:HG2	1.77	0.67
31:La:72:THR:HG22	31:La:110:LYS:HB3	1.76	0.67
50:SA:198:MET:HE3	50:SA:200:ASP:HB2	1.76	0.66
68:S2:1417:C:O2	68:S2:1422:G:O6	2.13	0.66
83:Sg:73:SER:H	83:Sg:117:ASN:HD21	1.43	0.66
3:L5:966:A:H5''	3:L5:2092:G:H22	1.61	0.66
25:LU:80:LYS:HZ1	25:LU:109:SER:H	1.44	0.66
68:S2:928:G:H2'	68:S2:929:G:C8	2.31	0.66
68:S2:1536:G:H2'	68:S2:1537:A:H8	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SG:227:GLN:HB3	54:SG:231:ARG:HH21	1.60	0.66
55:SH:137:SER:HB3	55:SH:162:GLN:HE21	1.61	0.66
68:S2:1433:C:H42	78:SU:92:HIS:HD2	1.43	0.66
3:L5:2362:U:H2'	3:L5:2363:A2M:H8	1.77	0.65
68:S2:1581:C:H5'	68:S2:1582:C:H5	1.61	0.65
50:SA:85:ARG:HH22	69:SR:83:ASN:HD22	1.43	0.65
68:S2:1277:C:H2'	68:S2:1278:A:H8	1.61	0.65
3:L5:4242:U:H3	3:L5:4281:A:H2	1.44	0.65
8:LC:340:ILE:HG21	10:LE:50:LEU:HD13	1.79	0.65
64:SY:55:ILE:HG23	64:SY:75:ILE:HG22	1.77	0.65
53:SE:191:ARG:HD2	53:SE:245:ARG:HH11	1.61	0.65
54:SG:137:ARG:HB3	54:SG:140:ARG:HG3	1.77	0.65
68:S2:1228:A:H2'	68:S2:1229:G:C8	2.32	0.65
6:LA:137:ILE:HD11	6:LA:149:LYS:HB2	1.78	0.65
25:LU:100:LEU:HD13	25:LU:112:LEU:HD23	1.78	0.65
3:L5:4611:A:H2	13:LH:120:GLU:HB3	1.62	0.65
68:S2:1829:G:H1'	68:S2:1850:MA6:H2	1.78	0.65
3:L5:659:G:H2'	3:L5:660:A:H8	1.62	0.65
6:LA:36:GLU:HG3	6:LA:91:GLY:HA2	1.79	0.65
38:Lh:73:TYR:HA	38:Lh:76:LYS:HD2	1.79	0.65
77:ST:104:LEU:HD23	77:ST:121:ARG:HD2	1.78	0.65
77:ST:143:LYS:HG2	77:ST:144:LYS:HG2	1.77	0.65
68:S2:1602:U:H4'	76:SS:24:ARG:HH22	1.62	0.64
68:S2:834:C:H42	68:S2:839:C:H42	1.45	0.64
85:CB:590:LEU:HD21	85:CB:603:TYR:HB3	1.77	0.64
49:Lt:83:LYS:HD2	49:Lt:86:LYS:HZ1	1.61	0.64
86:CA:189:GLN:HE21	86:CA:222:GLU:HB2	1.62	0.64
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.63	0.64
3:L5:1940:G:H22	3:L5:4434:C:H5''	1.62	0.64
25:LU:28:PRO:HB2	25:LU:34:MET:HG2	1.79	0.64
55:SH:53:VAL:HG21	55:SH:172:THR:HG22	1.79	0.64
3:L5:2020:U:H2'	3:L5:2021:G:H8	1.61	0.64
88:L5:5294:SPM:H112	19:LO:91:LYS:HD3	1.78	0.64
59:SN:55:ARG:HD3	68:S2:1017:U:H5'	1.79	0.64
71:SF:17:ILE:HG21	71:SF:46:ALA:HB1	1.80	0.64
3:L5:4302:U:H4'	24:LT:5:LYS:HD2	1.80	0.64
48:Ls:39:GLN:HG3	48:Ls:107:VAL:HG21	1.79	0.64
69:SR:28:PHE:HA	69:SR:55:THR:HG21	1.80	0.64
78:SU:21:ARG:HD3	78:SU:88:LEU:HD22	1.78	0.64
85:CB:524:LEU:HD22	85:CB:546:ILE:HD11	1.79	0.63
16:LL:64:VAL:HA	16:LL:67:HIS:CD2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1285:G:H5'	73:SM:35:ILE:HG12	1.80	0.63
70:SD:127:MET:HE1	70:SD:133:GLY:HA2	1.81	0.63
25:LU:18:VAL:HG13	25:LU:73:THR:HG23	1.79	0.63
52:SC:68:ARG:HG2	52:SC:277:HIS:HB2	1.80	0.63
3:L5:1820:C:H2'	3:L5:1822:U:H5'	1.80	0.63
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.34	0.63
3:L5:3697:U:H5''	3:L5:3698:G:H5'	1.79	0.63
3:L5:3774:A:H2'	3:L5:3775:A:C8	2.34	0.63
73:SM:89:VAL:HG21	73:SM:109:VAL:HG21	1.81	0.63
86:CA:11:THR:HG23	86:CA:13:ALA:H	1.64	0.63
74:SP:34:MET:HE2	74:SP:45:LEU:HB3	1.80	0.63
48:Ls:91:THR:HG21	48:Ls:98:ILE:HG13	1.80	0.63
55:SH:154:ILE:HB	55:SH:185:VAL:HG22	1.80	0.62
68:S2:1854:U:H2'	68:S2:1855:G:H8	1.64	0.62
3:L5:173:C:H5''	16:LL:129:ARG:HH12	1.62	0.62
20:LP:52:THR:HG23	20:LP:85:LYS:HG3	1.81	0.62
82:Sf:132:MET:HA	82:Sf:141:CYS:HA	1.80	0.62
51:SB:171:ILE:HA	51:SB:174:ARG:HG2	1.81	0.62
68:S2:1337:4AC:H2'	68:S2:1338:G:H8	1.65	0.62
68:S2:1550:G:H3'	68:S2:1579:A:H61	1.65	0.62
83:Sg:20:GLN:HG2	83:Sg:69:VAL:H	1.64	0.62
68:S2:1354:G:H2'	68:S2:1356:G:N2	2.15	0.62
68:S2:1752:C:H42	68:S2:1755:C:H41	1.48	0.62
70:SD:170:THR:HG23	70:SD:187:LYS:HG2	1.81	0.62
3:L5:502:C:H3'	3:L5:503:C:H3'	1.81	0.62
83:Sg:174:VAL:HB	83:Sg:188:HIS:HB2	1.80	0.62
85:CB:89:ILE:HB	85:CB:93:LYS:HD3	1.82	0.62
85:CB:110:ASP:HB3	85:CB:553:HIS:HB2	1.81	0.62
68:S2:508:A:H3'	68:S2:509:OMG:H8	1.64	0.62
75:SQ:97:GLN:HB2	75:SQ:105:LYS:HD2	1.80	0.62
86:CA:25:GLY:HA3	86:CA:333:ILE:HG22	1.82	0.62
14:LI:54:SER:HB3	14:LI:135:ILE:HD11	1.82	0.62
51:SB:88:THR:HG22	51:SB:98:THR:HG22	1.82	0.61
3:L5:2709:C:H42	86:CA:257:LEU:H	1.48	0.61
3:L5:3950:U:H3'	3:L5:3951:G:C8	2.35	0.61
51:SB:131:ASP:HB2	51:SB:180:ASP:HB2	1.82	0.61
51:SB:74:LEU:HD21	51:SB:86:LEU:HD11	1.82	0.61
86:CA:31:VAL:HG21	86:CA:56:ILE:HD11	1.83	0.61
7:LB:107:ALA:HB2	7:LB:201:LEU:HD22	1.83	0.61
50:SA:41:ARG:HE	50:SA:45:GLY:HA2	1.65	0.61
68:S2:1588:A:H2'	68:S2:1589:A:C8	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4363:A:H5''	45:Lo:36:GLN:HG2	1.81	0.61
13:LH:44:GLU:HG3	17:LM:2:VAL:HG12	1.83	0.61
48:Ls:127:ASN:HD21	48:Ls:151:THR:HG23	1.66	0.61
85:CB:642:ASP:HB3	85:CB:645:GLU:HG2	1.82	0.61
3:L5:268:G:H2'	3:L5:269:G:H8	1.65	0.61
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.66	0.61
64:SY:12:PHE:HZ	64:SY:21:LYS:HE2	1.64	0.60
28:LX:73:HIS:HB3	28:LX:116:LEU:HD23	1.83	0.60
86:CA:10:GLN:HB3	86:CA:117:PHE:HZ	1.64	0.60
3:L5:2517:A:H5'	37:Lg:62:LYS:HD3	1.83	0.60
3:L5:5024:C:H41	3:L5:5028:G:H21	1.47	0.60
52:SC:118:ALA:HB2	68:S2:1486:A:H4'	1.83	0.60
57:SJ:111:GLN:HE21	57:SJ:123:ILE:HG13	1.66	0.60
69:SR:16:ILE:HD11	69:SR:54:VAL:HG21	1.81	0.60
75:SQ:43:GLU:HB2	75:SQ:44:PRO:HD3	1.81	0.60
85:CB:327:ASP:HA	85:CB:330:LYS:HE3	1.82	0.60
52:SC:167:ARG:HB3	52:SC:177:PRO:HB2	1.84	0.60
71:SF:162:ALA:HB3	71:SF:169:ILE:HD13	1.83	0.60
68:S2:1228:A:H2'	68:S2:1229:G:H8	1.67	0.60
3:L5:1444:G:H22	3:L5:2104:G:H21	1.50	0.60
27:LW:97:LYS:HG3	27:LW:99:GLU:H	1.66	0.60
64:SY:37:LYS:HA	64:SY:40:ILE:HD12	1.83	0.60
51:SB:138:PHE:HD2	51:SB:214:LYS:HB3	1.67	0.60
7:LB:57:VAL:HG22	7:LB:73:VAL:HG12	1.82	0.60
86:CA:79:SER:HB3	86:CA:109:ASP:HB2	1.83	0.60
35:Le:89:LEU:HD13	35:Le:118:LEU:HD22	1.84	0.60
68:S2:851:C:H5''	68:S2:852:G:H5'	1.84	0.60
3:L5:1697:G:H22	3:L5:2084:C:P	2.25	0.59
68:S2:1536:G:H2'	68:S2:1537:A:C8	2.37	0.59
86:CA:185:MET:HG3	86:CA:229:LEU:HD23	1.84	0.59
3:L5:3868:G:H22	3:L5:3900:G:H1'	1.68	0.59
72:SK:14:LEU:HD23	72:SK:21:MET:HE1	1.84	0.59
85:CB:83:GLU:HA	85:CB:86:LEU:HD12	1.84	0.59
3:L5:1509:C:H5''	31:La:2:PRO:HD3	1.84	0.59
76:SS:22:GLY:HA2	76:SS:56:ALA:HB3	1.83	0.59
57:SJ:129:LEU:HB3	57:SJ:135:ILE:HD11	1.83	0.59
76:SS:20:ILE:HG22	76:SS:32:ALA:HB3	1.84	0.59
51:SB:85:LYS:HB2	51:SB:101:HIS:HB3	1.84	0.59
3:L5:3611:A:H2	3:L5:5016:A:H8	1.49	0.59
3:L5:3754:G:H1	3:L5:3770:U:H3	1.49	0.59
3:L5:4992:G:H2'	3:L5:4993:G:C8	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:Sa:51:ARG:HH12	80:Sc:63:ARG:HA	1.68	0.59
22:LR:160:GLU:HA	22:LR:163:ARG:HG2	1.85	0.59
76:SS:124:ARG:HE	76:SS:129:LEU:HB2	1.68	0.59
85:CB:27:HIS:HB2	85:CB:139:THR:HG23	1.84	0.59
70:SD:220:THR:HG22	70:SD:221:THR:H	1.66	0.58
8:LC:298:ILE:HD13	21:LQ:131:PRO:HB3	1.84	0.58
68:S2:874:G:H2'	68:S2:875:A:H8	1.68	0.58
56:SI:98:LYS:HB3	68:S2:377:G:H5'	1.84	0.58
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.33	0.58
68:S2:1513:C:H2'	68:S2:1514:G:H8	1.68	0.58
68:S2:1650:A:H5''	75:SQ:139:ALA:HB2	1.84	0.58
9:LD:64:ILE:HD13	9:LD:109:LEU:HD22	1.86	0.58
15:LJ:141:ILE:HA	15:LJ:144:LYS:HD2	1.85	0.58
48:Ls:120:GLU:HB2	48:Ls:163:THR:HG23	1.85	0.58
71:SF:102:LEU:HD11	79:SZ:110:THR:HB	1.85	0.58
75:SQ:32:ILE:HG23	75:SQ:68:ILE:HB	1.86	0.58
3:L5:4279:A:H5'	3:L5:4281:A:H1'	1.86	0.58
8:LC:324:ILE:HD13	8:LC:327:LYS:HE2	1.86	0.58
3:L5:411:G:H5''	3:L5:414:C:H1'	1.84	0.58
20:LP:138:PRO:HB3	20:LP:140:MET:HE2	1.83	0.58
64:SY:21:LYS:HD3	64:SY:75:ILE:HD11	1.85	0.58
85:CB:659:PRO:HG2	85:CB:698:ARG:HG2	1.86	0.58
11:LF:105:VAL:HG13	11:LF:136:VAL:HG12	1.86	0.58
51:SB:52:THR:HG23	51:SB:57:ILE:HA	1.86	0.58
3:L5:1175:A:H2	3:L5:1185:G:H22	1.52	0.58
48:Ls:30:VAL:HG21	48:Ls:187:LEU:HD13	1.85	0.58
60:SO:34:PHE:HB3	60:SO:41:PHE:HB2	1.86	0.58
66:Sb:19:HIS:HB3	66:Sb:22:LYS:HG3	1.85	0.58
3:L5:261:G:H2'	3:L5:262:G:C8	2.39	0.58
3:L5:1326:A2M:H2'	3:L5:1327:C:C6	2.38	0.58
66:Sb:72:ARG:HH12	68:S2:1120:U:H5'	1.69	0.58
3:L5:2745:A:H2'	3:L5:2746:A:C8	2.40	0.57
3:L5:4966:A:H5''	7:LB:128:LYS:HG3	1.84	0.57
6:LA:150:LEU:HD11	6:LA:156:LYS:HD2	1.86	0.57
62:SW:3:ARG:HD3	62:SW:6:VAL:HG12	1.85	0.57
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.38	0.57
68:S2:388:U:H2'	68:S2:389:A:H8	1.70	0.57
23:LS:161:ARG:HE	23:LS:164:LYS:HB2	1.69	0.57
53:SE:64:ILE:HD11	64:SY:18:LEU:HD11	1.84	0.57
69:SR:58:MET:HA	69:SR:61:ILE:HG12	1.86	0.57
3:L5:2303:C:H5''	35:Le:104:SER:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Lg:83:CYS:SG	37:Lg:86:CYS:HB2	2.44	0.57
85:CB:279:SER:HB3	85:CB:285:LEU:HD21	1.85	0.57
20:LP:131:ARG:HG3	20:LP:137:ASN:OD1	2.05	0.57
55:SH:33:ASN:HD21	55:SH:37:LYS:HG2	1.69	0.57
74:SP:108:LYS:HB2	74:SP:111:MET:HG3	1.85	0.57
3:L5:1995:G:H4'	49:Lt:128:THR:HB	1.87	0.57
8:LC:110:ARG:HB2	18:LN:204:ARG:HH21	1.69	0.57
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.39	0.57
15:LJ:56:THR:HG23	15:LJ:63:ARG:HA	1.87	0.57
50:SA:81:ASN:HA	50:SA:84:GLN:NE2	2.20	0.57
56:SI:91:VAL:HG21	56:SI:205:ARG:HH12	1.70	0.57
3:L5:1194:G:H2'	3:L5:1195:G:H8	1.69	0.57
50:SA:10:MET:HE3	50:SA:55:TRP:HB2	1.86	0.57
63:SX:88:ASP:HA	68:S2:617:G:H4'	1.87	0.57
78:SU:56:MET:HB2	78:SU:86:LYS:HB3	1.86	0.57
83:Sg:259:TRP:HB3	83:Sg:266:ILE:HA	1.86	0.57
85:CB:305:MET:HE3	85:CB:336:LEU:HD22	1.87	0.57
85:CB:408:GLY:HA2	85:CB:526:ARG:HD3	1.86	0.57
53:SE:36:HIS:ND1	53:SE:85:GLY:HA3	2.20	0.56
68:S2:996:A:H2'	68:S2:997:A:C8	2.39	0.56
3:L5:667:A:H5''	3:L5:668:C:H5''	1.87	0.56
50:SA:184:ARG:HD3	50:SA:191:ARG:HD3	1.87	0.56
85:CB:653:GLY:HA2	85:CB:660:ASN:HB2	1.88	0.56
3:L5:1997:U:H4'	48:Ls:44:ARG:HH12	1.70	0.56
3:L5:261:G:H2'	3:L5:262:G:H8	1.69	0.56
33:Lc:48:LEU:HD21	33:Lc:60:ILE:HG21	1.86	0.56
54:SG:32:MET:HE3	54:SG:100:CYS:HA	1.86	0.56
64:SY:9:THR:HG22	64:SY:25:ILE:HG22	1.88	0.56
68:S2:525:A:H2'	68:S2:526:A:H8	1.69	0.56
76:SS:80:PRO:HG2	77:ST:36:THR:HG21	1.86	0.56
86:CA:105:LEU:HD23	86:CA:139:LYS:HD2	1.87	0.56
3:L5:2745:A:H2'	3:L5:2746:A:H8	1.71	0.56
46:Lp:51:ALA:HB3	46:Lp:54:ILE:HD12	1.87	0.56
50:SA:145:ILE:HG13	50:SA:159:ILE:HD13	1.86	0.56
3:L5:1500:A:H5''	3:L5:1501:C:H5''	1.87	0.56
3:L5:4281:A:H2'	3:L5:4282:A:H2'	1.86	0.56
68:S2:106:C:H2'	68:S2:107:A:H8	1.71	0.56
3:L5:137:G:H2'	3:L5:138:G:H8	1.71	0.56
85:CB:20:ARG:HB2	85:CB:100:ILE:HD13	1.88	0.56
3:L5:2708:U:H3	86:CA:257:LEU:HD23	1.68	0.56
64:SY:10:ARG:HA	68:S2:839:C:H41	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1751:C:H42	68:S2:1782:G:N2	2.04	0.56
74:SP:108:LYS:H	74:SP:111:MET:HE2	1.69	0.56
51:SB:150:ILE:HD13	69:SR:129:LYS:HB2	1.88	0.56
56:SI:110:ARG:HH21	56:SI:123:ARG:HH11	1.52	0.56
68:S2:925:G:H1	68:S2:1017:U:H3	1.54	0.56
68:S2:1286:G:H21	68:S2:1313:A:H62	1.54	0.56
68:S2:1461:G:H3'	68:S2:1463:U:H3	1.70	0.56
85:CB:24:VAL:HG12	85:CB:126:LEU:HB3	1.87	0.56
3:L5:3950:U:H3	3:L5:4063:U:H3	1.52	0.56
70:SD:72:VAL:HG22	72:SK:68:TYR:HD1	1.70	0.56
19:LO:61:ARG:HA	19:LO:70:PRO:HD2	1.88	0.55
68:S2:1560:U:O2	68:S2:1575:G:O6	2.24	0.55
3:L5:1177:U:H3	3:L5:1183:C:N4	2.04	0.55
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.41	0.55
26:LV:37:LEU:HD23	26:LV:65:VAL:HG12	1.88	0.55
12:LG:103:ARG:HD3	12:LG:195:HIS:CE1	2.41	0.55
54:SG:162:LEU:HD21	68:S2:67:C:H6	1.71	0.55
57:SJ:7:TRP:NE1	68:S2:39:A:H5'	2.20	0.55
3:L5:462:G:H2'	3:L5:463:A:C8	2.42	0.55
51:SB:114:VAL:HG11	68:S2:987:A:H2'	1.89	0.55
69:SR:5:ARG:HB2	69:SR:10:LYS:HE2	1.87	0.55
83:Sg:113:PHE:HE2	83:Sg:117:ASN:HD22	1.54	0.55
12:LG:102:TYR:HE2	12:LG:207:VAL:HG23	1.70	0.55
19:LO:175:MET:HE3	19:LO:179:LYS:HD3	1.88	0.55
34:Ld:22:THR:HG23	34:Ld:122:VAL:HG23	1.87	0.55
57:SJ:63:LEU:HD23	57:SJ:70:ARG:HB2	1.89	0.55
86:CA:81:SER:HB2	86:CA:85:CYS:HB3	1.88	0.55
44:Ln:1:MET:HB2	68:S2:1706:G:H5'	1.87	0.55
86:CA:72:LYS:HG2	86:CA:114:VAL:HG12	1.89	0.55
60:SO:101:GLY:HA3	60:SO:134:PRO:HD2	1.89	0.55
3:L5:233:U:O2'	3:L5:234:G:H2'	2.07	0.55
51:SB:40:ASN:HD21	51:SB:76:ASN:HB2	1.72	0.55
86:CA:27:ILE:HD11	86:CA:59:GLU:HB3	1.89	0.55
3:L5:4063:U:H2'	3:L5:4064:C:C2	2.42	0.55
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.42	0.55
34:Ld:64:ILE:HG23	34:Ld:68:LEU:HD23	1.88	0.55
53:SE:44:LEU:HD11	53:SE:70:ILE:HG21	1.89	0.54
61:SV:14:PRO:HG2	61:SV:23:ILE:HD12	1.88	0.54
66:Sb:54:VAL:HG23	66:Sb:63:LEU:HB2	1.87	0.54
3:L5:1994:C:H2'	3:L5:1995:G:C8	2.43	0.54
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LB:14:LEU:HD22	7:LB:17:LEU:HD11	1.89	0.54
52:SC:105:GLU:HB2	52:SC:216:MET:HE1	1.88	0.54
56:SI:22:HIS:HB3	68:S2:433:A:H5''	1.89	0.54
85:CB:746:LEU:HB2	85:CB:815:ASP:OD2	2.07	0.54
3:L5:4910:G:H4'	7:LB:95:THR:HG22	1.88	0.54
56:SI:83:TYR:HB3	56:SI:101:ILE:HG12	1.88	0.54
63:SX:28:LYS:HD2	63:SX:32:LEU:HD22	1.88	0.54
68:S2:1679:A:H2'	71:SF:60:ARG:HD2	1.90	0.54
85:CB:5:THR:HG23	85:CB:7:ASP:H	1.71	0.54
60:SO:53:ILE:HG23	60:SO:88:LEU:HD22	1.88	0.54
68:S2:1845:A:H2'	68:S2:1846:G:C8	2.42	0.54
68:S2:1845:A:H2'	68:S2:1846:G:H8	1.72	0.54
69:SR:83:ASN:HB3	69:SR:85:VAL:HG13	1.89	0.54
56:SI:162:LEU:HD21	56:SI:191:GLU:HB3	1.89	0.54
85:CB:801:ARG:HG2	85:CB:806:GLY:HA2	1.89	0.54
86:CA:92:LEU:HD22	86:CA:290:ARG:HD3	1.88	0.54
3:L5:433:A:C2	3:L5:3867:A2M:H4'	2.42	0.54
9:LD:223:PHE:HB3	9:LD:226:TYR:HB2	1.90	0.54
49:Lt:16:ARG:HH12	49:Lt:28:LEU:HB3	1.72	0.54
54:SG:11:GLY:HA2	68:S2:166:A2M:HM'1	1.88	0.54
68:S2:1277:C:H5''	72:SK:55:ARG:HD2	1.90	0.54
68:S2:1714:U:H2'	68:S2:1715:A:C8	2.42	0.54
3:L5:659:G:H2'	3:L5:660:A:C8	2.41	0.54
3:L5:662:C:H2'	3:L5:663:G:C8	2.43	0.54
68:S2:557:U:H2'	68:S2:558:G:C8	2.42	0.54
85:CB:290:CYS:HA	85:CB:294:LEU:HB2	1.89	0.54
30:LZ:50:PRO:HD3	30:LZ:68:ILE:HG12	1.89	0.54
56:SI:87:ASN:HB3	56:SI:90:LEU:HD23	1.88	0.54
68:S2:24:C:HO2'	68:S2:25:A:H8	1.56	0.54
75:SQ:132:PHE:HD2	78:SU:79:ARG:HH12	1.56	0.54
3:L5:93:G:H2'	3:L5:94:A:C8	2.43	0.54
3:L5:3910:C:H2'	3:L5:3911:C:C6	2.42	0.54
12:LG:125:LYS:HG3	12:LG:126:GLY:H	1.72	0.54
68:S2:149:A:N7	68:S2:169:U:O2	2.40	0.54
3:L5:4860:G:H5'	19:LO:169:ARG:HD3	1.90	0.54
41:Lk:8:ILE:HD11	41:Lk:56:LEU:HD21	1.88	0.54
66:Sb:72:ARG:NH1	68:S2:1120:U:H5'	2.23	0.54
85:CB:609:PHE:CD2	85:CB:699:GLY:HA2	2.43	0.54
10:LE:222:LEU:HD21	10:LE:225:PRO:HG3	1.89	0.53
27:LW:9:SER:HA	27:LW:52:THR:HG23	1.89	0.53
50:SA:120:ARG:HD2	52:SC:266:TYR:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1775:U:H2'	68:S2:1776:G:C8	2.43	0.53
71:SF:204:ARG:HH21	80:Sc:63:ARG:HH22	1.53	0.53
85:CB:654:PRO:HD2	85:CB:658:GLY:HA3	1.90	0.53
4:L7:117:G:H5'	9:LD:256:LYS:HD2	1.91	0.53
42:L1:28:ARG:HA	42:L1:33:ASN:ND2	2.23	0.53
53:SE:146:THR:HG21	68:S2:122:G:H21	1.73	0.53
3:L5:2568:C:H2'	3:L5:2569:G:H8	1.73	0.53
52:SC:173:LYS:HD3	61:SV:3:ASN:HA	1.90	0.53
52:SC:207:ALA:HB2	68:S2:4:C:H4'	1.91	0.53
57:SJ:46:VAL:HG13	57:SJ:102:ILE:HD11	1.91	0.53
71:SF:19:LEU:HD11	71:SF:69:VAL:HG11	1.89	0.53
3:L5:257:C:H2'	3:L5:258:G:C8	2.43	0.53
3:L5:497:G:N2	3:L5:498:C:H41	2.06	0.53
9:LD:182:GLY:HA2	9:LD:194:VAL:HG23	1.90	0.53
28:LX:80:PRO:HG2	28:LX:155:ILE:HG21	1.90	0.53
3:L5:3641:U:H5	3:L5:3646:A:N7	2.05	0.53
10:LE:264:ILE:HD11	10:LE:267:LEU:HD22	1.89	0.53
59:SN:35:GLU:HA	59:SN:38:TYR:HD1	1.74	0.53
24:LT:27:LEU:HB3	24:LT:31:MET:HE3	1.90	0.53
68:S2:906:U:H2'	68:S2:907:G:C8	2.43	0.53
68:S2:1398:G:H1'	83:Sg:63:SER:HB2	1.89	0.53
84:Et:5:G:H2'	84:Et:6:G:H8	1.74	0.53
3:L5:256:G:H2'	3:L5:257:C:C6	2.44	0.53
68:S2:1407:U:H2'	68:S2:1408:U:C6	2.44	0.53
68:S2:1595:U:H2'	68:S2:1596:U:C6	2.44	0.53
3:L5:257:C:H2'	3:L5:258:G:H8	1.73	0.53
19:LO:126:VAL:HG13	19:LO:127:VAL:HG13	1.90	0.53
68:S2:28:U:H2'	68:S2:29:G:H8	1.73	0.53
85:CB:289:PHE:HA	85:CB:293:ILE:HD12	1.91	0.53
3:L5:1194:G:H2'	3:L5:1195:G:C8	2.43	0.53
3:L5:1281:G:N1	10:LE:128:HIS:HB2	2.24	0.53
3:L5:4239:A:H2'	3:L5:4240:G:C8	2.44	0.53
19:LO:9:LEU:HD23	19:LO:118:MET:HB2	1.90	0.53
23:LS:154:LEU:HB3	23:LS:157:ARG:HD3	1.91	0.53
68:S2:1388:A:H61	70:SD:161:GLY:HA3	1.74	0.53
84:Et:5:G:H2'	84:Et:6:G:C8	2.44	0.53
85:CB:365:GLN:HA	85:CB:368:ARG:HB2	1.91	0.53
5:L8:8:U:H2'	5:L8:9:A:C8	2.44	0.53
17:LM:119:ARG:HG3	19:LO:189:ILE:HG23	1.90	0.53
68:S2:496:C:H2'	68:S2:497:C:H6	1.74	0.53
84:Et:25:C:H3'	84:Et:26:A:H5''	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1503:A:H62	21:LQ:87:THR:HG21	1.71	0.52
34:Ld:23:ARG:HG2	34:Ld:121:ASN:HA	1.91	0.52
50:SA:50:ASN:HD22	50:SA:53:ARG:HH11	1.55	0.52
3:L5:208:A:H2	3:L5:233:U:H5''	1.74	0.52
3:L5:1419:G:H5''	21:LQ:71:LYS:NZ	2.24	0.52
53:SE:100:ARG:HB2	53:SE:114:ILE:HD13	1.90	0.52
11:LF:220:MET:HB3	11:LF:232:ASP:OD2	2.08	0.52
55:SH:91:HIS:CE1	55:SH:169:LYS:HG2	2.44	0.52
68:S2:640:A:H2'	68:S2:641:A:C8	2.43	0.52
68:S2:1221:G:H2'	68:S2:1222:G:H8	1.74	0.52
3:L5:3952:A:H2'	3:L5:3953:G:C4	2.45	0.52
25:LU:66:SER:HB2	25:LU:67:LYS:HZ2	1.75	0.52
59:SN:91:LEU:HB3	59:SN:122:ILE:HG12	1.92	0.52
78:SU:66:ARG:NH1	78:SU:75:LYS:HA	2.23	0.52
81:Sd:38:MET:HE1	81:Sd:50:ILE:HD11	1.90	0.52
84:Et:6:G:H22	84:Et:67:U:H3	1.58	0.52
84:Et:37:A:H3'	84:Et:38:A:C8	2.45	0.52
7:LB:163:ILE:HG22	7:LB:180:LEU:HD22	1.90	0.52
19:LO:168:TYR:CE2	19:LO:172:LYS:HD2	2.43	0.52
48:Ls:55:MET:HG2	48:Ls:87:GLY:HA3	1.92	0.52
57:SJ:142:VAL:HG12	57:SJ:144:ILE:H	1.73	0.52
68:S2:1713:C:H2'	68:S2:1714:U:C6	2.45	0.52
3:L5:215:C:H5''	3:L5:216:C:H5''	1.92	0.52
3:L5:1405:C:H2'	3:L5:1406:G:H8	1.73	0.52
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.44	0.52
53:SE:45:ILE:HG13	53:SE:61:VAL:HG11	1.92	0.52
58:SL:111:VAL:HG11	58:SL:128:VAL:HG11	1.91	0.52
62:SW:28:ARG:HD3	68:S2:921:G:C5	2.45	0.52
62:SW:39:THR:HG22	62:SW:43:LYS:HE2	1.92	0.52
70:SD:113:LEU:HD11	70:SD:117:ARG:HG2	1.91	0.52
73:SM:128:PHE:HA	73:SM:131:LYS:HG2	1.92	0.52
11:LF:157:ARG:HE	11:LF:248:ASN:HB2	1.75	0.52
54:SG:55:GLY:HA2	54:SG:110:ASN:HD22	1.75	0.52
57:SJ:134:HIS:CD2	57:SJ:163:SER:HB2	2.45	0.52
68:S2:1438:A:H2'	68:S2:1439:A:C8	2.45	0.52
85:CB:354:ILE:HG23	85:CB:358:LEU:HD12	1.90	0.52
3:L5:3937:C:H1'	18:LN:125:SER:HB3	1.92	0.52
15:LJ:146:ARG:HG2	15:LJ:147:ARG:HG3	1.92	0.52
54:SG:159:ARG:HG3	54:SG:173:ALA:HB2	1.91	0.52
68:S2:49:C:H2'	68:S2:472:C:H41	1.75	0.52
68:S2:388:U:H2'	68:S2:389:A:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:952:G:H2'	68:S2:953:C:C6	2.45	0.52
68:S2:1030:A:H2'	68:S2:1031:A2M:H8	1.92	0.52
20:LP:54:GLN:HA	20:LP:83:TRP:CD1	2.45	0.52
49:Lt:65:GLN:HG3	49:Lt:67:ARG:H	1.74	0.52
49:Lt:127:GLY:O	49:Lt:131:GLU:HG2	2.09	0.52
68:S2:1729:U:H3	68:S2:1805:G:H1	1.56	0.52
74:SP:85:ILE:HG23	74:SP:107:ILE:HD11	1.92	0.52
6:LA:180:LEU:HD22	46:Lp:18:TYR:HB3	1.91	0.52
23:LS:15:ARG:HB3	23:LS:27:LEU:HD23	1.92	0.52
60:SO:92:ALA:HA	60:SO:125:LYS:HB2	1.91	0.52
65:Sa:73:TYR:HE2	65:Sa:83:VAL:HG21	1.75	0.52
68:S2:145:G:H2'	68:S2:146:G:C8	2.45	0.52
68:S2:544:G:H2'	68:S2:545:A:C8	2.45	0.52
68:S2:1139:C:H5	68:S2:1149:A:H62	1.58	0.52
68:S2:1221:G:H2'	68:S2:1222:G:C8	2.45	0.52
83:Sg:152:SER:HB2	83:Sg:170:TRP:CD1	2.45	0.52
85:CB:157:MET:HE1	85:CB:178:PHE:HA	1.91	0.52
86:CA:187:SER:HB2	86:CA:201:ILE:HB	1.92	0.52
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.45	0.51
3:L5:4935:C:H2'	3:L5:4936:G:C8	2.45	0.51
8:LC:7:LEU:HG	8:LC:21:ASN:HB3	1.91	0.51
85:CB:429:ILE:HB	85:CB:443:TYR:HB2	1.90	0.51
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.46	0.51
6:LA:180:LEU:HD21	46:Lp:22:LEU:HB3	1.91	0.51
30:LZ:77:TYR:HD2	33:Lc:39:ARG:HD3	1.75	0.51
33:Lc:38:ILE:HD11	33:Lc:46:VAL:HG21	1.91	0.51
48:Ls:133:GLU:HG2	48:Ls:134:LYS:HD2	1.93	0.51
56:SI:172:LEU:HB3	56:SI:190:LEU:HD12	1.91	0.51
68:S2:166:A2M:H2'	68:S2:167:G:H8	1.75	0.51
7:LB:307:TYR:CD2	7:LB:366:LYS:HG2	2.44	0.51
27:LW:102:LYS:HA	27:LW:105:ARG:HG2	1.93	0.51
42:Ll:9:ILE:HD12	42:Ll:51:LEU:HD12	1.93	0.51
53:SE:11:ARG:HD2	53:SE:20:LEU:HB3	1.92	0.51
73:SM:92:CYS:HB3	73:SM:103:VAL:HG12	1.91	0.51
86:CA:80:ILE:HD12	86:CA:108:ILE:HG12	1.91	0.51
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.76	0.51
3:L5:1333:A:H2'	3:L5:1334:A:C8	2.45	0.51
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.46	0.51
3:L5:4457:PSU:H1'	7:LB:252:ALA:HB3	1.92	0.51
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.91	0.51
36:Lf:15:LYS:HB3	36:Lf:25:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ls:61:MET:O	48:Ls:65:ILE:HG12	2.11	0.51
68:S2:160:U:C4	68:S2:468:A2M:H4'	2.44	0.51
68:S2:327:G:H5''	68:S2:328:U:C2	2.45	0.51
68:S2:1651:A:H2'	68:S2:1652:G:H8	1.74	0.51
66:Sb:72:ARG:HH22	68:S2:1119:A:H2'	1.75	0.51
68:S2:649:PSU:H2'	68:S2:650:A:H8	1.76	0.51
71:SF:167:LYS:HD2	71:SF:172:CYS:SG	2.51	0.51
3:L5:3911:C:H2'	3:L5:3912:U:H6	1.76	0.51
3:L5:4251:A:H5''	15:LJ:108:GLY:HA3	1.93	0.51
49:Lt:123:ARG:HD2	49:Lt:129:ILE:HD11	1.92	0.51
50:SA:74:VAL:HG12	50:SA:121:LEU:HB3	1.93	0.51
68:S2:107:A:H2'	68:S2:108:G:C8	2.45	0.51
75:SQ:72:VAL:HG21	75:SQ:84:ILE:HD11	1.93	0.51
3:L5:3944:G:O6	3:L5:4069:U:O4	2.28	0.51
52:SC:70:VAL:HG21	52:SC:93:ILE:HG23	1.92	0.51
66:Sb:14:GLU:HB2	66:Sb:17:ARG:HH21	1.75	0.51
68:S2:496:C:H2'	68:S2:497:C:C6	2.46	0.51
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.46	0.51
3:L5:3720:G:H22	3:L5:3733:A:H2	1.59	0.51
3:L5:4591:U:H2'	3:L5:4592:C:C6	2.46	0.51
50:SA:158:ASP:HB2	50:SA:159:ILE:HD12	1.92	0.51
3:L5:425:U:H4'	20:LP:6:LEU:HD21	1.92	0.51
3:L5:2520:C:H2'	3:L5:2521:G:H8	1.76	0.51
3:L5:3898:G:H5'	7:LB:254:ILE:HG13	1.92	0.51
3:L5:4238:G:H2'	3:L5:4239:A:C8	2.46	0.51
9:LD:156:GLY:HA2	9:LD:181:PRO:HG3	1.93	0.51
10:LE:165:LEU:HD12	10:LE:174:LEU:HG	1.93	0.51
41:Lk:26:LYS:HB2	41:Lk:69:LEU:HD12	1.92	0.51
63:SX:9:THR:HG22	68:S2:681:PSU:H4'	1.93	0.51
68:S2:1037:G:H4'	68:S2:1845:A:H4'	1.92	0.51
68:S2:1856:C:H2'	68:S2:1857:G:C8	2.46	0.51
3:L5:318:A:H2'	3:L5:319:A:C8	2.46	0.51
68:S2:981:A:H2'	68:S2:982:G:C8	2.46	0.51
3:L5:137:G:H2'	3:L5:138:G:C8	2.46	0.50
3:L5:158:A:H5''	3:L5:159:C:H2'	1.92	0.50
3:L5:187:U:H2'	3:L5:245:C:H1'	1.94	0.50
3:L5:490:C:H2'	3:L5:491:G:C8	2.46	0.50
3:L5:691:C:H2'	3:L5:692:A:C8	2.45	0.50
3:L5:4524:G:C2	7:LB:252:ALA:HB1	2.46	0.50
57:SJ:145:PRO:HD2	68:S2:522:A:H5''	1.92	0.50
68:S2:1844:U:H2'	68:S2:1845:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:SQ:48:GLN:HA	75:SQ:51:LEU:HD23	1.93	0.50
85:CB:604:MET:HE2	85:CB:704:VAL:HG22	1.93	0.50
7:LB:173:LEU:HD22	7:LB:342:LYS:HD2	1.93	0.50
18:LN:169:ARG:HG3	18:LN:174:LEU:HD12	1.93	0.50
43:Lm:99:CYS:HB2	43:Lm:114:LYS:HE3	1.92	0.50
59:SN:20:ARG:HH21	62:SW:56:HIS:HB3	1.77	0.50
3:L5:268:G:H2'	3:L5:269:G:C8	2.44	0.50
3:L5:1942:A:H2'	3:L5:1943:A:H8	1.76	0.50
3:L5:4723:A:H2'	3:L5:4724:A:C8	2.46	0.50
58:SL:68:ILE:HG13	58:SL:143:LEU:HD11	1.94	0.50
60:SO:87:GLU:HG2	60:SO:88:LEU:HD12	1.91	0.50
68:S2:319:C:H2'	68:S2:320:G:H8	1.75	0.50
68:S2:1705:C:H2'	68:S2:1706:G:C8	2.46	0.50
3:L5:3932:U:H2'	3:L5:3933:G:C8	2.47	0.50
3:L5:4508:C:N3	3:L5:4512:U:H5	2.09	0.50
68:S2:1139:C:H2'	68:S2:1140:G:O4'	2.12	0.50
3:L5:106:A:H2'	3:L5:107:G:O4'	2.11	0.50
3:L5:208:A:C2	3:L5:233:U:H5''	2.47	0.50
3:L5:1327:C:H2'	3:L5:1328:G:C8	2.47	0.50
3:L5:2706:G:H22	3:L5:2709:C:H5''	1.75	0.50
68:S2:746:C:H2'	68:S2:747:U:C6	2.47	0.50
75:SQ:19:ALA:HB2	75:SQ:75:GLY:HA3	1.92	0.50
76:SS:24:ARG:HG3	76:SS:29:ALA:HB2	1.94	0.50
85:CB:385:ILE:HG22	85:CB:418:SER:HB2	1.92	0.50
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.46	0.50
3:L5:1992:U:H4'	3:L5:1993:C:H5''	1.93	0.50
3:L5:1994:C:H2'	3:L5:1995:G:H8	1.76	0.50
7:LB:258:HIS:HA	7:LB:260:ALA:N	2.26	0.50
54:SG:7:PHE:CD1	54:SG:113:ILE:HB	2.47	0.50
68:S2:525:A:H2'	68:S2:526:A:C8	2.45	0.50
77:ST:77:LYS:HG3	77:ST:94:ARG:HH21	1.77	0.50
86:CA:70:MET:HE3	86:CA:71:LYS:HG2	1.94	0.50
3:L5:173:C:H5''	16:LL:129:ARG:NH1	2.26	0.50
3:L5:1725:U:H2'	3:L5:1726:U:H6	1.77	0.50
3:L5:1855:G:OP1	32:Lb:4:SER:HB2	2.12	0.50
3:L5:3595:U:H5''	3:L5:3597:G:OP2	2.11	0.50
3:L5:4967:A:H2'	3:L5:4968:A:H8	1.77	0.50
17:LM:123:ILE:HG21	19:LO:178:ARG:HE	1.77	0.50
50:SA:5:LEU:HD13	61:SV:41:LYS:HA	1.93	0.50
53:SE:94:LYS:HE3	64:SY:16:ARG:HB2	1.93	0.50
65:Sa:79:ILE:HD11	68:S2:1864:U:H5'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1421:A:H3'	68:S2:1422:G:C8	2.47	0.50
77:ST:42:HIS:HB3	77:ST:93:SER:HB3	1.92	0.50
3:L5:182:G:H2'	3:L5:183:C:H4'	1.93	0.50
3:L5:4742:G:H2'	3:L5:4743:G:H8	1.76	0.50
64:SY:20:ARG:HD2	64:SY:74:MET:HE3	1.94	0.50
68:S2:323:C:H2'	68:S2:327:G:H1	1.77	0.50
68:S2:808:A:H2	68:S2:855:G:H22	1.60	0.50
78:SU:26:SER:HB3	78:SU:32:LEU:HD13	1.94	0.50
3:L5:1405:C:H2'	3:L5:1406:G:C8	2.47	0.50
7:LB:307:TYR:HD2	7:LB:366:LYS:HG2	1.75	0.50
68:S2:112:U:H3	68:S2:349:A:H61	1.60	0.50
3:L5:153:G:H2'	3:L5:154:G:H8	1.76	0.49
3:L5:4076:G:H5'	12:LG:73:ARG:HG3	1.92	0.49
12:LG:58:PRO:HD2	12:LG:61:ILE:HD12	1.94	0.49
15:LJ:15:LEU:HD12	15:LJ:165:TRP:HB2	1.93	0.49
51:SB:134:LEU:HB3	51:SB:218:LEU:HB2	1.94	0.49
68:S2:367:U:H4'	68:S2:371:A:C8	2.47	0.49
68:S2:527:C:H2'	68:S2:528:A:H8	1.77	0.49
68:S2:528:A:H2'	68:S2:529:A:C8	2.47	0.49
68:S2:1217:A:H2'	68:S2:1218:C:C6	2.47	0.49
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.47	0.49
6:LA:114:CYS:HB3	6:LA:165:VAL:HB	1.94	0.49
27:LW:34:ALA:HA	27:LW:37:GLU:HG2	1.93	0.49
55:SH:157:HIS:HB3	55:SH:190:PRO:HG3	1.94	0.49
56:SI:44:HIS:CG	68:S2:307:G:H1	2.30	0.49
57:SJ:138:ARG:HH21	57:SJ:153:SER:HA	1.76	0.49
68:S2:562:U:H2'	68:S2:563:G:C8	2.47	0.49
3:L5:457:G:H2'	3:L5:458:C:C6	2.47	0.49
3:L5:717:U:H2'	3:L5:718:C:C6	2.47	0.49
3:L5:1269:G:H21	3:L5:1441:C:H1'	1.77	0.49
17:LM:96:GLU:O	17:LM:100:ARG:HG2	2.12	0.49
30:LZ:41:ALA:HB2	30:LZ:77:TYR:HE1	1.77	0.49
48:Ls:28:PHE:CE1	48:Ls:192:VAL:HG23	2.46	0.49
52:SC:90:GLU:HB2	52:SC:93:ILE:HG13	1.93	0.49
62:SW:28:ARG:NH1	68:S2:921:G:H2'	2.27	0.49
68:S2:931:C:H2'	68:S2:932:G:C8	2.47	0.49
68:S2:980:A:H2'	68:S2:981:A:C8	2.46	0.49
85:CB:583:VAL:HG22	85:CB:700:VAL:HG22	1.94	0.49
3:L5:162:A:H2'	3:L5:163:A:C8	2.47	0.49
3:L5:2448:G:H2'	3:L5:2449:A:C8	2.48	0.49
3:L5:3599:A:H2'	3:L5:3600:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3611:A:C2	3:L5:5016:A:H8	2.29	0.49
23:LS:4:SER:HB3	23:LS:111:ARG:HH22	1.75	0.49
25:LU:23:LEU:HD11	25:LU:83:LEU:HD13	1.93	0.49
28:LX:82:THR:HG21	38:Lh:37:THR:HG22	1.93	0.49
54:SG:172:LYS:HE2	68:S2:65:C:H4'	1.93	0.49
59:SN:47:PRO:HG3	59:SN:75:LEU:HD12	1.93	0.49
68:S2:907:G:H2'	68:S2:908:A:C8	2.47	0.49
68:S2:943:U:H2'	68:S2:944:A:C8	2.44	0.49
68:S2:1423:C:H5	75:SQ:4:LYS:HE3	1.76	0.49
68:S2:1644:C:H4'	75:SQ:140:ARG:HB2	1.94	0.49
70:SD:109:LEU:HD12	70:SD:184:ILE:HD11	1.95	0.49
71:SF:33:ILE:HG22	80:Sc:11:LEU:HD13	1.94	0.49
3:L5:3954:A:H1'	3:L5:4058:U:H5'	1.94	0.49
3:L5:4389:C:H2'	3:L5:4390:A:C8	2.48	0.49
14:LI:184:MET:HA	14:LI:187:LYS:HZ3	1.77	0.49
51:SB:71:LEU:HD12	51:SB:84:PHE:HE1	1.78	0.49
54:SG:66:GLY:HA2	68:S2:1745:A:H1'	1.94	0.49
68:S2:1004:PSU:H2'	68:S2:1005:G:H8	1.76	0.49
68:S2:1417:C:N3	68:S2:1422:G:N1	2.46	0.49
70:SD:137:VAL:HG22	70:SD:151:LYS:HG3	1.94	0.49
85:CB:230:GLU:HG2	85:CB:249:ARG:HH12	1.78	0.49
85:CB:484:THR:HG21	85:CB:494:MET:H	1.77	0.49
3:L5:2696:A:H62	41:Lk:35:LYS:NZ	2.10	0.49
48:Ls:102:LEU:HD23	48:Ls:189:ILE:HD11	1.94	0.49
52:SC:174:ILE:HG21	57:SJ:96:TYR:HE1	1.77	0.49
61:SV:17:CYS:HB2	61:SV:56:CYS:HB3	1.94	0.49
68:S2:85:A:H2'	68:S2:86:C:H6	1.77	0.49
68:S2:1284:A:C8	73:SM:33:ARG:HG3	2.48	0.49
68:S2:1752:C:H42	68:S2:1755:C:N4	2.10	0.49
78:SU:67:LYS:HG2	78:SU:78:ASP:HB2	1.94	0.49
3:L5:1199:G:H2'	3:L5:1200:G:C8	2.48	0.49
3:L5:4064:C:H2'	3:L5:4065:G:H8	1.78	0.49
27:LW:47:ARG:HH11	27:LW:54:LEU:HD13	1.78	0.49
50:SA:41:ARG:HD2	50:SA:47:TYR:CZ	2.48	0.49
64:SY:90:ARG:HA	64:SY:93:ARG:HD2	1.95	0.49
81:Sd:6:LEU:HA	81:Sd:9:SER:HB3	1.95	0.49
86:CA:105:LEU:HD21	86:CA:315:PHE:HB3	1.95	0.49
3:L5:2676:A:OP2	3:L5:2676:A:H8	1.96	0.49
47:Lr:80:THR:HG21	47:Lr:96:MET:HE1	1.94	0.49
48:Ls:114:GLY:HA2	48:Ls:166:LYS:HE3	1.94	0.49
55:SH:145:ARG:HE	62:SW:51:GLU:HG2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63: SX:124: LYS: HG2	63: SX:129: SER: HA	1.95	0.49
68: S2:976: G: H2'	68: S2:977: C: C6	2.48	0.49
68: S2:1365: G: H2'	68: S2:1366: G: C8	2.47	0.49
68: S2:1540: G: H5'	77: ST:47: PRO: HB3	1.93	0.49
81: Sd:39: CYS: HB2	81: Sd:42: CYS: N	2.24	0.49
85: CB:40: VAL: HG13	85: CB:47: ALA: HB1	1.95	0.49
85: CB:539: GLU: HG2	85: CB:545: ILE: HG13	1.94	0.49
3: L5:4612: C: C2	13: LH:120: GLU: HB2	2.48	0.49
5: L8:70: G: H5''	29: LY:27: ARG: CZ	2.43	0.49
17: LM:25: VAL: HB	17: LM:38: VAL: HG22	1.95	0.49
19: LO:81: TRP: HB2	19: LO:104: VAL: HG21	1.93	0.49
68: S2:1277: C: H2'	68: S2:1278: A: C8	2.44	0.49
77: ST:22: LEU: HD13	77: ST:28: LEU: HD13	1.94	0.49
78: SU:20: ILE: HG22	78: SU:91: LEU: HB2	1.95	0.49
7: LB:117: ARG: HA	7: LB:177: LYS: HD2	1.95	0.49
50: SA:81: ASN: HA	50: SA:84: GLN: HE22	1.77	0.49
52: SC:166: ARG: HD2	52: SC:248: TYR: CE1	2.48	0.49
68: S2:795: A: H2'	68: S2:796: G: C8	2.48	0.49
68: S2:1405: A: H2'	68: S2:1406: G: O4'	2.13	0.49
78: SU:56: MET: HE3	78: SU:88: LEU: HD12	1.93	0.49
83: Sg:212: LYS: HA	83: Sg:235: ILE: HG23	1.95	0.49
85: CB:4: PHE: HB2	85: CB:8: GLN: NE2	2.28	0.49
3: L5:662: C: H2'	3: L5:663: G: H8	1.78	0.48
3: L5:1461: C: H2'	3: L5:1462: A: C8	2.48	0.48
3: L5:1617: G: H1'	3: L5:2513: A: N6	2.27	0.48
3: L5:4260: U: H2'	3: L5:4261: C: C6	2.48	0.48
3: L5:4459: U: H2'	3: L5:4460: U: C6	2.47	0.48
30: LZ:30: ASP: HA	30: LZ:39: SER: OG	2.12	0.48
48: Ls:192: VAL: HG12	48: Ls:199: TYR: H	1.78	0.48
57: SJ:114: VAL: HG21	57: SJ:135: ILE: HG12	1.93	0.48
66: Sb:22: LYS: HE3	68: S2:1129: G: H5''	1.95	0.48
68: S2:550: C: H2'	68: S2:551: U: C6	2.48	0.48
68: S2:835: C: H4'	68: S2:836: G: C8	2.47	0.48
82: Sf:103: LEU: HG	82: Sf:104: LYS: H	1.78	0.48
3: L5:2656: U: H5''	30: LZ:38: TYR: HB3	1.95	0.48
3: L5:3664: G: H2'	3: L5:3665: G: H8	1.78	0.48
7: LB:132: LYS: HA	7: LB:135: LYS: HE2	1.95	0.48
74: SP:118: GLU: HG2	76: SS:120: HIS: H	1.77	0.48
84: Et:2: C: H2'	84: Et:3: C: C6	2.47	0.48
3: L5:965: G: N2	3: L5:2092: G: H1'	2.29	0.48
3: L5:1647: U: OP1	89: L5:5291: SPD: H51	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LA:101:VAL:HG22	6:LA:165:VAL:HG22	1.95	0.48
54:SG:10:THR:HA	54:SG:128:THR:HG23	1.95	0.48
60:SO:95:ILE:HD13	60:SO:116:LEU:HD11	1.94	0.48
68:S2:291:G:H2'	68:S2:292:A:C8	2.48	0.48
68:S2:1365:G:H2'	68:S2:1366:G:H8	1.78	0.48
3:L5:2101:C:H2'	3:L5:2102:G:H2'	1.95	0.48
31:La:100:ILE:HG13	31:La:123:ILE:HB	1.95	0.48
64:SY:9:THR:H	68:S2:837:A:N6	2.09	0.48
68:S2:1457:U:H2'	68:S2:1458:G:H8	1.79	0.48
71:SF:95:HIS:CD2	79:SZ:106:GLN:HB3	2.49	0.48
3:L5:2539:C:H2'	3:L5:2540:C:C6	2.49	0.48
3:L5:4250:G:H5''	15:LJ:98:ASN:HD22	1.78	0.48
5:L8:92:U:H2'	5:L8:93:C:O4'	2.14	0.48
63:SX:17:ARG:HH22	68:S2:659:G:H21	1.60	0.48
68:S2:835:C:H4'	68:S2:836:G:H8	1.77	0.48
68:S2:1222:G:H5''	71:SF:78:MET:HE1	1.95	0.48
68:S2:1588:A:H2'	68:S2:1589:A:H8	1.78	0.48
3:L5:907:C:H2'	3:L5:908:G:H8	1.79	0.48
3:L5:5057:C:H2'	3:L5:5058:A:C8	2.49	0.48
9:LD:51:MET:HE1	9:LD:163:LEU:HA	1.96	0.48
27:LW:83:THR:HG22	54:SG:160:LYS:HE2	1.95	0.48
48:Ls:34:ASN:HB2	48:Ls:185:PHE:CE2	2.48	0.48
49:Lt:61:LYS:HD2	49:Lt:72:GLU:HB3	1.96	0.48
68:S2:186:C:H2'	68:S2:187:G:C8	2.48	0.48
68:S2:455:A:H2'	68:S2:456:C:C6	2.49	0.48
68:S2:907:G:H2'	68:S2:908:A:H8	1.78	0.48
68:S2:1533:A:H2	68:S2:1536:G:N3	2.11	0.48
85:CB:292:LEU:HD12	85:CB:293:ILE:HG13	1.95	0.48
45:Lo:33:LEU:HA	45:Lo:38:LYS:HG2	1.95	0.48
68:S2:115:U:H2'	68:S2:116:OMU:C6	2.44	0.48
68:S2:329:G:H2'	68:S2:330:G:H8	1.79	0.48
68:S2:1144:A:H2'	68:S2:1145:A:C8	2.48	0.48
70:SD:55:THR:H	70:SD:90:LYS:HZ3	1.62	0.48
72:SK:16:PHE:HZ	72:SK:80:ARG:HE	1.60	0.48
76:SS:40:TYR:CZ	76:SS:97:GLN:HG2	2.48	0.48
85:CB:147:ILE:HD11	85:CB:192:TYR:HB2	1.96	0.48
3:L5:267:G:H2'	3:L5:268:G:H8	1.78	0.48
3:L5:2543:A:H2	3:L5:2773:G:H22	1.60	0.48
3:L5:4069:U:H2'	3:L5:4070:U:C6	2.49	0.48
33:Lc:38:ILE:HG21	33:Lc:63:TYR:HB3	1.95	0.48
68:S2:1692:U:H2'	68:S2:1693:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:SF:61:PHE:HB3	80:Sc:51:ARG:HH21	1.78	0.48
85:CB:609:PHE:CZ	85:CB:661:ILE:HG12	2.49	0.48
3:L5:1773:U:H2'	3:L5:1774:C:C6	2.49	0.48
6:LA:188:LYS:HZ2	6:LA:192:LYS:HE3	1.78	0.48
48:Ls:77:LYS:HG2	48:Ls:198:ILE:HD11	1.94	0.48
50:SA:198:MET:HE1	69:SR:86:PRO:HD2	1.96	0.48
54:SG:87:ARG:HH22	68:S2:162:C:H5''	1.78	0.48
55:SH:69:LEU:HD12	55:SH:96:ALA:HB2	1.96	0.48
76:SS:26:ILE:HG13	76:SS:56:ALA:HA	1.94	0.48
85:CB:70:ILE:HG21	85:CB:556:ILE:HG21	1.96	0.48
11:LF:127:LYS:HB2	24:LT:133:ALA:HB3	1.96	0.48
71:SF:33:ILE:HG23	80:Sc:55:VAL:HG11	1.96	0.48
3:L5:491:G:H2'	3:L5:492:U:C6	2.49	0.47
3:L5:2709:C:N4	86:CA:257:LEU:H	2.12	0.47
5:L8:8:U:H2'	5:L8:9:A:H8	1.79	0.47
50:SA:144:THR:HG23	61:SV:60:ARG:HH22	1.79	0.47
3:L5:4062:A:H2'	3:L5:4063:U:C6	2.49	0.47
3:L5:4098:A:N7	3:L5:4099:G:H1'	2.30	0.47
88:L5:5294:SPM:H31	88:L5:5294:SPM:H62	1.70	0.47
63:SX:90:CYS:HA	63:SX:93:PHE:HD2	1.78	0.47
68:S2:1653:U:H2'	68:S2:1654:G:C8	2.48	0.47
79:SZ:99:LEU:HD11	79:SZ:102:LYS:HB2	1.96	0.47
3:L5:497:G:H1	3:L5:657:C:H42	1.63	0.47
3:L5:1254:A:H5''	3:L5:1255:A:H5''	1.95	0.47
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.48	0.47
3:L5:3732:A:H2'	3:L5:3733:A:C8	2.49	0.47
51:SB:34:LYS:HD2	51:SB:95:ASN:HB3	1.96	0.47
61:SV:15:ARG:HH21	61:SV:24:ILE:HG21	1.79	0.47
68:S2:1775:U:H2'	68:S2:1776:G:H8	1.79	0.47
76:SS:64:VAL:O	76:SS:68:ILE:HG12	2.15	0.47
83:Sg:156:PHE:HA	83:Sg:165:ILE:HD12	1.97	0.47
85:CB:426:LYS:NZ	85:CB:444:LEU:HB3	2.29	0.47
3:L5:223:G:H4'	3:L5:225:G:N7	2.28	0.47
3:L5:679:C:H2'	3:L5:680:G:H8	1.79	0.47
3:L5:1188:C:H2'	3:L5:1189:G:C8	2.50	0.47
3:L5:1461:C:H2'	3:L5:1462:A:H8	1.78	0.47
3:L5:2411:C:H2'	3:L5:2412:A:H8	1.79	0.47
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.50	0.47
10:LE:190:HIS:HB3	10:LE:193:PHE:HD2	1.80	0.47
48:Ls:107:VAL:O	48:Ls:184:SER:HB3	2.13	0.47
83:Sg:165:ILE:HG22	83:Sg:177:TRP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:CB:323:LEU:HA	85:CB:342:ARG:NH1	2.28	0.47
86:CA:64:PHE:HD2	86:CA:72:LYS:HZ1	1.62	0.47
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.49	0.47
3:L5:4927:G:H5''	3:L5:4928:C:H5	1.80	0.47
12:LG:103:ARG:HG3	12:LG:193:LEU:O	2.15	0.47
31:La:87:ARG:NH1	31:La:118:PRO:HG3	2.27	0.47
53:SE:42:LEU:HG	53:SE:46:ILE:HD11	1.95	0.47
56:SI:25:ARG:HA	68:S2:448:A:H5''	1.96	0.47
68:S2:1535:U:P	71:SF:169:ILE:HG12	2.55	0.47
1:CD:195:ARG:HD3	68:S2:1489:A:OP2	2.14	0.47
3:L5:138:G:H2'	3:L5:139:G:H8	1.78	0.47
3:L5:455:C:H2'	3:L5:456:C:C6	2.49	0.47
3:L5:4238:G:H2'	3:L5:4239:A:H8	1.80	0.47
3:L5:4680:G:H2'	3:L5:4681:A:C8	2.49	0.47
6:LA:229:ALA:HB3	6:LA:234:LYS:HB3	1.96	0.47
49:Lt:16:ARG:HE	49:Lt:17:CYS:H	1.61	0.47
54:SG:49:VAL:HB	54:SG:115:LYS:HB3	1.97	0.47
68:S2:595:U:H2'	68:S2:596:U:C6	2.50	0.47
68:S2:690:G:H3'	68:S2:691:G:H21	1.79	0.47
85:CB:672:LEU:HD13	85:CB:707:VAL:HG21	1.96	0.47
3:L5:711:A:H2'	3:L5:712:C:C6	2.50	0.47
3:L5:737:C:C5	3:L5:739:G:H5''	2.49	0.47
3:L5:979:C:OP2	10:LE:66:LYS:HD3	2.15	0.47
3:L5:1577:G:H5'	3:L5:1578:U:H5''	1.97	0.47
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.14	0.47
3:L5:1705:G:H2'	3:L5:1706:A:O4'	2.15	0.47
3:L5:3951:G:H2'	3:L5:3952:A:C4	2.50	0.47
10:LE:226:ARG:HD3	10:LE:226:ARG:H	1.79	0.47
12:LG:182:CYS:HB3	12:LG:222:ILE:HD12	1.96	0.47
14:LI:152:LEU:HB3	14:LI:165:ILE:HD12	1.97	0.47
16:LL:47:ALA:HB3	16:LL:48:PRO:HD3	1.96	0.47
18:LN:200:LEU:HB3	18:LN:204:ARG:NH1	2.29	0.47
41:Lk:13:LEU:HA	41:Lk:16:ARG:HG2	1.96	0.47
53:SE:19:MET:HB2	53:SE:51:ARG:HH22	1.80	0.47
68:S2:16:G:H2'	68:S2:17:C:C6	2.50	0.47
68:S2:159:A2M:H1'	68:S2:159:A2M:HM'3	1.55	0.47
68:S2:573:U:O2	68:S2:576:A2M:H8	2.15	0.47
71:SF:39:ILE:HG22	71:SF:41:VAL:HG23	1.97	0.47
74:SP:22:LEU:HA	74:SP:25:LEU:HD12	1.97	0.47
79:SZ:99:LEU:HD21	79:SZ:102:LYS:HB2	1.97	0.47
85:CB:10:ARG:NH1	85:CB:465:PRO:HD3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:CB:33:SER:HB3	85:CB:54:THR:HG23	1.96	0.47
86:CA:56:ILE:HD12	86:CA:112:VAL:HG11	1.96	0.47
3:L5:982:U:H2'	3:L5:983:C:C6	2.50	0.47
3:L5:1307:A:H2'	3:L5:1308:C:C6	2.49	0.47
3:L5:1683:PSU:H2'	3:L5:1684:A:C8	2.49	0.47
3:L5:1976:G:H21	49:Lt:139:VAL:HG12	1.80	0.47
3:L5:4163:U:H5'	3:L5:4164:C:H5''	1.95	0.47
3:L5:4401:G:H2'	3:L5:4402:C:H6	1.80	0.47
3:L5:4742:G:H2'	3:L5:4743:G:C8	2.49	0.47
8:LC:315:LYS:HD2	11:LF:168:ALA:HB1	1.97	0.47
22:LR:172:ARG:HH22	68:S2:908:A:H5''	1.80	0.47
49:Lt:61:LYS:HA	49:Lt:75:PRO:HD2	1.97	0.47
68:S2:1203:G:H2'	68:S2:1204:A:C8	2.50	0.47
68:S2:1752:C:N4	68:S2:1755:C:H41	2.10	0.47
79:SZ:49:LEU:HD23	79:SZ:83:LEU:HD21	1.97	0.47
85:CB:382:ALA:O	85:CB:386:LYS:HG2	2.15	0.47
3:L5:10:A:H2'	3:L5:11:G:C8	2.50	0.47
3:L5:1190:C:H2'	3:L5:1191:C:C6	2.50	0.47
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.50	0.47
3:L5:2741:U:H2'	6:LA:50:HIS:CD2	2.49	0.47
14:LI:43:VAL:HG21	14:LI:197:VAL:HG13	1.97	0.47
45:Lo:22:LYS:HG2	45:Lo:73:VAL:HG12	1.97	0.47
54:SG:181:THR:H	54:SG:184:VAL:HG12	1.80	0.47
68:S2:5:U:H2'	68:S2:6:G:H8	1.80	0.47
71:SF:162:ALA:HB2	71:SF:172:CYS:SG	2.54	0.47
3:L5:325:U:H2'	3:L5:326:C:C6	2.50	0.47
6:LA:27:ALA:HB1	6:LA:77:ILE:HG13	1.96	0.47
7:LB:71:GLU:OE1	27:LW:2:LYS:HG2	2.15	0.47
51:SB:64:GLY:HA2	51:SB:87:ILE:HD11	1.97	0.47
68:S2:1468:C:H2'	68:S2:1469:A:H8	1.80	0.47
83:Sg:234:ASP:H	83:Sg:252:THR:HB	1.79	0.47
85:CB:537:ILE:HG13	85:CB:545:ILE:HB	1.97	0.47
3:L5:178:C:H2'	3:L5:179:G:C8	2.50	0.46
3:L5:2079:G:H2'	3:L5:2080:U:C6	2.50	0.46
3:L5:2568:C:H2'	3:L5:2569:G:C8	2.50	0.46
3:L5:4088:C:H2'	3:L5:4089:G:C8	2.50	0.46
3:L5:4688:C:H2'	3:L5:4689:PSU:C6	2.50	0.46
3:L5:4927:G:H5''	3:L5:4928:C:C5	2.50	0.46
6:LA:13:GLY:O	6:LA:17:ARG:HG3	2.15	0.46
68:S2:118:C:H1'	68:S2:445:A:C5	2.50	0.46
68:S2:329:G:H2'	68:S2:330:G:C8	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:458:A:H2'	68:S2:459:C:C6	2.50	0.46
68:S2:495:U:H2'	68:S2:496:C:O4'	2.15	0.46
68:S2:656:G:H5'	68:S2:662:G:N2	2.30	0.46
68:S2:876:C:H2'	68:S2:877:C:C6	2.50	0.46
84:Et:9:A:H2'	84:Et:11:C:H41	1.79	0.46
85:CB:189:ILE:HD12	85:CB:203:ILE:HG22	1.97	0.46
85:CB:226:LYS:HA	85:CB:257:MET:HE2	1.96	0.46
3:L5:262:G:H2'	3:L5:263:G:C8	2.50	0.46
3:L5:5027:C:O2'	3:L5:5028:G:H5''	2.15	0.46
12:LG:102:TYR:CE2	12:LG:207:VAL:HG23	2.50	0.46
50:SA:76:VAL:HG12	50:SA:123:VAL:HB	1.97	0.46
50:SA:184:ARG:HA	50:SA:189:ILE:HB	1.96	0.46
52:SC:149:THR:HG22	52:SC:152:ARG:HH12	1.80	0.46
68:S2:1562:C:H2'	68:S2:1563:G:C8	2.50	0.46
3:L5:460:C:H2'	3:L5:461:G:C8	2.51	0.46
3:L5:3597:G:H2'	3:L5:3598:C:H6	1.81	0.46
9:LD:179:ARG:HD3	9:LD:179:ARG:HA	1.69	0.46
11:LF:29:LYS:NZ	11:LF:32:ARG:HH12	2.13	0.46
22:LR:105:LEU:HD23	22:LR:138:LEU:HD23	1.96	0.46
38:Lh:13:LYS:HD2	38:Lh:13:LYS:HA	1.71	0.46
45:Lo:6:LYS:HG3	45:Lo:94:GLY:HA3	1.96	0.46
50:SA:123:VAL:HA	50:SA:145:ILE:O	2.14	0.46
62:SW:53:ILE:HG12	66:Sb:24:LEU:HD21	1.97	0.46
63:SX:107:ARG:HG2	63:SX:112:VAL:HG22	1.98	0.46
63:SX:140:ARG:HD2	63:SX:142:ARG:HH21	1.79	0.46
68:S2:1201:U:H2'	68:S2:1202:U:C6	2.50	0.46
71:SF:175:ASP:HA	71:SF:178:ILE:HG12	1.96	0.46
85:CB:27:HIS:ND1	85:CB:138:GLN:HB2	2.30	0.46
85:CB:121:VAL:HG13	85:CB:415:ARG:HB2	1.97	0.46
86:CA:310:GLU:HG3	86:CA:314:GLU:HB2	1.98	0.46
3:L5:92:C:C2	31:La:55:LYS:HE2	2.50	0.46
3:L5:1419:G:H5''	21:LQ:71:LYS:HZ2	1.80	0.46
3:L5:3606:U:H2'	3:L5:3607:U:C6	2.51	0.46
3:L5:3732:A:H2'	3:L5:3733:A:H8	1.79	0.46
3:L5:4347:G:H2'	3:L5:4348:A:C8	2.51	0.46
3:L5:4619:U:H2'	3:L5:4620:OMU:H6	1.97	0.46
3:L5:4622:A:H4'	7:LB:13:SER:HB2	1.97	0.46
17:LM:122:ILE:HB	19:LO:189:ILE:HD11	1.98	0.46
20:LP:117:ILE:HD12	20:LP:148:MET:HE2	1.96	0.46
57:SJ:164:PRO:HB3	57:SJ:170:PRO:HA	1.97	0.46
64:SY:111:LYS:HA	64:SY:114:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:29:G:H2'	68:S2:30:C:C6	2.50	0.46
77:ST:104:LEU:HD23	77:ST:121:ARG:HH11	1.80	0.46
86:CA:27:ILE:HG13	86:CA:30:ARG:HE	1.81	0.46
3:L5:99:A:H2'	3:L5:100:C:O2	2.15	0.46
3:L5:267:G:H2'	3:L5:268:G:C8	2.51	0.46
3:L5:1733:G:N3	3:L5:4214:A:H2'	2.29	0.46
3:L5:1960:A:H1'	48:Ls:60:MET:HE1	1.97	0.46
6:LA:158:ILE:HB	6:LA:162:ASN:ND2	2.30	0.46
8:LC:154:VAL:HG11	8:LC:174:LEU:HD11	1.98	0.46
64:SY:104:ARG:HG3	64:SY:107:ARG:NH2	2.31	0.46
68:S2:207:G:H3'	68:S2:208:G:H8	1.81	0.46
68:S2:1562:C:H2'	68:S2:1563:G:H8	1.80	0.46
77:ST:39:LEU:HD23	77:ST:39:LEU:HA	1.78	0.46
85:CB:533:MET:HE3	85:CB:533:MET:HB3	1.86	0.46
3:L5:498:C:C2	3:L5:499:G:H1'	2.50	0.46
3:L5:1732:C:H5''	24:LT:43:LYS:HE2	1.98	0.46
3:L5:1997:U:H4'	48:Ls:44:ARG:NH1	2.30	0.46
3:L5:4637:OMG:HM23	3:L5:4637:OMG:H1'	1.78	0.46
3:L5:4996:C:H4'	34:Ld:26:THR:HG23	1.97	0.46
51:SB:111:CYS:HB3	65:Sa:68:TYR:HB2	1.97	0.46
68:S2:154:U:H2'	68:S2:155:G:O4'	2.16	0.46
68:S2:834:C:N4	68:S2:839:C:H42	2.12	0.46
68:S2:1424:G:H2'	68:S2:1425:G:H8	1.80	0.46
68:S2:1764:G:H5''	68:S2:1765:C:H5''	1.97	0.46
83:Sg:69:VAL:HG12	83:Sg:80:SER:HB3	1.98	0.46
83:Sg:163:PRO:HB2	83:Sg:179:LEU:HD21	1.97	0.46
3:L5:1702:C:H4'	8:LC:308:LYS:HD2	1.98	0.46
3:L5:1962:A:H2	3:L5:2024:G:H21	1.63	0.46
3:L5:3726:A:H2'	3:L5:3727:A:C8	2.50	0.46
6:LA:206:PRO:HG3	6:LA:213:GLY:HA3	1.97	0.46
20:LP:116:HIS:HB3	20:LP:149:ILE:HB	1.96	0.46
68:S2:1010:G:H2'	68:S2:1011:A:C8	2.51	0.46
83:Sg:236:ILE:HG13	83:Sg:252:THR:HG22	1.98	0.46
85:CB:649:ILE:HA	85:CB:663:THR:HG22	1.97	0.46
85:CB:683:PHE:HD2	85:CB:684:GLN:HE21	1.62	0.46
85:CB:745:TYR:CE2	85:CB:812:CYS:HB3	2.45	0.46
86:CA:12:ILE:HG21	86:CA:324:LEU:HD11	1.98	0.46
3:L5:1084:C:H2'	3:L5:1085:C:H6	1.81	0.46
3:L5:4739:C:H2'	3:L5:4740:G:H5'	1.98	0.46
4:L7:112:U:H2'	4:L7:113:G:H8	1.81	0.46
7:LB:161:ARG:HG2	7:LB:184:GLN:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LW:52:THR:HG22	27:LW:54:LEU:H	1.80	0.46
49:Lt:19:GLY:HA2	49:Lt:48:LYS:NZ	2.31	0.46
68:S2:149:A:H3'	68:S2:150:A:H8	1.80	0.46
86:CA:155:ARG:HD2	86:CA:357:LEU:HB2	1.97	0.46
3:L5:455:C:O2'	3:L5:456:C:H5'	2.15	0.46
3:L5:1514:U:H2'	3:L5:1515:A:C8	2.49	0.46
3:L5:1788:A:H2'	14:LI:22:PHE:CZ	2.51	0.46
14:LI:73:ASN:HB2	14:LI:87:MET:HE1	1.98	0.46
49:Lt:11:LYS:HA	49:Lt:11:LYS:HD2	1.64	0.46
53:SE:31:PRO:HG2	53:SE:38:LEU:HB2	1.97	0.46
57:SJ:131:ARG:HA	57:SJ:131:ARG:HD2	1.72	0.46
58:SL:88:ILE:HD11	58:SL:109:MET:HE2	1.98	0.46
68:S2:1470:C:H2'	68:S2:1471:C:H6	1.81	0.46
86:CA:18:VAL:HG12	86:CA:22:LYS:HE2	1.96	0.46
3:L5:71:C:H1'	16:LL:62:PRO:O	2.16	0.46
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.16	0.46
7:LB:299:ILE:HB	7:LB:313:SER:HB3	1.97	0.46
50:SA:52:LYS:HB2	69:SR:109:LEU:HD13	1.98	0.46
68:S2:1010:G:H2'	68:S2:1011:A:H8	1.81	0.46
70:SD:195:THR:HG23	70:SD:197:LYS:H	1.81	0.46
85:CB:434:TYR:HB3	85:CB:493:ASN:HD21	1.80	0.46
85:CB:727:ARG:HG2	85:CB:854:PHE:HD1	1.81	0.46
3:L5:1867:A:H2'	3:L5:1868:A:C8	2.51	0.45
3:L5:1974:U:H4'	3:L5:1975:G:H3'	1.99	0.45
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.52	0.45
3:L5:4563:U:H2'	3:L5:4564:A:C8	2.51	0.45
3:L5:5002:U:H2'	3:L5:5003:U:C6	2.51	0.45
7:LB:165:HIS:HB3	7:LB:180:LEU:HD23	1.97	0.45
29:LY:13:LYS:O	29:LY:17:ARG:HD3	2.16	0.45
56:SI:43:ILE:HD13	68:S2:305:U:H1'	1.98	0.45
56:SI:57:ALA:HB2	56:SI:183:GLY:HA2	1.98	0.45
57:SJ:150:ARG:HG3	68:S2:821:G:C6	2.52	0.45
68:S2:185:G:H2'	68:S2:186:C:H6	1.80	0.45
68:S2:319:C:H2'	68:S2:320:G:C8	2.50	0.45
68:S2:494:C:H42	68:S2:509:OMG:HN22	1.64	0.45
79:SZ:102:LYS:HA	79:SZ:107:VAL:HG23	1.97	0.45
3:L5:1266:G:C5	32:Lb:95:ARG:HB3	2.51	0.45
3:L5:1278:C:H2'	3:L5:1279:A:O4'	2.17	0.45
3:L5:3856:A:H5''	20:LP:83:TRP:O	2.16	0.45
3:L5:5004:C:H2'	3:L5:5005:G:O4'	2.16	0.45
19:LO:191:LYS:HE3	19:LO:192:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:Lm:98:LYS:HG3	43:Lm:118:THR:HG21	1.98	0.45
51:SB:109:LYS:HD2	51:SB:113:MET:HE3	1.99	0.45
60:SO:134:PRO:HB3	68:S2:944:A:H5''	1.98	0.45
62:SW:57:ARG:HD2	68:S2:919:A:H4'	1.98	0.45
68:S2:543:C:H3'	68:S2:544:G:H8	1.81	0.45
68:S2:1399:C:H5''	83:Sg:100:ARG:CZ	2.46	0.45
79:SZ:49:LEU:HD23	79:SZ:49:LEU:HA	1.86	0.45
86:CA:123:HIS:HA	86:CA:319:PHE:HD1	1.80	0.45
3:L5:4685:U:H2'	3:L5:4686:G:C8	2.51	0.45
6:LA:107:MET:HE1	6:LA:113:VAL:HG11	1.98	0.45
7:LB:288:GLY:HA3	7:LB:330:PHE:CE1	2.50	0.45
36:Lf:46:ARG:HH21	36:Lf:89:ARG:HH22	1.64	0.45
51:SB:164:ILE:HD11	51:SB:204:ILE:HB	1.98	0.45
68:S2:166:A2M:H2'	68:S2:167:G:C8	2.50	0.45
68:S2:323:C:H4'	68:S2:324:C:C5	2.51	0.45
68:S2:1240:A:C5	74:SP:100:LYS:HD2	2.51	0.45
85:CB:381:ALA:HB1	85:CB:395:MET:SD	2.56	0.45
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.98	0.45
3:L5:4069:U:H2'	3:L5:4070:U:H6	1.80	0.45
3:L5:4389:C:H2'	3:L5:4390:A:H8	1.81	0.45
9:LD:83:LEU:HB3	9:LD:88:VAL:HG13	1.98	0.45
26:LV:69:LYS:HB2	26:LV:72:LEU:HD12	1.97	0.45
49:Lt:57:ARG:HG3	49:Lt:83:LYS:HB3	1.97	0.45
50:SA:51:LEU:HA	50:SA:54:THR:HG22	1.98	0.45
51:SB:25:PHE:HA	51:SB:28:LYS:HG2	1.98	0.45
52:SC:79:GLU:HB3	61:SV:12:TYR:HB3	1.98	0.45
52:SC:191:VAL:HG11	52:SC:236:PHE:HA	1.97	0.45
55:SH:36:LEU:HA	55:SH:39:GLN:HE22	1.81	0.45
55:SH:73:GLN:HA	55:SH:76:GLN:HB2	1.98	0.45
56:SI:141:ARG:HD3	56:SI:145:ILE:HG21	1.98	0.45
85:CB:77:LEU:HB2	85:CB:100:ILE:HB	1.98	0.45
3:L5:494:U:H2'	3:L5:495:C:C6	2.52	0.45
3:L5:3944:G:N2	3:L5:4069:U:O2	2.39	0.45
3:L5:4600:G:H4'	3:L5:4601:U:O5'	2.17	0.45
51:SB:27:LYS:HG3	51:SB:51:ARG:HH21	1.82	0.45
53:SE:11:ARG:HH11	53:SE:20:LEU:HB3	1.81	0.45
56:SI:154:LYS:HB3	56:SI:154:LYS:HE3	1.79	0.45
68:S2:1831:A:H2'	68:S2:1832:6MZ:H8	1.98	0.45
3:L5:37:U:H2'	3:L5:38:A:O4'	2.17	0.45
3:L5:964:A:H2'	3:L5:965:G:H4'	1.97	0.45
3:L5:1669:A:H4'	3:L5:1685:G:N2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3610:A:H2'	3:L5:3611:A:C8	2.51	0.45
3:L5:3825:A2M:H2'	3:L5:3826:C:O4'	2.17	0.45
10:LE:261:ILE:HG23	10:LE:267:LEU:HD23	1.98	0.45
13:LH:4:ILE:HG12	13:LH:61:TRP:CH2	2.52	0.45
29:LY:115:ARG:HA	29:LY:115:ARG:HD2	1.79	0.45
40:Lj:60:GLY:HA2	40:Lj:64:MET:SD	2.56	0.45
55:SH:160:LYS:HA	55:SH:163:GLN:NE2	2.32	0.45
82:Sf:103:LEU:HB2	82:Sf:105:TYR:CE2	2.51	0.45
85:CB:648:LYS:HB3	85:CB:664:ASP:OD1	2.17	0.45
3:L5:178:C:H2'	3:L5:179:G:H8	1.82	0.45
3:L5:1300:G:H2'	3:L5:1301:C:C6	2.52	0.45
3:L5:4392:OMG:HM21	3:L5:4394:A:H2'	1.99	0.45
35:Le:78:LEU:HB3	47:Lr:20:ARG:HD2	1.98	0.45
50:SA:111:GLN:HA	50:SA:116:PHE:CG	2.52	0.45
63:SX:140:ARG:HG3	63:SX:142:ARG:HE	1.80	0.45
68:S2:508:A:H3'	68:S2:509:OMG:C8	2.50	0.45
68:S2:629:A:H4'	70:SD:143:ARG:HH12	1.82	0.45
76:SS:36:VAL:HG23	76:SS:40:TYR:HB3	1.99	0.45
82:Sf:121:CYS:HB3	82:Sf:141:CYS:HB2	1.50	0.45
85:CB:358:LEU:HD23	85:CB:358:LEU:HA	1.85	0.45
3:L5:121:A:H62	3:L5:152:U:H3	1.65	0.45
3:L5:400:A2M:HM'3	3:L5:400:A2M:H1'	1.76	0.45
3:L5:499:G:H2'	3:L5:499:G:N3	2.32	0.45
3:L5:1213:G:H5''	3:L5:1214:C:H5'	1.98	0.45
3:L5:2385:U:H4'	22:LR:3:MET:HG3	1.98	0.45
3:L5:4536:OMC:HM22	3:L5:4537:C:O4'	2.17	0.45
14:LI:61:SER:HA	14:LI:126:VAL:HG12	1.97	0.45
50:SA:146:ALA:HB3	50:SA:157:VAL:HG13	1.98	0.45
54:SG:14:LYS:HE2	54:SG:16:ILE:HD11	1.98	0.45
56:SI:110:ARG:O	56:SI:114:GLU:HG2	2.16	0.45
68:S2:389:A:H2'	68:S2:390:C:C6	2.52	0.45
68:S2:884:C:H2'	68:S2:885:U:C6	2.52	0.45
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.52	0.45
3:L5:2415:U:H2'	3:L5:2416:G:C8	2.52	0.45
3:L5:4405:G:H5'	14:LI:8:CYS:SG	2.57	0.45
3:L5:4504:C:H2'	3:L5:4505:C:C6	2.52	0.45
3:L5:4991:U:H2'	3:L5:4992:G:C8	2.52	0.45
12:LG:73:ARG:HD3	12:LG:73:ARG:HA	1.81	0.45
12:LG:83:PHE:HA	12:LG:183:ILE:HD13	1.98	0.45
14:LI:47:PRO:HB3	14:LI:171:TRP:CZ2	2.51	0.45
21:LQ:43:PHE:CD2	21:LQ:133:GLY:HA3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LS:16:CYS:SG	23:LS:54:MET:HG2	2.57	0.45
28:LX:82:THR:HA	28:LX:87:MET:HE3	1.98	0.45
48:Ls:29:ILE:HD11	48:Ls:78:LEU:HD22	1.99	0.45
68:S2:223:C:H2'	68:S2:224:A:C8	2.52	0.45
68:S2:1778:C:H2'	68:S2:1779:G:O4'	2.17	0.45
79:SZ:50:PHE:CE1	79:SZ:79:ILE:HG21	2.52	0.45
84:Et:22:G:N7	84:Et:46:G:O6	2.50	0.45
3:L5:318:A:H2'	3:L5:319:A:H8	1.80	0.45
3:L5:460:C:H2'	3:L5:461:G:H8	1.82	0.45
3:L5:469:C:H2'	3:L5:470:A:H8	1.81	0.45
3:L5:1199:G:H2'	3:L5:1200:G:H8	1.82	0.45
3:L5:1725:U:H2'	3:L5:1726:U:C6	2.52	0.45
3:L5:3861:A:H2'	3:L5:3862:A:C8	2.52	0.45
5:L8:141:C:H2'	5:L8:142:U:C6	2.51	0.45
10:LE:148:THR:HA	10:LE:200:LYS:HG2	1.97	0.45
13:LH:140:GLN:HB2	13:LH:143:GLU:HB2	1.99	0.45
14:LI:87:MET:HG2	14:LI:138:ILE:HG12	1.99	0.45
35:Le:76:LYS:HE2	35:Le:98:GLU:OE2	2.17	0.45
54:SG:50:VAL:HG21	54:SG:111:LEU:HD13	1.99	0.45
68:S2:874:G:H2'	68:S2:875:A:C8	2.50	0.45
68:S2:909:G:H2'	68:S2:910:G:C8	2.52	0.45
68:S2:1328:OMG:HM23	68:S2:1328:OMG:H1'	1.68	0.45
80:Sc:20:ARG:HD3	80:Sc:28:THR:HB	1.99	0.45
86:CA:159:PRO:HD3	86:CA:325:LEU:HD11	1.98	0.45
3:L5:300:A:H2'	3:L5:301:G:H8	1.82	0.44
3:L5:1468:C:H2'	3:L5:1469:C:C6	2.52	0.44
3:L5:1534:A2M:HM'3	3:L5:1637:A:C4	2.52	0.44
3:L5:4441:A:H5''	14:LI:114:GLY:HA2	1.98	0.44
3:L5:4935:C:H2'	3:L5:4936:G:H8	1.81	0.44
8:LC:144:ILE:HG22	8:LC:147:VAL:HG21	1.98	0.44
9:LD:181:PRO:HD2	9:LD:195:HIS:CD2	2.52	0.44
14:LI:38:ARG:HD3	14:LI:83:ASP:OD1	2.16	0.44
50:SA:137:ALA:HB1	50:SA:142:LEU:HB3	1.99	0.44
51:SB:65:ARG:HG2	60:SO:50:LYS:HD3	1.98	0.44
56:SI:36:THR:O	56:SI:95:THR:HA	2.17	0.44
58:SL:126:VAL:HG13	58:SL:142:VAL:HG13	1.99	0.44
68:S2:484:A2M:H8	68:S2:484:A2M:O5'	2.17	0.44
68:S2:1661:A:H8	81:Sd:14:PHE:HB2	1.82	0.44
68:S2:1792:G:H2'	68:S2:1793:A:H8	1.81	0.44
68:S2:1839:U:H2'	68:S2:1840:U:C6	2.52	0.44
84:Et:6:G:H1	84:Et:67:U:H3	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:CA:86:VAL:HG11	86:CA:185:MET:HE3	1.99	0.44
3:L5:3709:U:H2'	3:L5:3710:G:O4'	2.17	0.44
3:L5:4196:OMG:HM23	3:L5:4196:OMG:H1'	1.65	0.44
3:L5:4274:A:H2'	3:L5:4275:G:H8	1.79	0.44
38:Lh:70:ARG:HG2	38:Lh:83:LEU:HD22	1.99	0.44
50:SA:8:LEU:HD11	61:SV:39:VAL:HG21	1.99	0.44
56:SI:124:LYS:HE3	56:SI:167:GLN:HE21	1.82	0.44
65:Sa:45:VAL:HG13	65:Sa:50:VAL:HG12	1.99	0.44
68:S2:1658:G:H5'	81:Sd:33:LYS:HD2	1.99	0.44
77:ST:42:HIS:NE2	77:ST:43:LYS:HE3	2.33	0.44
78:SU:51:LYS:HD3	78:SU:51:LYS:HA	1.78	0.44
85:CB:584:SER:HB3	85:CB:739:ARG:HG3	1.99	0.44
3:L5:2611:A:H2'	3:L5:2612:G:C8	2.52	0.44
3:L5:3652:A:H2'	3:L5:3653:A:C5	2.52	0.44
3:L5:3861:A:H2'	3:L5:3862:A:H8	1.82	0.44
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.53	0.44
3:L5:4601:U:H2'	3:L5:4602:A:H8	1.81	0.44
3:L5:4754:G:N7	10:LE:278:THR:HG23	2.33	0.44
34:Ld:90:ARG:HD3	34:Ld:102:LEU:HD13	1.99	0.44
48:Ls:34:ASN:HB2	48:Ls:185:PHE:HE2	1.81	0.44
68:S2:15:U:H2'	68:S2:16:G:O4'	2.18	0.44
68:S2:17:C:H2'	68:S2:18:C:C6	2.52	0.44
68:S2:886:A:H2'	68:S2:887:U:O4'	2.16	0.44
68:S2:1543:U:H4'	75:SQ:43:GLU:CD	2.42	0.44
78:SU:66:ARG:HH12	78:SU:75:LYS:HD3	1.83	0.44
85:CB:259:LYS:HD2	85:CB:273:PHE:CD2	2.52	0.44
85:CB:498:LYS:HE3	85:CB:498:LYS:HB3	1.74	0.44
1:CD:195:ARG:HA	1:CD:195:ARG:HD2	1.85	0.44
3:L5:7:C:H2'	3:L5:8:U:C6	2.52	0.44
3:L5:2554:U:C2	3:L5:2764:A:N7	2.86	0.44
3:L5:3619:G:H22	3:L5:3624:A:H1'	1.81	0.44
3:L5:4913:G:H4'	3:L5:4914:C:O5'	2.16	0.44
7:LB:50:LYS:HB2	7:LB:345:LEU:HD11	1.98	0.44
16:LL:110:LEU:O	16:LL:114:VAL:HG13	2.18	0.44
49:Lt:108:GLU:HG2	49:Lt:109:ILE:HD12	1.99	0.44
51:SB:145:LYS:HB2	51:SB:145:LYS:HE3	1.81	0.44
52:SC:196:ILE:HB	52:SC:223:TYR:HB2	2.00	0.44
68:S2:864:A:H2'	68:S2:865:A:H8	1.82	0.44
68:S2:929:G:H2'	68:S2:930:C:O4'	2.18	0.44
68:S2:948:C:H2'	68:S2:949:G:H8	1.82	0.44
68:S2:1670:C:H2'	68:S2:1671:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SD:141:LYS:HE2	70:SD:179:GLN:HB3	1.98	0.44
71:SF:61:PHE:HB3	80:Sc:51:ARG:NH2	2.32	0.44
73:SM:19:GLN:O	73:SM:23:LYS:HG2	2.17	0.44
3:L5:1095:A:H2	3:L5:1200:G:H1	1.57	0.44
3:L5:1356:U:H2'	3:L5:1357:C:C6	2.53	0.44
3:L5:2465:C:H2'	3:L5:2466:G:O4'	2.18	0.44
3:L5:3923:A:H2'	3:L5:3924:C:C6	2.53	0.44
3:L5:3946:G:H2'	3:L5:3947:A:H8	1.82	0.44
3:L5:4277:G:H5''	24:LT:17:ARG:HG2	1.98	0.44
18:LN:140:LYS:HD3	18:LN:140:LYS:HA	1.64	0.44
60:SO:57:THR:O	60:SO:60:MET:HG2	2.18	0.44
62:SW:119:LYS:HG3	62:SW:121:THR:HG22	2.00	0.44
65:Sa:21:ILE:HD12	65:Sa:72:HIS:HB3	1.99	0.44
68:S2:194:C:H2'	68:S2:195:C:C6	2.53	0.44
68:S2:656:G:N2	68:S2:663:C:H5''	2.32	0.44
68:S2:1199:A:H2'	68:S2:1200:A:C8	2.53	0.44
68:S2:1711:U:H2'	68:S2:1712:A:H8	1.82	0.44
68:S2:1780:G:H3'	68:S2:1781:A:C8	2.52	0.44
83:Sg:24:THR:HG23	83:Sg:27:PHE:H	1.82	0.44
83:Sg:129:ILE:HB	83:Sg:142:VAL:HB	1.98	0.44
84:Et:26:A:H4'	84:Et:26:A:OP1	2.18	0.44
85:CB:442:LEU:HD23	85:CB:442:LEU:HA	1.84	0.44
86:CA:194:VAL:HG22	86:CA:196:ASP:H	1.83	0.44
3:L5:4489:G:H4'	89:L5:5290:SPD:H91	1.99	0.44
3:L5:4571:A2M:H2'	3:L5:4572:U:C6	2.44	0.44
39:Li:76:ARG:HD3	39:Li:76:ARG:HA	1.65	0.44
61:SV:37:ALA:HB1	61:SV:46:PHE:CD1	2.52	0.44
68:S2:348:A:H2'	68:S2:349:A:C8	2.53	0.44
68:S2:601:OMG:HM23	68:S2:601:OMG:H1'	1.75	0.44
68:S2:1457:U:H2'	68:S2:1458:G:C8	2.52	0.44
3:L5:258:G:H2'	3:L5:259:C:O4'	2.18	0.44
3:L5:1359:G:H4'	18:LN:203:TYR:HB2	1.99	0.44
3:L5:2474:G:H2'	3:L5:2502:G:N2	2.33	0.44
4:L7:120:U:H4'	9:LD:262:LYS:HG2	2.00	0.44
20:LP:76:TRP:CD1	20:LP:76:TRP:H	2.35	0.44
20:LP:126:ARG:CZ	20:LP:140:MET:HE1	2.48	0.44
30:LZ:115:LYS:O	30:LZ:119:GLU:HG2	2.18	0.44
51:SB:59:SER:O	51:SB:63:LYS:HG2	2.18	0.44
53:SE:127:ARG:HD2	53:SE:142:HIS:HA	2.00	0.44
68:S2:1468:C:H2'	68:S2:1469:A:C8	2.52	0.44
68:S2:1540:G:H2'	68:S2:1541:G:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1593:C:H2'	68:S2:1594:A:H8	1.83	0.44
75:SQ:8:GLN:HB3	75:SQ:27:ARG:HE	1.83	0.44
75:SQ:42:ILE:HG13	75:SQ:43:GLU:H	1.82	0.44
83:Sg:249:CYS:HB3	83:Sg:258:ILE:HD13	1.98	0.44
85:CB:388:CYS:HB2	85:CB:466:CYS:HB2	1.46	0.44
86:CA:144:LYS:HG3	86:CA:343:TYR:HD2	1.83	0.44
3:L5:4280:A:C8	15:LJ:145:LYS:HE3	2.52	0.44
3:L5:4749:C:H2'	3:L5:4750:G:O4'	2.17	0.44
3:L5:4887:C:H42	3:L5:4932:U:H3	1.64	0.44
5:L8:90:C:H1'	29:LY:24:HIS:HB3	2.00	0.44
7:LB:117:ARG:NH2	7:LB:177:LYS:HG2	2.33	0.44
20:LP:107:LEU:HB2	20:LP:152:GLU:OE2	2.18	0.44
49:Lt:131:GLU:OE2	49:Lt:155:ILE:HD13	2.18	0.44
52:SC:74:LYS:HD3	52:SC:74:LYS:HA	1.85	0.44
56:SI:133:GLU:HA	56:SI:136:ILE:HG12	2.00	0.44
65:Sa:12:LYS:HG3	65:Sa:15:ARG:HB2	2.00	0.44
68:S2:882:U:H1'	68:S2:905:C:N3	2.33	0.44
70:SD:163:PRO:O	70:SD:167:TYR:HB2	2.18	0.44
75:SQ:10:VAL:HG22	75:SQ:25:CYS:HB3	1.98	0.44
85:CB:311:GLU:HG3	85:CB:314:LYS:HE3	2.00	0.44
85:CB:420:LEU:HD11	85:CB:463:ASP:HB2	1.99	0.44
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.53	0.44
3:L5:1645:C:H2'	3:L5:1646:A:C8	2.53	0.44
3:L5:1968:G:H4'	48:Ls:34:ASN:OD1	2.17	0.44
3:L5:3610:A:H2'	3:L5:3611:A:H8	1.82	0.44
25:LU:43:LEU:O	25:LU:47:ILE:HG12	2.17	0.44
50:SA:63:ARG:HH21	61:SV:38:GLU:HA	1.83	0.44
57:SJ:5:ARG:HG3	68:S2:38:A:OP1	2.17	0.44
68:S2:432:G:H2'	68:S2:433:A:C8	2.53	0.44
68:S2:800:U:H2'	68:S2:801:PSU:O4'	2.17	0.44
68:S2:835:C:H5'	68:S2:836:G:H5'	1.99	0.44
85:CB:85:ASP:HA	85:CB:88:PHE:HD2	1.83	0.44
85:CB:686:ALA:HB3	85:CB:729:LEU:HD12	2.00	0.44
3:L5:1464:C:H5''	32:Lb:32:LEU:HD12	2.00	0.43
3:L5:1588:U:H2'	3:L5:1589:C:C6	2.53	0.43
3:L5:3690:U:H2'	3:L5:3691:G:O4'	2.18	0.43
5:L8:37:A:OP2	38:Lh:89:ARG:HD2	2.18	0.43
5:L8:52:A:H4'	42:Ll:19:GLN:HA	1.99	0.43
13:LH:102:ASN:HB2	13:LH:115:ARG:HB2	2.00	0.43
15:LJ:78:LYS:HE3	15:LJ:82:ILE:HD11	2.00	0.43
32:Lb:109:ARG:HA	32:Lb:112:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SG:50:VAL:HG12	54:SG:113:ILE:HA	2.00	0.43
55:SH:33:ASN:ND2	55:SH:37:LYS:HG2	2.33	0.43
58:SL:111:VAL:HG12	58:SL:140:PHE:HB2	2.00	0.43
68:S2:940:U:H2'	68:S2:941:C:C6	2.53	0.43
68:S2:1706:G:H2'	68:S2:1707:U:H6	1.82	0.43
70:SD:109:LEU:HD13	70:SD:182:LEU:HD23	2.00	0.43
83:Sg:183:LYS:HD2	83:Sg:183:LYS:HA	1.77	0.43
84:Et:37:A:H3'	84:Et:38:A:H8	1.83	0.43
85:CB:89:ILE:HG13	85:CB:356:ILE:HG12	2.00	0.43
3:L5:4625:C:O2'	3:L5:4626:A:H5'	2.19	0.43
5:L8:5:U:H2'	5:L8:6:C:H6	1.83	0.43
7:LB:28:LYS:HE3	7:LB:28:LYS:HB2	1.79	0.43
14:LI:53:VAL:HG11	24:LT:158:PHE:HZ	1.82	0.43
18:LN:178:HIS:HA	18:LN:181:HIS:NE2	2.33	0.43
72:SK:3:MET:SD	72:SK:48:ALA:HB2	2.57	0.43
77:ST:131:LEU:HD23	77:ST:131:LEU:HA	1.79	0.43
81:Sd:39:CYS:H	81:Sd:42:CYS:HB2	1.83	0.43
85:CB:666:THR:HG22	85:CB:706:ASP:HA	1.99	0.43
3:L5:186:G:H4'	3:L5:187:U:O4'	2.19	0.43
3:L5:1978:C:H2'	3:L5:1979:A:O4'	2.17	0.43
3:L5:2481:G:H2'	3:L5:2482:C:C6	2.53	0.43
10:LE:243:THR:HG22	10:LE:245:GLN:H	1.83	0.43
16:LL:48:PRO:HB2	38:Lh:120:ALA:HB2	2.00	0.43
33:Lc:47:ILE:HB	33:Lc:94:LEU:HG	2.01	0.43
35:Le:35:TRP:CZ2	35:Le:56:PRO:HD2	2.53	0.43
49:Lt:114:ARG:HH21	49:Lt:117:ARG:HG3	1.82	0.43
50:SA:117:ARG:HG3	50:SA:119:PRO:HD3	2.00	0.43
51:SB:113:MET:HB3	51:SB:142:PHE:CZ	2.53	0.43
56:SI:199:LEU:HD23	56:SI:199:LEU:HA	1.84	0.43
58:SL:133:PRO:HG2	68:S2:383:G:H21	1.83	0.43
68:S2:554:A:O2'	68:S2:555:A:H8	2.01	0.43
68:S2:649:PSU:H2'	68:S2:650:A:C8	2.53	0.43
68:S2:1803:U:H2'	68:S2:1804:U:H6	1.83	0.43
86:CA:157:VAL:HG22	86:CA:325:LEU:HD13	1.99	0.43
1:CD:195:ARG:HH11	68:S2:1489:A:H5''	1.83	0.43
3:L5:381:U:H4'	3:L5:415:G:H5'	1.99	0.43
3:L5:424:U:H2'	3:L5:425:U:C6	2.53	0.43
3:L5:2538:U:H2'	3:L5:2539:C:C6	2.54	0.43
3:L5:4523:A2M:HM'3	3:L5:4523:A2M:H1'	1.83	0.43
5:L8:75:OMG:HM23	5:L8:75:OMG:H1'	1.75	0.43
5:L8:96:C:H5''	38:Lh:66:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LR:174:GLU:HA	22:LR:177:LEU:HB2	1.99	0.43
31:La:93:ASN:ND2	31:La:97:ALA:HB3	2.33	0.43
33:Lc:26:LYS:HB2	33:Lc:98:ASP:HB3	2.00	0.43
38:Lh:80:PRO:HD2	38:Lh:83:LEU:HD12	2.00	0.43
53:SE:38:LEU:HD23	68:S2:346:C:H5'	2.00	0.43
53:SE:66:MET:HG3	68:S2:502:C:O4'	2.18	0.43
54:SG:176:ILE:H	54:SG:176:ILE:HD12	1.84	0.43
71:SF:91:ARG:HD2	79:SZ:103:HIS:CE1	2.52	0.43
75:SQ:80:GLN:O	75:SQ:84:ILE:HG12	2.18	0.43
76:SS:102:GLY:HA2	76:SS:105:ASN:HD21	1.83	0.43
85:CB:74:ALA:HA	85:CB:103:ILE:HG22	2.01	0.43
85:CB:361:PRO:O	85:CB:365:GLN:HG2	2.19	0.43
1:CD:201:ARG:HD3	68:S2:626:G:H2'	2.00	0.43
3:L5:510:U:OP1	16:LL:163:LYS:HE3	2.19	0.43
3:L5:4563:U:H2'	3:L5:4564:A:H8	1.84	0.43
3:L5:4611:A:H2'	3:L5:4612:C:H6	1.82	0.43
3:L5:4934:A:H2'	3:L5:4935:C:H6	1.82	0.43
3:L5:4981:G:H3'	3:L5:4982:A:H8	1.84	0.43
13:LH:94:SER:OG	13:LH:142:ASP:HB3	2.19	0.43
33:Lc:52:CYS:HB3	33:Lc:57:LYS:HG3	1.99	0.43
36:Lf:29:LYS:HB2	36:Lf:83:MET:HE1	2.01	0.43
38:Lh:89:ARG:O	38:Lh:93:ARG:HG2	2.19	0.43
48:Ls:66:ARG:HG2	48:Ls:79:LEU:HD21	1.99	0.43
66:Sb:64:CYS:HB3	66:Sb:71:ALA:HB1	2.00	0.43
68:S2:587:A:H5'	68:S2:592:C:H41	1.84	0.43
69:SR:24:LEU:HD23	69:SR:54:VAL:HG11	2.00	0.43
85:CB:207:PRO:HG2	85:CB:261:TRP:CE2	2.53	0.43
3:L5:73:A:H62	16:LL:103:ARG:HH22	1.66	0.43
3:L5:136:C:H41	38:Lh:77:LYS:HA	1.84	0.43
3:L5:1244:G:H2'	3:L5:1245:C:H6	1.84	0.43
3:L5:2844:A:O2'	3:L5:4631:G:H4'	2.18	0.43
3:L5:3911:C:H2'	3:L5:3912:U:C6	2.53	0.43
5:L8:19:C:H2'	5:L8:20:A:C8	2.52	0.43
5:L8:81:C:H5'	38:Lh:3:LYS:NZ	2.33	0.43
7:LB:217:ILE:HD12	7:LB:347:LEU:HB3	2.00	0.43
17:LM:100:ARG:HA	17:LM:103:LYS:HG2	2.00	0.43
28:LX:64:SER:HB2	38:Lh:69:LEU:HD13	2.01	0.43
38:Lh:6:ALA:O	38:Lh:10:ARG:HG3	2.17	0.43
56:SI:81:VAL:HA	56:SI:102:VAL:HG23	2.01	0.43
62:SW:107:SER:HB2	68:S2:860:G:H21	1.84	0.43
68:S2:5:U:H2'	68:S2:6:G:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1304:U:H5''	82:Sf:95:ARG:HB2	2.01	0.43
71:SF:121:PRO:HA	71:SF:193:LYS:HG3	1.99	0.43
74:SP:68:PRO:O	74:SP:71:GLU:HG2	2.19	0.43
75:SQ:34:VAL:HG12	75:SQ:70:VAL:HB	2.01	0.43
76:SS:50:ILE:HG21	76:SS:59:LEU:HD21	1.99	0.43
82:Sf:123:SER:HB3	82:Sf:126:CYS:SG	2.59	0.43
83:Sg:118:ARG:HG3	83:Sg:119:GLN:HG3	2.00	0.43
3:L5:978:G:H2'	3:L5:979:C:C6	2.53	0.43
3:L5:1071:C:C5	10:LE:67:ALA:HB2	2.54	0.43
3:L5:1298:C:H2'	3:L5:1299:G:C8	2.53	0.43
3:L5:2256:C:H2'	3:L5:2257:C:O4'	2.19	0.43
7:LB:279:GLU:HB3	7:LB:282:LYS:HZ3	1.83	0.43
7:LB:341:LYS:O	7:LB:342:LYS:HG2	2.19	0.43
8:LC:318:PRO:C	8:LC:320:LYS:H	2.25	0.43
13:LH:95:VAL:HG12	43:Lm:82:LEU:HD22	2.01	0.43
15:LJ:115:LEU:HD23	15:LJ:115:LEU:HA	1.89	0.43
50:SA:148:CYS:SG	50:SA:163:CYS:N	2.92	0.43
50:SA:205:ARG:HE	69:SR:81:ARG:NH1	2.17	0.43
55:SH:145:ARG:HB2	62:SW:51:GLU:OE2	2.18	0.43
56:SI:141:ARG:HD3	56:SI:145:ILE:HD13	2.00	0.43
68:S2:674:C:H2'	68:S2:675:U:C6	2.54	0.43
69:SR:14:ARG:O	69:SR:18:GLU:HG2	2.19	0.43
3:L5:750:U:H1'	3:L5:917:A:C8	2.53	0.43
3:L5:1468:C:H2'	3:L5:1469:C:H6	1.84	0.43
3:L5:3722:G:H2'	3:L5:3723:A:H8	1.83	0.43
3:L5:3920:PSU:H2'	3:L5:3921:U:C6	2.54	0.43
3:L5:4364:G:H2'	3:L5:4365:C:H6	1.84	0.43
3:L5:4524:G:N3	7:LB:252:ALA:HB1	2.33	0.43
3:L5:5053:U:H3'	3:L5:5054:C:C6	2.53	0.43
5:L8:36:G:C5	38:Lh:89:ARG:HD3	2.53	0.43
28:LX:148:ASP:HA	28:LX:151:ASN:HB2	2.01	0.43
52:SC:107:LEU:HB3	52:SC:233:LEU:HD21	2.00	0.43
53:SE:128:LYS:HG2	53:SE:140:VAL:HG22	2.00	0.43
68:S2:867:OMG:HM23	68:S2:867:OMG:H1'	1.86	0.43
68:S2:1237:C:H5'	74:SP:131:PRO:HA	2.00	0.43
68:S2:1617:G:O6	74:SP:43:ARG:HD3	2.19	0.43
74:SP:133:ILE:HG22	74:SP:134:GLY:H	1.82	0.43
83:Sg:40:ILE:HD11	83:Sg:66:VAL:HG21	2.00	0.43
3:L5:52:G:H4'	3:L5:1529:G:H4'	2.01	0.43
3:L5:469:C:H2'	3:L5:470:A:C8	2.54	0.43
3:L5:4344:U:H2'	3:L5:4345:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4456:OMC:HM21	7:LB:241:PRO:HD3	2.00	0.43
3:L5:4481:U:H2'	3:L5:4482:U:C6	2.54	0.43
11:LF:60:GLU:O	11:LF:64:MET:HG3	2.19	0.43
14:LI:99:ILE:HG22	14:LI:123:GLN:HB2	2.00	0.43
30:LZ:11:VAL:HG12	30:LZ:82:PRO:HA	2.01	0.43
48:Ls:39:GLN:CG	48:Ls:107:VAL:HG21	2.48	0.43
50:SA:166:LYS:HA	50:SA:166:LYS:HD2	1.92	0.43
51:SB:86:LEU:HD23	51:SB:100:PHE:HA	2.01	0.43
68:S2:468:A2M:HM'3	68:S2:468:A2M:H1'	1.61	0.43
68:S2:1491:G:H2'	68:S2:1492:U:C6	2.53	0.43
75:SQ:53:GLU:HA	75:SQ:56:LEU:HD12	1.99	0.43
85:CB:76:SER:HB2	85:CB:454:MET:HE1	2.01	0.43
85:CB:438:LYS:HA	85:CB:438:LYS:HD3	1.78	0.43
3:L5:1084:C:H2'	3:L5:1085:C:C6	2.53	0.43
3:L5:1195:G:H2'	3:L5:1196:G:H8	1.83	0.43
3:L5:1534:A2M:N3	40:Lj:11:ARG:HB2	2.34	0.43
3:L5:2380:G:N2	3:L5:2424:OMG:H5''	2.34	0.43
3:L5:2894:A:H2'	3:L5:2895:A:C8	2.54	0.43
24:LT:39:ILE:HG22	24:LT:61:THR:HG22	2.01	0.43
25:LU:84:LYS:HB2	25:LU:110:TYR:CZ	2.54	0.43
43:Lm:93:LYS:HD3	43:Lm:102:ARG:HG2	2.01	0.43
45:Lo:33:LEU:HD12	45:Lo:38:LYS:HE3	2.00	0.43
49:Lt:147:HIS:HA	49:Lt:148:PRO:HD3	1.89	0.43
50:SA:126:ASP:HB3	50:SA:129:ALA:HB3	2.01	0.43
62:SW:69:LEU:HD21	62:SW:72:CYS:HB3	2.01	0.43
68:S2:494:C:N4	68:S2:509:OMG:HN22	2.17	0.43
68:S2:959:G:H2'	68:S2:960:U:C6	2.52	0.43
68:S2:1101:U:H2'	68:S2:1102:G:H8	1.83	0.43
68:S2:1599:U:H3'	79:SZ:44:LEU:HD22	2.01	0.43
71:SF:178:ILE:O	71:SF:182:LYS:HG2	2.19	0.43
71:SF:192:LYS:HA	71:SF:192:LYS:HD2	1.80	0.43
85:CB:89:ILE:HG22	85:CB:91:GLN:H	1.84	0.43
3:L5:2696:A:H62	41:Lk:35:LYS:HZ2	1.67	0.42
3:L5:2714:G:H2'	3:L5:2715:G:H8	1.83	0.42
3:L5:3867:A2M:H2'	3:L5:3868:G:O4'	2.18	0.42
3:L5:3870:C:H2'	3:L5:3871:A:C8	2.54	0.42
3:L5:4103:C:H2'	3:L5:4105:A:C2	2.53	0.42
3:L5:4770:U:H2'	3:L5:4771:C:C5	2.54	0.42
3:L5:4934:A:H2'	3:L5:4935:C:C6	2.54	0.42
14:LI:91:LEU:HD12	14:LI:135:ILE:HG23	2.00	0.42
29:LY:50:ARG:HG3	29:LY:51:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LZ:77:TYR:CD2	33:Lc:39:ARG:HD3	2.54	0.42
53:SE:38:LEU:HA	53:SE:41:CYS:SG	2.59	0.42
53:SE:79:ASP:HB3	53:SE:82:TYR:HB2	2.01	0.42
54:SG:71:GLY:O	54:SG:98:ARG:HD2	2.19	0.42
68:S2:349:A:H2'	68:S2:350:C:C6	2.54	0.42
68:S2:441:C:H2'	68:S2:442:C:C6	2.54	0.42
68:S2:609:U:H2'	68:S2:610:G:H8	1.85	0.42
68:S2:656:G:H21	68:S2:663:C:H5''	1.83	0.42
68:S2:677:G:H21	68:S2:1028:A:H62	1.65	0.42
68:S2:945:U:H2'	68:S2:946:U:C6	2.54	0.42
71:SF:103:LEU:HD11	79:SZ:67:LEU:HD22	2.01	0.42
72:SK:41:PRO:HG2	72:SK:44:HIS:ND1	2.34	0.42
85:CB:531:ASP:HB3	85:CB:534:VAL:HG12	2.00	0.42
3:L5:260:C:H2'	3:L5:261:G:C8	2.55	0.42
3:L5:385:A:N3	3:L5:387:G:H5''	2.34	0.42
3:L5:4113:U:H4'	3:L5:4115:G:C5	2.53	0.42
3:L5:4273:A:H2'	3:L5:4274:A:C8	2.54	0.42
3:L5:4771:C:H2'	3:L5:4772:C:C6	2.53	0.42
4:L7:24:C:H2'	4:L7:25:G:O4'	2.19	0.42
6:LA:83:HIS:HB3	46:Lp:64:VAL:HG22	2.01	0.42
15:LJ:68:ILE:HD13	15:LJ:68:ILE:HA	1.88	0.42
58:SL:80:MET:HA	58:SL:86:ILE:HG22	2.01	0.42
62:SW:111:MET:HE1	62:SW:119:LYS:HD2	2.00	0.42
68:S2:166:A2M:HM'3	68:S2:166:A2M:H1'	1.48	0.42
68:S2:527:C:H2'	68:S2:528:A:C8	2.53	0.42
68:S2:1803:U:H2'	68:S2:1804:U:C6	2.53	0.42
71:SF:97:PHE:HZ	71:SF:112:LEU:HD22	1.84	0.42
85:CB:79:TYR:CZ	85:CB:351:LEU:HB3	2.53	0.42
3:L5:2709:C:H1'	22:LR:40:GLN:HG3	2.02	0.42
3:L5:4481:U:H2'	3:L5:4482:U:H6	1.83	0.42
4:L7:4:U:H2'	4:L7:5:A:C8	2.55	0.42
7:LB:27:GLY:HA2	7:LB:276:HIS:CD2	2.54	0.42
9:LD:65:ALA:HB2	9:LD:74:ILE:HG13	2.00	0.42
13:LH:93:ARG:HG2	13:LH:182:SER:HB3	2.01	0.42
23:LS:127:MET:HB3	24:LT:153:PRO:HG2	2.01	0.42
35:Le:81:ASN:OD1	35:Le:84:GLU:HG3	2.19	0.42
40:Lj:67:LEU:HD23	40:Lj:67:LEU:HA	1.88	0.42
56:SI:5:ARG:HD2	68:S2:386:C:H1'	2.00	0.42
56:SI:193:LYS:HE2	58:SL:30:LYS:NZ	2.35	0.42
57:SJ:136:ARG:HA	57:SJ:141:VAL:HA	2.02	0.42
62:SW:94:LEU:HD21	62:SW:102:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63: SX:54: LYS: HE3	63: SX:91: LEU: HG	2.01	0.42
65: Sa:46: GLU: O	65: Sa:50: VAL: HG13	2.19	0.42
68: S2:1856: C: H2'	68: S2:1857: G: H8	1.84	0.42
69: SR:24: LEU: HG	69: SR:34: VAL: HG21	2.01	0.42
72: SK:90: VAL: HB	72: SK:94: LEU: HD23	2.00	0.42
75: SQ:58: LEU: HD23	75: SQ:58: LEU: HA	1.87	0.42
75: SQ:58: LEU: HD13	75: SQ:92: LEU: HD11	2.00	0.42
3: L5:372: A: OP1	40: Lj:36: LYS: HE2	2.20	0.42
3: L5:2683: C: H2'	3: L5:2684: C: C6	2.55	0.42
7: LB:28: LYS: HG3	7: LB:30: LYS: HG3	2.00	0.42
30: LZ:135: ARG: HA	30: LZ:135: ARG: HD2	1.83	0.42
50: SA:80: ARG: HH22	50: SA:166: LYS: HA	1.84	0.42
60: SO:98: ARG: HB2	60: SO:132: VAL: HG23	2.01	0.42
68: S2:352: U: H2'	68: S2:353: C: C6	2.54	0.42
68: S2:1538: C: H2'	68: S2:1539: U: C6	2.53	0.42
68: S2:1683: C: H2'	68: S2:1684: C: H6	1.85	0.42
68: S2:1703: OMC: H2'	68: S2:1704: C: O4'	2.19	0.42
68: S2:1801: A: H2'	68: S2:1802: C: H6	1.84	0.42
73: SM:53: ALA: HA	73: SM:79: VAL: HG12	2.01	0.42
74: SP:61: ARG: O	74: SP:65: LYS: HD3	2.19	0.42
85: CB:304: ILE: HD13	85: CB:336: LEU: HA	2.02	0.42
3: L5:264: C: H2'	3: L5:265: C: C5	2.54	0.42
3: L5:423: G: H5'	20: LP:26: PHE: HZ	1.85	0.42
3: L5:908: G: H2'	3: L5:909: A: H8	1.84	0.42
3: L5:1545: G: H2'	3: L5:1546: C: C6	2.54	0.42
3: L5:1601: A: O2'	40: Lj:2: THR: HG21	2.20	0.42
3: L5:1971: C: O3'	48: Ls:38: LYS: HE3	2.19	0.42
3: L5:2095: A: H1'	3: L5:2096: G: N2	2.35	0.42
9: LD:118: ILE: HG13	9: LD:135: ILE: HD12	2.01	0.42
17: LM:71: LYS: O	17: LM:75: GLN: HG3	2.20	0.42
22: LR:19: LYS: HB2	22: LR:19: LYS: HE2	1.79	0.42
47: Lr:16: PHE: HB3	47: Lr:27: THR: H	1.84	0.42
48: Ls:141: LEU: HD11	48: Ls:171: GLU: HG3	2.02	0.42
53: SE:49: ARG: HE	53: SE:49: ARG: HB3	1.64	0.42
60: SO:15: ILE: HG12	60: SO:16: SER: H	1.84	0.42
61: SV:11: LEU: HD12	61: SV:12: TYR: HD1	1.85	0.42
64: SY:110: ARG: HG3	64: SY:114: MET: HE1	2.02	0.42
68: S2:919: A: H8	68: S2:919: A: OP2	2.01	0.42
68: S2:1667: U: H2'	68: S2:1668: U: C6	2.54	0.42
68: S2:1758: G: H1	68: S2:1771: G: H3'	1.85	0.42
69: SR:80: ARG: HG2	69: SR:81: ARG: H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:SZ:84:ALA:O	79:SZ:88:LEU:HB2	2.20	0.42
85:CB:321:ILE:HD13	85:CB:343:TRP:HB2	2.00	0.42
3:L5:2109:G:H2'	3:L5:2110:C:C6	2.54	0.42
3:L5:3606:U:H2'	3:L5:3607:U:H6	1.84	0.42
5:L8:40:A:H2'	5:L8:41:A:C8	2.54	0.42
7:LB:206:PRO:HG2	7:LB:209:GLN:HG2	2.00	0.42
7:LB:291:TYR:CD2	7:LB:327:THR:HG23	2.55	0.42
19:LO:47:PHE:HA	19:LO:136:ALA:HB2	2.00	0.42
26:LV:92:ASP:HB2	27:LW:2:LYS:NZ	2.35	0.42
28:LX:156:ILE:HD12	28:LX:156:ILE:HA	1.92	0.42
50:SA:77:ILE:HG12	50:SA:99:ILE:HB	2.01	0.42
60:SO:83:GLN:HA	60:SO:86:LYS:HE2	2.02	0.42
68:S2:878:G:H22	68:S2:908:A:H2	1.67	0.42
72:SK:76:ILE:O	72:SK:80:ARG:HG2	2.19	0.42
73:SM:121:LYS:O	73:SM:125:GLU:HG2	2.20	0.42
3:L5:163:A:H2'	3:L5:164:G:H8	1.84	0.42
3:L5:490:C:H2'	3:L5:491:G:H8	1.83	0.42
3:L5:705:G:H2'	3:L5:706:C:C6	2.55	0.42
3:L5:729:G:H5''	11:LF:76:ARG:HD2	2.01	0.42
3:L5:1751:A:H2'	3:L5:1752:G:C8	2.54	0.42
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	2.02	0.42
3:L5:3661:G:C4	6:LA:150:LEU:HD13	2.54	0.42
3:L5:3928:A:H2'	3:L5:3929:G:O4'	2.19	0.42
3:L5:4578:G:H2'	3:L5:4579:PSU:C6	2.54	0.42
7:LB:258:HIS:HA	7:LB:260:ALA:H	1.83	0.42
11:LF:216:PRO:HD3	11:LF:247:MET:HE2	2.01	0.42
11:LF:236:ARG:HB2	11:LF:239:GLN:HB2	2.01	0.42
38:Lh:52:LYS:HA	38:Lh:52:LYS:HD3	1.71	0.42
52:SC:112:VAL:HG11	68:S2:1357:A:H5'	2.01	0.42
57:SJ:130:ILE:HG13	57:SJ:135:ILE:HD13	2.01	0.42
59:SN:109:LYS:HD2	68:S2:1032:C:H5''	2.01	0.42
64:SY:41:ARG:HH21	64:SY:53:ASP:HA	1.83	0.42
68:S2:569:A:H2'	68:S2:570:C:O4'	2.20	0.42
68:S2:1298:G:H1'	74:SP:79:HIS:HB2	2.02	0.42
68:S2:1406:G:H2'	68:S2:1407:U:C6	2.55	0.42
71:SF:22:LYS:HG3	71:SF:23:TRP:CD2	2.54	0.42
83:Sg:8:ARG:HD2	83:Sg:311:GLN:CG	2.38	0.42
83:Sg:153:CYS:SG	83:Sg:198:VAL:HG12	2.59	0.42
84:Et:52:G:H2'	84:Et:53:G:H8	1.84	0.42
85:CB:50:ARG:NH2	85:CB:456:ARG:HH12	2.17	0.42
85:CB:369:CYS:SG	85:CB:385:ILE:HG13	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:CB:680:VAL:O	85:CB:684:GLN:HG2	2.18	0.42
3:L5:135:G:H5''	38:Lh:96:ASN:HB2	2.02	0.42
3:L5:513:U:H3'	3:L5:514:U:H4'	2.02	0.42
3:L5:1345:A:H2'	3:L5:1346:C:C6	2.54	0.42
3:L5:1593:A:H5''	3:L5:2839:PSU:H5'	2.01	0.42
3:L5:3910:C:H2'	3:L5:3911:C:H6	1.81	0.42
3:L5:4095:G:H2'	3:L5:4096:C:C6	2.55	0.42
3:L5:5006:U:H4'	3:L5:5007:A:H5'	2.01	0.42
11:LF:182:TYR:CZ	11:LF:203:GLU:HG2	2.55	0.42
12:LG:218:LEU:O	12:LG:222:ILE:HG12	2.19	0.42
34:Ld:24:GLU:HG3	34:Ld:122:VAL:HG11	2.00	0.42
50:SA:220:LYS:HA	50:SA:220:LYS:HD3	1.84	0.42
55:SH:53:VAL:HG12	55:SH:175:GLY:HA3	2.01	0.42
63:SX:17:ARG:HH12	68:S2:659:G:N2	2.17	0.42
68:S2:940:U:H3	68:S2:1002:U:H3	1.68	0.42
68:S2:1213:C:H2'	68:S2:1214:A:C8	2.54	0.42
68:S2:1227:G:C2	68:S2:1228:A:C8	3.07	0.42
68:S2:1278:A:H2'	68:S2:1279:C:C6	2.54	0.42
71:SF:49:LEU:HD12	75:SQ:50:LYS:HG2	2.01	0.42
80:Sc:16:LYS:HB3	80:Sc:16:LYS:HE2	1.77	0.42
85:CB:829:SER:HB2	85:CB:831:PRO:HD2	2.01	0.42
86:CA:107:LYS:HG2	86:CA:124:THR:OG1	2.19	0.42
3:L5:2654:C:H2'	3:L5:2655:C:H6	1.85	0.42
3:L5:2709:C:H42	86:CA:256:GLY:HA2	1.84	0.42
3:L5:4991:U:H2'	3:L5:4992:G:H8	1.83	0.42
3:L5:5001:PSU:H2'	3:L5:5002:U:O4'	2.19	0.42
4:L7:110:G:H2'	4:L7:111:C:C6	2.55	0.42
24:LT:116:LYS:HG3	24:LT:128:LEU:HD11	2.00	0.42
59:SN:5:HIS:HD2	68:S2:676:C:H5''	1.84	0.42
68:S2:348:A:H2'	68:S2:349:A:H8	1.84	0.42
74:SP:93:MET:HB3	74:SP:104:GLN:HE22	1.85	0.42
83:Sg:10:THR:HB	83:Sg:306:LEU:HD21	2.01	0.42
85:CB:110:ASP:OD2	85:CB:552:LEU:HB3	2.19	0.42
3:L5:269:G:H2'	3:L5:270:U:C6	2.55	0.42
3:L5:702:U:H2'	3:L5:703:G:O4'	2.19	0.42
3:L5:1397:A:H8	31:La:114:LYS:HG3	1.84	0.42
3:L5:2743:A:H2'	3:L5:2744:A:C8	2.55	0.42
3:L5:2765:A:H2'	3:L5:2766:A:C8	2.54	0.42
3:L5:4965:U:H4'	3:L5:4966:A:H5'	2.02	0.42
4:L7:7:G:OP1	9:LD:33:ARG:HD2	2.20	0.42
8:LC:57:LEU:HB3	8:LC:61:GLN:HE21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LZ:46:ILE:HA	30:LZ:70:SER:HA	2.02	0.42
51:SB:115:LYS:HE2	68:S2:1869:A:C2	2.53	0.42
52:SC:166:ARG:HG2	52:SC:181:PRO:HG3	2.02	0.42
56:SI:139:LYS:HB2	56:SI:139:LYS:HE2	1.68	0.42
62:SW:11:LEU:HD12	62:SW:74:VAL:HB	2.02	0.42
68:S2:900:C:H3'	68:S2:901:G:H8	1.84	0.42
68:S2:1004:PSU:H2'	68:S2:1005:G:C8	2.54	0.42
70:SD:151:LYS:HE2	70:SD:153:VAL:HG11	2.02	0.42
3:L5:175:C:H2'	3:L5:176:G:C8	2.55	0.41
3:L5:218:A:H1'	3:L5:219:G:C8	2.55	0.41
3:L5:1504:G:H2'	3:L5:1505:C:C6	2.55	0.41
3:L5:3588:C:H2'	3:L5:3589:G:O4'	2.20	0.41
3:L5:3722:G:H2'	3:L5:3723:A:C8	2.55	0.41
3:L5:4088:C:H2'	3:L5:4089:G:H8	1.85	0.41
3:L5:5062:G:C2	3:L5:5063:G:C8	3.08	0.41
5:L8:144:U:H2'	5:L8:145:C:C6	2.54	0.41
12:LG:35:ARG:HH22	30:LZ:52:LYS:HG3	1.84	0.41
26:LV:45:ILE:HG21	26:LV:53:PRO:HB3	2.02	0.41
30:LZ:9:LYS:HD2	30:LZ:83:THR:O	2.19	0.41
36:Lf:46:ARG:HH21	36:Lf:89:ARG:NH2	2.18	0.41
50:SA:38:ILE:HD11	50:SA:150:THR:HG22	2.02	0.41
55:SH:118:ARG:HA	55:SH:118:ARG:HD3	1.87	0.41
56:SI:27:TYR:HB2	68:S2:381:C:N4	2.35	0.41
56:SI:150:ASP:O	56:SI:153:LYS:HG2	2.20	0.41
68:S2:12:U:O2'	68:S2:1356:G:C8	2.73	0.41
68:S2:140:C:H42	68:S2:313:A:H61	1.68	0.41
68:S2:882:U:H1'	68:S2:905:C:C2	2.54	0.41
3:L5:162:A:H2'	3:L5:163:A:H8	1.84	0.41
3:L5:1309:C:H2'	3:L5:1310:C:C6	2.55	0.41
3:L5:1876:U:O3'	11:LF:103:PRO:HD3	2.20	0.41
3:L5:2730:U:H2'	3:L5:2731:C:C6	2.54	0.41
3:L5:3848:U:H2'	3:L5:3849:A:C8	2.55	0.41
6:LA:115:CYS:SG	6:LA:124:GLY:HA3	2.60	0.41
12:LG:70:LEU:HD23	12:LG:70:LEU:HA	1.85	0.41
13:LH:107:GLU:O	13:LH:107:GLU:HG2	2.20	0.41
14:LI:36:LEU:HD11	14:LI:69:ARG:HD2	2.01	0.41
20:LP:114:ILE:HG12	20:LP:150:LEU:HD22	2.01	0.41
25:LU:88:LYS:HD2	25:LU:97:ARG:CZ	2.50	0.41
54:SG:224:ARG:HA	54:SG:227:GLN:OE1	2.20	0.41
62:SW:42:MET:HE3	62:SW:42:MET:HB3	1.87	0.41
68:S2:455:A:H2'	68:S2:456:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1598:G:H5''	79:SZ:80:ARG:HH11	1.84	0.41
68:S2:1610:G:H2'	68:S2:1611:G:C8	2.56	0.41
68:S2:1610:G:H2'	68:S2:1611:G:H8	1.84	0.41
71:SF:101:HIS:HB2	71:SF:108:PRO:HG3	2.02	0.41
77:ST:18:LEU:HD22	77:ST:58:ALA:HA	2.02	0.41
77:ST:56:ARG:HG3	77:ST:103:VAL:HG21	2.01	0.41
84:Et:10:G:C2	84:Et:26:A:H1'	2.55	0.41
85:CB:12:ILE:HG13	85:CB:15:LYS:HD2	2.01	0.41
85:CB:222:ALA:HB3	85:CB:346:ALA:HA	2.02	0.41
86:CA:181:PRO:HB2	86:CA:204:ASN:HB2	2.02	0.41
3:L5:679:C:H2'	3:L5:680:G:C8	2.55	0.41
3:L5:751:G:H2'	3:L5:752:G:O4'	2.20	0.41
3:L5:3597:G:H2'	3:L5:3598:C:C6	2.55	0.41
3:L5:3867:A2M:HM'3	3:L5:3867:A2M:H1'	1.70	0.41
3:L5:4392:OMG:N3	3:L5:4447:5MC:HM52	2.36	0.41
7:LB:29:VAL:HG12	7:LB:31:SER:H	1.84	0.41
8:LC:5:ARG:NH2	8:LC:266:THR:HG23	2.30	0.41
8:LC:207:PRO:HB3	8:LC:249:PHE:CD2	2.56	0.41
11:LF:54:ALA:HB2	11:LF:188:GLU:HG3	2.02	0.41
20:LP:105:LYS:HE2	20:LP:105:LYS:HB3	1.92	0.41
56:SI:38:ILE:HD13	56:SI:80:ASP:HA	2.03	0.41
56:SI:174:CYS:HB2	56:SI:190:LEU:HD21	2.02	0.41
58:SL:17:PHE:CD2	68:S2:222:U:H5''	2.56	0.41
68:S2:102:A:H4'	68:S2:104:A:C8	2.55	0.41
68:S2:944:A:H2'	68:S2:945:U:C6	2.55	0.41
73:SM:20:GLU:HG2	73:SM:119:GLN:HB2	2.03	0.41
84:Et:46:G:H4'	84:Et:47:U:OP2	2.20	0.41
86:CA:89:PHE:CZ	86:CA:91:PRO:HG3	2.54	0.41
3:L5:674:G:H2'	3:L5:675:C:C6	2.55	0.41
3:L5:959:G:C8	10:LE:123:ARG:HG2	2.55	0.41
3:L5:1625:OMG:HM23	18:LN:81:TYR:HE2	1.85	0.41
3:L5:1912:G:N2	19:LO:87:MET:HE2	2.35	0.41
3:L5:2421:G:OP2	3:L5:2828:U:H1'	2.20	0.41
3:L5:2491:C:H2'	3:L5:2492:C:C6	2.55	0.41
3:L5:3951:G:H21	3:L5:4062:A:N6	2.18	0.41
3:L5:4095:G:H2'	3:L5:4096:C:C5	2.55	0.41
5:L8:106:G:H4'	5:L8:137:A:H5'	2.01	0.41
6:LA:132:ASN:O	6:LA:169:VAL:HG12	2.20	0.41
13:LH:137:SER:OG	13:LH:143:GLU:HB3	2.20	0.41
17:LM:139:SER:HA	17:LM:140:PRO:HD3	1.95	0.41
25:LU:19:LEU:HD23	25:LU:19:LEU:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LU:86:LEU:HD23	25:LU:86:LEU:HA	1.88	0.41
31:La:36:GLY:HA3	31:La:40:HIS:CE1	2.55	0.41
55:SH:172:THR:O	55:SH:176:VAL:HG12	2.20	0.41
68:S2:639:C:H2'	68:S2:640:A:C8	2.56	0.41
68:S2:1541:G:H2'	68:S2:1542:C:C6	2.55	0.41
68:S2:1597:C:H4'	68:S2:1603:G:O6	2.20	0.41
68:S2:1603:G:H4'	76:SS:38:ARG:NH2	2.36	0.41
68:S2:1616:U:H2'	68:S2:1617:G:C8	2.55	0.41
83:Sg:120:ILE:O	83:Sg:131:LEU:HD12	2.20	0.41
83:Sg:152:SER:HB2	83:Sg:170:TRP:HD1	1.83	0.41
3:L5:272:U:H2'	3:L5:273:U:C6	2.55	0.41
3:L5:2726:G:H2'	3:L5:2727:C:C6	2.56	0.41
6:LA:225:ILE:HG12	6:LA:234:LYS:HA	2.03	0.41
7:LB:348:ARG:HG2	7:LB:349:LYS:O	2.21	0.41
8:LC:159:GLU:HA	8:LC:217:ILE:HB	2.02	0.41
9:LD:62:CYS:HB3	9:LD:105:LEU:HD22	2.02	0.41
16:LL:210:LYS:HD3	16:LL:210:LYS:HA	1.89	0.41
53:SE:186:GLY:HA3	68:S2:809:A:OP1	2.21	0.41
54:SG:174:PRO:HB3	68:S2:65:C:C6	2.56	0.41
54:SG:228:ILE:HA	54:SG:231:ARG:HG2	2.02	0.41
65:Sa:44:ILE:HD13	65:Sa:67:LEU:HG	2.02	0.41
68:S2:116:OMU:O5'	68:S2:116:OMU:H6	2.20	0.41
68:S2:696:G:H21	68:S2:737:G:N2	2.18	0.41
68:S2:1101:U:H2'	68:S2:1102:G:C8	2.55	0.41
68:S2:1291:A:H62	82:Sf:95:ARG:HH12	1.69	0.41
68:S2:1383:A2M:HM'3	68:S2:1383:A2M:H1'	1.87	0.41
82:Sf:89:LYS:HE2	82:Sf:89:LYS:HB3	1.90	0.41
85:CB:313:ALA:O	85:CB:317:GLU:HG2	2.21	0.41
85:CB:687:THR:HG22	85:CB:697:MET:HE2	2.01	0.41
3:L5:398:A2M:O5'	3:L5:398:A2M:H8	2.20	0.41
3:L5:1307:A:H2'	3:L5:1308:C:H6	1.86	0.41
3:L5:3841:OMC:HM23	3:L5:3841:OMC:H1'	1.86	0.41
3:L5:4743:G:H2'	3:L5:4744:A:C8	2.56	0.41
3:L5:4775:C:H41	3:L5:4859:C:N4	2.10	0.41
7:LB:36:ASP:HA	7:LB:37:PRO:HD3	1.94	0.41
14:LI:51:HIS:CD2	14:LI:168:SER:HB3	2.55	0.41
27:LW:2:LYS:HE2	27:LW:15:PRO:HB3	2.02	0.41
28:LX:129:ARG:HE	28:LX:133:GLU:HB2	1.86	0.41
41:Lk:14:THR:HA	41:Lk:17:ARG:HD3	2.01	0.41
59:SN:139:TRP:CZ2	59:SN:149:LEU:HD21	2.55	0.41
60:SO:95:ILE:HD12	60:SO:126:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:378:U:H2'	68:S2:379:C:C6	2.56	0.41
68:S2:391:C:H2'	68:S2:392:A:H8	1.85	0.41
68:S2:434:G:H2'	68:S2:435:A:C8	2.56	0.41
68:S2:644:OMG:HM23	68:S2:644:OMG:H1'	1.80	0.41
71:SF:81:ARG:HG3	71:SF:82:ASN:OD1	2.21	0.41
73:SM:124:ILE:HD13	73:SM:124:ILE:HA	1.92	0.41
76:SS:102:GLY:HA2	76:SS:105:ASN:ND2	2.36	0.41
78:SU:49:LYS:HE3	78:SU:49:LYS:HB2	1.90	0.41
83:Sg:76:GLN:OE1	83:Sg:91:ASP:HB2	2.21	0.41
85:CB:265:TYR:HA	85:CB:287:ARG:HA	2.03	0.41
3:L5:1092:G:H2'	3:L5:1093:C:C6	2.56	0.41
3:L5:1341:U:H2'	3:L5:1342:A:C8	2.56	0.41
3:L5:1703:C:H2'	3:L5:1704:C:O4'	2.21	0.41
3:L5:2490:U:H3'	3:L5:2491:C:C6	2.56	0.41
3:L5:2696:A:H5'	41:Lk:70:LYS:HE2	2.03	0.41
3:L5:2764:A:H2'	3:L5:2765:A:H8	1.84	0.41
3:L5:3867:A2M:HM'3	3:L5:3880:G:N2	2.35	0.41
3:L5:4220:6MZ:H2'	3:L5:4222:G:H5''	2.02	0.41
3:L5:4530:UR3:H2'	3:L5:4531:U:H2'	2.02	0.41
3:L5:5025:C:H42	3:L5:5027:C:H42	1.67	0.41
4:L7:3:C:H2'	4:L7:4:U:H6	1.86	0.41
9:LD:126:THR:HA	9:LD:196:ARG:HG3	2.02	0.41
10:LE:222:LEU:H	10:LE:237:LYS:NZ	2.19	0.41
10:LE:264:ILE:HA	10:LE:265:PRO:HD3	1.94	0.41
14:LI:87:MET:HB2	14:LI:87:MET:HE3	1.77	0.41
30:LZ:73:LYS:HE3	30:LZ:73:LYS:HB3	1.75	0.41
31:La:2:PRO:HG2	31:La:5:LEU:HD12	2.03	0.41
34:Ld:33:ILE:HD13	34:Ld:33:ILE:HA	1.80	0.41
45:Lo:24:THR:HA	45:Lo:93:LEU:HD21	2.02	0.41
49:Lt:151:ILE:O	49:Lt:155:ILE:HB	2.20	0.41
53:SE:248:ILE:HA	53:SE:251:GLU:OE2	2.20	0.41
54:SG:223:LYS:HA	54:SG:223:LYS:HD2	1.88	0.41
56:SI:198:TYR:O	56:SI:202:ILE:HG12	2.20	0.41
68:S2:323:C:H5'	68:S2:324:C:OP1	2.21	0.41
68:S2:917:U:H2'	68:S2:918:U:C6	2.54	0.41
68:S2:1330:G:H4'	68:S2:1331:C:H3'	2.02	0.41
68:S2:1448:A:H2'	68:S2:1449:G:O4'	2.20	0.41
68:S2:1453:C:O2'	69:SR:52:GLY:HA3	2.21	0.41
68:S2:1709:G:H1	68:S2:1824:A:N6	2.19	0.41
83:Sg:107:ASP:HB2	83:Sg:125:ARG:HD2	2.02	0.41
83:Sg:155:ARG:NH1	83:Sg:200:VAL:H	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:CB:305:MET:HE1	85:CB:333:LYS:HA	2.02	0.41
3:L5:2335:C:H2'	3:L5:2336:G:H8	1.86	0.41
3:L5:2709:C:N4	86:CA:256:GLY:HA2	2.36	0.41
3:L5:3664:G:H2'	3:L5:3665:G:C8	2.55	0.41
3:L5:3771:C:H2'	3:L5:3772:U:C6	2.56	0.41
3:L5:4892:A:H2'	3:L5:4893:A:O4'	2.21	0.41
4:L7:23:A:H2'	4:L7:24:C:C6	2.56	0.41
8:LC:106:LYS:HD3	8:LC:108:TRP:CZ2	2.55	0.41
30:LZ:95:VAL:HG12	30:LZ:110:ALA:HA	2.03	0.41
42:Ll:12:PHE:HE2	42:Ll:51:LEU:HD22	1.85	0.41
47:Lr:47:LYS:HB2	47:Lr:102:TYR:CZ	2.56	0.41
50:SA:73:ASP:HB3	50:SA:120:ARG:HB2	2.03	0.41
53:SE:182:MET:HE2	53:SE:192:ILE:HD11	2.02	0.41
56:SI:114:GLU:HB3	56:SI:136:ILE:HD12	2.03	0.41
59:SN:5:HIS:HD1	59:SN:121:ARG:HH11	1.69	0.41
61:SV:16:LYS:HG2	61:SV:23:ILE:HD13	2.03	0.41
65:Sa:10:ARG:HB2	65:Sa:33:ASP:OD2	2.20	0.41
78:SU:55:ARG:HG2	78:SU:87:ARG:HD3	2.01	0.41
84:Et:2:C:H2'	84:Et:3:C:H6	1.86	0.41
85:CB:9:ILE:O	85:CB:13:MET:HB2	2.21	0.41
3:L5:348:G:O4'	8:LC:50:GLN:HG3	2.21	0.41
3:L5:457:G:H2'	3:L5:458:C:H6	1.83	0.41
3:L5:497:G:H21	3:L5:498:C:H41	1.66	0.41
3:L5:1190:C:H2'	3:L5:1191:C:H6	1.86	0.41
3:L5:1340:OMC:HM23	3:L5:1340:OMC:H1'	1.77	0.41
3:L5:1431:C:H2'	3:L5:1432:G:O4'	2.21	0.41
3:L5:1479:G:O2'	3:L5:1480:C:H5'	2.21	0.41
3:L5:1538:U:H2'	3:L5:1539:G:H8	1.86	0.41
3:L5:1762:C:H41	3:L5:1770:A:H2	1.68	0.41
3:L5:1895:G:H2'	3:L5:1896:A:O4'	2.21	0.41
3:L5:2254:G:H4'	3:L5:2255:C:C5	2.56	0.41
3:L5:3952:A:H2'	3:L5:3953:G:N9	2.36	0.41
3:L5:5029:C:HO2'	3:L5:5030:U:H6	1.69	0.41
4:L7:75:G:H5''	23:LS:49:SER:O	2.21	0.41
6:LA:20:VAL:HA	6:LA:23:ARG:HG3	2.01	0.41
6:LA:131:GLY:H	6:LA:169:VAL:HG13	1.86	0.41
8:LC:326:LEU:HD23	8:LC:326:LEU:HA	1.85	0.41
9:LD:53:VAL:HG11	9:LD:159:VAL:HA	2.02	0.41
9:LD:238:GLU:O	9:LD:242:LYS:HG2	2.20	0.41
35:Le:88:LEU:HB2	35:Le:120:ILE:HD13	2.02	0.41
49:Lt:16:ARG:HH22	49:Lt:28:LEU:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SA:127:PRO:HB2	50:SA:153:PRO:HD2	2.03	0.41
51:SB:113:MET:HB3	51:SB:142:PHE:CE2	2.56	0.41
51:SB:113:MET:SD	51:SB:209:ASP:HB3	2.61	0.41
51:SB:152:LYS:HD3	69:SR:133:GLY:HA3	2.03	0.41
54:SG:218:LYS:HB3	54:SG:218:LYS:HE3	1.84	0.41
58:SL:105:ARG:HG3	63:SX:11:ARG:HH22	1.84	0.41
59:SN:14:SER:HB2	68:S2:1016:U:H5''	2.02	0.41
60:SO:47:LEU:HD23	60:SO:47:LEU:HA	1.93	0.41
60:SO:72:TYR:O	60:SO:75:MET:HG3	2.21	0.41
68:S2:28:U:H2'	68:S2:29:G:C8	2.53	0.41
68:S2:194:C:H2'	68:S2:195:C:H6	1.85	0.41
68:S2:1217:A:H2'	68:S2:1218:C:H6	1.85	0.41
70:SD:133:GLY:HA3	70:SD:156:LEU:O	2.21	0.41
76:SS:4:VAL:HA	79:SZ:50:PHE:O	2.21	0.41
82:Sf:108:VAL:HB	82:Sf:112:GLY:HA2	2.02	0.41
85:CB:56:PHE:HB3	85:CB:455:GLY:HA3	2.03	0.41
85:CB:743:PRO:O	85:CB:790:VAL:HG23	2.21	0.41
86:CA:325:LEU:HD12	86:CA:325:LEU:HA	1.88	0.41
2:CI:55:LEU:HD22	25:LU:99:TRP:CG	2.56	0.41
3:L5:138:G:H2'	3:L5:139:G:C8	2.54	0.41
3:L5:254:G:H8	3:L5:254:G:O5'	2.04	0.41
3:L5:1510:G:H2'	3:L5:1511:U:C6	2.56	0.41
3:L5:1806:G:H2'	3:L5:1807:C:H6	1.85	0.41
3:L5:2870:A:H2'	3:L5:2871:A:C8	2.56	0.41
3:L5:3932:U:H2'	3:L5:3933:G:H8	1.84	0.41
3:L5:4236:G:H4'	3:L5:4328:G:O2'	2.20	0.41
3:L5:4741:C:H3'	3:L5:4900:C:N3	2.35	0.41
4:L7:4:U:H2'	4:L7:5:A:H8	1.86	0.41
7:LB:47:LEU:HD23	7:LB:47:LEU:HA	1.92	0.41
10:LE:183:ARG:HD2	10:LE:183:ARG:HA	1.73	0.41
21:LQ:27:LEU:HD23	21:LQ:27:LEU:HA	1.95	0.41
27:LW:93:LYS:HA	27:LW:96:GLN:HG3	2.02	0.41
42:Ll:11:ARG:HE	42:Ll:11:ARG:HB3	1.65	0.41
51:SB:24:PRO:HG2	68:S2:953:C:H5''	2.03	0.41
51:SB:35:ALA:HB2	51:SB:44:ILE:HD11	2.02	0.41
58:SL:22:ARG:HB3	58:SL:28:THR:HG22	2.03	0.41
63:SX:17:ARG:NH1	68:S2:658:U:H1'	2.36	0.41
68:S2:639:C:H2'	68:S2:640:A:H8	1.86	0.41
68:S2:1354:G:H2'	68:S2:1356:G:H22	1.82	0.41
68:S2:1560:U:H2'	68:S2:1561:A:H8	1.86	0.41
81:Sd:21:CYS:SG	81:Sd:39:CYS:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Sf:141:CYS:HB2	82:Sf:145:CYS:HB2	1.87	0.41
83:Sg:11:LEU:HB3	83:Sg:43:TRP:CZ3	2.56	0.41
83:Sg:34:ALA:HB1	83:Sg:66:VAL:HG13	2.03	0.41
85:CB:692:LEU:HD22	85:CB:848:ILE:HD13	2.03	0.41
85:CB:820:LEU:HD23	85:CB:831:PRO:HB3	2.03	0.41
3:L5:1494:U:H2'	3:L5:1495:G:H8	1.85	0.40
3:L5:1980:U:O2'	3:L5:1981:G:H5''	2.21	0.40
3:L5:2323:C:H2'	3:L5:2324:C:C6	2.56	0.40
3:L5:4872:G:C2	19:LO:203:VAL:HG23	2.55	0.40
3:L5:4957:C:H2'	3:L5:4958:C:C6	2.56	0.40
3:L5:5027:C:H2'	56:SI:170:LYS:HZ1	1.87	0.40
4:L7:3:C:H2'	4:L7:4:U:C6	2.56	0.40
12:LG:207:VAL:HG13	12:LG:212:LYS:HG2	2.02	0.40
31:La:71:PRO:HG2	31:La:108:TYR:HA	2.03	0.40
36:Lf:48:ALA:HB2	36:Lf:71:TRP:CZ3	2.56	0.40
53:SE:45:ILE:HD12	53:SE:80:ILE:HD11	2.03	0.40
54:SG:16:ILE:HD13	54:SG:16:ILE:HA	1.93	0.40
61:SV:51:LYS:HE2	61:SV:51:LYS:HB2	1.87	0.40
68:S2:116:OMU:HM23	68:S2:116:OMU:H1'	1.92	0.40
68:S2:857:U:H2'	68:S2:858:A:C8	2.55	0.40
68:S2:1289:U:C5	82:Sf:97:LYS:HE2	2.57	0.40
68:S2:1339:U:H2'	68:S2:1340:U:C6	2.56	0.40
68:S2:1470:C:H2'	68:S2:1471:C:C6	2.57	0.40
68:S2:1630:A:H5'	76:SS:37:GLY:N	2.36	0.40
69:SR:57:LEU:O	69:SR:61:ILE:HG23	2.21	0.40
70:SD:25:LEU:HD23	70:SD:25:LEU:HA	1.88	0.40
73:SM:99:LYS:HG3	73:SM:101:ARG:H	1.86	0.40
75:SQ:13:PHE:HE1	75:SQ:15:ARG:HE	1.68	0.40
78:SU:67:LYS:HB2	78:SU:76:THR:HG23	2.03	0.40
83:Sg:42:MET:HG2	83:Sg:57:ARG:HB3	2.03	0.40
83:Sg:57:ARG:HH12	83:Sg:94:THR:C	2.28	0.40
83:Sg:181:ASN:ND2	83:Sg:183:LYS:HB3	2.36	0.40
84:Et:14:A:H2'	84:Et:15:G:O4'	2.20	0.40
85:CB:214:PHE:HB2	85:CB:223:PHE:CE1	2.56	0.40
86:CA:224:TYR:HB3	86:CA:226:VAL:HG13	2.03	0.40
3:L5:128:C:H2'	3:L5:129:C:C6	2.56	0.40
3:L5:173:C:H2'	3:L5:174:C:C6	2.56	0.40
3:L5:253:G:H2'	3:L5:254:G:C8	2.56	0.40
3:L5:1081:C:O2'	3:L5:1082:C:H5'	2.20	0.40
3:L5:1914:C:H4'	19:LO:89:PRO:HD3	2.03	0.40
3:L5:2461:G:H2'	3:L5:2462:C:C6	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3887:OMC:O2	88:L5:5294:SPM:H71	2.21	0.40
17:LM:33:GLN:HB2	23:LS:145:PHE:HZ	1.86	0.40
27:LW:104:GLN:O	27:LW:107:GLN:HG3	2.20	0.40
53:SE:57:THR:HG21	68:S2:494:C:H5''	2.02	0.40
55:SH:142:LYS:HB3	62:SW:54:ASP:HB3	2.03	0.40
58:SL:93:LEU:HB3	58:SL:102:PHE:HB3	2.02	0.40
68:S2:531:A:N6	68:S2:554:A:H61	2.19	0.40
68:S2:564:A:H2'	68:S2:565:G:O4'	2.21	0.40
68:S2:1621:U:O2'	68:S2:1622:U:H2'	2.21	0.40
71:SF:122:ARG:HE	80:Sc:59:LEU:HD21	1.86	0.40
71:SF:204:ARG:HH21	80:Sc:63:ARG:HH12	1.68	0.40
74:SP:56:LEU:HD22	74:SP:80:LEU:HD11	2.04	0.40
75:SQ:84:ILE:HA	75:SQ:84:ILE:HD13	1.85	0.40
80:Sc:44:ARG:HD2	80:Sc:44:ARG:HA	1.88	0.40
85:CB:50:ARG:HG2	85:CB:52:GLY:H	1.86	0.40
85:CB:189:ILE:HD11	85:CB:204:MET:HA	2.03	0.40
3:L5:223:G:H4'	3:L5:225:G:C8	2.57	0.40
3:L5:677:G:H2'	3:L5:678:C:C6	2.56	0.40
3:L5:937:U:C6	17:LM:46:ARG:HD2	2.57	0.40
3:L5:2385:U:H2'	3:L5:2386:U:C6	2.56	0.40
3:L5:2464:C:HO2'	3:L5:2465:C:H6	1.64	0.40
3:L5:4291:G:H5'	3:L5:4293:PSU:C6	2.56	0.40
17:LM:100:ARG:HD3	19:LO:198:THR:O	2.21	0.40
18:LN:148:THR:O	18:LN:151:ILE:HG22	2.22	0.40
23:LS:83:ARG:HG3	23:LS:125:GLN:HB3	2.03	0.40
24:LT:44:GLY:HA2	24:LT:95:HIS:HB3	2.03	0.40
32:Lb:105:GLY:O	32:Lb:109:ARG:HG2	2.21	0.40
68:S2:27:A2M:HM'3	68:S2:27:A2M:H1'	1.87	0.40
68:S2:85:A:H2'	68:S2:86:C:C6	2.54	0.40
68:S2:159:A2M:O5'	68:S2:159:A2M:H8	2.21	0.40
68:S2:979:C:H2'	68:S2:980:A:C8	2.56	0.40
68:S2:1058:A:H2'	68:S2:1059:G:C8	2.56	0.40
68:S2:1174:PSU:H2'	68:S2:1175:G:H8	1.85	0.40
68:S2:1214:A:H2'	68:S2:1217:A:N7	2.36	0.40
68:S2:1542:C:H2'	68:S2:1543:U:O4'	2.22	0.40
71:SF:30:ILE:HG13	71:SF:113:VAL:HG11	2.03	0.40
71:SF:76:MET:HE1	71:SF:173:LEU:HD22	2.04	0.40
74:SP:75:VAL:HG22	74:SP:93:MET:HB3	2.04	0.40
3:L5:2374:A:H5'	34:Ld:64:ILE:O	2.21	0.40
3:L5:4627:U:H5''	7:LB:373:LYS:HG2	2.02	0.40
3:L5:4653:C:H2'	3:L5:4654:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:5003:U:H2'	3:L5:5004:C:C6	2.56	0.40
10:LE:244:GLU:O	10:LE:248:ILE:HG12	2.22	0.40
18:LN:146:PRO:HB2	38:Lh:104:THR:HG23	2.03	0.40
26:LV:65:VAL:HG22	26:LV:73:ARG:HA	2.03	0.40
36:Lf:78:HIS:O	36:Lf:83:MET:HB2	2.22	0.40
46:Lp:62:LYS:HE2	46:Lp:62:LYS:HB2	1.91	0.40
49:Lt:77:ALA:O	49:Lt:81:ILE:HG12	2.21	0.40
50:SA:158:ASP:O	61:SV:66:ASP:HA	2.21	0.40
51:SB:90:ASP:HB2	51:SB:228:LEU:HD23	2.04	0.40
55:SH:12:ASN:ND2	55:SH:14:GLU:H	2.19	0.40
63:SX:107:ARG:HG3	63:SX:110:HIS:HB3	2.03	0.40
68:S2:1238:U:O2	68:S2:1242:U:H5	2.04	0.40
68:S2:1408:U:H2'	68:S2:1409:A:C8	2.57	0.40
70:SD:219:PRO:HB2	83:Sg:192:THR:HG22	2.02	0.40
78:SU:40:ILE:O	78:SU:44:LYS:HG2	2.22	0.40
78:SU:81:GLN:HE21	78:SU:83:ARG:HE	1.69	0.40
79:SZ:50:PHE:HE1	79:SZ:79:ILE:HG21	1.85	0.40
80:Sc:11:LEU:HD23	80:Sc:57:THR:HA	2.03	0.40
83:Sg:230:LEU:HD22	83:Sg:259:TRP:CE2	2.56	0.40
85:CB:43:ALA:HB3	85:CB:77:LEU:HD12	2.03	0.40
1:CD:205:LYS:HD2	68:S2:1698:C:H5'	2.04	0.40
3:L5:976:G:H4'	8:LC:326:LEU:HD13	2.03	0.40
3:L5:1786:A:H2'	3:L5:1789:C:C5	2.57	0.40
3:L5:1847:C:H2'	3:L5:1848:C:C6	2.56	0.40
3:L5:2422:OMC:HM23	3:L5:2422:OMC:H1'	1.93	0.40
3:L5:2864:A:H2'	3:L5:2865:U:C6	2.56	0.40
10:LE:50:LEU:HD12	10:LE:51:VAL:N	2.36	0.40
10:LE:164:PHE:HA	10:LE:175:VAL:HG12	2.03	0.40
17:LM:135:LEU:HD12	17:LM:135:LEU:HA	1.97	0.40
18:LN:104:GLU:HA	18:LN:160:GLU:HG3	2.03	0.40
19:LO:12:ARG:HB2	19:LO:37:ARG:HD2	2.03	0.40
19:LO:76:PRO:HB3	19:LO:138:LEU:HG	2.04	0.40
53:SE:182:MET:HE3	53:SE:228:ILE:HD13	2.04	0.40
60:SO:45:THR:HA	60:SO:52:THR:HA	2.04	0.40
62:SW:62:VAL:HG11	66:Sb:8:LEU:HG	2.03	0.40
68:S2:24:C:O2'	68:S2:25:A:H8	2.05	0.40
68:S2:399:C:H5	68:S2:680:G:H5''	1.86	0.40
68:S2:1628:C:H2'	68:S2:1629:C:C6	2.56	0.40
68:S2:1751:C:H1'	68:S2:1784:G:N2	2.35	0.40
70:SD:1:MET:HB3	70:SD:2:ALA:H	1.79	0.40
76:SS:55:ARG:HA	76:SS:55:ARG:HD2	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
77:ST:51:ASN:HB3	77:ST:54:TYR:CD2	2.57	0.40
85:CB:365:GLN:HB2	85:CB:369:CYS:SG	2.61	0.40
85:CB:750:GLN:HG2	85:CB:783:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CD	51/408 (12%)	51 (100%)	0	0	100	100
2	CI	29/31 (94%)	29 (100%)	0	0	100	100
6	LA	246/248 (99%)	236 (96%)	10 (4%)	0	100	100
7	LB	400/402 (100%)	387 (97%)	13 (3%)	0	100	100
8	LC	366/368 (100%)	350 (96%)	16 (4%)	0	100	100
9	LD	291/293 (99%)	279 (96%)	12 (4%)	0	100	100
10	LE	236/250 (94%)	218 (92%)	18 (8%)	0	100	100
11	LF	223/225 (99%)	217 (97%)	6 (3%)	0	100	100
12	LG	239/241 (99%)	229 (96%)	9 (4%)	1 (0%)	30	49
13	LH	188/190 (99%)	182 (97%)	6 (3%)	0	100	100
14	LI	201/213 (94%)	201 (100%)	0	0	100	100
15	LJ	168/176 (96%)	163 (97%)	5 (3%)	0	100	100
16	LL	208/210 (99%)	201 (97%)	7 (3%)	0	100	100
17	LM	137/139 (99%)	134 (98%)	3 (2%)	0	100	100
18	LN	201/203 (99%)	197 (98%)	4 (2%)	0	100	100
19	LO	199/201 (99%)	198 (100%)	1 (0%)	0	100	100
20	LP	151/153 (99%)	144 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	LQ	185/187 (99%)	183 (99%)	2 (1%)	0	100	100
22	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
23	LS	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
24	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
25	LU	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
26	LV	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
27	LW	112/124 (90%)	111 (99%)	1 (1%)	0	100	100
28	LX	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
29	LY	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
30	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
31	La	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
32	Lb	105/121 (87%)	101 (96%)	4 (4%)	0	100	100
33	Lc	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
34	Ld	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
35	Le	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
36	Lf	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
37	Lg	112/114 (98%)	112 (100%)	0	0	100	100
38	Lh	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
39	Li	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
40	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
41	Lk	67/69 (97%)	67 (100%)	0	0	100	100
42	Ll	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
43	Lm	50/52 (96%)	50 (100%)	0	0	100	100
44	Ln	22/24 (92%)	22 (100%)	0	0	100	100
45	Lo	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
46	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
47	Lr	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
48	Ls	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
49	Lt	128/157 (82%)	105 (82%)	23 (18%)	0	100	100
50	SA	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
51	SB	212/214 (99%)	204 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	SC	218/222 (98%)	206 (94%)	12 (6%)	0	100	100
53	SE	260/262 (99%)	251 (96%)	9 (4%)	0	100	100
54	SG	235/237 (99%)	223 (95%)	12 (5%)	0	100	100
55	SH	182/189 (96%)	164 (90%)	18 (10%)	0	100	100
56	SI	204/206 (99%)	191 (94%)	13 (6%)	0	100	100
57	SJ	183/185 (99%)	174 (95%)	9 (5%)	0	100	100
58	SL	151/153 (99%)	139 (92%)	12 (8%)	0	100	100
59	SN	148/150 (99%)	144 (97%)	4 (3%)	0	100	100
60	SO	135/140 (96%)	129 (96%)	6 (4%)	0	100	100
61	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
62	SW	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
63	SX	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
64	SY	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
65	Sa	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
66	Sb	81/83 (98%)	73 (90%)	8 (10%)	0	100	100
67	Se	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
69	SR	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
70	SD	225/227 (99%)	221 (98%)	4 (2%)	0	100	100
71	SF	187/189 (99%)	179 (96%)	8 (4%)	0	100	100
72	SK	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
73	SM	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
74	SP	119/121 (98%)	117 (98%)	2 (2%)	0	100	100
75	SQ	142/144 (99%)	132 (93%)	10 (7%)	0	100	100
76	SS	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
77	ST	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
78	SU	102/104 (98%)	96 (94%)	6 (6%)	0	100	100
79	SZ	73/75 (97%)	67 (92%)	6 (8%)	0	100	100
80	Sc	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
81	Sd	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
82	Sf	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
83	Sg	311/313 (99%)	295 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
85	CB	842/856 (98%)	813 (97%)	29 (3%)	0	100	100
86	CA	350/356 (98%)	334 (95%)	16 (5%)	0	100	100
All	All	12905/13527 (95%)	12387 (96%)	517 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	LG	124	GLY

5.3.2 Protein sidechains [i](#)

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	CD	46/328 (14%)	46 (100%)	0	100	100
2	CI	25/25 (100%)	25 (100%)	0	100	100
6	LA	190/190 (100%)	189 (100%)	1 (0%)	81	91
7	LB	348/348 (100%)	348 (100%)	0	100	100
8	LC	306/306 (100%)	306 (100%)	0	100	100
9	LD	246/247 (100%)	246 (100%)	0	100	100
10	LE	212/222 (96%)	212 (100%)	0	100	100
11	LF	194/194 (100%)	194 (100%)	0	100	100
12	LG	203/205 (99%)	203 (100%)	0	100	100
13	LH	169/169 (100%)	169 (100%)	0	100	100
14	LI	175/180 (97%)	175 (100%)	0	100	100
15	LJ	143/148 (97%)	143 (100%)	0	100	100
16	LL	176/176 (100%)	176 (100%)	0	100	100
17	LM	118/118 (100%)	118 (100%)	0	100	100
18	LN	171/171 (100%)	171 (100%)	0	100	100
19	LO	173/173 (100%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	LP	134/134 (100%)	134 (100%)	0	100	100
21	LQ	164/164 (100%)	164 (100%)	0	100	100
22	LR	166/166 (100%)	166 (100%)	0	100	100
23	LS	156/156 (100%)	156 (100%)	0	100	100
24	LT	139/139 (100%)	139 (100%)	0	100	100
25	LU	91/91 (100%)	91 (100%)	0	100	100
26	LV	101/101 (100%)	101 (100%)	0	100	100
27	LW	95/103 (92%)	95 (100%)	0	100	100
28	LX	108/108 (100%)	108 (100%)	0	100	100
29	LY	124/124 (100%)	124 (100%)	0	100	100
30	LZ	117/117 (100%)	117 (100%)	0	100	100
31	La	120/120 (100%)	120 (100%)	0	100	100
32	Lb	88/101 (87%)	88 (100%)	0	100	100
33	Lc	83/83 (100%)	83 (100%)	0	100	100
34	Ld	98/98 (100%)	98 (100%)	0	100	100
35	Le	114/114 (100%)	114 (100%)	0	100	100
36	Lf	88/88 (100%)	88 (100%)	0	100	100
37	Lg	98/98 (100%)	98 (100%)	0	100	100
38	Lh	109/109 (100%)	109 (100%)	0	100	100
39	Li	86/86 (100%)	86 (100%)	0	100	100
40	Lj	73/73 (100%)	73 (100%)	0	100	100
41	Lk	64/64 (100%)	64 (100%)	0	100	100
42	Ll	47/47 (100%)	47 (100%)	0	100	100
43	Lm	48/48 (100%)	48 (100%)	0	100	100
44	Ln	23/23 (100%)	23 (100%)	0	100	100
45	Lo	93/93 (100%)	93 (100%)	0	100	100
46	Lp	74/74 (100%)	74 (100%)	0	100	100
47	Lr	109/109 (100%)	109 (100%)	0	100	100
48	Ls	162/164 (99%)	162 (100%)	0	100	100
49	Lt	107/130 (82%)	107 (100%)	0	100	100
50	SA	183/183 (100%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	SB	195/195 (100%)	195 (100%)	0	100	100
52	SC	186/188 (99%)	186 (100%)	0	100	100
53	SE	224/224 (100%)	224 (100%)	0	100	100
54	SG	207/207 (100%)	207 (100%)	0	100	100
55	SH	166/169 (98%)	166 (100%)	0	100	100
56	SI	178/178 (100%)	178 (100%)	0	100	100
57	SJ	161/161 (100%)	161 (100%)	0	100	100
58	SL	137/137 (100%)	137 (100%)	0	100	100
59	SN	130/130 (100%)	130 (100%)	0	100	100
60	SO	107/110 (97%)	107 (100%)	0	100	100
61	SV	67/67 (100%)	67 (100%)	0	100	100
62	SW	112/112 (100%)	112 (100%)	0	100	100
63	SX	113/113 (100%)	113 (100%)	0	100	100
64	SY	113/113 (100%)	113 (100%)	0	100	100
65	Sa	89/89 (100%)	89 (100%)	0	100	100
66	Sb	75/75 (100%)	75 (100%)	0	100	100
67	Se	47/47 (100%)	47 (100%)	0	100	100
69	SR	122/122 (100%)	121 (99%)	1 (1%)	73	87
70	SD	190/190 (100%)	190 (100%)	0	100	100
71	SF	159/159 (100%)	159 (100%)	0	100	100
72	SK	89/89 (100%)	89 (100%)	0	100	100
73	SM	102/104 (98%)	102 (100%)	0	100	100
74	SP	107/107 (100%)	107 (100%)	0	100	100
75	SQ	119/119 (100%)	119 (100%)	0	100	100
76	SS	126/126 (100%)	126 (100%)	0	100	100
77	ST	113/113 (100%)	113 (100%)	0	100	100
78	SU	94/94 (100%)	94 (100%)	0	100	100
79	SZ	66/66 (100%)	66 (100%)	0	100	100
80	Sc	57/57 (100%)	57 (100%)	0	100	100
81	Sd	48/48 (100%)	48 (100%)	0	100	100
82	Sf	60/60 (100%)	60 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
83	Sg	272/272 (100%)	272 (100%)	0	100	100
85	CB	722/728 (99%)	722 (100%)	0	100	100
86	CA	303/305 (99%)	303 (100%)	0	100	100
All	All	11213/11582 (97%)	11211 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	LA	208	GLU
69	SR	76	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	CD	206	HIS
6	LA	140	ASN
7	LB	68	ASN
7	LB	184	GLN
7	LB	208	ASN
8	LC	286	ASN
8	LC	329	ASN
9	LD	225	GLN
9	LD	229	ASN
10	LE	182	ASN
10	LE	266	GLN
11	LF	80	ASN
12	LG	225	ASN
13	LH	102	ASN
13	LH	138	GLN
13	LH	188	GLN
13	LH	189	GLN
14	LI	59	GLN
14	LI	73	ASN
14	LI	147	HIS
15	LJ	23	ASN
15	LJ	65	ASN
17	LM	20	HIS
17	LM	34	ASN
17	LM	125	ASN
18	LN	8	GLN

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Mol	Chain	Res	Type
18	LN	199	GLN
19	LO	26	GLN
19	LO	180	GLN
20	LP	21	ASN
20	LP	34	GLN
21	LQ	44	ASN
21	LQ	57	ASN
23	LS	108	GLN
24	LT	131	GLN
25	LU	50	ASN
26	LV	135	ASN
31	La	34	ASN
31	La	60	HIS
32	Lb	6	ASN
32	Lb	11	ASN
32	Lb	27	GLN
32	Lb	60	ASN
35	Le	52	GLN
36	Lf	20	ASN
36	Lf	21	GLN
38	Lh	107	GLN
39	Li	15	HIS
40	Lj	66	HIS
42	Ll	33	ASN
43	Lm	87	GLN
44	Ln	22	GLN
47	Lr	4	HIS
47	Lr	30	ASN
48	Ls	179	ASN
48	Ls	190	GLN
50	SA	84	GLN
50	SA	132	GLN
51	SB	159	GLN
51	SB	179	ASN
54	SG	81	HIS
54	SG	105	ASN
55	SH	162	GLN
55	SH	168	HIS
55	SH	186	ASN
56	SI	52	ASN
57	SJ	134	HIS
57	SJ	140	GLN

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Mol	Chain	Res	Type
57	SJ	154	GLN
58	SL	11	GLN
58	SL	39	ASN
58	SL	100	ASN
59	SN	13	GLN
63	SX	16	HIS
64	SY	89	HIS
65	Sa	80	HIS
67	Se	39	ASN
69	SR	83	ASN
69	SR	116	ASN
70	SD	165	ASN
72	SK	66	HIS
73	SM	55	ASN
73	SM	119	GLN
74	SP	103	ASN
76	SS	11	HIS
77	ST	10	ASN
79	SZ	112	ASN
83	Sg	117	ASN
85	CB	8	GLN
85	CB	108	HIS
85	CB	168	GLN
85	CB	202	ASN
85	CB	227	GLN
85	CB	357	HIS
85	CB	565	HIS
85	CB	715	HIS
85	CB	803	ASN
86	CA	10	GLN
86	CA	189	GLN
86	CA	192	GLN
86	CA	318	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3643/5070 (71%)	740 (20%)	18 (0%)
4	L7	119/120 (99%)	11 (9%)	0
5	L8	155/156 (99%)	26 (16%)	0
68	S2	1715/1740 (98%)	392 (22%)	5 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
84	Et	73/75 (97%)	30 (41%)	0
All	All	5705/7161 (79%)	1199 (21%)	23 (0%)

All (1199) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L5	25	A
3	L5	30	C
3	L5	39	A
3	L5	42	A
3	L5	48	G
3	L5	56	A
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	66	A
3	L5	73	A
3	L5	91	G
3	L5	104	G
3	L5	108	A
3	L5	109	G
3	L5	110	C
3	L5	119	G
3	L5	120	A
3	L5	132	G
3	L5	133	C
3	L5	134	G
3	L5	135	G
3	L5	136	C
3	L5	139	G
3	L5	159	C
3	L5	165	A
3	L5	172	C
3	L5	181	C
3	L5	182	G
3	L5	183	C
3	L5	184	U
3	L5	185	C
3	L5	186	G
3	L5	188	G
3	L5	189	G
3	L5	200	U

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Mol	Chain	Res	Type
3	L5	209	U
3	L5	210	C
3	L5	216	C
3	L5	218	A
3	L5	220	C
3	L5	237	G
3	L5	254	G
3	L5	255	C
3	L5	256	G
3	L5	261	G
3	L5	263	G
3	L5	264	C
3	L5	265	C
3	L5	266	C
3	L5	267	G
3	L5	275	C
3	L5	280	G
3	L5	297	U
3	L5	306	A
3	L5	315	G
3	L5	316	U
3	L5	326	C
3	L5	340	C
3	L5	373	G
3	L5	385	A
3	L5	387	G
3	L5	388	A
3	L5	407	A
3	L5	409	G
3	L5	410	A
3	L5	411	G
3	L5	412	G
3	L5	413	G
3	L5	432	U
3	L5	440	U
3	L5	449	C
3	L5	452	A
3	L5	453	G
3	L5	454	U
3	L5	456	C
3	L5	457	G
3	L5	467	U

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Mol	Chain	Res	Type
3	L5	468	U
3	L5	479	G
3	L5	484	U
3	L5	485	C
3	L5	486	C
3	L5	489	C
3	L5	494	U
3	L5	496	G
3	L5	497	G
3	L5	498	C
3	L5	499	G
3	L5	502	C
3	L5	503	C
3	L5	504	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	518	G
3	L5	519	C
3	L5	643	C
3	L5	644	G
3	L5	654	C
3	L5	655	C
3	L5	657	C
3	L5	659	G
3	L5	665	C
3	L5	667	A
3	L5	668	C
3	L5	669	C
3	L5	673	C
3	L5	685	C
3	L5	686	A
3	L5	687	U
3	L5	696	C
3	L5	704	C
3	L5	708	G
3	L5	730	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	746	A
3	L5	759	G
3	L5	904	C
3	L5	905	C
3	L5	913	U
3	L5	914	U
3	L5	915	A
3	L5	917	A
3	L5	923	C
3	L5	924	C
3	L5	926	G
3	L5	932	A
3	L5	933	G
3	L5	935	A
3	L5	936	C
3	L5	942	G
3	L5	943	A
3	L5	945	U
3	L5	946	C
3	L5	958	G
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	965	G
3	L5	966	A
3	L5	967	C
3	L5	968	C
3	L5	969	C
3	L5	970	G
3	L5	977	C
3	L5	982	U
3	L5	985	C
3	L5	989	U
3	L5	1066	G
3	L5	1070	G
3	L5	1072	C
3	L5	1075	G
3	L5	1082	C
3	L5	1083	U

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Mol	Chain	Res	Type
3	L5	1095	A
3	L5	1168	G
3	L5	1171	G
3	L5	1172	C
3	L5	1173	G
3	L5	1179	U
3	L5	1180	C
3	L5	1181	C
3	L5	1182	C
3	L5	1183	C
3	L5	1187	G
3	L5	1202	C
3	L5	1203	G
3	L5	1210	C
3	L5	1211	G
3	L5	1214	C
3	L5	1215	C
3	L5	1216	C
3	L5	1218	G
3	L5	1219	G
3	L5	1222	A
3	L5	1241	C
3	L5	1242	G
3	L5	1253	G
3	L5	1254	A
3	L5	1257	A
3	L5	1258	G
3	L5	1266	G
3	L5	1267	C
3	L5	1269	G
3	L5	1270	A
3	L5	1271	G
3	L5	1272	C
3	L5	1273	G
3	L5	1275	G
3	L5	1277	G
3	L5	1280	C
3	L5	1284	G
3	L5	1285	U
3	L5	1287	G
3	L5	1293	G
3	L5	1294	A

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Mol	Chain	Res	Type
3	L5	1295	C
3	L5	1296	G
3	L5	1301	C
3	L5	1326	A2M
3	L5	1337	A
3	L5	1354	A
3	L5	1359	G
3	L5	1365	C
3	L5	1366	G
3	L5	1381	U
3	L5	1387	A
3	L5	1394	G
3	L5	1397	A
3	L5	1398	A
3	L5	1404	G
3	L5	1407	C
3	L5	1408	G
3	L5	1409	C
3	L5	1410	U
3	L5	1415	G
3	L5	1416	G
3	L5	1417	C
3	L5	1418	C
3	L5	1420	A
3	L5	1437	C
3	L5	1439	C
3	L5	1442	C
3	L5	1443	A
3	L5	1444	G
3	L5	1446	C
3	L5	1447	C
3	L5	1480	C
3	L5	1483	C
3	L5	1497	A
3	L5	1498	G
3	L5	1502	G
3	L5	1517	G
3	L5	1524	A2M
3	L5	1534	A2M
3	L5	1535	C
3	L5	1537	A
3	L5	1547	A

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Mol	Chain	Res	Type
3	L5	1552	G
3	L5	1566	C
3	L5	1574	G
3	L5	1578	U
3	L5	1586	G
3	L5	1587	G
3	L5	1591	U
3	L5	1596	U
3	L5	1613	A
3	L5	1621	A
3	L5	1624	G
3	L5	1625	OMG
3	L5	1626	G
3	L5	1631	A
3	L5	1633	G
3	L5	1634	A
3	L5	1638	A
3	L5	1640	C
3	L5	1641	G
3	L5	1642	A
3	L5	1654	G
3	L5	1661	C
3	L5	1676	C
3	L5	1677	PSU
3	L5	1697	G
3	L5	1698	C
3	L5	1699	A
3	L5	1700	G
3	L5	1702	C
3	L5	1704	C
3	L5	1705	G
3	L5	1717	C
3	L5	1718	C
3	L5	1719	A
3	L5	1721	G
3	L5	1731	C
3	L5	1734	G
3	L5	1740	C
3	L5	1741	G
3	L5	1742	A
3	L5	1757	U
3	L5	1760	G

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Mol	Chain	Res	Type
3	L5	1761	G
3	L5	1762	C
3	L5	1763	C
3	L5	1764	G
3	L5	1765	A
3	L5	1766	A
3	L5	1767	A
3	L5	1768	C
3	L5	1770	A
3	L5	1787	A
3	L5	1804	A
3	L5	1806	G
3	L5	1810	G
3	L5	1821	G
3	L5	1834	U
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1855	G
3	L5	1869	G
3	L5	1882	U
3	L5	1892	A
3	L5	1893	C
3	L5	1897	A
3	L5	1917	A
3	L5	1918	U
3	L5	1919	G
3	L5	1920	C
3	L5	1921	C
3	L5	1922	G
3	L5	1925	G
3	L5	1930	U
3	L5	1931	C
3	L5	1932	A
3	L5	1936	C
3	L5	1948	G
3	L5	1962	A
3	L5	1974	U
3	L5	1975	G
3	L5	1978	C
3	L5	1980	U
3	L5	1981	G

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Mol	Chain	Res	Type
3	L5	1982	G
3	L5	1984	A
3	L5	1985	G
3	L5	1991	A
3	L5	1992	U
3	L5	1993	C
3	L5	1997	U
3	L5	2002	A
3	L5	2003	G
3	L5	2005	G
3	L5	2011	C
3	L5	2024	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	2092	G
3	L5	2093	A
3	L5	2095	A
3	L5	2097	U
3	L5	2098	G
3	L5	2101	C
3	L5	2102	G
3	L5	2103	G
3	L5	2107	C
3	L5	2112	G
3	L5	2250	C
3	L5	2252	G
3	L5	2253	A
3	L5	2254	G
3	L5	2256	C
3	L5	2258	C
3	L5	2259	G
3	L5	2269	C
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2306	G

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Mol	Chain	Res	Type
3	L5	2313	A
3	L5	2333	G
3	L5	2345	G
3	L5	2348	G
3	L5	2351	OMC
3	L5	2360	A
3	L5	2364	OMG
3	L5	2383	C
3	L5	2389	A
3	L5	2395	A
3	L5	2397	G
3	L5	2411	C
3	L5	2417	A
3	L5	2425	U
3	L5	2450	G
3	L5	2453	A
3	L5	2464	C
3	L5	2465	C
3	L5	2469	C
3	L5	2471	G
3	L5	2474	G
3	L5	2475	G
3	L5	2478	C
3	L5	2479	G
3	L5	2483	G
3	L5	2484	A
3	L5	2485	U
3	L5	2487	G
3	L5	2488	C
3	L5	2489	C
3	L5	2490	U
3	L5	2491	C
3	L5	2494	U
3	L5	2504	C
3	L5	2505	C
3	L5	2506	G
3	L5	2513	A
3	L5	2514	G
3	L5	2518	G
3	L5	2519	U
3	L5	2520	C
3	L5	2537	A

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Mol	Chain	Res	Type
3	L5	2544	G
3	L5	2546	G
3	L5	2547	G
3	L5	2554	U
3	L5	2555	G
3	L5	2559	G
3	L5	2560	C
3	L5	2565	A
3	L5	2573	A
3	L5	2583	C
3	L5	2587	A
3	L5	2589	C
3	L5	2591	A
3	L5	2606	G
3	L5	2611	A
3	L5	2618	G
3	L5	2627	C
3	L5	2638	G
3	L5	2653	C
3	L5	2662	G
3	L5	2669	C
3	L5	2675	G
3	L5	2676	A
3	L5	2687	U
3	L5	2694	G
3	L5	2695	A
3	L5	2696	A
3	L5	2702	C
3	L5	2703	G
3	L5	2707	U
3	L5	2708	U
3	L5	2709	C
3	L5	2710	C
3	L5	2711	G
3	L5	2712	G
3	L5	2721	G
3	L5	2724	G
3	L5	2726	G
3	L5	2739	C
3	L5	2742	G
3	L5	2743	A
3	L5	2746	A

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Mol	Chain	Res	Type
3	L5	2754	G
3	L5	2761	U
3	L5	2763	U
3	L5	2764	A
3	L5	2769	U
3	L5	2770	C
3	L5	2788	U
3	L5	2790	U
3	L5	2806	A
3	L5	2815	A2M
3	L5	2826	U
3	L5	2827	G
3	L5	2848	G
3	L5	2855	G
3	L5	2867	C
3	L5	2877	G
3	L5	2892	C
3	L5	2897	G
3	L5	2900	U
3	L5	2901	G
3	L5	2902	G
3	L5	2903	G
3	L5	2904	U
3	L5	2905	C
3	L5	2906	G
3	L5	2907	G
3	L5	2908	U
3	L5	3590	G
3	L5	3591	C
3	L5	3594	C
3	L5	3595	U
3	L5	3596	A
3	L5	3597	G
3	L5	3599	A
3	L5	3605	C
3	L5	3615	G
3	L5	3616	U
3	L5	3626	G
3	L5	3630	A
3	L5	3635	A
3	L5	3644	U
3	L5	3646	A

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Mol	Chain	Res	Type
3	L5	3648	A
3	L5	3662	A
3	L5	3664	G
3	L5	3670	C
3	L5	3673	C
3	L5	3674	G
3	L5	3701	OMC
3	L5	3710	G
3	L5	3711	A
3	L5	3713	U
3	L5	3727	A
3	L5	3756	A
3	L5	3764	U
3	L5	3770	U
3	L5	3775	A
3	L5	3776	G
3	L5	3777	G
3	L5	3785	A2M
3	L5	3786	U
3	L5	3792	OMG
3	L5	3811	G
3	L5	3814	U
3	L5	3817	A
3	L5	3819	G
3	L5	3824	A
3	L5	3827	G
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3867	A2M
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3880	G
3	L5	3885	G
3	L5	3890	A
3	L5	3892	U
3	L5	3897	G
3	L5	3901	A
3	L5	3906	A
3	L5	3907	G
3	L5	3908	A

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Mol	Chain	Res	Type
3	L5	3915	U
3	L5	3923	A
3	L5	3930	U
3	L5	3938	G
3	L5	3942	A
3	L5	3944	G
3	L5	3947	A
3	L5	3948	C
3	L5	3949	A
3	L5	3950	U
3	L5	3951	G
3	L5	3953	G
3	L5	4057	C
3	L5	4058	U
3	L5	4059	C
3	L5	4060	U
3	L5	4061	G
3	L5	4062	A
3	L5	4064	C
3	L5	4068	U
3	L5	4069	U
3	L5	4076	G
3	L5	4095	G
3	L5	4097	G
3	L5	4099	G
3	L5	4101	C
3	L5	4104	G
3	L5	4108	G
3	L5	4111	U
3	L5	4114	C
3	L5	4115	G
3	L5	4116	C
3	L5	4119	C
3	L5	4122	G
3	L5	4127	A
3	L5	4141	G
3	L5	4142	C
3	L5	4143	G
3	L5	4144	C
3	L5	4146	G
3	L5	4150	G
3	L5	4162	C

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Mol	Chain	Res	Type
3	L5	4163	U
3	L5	4170	A
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4201	G
3	L5	4203	A
3	L5	4220	6MZ
3	L5	4222	G
3	L5	4225	G
3	L5	4228	OMG
3	L5	4229	U
3	L5	4232	U
3	L5	4233	A
3	L5	4238	G
3	L5	4251	A
3	L5	4254	G
3	L5	4257	A
3	L5	4258	C
3	L5	4265	U
3	L5	4268	A
3	L5	4273	A
3	L5	4281	A
3	L5	4291	G
3	L5	4295	U
3	L5	4304	A
3	L5	4305	G
3	L5	4314	C
3	L5	4319	C
3	L5	4329	G
3	L5	4330	G
3	L5	4332	C
3	L5	4338	G
3	L5	4349	C
3	L5	4350	C
3	L5	4354	U
3	L5	4371	G
3	L5	4373	G
3	L5	4376	A
3	L5	4377	G
3	L5	4378	A
3	L5	4379	A

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Mol	Chain	Res	Type
3	L5	4387	C
3	L5	4391	G
3	L5	4394	A
3	L5	4405	G
3	L5	4415	A
3	L5	4420	U
3	L5	4421	C
3	L5	4422	A
3	L5	4444	C
3	L5	4448	G
3	L5	4449	A
3	L5	4452	U
3	L5	4464	A
3	L5	4466	C
3	L5	4475	G
3	L5	4488	A
3	L5	4500	PSU
3	L5	4512	U
3	L5	4513	A
3	L5	4515	G
3	L5	4519	C
3	L5	4524	G
3	L5	4525	C
3	L5	4545	G
3	L5	4548	A
3	L5	4549	G
3	L5	4560	C
3	L5	4567	G
3	L5	4572	U
3	L5	4573	G
3	L5	4575	G
3	L5	4589	A
3	L5	4590	A2M
3	L5	4600	G
3	L5	4601	U
3	L5	4623	OMG
3	L5	4635	A
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4656	A
3	L5	4657	U
3	L5	4670	C

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Mol	Chain	Res	Type
3	L5	4672	A
3	L5	4679	G
3	L5	4687	A
3	L5	4694	G
3	L5	4695	C
3	L5	4700	A
3	L5	4708	A
3	L5	4709	U
3	L5	4719	G
3	L5	4734	A
3	L5	4740	G
3	L5	4741	C
3	L5	4742	G
3	L5	4745	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4764	A
3	L5	4765	G
3	L5	4771	C
3	L5	4772	C
3	L5	4775	C
3	L5	4859	C
3	L5	4863	G
3	L5	4870	G
3	L5	4871	C
3	L5	4875	G
3	L5	4881	U
3	L5	4882	U
3	L5	4883	C
3	L5	4889	G
3	L5	4895	C
3	L5	4896	G
3	L5	4900	C
3	L5	4901	G
3	L5	4910	G
3	L5	4912	G
3	L5	4914	C
3	L5	4915	G
3	L5	4925	U
3	L5	4926	C

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Mol	Chain	Res	Type
3	L5	4927	G
3	L5	4928	C
3	L5	4934	A
3	L5	4940	C
3	L5	4941	G
3	L5	4943	A
3	L5	4947	U
3	L5	4951	G
3	L5	4960	G
3	L5	4975	G
3	L5	4976	U
3	L5	4979	A
3	L5	4988	U
3	L5	4989	U
3	L5	4990	C
3	L5	4991	U
3	L5	4995	U
3	L5	5013	C
3	L5	5014	A
3	L5	5017	G
3	L5	5022	U
3	L5	5023	C
3	L5	5024	C
3	L5	5027	C
3	L5	5028	G
3	L5	5030	U
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	24	C
4	L7	33	U
4	L7	38	U
4	L7	53	U
4	L7	54	A
4	L7	64	G
4	L7	97	G
4	L7	100	A
4	L7	102	U
4	L7	110	G

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Mol	Chain	Res	Type
4	L7	111	C
5	L8	23	C
5	L8	25	G
5	L8	34	U
5	L8	35	C
5	L8	59	A
5	L8	62	A
5	L8	63	U
5	L8	75	OMG
5	L8	80	A
5	L8	82	A
5	L8	83	C
5	L8	84	A
5	L8	85	U
5	L8	86	U
5	L8	87	G
5	L8	94	G
5	L8	103	A
5	L8	105	C
5	L8	111	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
5	L8	147	G
68	S2	4	C
68	S2	13	C
68	S2	14	C
68	S2	25	A
68	S2	33	G
68	S2	41	G
68	S2	42	A
68	S2	46	A
68	S2	56	G
68	S2	58	C
68	S2	59	U
68	S2	65	C
68	S2	67	C
68	S2	68	A
68	S2	72	C

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Mol	Chain	Res	Type
68	S2	73	C
68	S2	74	G
68	S2	76	U
68	S2	92	A
68	S2	93	PSU
68	S2	99	A2M
68	S2	103	A
68	S2	113	G
68	S2	115	U
68	S2	126	G
68	S2	130	G
68	S2	142	C
68	S2	143	U
68	S2	147	A
68	S2	148	U
68	S2	149	A
68	S2	158	A
68	S2	160	U
68	S2	162	C
68	S2	163	U
68	S2	170	A
68	S2	179	C
68	S2	190	G
68	S2	196	C
68	S2	197	U
68	S2	198	U
68	S2	200	G
68	S2	203	G
68	S2	204	G
68	S2	206	G
68	S2	207	G
68	S2	208	G
68	S2	213	G
68	S2	214	U
68	S2	291	G
68	S2	292	A
68	S2	294	U
68	S2	295	C
68	S2	302	A
68	S2	303	C
68	S2	305	U
68	S2	306	C

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Mol	Chain	Res	Type
68	S2	307	G
68	S2	308	G
68	S2	309	G
68	S2	312	G
68	S2	318	A
68	S2	319	C
68	S2	320	G
68	S2	323	C
68	S2	324	C
68	S2	325	C
68	S2	326	C
68	S2	328	U
68	S2	329	G
68	S2	332	G
68	S2	339	A
68	S2	347	G
68	S2	360	A
68	S2	361	U
68	S2	362	C
68	S2	363	A
68	S2	364	A
68	S2	368	U
68	S2	370	G
68	S2	373	G
68	S2	381	C
68	S2	383	G
68	S2	385	G
68	S2	386	C
68	S2	408	A
68	S2	409	C
68	S2	426	A
68	S2	428	OMU
68	S2	448	A
68	S2	449	A
68	S2	450	C
68	S2	452	G
68	S2	464	A
68	S2	465	A
68	S2	466	G
68	S2	471	G
68	S2	472	C
68	S2	473	A

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Mol	Chain	Res	Type
68	S2	474	G
68	S2	482	G
68	S2	487	U
68	S2	488	U
68	S2	492	C
68	S2	493	A
68	S2	502	C
68	S2	516	A
68	S2	531	A
68	S2	532	C
68	S2	536	A
68	S2	537	C
68	S2	540	U
68	S2	542	U
68	S2	544	G
68	S2	546	G
68	S2	547	G
68	S2	557	U
68	S2	558	G
68	S2	563	G
68	S2	564	A
68	S2	576	A2M
68	S2	583	A
68	S2	587	A
68	S2	589	G
68	S2	590	A
68	S2	591	U
68	S2	592	C
68	S2	593	C
68	S2	604	A
68	S2	606	G
68	S2	613	G
68	S2	614	C
68	S2	617	G
68	S2	623	G
68	S2	627	OMU
68	S2	628	A
68	S2	631	U
68	S2	634	A
68	S2	643	A
68	S2	644	OMG
68	S2	655	A

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Mol	Chain	Res	Type
68	S2	659	G
68	S2	660	C
68	S2	664	A
68	S2	668	A2M
68	S2	669	A
68	S2	670	A
68	S2	671	A
68	S2	672	A
68	S2	673	G
68	S2	684	G
68	S2	688	U
68	S2	689	U
68	S2	690	G
68	S2	692	G
68	S2	693	A
68	S2	695	C
68	S2	696	G
68	S2	697	G
68	S2	698	G
68	S2	732	U
68	S2	733	C
68	S2	736	C
68	S2	738	C
68	S2	749	U
68	S2	751	G
68	S2	752	G
68	S2	753	C
68	S2	788	G
68	S2	791	C
68	S2	792	C
68	S2	793	G
68	S2	798	G
68	S2	799	OMU
68	S2	801	PSU
68	S2	821	G
68	S2	822	U
68	S2	823	U
68	S2	824	C
68	S2	827	A
68	S2	830	A
68	S2	834	C
68	S2	835	C

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Mol	Chain	Res	Type
68	S2	836	G
68	S2	837	A
68	S2	838	G
68	S2	839	C
68	S2	840	C
68	S2	847	A
68	S2	867	OMG
68	S2	868	G
68	S2	869	A
68	S2	870	A
68	S2	873	G
68	S2	878	G
68	S2	888	U
68	S2	889	U
68	S2	891	G
68	S2	894	G
68	S2	896	U
68	S2	897	U
68	S2	898	U
68	S2	899	U
68	S2	900	C
68	S2	901	G
68	S2	903	A
68	S2	909	G
68	S2	913	A
68	S2	917	U
68	S2	920	A
68	S2	922	A
68	S2	930	C
68	S2	933	G
68	S2	934	G
68	S2	950	C
68	S2	959	G
68	S2	963	A
68	S2	970	G
68	S2	971	G
68	S2	972	A
68	S2	982	G
68	S2	990	A
68	S2	992	A
68	S2	997	A
68	S2	999	G

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Mol	Chain	Res	Type
68	S2	1001	A
68	S2	1002	U
68	S2	1008	A
68	S2	1017	U
68	S2	1023	A
68	S2	1027	A
68	S2	1045	PSU
68	S2	1060	A
68	S2	1061	U
68	S2	1062	A
68	S2	1067	C
68	S2	1080	A
68	S2	1083	A
68	S2	1085	C
68	S2	1107	G
68	S2	1108	G
68	S2	1109	C
68	S2	1113	A
68	S2	1114	U
68	S2	1116	C
68	S2	1119	A
68	S2	1121	G
68	S2	1123	C
68	S2	1133	A
68	S2	1138	C
68	S2	1139	C
68	S2	1148	A
68	S2	1153	C
68	S2	1154	U
68	S2	1155	U
68	S2	1161	U
68	S2	1195	A
68	S2	1207	G
68	S2	1208	A
68	S2	1215	C
68	S2	1217	A
68	S2	1220	A
68	S2	1224	G
68	S2	1227	G
68	S2	1242	U
68	S2	1243	U
68	S2	1251	A

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Mol	Chain	Res	Type
68	S2	1253	A
68	S2	1255	G
68	S2	1256	G
68	S2	1257	G
68	S2	1259	A
68	S2	1274	G
68	S2	1275	G
68	S2	1284	A
68	S2	1286	G
68	S2	1294	G
68	S2	1295	A
68	S2	1301	A
68	S2	1302	G
68	S2	1303	C
68	S2	1304	U
68	S2	1308	U
68	S2	1341	C
68	S2	1342	U
68	S2	1354	G
68	S2	1356	G
68	S2	1357	A
68	S2	1371	U
68	S2	1372	U
68	S2	1376	A
68	S2	1378	A
68	S2	1382	A
68	S2	1402	A
68	S2	1408	U
68	S2	1413	G
68	S2	1414	A
68	S2	1417	C
68	S2	1418	C
68	S2	1419	C
68	S2	1421	A
68	S2	1423	C
68	S2	1428	G
68	S2	1429	G
68	S2	1433	C
68	S2	1434	C
68	S2	1435	C
68	S2	1437	C
68	S2	1438	A

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Mol	Chain	Res	Type
68	S2	1439	A
68	S2	1442	OMU
68	S2	1449	G
68	S2	1454	A
68	S2	1463	U
68	S2	1464	C
68	S2	1466	G
68	S2	1480	A
68	S2	1484	A
68	S2	1489	A
68	S2	1490	OMG
68	S2	1492	U
68	S2	1494	U
68	S2	1495	G
68	S2	1497	G
68	S2	1498	A
68	S2	1521	C
68	S2	1522	A
68	S2	1533	A
68	S2	1536	G
68	S2	1544	C
68	S2	1546	G
68	S2	1552	G
68	S2	1553	C
68	S2	1555	U
68	S2	1558	C
68	S2	1560	U
68	S2	1575	G
68	S2	1579	A
68	S2	1580	A
68	S2	1581	C
68	S2	1585	U
68	S2	1587	G
68	S2	1588	A
68	S2	1601	A
68	S2	1604	G
68	S2	1606	G
68	S2	1621	U
68	S2	1623	A
68	S2	1632	G
68	S2	1633	A
68	S2	1634	A

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Mol	Chain	Res	Type
68	S2	1637	A
68	S2	1646	C
68	S2	1648	G
68	S2	1654	G
68	S2	1663	A
68	S2	1664	A
68	S2	1665	G
68	S2	1680	G
68	S2	1683	C
68	S2	1698	C
68	S2	1699	A
68	S2	1722	G
68	S2	1744	G
68	S2	1745	A
68	S2	1752	C
68	S2	1753	C
68	S2	1754	G
68	S2	1756	C
68	S2	1757	G
68	S2	1758	G
68	S2	1759	G
68	S2	1761	U
68	S2	1772	C
68	S2	1773	C
68	S2	1774	C
68	S2	1775	U
68	S2	1783	C
68	S2	1784	G
68	S2	1786	U
68	S2	1810	U
68	S2	1824	A
68	S2	1826	G
68	S2	1831	A
68	S2	1835	A
68	S2	1838	U
68	S2	1849	G
68	S2	1851	MA6
68	S2	1861	G
68	S2	1862	G
68	S2	1863	A
68	S2	1865	C
84	Et	9	A

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Mol	Chain	Res	Type
84	Et	11	C
84	Et	16	C
84	Et	19	G
84	Et	20	U
84	Et	21	A
84	Et	26	A
84	Et	31	A
84	Et	32	C
84	Et	33	U
84	Et	35	U
84	Et	36	U
84	Et	37	A
84	Et	38	A
84	Et	39	U
84	Et	43	A
84	Et	45	G
84	Et	46	G
84	Et	47	U
84	Et	49	C
84	Et	50	A
84	Et	55	U
84	Et	56	C
84	Et	58	A
84	Et	61	C
84	Et	63	C
84	Et	66	U
84	Et	70	G
84	Et	73	G
84	Et	76	A

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	254	G
3	L5	406	C
3	L5	493	G
3	L5	914	U
3	L5	1082	C
3	L5	1590	C
3	L5	1633	G
3	L5	1698	C
3	L5	1703	C

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Mol	Chain	Res	Type
3	L5	1977	C
3	L5	2416	G
3	L5	2675	G
3	L5	2760	G
3	L5	2763	U
3	L5	3673	C
3	L5	4600	G
3	L5	4699	U
3	L5	4913	G
68	S2	291	G
68	S2	531	A
68	S2	563	G
68	S2	688	U
68	S2	867	OMG

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

178 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	PSU	L5	4552	3	18,21,22	1.13	2 (11%)	21,30,33	2.03	4 (19%)
3	A2M	L5	1871	3,87	22,25,26	1.31	2 (9%)	30,36,39	1.64	6 (20%)
68	OMU	S2	627	68	19,22,23	3.33	7 (36%)	25,31,34	1.85	5 (20%)
68	PSU	S2	1045	68	18,21,22	1.08	1 (5%)	21,30,33	1.93	4 (19%)
3	PSU	L5	4471	3	18,21,22	1.10	2 (11%)	21,30,33	1.89	4 (19%)
3	OMU	L5	4620	3	19,22,23	3.12	7 (36%)	25,31,34	1.72	4 (16%)
5	OMG	L8	75	5	23,26,27	0.57	0	32,38,41	0.49	0
3	OMC	L5	3701	3	19,22,23	0.73	1 (5%)	25,31,34	1.80	4 (16%)
68	OMC	S2	462	68	19,22,23	0.55	0	25,31,34	0.65	0
3	PSU	L5	4299	3	18,21,22	1.05	1 (5%)	21,30,33	1.82	4 (19%)
68	PSU	S2	1046	68	18,21,22	1.05	1 (5%)	21,30,33	1.84	4 (19%)
3	PSU	L5	2839	3	18,21,22	1.11	2 (11%)	21,30,33	1.93	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	PSU	S2	1244	68	18,21,22	1.07	1 (5%)	21,30,33	1.89	4 (19%)
3	PSU	L5	3851	3	18,21,22	1.04	1 (5%)	21,30,33	1.90	4 (19%)
3	OMU	L5	4227	3	19,22,23	3.23	7 (36%)	25,31,34	1.88	5 (20%)
3	A2M	L5	3785	3,87	22,25,26	1.18	1 (4%)	30,36,39	1.62	10 (33%)
68	PSU	S2	1174	68	18,21,22	1.05	2 (11%)	21,30,33	1.90	4 (19%)
68	PSU	S2	1004	68	18,21,22	1.10	1 (5%)	21,30,33	1.84	4 (19%)
3	OMC	L5	2365	3,87	19,22,23	0.68	0	25,31,34	0.54	0
3	OMC	L5	2804	3	19,22,23	0.69	0	25,31,34	0.64	0
3	OMC	L5	3869	3	19,22,23	0.67	0	25,31,34	0.62	0
3	OMG	L5	3792	3	23,26,27	0.59	0	32,38,41	0.49	0
68	6MZ	S2	1832	68,87	22,25,26	3.07	5 (22%)	29,36,39	2.31	10 (34%)
68	A2M	S2	1031	68	22,25,26	1.17	1 (4%)	30,36,39	1.52	7 (23%)
3	OMG	L5	3744	3	23,26,27	0.59	0	32,38,41	0.47	0
3	PSU	L5	4431	3	18,21,22	1.09	2 (11%)	21,30,33	1.93	4 (19%)
3	PSU	L5	4579	3	18,21,22	1.09	2 (11%)	21,30,33	1.94	4 (19%)
3	OMG	L5	4499	3	23,26,27	0.59	0	32,38,41	0.52	0
68	OMC	S2	174	68	19,22,23	0.52	0	25,31,34	0.68	0
3	A2M	L5	1534	3,87	22,25,26	1.23	2 (9%)	30,36,39	1.47	7 (23%)
3	PSU	L5	1781	3	18,21,22	1.04	1 (5%)	21,30,33	1.83	4 (19%)
68	OMU	S2	172	68	19,22,23	3.30	7 (36%)	25,31,34	1.86	5 (20%)
3	A2M	L5	2787	3	22,25,26	1.16	1 (4%)	30,36,39	1.48	8 (26%)
3	5MC	L5	4447	3	19,22,23	0.98	2 (10%)	26,32,35	0.83	0
3	OMC	L5	2861	3	19,22,23	0.67	0	25,31,34	0.82	1 (4%)
68	A2M	S2	166	68	22,25,26	1.27	1 (4%)	30,36,39	1.53	7 (23%)
68	A2M	S2	668	68,87	22,25,26	1.37	2 (9%)	30,36,39	1.67	7 (23%)
68	PSU	S2	1177	68	18,21,22	1.08	1 (5%)	21,30,33	1.95	4 (19%)
68	OMU	S2	1288	68	19,22,23	3.38	7 (36%)	25,31,34	1.70	4 (16%)
68	G7M	S2	1639	84,68	23,26,27	2.66	8 (34%)	34,39,42	2.61	11 (32%)
3	A2M	L5	4571	3	22,25,26	1.34	3 (13%)	30,36,39	1.64	9 (30%)
68	OMU	S2	799	68	19,22,23	3.38	7 (36%)	25,31,34	1.81	5 (20%)
68	A2M	S2	468	68	22,25,26	1.24	1 (4%)	30,36,39	1.56	7 (23%)
68	OMG	S2	601	68	23,26,27	0.56	0	32,38,41	0.44	0
68	OMG	S2	683	68	23,26,27	0.53	0	32,38,41	0.52	0
3	OMG	L5	4370	3	23,26,27	0.62	0	32,38,41	0.54	0
3	OMG	L5	4623	3	23,26,27	0.61	0	32,38,41	0.58	0
3	OMG	L5	4228	3	23,26,27	0.62	0	32,38,41	0.67	0
68	PSU	S2	866	68	18,21,22	1.10	1 (5%)	21,30,33	1.92	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	5001	3	18,21,22	1.05	1 (5%)	21,30,33	1.90	4 (19%)
3	PSU	L5	4521	3,87	18,21,22	1.12	2 (11%)	21,30,33	2.04	5 (23%)
3	A2M	L5	400	3	22,25,26	1.26	3 (13%)	30,36,39	1.56	9 (30%)
3	PSU	L5	1860	3	18,21,22	1.10	2 (11%)	21,30,33	1.87	4 (19%)
68	OMU	S2	354	68	19,22,23	3.27	7 (36%)	25,31,34	1.81	5 (20%)
3	PSU	L5	1792	3	18,21,22	1.02	1 (5%)	21,30,33	1.91	4 (19%)
3	OMC	L5	3808	3	19,22,23	0.74	1 (5%)	25,31,34	0.77	1 (4%)
3	OMC	L5	2351	3,87	19,22,23	0.77	1 (5%)	25,31,34	0.79	1 (4%)
3	PSU	L5	1862	3	18,21,22	1.04	1 (5%)	21,30,33	1.95	4 (19%)
68	A2M	S2	27	68	22,25,26	1.24	1 (4%)	30,36,39	1.51	7 (23%)
68	OMG	S2	1328	68	23,26,27	0.52	0	32,38,41	0.44	0
3	OMG	L5	4494	3	23,26,27	0.62	0	32,38,41	0.50	0
3	OMG	L5	1625	3	23,26,27	0.63	0	32,38,41	0.46	0
68	A2M	S2	576	68	22,25,26	1.18	1 (4%)	30,36,39	1.53	5 (16%)
68	PSU	S2	651	68	18,21,22	1.08	1 (5%)	21,30,33	1.99	5 (23%)
68	PSU	S2	814	68	18,21,22	1.06	1 (5%)	21,30,33	1.90	4 (19%)
68	PSU	S2	801	68	18,21,22	1.10	1 (5%)	21,30,33	1.80	4 (19%)
68	PSU	S2	1056	68	18,21,22	1.10	1 (5%)	21,30,33	1.94	5 (23%)
68	OMU	S2	121	68	19,22,23	3.27	7 (36%)	25,31,34	1.75	5 (20%)
3	PSU	L5	5010	3	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
68	PSU	S2	1081	68	18,21,22	1.06	1 (5%)	21,30,33	1.93	5 (23%)
3	PSU	L5	3822	3	18,21,22	1.08	2 (11%)	21,30,33	1.98	6 (28%)
68	OMU	S2	116	68	19,22,23	3.27	7 (36%)	25,31,34	1.71	5 (20%)
3	UY1	L5	3818	3	19,22,23	4.77	9 (47%)	21,31,34	2.00	6 (28%)
3	5MC	L5	3782	3,87	19,22,23	0.75	0	26,32,35	0.77	1 (3%)
3	OMC	L5	2422	3,87	19,22,23	0.68	0	25,31,34	0.71	0
68	4AC	S2	1842	68	21,24,25	0.40	0	28,34,37	0.46	0
3	A2M	L5	4523	3,87	22,25,26	1.26	3 (13%)	30,36,39	1.52	7 (23%)
3	OMG	L5	2876	3	23,26,27	0.62	0	32,38,41	0.49	0
68	OMU	S2	1326	68	19,22,23	3.29	7 (36%)	25,31,34	1.83	5 (20%)
3	PSU	L5	1536	3	18,21,22	1.06	2 (11%)	21,30,33	1.92	4 (19%)
3	6MZ	L5	4220	3	22,25,26	2.93	6 (27%)	29,36,39	2.44	11 (37%)
3	PSU	L5	4312	3	18,21,22	1.06	2 (11%)	21,30,33	1.81	4 (19%)
3	PSU	L5	4689	3	18,21,22	1.11	2 (11%)	21,30,33	1.93	4 (19%)
68	PSU	S2	681	68	18,21,22	1.04	1 (5%)	21,30,33	1.88	4 (19%)
68	A2M	S2	99	68,87	22,25,26	1.26	2 (9%)	30,36,39	1.58	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMU	L5	3925	3	19,22,23	3.12	7 (36%)	25,31,34	1.85	5 (20%)
3	OMG	L5	4637	3	23,26,27	0.59	0	32,38,41	0.49	0
3	OMU	L5	2837	3	19,22,23	3.23	7 (36%)	25,31,34	1.89	5 (20%)
3	PSU	L5	2632	3	18,21,22	1.04	1 (5%)	21,30,33	1.95	4 (19%)
3	A2M	L5	2363	3,87	22,25,26	1.25	2 (9%)	30,36,39	1.58	8 (26%)
3	A2M	L5	3825	3	22,25,26	1.22	2 (9%)	30,36,39	1.57	7 (23%)
3	PSU	L5	4457	3	18,21,22	1.06	2 (11%)	21,30,33	2.05	4 (19%)
68	OMG	S2	867	68	23,26,27	0.53	0	32,38,41	0.54	0
3	PSU	L5	4442	3	18,21,22	1.09	1 (5%)	21,30,33	2.07	6 (28%)
3	OMC	L5	3841	3	19,22,23	0.71	0	25,31,34	0.57	0
68	B8N	S2	1248	68	25,29,30	3.24	6 (24%)	28,42,45	2.08	8 (28%)
3	PSU	L5	4500	3	18,21,22	1.11	3 (16%)	21,30,33	2.12	5 (23%)
5	PSU	L8	55	5	18,21,22	1.07	2 (11%)	21,30,33	1.85	4 (19%)
3	OMG	L5	3627	3	23,26,27	0.59	0	32,38,41	0.64	0
68	OMG	S2	509	68	23,26,27	0.51	0	32,38,41	0.50	0
3	A2M	L5	2815	3	22,25,26	1.20	2 (9%)	30,36,39	1.54	9 (30%)
3	PSU	L5	3884	3	18,21,22	1.09	2 (11%)	21,30,33	1.99	5 (23%)
3	OMG	L5	3899	3	23,26,27	0.71	0	32,38,41	0.56	0
3	PSU	L5	3637	3	18,21,22	1.09	1 (5%)	21,30,33	2.06	5 (23%)
3	PSU	L5	4636	3	18,21,22	1.11	3 (16%)	21,30,33	2.28	7 (33%)
68	PSU	S2	109	68	18,21,22	1.11	2 (11%)	21,30,33	1.98	5 (23%)
3	PSU	L5	4673	3,87	18,21,22	1.07	2 (11%)	21,30,33	1.86	4 (19%)
3	PSU	L5	4628	3	18,21,22	1.03	2 (11%)	21,30,33	1.89	4 (19%)
3	PSU	L5	1677	3	18,21,22	1.07	3 (16%)	21,30,33	2.01	5 (23%)
5	PSU	L8	69	5	18,21,22	1.05	1 (5%)	21,30,33	2.03	6 (28%)
3	1MA	L5	1322	3,87	21,25,26	0.73	0	30,37,40	0.82	2 (6%)
68	A2M	S2	1383	68	22,25,26	1.18	1 (4%)	30,36,39	1.60	7 (23%)
3	OMG	L5	1522	3	23,26,27	0.64	0	32,38,41	0.62	0
3	A2M	L5	1323	3	22,25,26	1.30	3 (13%)	30,36,39	1.60	9 (30%)
3	PSU	L5	1782	3	18,21,22	1.08	2 (11%)	21,30,33	1.92	4 (19%)
3	PSU	L5	4361	3	18,21,22	1.05	1 (5%)	21,30,33	1.86	4 (19%)
3	A2M	L5	2401	3	22,25,26	1.17	2 (9%)	30,36,39	1.56	8 (26%)
3	OMU	L5	4306	3	19,22,23	3.16	7 (36%)	25,31,34	1.74	4 (16%)
3	PSU	L5	1582	3	18,21,22	1.09	2 (11%)	21,30,33	1.90	4 (19%)
3	PSU	L5	4353	3	18,21,22	1.06	2 (11%)	21,30,33	1.99	5 (23%)
68	OMC	S2	1272	68	19,22,23	0.56	0	25,31,34	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	OMG	S2	1490	68	23,26,27	0.51	0	32,38,41	0.46	0
68	PSU	S2	966	68,87	18,21,22	1.07	1 (5%)	21,30,33	1.85	4 (19%)
3	OMG	L5	4618	3	23,26,27	0.64	0	32,38,41	0.52	0
3	PSU	L5	4493	3	18,21,22	1.10	1 (5%)	21,30,33	1.88	4 (19%)
3	A2M	L5	398	3	22,25,26	1.20	3 (13%)	30,36,39	1.65	6 (20%)
3	PSU	L5	3920	3,87	18,21,22	1.10	2 (11%)	21,30,33	2.02	6 (28%)
68	OMG	S2	436	68	23,26,27	0.52	0	32,38,41	0.55	0
68	OMG	S2	644	68	23,26,27	0.53	0	32,38,41	0.52	0
3	PSU	L5	1683	3	18,21,22	1.07	2 (11%)	21,30,33	2.02	4 (19%)
68	PSU	S2	1232	68	18,21,22	1.05	1 (5%)	21,30,33	1.98	5 (23%)
68	OMU	S2	428	68	19,22,23	3.34	7 (36%)	25,31,34	1.82	5 (20%)
3	PSU	L5	4296	3	18,21,22	1.04	1 (5%)	21,30,33	1.95	4 (19%)
3	OMG	L5	2424	3	23,26,27	0.61	0	32,38,41	0.45	0
68	OMC	S2	1703	68	19,22,23	0.57	0	25,31,34	0.68	0
68	PSU	S2	1367	68	18,21,22	1.09	1 (5%)	21,30,33	1.95	5 (23%)
3	PSU	L5	3853	3,87	18,21,22	1.04	1 (5%)	21,30,33	1.85	4 (19%)
3	OMG	L5	4196	3	23,26,27	0.60	0	32,38,41	0.45	0
3	PSU	L5	4403	3	18,21,22	1.11	3 (16%)	21,30,33	2.03	6 (28%)
3	PSU	L5	3639	3	18,21,22	1.16	3 (16%)	21,30,33	1.88	4 (19%)
3	OMG	L5	4392	3	23,26,27	0.67	0	32,38,41	0.50	0
68	A2M	S2	484	68	22,25,26	1.18	1 (4%)	30,36,39	1.50	7 (23%)
3	OMU	L5	4498	3	19,22,23	3.20	7 (36%)	25,31,34	1.92	5 (20%)
68	OMC	S2	1391	68	19,22,23	0.58	0	25,31,34	0.70	0
3	PSU	L5	4972	3	18,21,22	1.02	1 (5%)	21,30,33	1.86	4 (19%)
3	OMC	L5	4536	3	19,22,23	0.70	0	25,31,34	0.71	0
68	PSU	S2	863	68	18,21,22	1.10	1 (5%)	21,30,33	1.85	4 (19%)
3	PSU	L5	3695	3	18,21,22	1.05	2 (11%)	21,30,33	1.97	4 (19%)
68	PSU	S2	93	68	18,21,22	1.04	1 (5%)	21,30,33	1.78	4 (19%)
68	PSU	S2	105	68	18,21,22	1.11	1 (5%)	21,30,33	2.01	5 (23%)
68	PSU	S2	406	68	18,21,22	1.11	2 (11%)	21,30,33	1.98	5 (23%)
3	PSU	L5	4532	3	18,21,22	1.09	1 (5%)	21,30,33	1.94	4 (19%)
3	PSU	L5	3844	3	18,21,22	1.15	2 (11%)	21,30,33	1.86	4 (19%)
3	OMG	L5	1316	3	23,26,27	0.73	0	32,38,41	0.61	0
3	OMC	L5	3887	3	19,22,23	0.68	0	25,31,34	0.61	0
68	A2M	S2	159	68	22,25,26	1.17	1 (4%)	30,36,39	1.53	6 (20%)
68	PSU	S2	686	68	18,21,22	1.10	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L5	4576	3	18,21,22	1.10	2 (11%)	21,30,33	1.89	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	MA6	S2	1850	68	23,26,27	1.28	2 (8%)	33,38,41	3.33	12 (36%)
3	OMC	L5	1340	3	19,22,23	0.69	0	25,31,34	0.68	0
3	OMC	L5	4456	3	19,22,23	0.76	1 (5%)	25,31,34	0.61	0
3	A2M	L5	4590	3	22,25,26	1.23	2 (9%)	30,36,39	1.55	5 (16%)
3	PSU	L5	4973	3	18,21,22	1.05	2 (11%)	21,30,33	1.89	4 (19%)
68	MA6	S2	1851	68	23,26,27	1.27	2 (8%)	33,38,41	3.38	12 (36%)
3	A2M	L5	3718	3	22,25,26	1.13	2 (9%)	30,36,39	1.55	6 (20%)
3	PSU	L5	1744	3,87	18,21,22	1.08	1 (5%)	21,30,33	1.95	4 (19%)
3	PSU	L5	4293	3	18,21,22	1.06	2 (11%)	21,30,33	1.97	4 (19%)
3	A2M	L5	1326	3	22,25,26	1.24	2 (9%)	30,36,39	1.49	9 (30%)
3	OMG	L5	2364	3,87	23,26,27	0.65	0	32,38,41	0.44	0
68	PSU	S2	649	68	18,21,22	1.09	2 (11%)	21,30,33	1.88	4 (19%)
68	4AC	S2	1337	68	21,24,25	0.40	0	28,34,37	0.62	0
68	OMC	S2	517	68	19,22,23	0.56	0	25,31,34	0.68	0
3	A2M	L5	3867	3	22,25,26	1.30	2 (9%)	30,36,39	1.51	9 (30%)
3	UR3	L5	4530	3	19,22,23	2.61	7 (36%)	26,32,35	1.54	3 (11%)
3	A2M	L5	1524	3	22,25,26	1.33	2 (9%)	30,36,39	1.50	7 (23%)
3	OMC	L5	2824	3	19,22,23	0.65	0	25,31,34	0.68	0
3	A2M	L5	3830	3	22,25,26	1.19	1 (4%)	30,36,39	1.58	6 (20%)
68	OMU	S2	1442	68	19,22,23	3.34	7 (36%)	25,31,34	1.78	4 (16%)

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	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1871	3,87	-	0/9/27/28	0/3/3/3
68	OMU	S2	627	68	-	2/9/27/28	0/2/2/2
68	PSU	S2	1045	68	-	2/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
5	OMG	L8	75	5	-	2/9/27/28	0/3/3/3
3	OMC	L5	3701	3	-	6/9/27/28	0/2/2/2
68	OMC	S2	462	68	-	1/9/27/28	0/2/2/2
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1046	68	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	2839	3	-	2/7/25/26	0/2/2/2
68	PSU	S2	1244	68	-	1/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3785	3,87	-	1/9/27/28	0/3/3/3
68	PSU	S2	1174	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	1004	68	-	0/7/25/26	0/2/2/2
3	OMC	L5	2365	3,87	-	0/9/27/28	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	3869	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
68	6MZ	S2	1832	68,87	-	2/9/27/28	0/3/3/3
68	A2M	S2	1031	68	-	0/9/27/28	0/3/3/3
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
68	OMC	S2	174	68	-	0/9/27/28	0/2/2/2
3	A2M	L5	1534	3,87	-	1/9/27/28	0/3/3/3
3	PSU	L5	1781	3	-	1/7/25/26	0/2/2/2
68	OMU	S2	172	68	-	2/9/27/28	0/2/2/2
3	A2M	L5	2787	3	-	6/9/27/28	0/3/3/3
3	5MC	L5	4447	3	-	3/7/25/26	0/2/2/2
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
68	A2M	S2	166	68	-	1/9/27/28	0/3/3/3
68	A2M	S2	668	68,87	-	4/9/27/28	0/3/3/3
68	PSU	S2	1177	68	-	0/7/25/26	0/2/2/2
68	OMU	S2	1288	68	-	0/9/27/28	0/2/2/2
68	G7M	S2	1639	84,68	-	0/7/25/26	0/3/3/3
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
68	OMU	S2	799	68	-	2/9/27/28	0/2/2/2
68	A2M	S2	468	68	-	1/9/27/28	0/3/3/3
68	OMG	S2	601	68	-	1/9/27/28	0/3/3/3
68	OMG	S2	683	68	-	0/9/27/28	0/3/3/3
3	OMG	L5	4370	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	4623	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	4228	3	-	2/9/27/28	0/3/3/3
68	PSU	S2	866	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4521	3,87	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	354	68	-	0/9/27/28	0/2/2/2
3	PSU	L5	1792	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	2351	3,87	-	2/9/27/28	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	27	68	-	0/9/27/28	0/3/3/3
68	OMG	S2	1328	68	-	1/9/27/28	0/3/3/3
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1625	3	-	2/9/27/28	0/3/3/3
68	A2M	S2	576	68	-	3/9/27/28	0/3/3/3
68	PSU	S2	651	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	814	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	801	68	-	2/7/25/26	0/2/2/2
68	PSU	S2	1056	68	-	0/7/25/26	0/2/2/2
68	OMU	S2	121	68	-	0/9/27/28	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1081	68	-	1/7/25/26	0/2/2/2
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	116	68	-	0/9/27/28	0/2/2/2
3	UY1	L5	3818	3	-	3/9/27/28	0/2/2/2
3	5MC	L5	3782	3,87	-	1/7/25/26	0/2/2/2
3	OMC	L5	2422	3,87	-	2/9/27/28	0/2/2/2
68	4AC	S2	1842	68	-	0/11/29/30	0/2/2/2
3	A2M	L5	4523	3,87	-	0/9/27/28	0/3/3/3
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
68	OMU	S2	1326	68	-	0/9/27/28	0/2/2/2
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
3	6MZ	L5	4220	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	681	68	-	0/7/25/26	0/2/2/2
68	A2M	S2	99	68,87	-	2/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	2632	3	-	1/7/25/26	0/2/2/2
3	A2M	L5	2363	3,87	-	0/9/27/28	0/3/3/3
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
68	OMG	S2	867	68	-	2/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
68	B8N	S2	1248	68	-	3/16/34/35	0/2/2/2
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
68	OMG	S2	509	68	-	0/9/27/28	0/3/3/3
3	A2M	L5	2815	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4636	3	-	1/7/25/26	0/2/2/2
68	PSU	S2	109	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	3,87	-	0/7/25/26	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
5	PSU	L8	69	5	-	1/7/25/26	0/2/2/2
3	1MA	L5	1322	3,87	-	2/7/25/26	0/3/3/3
68	A2M	S2	1383	68	-	0/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1323	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2401	3	-	1/9/27/28	0/3/3/3
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1582	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
68	OMC	S2	1272	68	-	0/9/27/28	0/2/2/2
68	OMG	S2	1490	68	-	1/9/27/28	0/3/3/3
68	PSU	S2	966	68,87	-	0/7/25/26	0/2/2/2
3	OMG	L5	4618	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3920	3,87	-	0/7/25/26	0/2/2/2
68	OMG	S2	436	68	-	0/9/27/28	0/3/3/3
68	OMG	S2	644	68	-	3/9/27/28	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1232	68	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	OMU	S2	428	68	-	6/9/27/28	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
68	OMC	S2	1703	68	-	0/9/27/28	0/2/2/2
68	PSU	S2	1367	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	3853	3,87	-	0/7/25/26	0/2/2/2
3	OMG	L5	4196	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
68	A2M	S2	484	68	-	0/9/27/28	0/3/3/3
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
68	OMC	S2	1391	68	-	0/9/27/28	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	863	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	93	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	105	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	406	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
68	A2M	S2	159	68	-	1/9/27/28	0/3/3/3
68	PSU	S2	686	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
68	MA6	S2	1850	68	-	0/11/29/30	0/3/3/3
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	4590	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
68	MA6	S2	1851	68	-	1/11/29/30	0/3/3/3
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1744	3,87	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	3/9/27/28	0/3/3/3
3	OMG	L5	2364	3,87	-	2/9/27/28	0/3/3/3
68	PSU	S2	649	68	-	0/7/25/26	0/2/2/2
68	4AC	S2	1337	68	-	0/11/29/30	0/2/2/2
68	OMC	S2	517	68	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	3867	3	-	2/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
68	OMU	S2	1442	68	-	2/9/27/28	0/2/2/2

All (327) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	1832	6MZ	C6-N6	12.74	1.48	1.34
3	L5	3818	UY1	C6-C5	12.42	1.49	1.35
3	L5	4220	6MZ	C6-N6	11.66	1.47	1.34
3	L5	3818	UY1	C2-N1	11.39	1.51	1.36
68	S2	799	OMU	C2-N1	8.43	1.51	1.38
68	S2	1288	OMU	C2-N1	8.41	1.51	1.38
68	S2	1442	OMU	C2-N1	8.11	1.51	1.38
68	S2	172	OMU	C2-N1	8.04	1.51	1.38
68	S2	627	OMU	C2-N1	8.03	1.51	1.38
68	S2	428	OMU	C2-N1	8.01	1.51	1.38
68	S2	1326	OMU	C2-N1	7.98	1.51	1.38
68	S2	116	OMU	C2-N1	7.91	1.50	1.38
68	S2	121	OMU	C2-N1	7.90	1.50	1.38
3	L5	4227	OMU	C2-N1	7.88	1.50	1.38
68	S2	354	OMU	C2-N1	7.84	1.50	1.38
3	L5	2837	OMU	C2-N1	7.81	1.50	1.38
68	S2	1248	B8N	C6-N1	7.73	1.55	1.36
68	S2	1248	B8N	C4-N3	-7.64	1.26	1.40
3	L5	3818	UY1	C2-N3	7.56	1.49	1.37
3	L5	3925	OMU	C2-N1	7.55	1.50	1.38
3	L5	4498	OMU	C2-N1	7.54	1.50	1.38
3	L5	4306	OMU	C2-N1	7.52	1.50	1.38
3	L5	4620	OMU	C2-N1	7.38	1.50	1.38
68	S2	1248	B8N	C4-C5	7.18	1.63	1.47
68	S2	428	OMU	C2-N3	6.94	1.50	1.38
68	S2	799	OMU	C2-N3	6.91	1.50	1.38
68	S2	1288	OMU	C2-N3	6.87	1.49	1.38
68	S2	116	OMU	C2-N3	6.84	1.49	1.38
68	S2	627	OMU	C2-N3	6.81	1.49	1.38
68	S2	1442	OMU	C2-N3	6.81	1.49	1.38
68	S2	172	OMU	C2-N3	6.78	1.49	1.38
68	S2	1326	OMU	C2-N3	6.70	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	121	OMU	C2-N3	6.68	1.49	1.38
68	S2	354	OMU	C2-N3	6.65	1.49	1.38
68	S2	1639	G7M	C4-N3	6.59	1.49	1.34
3	L5	2837	OMU	C2-N3	6.58	1.49	1.38
3	L5	4227	OMU	C2-N3	6.56	1.49	1.38
3	L5	4498	OMU	C2-N3	6.47	1.49	1.38
3	L5	4306	OMU	C2-N3	6.42	1.49	1.38
3	L5	4620	OMU	C2-N3	6.26	1.48	1.38
3	L5	3925	OMU	C2-N3	6.17	1.48	1.38
3	L5	4530	UR3	C6-C5	6.09	1.49	1.35
3	L5	4530	UR3	C2-N1	5.97	1.46	1.38
68	S2	428	OMU	C6-C5	5.87	1.48	1.35
68	S2	1288	OMU	C6-C5	5.86	1.48	1.35
68	S2	1248	B8N	C2-N1	5.85	1.56	1.39
68	S2	172	OMU	C6-C5	5.82	1.48	1.35
3	L5	4620	OMU	O4-C4	-5.81	1.13	1.24
68	S2	799	OMU	C6-C5	5.80	1.48	1.35
68	S2	1442	OMU	C6-C5	5.80	1.48	1.35
68	S2	627	OMU	C6-C5	5.79	1.48	1.35
68	S2	121	OMU	C6-C5	5.78	1.48	1.35
68	S2	354	OMU	C6-C5	5.74	1.48	1.35
68	S2	1326	OMU	C6-C5	5.74	1.48	1.35
3	L5	3925	OMU	O4-C4	-5.73	1.13	1.24
3	L5	4306	OMU	O4-C4	-5.73	1.13	1.24
3	L5	4498	OMU	O4-C4	-5.70	1.13	1.24
3	L5	4227	OMU	O4-C4	-5.69	1.13	1.24
3	L5	4498	OMU	C6-C5	5.67	1.48	1.35
3	L5	2837	OMU	C6-C5	5.65	1.48	1.35
68	S2	116	OMU	C6-C5	5.64	1.48	1.35
68	S2	354	OMU	O4-C4	-5.61	1.13	1.24
3	L5	2837	OMU	O4-C4	-5.60	1.13	1.24
3	L5	4227	OMU	C6-C5	5.59	1.48	1.35
3	L5	4306	OMU	C6-C5	5.56	1.48	1.35
68	S2	1442	OMU	O4-C4	-5.55	1.13	1.24
3	L5	4620	OMU	C6-C5	5.54	1.47	1.35
68	S2	116	OMU	O4-C4	-5.53	1.13	1.24
3	L5	3925	OMU	C6-C5	5.52	1.47	1.35
68	S2	799	OMU	O4-C4	-5.49	1.13	1.24
68	S2	1326	OMU	O4-C4	-5.48	1.13	1.24
68	S2	627	OMU	O4-C4	-5.47	1.13	1.24
68	S2	121	OMU	O4-C4	-5.46	1.13	1.24
68	S2	1639	G7M	C2-N3	5.45	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	428	OMU	O4-C4	-5.44	1.13	1.24
3	L5	4530	UR3	C2-N3	5.42	1.49	1.39
68	S2	172	OMU	O4-C4	-5.42	1.13	1.24
68	S2	1288	OMU	O4-C4	-5.40	1.14	1.24
68	S2	1248	B8N	C6-C5	5.23	1.42	1.35
3	L5	3818	UY1	C6-N1	5.14	1.44	1.36
68	S2	1639	G7M	C5-N7	-4.96	1.33	1.39
68	S2	1639	G7M	C2-N2	4.89	1.45	1.34
68	S2	627	OMU	C4-N3	4.47	1.46	1.38
68	S2	428	OMU	C4-N3	4.36	1.46	1.38
68	S2	1326	OMU	C4-N3	4.35	1.46	1.38
68	S2	1442	OMU	C4-N3	4.35	1.46	1.38
68	S2	1288	OMU	C4-N3	4.32	1.46	1.38
68	S2	799	OMU	C4-N3	4.24	1.45	1.38
3	L5	3818	UY1	C4-N3	4.22	1.46	1.38
68	S2	172	OMU	C4-N3	4.21	1.45	1.38
68	S2	116	OMU	C4-N3	4.19	1.45	1.38
68	S2	121	OMU	C4-N3	4.18	1.45	1.38
68	S2	354	OMU	C4-N3	4.12	1.45	1.38
3	L5	2837	OMU	C4-N3	4.00	1.45	1.38
3	L5	4498	OMU	C4-N3	3.97	1.45	1.38
68	S2	1639	G7M	C5-C6	3.84	1.54	1.43
3	L5	4227	OMU	C4-N3	3.83	1.45	1.38
3	L5	3818	UY1	O4-C4	-3.77	1.16	1.23
3	L5	4306	OMU	C4-N3	3.76	1.45	1.38
68	S2	1248	B8N	C1'-C5	3.70	1.58	1.50
3	L5	4620	OMU	C4-N3	3.64	1.44	1.38
3	L5	1524	A2M	O5'-C5'	-3.63	1.33	1.44
3	L5	1871	A2M	O5'-C5'	-3.62	1.33	1.44
3	L5	3830	A2M	O5'-C5'	-3.61	1.33	1.44
3	L5	4220	6MZ	C5-C4	-3.61	1.32	1.39
3	L5	1323	A2M	O5'-C5'	-3.56	1.33	1.44
3	L5	3825	A2M	O5'-C5'	-3.56	1.33	1.44
3	L5	1326	A2M	O5'-C5'	-3.56	1.33	1.44
68	S2	801	PSU	C6-C5	3.56	1.39	1.35
68	S2	99	A2M	O5'-C5'	-3.55	1.33	1.44
68	S2	1004	PSU	C6-C5	3.55	1.39	1.35
3	L5	400	A2M	O5'-C5'	-3.55	1.33	1.44
68	S2	866	PSU	C6-C5	3.53	1.39	1.35
3	L5	3785	A2M	O5'-C5'	-3.53	1.33	1.44
3	L5	2363	A2M	O5'-C5'	-3.53	1.33	1.44
68	S2	668	A2M	O5'-C5'	-3.51	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3925	OMU	C4-N3	3.51	1.44	1.38
68	S2	1056	PSU	C6-C5	3.51	1.39	1.35
68	S2	1367	PSU	C6-C5	3.50	1.39	1.35
68	S2	27	A2M	O5'-C5'	-3.49	1.34	1.44
3	L5	4571	A2M	O5'-C5'	-3.49	1.34	1.44
3	L5	2815	A2M	O5'-C5'	-3.49	1.34	1.44
68	S2	406	PSU	C6-C5	3.49	1.39	1.35
68	S2	686	PSU	C6-C5	3.48	1.39	1.35
3	L5	2787	A2M	O5'-C5'	-3.45	1.34	1.44
68	S2	966	PSU	C6-C5	3.45	1.39	1.35
68	S2	105	PSU	C6-C5	3.44	1.39	1.35
3	L5	3844	PSU	C6-C5	3.43	1.39	1.35
68	S2	109	PSU	C6-C5	3.43	1.39	1.35
3	L5	3867	A2M	O5'-C5'	-3.43	1.34	1.44
68	S2	1383	A2M	O5'-C5'	-3.42	1.34	1.44
68	S2	1244	PSU	C6-C5	3.40	1.39	1.35
68	S2	863	PSU	C6-C5	3.40	1.39	1.35
68	S2	468	A2M	O5'-C5'	-3.40	1.34	1.44
68	S2	484	A2M	O5'-C5'	-3.39	1.34	1.44
3	L5	4590	A2M	O5'-C5'	-3.39	1.34	1.44
68	S2	1031	A2M	O5'-C5'	-3.38	1.34	1.44
68	S2	1045	PSU	C6-C5	3.38	1.39	1.35
3	L5	2401	A2M	O5'-C5'	-3.37	1.34	1.44
68	S2	651	PSU	C6-C5	3.36	1.39	1.35
68	S2	814	PSU	C6-C5	3.36	1.39	1.35
68	S2	1177	PSU	C6-C5	3.36	1.39	1.35
3	L5	3718	A2M	O5'-C5'	-3.35	1.34	1.44
68	S2	576	A2M	O5'-C5'	-3.34	1.34	1.44
3	L5	4552	PSU	C6-C5	3.33	1.39	1.35
68	S2	93	PSU	C6-C5	3.33	1.39	1.35
3	L5	4493	PSU	C6-C5	3.33	1.39	1.35
68	S2	649	PSU	C6-C5	3.33	1.39	1.35
3	L5	5010	PSU	C6-C5	3.32	1.39	1.35
68	S2	166	A2M	O5'-C5'	-3.32	1.34	1.44
3	L5	4523	A2M	O5'-C5'	-3.31	1.34	1.44
3	L5	1860	PSU	C6-C5	3.31	1.39	1.35
3	L5	398	A2M	O5'-C5'	-3.31	1.34	1.44
3	L5	1534	A2M	O5'-C5'	-3.27	1.34	1.44
3	L5	4220	6MZ	C5-N7	-3.27	1.33	1.39
3	L5	4220	6MZ	C8-N9	-3.26	1.32	1.37
68	S2	668	A2M	O4'-C4'	-3.26	1.37	1.45
68	S2	1081	PSU	C6-C5	3.24	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L8	55	PSU	C6-C5	3.23	1.38	1.35
68	S2	1046	PSU	C6-C5	3.22	1.38	1.35
3	L5	1744	PSU	C6-C5	3.21	1.38	1.35
3	L5	3818	UY1	O2-C2	-3.21	1.16	1.23
3	L5	4500	PSU	C6-C5	3.21	1.38	1.35
3	L5	4576	PSU	C6-C5	3.21	1.38	1.35
3	L5	3639	PSU	C6-C5	3.19	1.38	1.35
3	L5	4579	PSU	C6-C5	3.18	1.38	1.35
68	S2	1232	PSU	C6-C5	3.17	1.38	1.35
3	L5	4431	PSU	C6-C5	3.17	1.38	1.35
3	L5	1782	PSU	C6-C5	3.17	1.38	1.35
68	S2	1832	6MZ	C5-N7	-3.17	1.33	1.39
3	L5	4521	PSU	C6-C5	3.16	1.38	1.35
68	S2	1832	6MZ	C5-C4	-3.16	1.33	1.39
3	L5	4532	PSU	C6-C5	3.16	1.38	1.35
3	L5	3818	UY1	C1'-C5	3.15	1.57	1.50
3	L5	4442	PSU	C6-C5	3.15	1.38	1.35
68	S2	159	A2M	O5'-C5'	-3.14	1.35	1.44
3	L5	1781	PSU	C6-C5	3.11	1.38	1.35
3	L5	4312	PSU	C6-C5	3.11	1.38	1.35
3	L5	4471	PSU	C6-C5	3.10	1.38	1.35
3	L5	2632	PSU	C6-C5	3.10	1.38	1.35
3	L5	2839	PSU	C6-C5	3.09	1.38	1.35
3	L5	1862	PSU	C6-C5	3.09	1.38	1.35
3	L5	3822	PSU	C6-C5	3.09	1.38	1.35
3	L5	4296	PSU	C6-C5	3.09	1.38	1.35
68	S2	1832	6MZ	C8-N9	-3.08	1.32	1.37
68	S2	1851	MA6	C6-N6	3.08	1.45	1.36
3	L5	4673	PSU	C6-C5	3.07	1.38	1.35
3	L5	4689	PSU	C6-C5	3.07	1.38	1.35
3	L5	1582	PSU	C6-C5	3.07	1.38	1.35
3	L5	4353	PSU	C6-C5	3.06	1.38	1.35
68	S2	1850	MA6	C6-N6	3.05	1.45	1.36
68	S2	1174	PSU	C6-C5	3.02	1.38	1.35
3	L5	3695	PSU	C6-C5	3.01	1.38	1.35
3	L5	4299	PSU	C6-C5	3.00	1.38	1.35
3	L5	4293	PSU	C6-C5	2.99	1.38	1.35
3	L5	3637	PSU	C6-C5	2.99	1.38	1.35
3	L5	4361	PSU	C6-C5	2.96	1.38	1.35
3	L5	4636	PSU	C6-C5	2.96	1.38	1.35
5	L8	69	PSU	C6-C5	2.96	1.38	1.35
3	L5	4973	PSU	C6-C5	2.95	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4972	PSU	C6-C5	2.95	1.38	1.35
3	L5	3851	PSU	C6-C5	2.94	1.38	1.35
68	S2	681	PSU	C6-C5	2.93	1.38	1.35
3	L5	1683	PSU	C6-C5	2.93	1.38	1.35
3	L5	3920	PSU	C6-C5	2.92	1.38	1.35
3	L5	5001	PSU	C6-C5	2.91	1.38	1.35
3	L5	1792	PSU	C6-C5	2.89	1.38	1.35
3	L5	3853	PSU	C6-C5	2.89	1.38	1.35
3	L5	4530	UR3	O2-C2	-2.88	1.17	1.22
3	L5	1536	PSU	C6-C5	2.87	1.38	1.35
3	L5	4403	PSU	C6-C5	2.86	1.38	1.35
68	S2	428	OMU	C5-C4	2.85	1.49	1.43
68	S2	1288	OMU	C5-C4	2.83	1.49	1.43
3	L5	4571	A2M	O4'-C4'	-2.83	1.38	1.45
3	L5	1524	A2M	O4'-C4'	-2.82	1.38	1.45
3	L5	4457	PSU	C6-C5	2.81	1.38	1.35
68	S2	627	OMU	C5-C4	2.80	1.49	1.43
3	L5	3884	PSU	C6-C5	2.79	1.38	1.35
3	L5	1323	A2M	O4'-C4'	-2.79	1.38	1.45
68	S2	1442	OMU	C5-C4	2.78	1.49	1.43
68	S2	799	OMU	C5-C4	2.76	1.49	1.43
3	L5	4628	PSU	C6-C5	2.76	1.38	1.35
68	S2	172	OMU	C5-C4	2.75	1.49	1.43
68	S2	1326	OMU	C5-C4	2.75	1.49	1.43
68	S2	121	OMU	C5-C4	2.74	1.49	1.43
3	L5	2363	A2M	O4'-C4'	-2.74	1.38	1.45
68	S2	1288	OMU	C6-N1	2.73	1.44	1.38
68	S2	1639	G7M	C2-N1	2.72	1.44	1.37
3	L5	4227	OMU	C5-C4	2.71	1.49	1.43
68	S2	799	OMU	C6-N1	2.69	1.44	1.38
68	S2	354	OMU	C5-C4	2.63	1.49	1.43
3	L5	3867	A2M	O4'-C4'	-2.62	1.39	1.45
68	S2	1442	OMU	C6-N1	2.62	1.44	1.38
3	L5	1677	PSU	O4'-C1'	-2.61	1.40	1.43
3	L5	3818	UY1	O4'-C1'	-2.60	1.40	1.43
3	L5	4498	OMU	C5-C4	2.58	1.49	1.43
68	S2	627	OMU	C6-N1	2.57	1.44	1.38
3	L5	1326	A2M	O4'-C4'	-2.57	1.39	1.45
68	S2	121	OMU	C6-N1	2.57	1.44	1.38
68	S2	1851	MA6	C5-C4	-2.56	1.34	1.39
3	L5	4220	6MZ	C6-N1	-2.55	1.31	1.35
68	S2	428	OMU	C6-N1	2.55	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	1639	G7M	O6-C6	-2.55	1.18	1.23
3	L5	2837	OMU	C5-C4	2.55	1.49	1.43
3	L5	1534	A2M	O4'-C4'	-2.55	1.39	1.45
68	S2	354	OMU	C6-N1	2.54	1.44	1.38
68	S2	116	OMU	C5-C4	2.52	1.49	1.43
68	S2	1850	MA6	C5-C4	-2.51	1.34	1.39
68	S2	1326	OMU	C6-N1	2.49	1.44	1.38
3	L5	4530	UR3	C6-N1	2.46	1.43	1.38
3	L5	4498	OMU	C6-N1	2.45	1.43	1.38
3	L5	3925	OMU	C5-C4	2.41	1.48	1.43
68	S2	116	OMU	C6-N1	2.41	1.43	1.38
68	S2	172	OMU	C6-N1	2.40	1.43	1.38
3	L5	4306	OMU	C6-N1	2.40	1.43	1.38
3	L5	2837	OMU	C6-N1	2.38	1.43	1.38
3	L5	4620	OMU	C5-C4	2.37	1.48	1.43
3	L5	1871	A2M	O4'-C4'	-2.37	1.39	1.45
3	L5	4620	OMU	C6-N1	2.37	1.43	1.38
3	L5	4306	OMU	C5-C4	2.36	1.48	1.43
3	L5	4227	OMU	C6-N1	2.34	1.43	1.38
3	L5	1323	A2M	O3'-C3'	-2.32	1.37	1.43
3	L5	4447	5MC	C4-N3	-2.31	1.30	1.34
3	L5	3925	OMU	C6-N1	2.31	1.43	1.38
68	S2	1639	G7M	C6-N1	2.31	1.43	1.38
3	L5	3884	PSU	C4-C5	-2.29	1.38	1.44
68	S2	1832	6MZ	C6-N1	-2.29	1.31	1.35
3	L5	2815	A2M	O4'-C4'	-2.29	1.39	1.45
3	L5	1677	PSU	C6-C5	2.29	1.37	1.35
3	L5	2839	PSU	C4-C5	-2.28	1.38	1.44
3	L5	4523	A2M	O4'-C4'	-2.28	1.39	1.45
3	L5	3920	PSU	C4-C5	-2.27	1.38	1.44
3	L5	4220	6MZ	C4-N9	-2.24	1.33	1.37
3	L5	400	A2M	O4'-C4'	-2.24	1.40	1.45
3	L5	4403	PSU	C4-C5	-2.20	1.38	1.44
3	L5	3639	PSU	C4-C5	-2.19	1.38	1.44
3	L5	4689	PSU	C4-C5	-2.19	1.38	1.44
3	L5	4521	PSU	C4-C5	-2.16	1.38	1.44
3	L5	4590	A2M	O4'-C4'	-2.16	1.40	1.45
3	L5	400	A2M	O3'-C3'	-2.14	1.37	1.43
3	L5	4447	5MC	C5-C4	-2.14	1.42	1.44
3	L5	4636	PSU	C4-C5	-2.14	1.38	1.44
3	L5	4973	PSU	C4-C5	-2.13	1.38	1.44
3	L5	4293	PSU	C4-C5	-2.13	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4571	A2M	O3'-C3'	-2.13	1.37	1.43
3	L5	4552	PSU	C4-C5	-2.12	1.38	1.44
3	L5	3825	A2M	O4'-C4'	-2.12	1.40	1.45
68	S2	99	A2M	O4'-C4'	-2.12	1.40	1.45
3	L5	4431	PSU	C4-C5	-2.11	1.38	1.44
3	L5	4523	A2M	O3'-C3'	-2.11	1.37	1.43
3	L5	4636	PSU	O4'-C1'	-2.11	1.40	1.43
3	L5	4530	UR3	C5-C4	2.10	1.49	1.43
3	L5	398	A2M	O3'-C3'	-2.10	1.37	1.43
3	L5	1677	PSU	C4-C5	-2.09	1.38	1.44
3	L5	4673	PSU	C4-C5	-2.08	1.38	1.44
5	L8	55	PSU	C4-C5	-2.08	1.38	1.44
68	S2	649	PSU	C4-C5	-2.07	1.38	1.44
3	L5	2351	OMC	C4-N3	-2.07	1.30	1.34
3	L5	4456	OMC	C4-N3	-2.07	1.30	1.34
3	L5	1860	PSU	C4-C5	-2.07	1.38	1.44
68	S2	1174	PSU	C4-C5	-2.06	1.38	1.44
3	L5	4353	PSU	C4-C5	-2.06	1.38	1.44
3	L5	398	A2M	O4'-C4'	-2.06	1.40	1.45
3	L5	3808	OMC	C4-N3	-2.05	1.30	1.34
3	L5	3639	PSU	O4'-C1'	-2.05	1.41	1.43
3	L5	1683	PSU	C4-C5	-2.05	1.38	1.44
3	L5	1536	PSU	C4-C5	-2.04	1.38	1.44
3	L5	4576	PSU	C4-C5	-2.04	1.38	1.44
3	L5	4312	PSU	C4-C5	-2.04	1.38	1.44
3	L5	4500	PSU	C4-C5	-2.03	1.38	1.44
3	L5	4579	PSU	C4-C5	-2.03	1.38	1.44
3	L5	2401	A2M	O4'-C4'	-2.03	1.40	1.45
3	L5	3701	OMC	C4-N3	-2.03	1.30	1.34
3	L5	1582	PSU	C4-C5	-2.03	1.38	1.44
3	L5	4403	PSU	O4'-C1'	-2.03	1.41	1.43
3	L5	3844	PSU	C4-C5	-2.03	1.38	1.44
68	S2	109	PSU	C4-C5	-2.03	1.38	1.44
3	L5	1782	PSU	C4-C5	-2.02	1.38	1.44
68	S2	406	PSU	C4-C5	-2.02	1.38	1.44
3	L5	3695	PSU	C4-C5	-2.01	1.38	1.44
3	L5	4457	PSU	C4-C5	-2.01	1.38	1.44
3	L5	3822	PSU	C4-C5	-2.01	1.38	1.44
3	L5	3718	A2M	O4'-C4'	-2.01	1.40	1.45
3	L5	4500	PSU	O4'-C1'	-2.01	1.41	1.43
3	L5	4628	PSU	C4-C5	-2.01	1.38	1.44
3	L5	4471	PSU	C4-C5	-2.01	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4530	UR3	C3U-N3	2.00	1.50	1.47

All (688) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1851	MA6	N1-C6-N6	-12.07	102.16	116.86
68	S2	1850	MA6	N1-C6-N6	-11.71	102.59	116.86
68	S2	1851	MA6	C5-C6-N6	7.85	137.76	125.33
68	S2	1850	MA6	C5-C6-N6	7.66	137.46	125.33
68	S2	1639	G7M	C1'-N9-C4	7.59	148.89	126.49
68	S2	1639	G7M	C1'-N9-C8	-7.42	101.70	126.74
3	L5	4220	6MZ	N1-C2-N3	-6.01	119.48	128.58
3	L5	4498	OMU	C4-N3-C2	-5.99	119.17	126.61
3	L5	4227	OMU	C4-N3-C2	-5.99	119.18	126.61
68	S2	627	OMU	C4-N3-C2	-5.80	119.41	126.61
3	L5	2837	OMU	C4-N3-C2	-5.77	119.45	126.61
68	S2	1326	OMU	C4-N3-C2	-5.77	119.45	126.61
68	S2	1851	MA6	N1-C2-N3	-5.76	119.87	128.58
3	L5	3925	OMU	C4-N3-C2	-5.72	119.51	126.61
68	S2	428	OMU	C4-N3-C2	-5.72	119.52	126.61
68	S2	1832	6MZ	N1-C2-N3	-5.70	119.95	128.58
3	L5	4636	PSU	C4-N3-C2	-5.66	118.58	126.37
68	S2	172	OMU	C4-N3-C2	-5.63	119.62	126.61
68	S2	1850	MA6	N1-C2-N3	-5.60	120.11	128.58
3	L5	4636	PSU	N1-C2-N3	5.58	121.06	115.17
3	L5	3701	OMC	C1'-N1-C2	5.58	130.77	118.44
68	S2	1442	OMU	C4-N3-C2	-5.57	119.69	126.61
68	S2	354	OMU	C4-N3-C2	-5.55	119.72	126.61
68	S2	799	OMU	C4-N3-C2	-5.48	119.81	126.61
68	S2	1850	MA6	N9-C8-N7	-5.46	106.18	113.94
68	S2	1851	MA6	N9-C8-N7	-5.41	106.25	113.94
68	S2	121	OMU	C4-N3-C2	-5.39	119.92	126.61
3	L5	3637	PSU	N1-C2-N3	5.39	120.86	115.17
68	S2	1248	B8N	C5-C4-N3	5.38	125.92	116.15
3	L5	4500	PSU	N1-C2-N3	5.36	120.83	115.17
3	L5	4220	6MZ	C9-N6-C6	-5.27	117.96	122.85
3	L5	4442	PSU	N1-C2-N3	5.26	120.72	115.17
3	L5	3637	PSU	C4-N3-C2	-5.26	119.13	126.37
3	L5	4552	PSU	N1-C2-N3	5.24	120.69	115.17
3	L5	1683	PSU	N1-C2-N3	5.24	120.69	115.17
3	L5	4530	UR3	C4-N3-C2	-5.24	120.37	124.58
3	L5	1677	PSU	C4-N3-C2	-5.23	119.16	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4457	PSU	C4-N3-C2	-5.23	119.17	126.37
3	L5	4306	OMU	C4-N3-C2	-5.19	120.17	126.61
68	S2	105	PSU	N1-C2-N3	5.19	120.64	115.17
3	L5	4353	PSU	N1-C2-N3	5.17	120.62	115.17
3	L5	4521	PSU	N1-C2-N3	5.17	120.62	115.17
3	L5	4457	PSU	N1-C2-N3	5.15	120.60	115.17
5	L8	69	PSU	N1-C2-N3	5.11	120.55	115.17
68	S2	1288	OMU	C4-N3-C2	-5.10	120.28	126.61
3	L5	4403	PSU	N1-C2-N3	5.09	120.54	115.17
3	L5	4220	6MZ	N9-C8-N7	-5.08	106.73	113.94
3	L5	3884	PSU	N1-C2-N3	5.07	120.52	115.17
3	L5	3920	PSU	N1-C2-N3	5.06	120.51	115.17
68	S2	651	PSU	N1-C2-N3	5.05	120.49	115.17
3	L5	3920	PSU	C4-N3-C2	-5.05	119.42	126.37
3	L5	4620	OMU	C4-N3-C2	-5.04	120.36	126.61
68	S2	1232	PSU	N1-C2-N3	5.03	120.47	115.17
3	L5	3822	PSU	N1-C2-N3	5.02	120.47	115.17
3	L5	3695	PSU	C4-N3-C2	-5.02	119.45	126.37
68	S2	116	OMU	C4-N3-C2	-5.02	120.38	126.61
68	S2	1248	B8N	C4-N3-C2	-5.01	119.45	125.62
3	L5	4293	PSU	C4-N3-C2	-5.01	119.48	126.37
3	L5	4579	PSU	N1-C2-N3	5.00	120.44	115.17
3	L5	1744	PSU	N1-C2-N3	4.99	120.44	115.17
3	L5	3695	PSU	N1-C2-N3	4.99	120.44	115.17
3	L5	1862	PSU	N1-C2-N3	4.99	120.43	115.17
3	L5	4689	PSU	N1-C2-N3	4.99	120.43	115.17
68	S2	814	PSU	C4-N3-C2	-4.99	119.50	126.37
3	L5	1683	PSU	C4-N3-C2	-4.99	119.50	126.37
3	L5	1582	PSU	C4-N3-C2	-4.99	119.50	126.37
68	S2	1832	6MZ	N9-C8-N7	-4.98	106.86	113.94
3	L5	4521	PSU	C4-N3-C2	-4.98	119.51	126.37
68	S2	1081	PSU	C4-N3-C2	-4.97	119.52	126.37
68	S2	406	PSU	N1-C2-N3	4.97	120.41	115.17
68	S2	109	PSU	C4-N3-C2	-4.97	119.52	126.37
3	L5	4442	PSU	C4-N3-C2	-4.97	119.52	126.37
3	L5	4500	PSU	C4-N3-C2	-4.97	119.53	126.37
3	L5	2632	PSU	N1-C2-N3	4.95	120.39	115.17
3	L5	4403	PSU	C4-N3-C2	-4.95	119.55	126.37
3	L5	4296	PSU	N1-C2-N3	4.95	120.39	115.17
68	S2	1056	PSU	N1-C2-N3	4.94	120.38	115.17
3	L5	4552	PSU	C4-N3-C2	-4.93	119.58	126.37
68	S2	1232	PSU	C4-N3-C2	-4.93	119.58	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4532	PSU	N1-C2-N3	4.93	120.36	115.17
68	S2	1177	PSU	N1-C2-N3	4.92	120.36	115.17
3	L5	3818	UY1	C4-N3-C2	-4.92	119.59	126.37
3	L5	1782	PSU	N1-C2-N3	4.92	120.36	115.17
68	S2	1367	PSU	N1-C2-N3	4.92	120.36	115.17
68	S2	109	PSU	N1-C2-N3	4.91	120.34	115.17
68	S2	651	PSU	C4-N3-C2	-4.90	119.62	126.37
3	L5	4293	PSU	N1-C2-N3	4.90	120.34	115.17
3	L5	4296	PSU	C4-N3-C2	-4.90	119.62	126.37
3	L5	1536	PSU	N1-C2-N3	4.90	120.33	115.17
3	L5	4431	PSU	C4-N3-C2	-4.89	119.63	126.37
68	S2	406	PSU	C4-N3-C2	-4.89	119.64	126.37
3	L5	3884	PSU	C4-N3-C2	-4.89	119.64	126.37
3	L5	1862	PSU	C4-N3-C2	-4.89	119.64	126.37
68	S2	1367	PSU	C4-N3-C2	-4.89	119.64	126.37
3	L5	5001	PSU	C4-N3-C2	-4.88	119.64	126.37
68	S2	1045	PSU	N1-C2-N3	4.88	120.32	115.17
3	L5	4471	PSU	N1-C2-N3	4.88	120.31	115.17
3	L5	4973	PSU	C4-N3-C2	-4.87	119.66	126.37
68	S2	1177	PSU	C4-N3-C2	-4.87	119.66	126.37
3	L5	4532	PSU	C4-N3-C2	-4.86	119.67	126.37
3	L5	4493	PSU	C4-N3-C2	-4.85	119.69	126.37
68	S2	105	PSU	C4-N3-C2	-4.85	119.69	126.37
3	L5	4353	PSU	C4-N3-C2	-4.85	119.69	126.37
68	S2	1081	PSU	N1-C2-N3	4.85	120.28	115.17
3	L5	4972	PSU	C4-N3-C2	-4.85	119.69	126.37
68	S2	686	PSU	C4-N3-C2	-4.84	119.70	126.37
3	L5	4431	PSU	N1-C2-N3	4.84	120.27	115.17
68	S2	1045	PSU	C4-N3-C2	-4.84	119.70	126.37
3	L5	1792	PSU	N1-C2-N3	4.84	120.27	115.17
3	L5	3851	PSU	C4-N3-C2	-4.83	119.72	126.37
68	S2	1174	PSU	C4-N3-C2	-4.82	119.73	126.37
3	L5	1792	PSU	C4-N3-C2	-4.82	119.73	126.37
3	L5	1582	PSU	N1-C2-N3	4.82	120.25	115.17
3	L5	3851	PSU	N1-C2-N3	4.82	120.25	115.17
5	L8	69	PSU	C4-N3-C2	-4.82	119.74	126.37
3	L5	3822	PSU	C4-N3-C2	-4.82	119.74	126.37
68	S2	866	PSU	N1-C2-N3	4.80	120.24	115.17
3	L5	2632	PSU	C4-N3-C2	-4.80	119.75	126.37
68	S2	681	PSU	N1-C2-N3	4.80	120.23	115.17
3	L5	1744	PSU	C4-N3-C2	-4.79	119.77	126.37
3	L5	2839	PSU	N1-C2-N3	4.79	120.22	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3844	PSU	N1-C2-N3	4.79	120.22	115.17
68	S2	863	PSU	C4-N3-C2	-4.79	119.78	126.37
3	L5	4361	PSU	C4-N3-C2	-4.78	119.78	126.37
3	L5	3853	PSU	N1-C2-N3	4.78	120.21	115.17
68	S2	1244	PSU	C4-N3-C2	-4.78	119.79	126.37
68	S2	866	PSU	C4-N3-C2	-4.78	119.79	126.37
5	L8	55	PSU	N1-C2-N3	4.77	120.20	115.17
3	L5	5001	PSU	N1-C2-N3	4.77	120.20	115.17
3	L5	5010	PSU	N1-C2-N3	4.77	120.20	115.17
3	L5	1860	PSU	N1-C2-N3	4.77	120.20	115.17
68	S2	1056	PSU	C4-N3-C2	-4.77	119.81	126.37
3	L5	4628	PSU	C4-N3-C2	-4.76	119.81	126.37
3	L5	3639	PSU	N1-C2-N3	4.76	120.19	115.17
3	L5	1536	PSU	C4-N3-C2	-4.75	119.83	126.37
3	L5	1782	PSU	C4-N3-C2	-4.74	119.84	126.37
68	S2	1244	PSU	N1-C2-N3	4.74	120.17	115.17
3	L5	4579	PSU	C4-N3-C2	-4.74	119.84	126.37
68	S2	1174	PSU	N1-C2-N3	4.74	120.16	115.17
3	L5	4972	PSU	N1-C2-N3	4.73	120.15	115.17
68	S2	814	PSU	N1-C2-N3	4.72	120.15	115.17
3	L5	4361	PSU	N1-C2-N3	4.72	120.15	115.17
68	S2	1832	6MZ	C5-C4-N3	-4.72	120.22	126.72
3	L5	4673	PSU	N1-C2-N3	4.71	120.14	115.17
3	L5	4628	PSU	N1-C2-N3	4.70	120.13	115.17
3	L5	1781	PSU	C4-N3-C2	-4.70	119.90	126.37
68	S2	686	PSU	N1-C2-N3	4.70	120.12	115.17
3	L5	4493	PSU	N1-C2-N3	4.69	120.12	115.17
3	L5	1781	PSU	N1-C2-N3	4.69	120.11	115.17
3	L5	4576	PSU	C4-N3-C2	-4.68	119.92	126.37
3	L5	4576	PSU	N1-C2-N3	4.68	120.11	115.17
68	S2	649	PSU	N1-C2-N3	4.68	120.11	115.17
68	S2	1004	PSU	N1-C2-N3	4.68	120.10	115.17
68	S2	801	PSU	N1-C2-N3	4.67	120.09	115.17
3	L5	4471	PSU	C4-N3-C2	-4.66	119.95	126.37
3	L5	4973	PSU	N1-C2-N3	4.66	120.08	115.17
3	L5	1677	PSU	N1-C2-N3	4.64	120.07	115.17
3	L5	4299	PSU	N1-C2-N3	4.64	120.06	115.17
68	S2	966	PSU	N1-C2-N3	4.64	120.06	115.17
68	S2	649	PSU	C4-N3-C2	-4.63	119.99	126.37
68	S2	863	PSU	N1-C2-N3	4.63	120.05	115.17
3	L5	2839	PSU	C4-N3-C2	-4.63	119.99	126.37
68	S2	966	PSU	C4-N3-C2	-4.62	120.01	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	681	PSU	C4-N3-C2	-4.61	120.02	126.37
68	S2	93	PSU	C4-N3-C2	-4.61	120.03	126.37
3	L5	3639	PSU	C4-N3-C2	-4.61	120.03	126.37
3	L5	5010	PSU	C4-N3-C2	-4.60	120.03	126.37
3	L5	4312	PSU	C4-N3-C2	-4.60	120.03	126.37
68	S2	1639	G7M	C2-N3-C4	4.60	120.22	112.30
68	S2	1046	PSU	C4-N3-C2	-4.59	120.05	126.37
68	S2	1004	PSU	C4-N3-C2	-4.58	120.07	126.37
68	S2	1046	PSU	N1-C2-N3	4.57	119.98	115.17
3	L5	4673	PSU	C4-N3-C2	-4.56	120.09	126.37
68	S2	93	PSU	N1-C2-N3	4.55	119.97	115.17
3	L5	4299	PSU	C4-N3-C2	-4.54	120.12	126.37
3	L5	1860	PSU	C4-N3-C2	-4.53	120.13	126.37
3	L5	4312	PSU	N1-C2-N3	4.51	119.92	115.17
68	S2	1851	MA6	C5-C4-N3	-4.51	120.51	126.72
3	L5	3853	PSU	C4-N3-C2	-4.50	120.18	126.37
68	S2	1850	MA6	C4-N9-C8	4.45	110.41	105.74
68	S2	1850	MA6	C5-C4-N3	-4.43	120.61	126.72
3	L5	3701	OMC	C1'-N1-C6	-4.42	111.33	120.78
3	L5	3844	PSU	C4-N3-C2	-4.40	120.32	126.37
3	L5	4689	PSU	C4-N3-C2	-4.39	120.32	126.37
5	L8	55	PSU	C4-N3-C2	-4.36	120.37	126.37
68	S2	801	PSU	C4-N3-C2	-4.36	120.37	126.37
3	L5	3818	UY1	N1-C2-N3	4.34	119.74	115.17
68	S2	1248	B8N	C1'-C5-C4	4.26	124.06	117.61
3	L5	398	A2M	C3'-C2'-C1'	-4.23	94.70	102.81
68	S2	1639	G7M	C5-C4-N3	-4.22	120.17	128.15
3	L5	1871	A2M	C3'-C2'-C1'	-4.22	94.73	102.81
3	L5	4498	OMU	N3-C2-N1	4.22	120.38	114.89
3	L5	4220	6MZ	C5-C4-N3	-4.21	120.92	126.72
3	L5	3830	A2M	C3'-C2'-C1'	-4.16	94.85	102.81
68	S2	1851	MA6	C4-N9-C8	4.14	110.09	105.74
3	L5	3925	OMU	N3-C2-N1	4.09	120.22	114.89
3	L5	2837	OMU	N3-C2-N1	4.03	120.14	114.89
68	S2	1639	G7M	C5-C6-N1	4.03	120.16	111.84
3	L5	4227	OMU	C5-C4-N3	3.94	120.32	114.80
3	L5	4227	OMU	N3-C2-N1	3.90	119.96	114.89
68	S2	172	OMU	N3-C2-N1	3.87	119.93	114.89
3	L5	4498	OMU	C5-C4-N3	3.85	120.19	114.80
68	S2	354	OMU	N3-C2-N1	3.85	119.90	114.89
68	S2	428	OMU	N3-C2-N1	3.84	119.89	114.89
68	S2	1442	OMU	C5-C4-N3	3.83	120.17	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1383	A2M	C3'-C2'-C1'	-3.83	95.47	102.81
68	S2	627	OMU	C5-C4-N3	3.82	120.15	114.80
3	L5	4571	A2M	C3'-C2'-C1'	-3.81	95.51	102.81
68	S2	1326	OMU	C5-C4-N3	3.80	120.12	114.80
3	L5	4523	A2M	C3'-C2'-C1'	-3.80	95.54	102.81
68	S2	799	OMU	N3-C2-N1	3.78	119.81	114.89
68	S2	1326	OMU	N3-C2-N1	3.74	119.76	114.89
3	L5	3925	OMU	C5-C4-N3	3.73	120.03	114.80
3	L5	4220	6MZ	C4-N9-C8	3.72	109.65	105.74
3	L5	4530	UR3	C5-C4-N3	3.72	119.94	115.04
3	L5	4620	OMU	N3-C2-N1	3.72	119.74	114.89
68	S2	121	OMU	N3-C2-N1	3.72	119.73	114.89
3	L5	3718	A2M	C3'-C2'-C1'	-3.70	95.73	102.81
68	S2	354	OMU	C5-C4-N3	3.69	119.97	114.80
3	L5	4306	OMU	N3-C2-N1	3.67	119.67	114.89
3	L5	398	A2M	O3'-C3'-C2'	3.66	121.43	111.19
3	L5	3825	A2M	C3'-C2'-C1'	-3.64	95.83	102.81
68	S2	99	A2M	C3'-C2'-C1'	-3.63	95.85	102.81
68	S2	627	OMU	N3-C2-N1	3.62	119.61	114.89
3	L5	2787	A2M	O3'-C3'-C2'	3.61	121.30	111.19
68	S2	799	OMU	C5-C4-N3	3.61	119.85	114.80
3	L5	4689	PSU	C6-N1-C2	-3.60	119.35	122.69
3	L5	2837	OMU	C5-C4-N3	3.59	119.83	114.80
68	S2	121	OMU	C5-C4-N3	3.59	119.83	114.80
68	S2	428	OMU	C5-C4-N3	3.59	119.83	114.80
68	S2	1442	OMU	N3-C2-N1	3.57	119.54	114.89
68	S2	172	OMU	C5-C4-N3	3.57	119.80	114.80
3	L5	4590	A2M	C3'-C2'-C1'	-3.56	95.99	102.81
68	S2	1288	OMU	N3-C2-N1	3.56	119.53	114.89
3	L5	4636	PSU	C6-C5-C4	3.56	120.58	118.17
3	L5	1323	A2M	C2'-C1'-N9	3.54	119.58	113.75
68	S2	1383	A2M	O3'-C3'-C2'	3.53	121.06	111.19
3	L5	4306	OMU	C5-C4-N3	3.52	119.73	114.80
68	S2	116	OMU	N3-C2-N1	3.50	119.45	114.89
68	S2	1851	MA6	C2-N1-C6	3.50	120.38	111.83
68	S2	1248	B8N	N3-C2-N1	3.49	120.99	116.72
68	S2	1850	MA6	C2-N1-C6	3.47	120.31	111.83
68	S2	1832	6MZ	C5-N7-C8	3.47	108.90	103.45
68	S2	1850	MA6	C4-C5-C6	3.44	119.47	115.91
3	L5	4620	OMU	C5-C4-N3	3.44	119.61	114.80
3	L5	3818	UY1	C6-C5-C4	3.42	120.48	118.17
68	S2	1288	OMU	C5-C4-N3	3.41	119.58	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	116	OMU	C5-C4-N3	3.41	119.57	114.80
68	S2	1850	MA6	N3-C4-N9	3.41	132.96	127.17
68	S2	1832	6MZ	C2-N3-C4	3.40	120.14	111.83
68	S2	1639	G7M	N9-C4-N3	3.38	132.72	125.95
68	S2	1832	6MZ	C4-N9-C8	3.35	109.25	105.74
3	L5	4220	6MZ	C2-N3-C4	3.35	120.00	111.83
68	S2	1031	A2M	C3'-C2'-C1'	-3.33	96.43	102.81
68	S2	668	A2M	C4-N9-C1'	-3.33	118.85	126.63
3	L5	1871	A2M	O3'-C3'-C2'	3.33	120.50	111.19
68	S2	576	A2M	O3'-C3'-C2'	3.32	120.48	111.19
68	S2	1851	MA6	N3-C4-N9	3.31	132.80	127.17
68	S2	1639	G7M	O6-C6-C5	-3.31	120.62	128.01
68	S2	1851	MA6	C4-C5-C6	3.29	119.31	115.91
68	S2	1851	MA6	C2-N3-C4	3.29	119.86	111.83
68	S2	468	A2M	C3'-C2'-C1'	-3.27	96.55	102.81
5	L8	69	PSU	O2-C2-N1	-3.26	119.43	122.79
3	L5	4500	PSU	O2-C2-N1	-3.26	119.43	122.79
3	L5	2815	A2M	C2'-C1'-N9	3.25	119.11	113.75
68	S2	576	A2M	C3'-C2'-C1'	-3.25	96.59	102.81
3	L5	3830	A2M	O3'-C3'-C2'	3.24	120.26	111.19
3	L5	2363	A2M	C2'-C1'-N9	3.20	119.02	113.75
3	L5	3718	A2M	O3'-C3'-C2'	3.20	120.14	111.19
68	S2	1851	MA6	C5-N7-C8	3.20	108.48	103.45
3	L5	3867	A2M	C2'-C1'-N9	3.20	119.01	113.75
68	S2	1832	6MZ	C4-C5-C6	3.19	119.43	116.78
3	L5	1534	A2M	C3'-C2'-C1'	-3.19	96.71	102.81
3	L5	4532	PSU	O2-C2-N1	-3.18	119.50	122.79
68	S2	99	A2M	O3'-C3'-C2'	3.17	120.06	111.19
68	S2	166	A2M	O3'-C3'-C2'	3.17	120.06	111.19
68	S2	159	A2M	O3'-C3'-C2'	3.17	120.05	111.19
68	S2	1046	PSU	O2-C2-N1	-3.17	119.52	122.79
3	L5	4571	A2M	O3'-C3'-C2'	3.16	120.04	111.19
68	S2	1850	MA6	C2-N3-C4	3.16	119.54	111.83
3	L5	2401	A2M	O3'-C3'-C2'	3.15	120.02	111.19
68	S2	627	OMU	O4-C4-C5	-3.15	119.73	125.16
68	S2	668	A2M	C1'-N9-C8	3.14	134.06	127.09
3	L5	1677	PSU	O2-C2-N1	-3.14	119.55	122.79
68	S2	468	A2M	O3'-C3'-C2'	3.12	119.92	111.19
68	S2	1850	MA6	C5-N7-C8	3.12	108.35	103.45
68	S2	1832	6MZ	N3-C4-N9	3.12	132.47	127.17
3	L5	1871	A2M	C4-N9-C1'	-3.11	119.36	126.63
3	L5	4628	PSU	O2-C2-N1	-3.10	119.59	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	27	A2M	C3'-C2'-C1'	-3.10	96.88	102.81
3	L5	1323	A2M	O3'-C3'-C2'	3.09	119.85	111.19
3	L5	4220	6MZ	C5-N7-C8	3.08	108.29	103.45
68	S2	1639	G7M	CN7-N7-C5	3.08	130.64	126.80
3	L5	4457	PSU	O2-C2-N1	-3.07	119.62	122.79
3	L5	1536	PSU	O2-C2-N1	-3.07	119.62	122.79
3	L5	2363	A2M	C3'-C2'-C1'	-3.07	96.94	102.81
68	S2	116	OMU	O4-C4-C5	-3.06	119.88	125.16
68	S2	1639	G7M	C2-N1-C6	-3.05	119.57	125.11
3	L5	2632	PSU	O2-C2-N1	-3.05	119.64	122.79
68	S2	1442	OMU	O4-C4-C5	-3.05	119.91	125.16
3	L5	4293	PSU	O2-C2-N1	-3.04	119.66	122.79
68	S2	668	A2M	O3'-C3'-C2'	3.03	119.66	111.19
5	L8	55	PSU	C6-N1-C2	-3.02	119.89	122.69
3	L5	2837	OMU	O4-C4-C5	-3.02	119.96	125.16
3	L5	4498	OMU	O4-C4-C5	-3.00	119.98	125.16
3	L5	4500	PSU	C6-N1-C2	-3.00	119.90	122.69
68	S2	468	A2M	C4-N9-C1'	-3.00	119.62	126.63
3	L5	3785	A2M	C4'-O4'-C1'	-3.00	102.85	109.47
68	S2	799	OMU	O4-C4-C5	-2.99	120.01	125.16
3	L5	1683	PSU	O2-C2-N1	-2.99	119.71	122.79
3	L5	1792	PSU	O2-C2-N1	-2.98	119.72	122.79
68	S2	105	PSU	O2-C2-N1	-2.97	119.72	122.79
3	L5	1860	PSU	C6-N1-C2	-2.97	119.93	122.69
68	S2	1326	OMU	O4-C4-C5	-2.96	120.06	125.16
3	L5	1323	A2M	C3'-C2'-C1'	-2.96	97.14	102.81
68	S2	651	PSU	O2-C2-N1	-2.95	119.74	122.79
3	L5	400	A2M	O3'-C3'-C2'	2.95	119.45	111.19
3	L5	3785	A2M	O3'-C3'-C2'	2.95	119.44	111.19
3	L5	3825	A2M	O3'-C3'-C2'	2.95	119.44	111.19
68	S2	428	OMU	O4-C4-C5	-2.95	120.07	125.16
3	L5	2401	A2M	C3'-C2'-C1'	-2.95	97.16	102.81
3	L5	3701	OMC	O2-C2-N3	-2.95	117.69	122.33
68	S2	484	A2M	O3'-C3'-C2'	2.94	119.41	111.19
68	S2	1031	A2M	O3'-C3'-C2'	2.93	119.39	111.19
68	S2	354	OMU	O4-C4-C5	-2.93	120.11	125.16
68	S2	109	PSU	O2-C2-N1	-2.93	119.77	122.79
3	L5	2401	A2M	C4-N9-C1'	-2.92	119.79	126.63
3	L5	1524	A2M	O3'-C3'-C2'	2.92	119.36	111.19
68	S2	1244	PSU	O2-C2-N1	-2.92	119.78	122.79
3	L5	3844	PSU	C6-N1-C2	-2.91	119.99	122.69
3	L5	4579	PSU	O2-C2-N1	-2.91	119.79	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4590	A2M	C4-N9-C1'	-2.91	119.83	126.63
3	L5	2839	PSU	C6-N1-C2	-2.91	120.00	122.69
68	S2	1248	B8N	O4-C4-N3	-2.90	115.28	119.99
68	S2	172	OMU	O4-C4-C5	-2.89	120.17	125.16
68	S2	1045	PSU	O2-C2-N1	-2.89	119.81	122.79
3	L5	1744	PSU	O2-C2-N1	-2.89	119.81	122.79
3	L5	4579	PSU	C6-N1-C2	-2.88	120.02	122.69
68	S2	668	A2M	C2'-C1'-N9	2.88	118.49	113.75
3	L5	4306	OMU	O4-C4-C5	-2.88	120.20	125.16
3	L5	4636	PSU	O2-C2-N1	-2.87	119.83	122.79
3	L5	3853	PSU	O2-C2-N1	-2.87	119.83	122.79
3	L5	1871	A2M	C1'-N9-C8	2.87	133.46	127.09
3	L5	4571	A2M	C4-N9-C1'	-2.86	119.93	126.63
68	S2	1177	PSU	O2-C2-N1	-2.86	119.83	122.79
3	L5	4523	A2M	O3'-C3'-C2'	2.86	119.20	111.19
3	L5	3844	PSU	O2-C2-N1	-2.86	119.84	122.79
3	L5	400	A2M	C3'-C2'-C1'	-2.86	97.33	102.81
68	S2	166	A2M	C3'-C2'-C1'	-2.86	97.33	102.81
3	L5	1326	A2M	O3'-C3'-C2'	2.85	119.17	111.19
68	S2	1288	OMU	O4-C4-C5	-2.84	120.26	125.16
3	L5	3884	PSU	O2-C2-N1	-2.84	119.86	122.79
3	L5	3818	UY1	C6-N1-C2	-2.84	120.06	122.69
3	L5	4552	PSU	O2-C2-N1	-2.83	119.86	122.79
68	S2	1174	PSU	O2-C2-N1	-2.83	119.86	122.79
3	L5	2839	PSU	O2-C2-N1	-2.83	119.87	122.79
3	L5	4296	PSU	O2-C2-N1	-2.83	119.87	122.79
68	S2	1031	A2M	C4-N9-C1'	-2.83	120.02	126.63
3	L5	4442	PSU	O2-C2-N1	-2.82	119.88	122.79
3	L5	4220	6MZ	N3-C4-N9	2.82	131.96	127.17
3	L5	4552	PSU	C6-N1-C2	-2.82	120.08	122.69
3	L5	1862	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L5	3925	OMU	O4-C4-C5	-2.81	120.31	125.16
3	L5	1683	PSU	C6-N1-C2	-2.80	120.09	122.69
3	L5	4353	PSU	C6-N1-C2	-2.80	120.09	122.69
68	S2	99	A2M	C4-N9-C1'	-2.80	120.09	126.63
68	S2	484	A2M	C4-N9-C1'	-2.79	120.10	126.63
3	L5	4227	OMU	O4-C4-C5	-2.79	120.34	125.16
68	S2	681	PSU	C6-N1-C2	-2.79	120.10	122.69
3	L5	3825	A2M	C4-N9-C1'	-2.79	120.12	126.63
68	S2	1383	A2M	C4-N9-C1'	-2.79	120.12	126.63
68	S2	121	OMU	O4-C4-C5	-2.79	120.36	125.16
3	L5	4521	PSU	O2-C2-N1	-2.78	119.92	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2815	A2M	O3'-C3'-C2'	2.78	118.97	111.19
3	L5	1536	PSU	C6-N1-C2	-2.78	120.11	122.69
68	S2	866	PSU	O2-C2-N1	-2.78	119.92	122.79
68	S2	1367	PSU	O2-C2-N1	-2.77	119.93	122.79
68	S2	801	PSU	C6-N1-C2	-2.77	120.12	122.69
68	S2	166	A2M	C4-N9-C1'	-2.77	120.16	126.63
3	L5	5010	PSU	O2-C2-N1	-2.76	119.94	122.79
68	S2	406	PSU	O2-C2-N1	-2.76	119.94	122.79
3	L5	4576	PSU	O2-C2-N1	-2.76	119.94	122.79
3	L5	3639	PSU	C6-N1-C2	-2.76	120.13	122.69
3	L5	3822	PSU	O2-C2-N1	-2.75	119.95	122.79
3	L5	2363	A2M	O3'-C3'-C2'	2.75	118.89	111.19
68	S2	105	PSU	C6-N1-C2	-2.75	120.14	122.69
3	L5	3884	PSU	C6-N1-C2	-2.74	120.14	122.69
68	S2	966	PSU	O2-C2-N1	-2.74	119.96	122.79
68	S2	1056	PSU	O2-C2-N1	-2.74	119.96	122.79
3	L5	4590	A2M	C1'-N9-C8	2.74	133.18	127.09
3	L5	5001	PSU	O2-C2-N1	-2.73	119.98	122.79
68	S2	814	PSU	O2-C2-N1	-2.72	119.98	122.79
3	L5	4500	PSU	C6-C5-C4	2.72	120.01	118.17
68	S2	1081	PSU	O2-C2-N1	-2.72	119.98	122.79
68	S2	649	PSU	O2-C2-N1	-2.71	119.99	122.79
68	S2	686	PSU	O2-C2-N1	-2.71	119.99	122.79
68	S2	1232	PSU	O2-C2-N1	-2.71	119.99	122.79
68	S2	484	A2M	C1'-N9-C8	2.71	133.11	127.09
3	L5	4471	PSU	O2-C2-N1	-2.71	120.00	122.79
3	L5	3785	A2M	C4-N9-C1'	-2.71	120.30	126.63
3	L5	1782	PSU	C6-N1-C2	-2.70	120.18	122.69
3	L5	4673	PSU	O2-C2-N1	-2.70	120.00	122.79
3	L5	3851	PSU	O2-C2-N1	-2.70	120.00	122.79
3	L5	2401	A2M	C1'-N9-C8	2.70	133.08	127.09
68	S2	1031	A2M	C1'-N9-C8	2.70	133.08	127.09
3	L5	3920	PSU	O2-C2-N1	-2.69	120.01	122.79
3	L5	3822	PSU	C6-N1-C2	-2.69	120.19	122.69
5	L8	69	PSU	C6-N1-C2	-2.69	120.19	122.69
3	L5	3853	PSU	C6-N1-C2	-2.69	120.20	122.69
68	S2	1046	PSU	C6-N1-C2	-2.69	120.20	122.69
68	S2	27	A2M	O3'-C3'-C2'	2.68	118.69	111.19
68	S2	1056	PSU	C6-N1-C2	-2.68	120.21	122.69
3	L5	4353	PSU	O2-C2-N1	-2.68	120.03	122.79
3	L5	1782	PSU	O2-C2-N1	-2.67	120.03	122.79
68	S2	468	A2M	C1'-N9-C8	2.67	133.02	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	5010	PSU	C6-N1-C2	-2.67	120.21	122.69
3	L5	1524	A2M	C4'-O4'-C1'	-2.67	103.57	109.47
3	L5	4471	PSU	C6-N1-C2	-2.67	120.22	122.69
68	S2	668	A2M	O4'-C1'-C2'	2.67	111.18	106.59
68	S2	159	A2M	C3'-C2'-C1'	-2.67	97.70	102.81
3	L5	398	A2M	C4-N9-C1'	-2.67	120.39	126.63
68	S2	159	A2M	C4-N9-C1'	-2.66	120.41	126.63
3	L5	4673	PSU	C6-N1-C2	-2.65	120.23	122.69
3	L5	1781	PSU	O2-C2-N1	-2.65	120.05	122.79
3	L5	4590	A2M	O3'-C3'-C2'	2.65	118.61	111.19
3	L5	400	A2M	C4-N9-C1'	-2.65	120.43	126.63
68	S2	27	A2M	C4-N9-C1'	-2.65	120.44	126.63
3	L5	1744	PSU	C6-N1-C2	-2.65	120.24	122.69
3	L5	4571	A2M	C1'-N9-C8	2.64	132.97	127.09
3	L5	4442	PSU	C6-N1-C2	-2.64	120.24	122.69
3	L5	3695	PSU	O2-C2-N1	-2.64	120.06	122.79
3	L5	4689	PSU	O2-C2-N1	-2.64	120.06	122.79
3	L5	3701	OMC	O2-C2-N1	2.64	124.07	118.90
3	L5	4442	PSU	C6-C5-C4	2.64	119.95	118.17
3	L5	3785	A2M	C3'-C2'-C1'	-2.64	97.76	102.81
68	S2	1639	G7M	CN7-N7-C8	-2.64	120.80	124.79
68	S2	159	A2M	C1'-N9-C8	2.63	132.93	127.09
3	L5	4431	PSU	O2-C2-N1	-2.62	120.08	122.79
3	L5	2632	PSU	C6-N1-C2	-2.62	120.26	122.69
68	S2	1177	PSU	C6-N1-C2	-2.62	120.26	122.69
3	L5	2363	A2M	C1'-N9-C8	2.62	132.91	127.09
3	L5	3830	A2M	C4-N9-C1'	-2.61	120.52	126.63
68	S2	576	A2M	C4-N9-C1'	-2.61	120.52	126.63
3	L5	1326	A2M	C3'-C2'-C1'	-2.61	97.80	102.81
68	S2	863	PSU	O2-C2-N1	-2.60	120.10	122.79
68	S2	651	PSU	C6-N1-C2	-2.59	120.29	122.69
3	L5	4620	OMU	O4-C4-C5	-2.59	120.69	125.16
3	L5	2363	A2M	C4-N9-C1'	-2.59	120.58	126.63
3	L5	2815	A2M	C3'-C2'-C1'	-2.59	97.86	102.81
3	L5	4523	A2M	C4-N9-C1'	-2.58	120.59	126.63
3	L5	398	A2M	C1'-N9-C8	2.58	132.82	127.09
68	S2	649	PSU	C6-N1-C2	-2.58	120.30	122.69
3	L5	4493	PSU	O2-C2-N1	-2.58	120.13	122.79
3	L5	4521	PSU	C6-N1-C2	-2.57	120.30	122.69
5	L8	55	PSU	O2-C2-N1	-2.57	120.14	122.79
68	S2	1383	A2M	C1'-N9-C8	2.57	132.80	127.09
3	L5	3867	A2M	C4-N9-C1'	-2.57	120.63	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2787	A2M	O4'-C1'-C2'	2.57	111.01	106.59
68	S2	406	PSU	C6-N1-C2	-2.56	120.31	122.69
3	L5	1860	PSU	O2-C2-N1	-2.56	120.15	122.79
68	S2	99	A2M	C1'-N9-C8	2.55	132.76	127.09
68	S2	166	A2M	C1'-N9-C8	2.55	132.76	127.09
3	L5	4403	PSU	C6-N1-C2	-2.55	120.33	122.69
3	L5	3639	PSU	O2-C2-N1	-2.54	120.17	122.79
3	L5	1862	PSU	C6-N1-C2	-2.54	120.33	122.69
3	L5	3825	A2M	C1'-N9-C8	2.54	132.73	127.09
68	S2	1832	6MZ	C4-C5-N7	-2.54	107.68	110.58
3	L5	3920	PSU	C6-N1-C2	-2.54	120.33	122.69
3	L5	4431	PSU	C6-N1-C2	-2.53	120.34	122.69
3	L5	4973	PSU	O2-C2-N1	-2.52	120.19	122.79
3	L5	2861	OMC	C1'-N1-C2	2.52	124.01	118.44
3	L5	4403	PSU	C6-C5-C4	2.51	119.87	118.17
3	L5	3818	UY1	O2-C2-N1	-2.51	120.20	122.79
3	L5	1534	A2M	C4-N9-C1'	-2.51	120.77	126.63
3	L5	3867	A2M	C1'-N9-C8	2.50	132.65	127.09
68	S2	1174	PSU	C6-N1-C2	-2.50	120.37	122.69
3	L5	4299	PSU	C6-N1-C2	-2.50	120.37	122.69
3	L5	3718	A2M	C1'-N9-C8	2.50	132.64	127.09
3	L5	1524	A2M	O4'-C1'-C2'	2.50	110.89	106.59
68	S2	1004	PSU	C6-N1-C2	-2.50	120.37	122.69
3	L5	400	A2M	C1'-N9-C8	2.49	132.63	127.09
68	S2	1367	PSU	C6-N1-C2	-2.49	120.38	122.69
68	S2	27	A2M	C1'-N9-C8	2.49	132.62	127.09
3	L5	4296	PSU	C6-N1-C2	-2.49	120.38	122.69
68	S2	576	A2M	C1'-N9-C8	2.49	132.61	127.09
68	S2	866	PSU	C6-N1-C2	-2.49	120.39	122.69
3	L5	3830	A2M	C1'-N9-C8	2.48	132.60	127.09
68	S2	93	PSU	C6-N1-C2	-2.48	120.39	122.69
68	S2	1232	PSU	C6-N1-C2	-2.48	120.39	122.69
3	L5	4498	OMU	O2-C2-N1	-2.48	119.57	122.80
68	S2	1045	PSU	C6-N1-C2	-2.48	120.39	122.69
3	L5	1792	PSU	C6-N1-C2	-2.47	120.40	122.69
3	L5	3785	A2M	C1'-N9-C8	2.47	132.57	127.09
68	S2	1244	PSU	C6-N1-C2	-2.46	120.41	122.69
3	L5	3718	A2M	C4-N9-C1'	-2.45	120.90	126.63
68	S2	863	PSU	C6-N1-C2	-2.45	120.42	122.69
68	S2	109	PSU	C6-N1-C2	-2.45	120.42	122.69
3	L5	4312	PSU	C6-N1-C2	-2.45	120.42	122.69
3	L5	4299	PSU	O2-C2-N1	-2.44	120.27	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1326	A2M	C4-N9-C1'	-2.43	120.94	126.63
3	L5	4532	PSU	C6-N1-C2	-2.43	120.44	122.69
3	L5	4628	PSU	C6-N1-C2	-2.43	120.44	122.69
3	L5	4361	PSU	O2-C2-N1	-2.42	120.29	122.79
3	L5	1524	A2M	C4-N9-C1'	-2.42	120.96	126.63
68	S2	801	PSU	O2-C2-N1	-2.42	120.29	122.79
3	L5	1534	A2M	C1'-N9-C8	2.42	132.47	127.09
3	L5	3695	PSU	C6-N1-C2	-2.42	120.45	122.69
3	L5	4576	PSU	C6-N1-C2	-2.41	120.45	122.69
68	S2	1850	MA6	C1'-N9-C8	-2.41	121.74	127.09
68	S2	93	PSU	O2-C2-N1	-2.41	120.31	122.79
68	S2	484	A2M	O4'-C1'-C2'	2.41	110.73	106.59
68	S2	681	PSU	O2-C2-N1	-2.40	120.31	122.79
68	S2	1004	PSU	O2-C2-N1	-2.39	120.32	122.79
3	L5	4523	A2M	C1'-N9-C8	2.39	132.41	127.09
3	L5	1326	A2M	C1'-N9-C8	2.39	132.40	127.09
3	L5	4590	A2M	C6-C5-C4	-2.39	113.92	117.18
5	L8	69	PSU	C6-C5-C4	2.38	119.78	118.17
68	S2	686	PSU	C6-N1-C2	-2.38	120.48	122.69
3	L5	4312	PSU	O2-C2-N1	-2.38	120.34	122.79
3	L5	4972	PSU	C6-N1-C2	-2.38	120.49	122.69
3	L5	1582	PSU	O2-C2-N1	-2.37	120.34	122.79
3	L5	1582	PSU	C6-N1-C2	-2.37	120.49	122.69
68	S2	966	PSU	C6-N1-C2	-2.37	120.49	122.69
3	L5	1871	A2M	C6-C5-C4	-2.37	113.95	117.18
3	L5	1781	PSU	C6-N1-C2	-2.36	120.50	122.69
3	L5	4403	PSU	O2-C2-N1	-2.36	120.36	122.79
68	S2	668	A2M	C6-C5-C4	-2.33	113.99	117.18
3	L5	2351	OMC	C1'-N1-C2	2.33	123.58	118.44
3	L5	3808	OMC	C1'-N1-C2	2.32	123.57	118.44
3	L5	3637	PSU	C6-N1-C2	-2.32	120.54	122.69
3	L5	3637	PSU	C6-C5-C4	2.32	119.74	118.17
3	L5	4220	6MZ	C4-C5-C6	2.32	118.71	116.78
68	S2	428	OMU	O2-C2-N1	-2.32	119.78	122.80
3	L5	4293	PSU	C6-N1-C2	-2.31	120.55	122.69
3	L5	1323	A2M	O4'-C1'-C2'	2.31	110.57	106.59
3	L5	2363	A2M	O4'-C1'-C2'	2.31	110.56	106.59
3	L5	4636	PSU	O4'-C1'-C2'	2.30	108.34	105.15
3	L5	1524	A2M	C1'-N9-C8	2.30	132.21	127.09
3	L5	4361	PSU	C6-N1-C2	-2.30	120.55	122.69
3	L5	4457	PSU	C6-N1-C2	-2.30	120.56	122.69
3	L5	4521	PSU	C6-C5-C4	2.29	119.72	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4973	PSU	C6-N1-C2	-2.29	120.56	122.69
68	S2	668	A2M	O3'-C3'-C4'	-2.29	104.50	111.08
3	L5	4571	A2M	C6-C5-C4	-2.29	114.06	117.18
3	L5	2401	A2M	C6-C5-C4	-2.28	114.06	117.18
3	L5	3785	A2M	C2-N1-C6	-2.28	114.98	118.73
3	L5	4403	PSU	O4'-C1'-C2'	2.28	108.31	105.15
3	L5	4220	6MZ	C5-C6-N1	2.28	120.60	118.15
3	L5	3825	A2M	C6-C5-C4	-2.28	114.07	117.18
3	L5	1534	A2M	O4'-C1'-C2'	2.28	110.51	106.59
3	L5	4636	PSU	C5-C6-N1	-2.27	118.98	122.14
68	S2	1248	B8N	O4'-C1'-C2'	2.27	108.29	105.15
68	S2	468	A2M	C6-C5-C4	-2.27	114.08	117.18
68	S2	1232	PSU	C6-C5-C4	2.26	119.70	118.17
68	S2	354	OMU	O2-C2-N1	-2.26	119.85	122.80
3	L5	1322	1MA	N1-C6-N6	2.26	125.38	119.71
68	S2	166	A2M	O4'-C1'-C2'	2.26	110.47	106.59
3	L5	4493	PSU	C6-N1-C2	-2.26	120.60	122.69
3	L5	3851	PSU	C6-N1-C2	-2.25	120.60	122.69
68	S2	468	A2M	O4'-C1'-C2'	2.25	110.47	106.59
3	L5	4972	PSU	O2-C2-N1	-2.25	120.47	122.79
68	S2	1639	G7M	N9-C8-N7	-2.25	107.02	112.48
3	L5	3822	PSU	O4'-C1'-C2'	2.25	108.26	105.15
68	S2	1081	PSU	C6-N1-C2	-2.24	120.61	122.69
3	L5	2787	A2M	C4-N9-C1'	-2.24	121.39	126.63
3	L5	400	A2M	C6-C5-C4	-2.24	114.12	117.18
3	L5	1326	A2M	O4'-C1'-C2'	2.23	110.42	106.59
3	L5	400	A2M	O4'-C1'-C2'	2.22	110.42	106.59
3	L5	4530	UR3	C6-N1-C2	-2.22	119.98	121.80
68	S2	1851	MA6	C1'-N9-C8	-2.22	122.17	127.09
3	L5	1326	A2M	C2'-C1'-N9	2.22	117.40	113.75
3	L5	2815	A2M	C4-N9-C1'	-2.22	121.45	126.63
3	L5	3867	A2M	C3'-C2'-C1'	-2.22	98.57	102.81
3	L5	3867	A2M	C6-C5-C4	-2.21	114.15	117.18
68	S2	105	PSU	C6-C5-C4	2.21	119.67	118.17
68	S2	799	OMU	C1'-N1-C2	2.21	121.57	117.59
3	L5	5001	PSU	C6-N1-C2	-2.21	120.64	122.69
3	L5	3830	A2M	C6-C5-C4	-2.21	114.16	117.18
3	L5	3867	A2M	O3'-C3'-C2'	2.21	117.36	111.19
3	L5	1323	A2M	C4-N9-C1'	-2.20	121.48	126.63
3	L5	3785	A2M	C5-C6-N1	2.20	123.09	117.51
68	S2	166	A2M	C6-C5-C4	-2.20	114.18	117.18
3	L5	400	A2M	C2'-C1'-N9	2.19	117.36	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	627	OMU	O2-C2-N1	-2.19	119.94	122.80
3	L5	3925	OMU	O2-C2-N1	-2.19	119.95	122.80
68	S2	116	OMU	O2-C2-N1	-2.19	119.95	122.80
3	L5	1677	PSU	C6-C5-C4	2.19	119.65	118.17
68	S2	1248	B8N	O4-C4-C5	-2.18	118.80	122.58
5	L8	69	PSU	O4'-C1'-C2'	2.17	108.16	105.15
68	S2	406	PSU	C6-C5-C4	2.17	119.64	118.17
3	L5	4227	OMU	O2-C2-N1	-2.17	119.98	122.80
3	L5	3785	A2M	C6-C5-C4	-2.16	114.22	117.18
68	S2	814	PSU	C6-N1-C2	-2.16	120.69	122.69
3	L5	1677	PSU	O4'-C1'-C2'	2.16	108.14	105.15
3	L5	2363	A2M	C6-C5-C4	-2.16	114.23	117.18
68	S2	99	A2M	C5-C6-N1	2.16	122.99	117.51
3	L5	2787	A2M	C1'-N9-C8	2.16	131.88	127.09
3	L5	2815	A2M	C1'-N9-C8	2.16	131.88	127.09
68	S2	159	A2M	C2'-C1'-N9	2.15	117.29	113.75
3	L5	1524	A2M	C6-C5-C4	-2.15	114.24	117.18
3	L5	1323	A2M	C1'-N9-C8	2.15	131.87	127.09
68	S2	1031	A2M	C6-C5-C4	-2.14	114.25	117.18
3	L5	2837	OMU	O2-C2-N1	-2.14	120.01	122.80
68	S2	99	A2M	C6-C5-C4	-2.14	114.26	117.18
68	S2	99	A2M	C2-N1-C6	-2.14	115.22	118.73
68	S2	1383	A2M	C6-C5-C4	-2.14	114.26	117.18
68	S2	576	A2M	C6-C5-C4	-2.14	114.26	117.18
3	L5	3867	A2M	C2-N1-C6	-2.14	115.22	118.73
68	S2	27	A2M	C6-C5-C4	-2.14	114.26	117.18
3	L5	3718	A2M	C6-C5-C4	-2.13	114.26	117.18
68	S2	172	OMU	O2-C2-N1	-2.13	120.02	122.80
3	L5	4442	PSU	O4'-C1'-C2'	2.13	108.10	105.15
3	L5	398	A2M	C6-C5-C4	-2.13	114.27	117.18
68	S2	651	PSU	C6-C5-C4	2.13	119.61	118.17
3	L5	1326	A2M	C6-C5-C4	-2.13	114.27	117.18
68	S2	1326	OMU	O2-C2-N1	-2.13	120.03	122.80
3	L5	2787	A2M	C3'-C2'-C1'	-2.12	98.74	102.81
3	L5	2815	A2M	C6-C5-C4	-2.12	114.28	117.18
3	L5	3785	A2M	O4'-C4'-C3'	2.12	109.36	105.15
3	L5	3637	PSU	O2-C2-N3	-2.12	118.10	121.86
68	S2	99	A2M	O4'-C1'-C2'	2.11	110.22	106.59
3	L5	3782	5MC	C1'-N1-C6	-2.11	117.68	121.15
3	L5	3785	A2M	O4'-C1'-N9	2.11	112.14	108.09
3	L5	1534	A2M	C6-C5-C4	-2.11	114.30	117.18
3	L5	4571	A2M	O4'-C1'-C2'	2.10	110.21	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1322	1MA	CM1-N1-C6	-2.10	116.89	120.15
3	L5	1871	A2M	C4'-O4'-C1'	-2.10	104.82	109.47
3	L5	2363	A2M	C5-C6-N1	2.09	122.83	117.51
68	S2	159	A2M	C2-N1-C6	-2.09	115.30	118.73
3	L5	4523	A2M	C6-C5-C4	-2.09	114.32	117.18
68	S2	1031	A2M	C5-C6-N1	2.09	122.82	117.51
3	L5	4523	A2M	C5-C6-N1	2.08	122.80	117.51
3	L5	2815	A2M	O4'-C1'-C2'	2.08	110.18	106.59
3	L5	1534	A2M	C2-N1-C6	-2.08	115.31	118.73
3	L5	3920	PSU	O4'-C1'-C2'	2.07	108.02	105.15
68	S2	1031	A2M	C2-N1-C6	-2.07	115.32	118.73
3	L5	4523	A2M	C2-N1-C6	-2.07	115.32	118.73
3	L5	400	A2M	C5-C6-N1	2.07	122.78	117.51
3	L5	4636	PSU	C6-N1-C2	-2.07	120.77	122.69
3	L5	4220	6MZ	C4-C5-N7	-2.07	108.21	110.58
3	L5	1323	A2M	C5-C6-N1	2.07	122.77	117.51
68	S2	166	A2M	C5-C6-N1	2.07	122.77	117.51
3	L5	1323	A2M	C2-N1-C6	-2.07	115.33	118.73
68	S2	121	OMU	O2-C2-N1	-2.07	120.11	122.80
3	L5	2815	A2M	C5-C6-N1	2.07	122.76	117.51
3	L5	3825	A2M	C2-N1-C6	-2.07	115.33	118.73
68	S2	484	A2M	C6-C5-C4	-2.07	114.36	117.18
3	L5	2401	A2M	C5-C6-N1	2.06	122.75	117.51
3	L5	4571	A2M	C5-C6-N1	2.06	122.75	117.51
3	L5	1326	A2M	C2-N1-C6	-2.06	115.35	118.73
3	L5	398	A2M	C5-C6-N1	2.06	122.74	117.51
3	L5	3867	A2M	C5-C6-N1	2.06	122.73	117.51
3	L5	2401	A2M	O4'-C1'-C2'	2.05	110.12	106.59
3	L5	1326	A2M	C5-C6-N1	2.05	122.73	117.51
68	S2	1832	6MZ	C1'-N9-C8	-2.05	122.54	127.09
3	L5	3718	A2M	C5-C6-N1	2.05	122.72	117.51
68	S2	1383	A2M	C2-N1-C6	-2.05	115.36	118.73
68	S2	109	PSU	C6-C5-C4	2.05	119.56	118.17
3	L5	2787	A2M	C6-C5-C4	-2.05	114.38	117.18
3	L5	3825	A2M	C5-C6-N1	2.04	122.70	117.51
3	L5	2401	A2M	C2-N1-C6	-2.04	115.37	118.73
68	S2	1248	B8N	C31-N3-C2	2.04	120.66	117.64
3	L5	2787	A2M	C5-C6-N1	2.04	122.70	117.51
3	L5	1323	A2M	C6-C5-C4	-2.04	114.39	117.18
3	L5	4571	A2M	C2'-C1'-N9	2.04	117.11	113.75
3	L5	3830	A2M	C5-C6-N1	2.04	122.69	117.51
68	S2	27	A2M	C5-C6-N1	2.04	122.69	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2787	A2M	C2-N1-C6	-2.04	115.39	118.73
3	L5	3884	PSU	C6-C5-C4	2.03	119.55	118.17
3	L5	3920	PSU	C6-C5-C4	2.03	119.54	118.17
68	S2	1383	A2M	C5-C6-N1	2.03	122.66	117.51
68	S2	484	A2M	O4'-C4'-C3'	2.03	109.18	105.15
3	L5	2815	A2M	C2-N1-C6	-2.03	115.40	118.73
68	S2	1367	PSU	C6-C5-C4	2.03	119.54	118.17
3	L5	3822	PSU	C6-C5-C4	2.02	119.54	118.17
68	S2	1081	PSU	O4'-C1'-C2'	2.02	107.95	105.15
3	L5	1534	A2M	C5-C6-N1	2.02	122.64	117.51
68	S2	484	A2M	C5-C6-N1	2.02	122.64	117.51
3	L5	3867	A2M	O4'-C1'-C2'	2.02	110.06	106.59
3	L5	4571	A2M	C2-N1-C6	-2.01	115.42	118.73
3	L5	400	A2M	C2-N1-C6	-2.01	115.43	118.73
68	S2	1056	PSU	O4'-C1'-C2'	2.01	107.93	105.15
68	S2	468	A2M	C5-C6-N1	2.01	122.61	117.51
3	L5	4576	PSU	O4'-C1'-C2'	2.01	107.93	105.15
68	S2	27	A2M	C2-N1-C6	-2.01	115.43	118.73
3	L5	4353	PSU	C6-C5-C4	2.01	119.53	118.17
3	L5	1524	A2M	C5-C6-N1	2.00	122.60	117.51
3	L5	3818	UY1	O4'-C1'-C2'	2.00	108.06	104.56

There are no chirality outliers.

All (130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L8	75	OMG	C1'-C2'-O2'-CM2
3	L5	1326	A2M	O4'-C4'-C5'-O5'
3	L5	1340	OMC	C1'-C2'-O2'-CM2
3	L5	1625	OMG	O4'-C4'-C5'-O5'
3	L5	2351	OMC	C1'-C2'-O2'-CM2
3	L5	2364	OMG	O4'-C4'-C5'-O5'
3	L5	2787	A2M	C1'-C2'-O2'-CM'
3	L5	3701	OMC	C2'-C1'-N1-C2
3	L5	3701	OMC	O4'-C4'-C5'-O5'
3	L5	3792	OMG	O4'-C4'-C5'-O5'
3	L5	4196	OMG	C1'-C2'-O2'-CM2
3	L5	4637	OMG	O4'-C4'-C5'-O5'
68	S2	159	A2M	C1'-C2'-O2'-CM'
68	S2	166	A2M	C1'-C2'-O2'-CM'
68	S2	428	OMU	C2'-C1'-N1-C6
68	S2	462	OMC	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
68	S2	468	A2M	C1'-C2'-O2'-CM'
68	S2	601	OMG	C1'-C2'-O2'-CM2
68	S2	644	OMG	O4'-C4'-C5'-O5'
68	S2	801	PSU	C3'-C4'-C5'-O5'
68	S2	867	OMG	O4'-C4'-C5'-O5'
68	S2	1248	B8N	N34-C33-C34-O35
68	S2	1328	OMG	C1'-C2'-O2'-CM2
68	S2	1832	6MZ	C5-C6-N6-C9
68	S2	1832	6MZ	N1-C6-N6-C9
68	S2	428	OMU	C2'-C1'-N1-C2
3	L5	1536	PSU	C3'-C4'-C5'-O5'
3	L5	2815	A2M	O4'-C4'-C5'-O5'
3	L5	3867	A2M	C3'-C4'-C5'-O5'
3	L5	3899	OMG	O4'-C4'-C5'-O5'
3	L5	3899	OMG	C3'-C4'-C5'-O5'
3	L5	4500	PSU	O4'-C4'-C5'-O5'
3	L5	4590	A2M	O4'-C4'-C5'-O5'
3	L5	4590	A2M	C3'-C4'-C5'-O5'
68	S2	99	A2M	O4'-C4'-C5'-O5'
68	S2	867	OMG	C3'-C4'-C5'-O5'
68	S2	1442	OMU	O4'-C4'-C5'-O5'
3	L5	3701	OMC	C2'-C1'-N1-C6
3	L5	1326	A2M	C3'-C4'-C5'-O5'
3	L5	1536	PSU	O4'-C4'-C5'-O5'
3	L5	1625	OMG	C3'-C4'-C5'-O5'
3	L5	3701	OMC	C3'-C4'-C5'-O5'
3	L5	4220	6MZ	O4'-C4'-C5'-O5'
3	L5	4220	6MZ	C3'-C4'-C5'-O5'
3	L5	4500	PSU	C3'-C4'-C5'-O5'
68	S2	428	OMU	C3'-C4'-C5'-O5'
68	S2	428	OMU	O4'-C4'-C5'-O5'
68	S2	799	OMU	C3'-C4'-C5'-O5'
68	S2	799	OMU	O4'-C4'-C5'-O5'
68	S2	801	PSU	O4'-C4'-C5'-O5'
68	S2	1045	PSU	C3'-C4'-C5'-O5'
68	S2	1045	PSU	O4'-C4'-C5'-O5'
68	S2	1442	OMU	C3'-C4'-C5'-O5'
68	S2	1248	B8N	N34-C33-C34-O36
3	L5	2787	A2M	C3'-C2'-O2'-CM'
3	L5	2364	OMG	C3'-C4'-C5'-O5'
3	L5	3792	OMG	C3'-C4'-C5'-O5'
3	L5	4637	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
68	S2	644	OMG	C3'-C4'-C5'-O5'
3	L5	2815	A2M	C3'-C4'-C5'-O5'
68	S2	99	A2M	C3'-C4'-C5'-O5'
68	S2	627	OMU	C3'-C4'-C5'-O5'
68	S2	668	A2M	O4'-C4'-C5'-O5'
3	L5	1524	A2M	O4'-C4'-C5'-O5'
3	L5	2787	A2M	C3'-C4'-C5'-O5'
3	L5	3867	A2M	O4'-C4'-C5'-O5'
68	S2	172	OMU	O4'-C4'-C5'-O5'
68	S2	627	OMU	O4'-C4'-C5'-O5'
68	S2	668	A2M	C3'-C4'-C5'-O5'
3	L5	1524	A2M	C3'-C4'-C5'-O5'
3	L5	1582	PSU	C3'-C4'-C5'-O5'
68	S2	576	A2M	O4'-C4'-C5'-O5'
68	S2	576	A2M	C3'-C4'-C5'-O5'
3	L5	2422	OMC	O4'-C4'-C5'-O5'
3	L5	2787	A2M	C2'-C1'-N9-C8
3	L5	2422	OMC	C3'-C4'-C5'-O5'
3	L5	4590	A2M	C4'-C5'-O5'-P
3	L5	1323	A2M	O4'-C4'-C5'-O5'
3	L5	3818	UY1	C4'-C5'-O5'-P
3	L5	2839	PSU	C3'-C4'-C5'-O5'
3	L5	4618	OMG	C3'-C4'-C5'-O5'
68	S2	172	OMU	C3'-C4'-C5'-O5'
3	L5	3782	5MC	O4'-C4'-C5'-O5'
3	L5	4228	OMG	O4'-C4'-C5'-O5'
68	S2	1244	PSU	O4'-C4'-C5'-O5'
68	S2	576	A2M	C4'-C5'-O5'-P
3	L5	1326	A2M	C4'-C5'-O5'-P
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	3818	UY1	O4'-C1'-C5-C4
68	S2	1248	B8N	O4'-C1'-C5-C4
3	L5	2787	A2M	C2'-C1'-N9-C4
68	S2	428	OMU	O4'-C1'-N1-C2
3	L5	2839	PSU	O4'-C4'-C5'-O5'
3	L5	4228	OMG	C3'-C4'-C5'-O5'
3	L5	3887	OMC	C4'-C5'-O5'-P
68	S2	644	OMG	C4'-C5'-O5'-P
68	S2	1081	PSU	C4'-C5'-O5'-P
3	L5	1322	1MA	C2'-C1'-N9-C8
68	S2	428	OMU	O4'-C1'-N1-C6
3	L5	4500	PSU	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
68	S2	1490	OMG	C4'-C5'-O5'-P
3	L5	2401	A2M	C3'-C2'-O2'-CM'
3	L5	1322	1MA	C2'-C1'-N9-C4
5	L8	69	PSU	O4'-C4'-C5'-O5'
3	L5	1582	PSU	O4'-C4'-C5'-O5'
3	L5	1781	PSU	C3'-C4'-C5'-O5'
3	L5	4447	5MC	O4'-C1'-N1-C6
5	L8	75	OMG	C4'-C5'-O5'-P
3	L5	3844	PSU	C4'-C5'-O5'-P
68	S2	1851	MA6	C4'-C5'-O5'-P
3	L5	398	A2M	O4'-C4'-C5'-O5'
3	L5	3701	OMC	O4'-C1'-N1-C6
3	L5	4637	OMG	C1'-C2'-O2'-CM2
68	S2	668	A2M	C1'-C2'-O2'-CM'
3	L5	4623	OMG	C3'-C4'-C5'-O5'
68	S2	1046	PSU	O4'-C4'-C5'-O5'
3	L5	3818	UY1	O4'-C1'-C5-C6
3	L5	4636	PSU	O4'-C1'-C5-C6
3	L5	4370	OMG	C3'-C2'-O2'-CM2
3	L5	4618	OMG	O4'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C6
3	L5	1792	PSU	O4'-C4'-C5'-O5'
3	L5	2787	A2M	O4'-C1'-N9-C8
3	L5	3785	A2M	C3'-C2'-O2'-CM'
3	L5	3869	OMC	C3'-C2'-O2'-CM2
3	L5	2632	PSU	C3'-C4'-C5'-O5'
3	L5	3701	OMC	O4'-C1'-N1-C2
3	L5	4447	5MC	O4'-C1'-N1-C2
68	S2	668	A2M	O4'-C1'-N9-C8
3	L5	2351	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

61 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	1871	A2M	1	0
3	L5	4620	OMU	1	0
5	L8	75	OMG	1	0
3	L5	3701	OMC	1	0
3	L5	2839	PSU	1	0
68	S2	1174	PSU	1	0
68	S2	1004	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	S2	1832	6MZ	1	0
68	S2	1031	A2M	1	0
3	L5	4579	PSU	1	0
3	L5	1534	A2M	2	0
3	L5	4447	5MC	1	0
68	S2	166	A2M	4	0
3	L5	4571	A2M	2	0
68	S2	468	A2M	2	0
68	S2	601	OMG	1	0
3	L5	5001	PSU	1	0
3	L5	400	A2M	1	0
3	L5	2351	OMC	1	0
68	S2	27	A2M	1	0
68	S2	1328	OMG	1	0
3	L5	1625	OMG	1	0
68	S2	576	A2M	1	0
68	S2	801	PSU	1	0
68	S2	116	OMU	4	0
3	L5	2422	OMC	1	0
3	L5	4523	A2M	1	0
3	L5	4220	6MZ	1	0
3	L5	4689	PSU	1	0
68	S2	681	PSU	1	0
3	L5	4637	OMG	1	0
3	L5	2363	A2M	1	0
3	L5	3825	A2M	1	0
3	L5	4457	PSU	1	0
68	S2	867	OMG	1	0
3	L5	3841	OMC	1	0
68	S2	509	OMG	4	0
68	S2	1383	A2M	1	0
3	L5	4618	OMG	1	0
3	L5	398	A2M	1	0
3	L5	3920	PSU	1	0
68	S2	644	OMG	1	0
3	L5	1683	PSU	1	0
3	L5	2424	OMG	1	0
68	S2	1703	OMC	1	0
3	L5	4196	OMG	1	0
3	L5	4392	OMG	2	0
68	S2	484	A2M	1	0
3	L5	4536	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3887	OMC	1	0
68	S2	159	A2M	2	0
68	S2	1850	MA6	1	0
3	L5	1340	OMC	2	0
3	L5	4456	OMC	1	0
3	L5	3718	A2M	2	0
3	L5	4293	PSU	1	0
3	L5	1326	A2M	1	0
68	S2	649	PSU	2	0
68	S2	1337	4AC	1	0
3	L5	3867	A2M	4	0
3	L5	4530	UR3	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 241 ligands modelled in this entry, 224 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
89	SPD	L5	5287	-	9,9,9	0.30	0	8,8,8	0.82	0
89	SPD	L5	5261	-	9,9,9	0.33	0	8,8,8	1.10	0
89	SPD	L5	5283	-	9,9,9	0.31	0	8,8,8	0.83	0
88	SPM	L5	5259	-	13,13,13	0.37	0	12,12,12	1.03	0
89	SPD	L5	5284	-	9,9,9	0.30	0	8,8,8	0.82	0
89	SPD	L5	5285	-	9,9,9	0.33	0	8,8,8	0.94	0
89	SPD	L5	5290	-	9,9,9	0.31	0	8,8,8	0.83	0
89	SPD	L5	5291	-	9,9,9	0.31	0	8,8,8	0.73	0
88	SPM	L5	5263	-	13,13,13	0.34	0	12,12,12	1.02	0
88	SPM	L5	5264	-	13,13,13	0.36	0	12,12,12	1.04	0
88	SPM	L5	5289	-	13,13,13	0.37	0	12,12,12	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	SPD	L5	5293	-	9,9,9	0.35	0	8,8,8	0.92	0
89	SPD	L5	5288	-	9,9,9	0.33	0	8,8,8	0.76	0
88	SPM	L5	5294	-	13,13,13	0.35	0	12,12,12	0.81	0
89	SPD	L5	5286	-	9,9,9	0.34	0	8,8,8	0.84	0
88	SPM	L5	5292	-	13,13,13	0.37	0	12,12,12	0.80	0
88	SPM	L5	5267	-	13,13,13	0.37	0	12,12,12	0.95	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPD	L5	5287	-	-	1/7/7/7	-
89	SPD	L5	5261	-	-	0/7/7/7	-
89	SPD	L5	5283	-	-	0/7/7/7	-
88	SPM	L5	5259	-	-	3/11/11/11	-
89	SPD	L5	5284	-	-	2/7/7/7	-
89	SPD	L5	5285	-	-	5/7/7/7	-
89	SPD	L5	5290	-	-	3/7/7/7	-
89	SPD	L5	5291	-	-	4/7/7/7	-
88	SPM	L5	5263	-	-	4/11/11/11	-
88	SPM	L5	5264	-	-	2/11/11/11	-
88	SPM	L5	5289	-	-	5/11/11/11	-
89	SPD	L5	5293	-	-	1/7/7/7	-
89	SPD	L5	5288	-	-	1/7/7/7	-
88	SPM	L5	5294	-	-	6/11/11/11	-
89	SPD	L5	5286	-	-	2/7/7/7	-
88	SPM	L5	5292	-	-	6/11/11/11	-
88	SPM	L5	5267	-	-	4/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	L5	5292	SPM	C7-C8-C9-N10

Continued on next page...

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Mol	Chain	Res	Type	Atoms
88	L5	5292	SPM	N5-C6-C7-C8
88	L5	5264	SPM	C2-C3-C4-N5
88	L5	5292	SPM	C6-C7-C8-C9
88	L5	5292	SPM	N10-C11-C12-C13
88	L5	5267	SPM	C7-C8-C9-N10
88	L5	5263	SPM	N10-C11-C12-C13
89	L5	5285	SPD	N6-C7-C8-C9
88	L5	5263	SPM	N5-C6-C7-C8
88	L5	5294	SPM	C8-C9-N10-C11
89	L5	5286	SPD	C3-C4-C5-N6
89	L5	5285	SPD	C3-C4-C5-N6
88	L5	5263	SPM	C7-C6-N5-C4
89	L5	5288	SPD	C2-C3-C4-C5
88	L5	5289	SPM	C12-C11-N10-C9
89	L5	5291	SPD	C8-C7-N6-C5
88	L5	5267	SPM	C6-C7-C8-C9
89	L5	5285	SPD	C2-C3-C4-C5
88	L5	5289	SPM	C2-C3-C4-N5
88	L5	5259	SPM	C6-C7-C8-C9
88	L5	5294	SPM	C6-C7-C8-C9
89	L5	5286	SPD	C2-C3-C4-C5
88	L5	5289	SPM	C7-C6-N5-C4
88	L5	5289	SPM	C8-C9-N10-C11
88	L5	5263	SPM	C11-C12-C13-N14
88	L5	5294	SPM	C11-C12-C13-N14
89	L5	5291	SPD	C7-C8-C9-N10
89	L5	5290	SPD	N1-C2-C3-C4
89	L5	5287	SPD	C4-C5-N6-C7
89	L5	5291	SPD	N6-C7-C8-C9
88	L5	5294	SPM	N10-C11-C12-C13
88	L5	5264	SPM	N1-C2-C3-C4
88	L5	5289	SPM	N1-C2-C3-C4
88	L5	5292	SPM	N1-C2-C3-C4
89	L5	5285	SPD	C7-C8-C9-N10
88	L5	5292	SPM	C3-C4-N5-C6
88	L5	5294	SPM	C3-C4-N5-C6
89	L5	5290	SPD	C2-C3-C4-C5
89	L5	5284	SPD	C3-C4-C5-N6
89	L5	5291	SPD	C4-C5-N6-C7
88	L5	5259	SPM	C3-C4-N5-C6
89	L5	5285	SPD	C4-C5-N6-C7
88	L5	5267	SPM	C8-C9-N10-C11

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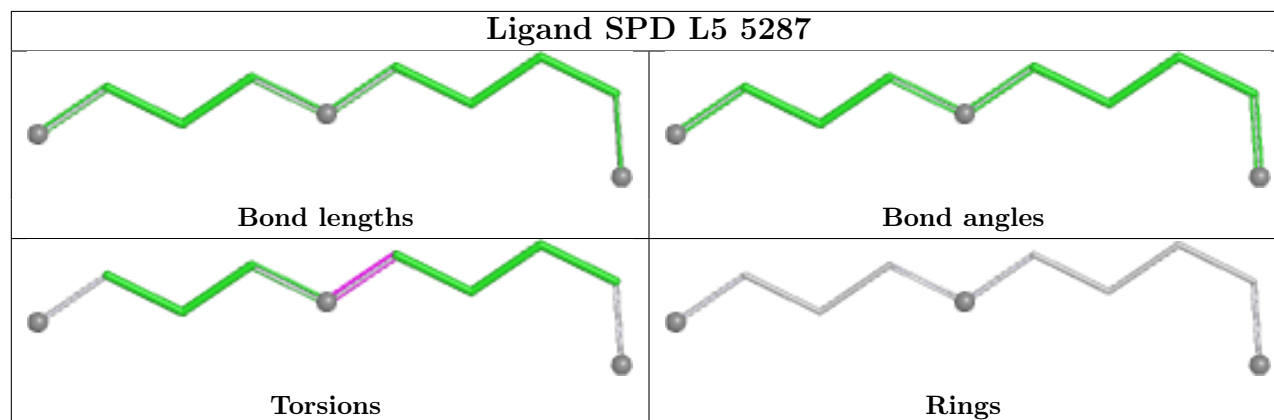
Mol	Chain	Res	Type	Atoms
88	L5	5294	SPM	C7-C6-N5-C4
89	L5	5284	SPD	C8-C7-N6-C5
89	L5	5293	SPD	C8-C7-N6-C5
88	L5	5259	SPM	N5-C6-C7-C8
88	L5	5267	SPM	C11-C12-C13-N14
89	L5	5290	SPD	N6-C7-C8-C9

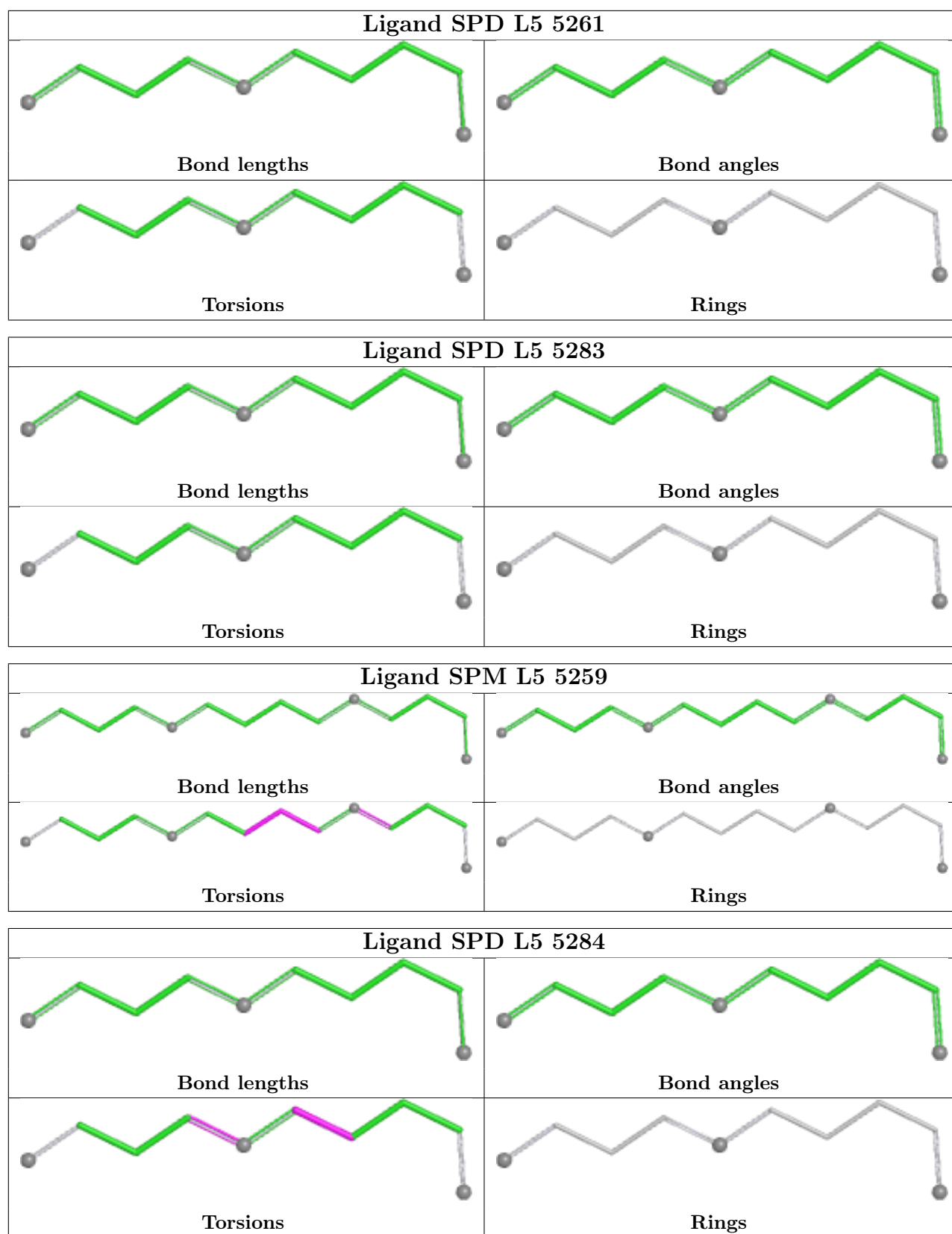
There are no ring outliers.

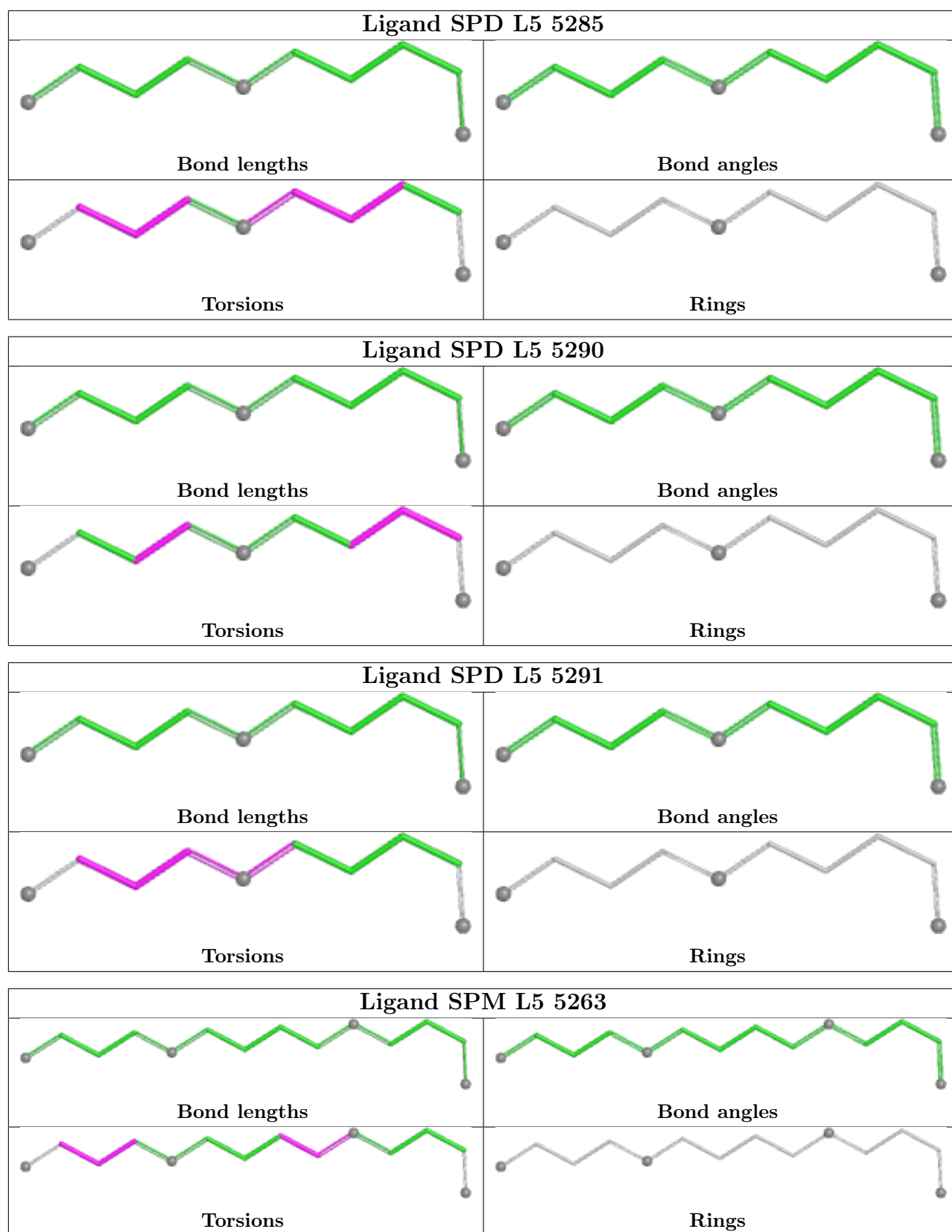
3 monomers are involved in 5 short contacts:

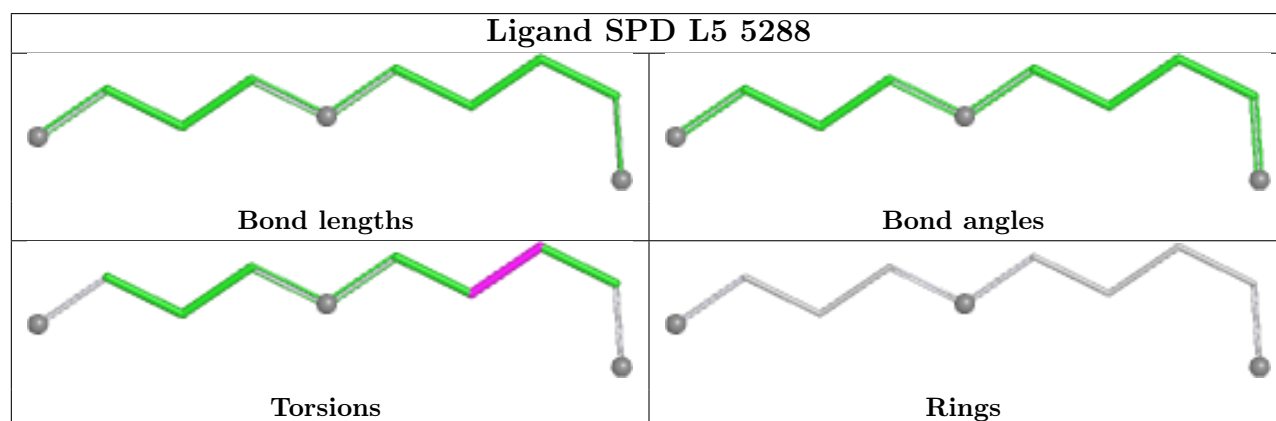
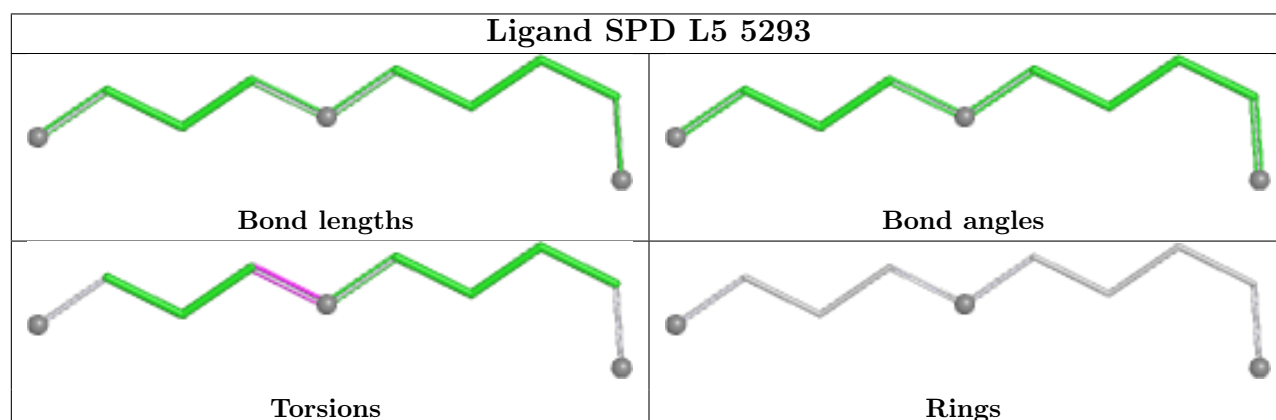
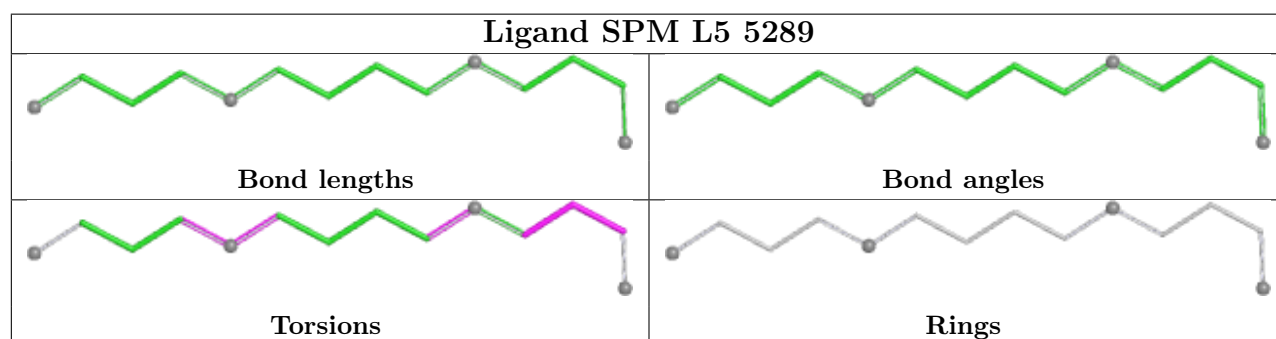
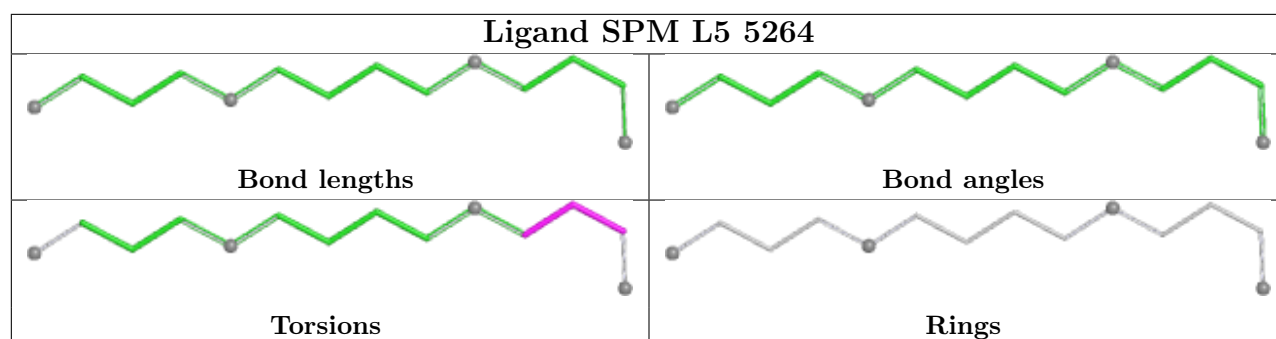
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	L5	5290	SPD	1	0
89	L5	5291	SPD	1	0
88	L5	5294	SPM	3	0

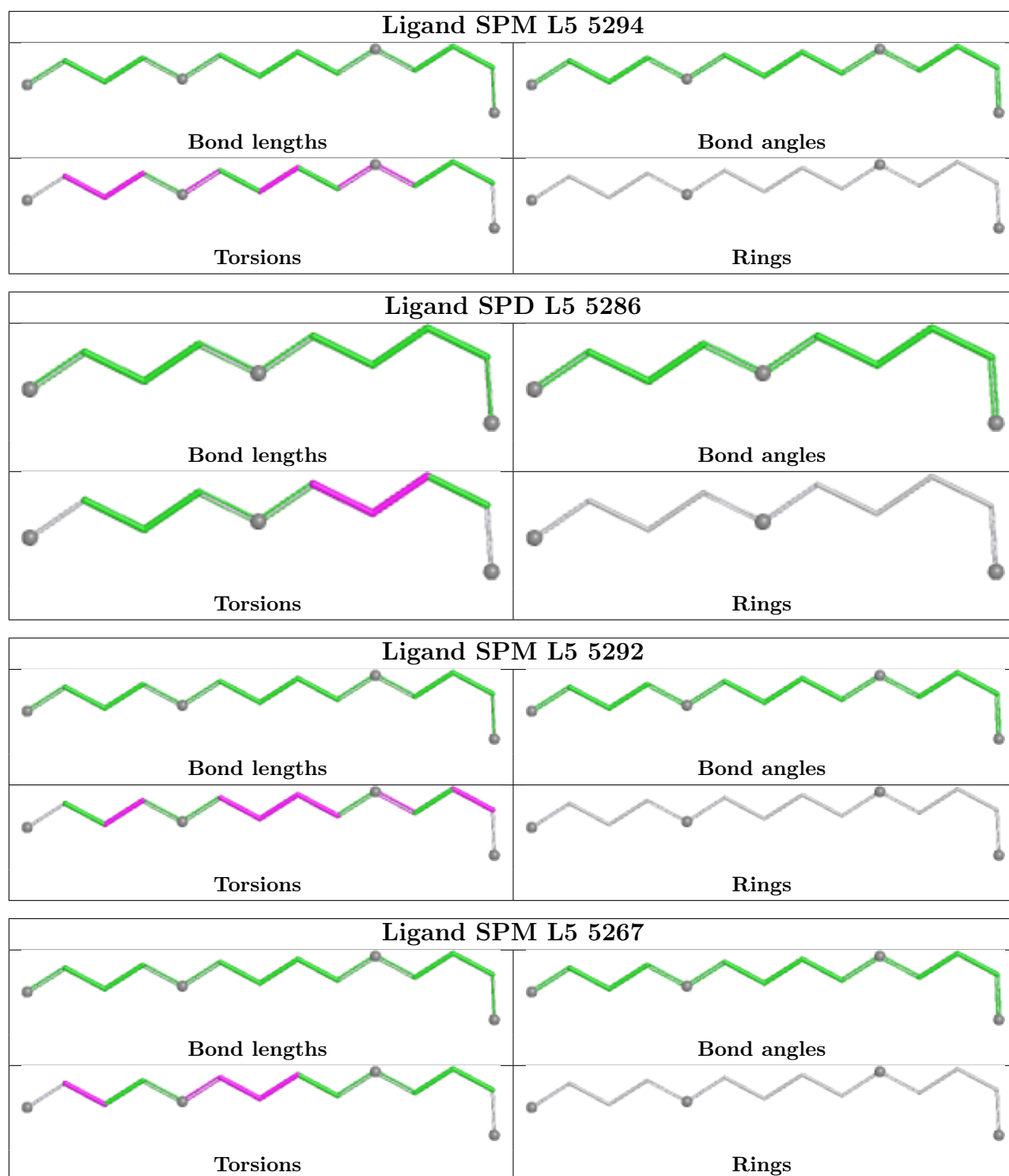
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
68	S2	4
84	Et	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	28.62
1	S2	698:G	O3'	730:C	P	14.26
1	S2	739:C	O3'	746:C	P	13.18
1	Et	16:C	O3'	18:U	P	7.21
1	S2	225:G	O3'	287:U	P	6.80

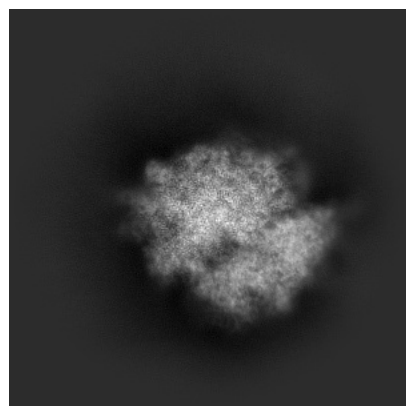
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71338. These allow visual inspection of the internal detail of the map and identification of artifacts.

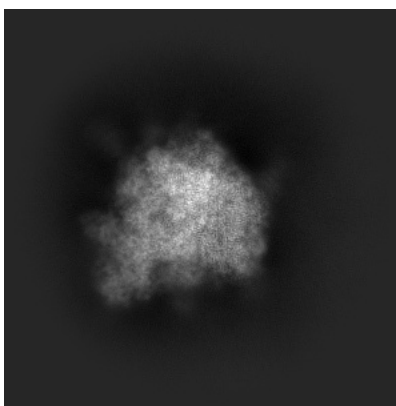
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

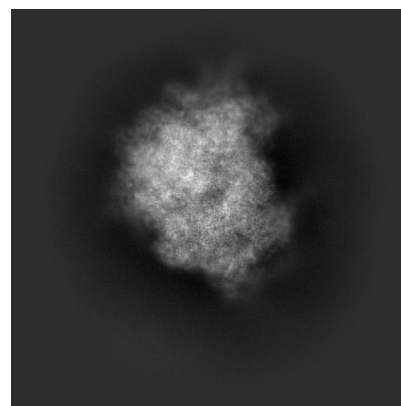
6.1.1 Primary map



X

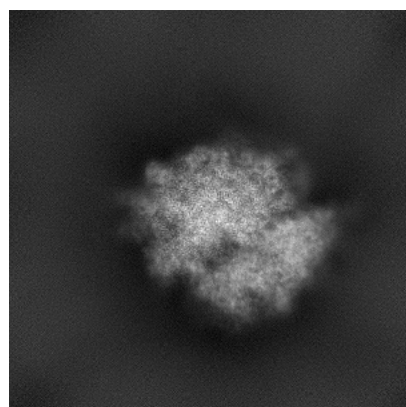


Y

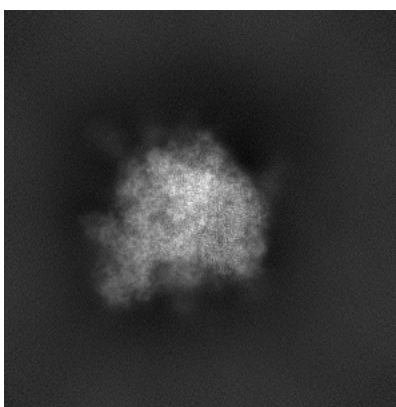


Z

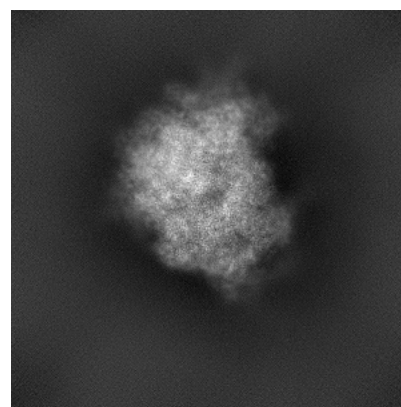
6.1.2 Raw map



X



Y

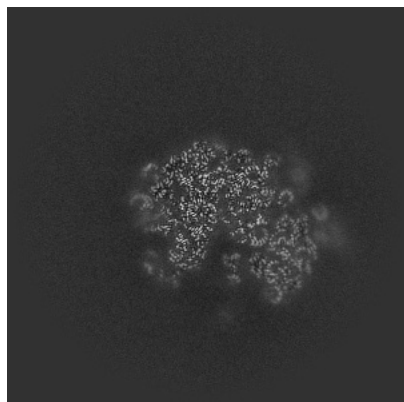


Z

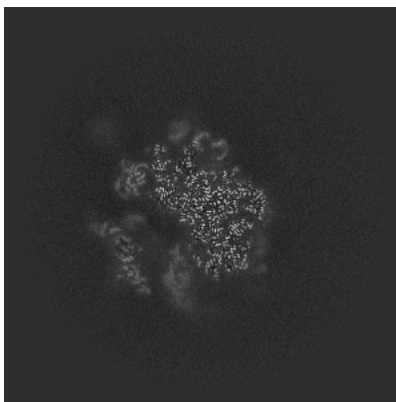
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

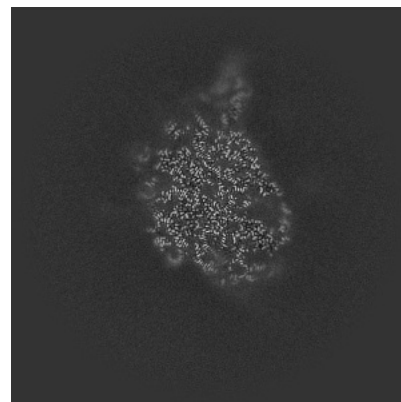
6.2.1 Primary map



X Index: 256

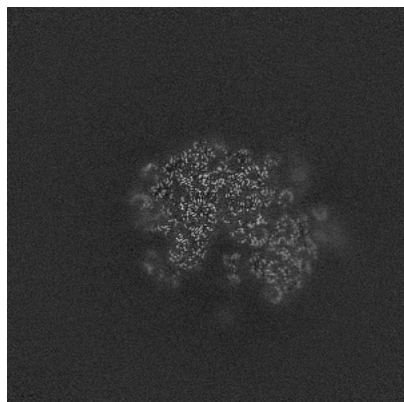


Y Index: 256

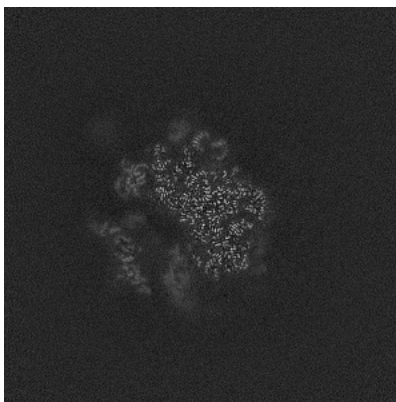


Z Index: 256

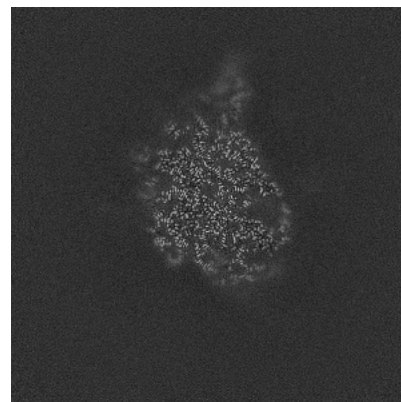
6.2.2 Raw map



X Index: 256



Y Index: 256

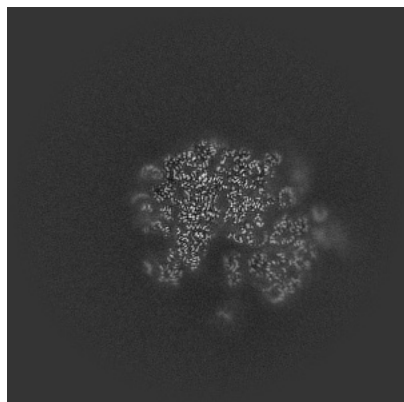


Z Index: 256

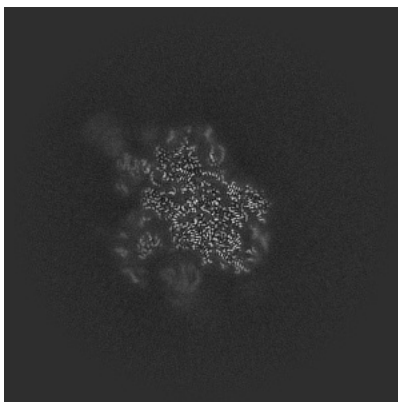
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

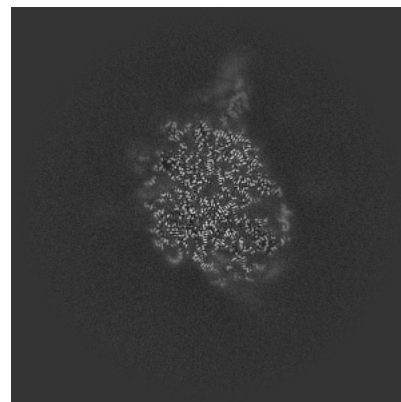
6.3.1 Primary map



X Index: 253

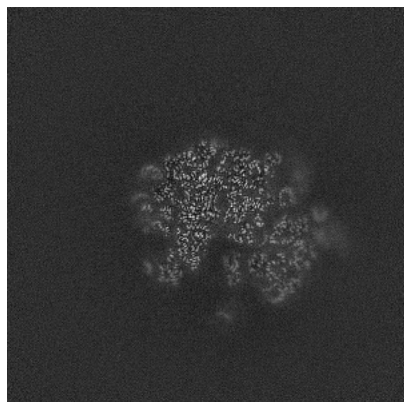


Y Index: 243

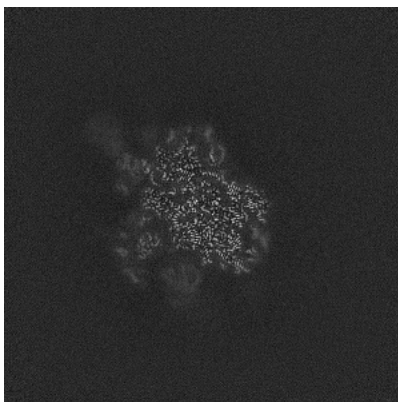


Z Index: 258

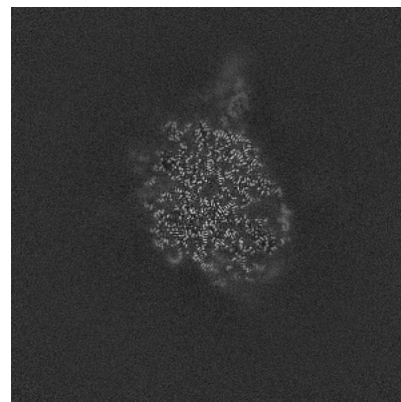
6.3.2 Raw map



X Index: 253



Y Index: 243

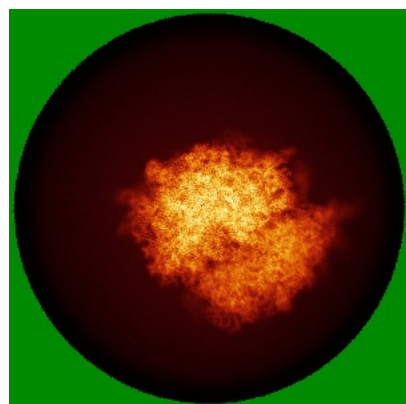


Z Index: 258

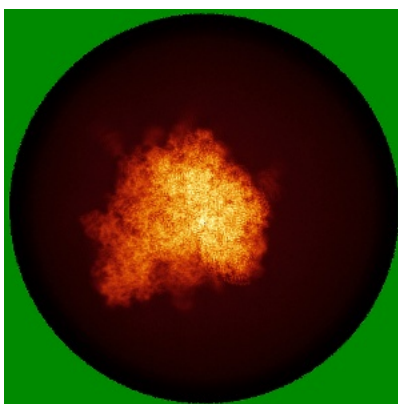
The images above show the largest variance slices of the map in three orthogonal directions.

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

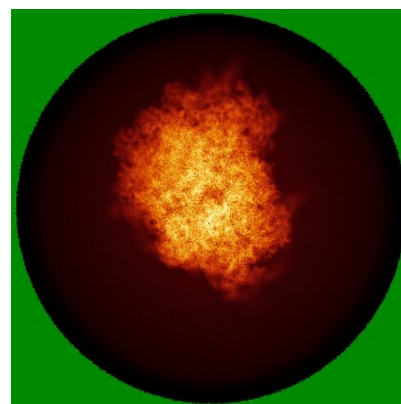
6.4.1 Primary map



X

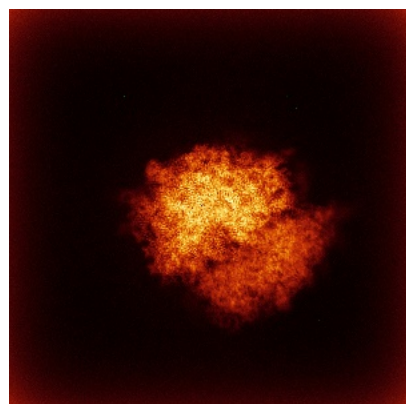


Y

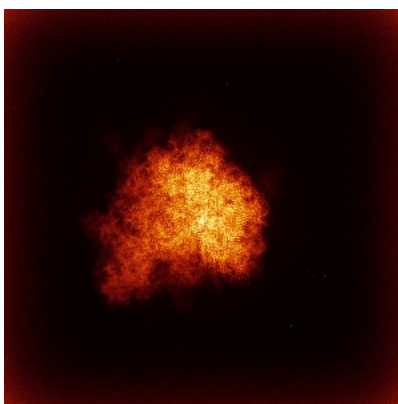


Z

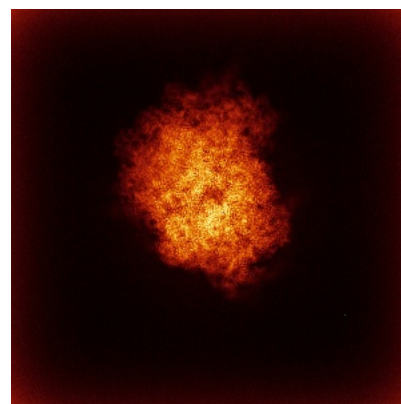
6.4.2 Raw map



X



Y

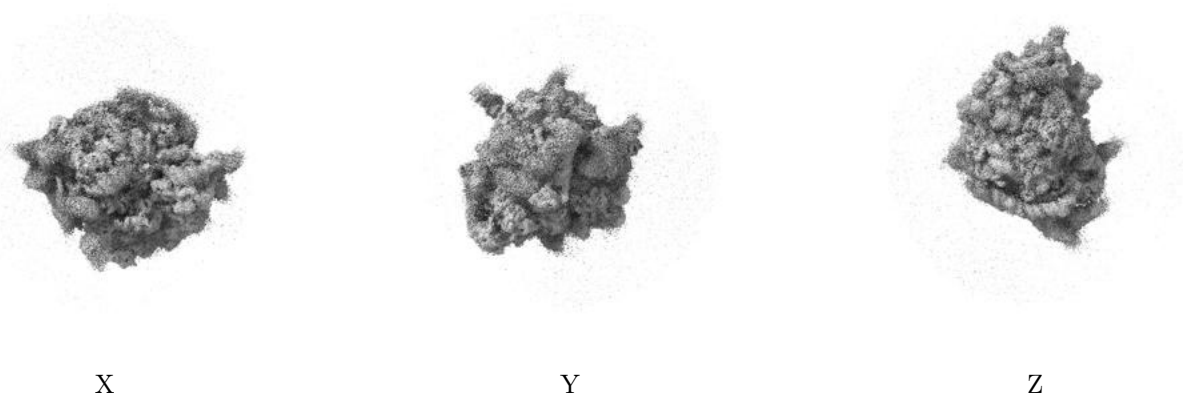


Z

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

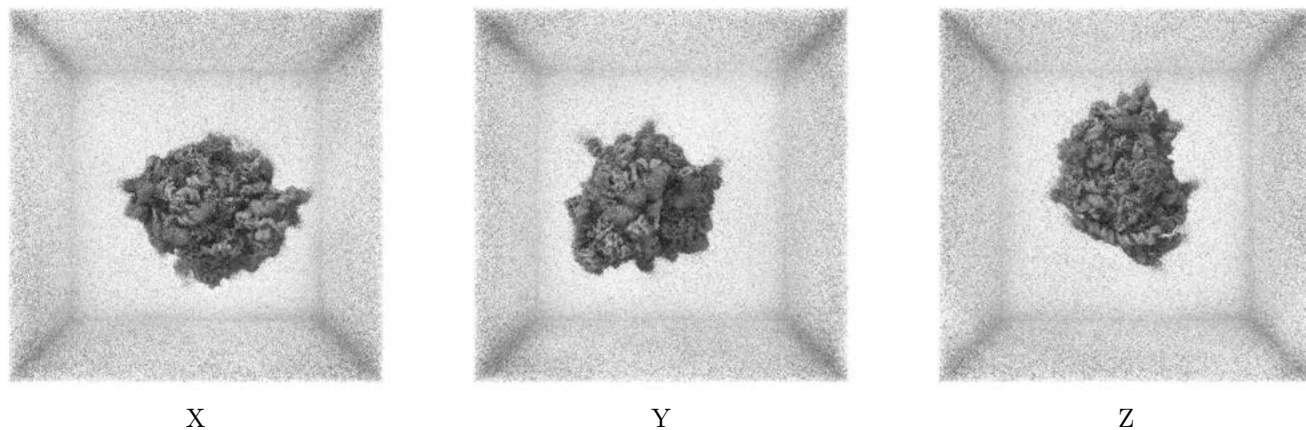
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0145. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

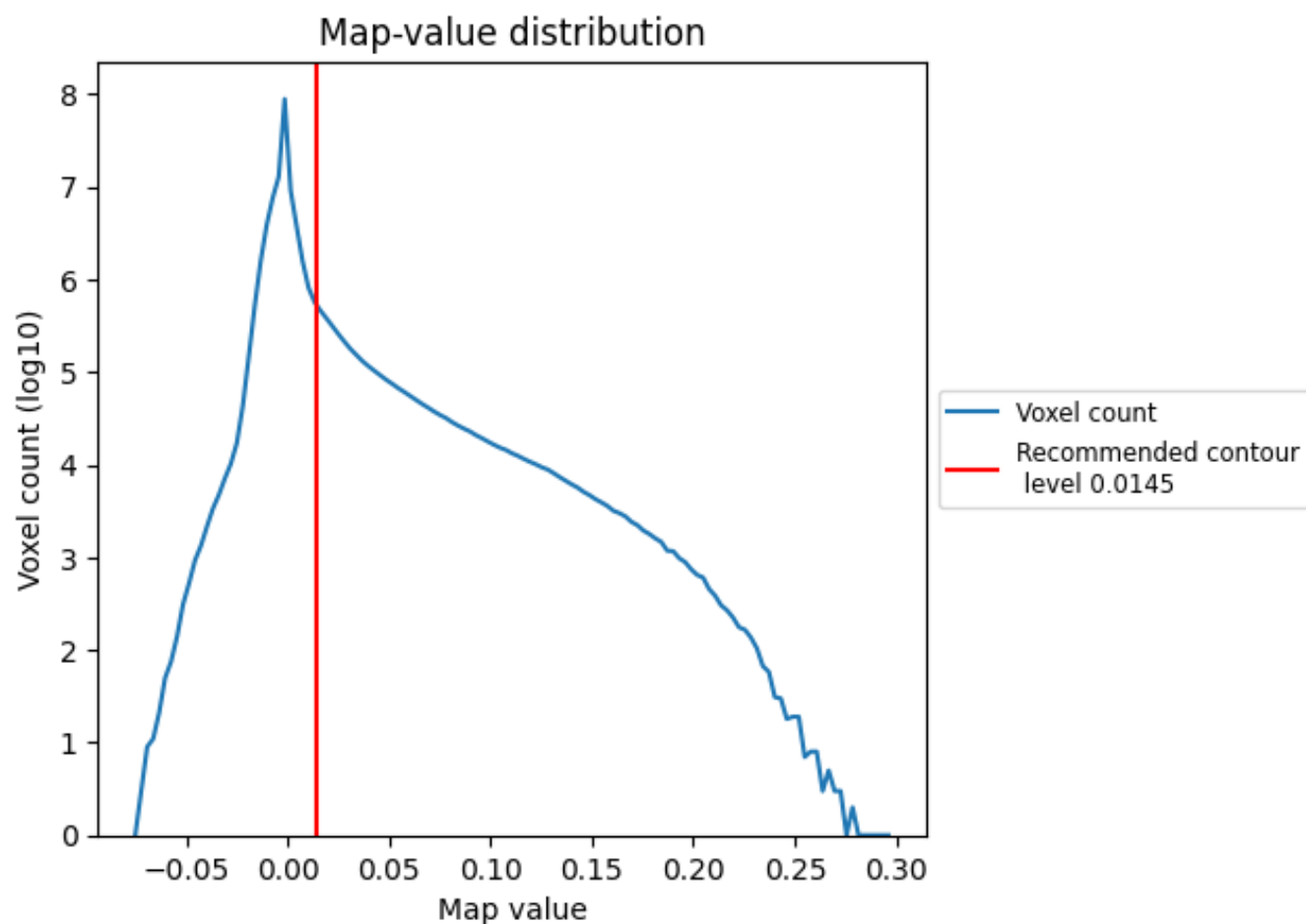
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

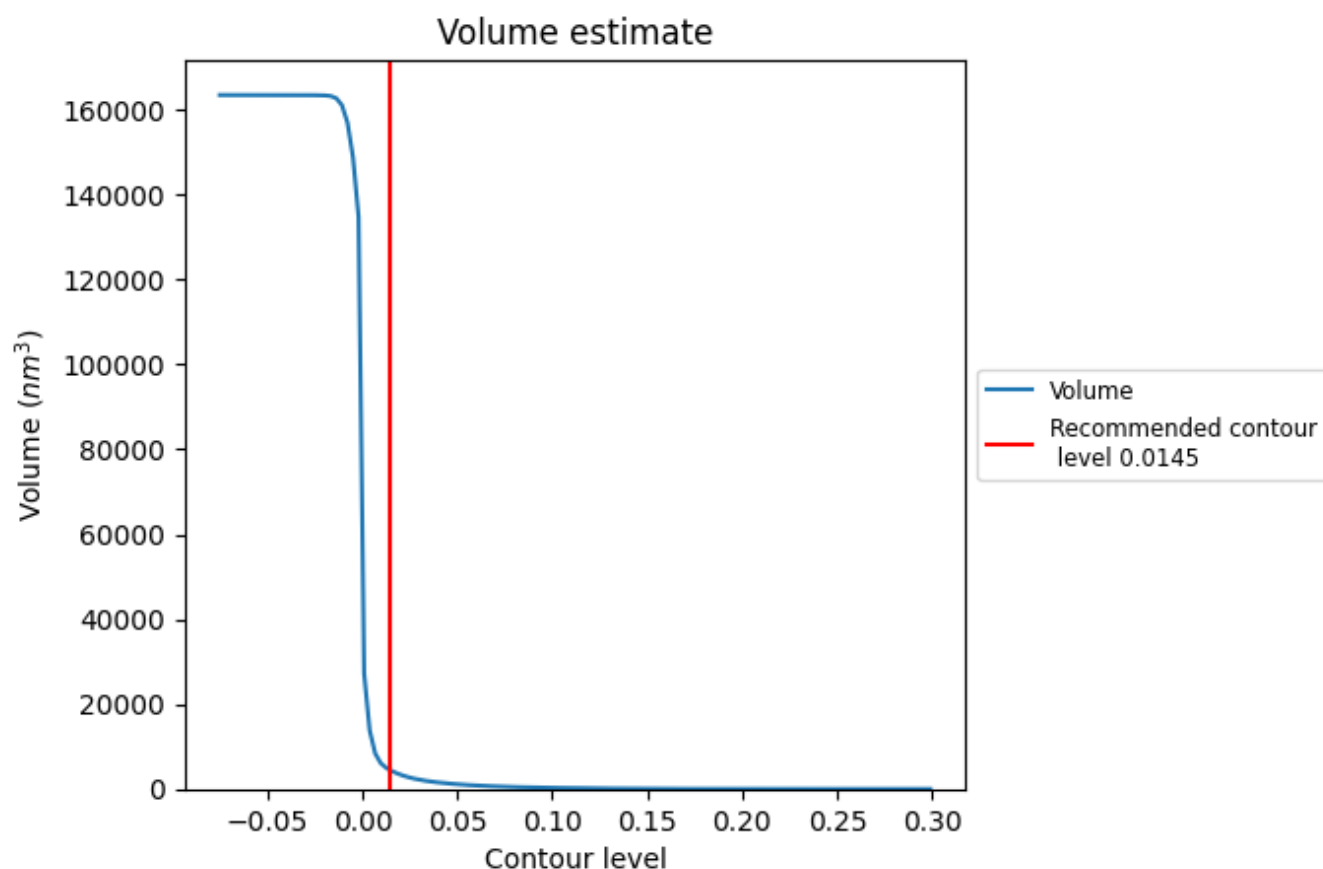
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

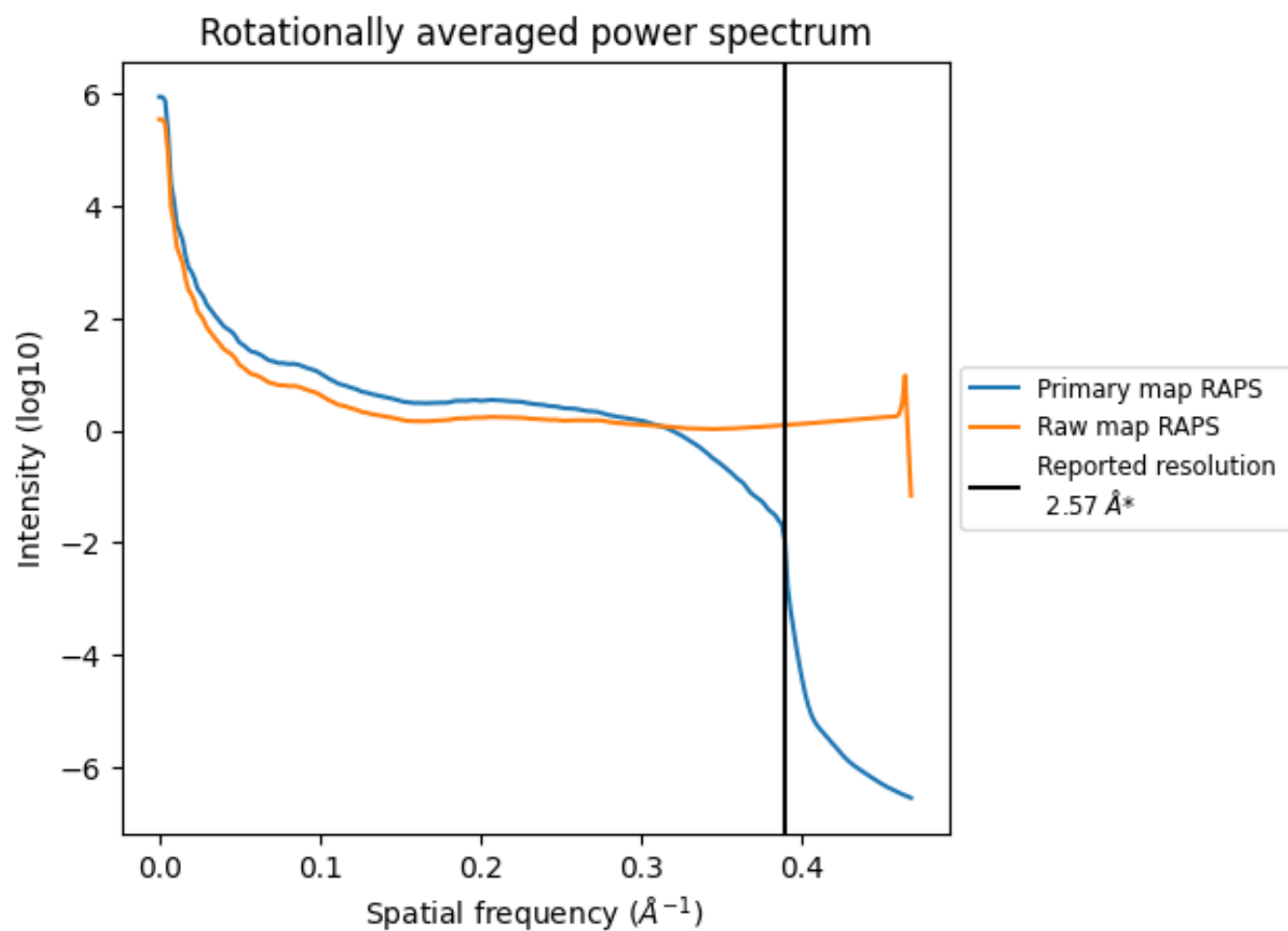
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4470 nm³; this corresponds to an approximate mass of 4038 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 ⓘ

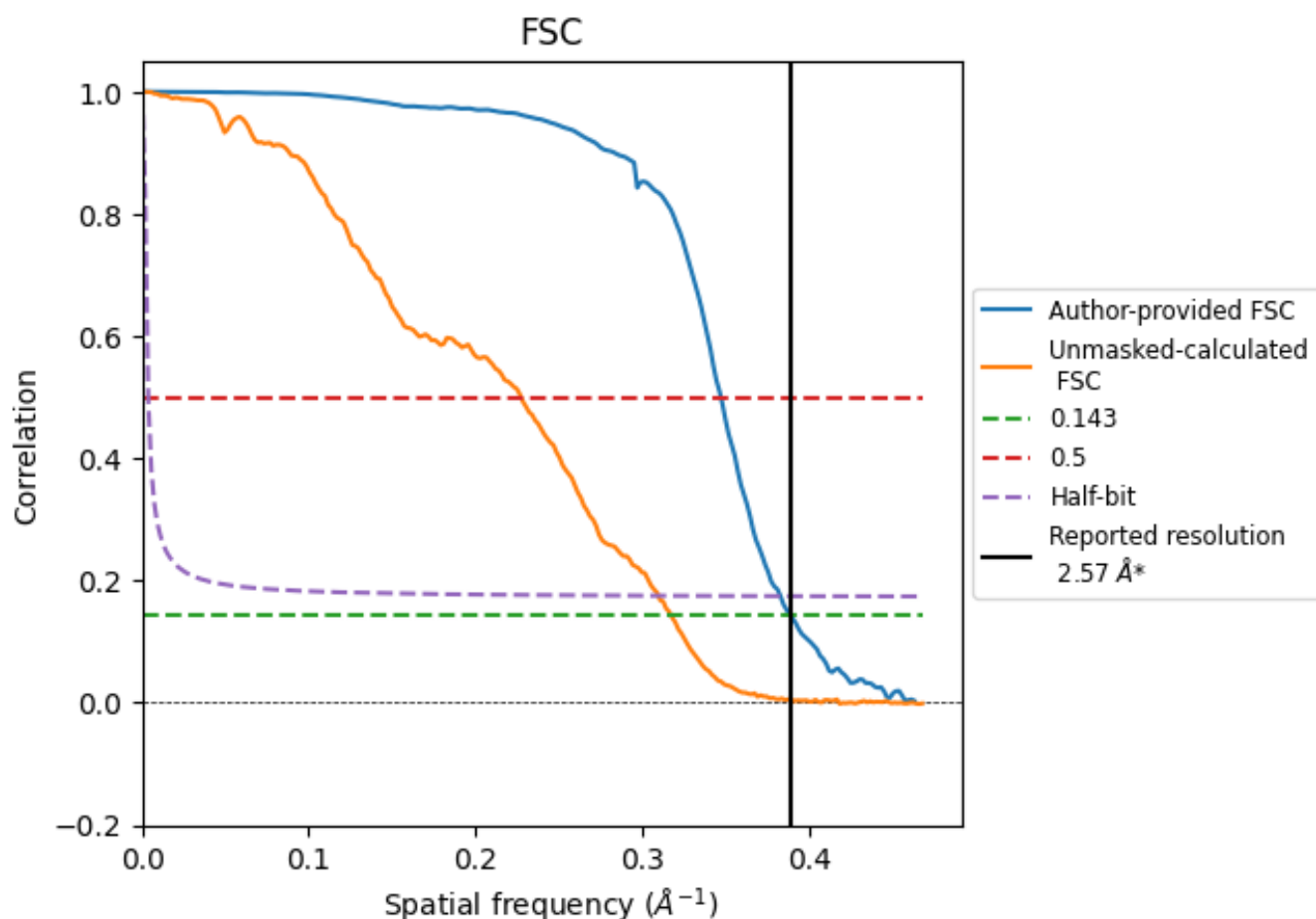


*Reported resolution corresponds to spatial frequency of 0.389 Å⁻¹

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 0.389 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

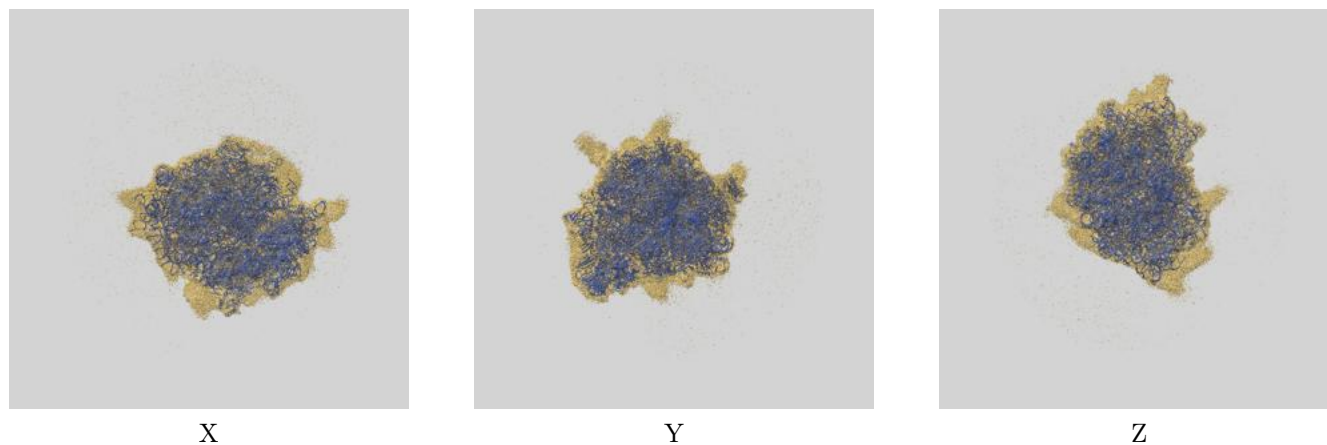
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.57	-	-
Author-provided FSC curve	2.57	2.88	2.61
Unmasked-calculated*	3.15	4.40	3.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.15 differs from the reported value 2.57 by more than 10 %

9 Map-model fit [i](#)

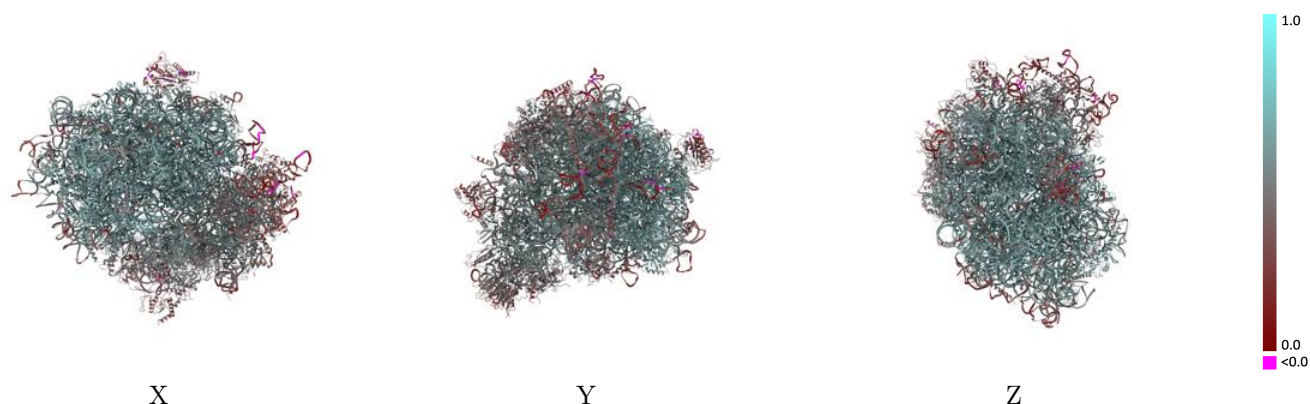
This section contains information regarding the fit between EMDB map EMD-71338 and PDB model 9P7D. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



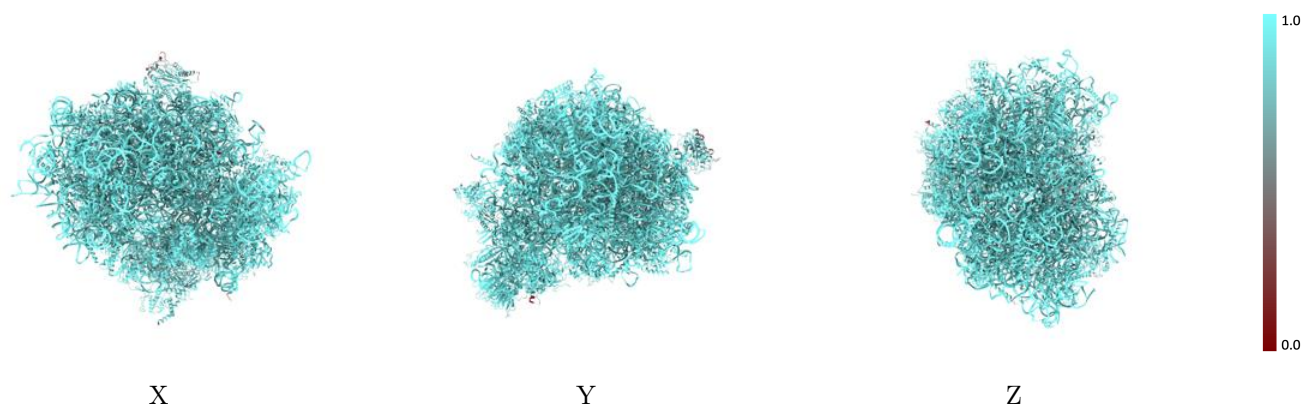
The images above show the 3D surface view of the map at the recommended contour level 0.0145 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



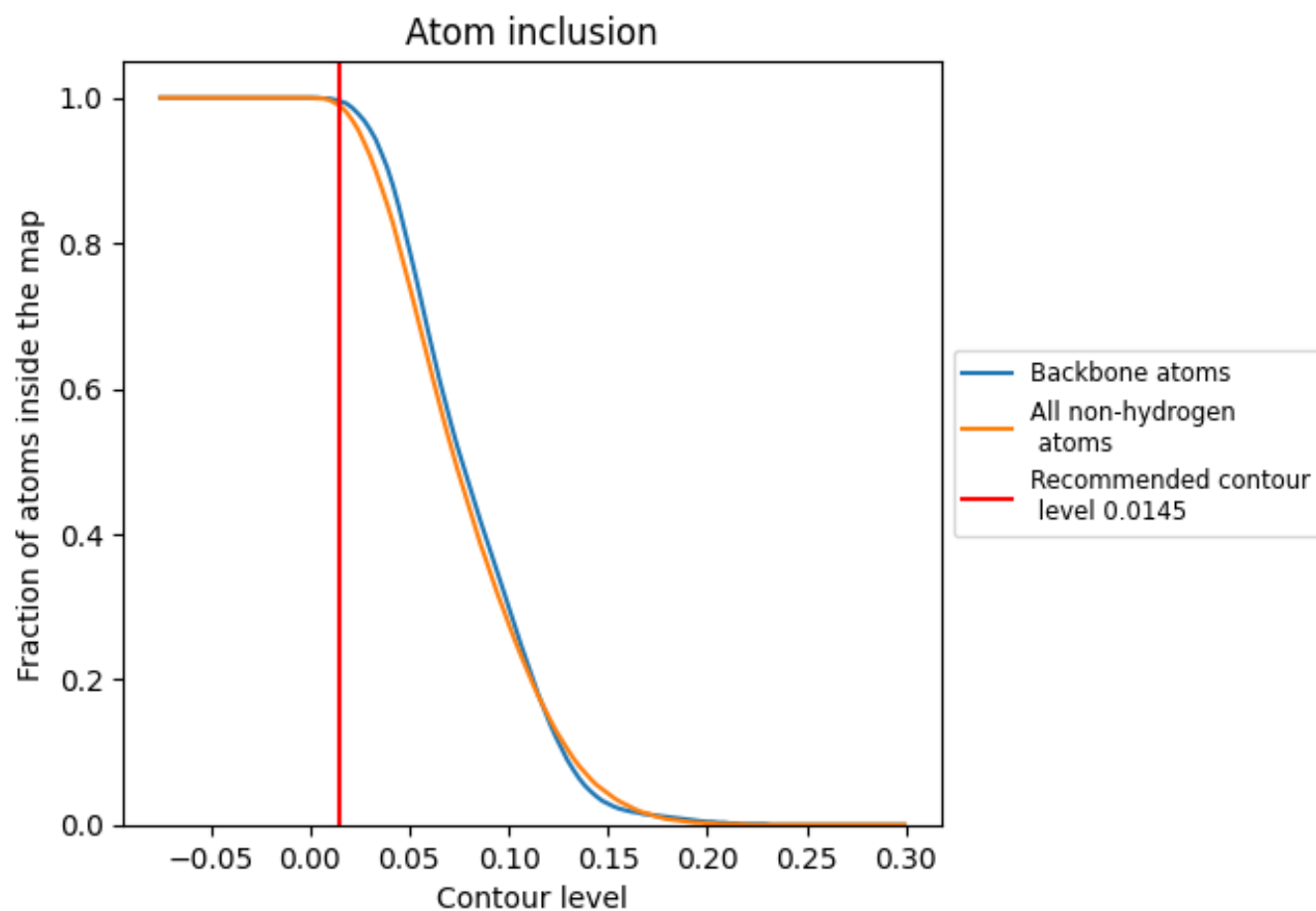
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0145).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% 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 (0.0145) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9900	 0.5380
CA	 0.8300	 0.3390
CB	 0.9730	 0.4960
CD	 0.9980	 0.4880
CI	 0.8950	 0.4690
Et	 0.9940	 0.4480
L5	 0.9970	 0.5720
L7	 1.0000	 0.6130
L8	 0.9960	 0.5900
LA	 1.0000	 0.6300
LB	 0.9880	 0.6140
LC	 0.9870	 0.6130
LD	 0.9870	 0.5820
LE	 0.9860	 0.5580
LF	 0.9980	 0.6160
LG	 0.9890	 0.5710
LH	 0.9930	 0.6030
LI	 0.9910	 0.6110
LJ	 0.9900	 0.5560
LL	 0.9750	 0.5910
LM	 0.9960	 0.6010
LN	 1.0000	 0.6400
LO	 0.9940	 0.6170
LP	 0.9940	 0.6230
LQ	 1.0000	 0.6340
LR	 0.9850	 0.5570
LS	 0.9990	 0.6280
LT	 0.9900	 0.6020
LU	 0.9810	 0.5360
LV	 0.9960	 0.6190
LW	 0.9800	 0.4630
LX	 0.9960	 0.5990
LY	 0.9920	 0.6040
LZ	 1.0000	 0.5880
La	 0.9960	 0.6330



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Chain	Atom inclusion	Q-score
Lb	 0.9710	 0.5590
Lc	 0.9890	 0.5690
Ld	 0.9940	 0.6030
Le	 0.9980	 0.6280
Lf	 0.9960	 0.6350
Lg	 0.9990	 0.6070
Lh	 0.9930	 0.5990
Li	 0.9940	 0.5950
Lj	 0.9970	 0.6290
Lk	 0.9770	 0.5530
Ll	 1.0000	 0.6190
Lm	 0.9900	 0.6130
Ln	 1.0000	 0.5980
Lo	 0.9900	 0.6150
Lp	 0.9930	 0.6050
Lr	 0.9960	 0.6160
Ls	 0.9740	 0.4480
Lt	 0.8770	 0.2800
S2	 0.9990	 0.4890
SA	 0.9690	 0.4860
SB	 0.9900	 0.4650
SC	 0.9990	 0.5420
SD	 0.9870	 0.4860
SE	 0.9970	 0.4920
SF	 0.9880	 0.4270
SG	 0.9780	 0.3780
SH	 0.9740	 0.4030
SI	 0.9830	 0.4510
SJ	 0.9850	 0.4980
SK	 0.9810	 0.4440
SL	 0.9880	 0.5060
SM	 0.9330	 0.2850
SN	 0.9970	 0.5150
SO	 0.9810	 0.4760
SP	 0.9850	 0.4670
SQ	 0.9850	 0.4420
SR	 0.9750	 0.4510
SS	 0.9780	 0.4350
ST	 0.9860	 0.4340
SU	 0.9930	 0.4570
SV	 0.9920	 0.5170
SW	 1.0000	 0.5500

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Chain	Atom inclusion	Q-score
SX	 0.9940	 0.5610
SY	 0.9650	 0.4170
SZ	 0.9470	 0.3720
Sa	 0.9960	 0.5190
Sb	 0.9840	 0.4530
Sc	 0.9860	 0.4220
Sd	 0.9980	 0.5330
Se	 0.9910	 0.4790
Sf	 0.9550	 0.3360
Sg	 0.9800	 0.3890