



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 07:26 AM EDT

PDB ID : 9P7C / pdb_00009p7c
EMDB ID : EMD-71337
Title : In situ human Hibernating class3 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 2.78 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

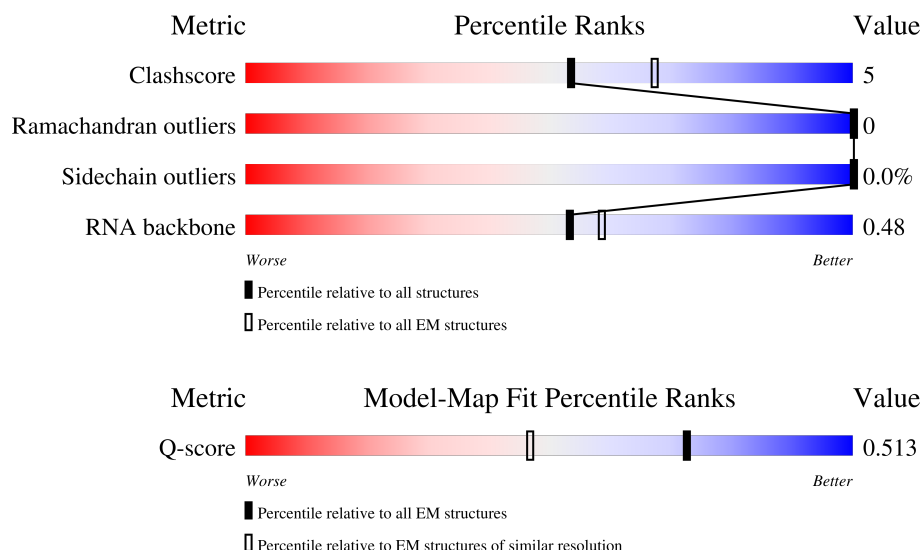
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.78 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.



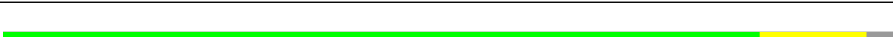
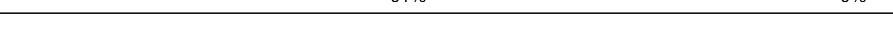
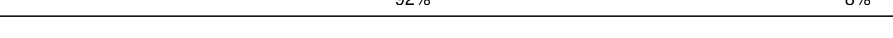
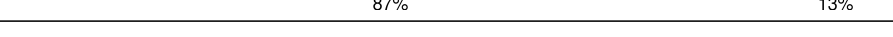
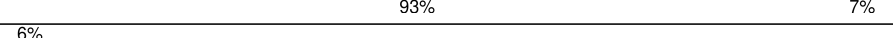
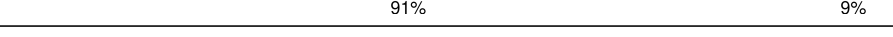
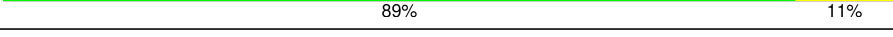
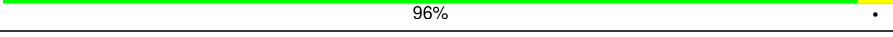
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10754 (2.28 - 3.28)

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	

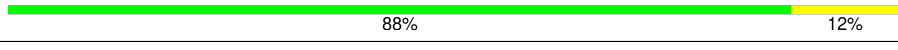
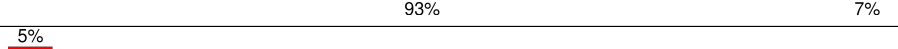
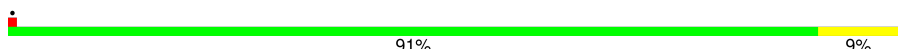
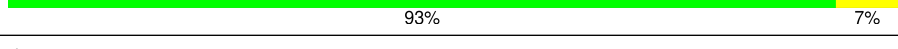
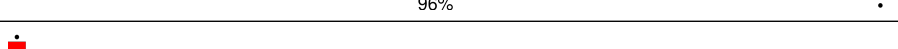
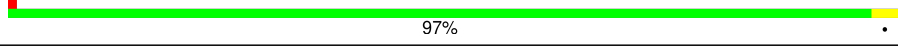
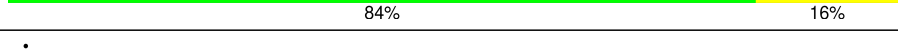
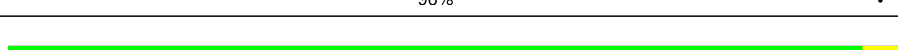
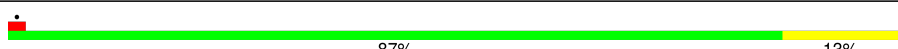
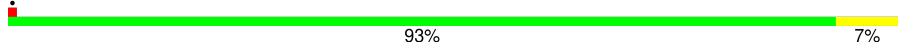
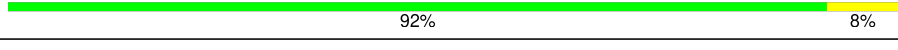
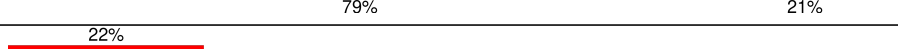
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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	156	
6	LA	248	
7	LB	402	
8	LC	368	
9	LD	293	
10	LE	250	
11	LF	225	
12	LG	241	
13	LH	190	
14	LI	213	
15	LJ	176	
16	LL	210	
17	LM	139	
18	LN	203	
19	LO	201	
20	LP	153	
21	LQ	187	
22	LR	187	
23	LS	175	
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	Sc	64	
81	Sd	55	
82	Sf	67	
83	Sg	313	
84	Et	75	
85	CB	856	
86	CA	356	

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.

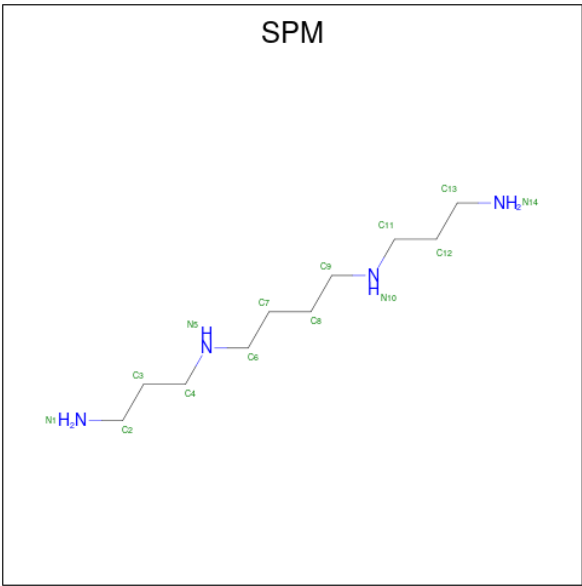
Mol	Chain	Residues	Atoms					AltConf	Trace
86	CA	354	Total	C	N	O	S	4	0
			2764	1744	475	528	17		

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

Mol	Chain	Residues	Atoms		AltConf
87	L5	177	Total	Mg	0
			177	177	
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	LB	1	Total	Mg	0
			1	1	
87	LI	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	SG	1	Total	Mg	0
			1	1	
87	S2	26	Total	Mg	0
			26	26	

- 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: C₇H₁₉N₃) (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	L8	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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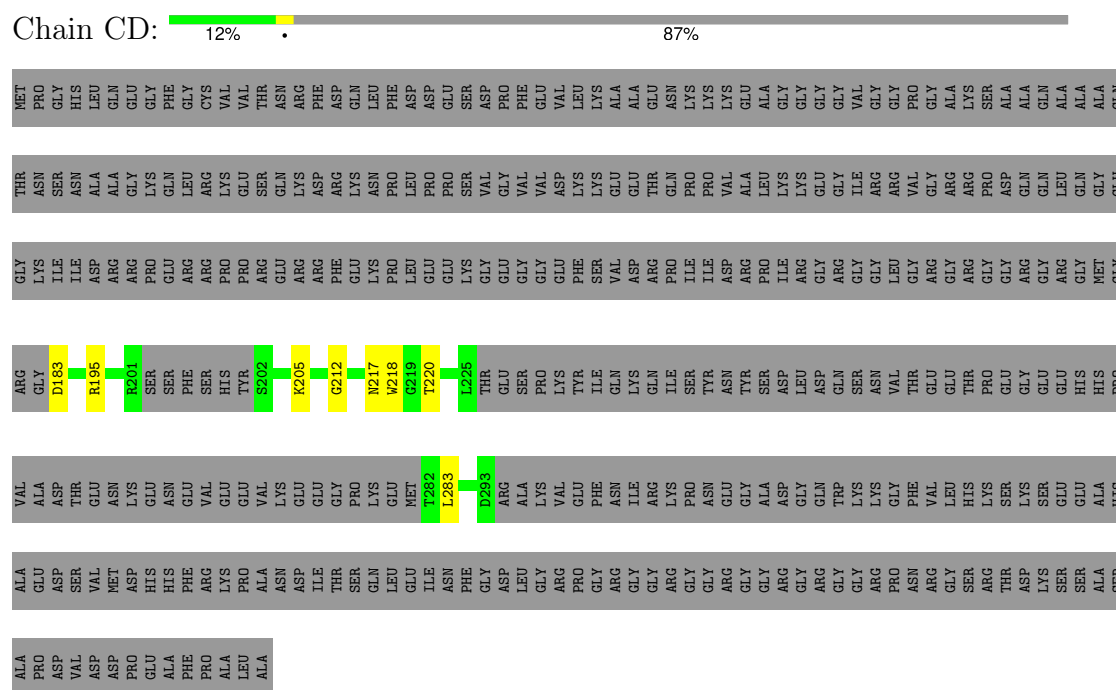
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Mol	Chain	Residues	Atoms		AltConf
90	Lj	1	Total 1	Zn 1	0
90	Lm	1	Total 1	Zn 1	0
90	Lo	1	Total 1	Zn 1	0
90	Lp	1	Total 1	Zn 1	0
90	Sa	1	Total 1	Zn 1	0

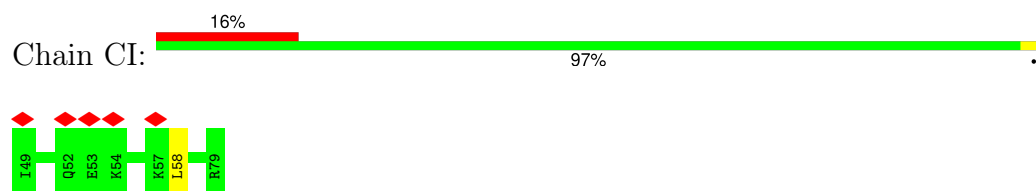
3 Residue-property plots

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

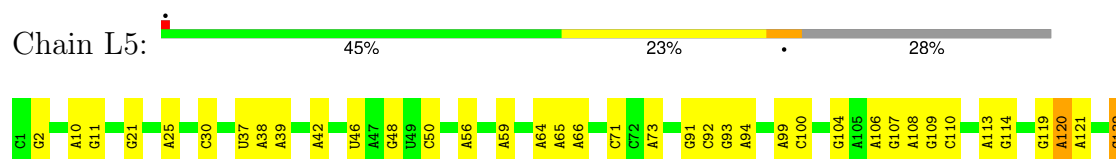
• Molecule 1: SERPINE1 mRNA-binding protein 1



• Molecule 2: Transcription factor BTF3



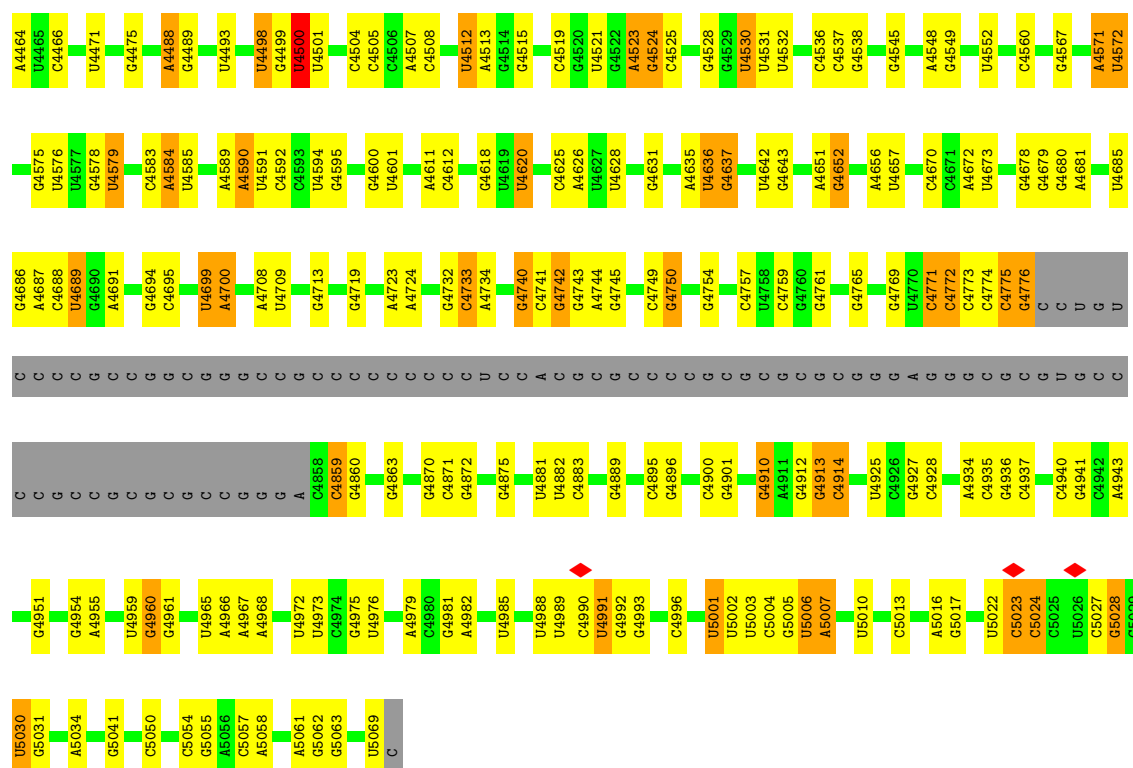
• Molecule 3: 28S rRNA











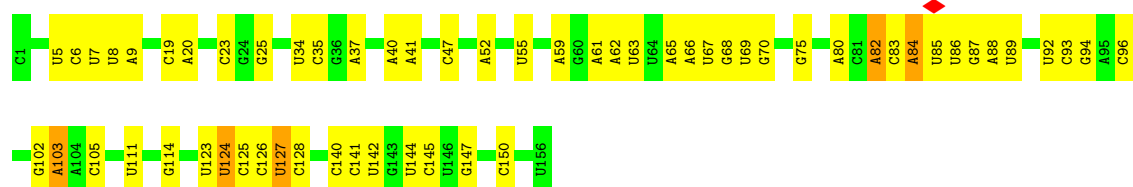
• Molecule 4: 5S rRNA

Chain L7: 82% 15% •



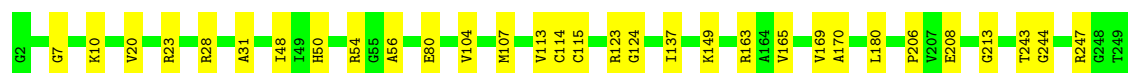
• Molecule 5: 5.8S rRNA

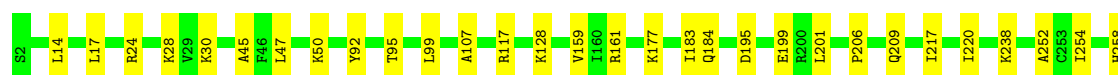
Chain L8: 62% 35% •



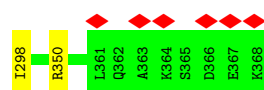
• Molecule 6: 60S ribosomal protein L8

Chain LA: 88% 12%





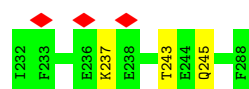
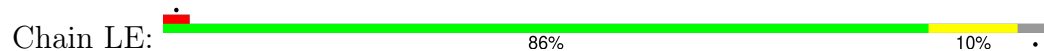
• Molecule 8: 60S ribosomal protein L4



• Molecule 9: Large ribosomal subunit protein uL18



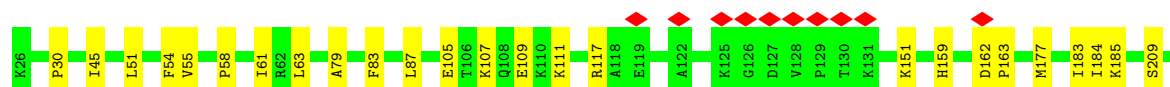
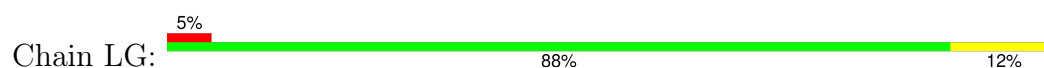
• Molecule 10: Large ribosomal subunit protein eL6

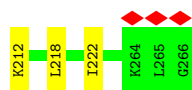


• Molecule 11: 60S ribosomal protein L7



• Molecule 12: 60S ribosomal protein L7a





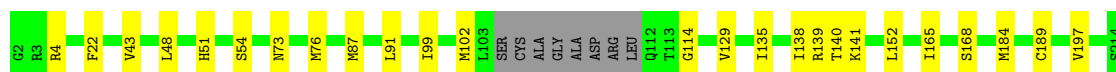
- Molecule 13: 60S ribosomal protein L9

Chain LH: 89% 11%



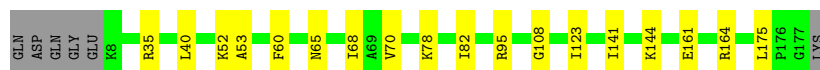
- Molecule 14: Ribosomal protein uL16-like

Chain LI: 85% 12% .



- Molecule 15: 60S ribosomal protein L11

Chain LJ: 86% 10% .



- Molecule 16: Large ribosomal subunit protein eL13

Chain LL: 91% 9%



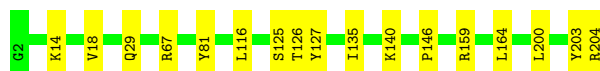
- Molecule 17: 60S ribosomal protein L14

Chain LM: 91% 9%



- Molecule 18: 60S ribosomal protein L15

Chain LN: 92% 8%



- Molecule 19: 60S ribosomal protein L13a

Chain LO: 87% 13%



- Molecule 20: 60S ribosomal protein L17

Chain LP: 87% 13%



- Molecule 21: 60S ribosomal protein L18

Chain LQ: 93% 7%



- Molecule 22: 60S ribosomal protein L19

Chain LR: 91% 6% 9%



- Molecule 23: 60S ribosomal protein L18a

Chain LS: 89% 11%



- Molecule 24: 60S ribosomal protein L21

Chain LT: 96% 4%



- Molecule 25: Heparin-binding protein HBp15

Chain LU: 83% 17%

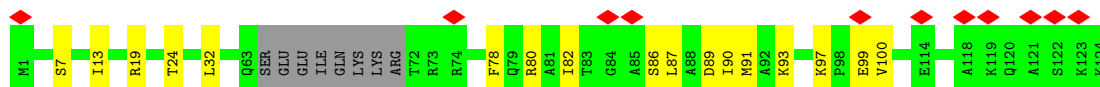
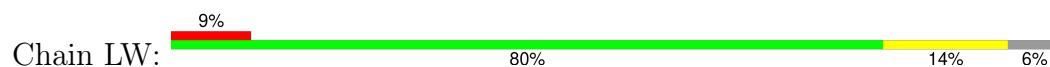


- Molecule 26: 60S ribosomal protein L23

Chain LV: 89% 11%



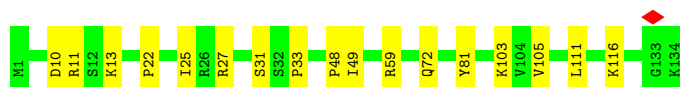
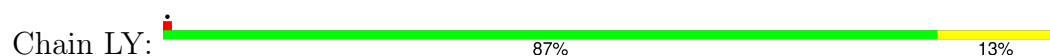
- Molecule 27: Ribosomal protein L24



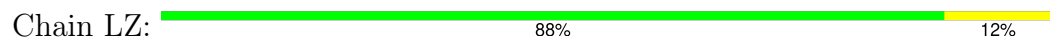
- Molecule 28: 60S ribosomal protein L23a



- Molecule 29: 60S ribosomal protein L26



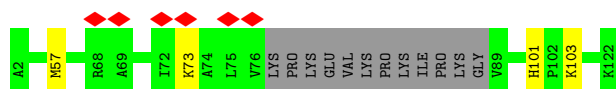
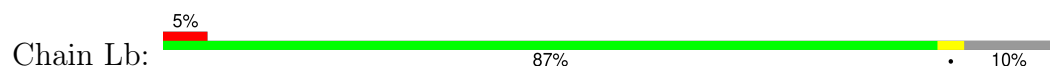
- Molecule 30: 60S ribosomal protein L27



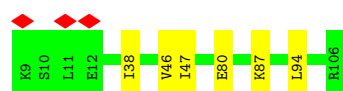
- Molecule 31: 60S ribosomal protein L27a



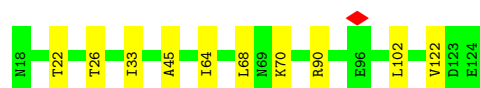
- Molecule 32: Large ribosomal subunit protein eL29



- Molecule 33: 60S ribosomal protein L30



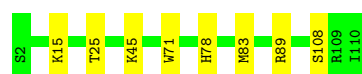
- Molecule 34: 60S ribosomal protein L31



- Molecule 35: 60S ribosomal protein L32



- Molecule 36: 60S ribosomal protein L35a



- Molecule 37: 60S ribosomal protein L34



- Molecule 38: 60S ribosomal protein L35



- Molecule 39: 60S ribosomal protein L36



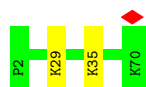
- Molecule 40: 60S ribosomal protein L37

Chain Lj:  91% 9%



- Molecule 41: 60S ribosomal protein L38

Chain Lk:  97%



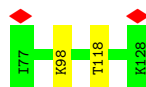
- Molecule 42: 60S ribosomal protein L39

Chain Ll:  84% 16%

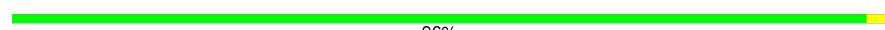


- Molecule 43: Large ribosomal subunit protein eL40

Chain Lm:  96%



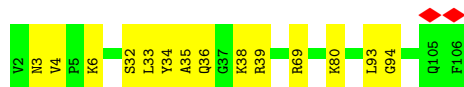
- Molecule 44: 60S ribosomal protein L41

Chain Ln:  96%



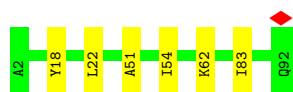
- Molecule 45: 60S ribosomal protein L36a

Chain Lo:  87% 13%



- Molecule 46: 60S ribosomal protein L37a

Chain Lp:  93% 7%



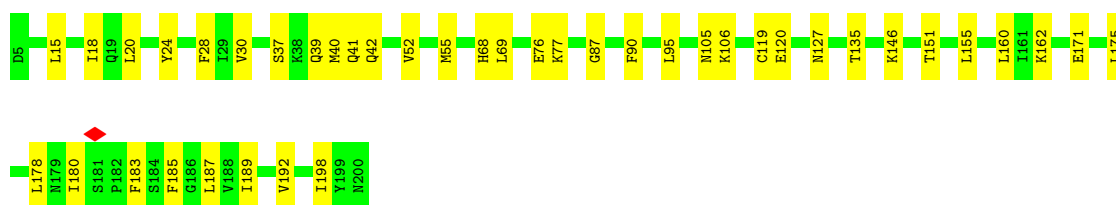
- Molecule 47: 60S ribosomal protein L28

Chain Lr: 92% 8%



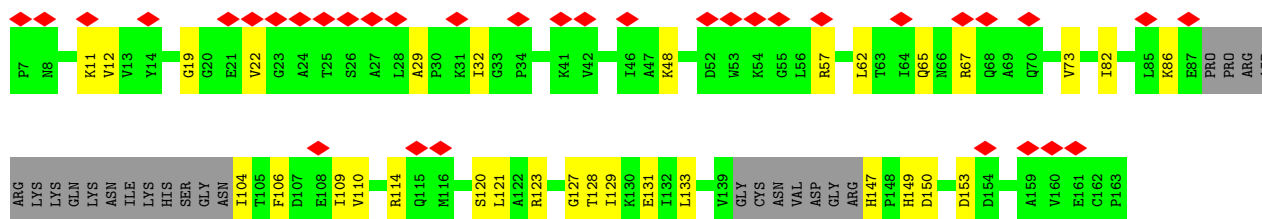
- Molecule 48: 60S acidic ribosomal protein P0

Chain Ls: 79% 21%



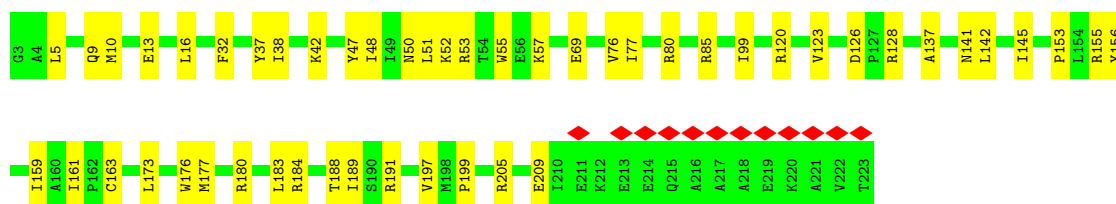
- Molecule 49: Large ribosomal subunit protein uL11

Chain Lt: 22% 66% 20% 15%



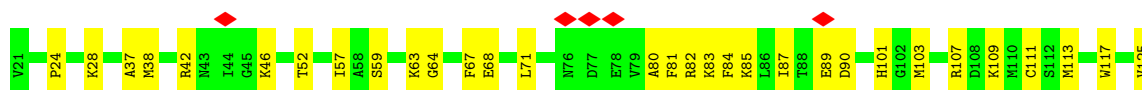
- Molecule 50: 40S ribosomal protein SA

Chain SA: 5% 77% 23%



- Molecule 51: 40S ribosomal protein S3a

Chain SB: 5% 71% 29%





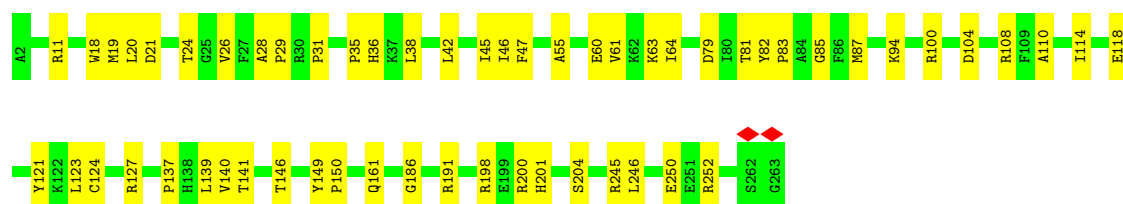
- Molecule 52: 40S ribosomal protein S2

Chain SC: 82% 17%



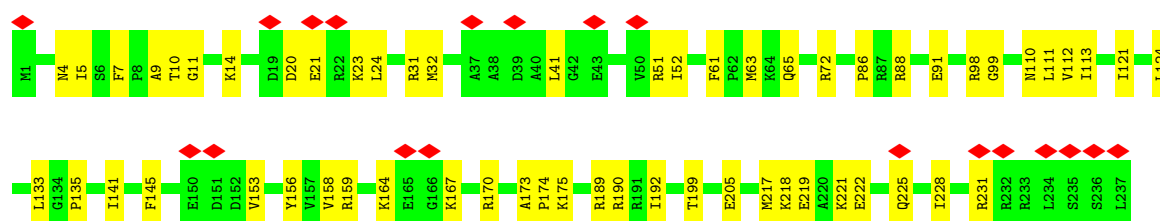
- Molecule 53: Small ribosomal subunit protein eS4, X isoform

Chain SE: 78% 22%



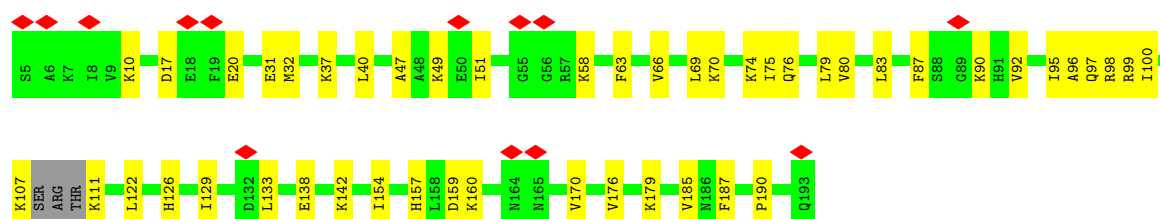
- Molecule 54: 40S ribosomal protein S6

Chain SG: 8% 76% 24%

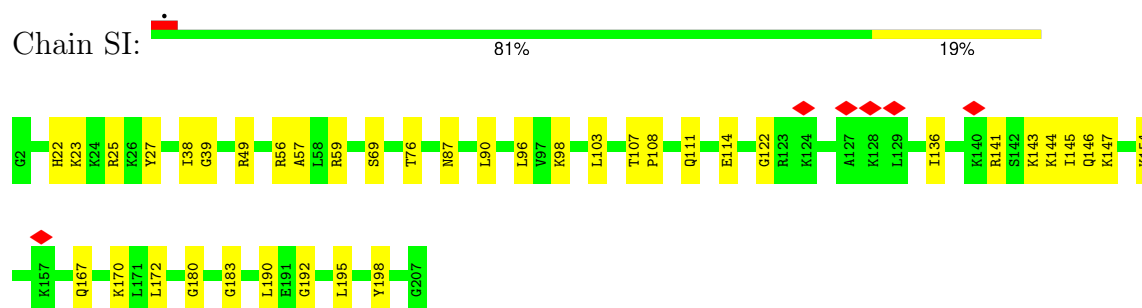


- Molecule 55: Small ribosomal subunit protein eS7

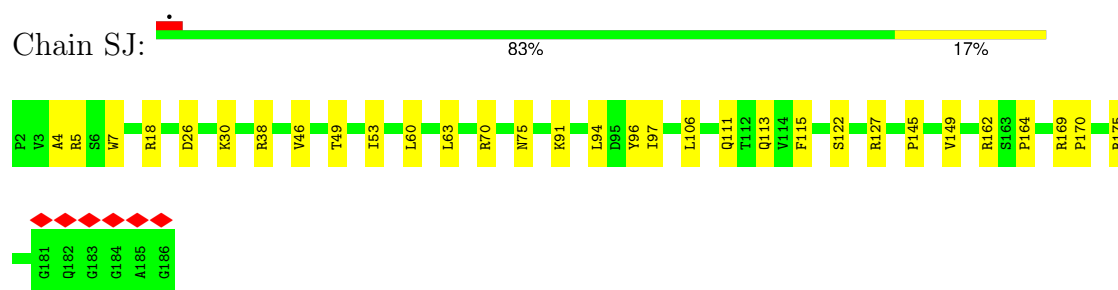
Chain SH: 7% 73% 25%



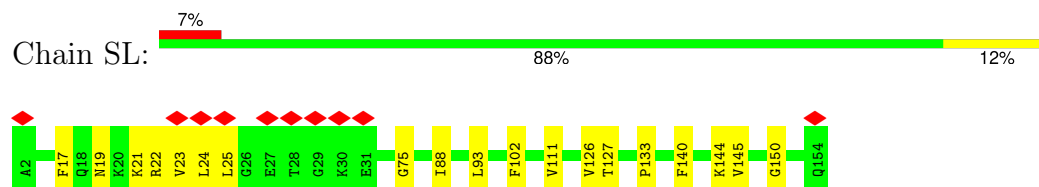
- Molecule 56: 40S ribosomal protein S8



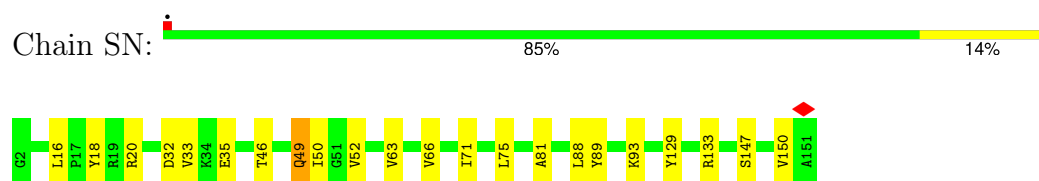
- Molecule 57: 40S ribosomal protein S9



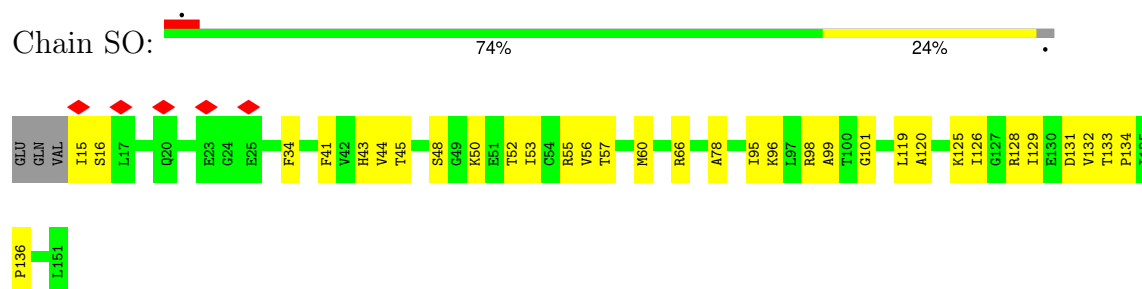
- Molecule 58: 40S ribosomal protein S11



- Molecule 59: 40S ribosomal protein S13



- Molecule 60: Small ribosomal subunit protein uS11



- Molecule 61: Small ribosomal subunit protein eS21

Chain SV:  83% 17%



- Molecule 62: 40S ribosomal protein S15a

Chain SW:  87% 13%



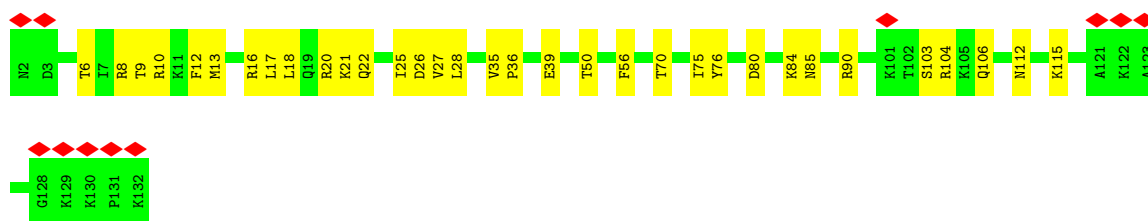
- Molecule 63: 40S ribosomal protein S23

Chain SX:  91% 9%



- Molecule 64: 40S ribosomal protein S24

Chain SY:  8% 75% 25%



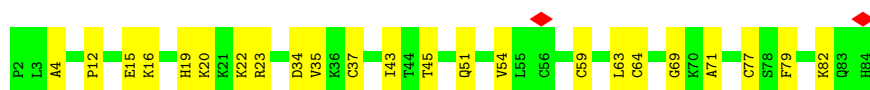
- Molecule 65: 40S ribosomal protein S26

Chain Sa:  89% 11%



- Molecule 66: Small ribosomal subunit protein eS27

Chain Sb:  72% 28%



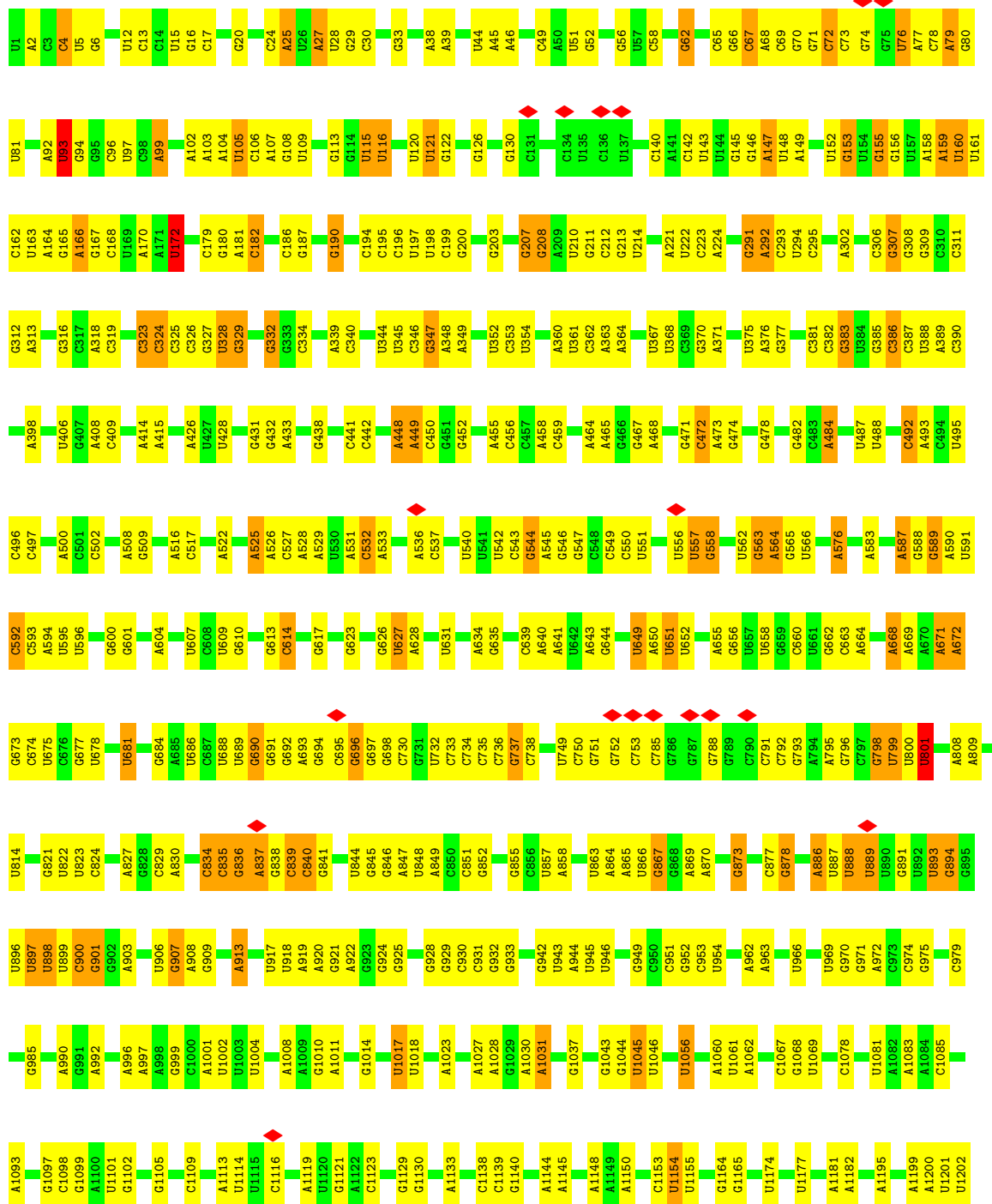
- Molecule 67: Small ribosomal subunit protein eS30

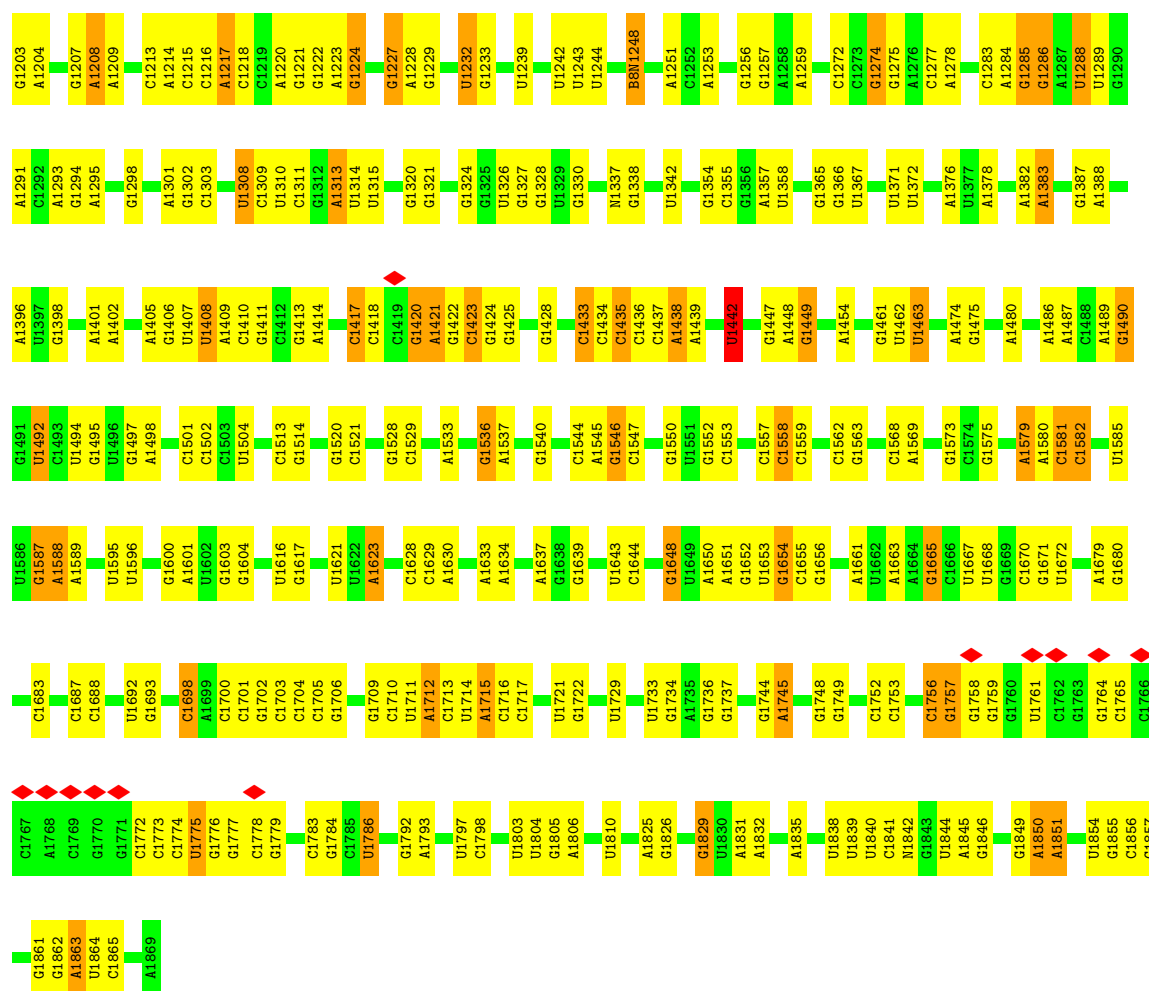
Chain Se:  5% 81% 19%



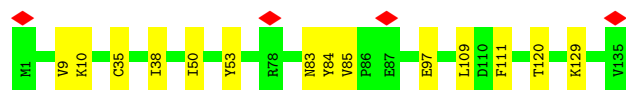
• Molecule 68: 18S rRNA [Homo sapiens]

Chain S2: 54% 38% 8%





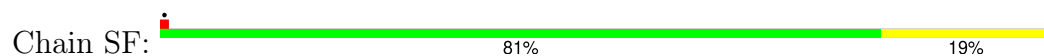
- Molecule 69: Small ribosomal subunit protein eS17

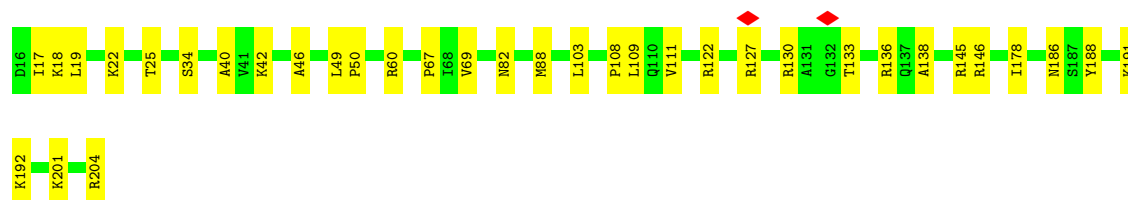


- Molecule 70: Small ribosomal subunit protein uS3

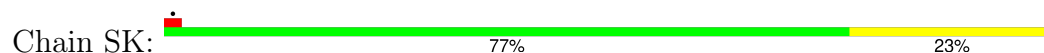


- Molecule 71: 40S ribosomal protein S5

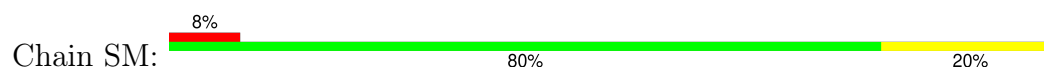




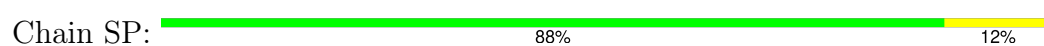
- Molecule 72: 40S ribosomal protein S10



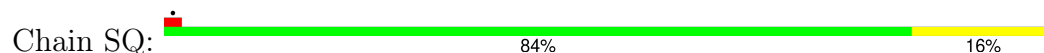
- Molecule 73: Small ribosomal subunit protein eS12



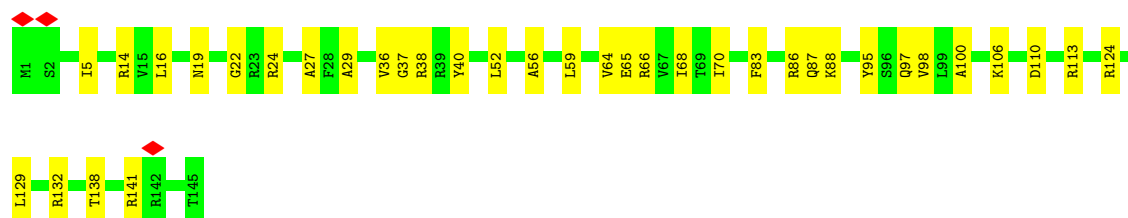
- Molecule 74: Small ribosomal subunit protein uS19



- Molecule 75: Small ribosomal subunit protein uS9

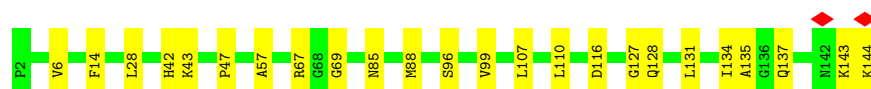


- Molecule 76: 40S ribosomal protein S18



- Molecule 77: 40S ribosomal protein S19

Chain ST:  83% 17%



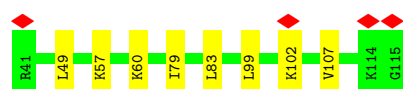
- Molecule 78: 40S ribosomal protein S20

Chain SU:  84% 16%



- Molecule 79: Small ribosomal subunit protein eS25

Chain SZ:  5% 89% 11%



- Molecule 80: 40S ribosomal protein S28

Chain Sc:  81% 19%



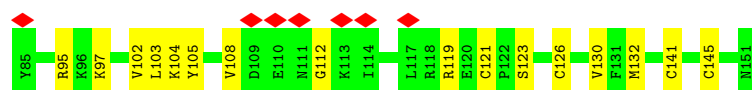
- Molecule 81: 40S ribosomal protein S29

Chain Sd:  75% 25%



- Molecule 82: Ubiquitin-40S ribosomal protein S27a

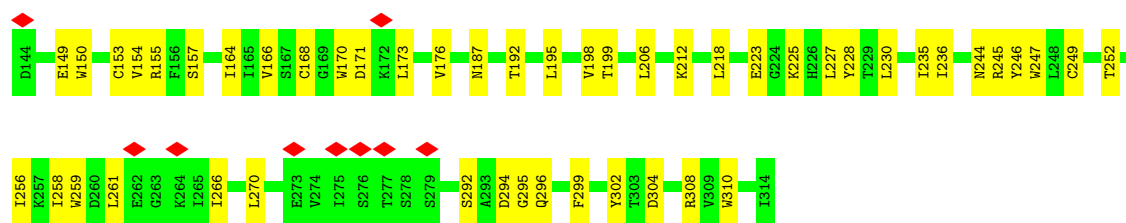
Chain Sf:  10% 76% 24%



- Molecule 83: Receptor of activated protein C kinase 1

Chain Sg:  74% 26%

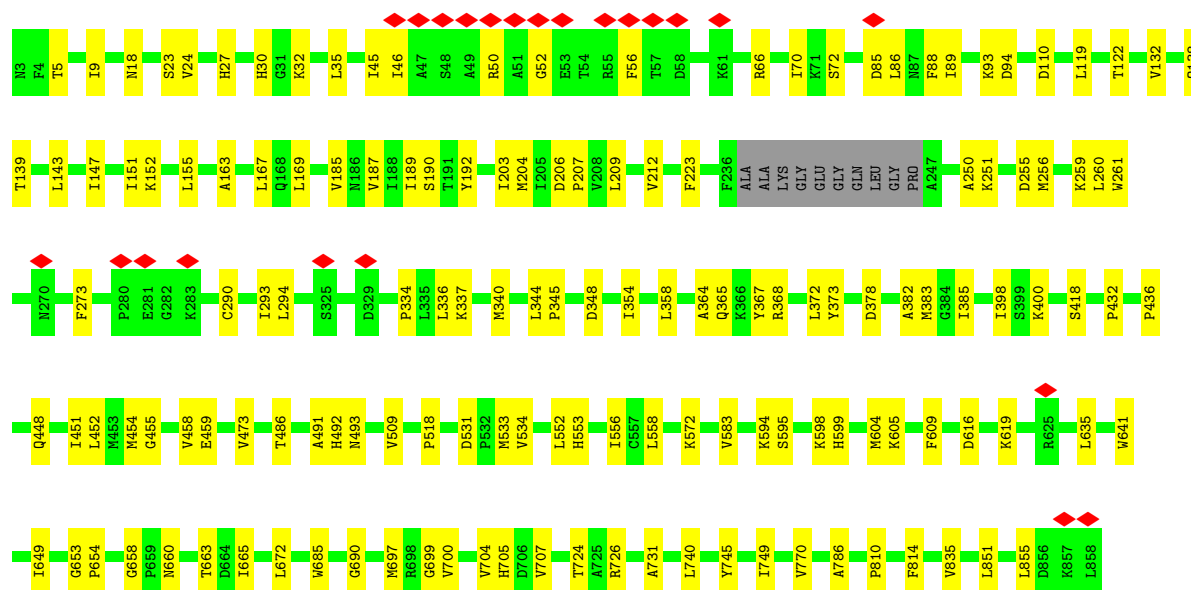
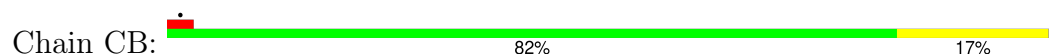




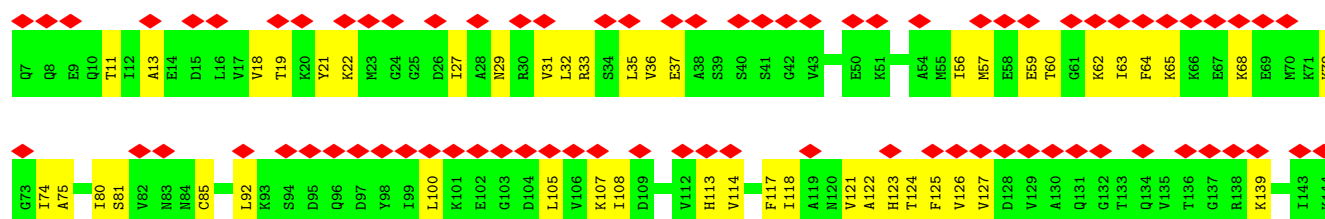
• Molecule 84: E site tRNA

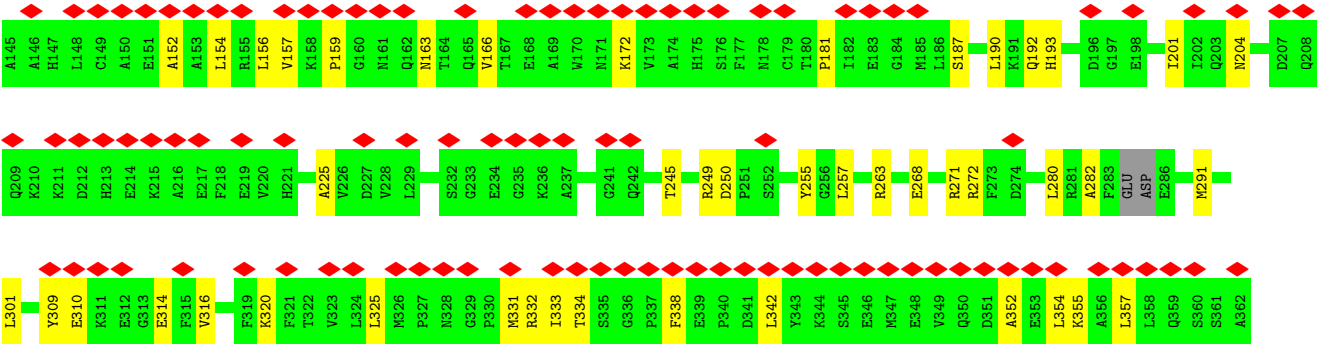


• Molecule 85: Elongation factor 2



• Molecule 86: Proliferation-associated protein 2G4





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54480	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	0.270	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.025	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.32	0/592
2	CI	0.13	0/247	0.30	0/323
3	L5	0.35	0/85098	0.33	0/132762
4	L7	0.34	0/2861	0.28	0/4459
5	L8	0.35	0/3631	0.30	0/5657
6	LA	0.34	0/1936	0.38	0/2596
7	LB	0.31	0/3306	0.35	0/4424
8	LC	0.32	0/2981	0.34	0/4002
9	LD	0.27	0/2428	0.32	0/3252
10	LE	0.25	0/1973	0.34	0/2645
11	LF	0.33	0/1905	0.32	0/2539
12	LG	0.27	0/1960	0.36	0/2637
13	LH	0.29	0/1537	0.34	0/2066
14	LI	0.29	0/1697	0.31	0/2266
15	LJ	0.23	0/1385	0.33	0/1852
16	LL	0.29	0/1732	0.32	0/2315
17	LM	0.29	0/1161	0.32	0/1554
18	LN	0.35	0/1746	0.35	0/2338
19	LO	0.32	0/1682	0.34	0/2250
20	LP	0.32	0/1268	0.35	0/1701
21	LQ	0.33	0/1537	0.36	0/2052
22	LR	0.27	0/1582	0.29	0/2091
23	LS	0.33	0/1493	0.35	0/2003
24	LT	0.30	0/1326	0.30	0/1770
25	LU	0.23	0/839	0.33	0/1126
26	LV	0.31	0/993	0.35	0/1332
27	LW	0.24	0/959	0.31	0/1270
28	LX	0.28	0/1002	0.30	0/1345
29	LY	0.29	0/1132	0.31	0/1504
30	LZ	0.27	0/1130	0.36	0/1507
31	La	0.32	0/1191	0.30	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.26	0/889	0.36	0/1175
33	Lc	0.27	0/774	0.36	0/1038
34	Ld	0.30	0/903	0.34	0/1216
35	Le	0.34	0/1071	0.32	0/1429
36	Lf	0.35	0/895	0.39	0/1198
37	Lg	0.29	0/916	0.33	0/1220
38	Lh	0.27	0/1023	0.33	0/1351
39	Li	0.25	0/843	0.30	0/1115
40	Lj	0.35	0/720	0.39	0/952
41	Lk	0.23	0/575	0.27	0/761
42	Ll	0.32	0/454	0.34	0/599
43	Lm	0.28	0/435	0.34	0/575
44	Ln	0.25	0/231	0.25	0/294
45	Lo	0.29	0/876	0.34	0/1156
46	Lp	0.31	0/718	0.31	0/953
47	Lr	0.32	0/1017	0.35	0/1364
48	Ls	0.16	0/1519	0.33	0/2052
49	Lt	0.20	0/1009	0.49	0/1363
50	SA	0.20	0/1778	0.33	0/2416
51	SB	0.18	0/1765	0.33	0/2362
52	SC	0.22	0/1744	0.36	0/2357
53	SE	0.19	0/2118	0.33	0/2849
54	SG	0.16	0/1946	0.36	0/2590
55	SH	0.18	0/1519	0.40	0/2033
56	SI	0.20	0/1715	0.34	0/2287
57	SJ	0.20	0/1550	0.34	0/2069
58	SL	0.21	0/1268	0.32	0/1696
59	SN	0.20	0/1232	0.30	0/1656
60	SO	0.19	0/1037	0.38	0/1391
61	SV	0.19	0/643	0.30	0/860
62	SW	0.23	0/1051	0.33	0/1406
63	SX	0.24	0/1116	0.39	0/1490
64	SY	0.16	0/1083	0.31	0/1438
65	Sa	0.23	0/836	0.34	0/1121
66	Sb	0.17	0/665	0.34	0/891
67	Se	0.18	0/465	0.35	0/612
68	S2	0.26	0/39756	0.30	0/61939
69	SR	0.19	0/1105	0.39	0/1484
70	SD	0.20	0/1793	0.32	0/2414
71	SF	0.18	0/1516	0.35	0/2037
72	SK	0.19	0/851	0.38	0/1147
73	SM	0.16	0/950	0.40	0/1275
74	SP	0.20	0/1003	0.33	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SQ	0.20	0/1160	0.36	0/1553
76	SS	0.17	0/1216	0.30	0/1628
77	ST	0.19	0/1131	0.33	0/1515
78	SU	0.20	0/831	0.35	0/1115
79	SZ	0.19	0/604	0.39	0/810
80	Sc	0.17	0/508	0.31	0/680
81	Sd	0.22	0/470	0.33	0/623
82	Sf	0.17	0/560	0.47	0/745
83	Sg	0.16	0/2493	0.35	0/3394
84	Et	0.20	0/1778	0.39	0/2767
85	CB	0.19	0/6734	0.34	0/9094
86	CA	0.14	0/2810	0.36	0/3780
All	All	0.29	0/239833	0.33	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	7	0
2	CI	247	0	283	1	0
3	L5	78444	0	39719	535	0
4	L7	2561	0	1295	9	0
5	L8	3315	0	1685	26	0
6	LA	1898	0	1993	23	0
7	LB	3238	0	3376	34	0
8	LC	2927	0	3104	24	0
9	LD	2382	0	2410	20	0
10	LE	1935	0	2096	18	0
11	LF	1870	0	1996	15	0
12	LG	1927	0	2074	18	0
13	LH	1518	0	1601	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	LI	1658	0	1697	15	0
15	LJ	1362	0	1399	10	0
16	LL	1701	0	1818	19	0
17	LM	1138	0	1204	7	0
18	LN	1701	0	1749	15	0
19	LO	1650	0	1794	15	0
20	LP	1242	0	1269	13	0
21	LQ	1513	0	1628	11	0
22	LR	1566	0	1729	15	0
23	LS	1453	0	1490	11	0
24	LT	1298	0	1366	5	0
25	LU	825	0	850	10	0
26	LV	979	0	1039	9	0
27	LW	945	0	1003	13	0
28	LX	985	0	1066	6	0
29	LY	1115	0	1205	10	0
30	LZ	1107	0	1182	10	0
31	La	1162	0	1213	7	0
32	Lb	876	0	948	3	0
33	Lc	764	0	804	4	0
34	Ld	888	0	930	6	0
35	Le	1053	0	1147	9	0
36	Lf	876	0	912	4	0
37	Lg	906	0	998	4	0
38	Lh	1015	0	1148	11	0
39	Li	832	0	917	7	0
40	Lj	705	0	737	6	0
41	Lk	569	0	637	2	0
42	Ll	444	0	483	5	0
43	Lm	429	0	465	1	0
44	Ln	230	0	276	1	0
45	Lo	862	0	929	8	0
46	Lp	708	0	756	5	0
47	Lr	1002	0	1068	7	0
48	Ls	1496	0	1540	25	0
49	Lt	998	0	1032	23	0
50	SA	1741	0	1746	35	0
51	SB	1738	0	1809	43	0
52	SC	1707	0	1791	29	0
53	SE	2076	0	2177	41	0
54	SG	1923	0	2089	48	0
55	SH	1497	0	1590	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	SI	1686	0	1772	27	0
57	SJ	1525	0	1640	23	0
58	SL	1247	0	1323	16	0
59	SN	1208	0	1294	14	0
60	SO	1024	0	1050	25	0
61	SV	636	0	637	9	0
62	SW	1034	0	1080	16	0
63	SX	1098	0	1167	9	0
64	SY	1065	0	1142	24	0
65	Sa	821	0	870	10	0
66	Sb	651	0	669	16	0
67	Se	459	0	503	10	0
68	S2	36952	0	18678	425	0
69	SR	1090	0	1149	11	0
70	SD	1765	0	1865	18	0
71	SF	1495	0	1549	24	0
72	SK	827	0	854	19	0
73	SM	940	0	965	16	0
74	SP	985	0	1031	11	0
75	SQ	1142	0	1213	17	0
76	SS	1198	0	1261	23	0
77	ST	1112	0	1146	16	0
78	SU	821	0	883	11	0
79	SZ	598	0	656	6	0
80	Sc	506	0	536	10	0
81	Sd	459	0	449	8	0
82	Sf	548	0	551	13	0
83	Sg	2436	0	2391	51	0
84	Et	1593	0	810	26	0
85	CB	6605	0	6679	89	0
86	CA	2764	0	2779	60	0
87	L5	177	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	LB	1	0	0	0	0
87	LI	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	26	0	0	0	0
87	SG	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	L5	98	0	182	5	0
89	L5	90	0	171	2	0
89	L8	10	0	19	0	0
90	Lg	1	0	0	0	0
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	172628	2072	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 (2072) 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)
84:Et:26:A:H62	84:Et:44:G:N2	1.48	1.12
84:Et:26:A:N6	84:Et:44:G:H21	1.50	1.10
68:S2:70:G:H21	68:S2:79:A:H62	1.08	0.95
68:S2:1417:C:H42	68:S2:1422:G:H22	1.02	0.93
68:S2:1748:G:H1	68:S2:1786:U:H3	1.19	0.87
3:L5:1175:A:H2	3:L5:1185:G:H1	1.21	0.85
68:S2:1417:C:N4	68:S2:1422:G:H22	1.77	0.82
68:S2:1417:C:H42	68:S2:1422:G:N2	1.80	0.79
56:SI:98:LYS:HB3	68:S2:377:G:H5'	1.64	0.79
68:S2:159:A2M:H2	68:S2:467:G:H21	1.49	0.78
68:S2:70:G:N2	68:S2:79:A:H62	1.80	0.78
83:Sg:127:LYS:HG2	83:Sg:150:TRP:H	1.50	0.77
50:SA:205:ARG:HH22	69:SR:84:TYR:H	1.31	0.76
42:Ll:23:ILE:HD11	42:Ll:28:ARG:HE	1.49	0.75
68:S2:851:C:H5''	68:S2:852:G:H5'	1.69	0.75
3:L5:690:C:H4'	47:Lr:85:ASN:HD22	1.49	0.75
3:L5:4775:C:H41	3:L5:4859:C:H42	1.33	0.75
86:CA:181:PRO:HB2	86:CA:204:ASN:HB2	1.69	0.74
16:LL:64:VAL:HA	16:LL:67:HIS:HD2	1.52	0.74
85:CB:336:LEU:HG	85:CB:340:MET:HE1	1.69	0.73
68:S2:1461:G:H3'	68:S2:1463:U:H3	1.52	0.73
3:L5:1404:G:N7	3:L5:1408:G:N2	2.36	0.73
70:SD:60:GLY:HA3	70:SD:65:ARG:H	1.54	0.72
50:SA:57:LYS:HG3	50:SA:161:ILE:HD13	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1820:C:H2'	3:L5:1822:U:H5'	1.70	0.72
7:LB:206:PRO:HD2	7:LB:209:GLN:HE21	1.54	0.71
83:Sg:247:TRP:HB3	83:Sg:258:ILE:HD11	1.72	0.71
3:L5:1995:G:H4'	49:Lt:128:THR:HB	1.72	0.71
76:SS:14:ARG:HD2	76:SS:19:ASN:HB3	1.72	0.71
86:CA:122:ALA:HB2	86:CA:320:LYS:HE3	1.73	0.70
85:CB:745:TYR:HB2	85:CB:814:PHE:HA	1.72	0.70
70:SD:105:LEU:HD11	70:SD:122:VAL:HG11	1.73	0.70
58:SL:150:GLY:HA2	59:SN:133:ARG:HH22	1.56	0.70
3:L5:4910:G:H4'	7:LB:95:THR:HG22	1.72	0.69
6:LA:31:ALA:HB2	6:LA:123:ARG:HH21	1.56	0.69
6:LA:104:VAL:HA	6:LA:107:MET:HE2	1.75	0.69
54:SG:175:LYS:HG3	68:S2:77:A:H2	1.56	0.69
3:L5:1270:A:H8	3:L5:2106:G:H21	1.39	0.69
3:L5:2554:U:O2	3:L5:2764:A:N7	2.25	0.69
55:SH:10:LYS:HE3	55:SH:20:GLU:HG2	1.75	0.69
68:S2:1679:A:H2'	71:SF:60:ARG:HD2	1.75	0.69
78:SU:24:LEU:HB3	78:SU:32:LEU:HD11	1.73	0.69
68:S2:70:G:H21	68:S2:79:A:N6	1.87	0.69
49:Lt:12:VAL:HG11	49:Lt:65:GLN:H	1.57	0.68
68:S2:1417:C:N3	68:S2:1422:G:N1	2.37	0.68
66:Sb:64:CYS:HB3	66:Sb:71:ALA:HB1	1.76	0.68
49:Lt:65:GLN:HG3	49:Lt:67:ARG:H	1.57	0.68
51:SB:127:VAL:HG11	51:SB:176:VAL:HG13	1.76	0.68
71:SF:49:LEU:HD12	75:SQ:50:LYS:HG3	1.76	0.68
3:L5:964:A:H2'	3:L5:965:G:H4'	1.76	0.68
64:SY:18:LEU:HD22	64:SY:20:ARG:HE	1.59	0.68
68:S2:1396:A:N7	68:S2:1449:G:O6	2.26	0.68
69:SR:83:ASN:HB3	69:SR:85:VAL:HG13	1.74	0.68
86:CA:75:ALA:HB2	86:CA:113:HIS:HB3	1.76	0.68
54:SG:23:LYS:HE2	54:SG:41:LEU:HA	1.75	0.67
54:SG:164:LYS:HB3	54:SG:167:LYS:HE3	1.76	0.67
3:L5:502:C:H3'	3:L5:503:C:H3'	1.76	0.67
3:L5:2709:C:H42	86:CA:257:LEU:H	1.42	0.67
13:LH:106:GLN:HB2	13:LH:111:LEU:HB3	1.77	0.67
34:Ld:90:ARG:HD3	34:Ld:102:LEU:HD13	1.76	0.67
63:SX:123:VAL:HG12	63:SX:124:LYS:HG3	1.76	0.67
86:CA:80:ILE:HG12	86:CA:108:ILE:HG12	1.75	0.67
67:Se:28:LYS:HE2	67:Se:32:ALA:HB1	1.77	0.67
85:CB:385:ILE:HG22	85:CB:418:SER:HB2	1.74	0.67
68:S2:1729:U:H3	68:S2:1805:G:H1	1.40	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LA:114:CYS:HB3	6:LA:165:VAL:HB	1.77	0.67
51:SB:71:LEU:HD13	51:SB:82:ARG:HH11	1.60	0.66
63:SX:50:ILE:HG13	85:CB:518:PRO:HB3	1.75	0.66
85:CB:595:SER:HA	85:CB:724:THR:HG21	1.77	0.66
68:S2:1228:A:H2'	68:S2:1229:G:C8	2.30	0.66
48:Ls:69:LEU:HD11	48:Ls:76:GLU:HB3	1.78	0.66
50:SA:184:ARG:HE	50:SA:191:ARG:HD3	1.59	0.66
68:S2:1652:G:H1	68:S2:1672:U:H3	1.42	0.66
83:Sg:87:LEU:HB2	83:Sg:101:PHE:HB2	1.77	0.66
68:S2:1030:A:H2'	68:S2:1031:A2M:H8	1.78	0.66
73:SM:92:CYS:HB3	73:SM:103:VAL:HG12	1.78	0.66
54:SG:218:LYS:HD2	54:SG:221:LYS:HE2	1.77	0.66
68:S2:508:A:H3'	68:S2:509:OMG:H8	1.59	0.66
77:ST:128:GLN:HA	77:ST:131:LEU:HB2	1.76	0.66
53:SE:139:LEU:HD22	53:SE:150:PRO:HB3	1.77	0.65
53:SE:38:LEU:HD22	68:S2:346:C:H5''	1.79	0.65
59:SN:20:ARG:HH21	62:SW:56:HIS:HB3	1.61	0.65
68:S2:1417:C:O2	68:S2:1422:G:O6	2.13	0.65
85:CB:672:LEU:HD13	85:CB:707:VAL:HG21	1.78	0.65
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.78	0.65
3:L5:3946:G:H1	3:L5:4067:U:H3	1.45	0.65
55:SH:10:LYS:HE2	55:SH:47:ALA:HA	1.77	0.65
3:L5:4571:A2M:H2'	3:L5:4572:U:H6	1.62	0.65
7:LB:28:LYS:HG3	7:LB:30:LYS:HG3	1.79	0.65
16:LL:64:VAL:HA	16:LL:67:HIS:CD2	2.30	0.65
86:CA:157:VAL:HG22	86:CA:325:LEU:HD21	1.78	0.65
9:LD:223:PHE:HB3	9:LD:226:TYR:HB2	1.78	0.65
57:SJ:113:GLN:HG2	57:SJ:149:VAL:HG21	1.79	0.65
76:SS:24:ARG:HB2	76:SS:29:ALA:HB2	1.79	0.65
86:CA:31:VAL:HG21	86:CA:56:ILE:HD11	1.79	0.64
85:CB:604:MET:HE2	85:CB:704:VAL:HG22	1.80	0.64
48:Ls:40:MET:HE1	48:Ls:187:LEU:HD23	1.80	0.64
55:SH:17:ASP:HB2	55:SH:20:GLU:HB3	1.79	0.64
68:S2:106:C:H2'	68:S2:107:A:H8	1.62	0.64
3:L5:3868:G:H22	3:L5:3900:G:H1'	1.63	0.64
48:Ls:30:VAL:HG21	48:Ls:187:LEU:HD13	1.80	0.64
72:SK:80:ARG:HH12	72:SK:87:PRO:HA	1.62	0.64
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.63	0.64
86:CA:100:LEU:HD21	86:CA:127:VAL:HG11	1.78	0.64
4:L7:49:A:H5''	9:LD:224:SER:HB3	1.80	0.64
61:SV:15:ARG:HH21	61:SV:24:ILE:HG21	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1729:U:O2	68:S2:1805:G:N2	2.29	0.63
68:S2:1536:G:H2'	68:S2:1537:A:H8	1.64	0.63
71:SF:201:LYS:HD3	71:SF:204:ARG:HH21	1.62	0.63
82:Sf:108:VAL:HB	82:Sf:112:GLY:HA2	1.80	0.63
83:Sg:246:TYR:HB3	83:Sg:261:LEU:HG	1.79	0.63
7:LB:107:ALA:HB2	7:LB:201:LEU:HD22	1.78	0.63
83:Sg:149:GLU:HB2	83:Sg:171:ASP:HB3	1.80	0.63
74:SP:37:TYR:HB3	74:SP:41:GLN:HB2	1.81	0.63
19:LO:34:VAL:HG22	19:LO:103:LYS:HB2	1.81	0.63
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.34	0.62
71:SF:17:ILE:HG21	71:SF:46:ALA:HB1	1.81	0.62
68:S2:120:U:H2'	68:S2:121:OMU:H6	1.81	0.62
54:SG:5:ILE:HD12	54:SG:124:LEU:HD22	1.81	0.62
55:SH:157:HIS:HB3	55:SH:190:PRO:HG3	1.80	0.62
71:SF:103:LEU:HD22	71:SF:178:ILE:HD13	1.82	0.62
83:Sg:120:ILE:HB	83:Sg:132:TRP:HB2	1.80	0.62
68:S2:1277:C:H2'	68:S2:1278:A:H8	1.64	0.62
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.64	0.62
56:SI:190:LEU:HD23	56:SI:195:LEU:HA	1.81	0.62
57:SJ:38:ARG:HA	67:Se:31:ARG:HB3	1.80	0.62
68:S2:928:G:H2'	68:S2:929:G:C8	2.35	0.62
68:S2:1562:C:H2'	68:S2:1563:G:H8	1.65	0.62
68:S2:1854:U:H2'	68:S2:1855:G:H8	1.65	0.62
85:CB:354:ILE:HG23	85:CB:358:LEU:HD12	1.81	0.62
56:SI:107:THR:HG23	56:SI:111:GLN:HE22	1.65	0.62
83:Sg:131:LEU:HD23	83:Sg:139:LYS:HD2	1.81	0.62
49:Lt:12:VAL:HG21	49:Lt:65:GLN:HB2	1.81	0.61
74:SP:22:LEU:HA	74:SP:25:LEU:HB2	1.82	0.61
76:SS:5:ILE:HG12	79:SZ:49:LEU:HB2	1.82	0.61
11:LF:127:LYS:HB2	24:LT:133:ALA:HB3	1.82	0.61
21:LQ:39:THR:HG22	21:LQ:41:SER:H	1.65	0.61
3:L5:2458:C:H5''	18:LN:67:ARG:HD2	1.81	0.61
20:LP:125:MET:HE3	20:LP:143:PRO:HG3	1.82	0.61
3:L5:2362:U:H2'	3:L5:2363:A2M:H8	1.82	0.61
23:LS:11:LYS:HE3	23:LS:29:ARG:HD3	1.81	0.61
57:SJ:111:GLN:HE22	57:SJ:127:ARG:HH11	1.49	0.61
68:S2:943:U:H2'	68:S2:944:A:H8	1.63	0.61
68:S2:1228:A:H2'	68:S2:1229:G:H8	1.63	0.61
3:L5:2708:U:H3	86:CA:257:LEU:HD23	1.64	0.61
3:L5:3937:C:H1'	18:LN:125:SER:HB3	1.82	0.61
47:Lr:63:VAL:HG12	47:Lr:79:ARG:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SB:63:LYS:HE2	51:SB:90:ASP:HA	1.82	0.61
60:SO:99:ALA:H	60:SO:133:THR:HG22	1.63	0.61
3:L5:1194:G:H2'	3:L5:1195:G:H8	1.65	0.61
49:Lt:106:PHE:HB2	49:Lt:109:ILE:HG12	1.82	0.61
68:S2:1422:G:H4'	68:S2:1423:C:H3'	1.81	0.61
85:CB:432:PRO:HA	85:CB:493:ASN:HD21	1.66	0.61
10:LE:165:LEU:HD11	10:LE:176:THR:HB	1.83	0.61
50:SA:42:LYS:HE3	50:SA:48:ILE:HD11	1.81	0.61
51:SB:87:ILE:H	51:SB:101:HIS:HB2	1.65	0.61
85:CB:18:ASN:HD21	85:CB:94:ASP:H	1.49	0.61
53:SE:191:ARG:HD2	53:SE:245:ARG:HH11	1.65	0.61
68:S2:834:C:H42	68:S2:839:C:H42	1.49	0.61
68:S2:1588:A:H2'	68:S2:1589:A:C8	2.36	0.61
3:L5:137:G:H2'	3:L5:138:G:H8	1.64	0.60
68:S2:925:G:H1	68:S2:1017:U:H3	1.47	0.60
3:L5:3950:U:H3'	3:L5:3951:G:C8	2.36	0.60
85:CB:558:LEU:HD13	85:CB:572:LYS:HE3	1.82	0.60
3:L5:257:C:H2'	3:L5:258:G:H8	1.67	0.60
3:L5:411:G:H5''	3:L5:414:C:H1'	1.83	0.60
14:LI:87:MET:HG2	14:LI:138:ILE:HG12	1.84	0.60
19:LO:61:ARG:HA	19:LO:70:PRO:HD2	1.84	0.60
64:SY:103:SER:H	64:SY:106:GLN:HE22	1.49	0.60
71:SF:50:PRO:HB3	71:SF:69:VAL:HG22	1.84	0.60
6:LA:137:ILE:HD11	6:LA:149:LYS:HB2	1.84	0.60
53:SE:87:MET:HE1	53:SE:123:LEU:HB2	1.83	0.60
86:CA:81:SER:HB2	86:CA:85:CYS:HB3	1.82	0.60
52:SC:118:ALA:HB2	68:S2:1486:A:H4'	1.82	0.60
55:SH:87:PHE:HB3	55:SH:90:LYS:HG3	1.83	0.60
82:Sf:119:ARG:HB3	82:Sf:132:MET:HB2	1.83	0.60
36:Lf:15:LYS:HB3	36:Lf:25:THR:HG23	1.84	0.60
3:L5:4363:A:H5''	45:Lo:36:GLN:HG2	1.83	0.59
3:L5:4691:A:H4'	13:LH:71:ARG:HG2	1.84	0.59
44:Ln:1:MET:HB2	68:S2:1706:G:H5'	1.84	0.59
68:S2:1324:G:H1	68:S2:1504:U:H3	1.50	0.59
86:CA:35:LEU:HD13	86:CA:108:ILE:HG21	1.83	0.59
49:Lt:114:ARG:HD3	49:Lt:129:ILE:HG22	1.83	0.59
85:CB:654:PRO:HD2	85:CB:658:GLY:HA3	1.84	0.59
3:L5:4302:U:H4'	24:LT:5:LYS:HD2	1.84	0.59
68:S2:1829:G:H1'	68:S2:1850:MA6:H2	1.83	0.59
14:LI:91:LEU:HD21	14:LI:129:VAL:HB	1.84	0.59
85:CB:605:LYS:HB2	85:CB:705:HIS:HE1	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LZ:46:ILE:HA	30:LZ:70:SER:HA	1.84	0.59
68:S2:51:U:H2'	68:S2:52:G:H8	1.68	0.59
68:S2:1841:C:H2'	68:S2:1842:4AC:H6	1.85	0.59
8:LC:218:ILE:HA	8:LC:229:LEU:HD13	1.84	0.59
14:LI:91:LEU:HD13	14:LI:135:ILE:HA	1.84	0.59
60:SO:55:ARG:HH12	68:S2:972:A:H61	1.49	0.59
85:CB:110:ASP:HB3	85:CB:553:HIS:HB2	1.83	0.59
86:CA:65:LYS:HA	86:CA:68:LYS:HD3	1.84	0.59
3:L5:2611:A:H5'	3:L5:2688:G:H4'	1.83	0.59
88:L5:5292:SPM:H112	19:LO:91:LYS:HD3	1.84	0.59
84:Et:26:A:H62	84:Et:44:G:H21	0.73	0.59
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.33	0.59
22:LR:169:ALA:HA	22:LR:172:ARG:HE	1.68	0.59
83:Sg:110:SER:HB2	83:Sg:154:VAL:HG12	1.85	0.59
3:L5:1629:G:H1	6:LA:208:GLU:HG2	1.67	0.58
3:L5:268:G:H2'	3:L5:269:G:H8	1.68	0.58
3:L5:4279:A:H5'	3:L5:4281:A:H1'	1.84	0.58
13:LH:44:GLU:HG3	17:LM:2:VAL:HG12	1.83	0.58
25:LU:18:VAL:HG13	25:LU:73:THR:HG23	1.84	0.58
57:SJ:26:ASP:HB2	67:Se:42:PHE:HZ	1.68	0.58
59:SN:63:VAL:HG11	59:SN:71:ILE:HD11	1.85	0.58
68:S2:1283:C:H4'	68:S2:1286:G:H4'	1.85	0.58
70:SD:197:LYS:HG2	70:SD:198:ILE:HG23	1.84	0.58
3:L5:1509:C:H5''	31:La:2:PRO:HD3	1.85	0.58
71:SF:19:LEU:HD23	71:SF:109:LEU:HD21	1.85	0.58
84:Et:6:G:H1	84:Et:67:U:H3	1.51	0.58
86:CA:21:TYR:HE1	86:CA:117:PHE:HB3	1.69	0.58
68:S2:207:G:H3'	68:S2:208:G:H8	1.68	0.58
3:L5:1414:C:H2'	3:L5:1415:G:H8	1.67	0.58
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.38	0.58
68:S2:525:A:H2'	68:S2:526:A:H8	1.68	0.58
68:S2:1547:C:H1'	68:S2:1670:C:H4'	1.86	0.58
3:L5:968:C:H5'	10:LE:110:ARG:HE	1.67	0.58
75:SQ:34:VAL:HG12	75:SQ:70:VAL:HB	1.86	0.58
83:Sg:40:ILE:HG13	83:Sg:59:LEU:HB2	1.84	0.58
86:CA:27:ILE:HD11	86:CA:59:GLU:HB3	1.86	0.58
68:S2:49:C:H2'	68:S2:472:C:H41	1.69	0.58
3:L5:4139:G:H21	3:L5:4140:C:H41	1.52	0.58
3:L5:4740:G:O6	3:L5:4959:U:O2	2.20	0.58
68:S2:152:U:H2'	68:S2:153:G:C8	2.38	0.58
68:S2:532:C:H2'	68:S2:533:A:H8	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:CB:509:VAL:HG12	85:CB:572:LYS:HG3	1.86	0.58
22:LR:172:ARG:HH12	68:S2:908:A:H5''	1.68	0.57
53:SE:100:ARG:HB2	53:SE:114:ILE:HD13	1.85	0.57
77:ST:143:LYS:HG3	77:ST:144:LYS:HG2	1.85	0.57
3:L5:2351:OMC:HM22	8:LC:95:MET:HG3	1.86	0.57
22:LR:170:ARG:HH22	22:LR:171:LYS:HD3	1.69	0.57
3:L5:1994:C:H2'	3:L5:1995:G:C8	2.39	0.57
12:LG:58:PRO:HD2	12:LG:61:ILE:HD12	1.86	0.57
53:SE:124:CYS:HB3	53:SE:141:THR:HB	1.86	0.57
56:SI:145:ILE:HD13	68:S2:190:G:H5'	1.85	0.57
60:SO:52:THR:HG21	68:S2:952:G:H21	1.68	0.57
68:S2:179:C:H3'	68:S2:180:G:H8	1.69	0.57
74:SP:133:ILE:HG22	74:SP:134:GLY:H	1.69	0.57
85:CB:27:HIS:HB3	85:CB:30:HIS:CD2	2.39	0.57
27:LW:97:LYS:HG3	27:LW:99:GLU:H	1.70	0.57
48:Ls:77:LYS:HB3	48:Ls:198:ILE:HD11	1.85	0.57
48:Ls:146:LYS:HD2	48:Ls:155:LEU:HD21	1.87	0.57
59:SN:75:LEU:HB3	59:SN:81:ALA:HB2	1.86	0.57
68:S2:1550:G:H3'	68:S2:1579:A:H61	1.70	0.57
51:SB:142:PHE:HB2	51:SB:209:ASP:HB3	1.85	0.57
51:SB:164:ILE:HD11	51:SB:204:ILE:HB	1.87	0.57
57:SJ:91:LYS:HB3	57:SJ:96:TYR:HD2	1.68	0.57
72:SK:27:VAL:HB	72:SK:43:LEU:HD12	1.85	0.57
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.69	0.57
52:SC:167:ARG:HB3	52:SC:177:PRO:HB2	1.87	0.57
85:CB:119:LEU:HD22	85:CB:151:ILE:HG13	1.87	0.57
11:LF:182:TYR:HB3	11:LF:200:ARG:HG3	1.85	0.57
25:LU:45:GLU:HG3	25:LU:46:ARG:HG2	1.86	0.57
54:SG:133:LEU:HB3	68:S2:65:C:H42	1.69	0.57
58:SL:75:GLY:HA3	58:SL:88:ILE:HD12	1.86	0.57
68:S2:1203:G:H2'	68:S2:1204:A:C8	2.39	0.57
84:Et:25:C:H3'	84:Et:26:A:H5''	1.86	0.57
1:CD:183:ASP:HB2	85:CB:599:HIS:HE2	1.69	0.57
3:L5:4611:A:H2	13:LH:120:GLU:HB3	1.69	0.57
68:S2:414:A:H2'	68:S2:415:A:H8	1.70	0.57
6:LA:115:CYS:SG	6:LA:124:GLY:HA3	2.44	0.57
35:Le:89:LEU:HD13	35:Le:118:LEU:HD22	1.86	0.57
57:SJ:164:PRO:HB3	57:SJ:170:PRO:HA	1.85	0.57
67:Se:2:VAL:HG23	67:Se:4:GLY:H	1.70	0.57
68:S2:145:G:H2'	68:S2:146:G:C8	2.39	0.57
48:Ls:42:GLN:HE22	48:Ls:105:ASN:HB2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SE:42:LEU:HG	53:SE:46:ILE:HD11	1.86	0.57
84:Et:37:A:H3'	84:Et:38:A:C8	2.40	0.57
85:CB:23:SER:HB3	85:CB:122:THR:HG21	1.87	0.57
3:L5:1333:A:H2'	3:L5:1334:A:C8	2.40	0.56
3:L5:1811:G:H21	32:Lb:57:MET:HE2	1.70	0.56
52:SC:102:LEU:HD12	52:SC:130:ILE:HG12	1.87	0.56
68:S2:527:C:H2'	68:S2:528:A:H8	1.70	0.56
68:S2:1536:G:H2'	68:S2:1537:A:C8	2.40	0.56
3:L5:3911:C:H2'	3:L5:3912:U:H6	1.70	0.56
68:S2:557:U:H2'	68:S2:558:G:C8	2.40	0.56
76:SS:124:ARG:HE	76:SS:129:LEU:HB2	1.70	0.56
3:L5:158:A:H5''	3:L5:159:C:H2'	1.88	0.56
48:Ls:135:THR:HG21	85:CB:187:VAL:HG11	1.88	0.56
75:SQ:19:ALA:HB2	75:SQ:75:GLY:HA3	1.87	0.56
86:CA:268:GLU:HG2	86:CA:271:ARG:HH22	1.71	0.56
52:SC:75:ILE:HD11	52:SC:265:PRO:HB3	1.87	0.56
64:SY:104:ARG:HH22	68:S2:492:C:H6	1.53	0.56
83:Sg:7:LEU:HA	83:Sg:310:TRP:HD1	1.71	0.56
30:LZ:50:PRO:HD3	30:LZ:68:ILE:HG12	1.88	0.56
55:SH:83:LEU:HB3	55:SH:92:VAL:HG11	1.88	0.56
69:SR:109:LEU:HG	69:SR:111:PHE:HD2	1.69	0.56
54:SG:31:ARG:HH22	68:S2:1745:A:H4'	1.69	0.56
25:LU:65:ARG:HG3	25:LU:70:ILE:HG12	1.88	0.56
28:LX:156:ILE:HD11	86:CA:291:MET:HB2	1.88	0.56
50:SA:10:MET:HE3	50:SA:55:TRP:HB2	1.87	0.56
68:S2:1407:U:H2'	68:S2:1408:U:C6	2.41	0.56
30:LZ:95:VAL:HG11	30:LZ:113:GLU:HG3	1.86	0.56
7:LB:92:TYR:HB2	7:LB:159:VAL:HB	1.88	0.56
3:L5:1326:A2M:H2'	3:L5:1327:C:C6	2.40	0.55
3:L5:3932:U:H2'	3:L5:3933:G:C8	2.41	0.55
12:LG:79:ALA:HB3	18:LN:18:VAL:HG11	1.88	0.55
56:SI:69:SER:HB2	58:SL:21:LYS:HB2	1.88	0.55
68:S2:996:A:H2'	68:S2:997:A:C8	2.41	0.55
54:SG:88:ARG:HG2	54:SG:91:GLU:HB2	1.87	0.55
54:SG:141:ILE:HD11	54:SG:153:VAL:HG13	1.88	0.55
3:L5:4992:G:H2'	3:L5:4993:G:C8	2.40	0.55
5:L8:67:U:H2'	5:L8:68:G:H8	1.71	0.55
68:S2:1398:G:H1'	83:Sg:63:SER:HB2	1.87	0.55
3:L5:4242:U:H3	3:L5:4281:A:H2	1.53	0.55
68:S2:808:A:H2	68:S2:855:G:H22	1.53	0.55
68:S2:1337:4AC:H2'	68:S2:1338:G:H8	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SD:158:ILE:HG23	70:SD:189:MET:HE1	1.88	0.55
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.42	0.55
48:Ls:120:GLU:HG2	48:Ls:162:LYS:HA	1.87	0.55
51:SB:170:GLU:HA	51:SB:173:THR:HG22	1.88	0.55
77:ST:14:PHE:HE1	77:ST:134:ILE:HG23	1.71	0.55
83:Sg:230:LEU:HD22	83:Sg:259:TRP:CE2	2.41	0.55
3:L5:2557:G:H1	3:L5:2570:U:H3	1.54	0.55
9:LD:182:GLY:HA2	9:LD:194:VAL:HG23	1.87	0.55
10:LE:95:PRO:HA	10:LE:104:THR:HG22	1.89	0.55
53:SE:137:PRO:HG2	53:SE:150:PRO:HD2	1.88	0.55
68:S2:734:C:N4	68:S2:737:G:H1	2.05	0.55
68:S2:1101:U:H2'	68:S2:1102:G:H8	1.72	0.55
57:SJ:46:VAL:HG11	57:SJ:106:LEU:HD21	1.89	0.55
85:CB:583:VAL:HG22	85:CB:700:VAL:HG22	1.89	0.55
68:S2:323:C:H2'	68:S2:327:G:H1	1.71	0.55
68:S2:1845:A:H2'	68:S2:1846:G:C8	2.41	0.55
68:S2:1562:C:H2'	68:S2:1563:G:C8	2.42	0.55
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.42	0.55
27:LW:87:LEU:HG	27:LW:91:MET:HE1	1.88	0.55
53:SE:31:PRO:HA	53:SE:81:THR:HB	1.89	0.55
54:SG:11:GLY:HA2	68:S2:166:A2M:HM'1	1.88	0.55
68:S2:677:G:H21	68:S2:1028:A:H62	1.55	0.55
86:CA:64:PHE:HD2	86:CA:72:LYS:HE2	1.72	0.55
3:L5:257:C:H2'	3:L5:258:G:C8	2.42	0.54
3:L5:1725:U:H2'	3:L5:1726:U:H6	1.72	0.54
3:L5:2480:G:H2'	3:L5:2481:G:H8	1.72	0.54
20:LP:131:ARG:HG3	20:LP:137:ASN:OD1	2.06	0.54
38:Lh:73:TYR:HA	38:Lh:76:LYS:HD2	1.88	0.54
3:L5:3748:A:H5''	6:LA:243:THR:HB	1.89	0.54
66:Sb:51:GLN:HE21	68:S2:1014:G:H21	1.55	0.54
68:S2:917:U:H2'	68:S2:918:U:H6	1.72	0.54
68:S2:1221:G:H2'	68:S2:1222:G:H8	1.73	0.54
71:SF:127:ARG:HA	71:SF:136:ARG:HD2	1.89	0.54
79:SZ:79:ILE:HB	79:SZ:83:LEU:HD23	1.90	0.54
83:Sg:37:ASP:HB3	83:Sg:39:THR:HG22	1.87	0.54
68:S2:888:U:H4'	68:S2:889:U:H5'	1.88	0.54
68:S2:1438:A:H2'	68:S2:1439:A:C8	2.42	0.54
78:SU:22:ILE:HD11	78:SU:112:VAL:HB	1.89	0.54
3:L5:432:U:H1'	88:L5:5292:SPM:H82	1.90	0.54
50:SA:38:ILE:HD12	50:SA:47:TYR:HB3	1.88	0.54
58:SL:111:VAL:HG12	58:SL:140:PHE:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:SS:22:GLY:HA2	76:SS:56:ALA:HB3	1.90	0.54
84:Et:8:U:H3	84:Et:14:A:H62	1.55	0.54
85:CB:345:PRO:HG2	85:CB:348:ASP:HB2	1.87	0.54
85:CB:770:VAL:HA	85:CB:786:ALA:HA	1.90	0.54
86:CA:333:ILE:HG13	86:CA:334:THR:HG23	1.89	0.54
13:LH:93:ARG:HD2	13:LH:143:GLU:HG3	1.90	0.54
15:LJ:35:ARG:HB3	15:LJ:123:ILE:HA	1.90	0.54
68:S2:1410:C:H2'	68:S2:1411:G:H8	1.72	0.54
68:S2:1845:A:H2'	68:S2:1846:G:H8	1.72	0.54
76:SS:16:LEU:HD23	76:SS:100:ALA:HB2	1.90	0.54
77:ST:6:VAL:HG12	77:ST:135:ALA:HB2	1.89	0.54
51:SB:150:ILE:HD13	69:SR:129:LYS:HB2	1.90	0.54
65:Sa:79:ILE:HD11	68:S2:1864:U:H5'	1.88	0.54
68:S2:28:U:H2'	68:S2:29:G:H8	1.73	0.54
68:S2:1221:G:H2'	68:S2:1222:G:C8	2.43	0.54
84:Et:36:U:H5''	84:Et:37:A:H2	1.73	0.54
10:LE:224:LYS:HG3	10:LE:227:HIS:HB3	1.89	0.54
50:SA:180:ARG:HD3	50:SA:184:ARG:HH11	1.73	0.54
54:SG:86:PRO:HB3	54:SG:91:GLU:HB3	1.90	0.54
68:S2:155:G:H2'	68:S2:156:G:H8	1.73	0.54
3:L5:659:G:H2'	3:L5:660:A:H8	1.72	0.54
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.43	0.54
68:S2:750:C:H42	68:S2:793:G:H1'	1.72	0.54
68:S2:1603:G:H4'	76:SS:38:ARG:HH22	1.73	0.54
84:Et:37:A:H3'	84:Et:38:A:H8	1.72	0.54
3:L5:700:G:O6	3:L5:701:G:O6	2.26	0.54
3:L5:1949:U:H5''	13:LH:64:ARG:HD3	1.90	0.54
69:SR:10:LYS:HG3	69:SR:53:TYR:CE2	2.43	0.54
73:SM:20:GLU:HG2	73:SM:119:GLN:HB2	1.89	0.54
48:Ls:175:LEU:HD22	48:Ls:180:ILE:HD11	1.90	0.54
51:SB:89:GLU:HB3	51:SB:223:PHE:HE1	1.73	0.54
83:Sg:259:TRP:HB3	83:Sg:266:ILE:HA	1.90	0.54
85:CB:189:ILE:HD12	85:CB:203:ILE:HG23	1.88	0.54
85:CB:206:ASP:HB2	85:CB:209:LEU:HB2	1.89	0.54
85:CB:605:LYS:HB2	85:CB:705:HIS:CE1	2.42	0.54
3:L5:691:C:H2'	3:L5:692:A:C8	2.43	0.53
3:L5:2539:C:H2'	3:L5:2540:C:C6	2.43	0.53
3:L5:3599:A:H2'	3:L5:3600:G:C8	2.43	0.53
3:L5:4508:C:N3	3:L5:4512:U:H5	2.06	0.53
12:LG:162:ASP:HB2	12:LG:163:PRO:HD3	1.89	0.53
58:SL:127:THR:HB	58:SL:144:LYS:HB3	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1748:G:O6	68:S2:1786:U:O4	2.26	0.53
71:SF:34:SER:HA	80:Sc:55:VAL:HG23	1.89	0.53
81:Sd:19:ARG:HH11	81:Sd:32:ARG:HD2	1.73	0.53
83:Sg:206:LEU:HD11	83:Sg:218:LEU:HD13	1.90	0.53
45:Lo:69:ARG:HE	45:Lo:80:LYS:HG2	1.72	0.53
51:SB:129:THR:HB	51:SB:133:TYR:H	1.72	0.53
68:S2:5:U:H2'	68:S2:6:G:H8	1.72	0.53
70:SD:67:ARG:HH11	72:SK:96:ARG:HG2	1.73	0.53
3:L5:1697:G:H22	3:L5:2084:C:P	2.31	0.53
3:L5:4139:G:N2	3:L5:4140:C:H41	2.05	0.53
3:L5:4220:6MZ:O5'	3:L5:4220:6MZ:H8	2.08	0.53
3:L5:4523:A2M:H5''	3:L5:4524:G:H5'	1.91	0.53
68:S2:12:U:H2'	68:S2:13:C:C6	2.43	0.53
68:S2:525:A:H2'	68:S2:526:A:C8	2.43	0.53
71:SF:122:ARG:HE	80:Sc:59:LEU:HD21	1.74	0.53
83:Sg:256:ILE:HB	83:Sg:270:LEU:HB2	1.90	0.53
3:L5:5006:U:H4'	3:L5:5007:A:H5'	1.90	0.53
6:LA:247:ARG:HB3	68:S2:1069:U:H4'	1.91	0.53
51:SB:129:THR:HG22	51:SB:131:ASP:H	1.73	0.53
68:S2:164:A:H3'	68:S2:165:G:H21	1.72	0.53
68:S2:886:A:H2'	68:S2:887:U:O4'	2.09	0.53
68:S2:1661:A:H8	81:Sd:14:PHE:HB2	1.73	0.53
70:SD:219:PRO:HB2	83:Sg:192:THR:HG22	1.91	0.53
14:LI:102:MET:HE1	14:LI:114:GLY:H	1.74	0.53
51:SB:117:TRP:HB3	51:SB:153:THR:HG22	1.89	0.53
3:L5:4742:G:H2'	3:L5:4743:G:H8	1.73	0.53
15:LJ:141:ILE:HA	15:LJ:144:LYS:HD2	1.91	0.53
56:SI:141:ARG:HB3	56:SI:145:ILE:HD11	1.91	0.53
60:SO:78:ALA:HB1	60:SO:119:LEU:HG	1.89	0.53
3:L5:3720:G:H22	3:L5:3733:A:H2	1.57	0.53
8:LC:110:ARG:HB2	18:LN:204:ARG:HH21	1.74	0.53
35:Le:7:LEU:HB2	35:Le:93:LYS:HB3	1.89	0.53
48:Ls:127:ASN:HD21	48:Ls:151:THR:HG23	1.74	0.53
49:Lt:82:ILE:HG22	49:Lt:86:LYS:HE2	1.91	0.53
61:SV:16:LYS:HG2	61:SV:23:ILE:HD13	1.90	0.53
71:SF:18:LYS:HD3	71:SF:22:LYS:HA	1.91	0.53
85:CB:9:ILE:HG13	85:CB:45:ILE:HD12	1.89	0.53
3:L5:2498:C:H2'	3:L5:2499:C:H6	1.74	0.53
27:LW:86:SER:HB3	27:LW:89:ASP:HB2	1.89	0.53
49:Lt:121:LEU:HD23	49:Lt:129:ILE:HA	1.89	0.53
62:SW:3:ARG:HD3	62:SW:6:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1421:A:N7	68:S2:1424:G:H1'	2.24	0.53
72:SK:80:ARG:NH1	72:SK:87:PRO:HA	2.24	0.53
3:L5:4153:C:H5''	28:LX:38:LYS:HD3	1.90	0.53
9:LD:204:VAL:HB	9:LD:236:MET:HE1	1.91	0.53
83:Sg:166:VAL:HG22	83:Sg:176:VAL:HG22	1.91	0.53
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.44	0.53
3:L5:2517:A:H5'	37:Lg:62:LYS:HD3	1.92	0.53
11:LF:105:VAL:HG13	11:LF:136:VAL:HG12	1.90	0.53
68:S2:907:G:H2'	68:S2:908:A:C8	2.44	0.53
68:S2:1764:G:H5''	68:S2:1765:C:H5''	1.90	0.53
73:SM:49:LEU:HG	73:SM:75:ASN:HB3	1.90	0.53
86:CA:121:VAL:HB	86:CA:334:THR:HB	1.89	0.53
3:L5:1503:A:H62	21:LQ:87:THR:HG21	1.74	0.52
58:SL:133:PRO:HG2	68:S2:383:G:H21	1.74	0.52
62:SW:53:ILE:HB	62:SW:60:LYS:HB2	1.91	0.52
85:CB:189:ILE:HD11	85:CB:204:MET:HA	1.90	0.52
14:LI:73:ASN:HB2	14:LI:87:MET:HE1	1.90	0.52
50:SA:77:ILE:HG12	50:SA:99:ILE:HB	1.90	0.52
53:SE:19:MET:HE3	53:SE:108:ARG:HD3	1.91	0.52
54:SG:228:ILE:HG22	54:SG:231:ARG:NH2	2.23	0.52
60:SO:101:GLY:HA3	60:SO:134:PRO:HD2	1.91	0.52
68:S2:13:C:H4'	68:S2:1355:C:H5	1.74	0.52
3:L5:3910:C:H2'	3:L5:3911:C:C6	2.44	0.52
8:LC:7:LEU:HG	8:LC:21:ASN:HB3	1.92	0.52
10:LE:190:HIS:HB3	10:LE:193:PHE:HD1	1.74	0.52
48:Ls:160:LEU:HD21	48:Ls:171:GLU:HB3	1.91	0.52
51:SB:107:ARG:HD2	60:SO:131:ASP:HB2	1.91	0.52
86:CA:60:THR:HA	86:CA:63:ILE:HG12	1.92	0.52
86:CA:190:LEU:HD22	86:CA:225:ALA:HB2	1.89	0.52
18:LN:159:ARG:HB3	18:LN:164:LEU:HB2	1.92	0.52
53:SE:36:HIS:CG	53:SE:85:GLY:HA3	2.44	0.52
10:LE:243:THR:HG22	10:LE:245:GLN:H	1.75	0.52
54:SG:231:ARG:HD2	68:S2:785:C:H5'	1.90	0.52
3:L5:433:A:C2	3:L5:3867:A2M:H4'	2.45	0.52
11:LF:222:LYS:HB3	11:LF:231:GLY:HA2	1.92	0.52
38:Lh:4:ILE:HD12	38:Lh:53:SER:HB3	1.91	0.52
49:Lt:104:ILE:HG13	49:Lt:106:PHE:HD2	1.75	0.52
64:SY:10:ARG:HA	68:S2:839:C:H41	1.75	0.52
64:SY:36:PRO:HG2	64:SY:39:GLU:HB2	1.91	0.52
68:S2:544:G:H2'	68:S2:545:A:C8	2.45	0.52
68:S2:1277:C:H2'	68:S2:1278:A:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.45	0.52
11:LF:162:ILE:HD12	11:LF:167:ILE:HB	1.92	0.52
51:SB:64:GLY:HA2	51:SB:87:ILE:HD11	1.92	0.52
56:SI:38:ILE:HD11	56:SI:96:LEU:HD21	1.90	0.52
68:S2:484:A2M:H8	68:S2:484:A2M:O5'	2.10	0.52
77:ST:28:LEU:HA	77:ST:110:LEU:HD21	1.91	0.52
3:L5:717:U:H2'	3:L5:718:C:C6	2.45	0.52
3:L5:1942:A:H2'	3:L5:1943:A:H8	1.72	0.52
3:L5:4935:C:H2'	3:L5:4936:G:C8	2.44	0.52
68:S2:639:C:H2'	68:S2:640:A:C8	2.45	0.52
71:SF:25:THR:HG22	71:SF:109:LEU:HG	1.92	0.52
71:SF:130:ARG:HG2	71:SF:133:THR:H	1.73	0.52
68:S2:640:A:H2'	68:S2:641:A:C8	2.45	0.52
85:CB:382:ALA:HA	85:CB:385:ILE:HG12	1.92	0.52
3:L5:2554:U:H3	3:L5:2764:A:H8	1.55	0.52
3:L5:4281:A:H2'	3:L5:4282:A:H2'	1.91	0.52
3:L5:4489:G:H4'	89:L5:5288:SPD:H91	1.91	0.52
40:Lj:19:CYS:SG	40:Lj:34:CYS:HB2	2.50	0.52
68:S2:694:G:H5''	68:S2:730:C:H5	1.74	0.52
78:SU:61:LEU:HB2	78:SU:82:MET:HB3	1.91	0.52
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.45	0.51
64:SY:12:PHE:HE1	64:SY:21:LYS:HB3	1.75	0.51
68:S2:674:C:H2'	68:S2:675:U:C6	2.45	0.51
76:SS:36:VAL:HG23	76:SS:40:TYR:HB3	1.92	0.51
85:CB:368:ARG:O	85:CB:372:LEU:HD13	2.11	0.51
3:L5:162:A:H2'	3:L5:163:A:C8	2.46	0.51
3:L5:4954:G:H2'	3:L5:4955:A:C8	2.45	0.51
52:SC:259:THR:HG21	61:SV:16:LYS:H	1.74	0.51
68:S2:1232:PSU:H2'	68:S2:1233:G:C8	2.45	0.51
68:S2:1643:U:H2'	68:S2:1644:C:C6	2.45	0.51
3:L5:138:G:H2'	3:L5:139:G:H8	1.74	0.51
3:L5:4401:G:H2'	3:L5:4402:C:H6	1.75	0.51
30:LZ:11:VAL:HG12	30:LZ:82:PRO:HA	1.93	0.51
34:Ld:22:THR:HG23	34:Ld:122:VAL:HB	1.92	0.51
59:SN:147:SER:HA	59:SN:150:VAL:HG12	1.92	0.51
68:S2:1423:C:H41	75:SQ:4:LYS:HG3	1.75	0.51
68:S2:1653:U:H2'	68:S2:1654:G:C8	2.45	0.51
83:Sg:129:ILE:HB	83:Sg:142:VAL:HB	1.93	0.51
85:CB:365:GLN:HA	85:CB:368:ARG:HB2	1.91	0.51
3:L5:667:A:H5''	3:L5:668:C:H5''	1.91	0.51
29:LY:111:LEU:HB3	29:LY:116:LYS:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:931:C:H2'	68:S2:932:G:C8	2.45	0.51
70:SD:59:LEU:HD23	70:SD:66:ILE:HG13	1.93	0.51
75:SQ:32:ILE:HG12	75:SQ:39:LEU:HD23	1.92	0.51
3:L5:2411:C:H2'	3:L5:2412:A:H8	1.74	0.51
51:SB:71:LEU:HD13	51:SB:82:ARG:HD2	1.92	0.51
51:SB:134:LEU:HG	51:SB:218:LEU:HD12	1.91	0.51
64:SY:56:PHE:HD1	64:SY:90:ARG:HG2	1.75	0.51
86:CA:57:MET:HE2	86:CA:74:ILE:HD12	1.92	0.51
86:CA:123:HIS:HE1	86:CA:338:PHE:HB2	1.76	0.51
3:L5:182:G:H2'	3:L5:183:C:H4'	1.93	0.51
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.26	0.51
23:LS:83:ARG:HG3	23:LS:125:GLN:HB3	1.93	0.51
50:SA:10:MET:HE1	50:SA:51:LEU:HG	1.92	0.51
68:S2:887:U:H3	68:S2:900:C:H5	1.58	0.51
68:S2:1037:G:H4'	68:S2:1845:A:H4'	1.92	0.51
83:Sg:212:LYS:HD2	83:Sg:235:ILE:HG12	1.92	0.51
84:Et:22:G:N7	84:Et:46:G:O6	2.43	0.51
53:SE:186:GLY:HA3	68:S2:809:A:OP1	2.11	0.51
56:SI:87:ASN:HB3	56:SI:90:LEU:HD13	1.91	0.51
68:S2:835:C:H4'	68:S2:836:G:C8	2.45	0.51
3:L5:490:C:H2'	3:L5:491:G:C8	2.46	0.51
3:L5:947:C:H5''	10:LE:51:VAL:HG21	1.92	0.51
3:L5:4723:A:H2'	3:L5:4724:A:C8	2.45	0.51
3:L5:5030:U:H2'	3:L5:5031:G:H8	1.74	0.51
50:SA:176:TRP:CD1	50:SA:199:PRO:HA	2.46	0.51
52:SC:68:ARG:HG2	52:SC:277:HIS:HB2	1.93	0.51
68:S2:165:G:H2'	68:S2:166:A2M:H8	1.93	0.51
72:SK:41:PRO:HD2	72:SK:44:HIS:HD2	1.76	0.51
83:Sg:32:LEU:HD21	83:Sg:71:ILE:HD11	1.92	0.51
86:CA:118:ILE:HG21	86:CA:190:LEU:HD23	1.93	0.51
3:L5:1327:C:H2'	3:L5:1328:G:C8	2.46	0.51
3:L5:1992:U:H4'	3:L5:1993:C:H5''	1.93	0.51
3:L5:3641:U:H5	3:L5:3646:A:N7	2.08	0.51
23:LS:15:ARG:HB3	23:LS:27:LEU:HD23	1.93	0.51
27:LW:7:SER:HB2	27:LW:13:ILE:HD11	1.92	0.51
51:SB:103:MET:HG3	51:SB:215:VAL:HG22	1.92	0.51
53:SE:42:LEU:HD21	53:SE:47:PHE:HB2	1.93	0.51
54:SG:61:PHE:CG	54:SG:72:ARG:HD2	2.45	0.51
68:S2:639:C:H2'	68:S2:640:A:H8	1.75	0.51
68:S2:1513:C:H2'	68:S2:1514:G:H8	1.75	0.51
75:SQ:68:ILE:HD12	75:SQ:88:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:SU:116:ILE:HB	78:SU:119:ALA:HB3	1.93	0.51
82:Sf:121:CYS:HB3	82:Sf:126:CYS:HB3	1.93	0.51
3:L5:4742:G:H2'	3:L5:4743:G:C8	2.46	0.51
54:SG:98:ARG:HH11	54:SG:99:GLY:H	1.56	0.51
55:SH:49:LYS:HD3	55:SH:179:LYS:HZ1	1.76	0.51
56:SI:103:LEU:HD22	56:SI:170:LYS:HB3	1.93	0.51
63:SX:9:THR:HG22	68:S2:681:PSU:H4'	1.93	0.51
79:SZ:99:LEU:HD11	79:SZ:102:LYS:HB2	1.92	0.51
85:CB:24:VAL:HG22	85:CB:32:LYS:HG2	1.93	0.51
3:L5:217:C:H5	3:L5:219:G:H4'	1.76	0.50
3:L5:256:G:H2'	3:L5:257:C:C6	2.45	0.50
3:L5:455:C:N4	3:L5:456:C:N4	2.59	0.50
3:L5:500:G:O2'	3:L5:504:G:H3'	2.11	0.50
3:L5:701:G:H2'	3:L5:702:U:C6	2.46	0.50
3:L5:1251:C:H2'	3:L5:1252:C:C6	2.46	0.50
5:L8:67:U:H2'	5:L8:68:G:C8	2.46	0.50
6:LA:7:GLY:HA2	6:LA:10:LYS:HG3	1.92	0.50
9:LD:65:ALA:HB2	9:LD:74:ILE:HD13	1.93	0.50
50:SA:145:ILE:HG12	50:SA:159:ILE:HD12	1.93	0.50
68:S2:1010:G:H2'	68:S2:1011:A:H8	1.76	0.50
56:SI:192:GLY:HA3	58:SL:19:ASN:HD21	1.76	0.50
66:Sb:45:THR:HG23	66:Sb:82:LYS:HE3	1.92	0.50
68:S2:223:C:H2'	68:S2:224:A:C8	2.46	0.50
68:S2:614:C:H2'	68:S2:626:G:C8	2.46	0.50
85:CB:259:LYS:HD3	85:CB:273:PHE:HE2	1.76	0.50
3:L5:2745:A:H2'	3:L5:2746:A:H8	1.77	0.50
3:L5:4769:G:H5''	19:LO:176:ARG:HD3	1.91	0.50
68:S2:877:C:H2'	68:S2:878:G:C8	2.46	0.50
3:L5:2485:U:H3	3:L5:2491:C:N4	2.08	0.50
50:SA:5:LEU:O	50:SA:9:GLN:HG2	2.12	0.50
51:SB:149:GLN:HE22	68:S2:1123:C:H4'	1.77	0.50
66:Sb:16:LYS:HA	66:Sb:23:ARG:HH21	1.75	0.50
68:S2:344:U:H2'	68:S2:345:U:H6	1.77	0.50
68:S2:929:G:H2'	68:S2:930:C:O4'	2.12	0.50
3:L5:1461:C:H2'	3:L5:1462:A:C8	2.47	0.50
3:L5:4612:C:C2	13:LH:120:GLU:HB2	2.45	0.50
7:LB:279:GLU:HB3	7:LB:282:LYS:HZ3	1.76	0.50
7:LB:354:GLN:HB3	7:LB:359:ALA:HB1	1.92	0.50
36:Lf:45:LYS:NZ	36:Lf:108:SER:HA	2.27	0.50
68:S2:1623:A:C6	76:SS:132:ARG:HD3	2.47	0.50
73:SM:31:LEU:HD21	73:SM:89:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Sg:34:ALA:HA	83:Sg:40:ILE:HG22	1.93	0.50
86:CA:21:TYR:CE1	86:CA:117:PHE:HB3	2.45	0.50
86:CA:107:LYS:NZ	86:CA:316:VAL:HG23	2.26	0.50
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.46	0.50
7:LB:288:GLY:HA3	7:LB:330:PHE:CE1	2.47	0.50
20:LP:54:GLN:HA	20:LP:83:TRP:CD1	2.46	0.50
56:SI:144:LYS:HG3	56:SI:145:ILE:HG23	1.94	0.50
68:S2:24:C:HO2'	68:S2:25:A:H8	1.58	0.50
6:LA:20:VAL:HA	6:LA:23:ARG:HG3	1.93	0.50
43:Lm:98:LYS:HG3	43:Lm:118:THR:HG21	1.94	0.50
55:SH:159:ASP:O	55:SH:160:LYS:HG2	2.11	0.50
60:SO:34:PHE:HB3	60:SO:41:PHE:HB2	1.94	0.50
68:S2:186:C:H2'	68:S2:187:G:C8	2.47	0.50
68:S2:690:G:H3'	68:S2:691:G:H21	1.76	0.50
68:S2:1587:G:C6	77:ST:67:ARG:HD2	2.47	0.50
3:L5:1428:U:H5''	21:LQ:42:THR:HB	1.94	0.50
3:L5:2745:A:H2'	3:L5:2746:A:C8	2.47	0.50
42:Ll:38:ASN:HB3	42:Ll:41:ARG:HG2	1.94	0.50
48:Ls:55:MET:HG2	48:Ls:87:GLY:HA3	1.94	0.50
51:SB:71:LEU:HD12	51:SB:84:PHE:HE1	1.77	0.50
60:SO:56:VAL:HG13	60:SO:60:MET:SD	2.52	0.50
64:SY:104:ARG:HH12	68:S2:492:C:H5	1.58	0.50
68:S2:106:C:H2'	68:S2:107:A:C8	2.45	0.50
68:S2:1284:A:H4'	68:S2:1285:G:H5''	1.94	0.50
68:S2:1650:A:H5''	75:SQ:139:ALA:HB2	1.94	0.50
85:CB:665:ILE:HD11	85:CB:705:HIS:CD2	2.47	0.50
86:CA:255:TYR:HB3	86:CA:301:LEU:HD11	1.92	0.50
3:L5:2542:G:H2'	3:L5:2543:A:C8	2.47	0.50
3:L5:4426:C:H2'	3:L5:4427:G:H5'	1.94	0.50
53:SE:79:ASP:HB3	53:SE:82:TYR:HB2	1.94	0.50
60:SO:125:LYS:HB3	65:Sa:58:VAL:HG13	1.94	0.50
68:S2:13:C:H4'	68:S2:1355:C:C5	2.46	0.50
68:S2:1232:PSU:H2'	68:S2:1233:G:H8	1.77	0.50
71:SF:138:ALA:HB2	71:SF:204:ARG:HA	1.94	0.50
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.94	0.49
54:SG:159:ARG:HG3	54:SG:173:ALA:HB2	1.93	0.49
58:SL:23:VAL:HG23	58:SL:25:LEU:HG	1.93	0.49
67:Se:48:THR:HG23	67:Se:50:GLY:H	1.76	0.49
68:S2:897:U:H2'	68:S2:898:U:H4'	1.93	0.49
68:S2:1274:G:H4'	72:SK:47:LYS:HE3	1.93	0.49
68:S2:1291:A:N6	82:Sf:95:ARG:HH12	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1655:C:H2'	68:S2:1656:G:H8	1.77	0.49
76:SS:66:ARG:O	76:SS:70:ILE:HG12	2.12	0.49
83:Sg:79:LEU:HD11	83:Sg:87:LEU:HD23	1.93	0.49
85:CB:290:CYS:HA	85:CB:294:LEU:HB2	1.92	0.49
3:L5:138:G:H2'	3:L5:139:G:C8	2.47	0.49
3:L5:2741:U:H2'	6:LA:50:HIS:CD2	2.48	0.49
50:SA:76:VAL:HG12	50:SA:123:VAL:HB	1.94	0.49
56:SI:154:LYS:HB2	58:SL:24:LEU:HD23	1.93	0.49
68:S2:595:U:H2'	68:S2:596:U:C6	2.47	0.49
68:S2:1644:C:H4'	75:SQ:140:ARG:HB2	1.94	0.49
78:SU:22:ILE:HG23	78:SU:89:ILE:HB	1.94	0.49
82:Sf:121:CYS:HB2	82:Sf:130:VAL:HG23	1.93	0.49
3:L5:1307:A:H2'	3:L5:1308:C:C6	2.46	0.49
7:LB:217:ILE:HD12	7:LB:347:LEU:HB3	1.94	0.49
7:LB:258:HIS:HA	7:LB:260:ALA:N	2.26	0.49
18:LN:146:PRO:HB2	38:Lh:104:THR:HG23	1.95	0.49
31:La:72:THR:HG22	31:La:110:LYS:HB3	1.95	0.49
49:Lt:110:VAL:O	49:Lt:114:ARG:HG2	2.13	0.49
51:SB:176:VAL:HG23	51:SB:184:VAL:HG21	1.94	0.49
64:SY:50:THR:HG21	64:SY:75:ILE:HD11	1.93	0.49
68:S2:163:U:H2'	68:S2:164:A:H8	1.75	0.49
77:ST:134:ILE:HA	77:ST:137:GLN:HG2	1.93	0.49
3:L5:2480:G:H2'	3:L5:2481:G:C8	2.47	0.49
51:SB:37:ALA:HA	51:SB:42:ARG:HH22	1.78	0.49
51:SB:67:PHE:CE1	60:SO:48:SER:HB3	2.47	0.49
52:SC:107:LEU:HB3	52:SC:233:LEU:HD21	1.93	0.49
68:S2:857:U:H2'	68:S2:858:A:C8	2.47	0.49
68:S2:867:OMG:H8	68:S2:867:OMG:H5''	1.77	0.49
76:SS:65:GLU:HA	76:SS:68:ILE:HG12	1.92	0.49
85:CB:259:LYS:HD3	85:CB:273:PHE:CE2	2.47	0.49
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.47	0.49
3:L5:4392:OMG:H2'	3:L5:4447:5MC:HM51	1.94	0.49
3:L5:5024:C:H41	3:L5:5028:G:H21	1.60	0.49
19:LO:76:PRO:HB3	19:LO:138:LEU:HG	1.94	0.49
54:SG:51:ARG:HH21	54:SG:112:VAL:HG11	1.76	0.49
66:Sb:22:LYS:HE3	68:S2:1129:G:H5''	1.94	0.49
68:S2:432:G:H2'	68:S2:433:A:C8	2.48	0.49
68:S2:1540:G:H5'	77:ST:47:PRO:HB3	1.94	0.49
72:SK:76:ILE:O	72:SK:80:ARG:HG2	2.12	0.49
86:CA:187:SER:HB2	86:CA:201:ILE:HB	1.94	0.49
12:LG:30:PRO:HG2	30:LZ:124:THR:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LN:116:LEU:HD22	18:LN:135:ILE:HD11	1.95	0.49
32:Lb:101:HIS:CE1	32:Lb:103:LYS:HG2	2.47	0.49
57:SJ:145:PRO:HD2	68:S2:522:A:H5''	1.94	0.49
60:SO:44:VAL:HG23	60:SO:53:ILE:HB	1.95	0.49
68:S2:1144:A:H2'	68:S2:1145:A:C8	2.47	0.49
83:Sg:87:LEU:HD11	83:Sg:108:VAL:HG11	1.94	0.49
85:CB:27:HIS:HB2	85:CB:139:THR:HG23	1.94	0.49
86:CA:172:LYS:HG2	86:CA:354:LEU:HD11	1.95	0.49
3:L5:2765:A:H2'	3:L5:2766:A:C8	2.46	0.49
51:SB:125:VAL:HG22	51:SB:137:LEU:HB2	1.94	0.49
68:S2:696:G:H4'	68:S2:735:C:C2	2.47	0.49
68:S2:1581:C:H5'	68:S2:1582:C:H5	1.78	0.49
75:SQ:42:ILE:HG13	75:SQ:43:GLU:H	1.78	0.49
76:SS:59:LEU:HD23	76:SS:64:VAL:HG22	1.94	0.49
1:CD:212:GLY:O	1:CD:220:THR:HG23	2.13	0.49
3:L5:4260:U:H2'	3:L5:4261:C:C6	2.48	0.49
49:Lt:121:LEU:HD23	49:Lt:129:ILE:HG12	1.94	0.49
51:SB:109:LYS:O	51:SB:113:MET:HG2	2.12	0.49
54:SG:192:ILE:HD11	68:S2:126:G:C2	2.48	0.49
68:S2:51:U:H2'	68:S2:52:G:C8	2.47	0.49
68:S2:834:C:N4	68:S2:839:C:H42	2.11	0.49
75:SQ:50:LYS:HE2	75:SQ:82:TYR:CZ	2.46	0.49
77:ST:85:ASN:HB3	77:ST:88:MET:HB2	1.93	0.49
3:L5:4146:G:H2'	3:L5:4147:G:C8	2.48	0.49
3:L5:4392:OMG:HM21	3:L5:4394:A:H2'	1.94	0.49
3:L5:4459:U:H2'	3:L5:4460:U:C6	2.47	0.49
8:LC:65:GLU:HG2	8:LC:80:ARG:HD3	1.95	0.49
48:Ls:119:CYS:HB3	48:Ls:183:PHE:HB3	1.95	0.49
50:SA:69:GLU:HB2	52:SC:270:THR:HG21	1.95	0.49
61:SV:1:MET:HA	61:SV:9:VAL:HG23	1.95	0.49
63:SX:107:ARG:HG3	63:SX:110:HIS:HB3	1.94	0.49
71:SF:122:ARG:HA	71:SF:146:ARG:HD3	1.95	0.49
85:CB:56:PHE:HB3	85:CB:455:GLY:HA3	1.95	0.49
15:LJ:78:LYS:HE3	15:LJ:82:ILE:HD11	1.95	0.49
55:SH:51:ILE:HD11	55:SH:176:VAL:HG12	1.95	0.49
55:SH:58:LYS:HG3	55:SH:90:LYS:HD3	1.95	0.49
68:S2:694:G:H5''	68:S2:730:C:C5	2.48	0.49
68:S2:1217:A:H2'	68:S2:1218:C:C6	2.48	0.49
3:L5:280:G:H5''	18:LN:14:LYS:HE2	1.95	0.48
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.48	0.48
3:L5:2020:U:H2'	3:L5:2021:G:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.47	0.48
3:L5:2709:C:H2'	86:CA:263:ARG:NE	2.27	0.48
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.48	0.48
15:LJ:40:LEU:HD12	15:LJ:70:VAL:HG22	1.93	0.48
68:S2:549:C:H2'	68:S2:550:C:C6	2.48	0.48
68:S2:1595:U:H2'	68:S2:1596:U:C6	2.48	0.48
83:Sg:7:LEU:HA	83:Sg:310:TRP:CD1	2.47	0.48
86:CA:156:LEU:HD11	86:CA:166:VAL:HG22	1.95	0.48
3:L5:121:A:H62	3:L5:152:U:H3	1.59	0.48
3:L5:233:U:O2'	3:L5:234:G:H2'	2.14	0.48
3:L5:737:C:C5	3:L5:739:G:H5''	2.48	0.48
3:L5:1177:U:H3	3:L5:1183:C:H42	1.61	0.48
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.49	0.48
3:L5:3861:A:H2'	3:L5:3862:A:H8	1.76	0.48
5:L8:141:C:H2'	5:L8:142:U:C6	2.48	0.48
21:LQ:39:THR:HG23	21:LQ:132:LYS:HE2	1.94	0.48
25:LU:23:LEU:HD23	25:LU:110:TYR:HB2	1.94	0.48
26:LV:97:TYR:CE1	27:LW:19:ARG:HD3	2.48	0.48
52:SC:207:ALA:HB2	68:S2:4:C:H4'	1.95	0.48
54:SG:170:ARG:HH12	68:S2:67:C:H5	1.59	0.48
65:Sa:79:ILE:HD13	68:S2:1863:A:H1'	1.94	0.48
68:S2:102:A:H4'	68:S2:104:A:C8	2.48	0.48
68:S2:414:A:H2'	68:S2:415:A:C8	2.48	0.48
68:S2:924:G:H1	68:S2:1018:U:H3	1.59	0.48
68:S2:1447:G:H2'	68:S2:1448:A:C8	2.49	0.48
84:Et:52:G:H2'	84:Et:53:G:H8	1.78	0.48
85:CB:448:GLN:HB2	85:CB:473:VAL:HG23	1.95	0.48
3:L5:46:U:H5''	16:LL:16:LYS:HG3	1.94	0.48
3:L5:93:G:H2'	3:L5:94:A:C8	2.49	0.48
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.48	0.48
53:SE:11:ARG:HA	53:SE:28:ALA:HB2	1.95	0.48
59:SN:89:TYR:CE2	59:SN:93:LYS:HD2	2.48	0.48
64:SY:80:ASP:O	64:SY:84:LYS:HG2	2.12	0.48
68:S2:1805:G:H2'	68:S2:1806:A:C8	2.48	0.48
69:SR:97:GLU:HG2	69:SR:120:THR:HG21	1.94	0.48
77:ST:42:HIS:NE2	77:ST:43:LYS:HE3	2.28	0.48
83:Sg:153:CYS:HB3	83:Sg:168:CYS:H	1.77	0.48
85:CB:378:ASP:HA	85:CB:383:MET:HE2	1.94	0.48
3:L5:425:U:H4'	20:LP:6:LEU:HD21	1.95	0.48
3:L5:1217:G:H2'	3:L5:1218:G:H8	1.78	0.48
3:L5:2303:C:H5''	35:Le:104:SER:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LC:204:ARG:HG2	8:LC:205:ARG:H	1.77	0.48
29:LY:10:ASP:HB3	29:LY:13:LYS:HB2	1.95	0.48
48:Ls:39:GLN:HG3	48:Ls:40:MET:HE2	1.93	0.48
57:SJ:60:LEU:HD22	57:SJ:70:ARG:HA	1.96	0.48
63:SX:129:SER:HB2	68:S2:29:G:H4'	1.94	0.48
68:S2:116:OMU:HN3	68:S2:347:G:H1	1.60	0.48
3:L5:1593:A:H5''	3:L5:2839:PSU:H5'	1.95	0.48
3:L5:1645:C:H2'	3:L5:1646:A:C8	2.48	0.48
3:L5:1867:A:H2'	3:L5:1868:A:C8	2.49	0.48
22:LR:99:MET:HE1	22:LR:127:VAL:HG12	1.95	0.48
27:LW:90:ILE:HB	54:SG:145:PHE:HE1	1.78	0.48
56:SI:22:HIS:HB3	68:S2:433:A:H5''	1.95	0.48
56:SI:25:ARG:HA	68:S2:448:A:H5''	1.94	0.48
64:SY:6:THR:HG23	64:SY:28:LEU:HD13	1.96	0.48
64:SY:20:ARG:HB3	64:SY:76:TYR:CE2	2.48	0.48
68:S2:455:A:H2'	68:S2:456:C:C6	2.48	0.48
68:S2:543:C:H3'	68:S2:544:G:H8	1.79	0.48
82:Sf:103:LEU:HD12	82:Sf:105:TYR:CZ	2.48	0.48
85:CB:334:PRO:HA	85:CB:337:LYS:HD2	1.95	0.48
16:LL:80:GLU:HG3	16:LL:110:LEU:HD12	1.94	0.48
26:LV:111:GLU:HG3	26:LV:131:ARG:HD3	1.96	0.48
29:LY:72:GLN:HB3	29:LY:81:TYR:HB2	1.96	0.48
51:SB:144:LYS:HD3	51:SB:208:HIS:CG	2.49	0.48
68:S2:1213:C:H2'	68:S2:1214:A:C8	2.48	0.48
68:S2:1424:G:H2'	68:S2:1425:G:H8	1.77	0.48
68:S2:1856:C:H2'	68:S2:1857:G:C8	2.49	0.48
70:SD:99:ILE:HG23	70:SD:173:ARG:HH21	1.78	0.48
3:L5:1333:A:H2'	3:L5:1334:A:H8	1.76	0.48
3:L5:2554:U:C2	3:L5:2764:A:N7	2.82	0.48
3:L5:4530:UR3:H2'	3:L5:4531:U:H2'	1.95	0.48
26:LV:37:LEU:HD23	26:LV:65:VAL:HG12	1.95	0.48
35:Le:82:VAL:O	35:Le:86:GLU:HG2	2.14	0.48
40:Lj:28:HIS:CD2	40:Lj:31:LYS:HE2	2.49	0.48
54:SG:52:ILE:HA	54:SG:111:LEU:HD13	1.96	0.48
62:SW:23:ARG:HB2	66:Sb:4:ALA:HA	1.94	0.48
84:Et:28:C:H2'	84:Et:29:A:H8	1.77	0.48
3:L5:4688:C:H2'	3:L5:4689:PSU:C6	2.49	0.48
6:LA:206:PRO:HG3	6:LA:213:GLY:HA3	1.95	0.48
19:LO:168:TYR:CE2	19:LO:172:LYS:HD2	2.49	0.48
49:Lt:114:ARG:NE	49:Lt:133:LEU:HD12	2.28	0.48
60:SO:134:PRO:HB3	68:S2:944:A:H5''	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1733:U:H2'	68:S2:1734:G:O4'	2.14	0.48
76:SS:110:ASP:HA	76:SS:113:ARG:HG2	1.95	0.48
3:L5:1461:C:H2'	3:L5:1462:A:H8	1.79	0.48
3:L5:1468:C:H2'	3:L5:1469:C:C6	2.48	0.48
3:L5:4680:G:H2'	3:L5:4681:A:C8	2.48	0.48
22:LR:28:GLU:O	22:LR:32:ILE:HG12	2.14	0.48
28:LX:81:LEU:HG	28:LX:83:THR:HG23	1.95	0.48
68:S2:367:U:H4'	68:S2:371:A:C8	2.49	0.48
85:CB:207:PRO:HG2	85:CB:261:TRP:CE2	2.49	0.48
3:L5:2090:U:H4'	3:L5:2091:C:H3'	1.96	0.48
3:L5:2543:A:H2	3:L5:2773:G:H22	1.61	0.48
3:L5:2709:C:N4	86:CA:257:LEU:H	2.11	0.48
3:L5:3952:A:H2'	3:L5:3953:G:C4	2.48	0.48
20:LP:122:ALA:HB3	20:LP:143:PRO:HG2	1.94	0.48
25:LU:28:PRO:HB2	25:LU:34:MET:HB3	1.96	0.48
68:S2:508:A:H3'	68:S2:509:OMG:C8	2.46	0.48
68:S2:1101:U:H2'	68:S2:1102:G:C8	2.48	0.48
68:S2:1420:G:H21	68:S2:1421:A:H1'	1.78	0.48
79:SZ:99:LEU:HD21	79:SZ:102:LYS:HB2	1.94	0.48
3:L5:137:G:H2'	3:L5:138:G:C8	2.48	0.47
3:L5:300:A:H2'	3:L5:301:G:H8	1.79	0.47
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.49	0.47
66:Sb:34:ASP:O	66:Sb:79:PHE:HA	2.13	0.47
68:S2:375:U:H2'	68:S2:376:A:C8	2.49	0.47
68:S2:845:G:H2'	68:S2:846:G:C8	2.49	0.47
68:S2:1129:G:H3'	68:S2:1130:G:H21	1.79	0.47
68:S2:1201:U:H2'	68:S2:1202:U:C6	2.48	0.47
68:S2:1712:A:H2'	68:S2:1713:C:C6	2.49	0.47
1:CD:205:LYS:HG3	68:S2:1698:C:H5'	1.96	0.47
1:CD:283:LEU:HD12	72:SK:16:PHE:HD2	1.79	0.47
3:L5:1359:G:H4'	18:LN:203:TYR:HB2	1.95	0.47
3:L5:2521:G:H5'	3:L5:2640:G:H1'	1.96	0.47
5:L8:52:A:H4'	42:L1:19:GLN:HA	1.96	0.47
7:LB:117:ARG:HA	7:LB:177:LYS:HD2	1.96	0.47
10:LE:178:PRO:HD2	10:LE:181:LEU:HD12	1.96	0.47
12:LG:209:SER:HA	12:LG:212:LYS:HG3	1.95	0.47
19:LO:81:TRP:HB2	19:LO:104:VAL:HG21	1.96	0.47
29:LY:31:SER:HA	29:LY:48:PRO:HA	1.94	0.47
52:SC:256:TRP:CE2	62:SW:68:ARG:HD3	2.50	0.47
55:SH:37:LYS:HA	55:SH:40:LEU:HB3	1.97	0.47
55:SH:75:ILE:HG23	55:SH:79:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:840:C:H5'	68:S2:841:G:H5''	1.95	0.47
3:L5:260:C:H2'	3:L5:261:G:H8	1.79	0.47
3:L5:1340:OMC:HM23	3:L5:1340:OMC:H1'	1.72	0.47
3:L5:3612:C:H1'	3:L5:5016:A:C8	2.49	0.47
9:LD:64:ILE:HD13	9:LD:109:LEU:HD22	1.96	0.47
26:LV:99:GLU:HB3	27:LW:24:THR:HG23	1.95	0.47
55:SH:138:GLU:HG2	55:SH:159:ASP:OD1	2.13	0.47
68:S2:528:A:H2'	68:S2:529:A:C8	2.49	0.47
85:CB:256:MET:O	85:CB:260:LEU:HD23	2.14	0.47
86:CA:105:LEU:HB3	86:CA:126:VAL:HG22	1.96	0.47
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.96	0.47
3:L5:4238:G:H2'	3:L5:4239:A:C8	2.49	0.47
3:L5:4426:C:C2'	3:L5:4427:G:H5'	2.44	0.47
3:L5:4637:OMG:HM23	3:L5:4637:OMG:H1'	1.64	0.47
29:LY:33:PRO:HG2	29:LY:105:VAL:HG12	1.96	0.47
68:S2:1289:U:C5	82:Sf:97:LYS:HE2	2.49	0.47
83:Sg:42:MET:SD	83:Sg:56:GLN:HB3	2.53	0.47
3:L5:4457:PSU:H1'	7:LB:252:ALA:HB3	1.97	0.47
3:L5:4996:C:H4'	34:Ld:26:THR:HG23	1.96	0.47
5:L8:47:C:H1'	5:L8:61:A:H2'	1.97	0.47
22:LR:105:LEU:HD23	22:LR:138:LEU:HD23	1.95	0.47
58:SL:17:PHE:CG	68:S2:222:U:H5''	2.49	0.47
60:SO:43:HIS:CE1	60:SO:55:ARG:HE	2.33	0.47
68:S2:1129:G:H2'	68:S2:1130:G:N3	2.29	0.47
68:S2:1298:G:H4'	74:SP:78:THR:HA	1.97	0.47
86:CA:11:THR:HG23	86:CA:13:ALA:H	1.80	0.47
3:L5:99:A:H2'	3:L5:100:C:O2	2.15	0.47
3:L5:139:G:H2'	3:L5:140:G:H8	1.80	0.47
3:L5:965:G:N2	3:L5:2092:G:H1'	2.29	0.47
3:L5:1468:C:H2'	3:L5:1469:C:H6	1.79	0.47
3:L5:3746:A:H5''	6:LA:244:GLY:HA3	1.97	0.47
12:LG:105:GLU:HB2	12:LG:109:GLU:HG2	1.96	0.47
13:LH:77:VAL:HA	13:LH:80:MET:HE3	1.95	0.47
68:S2:649:PSU:H2'	68:S2:650:A:H8	1.80	0.47
83:Sg:68:ASP:HB3	83:Sg:111:VAL:HG22	1.95	0.47
3:L5:162:A:H2'	3:L5:163:A:H8	1.78	0.47
3:L5:223:G:H4'	3:L5:225:G:N7	2.30	0.47
3:L5:711:A:H2'	3:L5:712:C:C6	2.50	0.47
3:L5:1354:A:OP2	21:LQ:87:THR:HG23	2.15	0.47
3:L5:1538:U:H2'	3:L5:1539:G:H8	1.80	0.47
3:L5:2906:G:H1'	3:L5:2908:U:C2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SE:31:PRO:HG2	53:SE:38:LEU:HB2	1.96	0.47
53:SE:35:PRO:HD2	53:SE:83:PRO:HG2	1.96	0.47
56:SI:76:THR:HG22	56:SI:108:PRO:HG2	1.96	0.47
68:S2:67:C:N3	68:S2:69:C:H5''	2.30	0.47
68:S2:77:A:H2'	68:S2:78:C:C6	2.50	0.47
68:S2:432:G:H2'	68:S2:433:A:H8	1.80	0.47
68:S2:562:U:H2'	68:S2:563:G:C8	2.50	0.47
68:S2:1288:OMU:OP2	68:S2:1288:OMU:H6	2.15	0.47
68:S2:1628:C:H2'	68:S2:1629:C:C6	2.50	0.47
85:CB:260:LEU:HD12	85:CB:293:ILE:HD11	1.96	0.47
86:CA:107:LYS:HG2	86:CA:124:THR:HG23	1.96	0.47
3:L5:469:C:H2'	3:L5:470:A:H8	1.80	0.47
3:L5:1764:G:H4'	3:L5:1769:G:C6	2.50	0.47
3:L5:4125:C:H5'	12:LG:45:ILE:HD12	1.97	0.47
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.50	0.47
4:L7:110:G:H2'	4:L7:111:C:C6	2.50	0.47
45:Lo:6:LYS:HG3	45:Lo:94:GLY:HA3	1.96	0.47
68:S2:186:C:H2'	68:S2:187:G:H8	1.80	0.47
72:SK:31:LYS:HA	72:SK:41:PRO:HA	1.95	0.47
75:SQ:43:GLU:HB2	75:SQ:44:PRO:HD3	1.95	0.47
3:L5:184:U:H3'	3:L5:185:C:O4'	2.15	0.47
3:L5:260:C:H2'	3:L5:261:G:C8	2.49	0.47
3:L5:1500:A:H5''	3:L5:1501:C:H5''	1.95	0.47
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.15	0.47
5:L8:5:U:H2'	5:L8:6:C:H6	1.80	0.47
50:SA:32:PHE:CG	68:S2:1097:G:H4'	2.50	0.47
54:SG:189:ARG:HH22	68:S2:332:G:H8	1.62	0.47
64:SY:112:ASN:HA	64:SY:115:LYS:HE2	1.97	0.47
68:S2:1705:C:H2'	68:S2:1706:G:C8	2.50	0.47
81:Sd:15:GLY:C	81:Sd:19:ARG:HH21	2.22	0.47
3:L5:1199:G:H2'	3:L5:1200:G:C8	2.50	0.47
3:L5:5004:C:H2'	3:L5:5005:G:O4'	2.14	0.47
6:LA:48:ILE:HG22	46:Lp:54:ILE:HG12	1.97	0.47
7:LB:24:ARG:HH11	7:LB:276:HIS:CD2	2.33	0.47
9:LD:181:PRO:HD2	9:LD:195:HIS:CD2	2.50	0.47
35:Le:35:TRP:CZ2	35:Le:56:PRO:HD2	2.50	0.47
57:SJ:115:PHE:HZ	57:SJ:122:SER:C	2.22	0.47
68:S2:221:A:H2'	68:S2:222:U:C6	2.49	0.47
68:S2:1288:OMU:HM21	68:S2:1315:U:H1'	1.97	0.47
68:S2:1628:C:H2'	68:S2:1629:C:H6	1.78	0.47
86:CA:152:ALA:HA	86:CA:357:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:132:G:H2'	3:L5:133:C:H4'	1.96	0.46
3:L5:215:C:H5''	3:L5:216:C:H5''	1.97	0.46
3:L5:268:G:H2'	3:L5:269:G:C8	2.50	0.46
3:L5:2008:U:H1'	3:L5:2011:C:H5	1.80	0.46
3:L5:3911:C:H2'	3:L5:3912:U:C6	2.48	0.46
3:L5:4232:U:H5'	45:Lo:3:ASN:HB3	1.97	0.46
18:LN:140:LYS:HD3	18:LN:140:LYS:HA	1.63	0.46
25:LU:80:LYS:HZ1	25:LU:109:SER:H	1.62	0.46
48:Ls:28:PHE:HB3	48:Ls:189:ILE:HD12	1.96	0.46
67:Se:35:ARG:O	67:Se:39:ASN:HB2	2.16	0.46
68:S2:291:G:H2'	68:S2:292:A:C8	2.50	0.46
68:S2:344:U:H2'	68:S2:345:U:C6	2.50	0.46
82:Sf:141:CYS:HB2	82:Sf:145:CYS:HB2	1.45	0.46
85:CB:594:LYS:HE2	85:CB:598:LYS:HD2	1.96	0.46
86:CA:352:ALA:HA	86:CA:355:LYS:HD3	1.98	0.46
3:L5:1733:G:N3	3:L5:4214:A:H2'	2.29	0.46
47:Lr:82:ILE:HG22	47:Lr:84:LYS:HG2	1.97	0.46
68:S2:164:A:H3'	68:S2:165:G:N2	2.29	0.46
69:SR:35:CYS:HA	69:SR:38:ILE:HG12	1.96	0.46
70:SD:135:GLU:HB2	70:SD:153:VAL:HG23	1.97	0.46
71:SF:40:ALA:HB3	71:SF:67:PRO:HA	1.97	0.46
3:L5:269:G:H2'	3:L5:270:U:C6	2.51	0.46
3:L5:4524:G:C2	7:LB:252:ALA:HB1	2.50	0.46
4:L7:4:U:H2'	4:L7:5:A:C8	2.50	0.46
7:LB:14:LEU:HD22	7:LB:17:LEU:HD11	1.97	0.46
16:LL:48:PRO:HG3	38:Lh:118:LYS:HE2	1.97	0.46
34:Ld:64:ILE:HG23	34:Ld:68:LEU:HD23	1.97	0.46
50:SA:145:ILE:HG23	50:SA:159:ILE:HB	1.97	0.46
57:SJ:162:ARG:HH21	57:SJ:169:ARG:HG2	1.79	0.46
59:SN:16:LEU:HD22	68:S2:919:A:H5''	1.98	0.46
66:Sb:19:HIS:HB3	66:Sb:22:LYS:HG3	1.97	0.46
68:S2:27:A2M:HM'3	68:S2:27:A2M:H1'	1.60	0.46
68:S2:600:G:H2'	68:S2:601:OMG:H8	1.81	0.46
82:Sf:123:SER:HB3	82:Sf:126:CYS:HB2	1.97	0.46
3:L5:229:G:H5''	29:LY:11:ARG:HG3	1.96	0.46
3:L5:4239:A:H2'	3:L5:4240:G:C8	2.50	0.46
3:L5:5057:C:H2'	3:L5:5058:A:C8	2.50	0.46
54:SG:135:PRO:HB2	54:SG:141:ILE:HG22	1.97	0.46
68:S2:1314:U:H2'	72:SK:2:LEU:HD12	1.96	0.46
83:Sg:249:CYS:SG	83:Sg:258:ILE:HD13	2.55	0.46
83:Sg:292:SER:HB3	83:Sg:299:PHE:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:CA:105:LEU:HD23	86:CA:139:LYS:HD3	1.98	0.46
3:L5:1514:U:H2'	3:L5:1515:A:C8	2.50	0.46
3:L5:2448:G:H2'	3:L5:2449:A:C8	2.51	0.46
3:L5:4088:C:H2'	3:L5:4089:G:C8	2.51	0.46
11:LF:187:MET:HE3	11:LF:187:MET:HB2	1.86	0.46
51:SB:167:LYS:O	51:SB:171:ILE:HG12	2.15	0.46
83:Sg:227:LEU:HD23	83:Sg:228:TYR:HB2	1.97	0.46
86:CA:59:GLU:HA	86:CA:62:LYS:HE3	1.98	0.46
3:L5:3856:A:H5''	20:LP:83:TRP:O	2.16	0.46
3:L5:3944:G:H1	3:L5:4069:U:H3	1.63	0.46
3:L5:4063:U:H2'	3:L5:4064:C:C2	2.50	0.46
4:L7:27:G:H5''	9:LD:57:ASN:OD1	2.15	0.46
4:L7:57:C:H2'	4:L7:58:A:H8	1.81	0.46
13:LH:44:GLU:HB3	13:LH:58:ASP:HB2	1.97	0.46
13:LH:137:SER:HB3	13:LH:145:ILE:HD11	1.98	0.46
50:SA:52:LYS:HB2	69:SR:109:LEU:HD13	1.97	0.46
68:S2:900:C:H3'	68:S2:901:G:C8	2.50	0.46
68:S2:1648:G:H5''	75:SQ:125:ARG:HB2	1.97	0.46
68:S2:1709:G:H2'	68:S2:1710:C:H6	1.80	0.46
73:SM:35:ILE:HD11	73:SM:61:TYR:CE1	2.51	0.46
86:CA:29:ASN:HD21	86:CA:334:THR:HA	1.81	0.46
3:L5:153:G:H2'	3:L5:154:G:H8	1.81	0.46
3:L5:3770:U:H2'	3:L5:3771:C:C6	2.51	0.46
3:L5:4618:OMG:H5'	26:LV:15:ARG:HB2	1.97	0.46
15:LJ:52:LYS:HB3	15:LJ:65:ASN:HA	1.96	0.46
37:Lg:5:LEU:HD11	37:Lg:30:ILE:HG22	1.98	0.46
57:SJ:63:LEU:HD23	57:SJ:70:ARG:HB2	1.97	0.46
68:S2:527:C:H2'	68:S2:528:A:C8	2.50	0.46
68:S2:1713:C:H2'	68:S2:1714:U:C6	2.50	0.46
78:SU:23:THR:HB	78:SU:113:GLU:HG2	1.96	0.46
84:Et:44:G:H2'	84:Et:45:G:C8	2.50	0.46
85:CB:223:PHE:HB3	85:CB:344:LEU:HD13	1.98	0.46
3:L5:683:C:H2'	3:L5:684:G:O4'	2.16	0.46
3:L5:1278:C:H2'	3:L5:1279:A:O4'	2.15	0.46
3:L5:1415:G:H2'	3:L5:1416:G:C8	2.51	0.46
3:L5:1683:PSU:H2'	3:L5:1684:A:C8	2.51	0.46
3:L5:1980:U:O2'	3:L5:1981:G:H5''	2.16	0.46
3:L5:2676:A:OP2	3:L5:2676:A:H8	1.98	0.46
3:L5:4872:G:C2	19:LO:203:VAL:HG23	2.51	0.46
7:LB:195:ASP:O	7:LB:199:GLU:HG2	2.15	0.46
8:LC:163:LYS:HB2	8:LC:166:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SE:149:TYR:HD2	54:SG:205:GLU:HG3	1.80	0.46
55:SH:97:GLN:C	55:SH:98:ARG:HD2	2.41	0.46
62:SW:3:ARG:HH12	62:SW:28:ARG:HH21	1.64	0.46
65:Sa:51:ARG:HG3	80:Sc:63:ARG:HH22	1.80	0.46
68:S2:1568:C:H2'	68:S2:1569:A:C8	2.50	0.46
74:SP:18:ARG:HE	76:SS:88:LYS:HZ2	1.64	0.46
76:SS:40:TYR:HA	76:SS:83:PHE:HE2	1.81	0.46
84:Et:66:U:H2'	84:Et:67:U:C6	2.51	0.46
85:CB:27:HIS:ND1	85:CB:138:GLN:HB2	2.31	0.46
3:L5:1508:A:H5''	8:LC:113:ARG:HD2	1.97	0.46
3:L5:2400:G:H21	37:Lg:6:THR:HG22	1.81	0.46
3:L5:3954:A:H1'	3:L5:4058:U:H5'	1.96	0.46
8:LC:298:ILE:HD13	21:LQ:131:PRO:HB3	1.96	0.46
10:LE:222:LEU:H	10:LE:237:LYS:NZ	2.14	0.46
23:LS:96:GLU:HG3	23:LS:139:ARG:HG2	1.98	0.46
30:LZ:92:ASP:HB3	30:LZ:95:VAL:HG12	1.98	0.46
35:Le:126:ASN:HA	35:Le:129:LEU:HD21	1.98	0.46
45:Lo:33:LEU:HA	45:Lo:38:LYS:HG2	1.97	0.46
48:Ls:24:TYR:CG	48:Ls:90:PHE:HB3	2.51	0.46
52:SC:187:ARG:HE	52:SC:192:LEU:HD12	1.80	0.46
53:SE:11:ARG:HH12	53:SE:24:THR:HG22	1.81	0.46
53:SE:149:TYR:CD2	54:SG:205:GLU:HG3	2.51	0.46
60:SO:96:LYS:HE3	60:SO:132:VAL:HG11	1.98	0.46
68:S2:166:A2M:HM'3	68:S2:166:A2M:H1'	1.64	0.46
68:S2:917:U:H2'	68:S2:918:U:C6	2.51	0.46
76:SS:138:THR:HA	76:SS:141:ARG:HH21	1.81	0.46
82:Sf:102:VAL:HG12	82:Sf:103:LEU:HD23	1.98	0.46
3:L5:518:G:H1	3:L5:643:C:H2'	1.81	0.46
3:L5:2521:G:H4'	37:Lg:26:PRO:HD2	1.97	0.46
3:L5:4238:G:H2'	3:L5:4239:A:H8	1.81	0.46
54:SG:174:PRO:HB3	68:S2:65:C:C6	2.51	0.46
62:SW:105:THR:HB	62:SW:126:LEU:HD11	1.97	0.46
68:S2:62:G:H1'	68:S2:172:OMU:HM23	1.98	0.46
68:S2:587:A:H5'	68:S2:592:C:H41	1.81	0.46
68:S2:945:U:H2'	68:S2:946:U:C6	2.51	0.46
73:SM:128:PHE:HA	73:SM:131:LYS:HG2	1.98	0.46
85:CB:163:ALA:HB1	85:CB:169:LEU:HD12	1.98	0.46
3:L5:710:G:H2'	3:L5:711:A:H8	1.81	0.45
3:L5:1743:A:O4'	9:LD:15:ARG:HD2	2.15	0.45
3:L5:1846:G:H2'	3:L5:1847:C:H6	1.80	0.45
16:LL:18:TRP:CD1	16:LL:18:TRP:H	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LV:72:LEU:HD21	26:LV:113:LYS:HE2	1.98	0.45
33:Lc:38:ILE:HD11	33:Lc:46:VAL:HG21	1.96	0.45
58:SL:17:PHE:CD2	68:S2:222:U:H5''	2.51	0.45
60:SO:136:PRO:HB3	68:S2:944:A:H1'	1.97	0.45
66:Sb:12:PRO:HA	66:Sb:15:GLU:HB2	1.98	0.45
68:S2:1298:G:H1'	74:SP:79:HIS:HB2	1.98	0.45
68:S2:1714:U:H2'	68:S2:1715:A:C8	2.52	0.45
83:Sg:206:LEU:HD21	83:Sg:218:LEU:HD22	1.98	0.45
85:CB:147:ILE:HD11	85:CB:192:TYR:HB2	1.98	0.45
85:CB:649:ILE:HD13	85:CB:663:THR:HB	1.98	0.45
86:CA:85:CYS:HB2	86:CA:309:TYR:HE1	1.80	0.45
3:L5:1961:G:H4'	3:L5:1962:A:H5''	1.97	0.45
3:L5:3932:U:H2'	3:L5:3933:G:H8	1.80	0.45
3:L5:4775:C:H41	3:L5:4859:C:N4	2.07	0.45
68:S2:5:U:H2'	68:S2:6:G:C8	2.51	0.45
68:S2:140:C:H42	68:S2:313:A:H61	1.64	0.45
68:S2:388:U:H2'	68:S2:389:A:H8	1.81	0.45
68:S2:1320:G:H2'	68:S2:1321:G:O4'	2.17	0.45
68:S2:1775:U:H2'	68:S2:1776:G:C8	2.51	0.45
78:SU:23:THR:HG23	78:SU:88:LEU:HD22	1.98	0.45
85:CB:690:GLY:HA2	85:CB:697:MET:HE3	1.98	0.45
3:L5:261:G:H2'	3:L5:262:G:C8	2.51	0.45
3:L5:677:G:H2'	3:L5:678:C:C6	2.52	0.45
3:L5:1788:A:H2'	14:LI:22:PHE:CZ	2.50	0.45
3:L5:2520:C:H2'	3:L5:2521:G:H8	1.82	0.45
3:L5:3861:A:H2'	3:L5:3862:A:C8	2.51	0.45
3:L5:4591:U:H2'	3:L5:4592:C:C6	2.51	0.45
3:L5:4743:G:H2'	3:L5:4744:A:C8	2.51	0.45
6:LA:107:MET:HE1	6:LA:113:VAL:HG11	1.98	0.45
34:Ld:70:LYS:HE2	34:Ld:70:LYS:HB3	1.78	0.45
39:Li:33:LEU:HD21	39:Li:38:LYS:HB2	1.99	0.45
68:S2:126:G:N3	68:S2:181:A:H1'	2.32	0.45
68:S2:601:OMG:HM23	68:S2:601:OMG:H1'	1.67	0.45
68:S2:1797:U:H2'	68:S2:1798:C:C6	2.51	0.45
68:S2:1804:U:H2'	68:S2:1805:G:C8	2.51	0.45
86:CA:59:GLU:HG2	86:CA:62:LYS:HE3	1.97	0.45
3:L5:173:C:H5''	16:LL:129:ARG:NH1	2.32	0.45
3:L5:325:U:H2'	3:L5:326:C:C6	2.51	0.45
3:L5:1095:A:H2	3:L5:1200:G:H22	1.65	0.45
3:L5:1186:U:H2'	3:L5:1187:G:N3	2.31	0.45
3:L5:1725:U:H2'	3:L5:1726:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3841:OMC:HM23	3:L5:3841:OMC:H1'	1.76	0.45
3:L5:4088:C:H2'	3:L5:4089:G:H8	1.82	0.45
3:L5:4913:G:H4'	3:L5:4914:C:O5'	2.16	0.45
19:LO:126:VAL:HG13	19:LO:127:VAL:HG13	1.98	0.45
50:SA:50:ASN:HD22	50:SA:53:ARG:HH11	1.63	0.45
55:SH:142:LYS:HB3	62:SW:54:ASP:HB3	1.97	0.45
59:SN:49:GLN:HA	59:SN:52:VAL:HG22	1.97	0.45
68:S2:496:C:H2'	68:S2:497:C:C6	2.51	0.45
68:S2:1010:G:H2'	68:S2:1011:A:C8	2.50	0.45
68:S2:1382:A:H2'	68:S2:1383:A2M:H8	1.98	0.45
84:Et:5:G:H2'	84:Et:6:G:H8	1.81	0.45
85:CB:155:LEU:HB3	85:CB:212:VAL:HG23	1.98	0.45
85:CB:731:ALA:HB1	85:CB:855:LEU:HD13	1.99	0.45
3:L5:4196:OMG:HM23	3:L5:4196:OMG:H1'	1.66	0.45
52:SC:256:TRP:CD2	62:SW:68:ARG:HD3	2.51	0.45
60:SO:43:HIS:HD2	60:SO:45:THR:HG23	1.82	0.45
68:S2:1337:4AC:H2'	68:S2:1338:G:C8	2.49	0.45
68:S2:1501:C:H2'	68:S2:1502:C:H6	1.82	0.45
68:S2:1775:U:H2'	68:S2:1776:G:H8	1.81	0.45
80:Sc:10:LYS:HE3	80:Sc:61:SER:HB2	1.98	0.45
85:CB:86:LEU:HD12	85:CB:89:ILE:HD12	1.99	0.45
3:L5:1751:A:H2'	3:L5:1752:G:C8	2.52	0.45
3:L5:2095:A:H1'	3:L5:2096:G:N2	2.31	0.45
3:L5:3619:G:H4'	22:LR:79:GLY:O	2.16	0.45
3:L5:4966:A:H5'	7:LB:128:LYS:HG3	1.98	0.45
14:LI:51:HIS:CD2	14:LI:168:SER:HB3	2.51	0.45
49:Lt:22:VAL:HA	49:Lt:48:LYS:HG2	1.99	0.45
49:Lt:147:HIS:ND1	49:Lt:149:HIS:HB3	2.31	0.45
50:SA:80:ARG:HH21	50:SA:126:ASP:HB2	1.82	0.45
3:L5:106:A:H2'	3:L5:107:G:O4'	2.16	0.45
3:L5:180:C:H2'	3:L5:181:C:O4'	2.17	0.45
3:L5:2544:G:H22	5:L8:124:U:H5'	1.82	0.45
3:L5:2823:G:N7	22:LR:20:LYS:HD3	2.31	0.45
3:L5:4498:OMU:HM22	3:L5:4499:OMG:C8	2.52	0.45
3:L5:4507:A:H2'	3:L5:4508:C:C6	2.52	0.45
9:LD:55:VAL:HG11	9:LD:158:LYS:HE3	1.99	0.45
13:LH:40:HIS:CD2	13:LH:40:HIS:H	2.34	0.45
27:LW:93:LYS:HZ1	54:SG:156:TYR:HB3	1.81	0.45
48:Ls:155:LEU:HD23	48:Ls:155:LEU:HA	1.82	0.45
60:SO:15:ILE:HG12	60:SO:16:SER:H	1.81	0.45
68:S2:152:U:H2'	68:S2:153:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1365:G:H2'	68:S2:1366:G:H8	1.82	0.45
85:CB:451:ILE:HD11	85:CB:458:VAL:HB	1.99	0.45
3:L5:701:G:H2'	3:L5:702:U:H6	1.82	0.45
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.51	0.45
3:L5:2570:U:H2'	3:L5:2571:C:C6	2.52	0.45
3:L5:5002:U:H2'	3:L5:5003:U:C6	2.51	0.45
6:LA:180:LEU:HD22	46:Lp:18:TYR:HB3	1.99	0.45
7:LB:220:ILE:HG12	7:LB:278:THR:HG23	1.99	0.45
7:LB:238:LYS:HE2	7:LB:238:LYS:HB2	1.74	0.45
40:Lj:27:TYR:HA	40:Lj:34:CYS:HA	1.99	0.45
51:SB:24:PRO:O	51:SB:28:LYS:HG2	2.17	0.45
51:SB:85:LYS:HB2	51:SB:101:HIS:HB3	1.99	0.45
52:SC:81:ILE:HG21	52:SC:88:ILE:HD11	1.99	0.45
68:S2:99:A2M:HM'3	68:S2:99:A2M:H1'	1.71	0.45
68:S2:1067:C:H2'	68:S2:1068:G:O4'	2.17	0.45
70:SD:32:ASP:HA	70:SD:54:ARG:HD2	1.98	0.45
85:CB:740:LEU:HD11	85:CB:835:VAL:HG23	1.99	0.45
6:LA:180:LEU:HD21	46:Lp:22:LEU:HB3	1.98	0.45
7:LB:45:ALA:HB3	7:LB:183:ILE:HG23	1.99	0.45
19:LO:108:ILE:HD12	19:LO:160:ARG:CZ	2.47	0.45
46:Lp:51:ALA:HB3	46:Lp:54:ILE:HD12	1.98	0.45
49:Lt:104:ILE:HG13	49:Lt:106:PHE:CD2	2.52	0.45
55:SH:154:ILE:HB	55:SH:185:VAL:HG23	1.98	0.45
63:SX:107:ARG:HG2	63:SX:112:VAL:HG22	1.98	0.45
68:S2:106:C:H5''	68:S2:431:G:O2'	2.17	0.45
68:S2:848:U:H2'	68:S2:849:A:H8	1.82	0.45
68:S2:1030:A:H2'	68:S2:1031:A2M:C8	2.46	0.45
68:S2:1383:A2M:HM'3	68:S2:1383:A2M:H1'	1.60	0.45
68:S2:1387:G:H2'	68:S2:1388:A:O4'	2.17	0.45
68:S2:1643:U:H1'	75:SQ:142:GLN:HE22	1.82	0.45
76:SS:98:VAL:HG11	76:SS:106:LYS:HG3	1.98	0.45
84:Et:10:G:C2	84:Et:26:A:H1'	2.52	0.45
84:Et:52:G:H2'	84:Et:53:G:C8	2.52	0.45
86:CA:19:THR:HA	86:CA:22:LYS:HE3	1.99	0.45
3:L5:462:G:H2'	3:L5:463:A:C8	2.52	0.45
3:L5:1761:G:H1'	3:L5:1764:G:H1	1.82	0.45
3:L5:2763:U:O2'	3:L5:2764:A:H4'	2.18	0.45
3:L5:4067:U:H2'	3:L5:4068:U:C6	2.52	0.45
3:L5:4678:G:N2	3:L5:4713:G:H1'	2.32	0.45
13:LH:59:LYS:HE2	13:LH:66:GLU:HG3	1.99	0.45
30:LZ:25:ILE:HD13	30:LZ:43:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Li:76:ARG:HD3	39:Li:76:ARG:HA	1.65	0.45
57:SJ:30:LYS:HD3	67:Se:42:PHE:CD1	2.52	0.45
68:S2:543:C:H3'	68:S2:544:G:C8	2.52	0.45
68:S2:1208:A:H2'	68:S2:1209:A:H8	1.82	0.45
68:S2:1486:A:H2'	68:S2:1487:A:C8	2.52	0.45
68:S2:1558:C:H2'	68:S2:1559:C:C6	2.52	0.45
68:S2:1736:G:H2'	68:S2:1737:G:C8	2.52	0.45
68:S2:1777:G:H2'	68:S2:1778:C:C6	2.52	0.45
71:SF:49:LEU:HD11	75:SQ:49:TYR:HB2	1.98	0.45
85:CB:86:LEU:HG	85:CB:93:LYS:HD2	1.99	0.45
3:L5:978:G:H2'	3:L5:979:C:C6	2.51	0.44
3:L5:1625:OMG:HM23	18:LN:81:TYR:HE2	1.81	0.44
9:LD:51:MET:HE3	9:LD:105:LEU:HD23	1.99	0.44
17:LM:36:ALA:HB3	17:LM:55:MET:HE1	1.99	0.44
34:Ld:33:ILE:HD11	34:Ld:45:ALA:HA	1.98	0.44
50:SA:177:MET:HE2	50:SA:177:MET:HB2	1.71	0.44
53:SE:118:GLU:HG2	53:SE:121:TYR:CE2	2.52	0.44
60:SO:57:THR:O	60:SO:60:MET:HG3	2.18	0.44
65:Sa:40:VAL:HG22	65:Sa:42:ARG:HG2	1.99	0.44
66:Sb:54:VAL:HG23	66:Sb:63:LEU:HB2	1.98	0.44
68:S2:293:C:O2'	68:S2:294:U:H3'	2.17	0.44
68:S2:795:A:H2'	68:S2:796:G:C8	2.51	0.44
68:S2:974:C:H2'	68:S2:975:G:H8	1.82	0.44
75:SQ:110:ASP:OD1	75:SQ:111:ILE:HD12	2.17	0.44
77:ST:96:SER:HB2	77:ST:99:VAL:HG12	1.99	0.44
2:CI:58:LEU:HD11	25:LU:115:PHE:HB2	1.99	0.44
3:L5:2824:OMC:HM23	3:L5:2824:OMC:H1'	1.64	0.44
11:LF:226:HIS:HB3	11:LF:229:GLU:HG2	1.98	0.44
45:Lo:4:VAL:HG23	45:Lo:93:LEU:HD12	1.99	0.44
50:SA:173:LEU:HD23	50:SA:177:MET:HE1	1.99	0.44
53:SE:45:ILE:HG13	53:SE:61:VAL:HG11	1.98	0.44
55:SH:133:LEU:HD11	55:SH:176:VAL:HG21	1.99	0.44
68:S2:307:G:P	68:S2:307:G:H8	2.40	0.44
68:S2:375:U:H2'	68:S2:376:A:H8	1.82	0.44
68:S2:564:A:H2'	68:S2:565:G:O4'	2.17	0.44
74:SP:18:ARG:HE	76:SS:88:LYS:NZ	2.16	0.44
86:CA:159:PRO:HD3	86:CA:325:LEU:HD22	1.99	0.44
3:L5:710:G:H2'	3:L5:711:A:C8	2.53	0.44
3:L5:724:C:OP1	8:LC:350:ARG:HD2	2.17	0.44
3:L5:1741:G:N3	3:L5:1781:PSU:H5''	2.33	0.44
3:L5:3920:PSU:H2'	3:L5:3921:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4251:A:H5''	15:LJ:108:GLY:HA3	1.99	0.44
31:La:36:GLY:HA3	31:La:40:HIS:CE1	2.53	0.44
53:SE:246:LEU:HD22	53:SE:250:GLU:HG3	1.99	0.44
53:SE:252:ARG:HH12	57:SJ:75:ASN:HB3	1.81	0.44
67:Se:39:ASN:HD21	68:S2:551:U:H5'	1.82	0.44
68:S2:588:G:H4'	68:S2:589:G:H5'	2.00	0.44
68:S2:1405:A:H2'	68:S2:1406:G:O4'	2.17	0.44
70:SD:175:VAL:HB	70:SD:182:LEU:HB3	1.99	0.44
77:ST:57:ALA:HB1	77:ST:107:LEU:HD21	1.99	0.44
83:Sg:101:PHE:CE2	83:Sg:136:GLY:HA2	2.52	0.44
85:CB:190:SER:HB2	85:CB:204:MET:HE2	1.98	0.44
85:CB:851:LEU:HD21	85:CB:855:LEU:HD23	1.99	0.44
3:L5:907:C:H2'	3:L5:908:G:H8	1.83	0.44
3:L5:2250:C:H2'	3:L5:2251:G:C8	2.52	0.44
3:L5:3714:G:H4'	84:Et:4:C:O2'	2.17	0.44
3:L5:3867:A2M:H2'	3:L5:3868:G:O4'	2.17	0.44
11:LF:104:LYS:HB2	11:LF:104:LYS:HE2	1.84	0.44
12:LG:63:LEU:HD11	18:LN:29:GLN:HG3	1.98	0.44
12:LG:159:HIS:ND1	12:LG:185:LYS:HA	2.32	0.44
18:LN:200:LEU:HB3	18:LN:204:ARG:NH1	2.32	0.44
52:SC:183:LYS:HA	52:SC:195:LEU:O	2.17	0.44
53:SE:198:ARG:NH2	53:SE:200:ARG:HH21	2.16	0.44
60:SO:50:LYS:NZ	68:S2:951:C:H1'	2.32	0.44
64:SY:9:THR:HG22	64:SY:25:ILE:HG22	1.99	0.44
68:S2:1545:A:H2'	68:S2:1546:G:C8	2.52	0.44
70:SD:29:LEU:HD13	70:SD:58:VAL:HG22	1.99	0.44
3:L5:190:G:H2'	3:L5:191:G:H8	1.82	0.44
3:L5:254:G:H8	3:L5:254:G:O5'	2.00	0.44
3:L5:1701:A:C8	3:L5:2096:G:C6	3.06	0.44
3:L5:2638:G:N1	3:L5:2718:U:H2'	2.32	0.44
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.52	0.44
3:L5:4139:G:H21	3:L5:4140:C:N4	2.15	0.44
3:L5:4524:G:N3	7:LB:252:ALA:HB1	2.33	0.44
9:LD:208:MET:HB2	9:LD:233:PRO:HG3	2.00	0.44
12:LG:107:LYS:O	12:LG:111:LYS:HG2	2.18	0.44
23:LS:76:LYS:HB2	23:LS:131:GLU:OE1	2.17	0.44
38:Lh:95:LEU:HB3	38:Lh:99:GLU:HG3	2.00	0.44
53:SE:36:HIS:CD2	53:SE:85:GLY:HA3	2.53	0.44
53:SE:104:ASP:HB3	53:SE:110:ALA:HB2	1.99	0.44
54:SG:7:PHE:CD1	54:SG:113:ILE:HB	2.53	0.44
62:SW:28:ARG:HB3	62:SW:29:PRO:HD3	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SD:161:GLY:O	70:SD:164:VAL:HG12	2.17	0.44
72:SK:3:MET:HE2	72:SK:8:ARG:HH11	1.82	0.44
73:SM:53:ALA:HB3	73:SM:107:SER:HB2	1.99	0.44
85:CB:685:TRP:CD2	85:CB:726:ARG:HD2	2.53	0.44
3:L5:318:A:H2'	3:L5:319:A:C8	2.53	0.44
3:L5:2554:U:N3	3:L5:2764:A:C8	2.81	0.44
3:L5:4174:U:H2'	3:L5:4175:G:H8	1.82	0.44
5:L8:70:G:H5''	29:LY:27:ARG:CZ	2.47	0.44
8:LC:209:ILE:HB	8:LC:229:LEU:HD23	1.98	0.44
14:LI:152:LEU:HB3	14:LI:165:ILE:HD12	1.99	0.44
27:LW:78:PHE:CD2	54:SG:9:ALA:HB2	2.52	0.44
50:SA:183:LEU:HD22	50:SA:188:THR:HG21	2.00	0.44
50:SA:184:ARG:NE	50:SA:191:ARG:HD3	2.29	0.44
68:S2:441:C:H2'	68:S2:442:C:C6	2.53	0.44
68:S2:609:U:H2'	68:S2:610:G:H8	1.82	0.44
68:S2:1616:U:H2'	68:S2:1617:G:C8	2.53	0.44
76:SS:40:TYR:CZ	76:SS:97:GLN:HG2	2.52	0.44
85:CB:855:LEU:HD12	85:CB:855:LEU:HA	1.85	0.44
86:CA:123:HIS:CD2	86:CA:125:PHE:HB3	2.53	0.44
3:L5:679:C:H2'	3:L5:680:G:H8	1.82	0.44
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.52	0.44
6:LA:28:ARG:HD3	6:LA:123:ARG:HH11	1.83	0.44
6:LA:247:ARG:HD3	6:LA:247:ARG:HA	1.76	0.44
21:LQ:43:PHE:CD2	21:LQ:133:GLY:HA3	2.53	0.44
22:LR:169:ALA:HA	22:LR:172:ARG:NE	2.31	0.44
53:SE:201:HIS:HB3	53:SE:204:SER:HB3	1.99	0.44
55:SH:111:LYS:HB3	68:S2:798:G:C8	2.52	0.44
56:SI:190:LEU:HD21	56:SI:198:TYR:HD2	1.82	0.44
59:SN:63:VAL:HG21	59:SN:71:ILE:HG12	2.00	0.44
66:Sb:35:VAL:HG13	66:Sb:77:CYS:HB3	1.99	0.44
68:S2:1711:U:H2'	68:S2:1712:A:H8	1.82	0.44
70:SD:140:GLY:HA3	70:SD:182:LEU:HD12	1.99	0.44
82:Sf:103:LEU:HG	82:Sf:104:LYS:H	1.83	0.44
84:Et:26:A:H4'	84:Et:26:A:OP1	2.17	0.44
85:CB:251:LYS:HE3	85:CB:255:ASP:HB3	1.99	0.44
3:L5:459:C:H5'	10:LE:110:ARG:HA	2.00	0.44
3:L5:3643:A:OP1	89:L5:5282:SPD:H32	2.17	0.44
3:L5:3690:U:H2'	3:L5:3691:G:O4'	2.17	0.44
3:L5:4227:OMU:H1'	3:L5:4227:OMU:HM23	1.78	0.44
5:L8:82:A:N7	5:L8:84:A:H3'	2.33	0.44
23:LS:30:MET:HE2	23:LS:30:MET:HB3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Sb:37:CYS:HB3	66:Sb:59:CYS:HB3	1.60	0.44
68:S2:656:G:N2	68:S2:663:C:H5''	2.33	0.44
76:SS:87:GLN:HB3	76:SS:95:TYR:HD2	1.82	0.44
86:CA:310:GLU:HG3	86:CA:314:GLU:HB2	1.99	0.44
3:L5:4508:C:H5''	26:LV:43:LYS:HD3	2.00	0.44
5:L8:141:C:H2'	5:L8:142:U:H6	1.83	0.44
8:LC:204:ARG:HG2	8:LC:205:ARG:N	2.33	0.44
23:LS:82:LEU:HD12	23:LS:124:ILE:HG23	1.99	0.44
51:SB:80:ALA:HB1	60:SO:128:ARG:NH2	2.32	0.44
53:SE:11:ARG:NE	53:SE:20:LEU:HD23	2.33	0.44
68:S2:210:U:H2'	68:S2:211:G:H8	1.83	0.44
68:S2:212:C:H2'	68:S2:213:G:C8	2.53	0.44
68:S2:800:U:H2'	68:S2:801:PSU:O4'	2.18	0.44
68:S2:1703:OMC:H2'	68:S2:1704:C:O4'	2.18	0.44
77:ST:127:GLY:O	77:ST:131:LEU:HD23	2.17	0.44
81:Sd:23:VAL:HG21	81:Sd:38:MET:HE3	2.00	0.44
86:CA:36:VAL:HG12	86:CA:125:PHE:CE1	2.52	0.44
3:L5:677:G:H2'	3:L5:678:C:H6	1.83	0.43
3:L5:1238:A:H5''	10:LE:60:SER:HB3	2.00	0.43
3:L5:1669:A:H4'	3:L5:1685:G:N2	2.32	0.43
3:L5:2481:G:H2'	3:L5:2482:C:C6	2.53	0.43
3:L5:2861:OMC:HM23	3:L5:2861:OMC:HI'	1.68	0.43
6:LA:114:CYS:SG	6:LA:169:VAL:HG22	2.57	0.43
12:LG:218:LEU:O	12:LG:222:ILE:HG12	2.17	0.43
30:LZ:135:ARG:HD2	30:LZ:135:ARG:HA	1.80	0.43
49:Lt:11:LYS:HA	49:Lt:11:LYS:HD2	1.73	0.43
50:SA:85:ARG:HH22	69:SR:83:ASN:HA	1.82	0.43
51:SB:52:THR:HG23	51:SB:57:ILE:HA	2.00	0.43
56:SI:57:ALA:HB2	56:SI:183:GLY:HA2	2.00	0.43
57:SJ:60:LEU:HD23	57:SJ:60:LEU:HA	1.82	0.43
60:SO:129:ILE:HG21	65:Sa:44:ILE:HG21	2.00	0.43
61:SV:55:ILE:HG23	61:SV:59:ILE:HD11	1.99	0.43
61:SV:60:ARG:HA	61:SV:65:SER:HB3	2.00	0.43
68:S2:93:PSU:H2'	68:S2:94:G:O4'	2.18	0.43
68:S2:115:U:H2'	68:S2:116:OMU:C6	2.47	0.43
83:Sg:153:CYS:SG	83:Sg:198:VAL:HG12	2.58	0.43
3:L5:1081:C:C2'	3:L5:1082:C:H5'	2.48	0.43
3:L5:2709:C:H5'	22:LR:43:LYS:HD3	1.99	0.43
22:LR:158:GLN:HB3	22:LR:162:ARG:HH12	1.82	0.43
27:LW:82:ILE:HG21	54:SG:158:VAL:HG21	2.01	0.43
36:Lf:71:TRP:HB2	36:Lf:89:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Li:73:ILE:O	39:Li:77:VAL:HG22	2.18	0.43
50:SA:120:ARG:HD2	52:SC:266:TYR:HB3	2.00	0.43
52:SC:74:LYS:HA	52:SC:74:LYS:HD2	1.80	0.43
54:SG:228:ILE:HG22	54:SG:231:ARG:HH21	1.83	0.43
59:SN:46:THR:O	59:SN:50:ILE:HG12	2.18	0.43
68:S2:1208:A:H2'	68:S2:1209:A:C8	2.53	0.43
68:S2:1438:A:H2'	68:S2:1439:A:H8	1.81	0.43
68:S2:1711:U:H2'	68:S2:1712:A:C8	2.53	0.43
71:SF:108:PRO:HA	71:SF:111:VAL:HG12	2.00	0.43
72:SK:14:LEU:HD22	72:SK:35:LEU:HD23	2.00	0.43
85:CB:132:VAL:HG13	85:CB:167:LEU:HD11	2.00	0.43
85:CB:616:ASP:HA	85:CB:619:LYS:HG2	1.99	0.43
3:L5:276:C:OP1	39:Li:36:HIS:HB3	2.18	0.43
3:L5:700:G:C6	3:L5:701:G:O6	2.71	0.43
3:L5:1811:G:H2'	3:L5:1812:C:C6	2.53	0.43
3:L5:1972:G:H21	49:Lt:121:LEU:HD11	1.83	0.43
3:L5:2568:C:H2'	3:L5:2569:G:C8	2.53	0.43
3:L5:2693:G:OP1	41:Lk:35:LYS:HD3	2.18	0.43
3:L5:3606:U:H2'	3:L5:3607:U:C6	2.54	0.43
3:L5:4103:C:H4'	3:L5:4104:G:N7	2.33	0.43
3:L5:4965:U:H4'	3:L5:4966:A:H5'	2.01	0.43
7:LB:297:LYS:HG3	7:LB:299:ILE:HG23	2.01	0.43
12:LG:51:LEU:O	12:LG:55:VAL:HG23	2.18	0.43
14:LI:43:VAL:HG21	14:LI:197:VAL:HG13	2.01	0.43
14:LI:54:SER:HB3	14:LI:135:ILE:HD11	2.00	0.43
16:LL:48:PRO:HB2	38:Lh:120:ALA:HB2	2.00	0.43
56:SI:39:GLY:HA3	56:SI:59:ARG:HE	1.84	0.43
68:S2:900:C:H3'	68:S2:901:G:H8	1.82	0.43
68:S2:919:A:H8	68:S2:919:A:OP2	2.00	0.43
68:S2:1778:C:H3'	68:S2:1779:G:H8	1.82	0.43
3:L5:37:U:H2'	3:L5:38:A:O4'	2.18	0.43
3:L5:4070:U:H2'	3:L5:4071:U:C6	2.54	0.43
3:L5:4389:C:H2'	3:L5:4390:A:C8	2.53	0.43
3:L5:4393:G:O4'	3:L5:4447:5MC:HM52	2.18	0.43
3:L5:4611:A:H2'	3:L5:4612:C:H6	1.82	0.43
5:L8:52:A:H5'	42:Ll:21:ARG:HD3	1.99	0.43
48:Ls:178:LEU:HD23	48:Ls:178:LEU:HA	1.84	0.43
51:SB:193:ILE:O	51:SB:197:ILE:HG12	2.18	0.43
55:SH:170:VAL:HG13	55:SH:187:PHE:HB2	2.00	0.43
61:SV:32:ILE:HD12	61:SV:34:MET:HB3	2.01	0.43
64:SY:27:VAL:HG21	64:SY:35:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1031:A2M:HM'3	68:S2:1031:A2M:H1'	1.57	0.43
68:S2:1839:U:H2'	68:S2:1840:U:C6	2.53	0.43
73:SM:17:ALA:HB2	73:SM:122:ASP:HB3	2.00	0.43
86:CA:272:ARG:NH2	86:CA:282:ALA:HB1	2.33	0.43
3:L5:50:C:H5'	16:LL:20:ARG:HH12	1.83	0.43
3:L5:434:A:H3'	3:L5:435:A:H8	1.82	0.43
3:L5:705:G:H2'	3:L5:706:C:C6	2.53	0.43
3:L5:1366:G:H5''	16:LL:36:ARG:HH12	1.84	0.43
3:L5:2903:G:H1'	3:L5:2904:U:C5	2.54	0.43
3:L5:4098:A:N7	3:L5:4099:G:H1'	2.33	0.43
3:L5:4504:C:H2'	3:L5:4505:C:C6	2.54	0.43
5:L8:92:U:H2'	5:L8:93:C:O4'	2.18	0.43
16:LL:47:ALA:HB3	16:LL:48:PRO:HD3	2.00	0.43
29:LY:59:ARG:HB2	29:LY:103:LYS:HD2	1.99	0.43
53:SE:63:LYS:HE2	64:SY:85:ASN:HA	1.99	0.43
53:SE:94:LYS:HG3	64:SY:16:ARG:HG3	1.99	0.43
55:SH:63:PHE:HA	55:SH:95:ILE:O	2.17	0.43
55:SH:126:HIS:HA	55:SH:129:ILE:HG12	2.00	0.43
56:SI:27:TYR:HB3	56:SI:49:ARG:NH2	2.33	0.43
57:SJ:46:VAL:HA	57:SJ:49:THR:HG22	2.00	0.43
68:S2:28:U:H2'	68:S2:29:G:C8	2.52	0.43
68:S2:181:A:H2'	68:S2:182:C:C5	2.53	0.43
68:S2:194:C:H2'	68:S2:195:C:H6	1.83	0.43
68:S2:651:PSU:H2'	68:S2:652:U:C6	2.54	0.43
68:S2:1748:G:H2'	68:S2:1749:G:H8	1.83	0.43
68:S2:1844:U:H2'	68:S2:1845:A:C8	2.54	0.43
73:SM:33:ARG:HD2	73:SM:91:LEU:HD12	2.00	0.43
86:CA:33:ARG:O	86:CA:37:GLU:HG2	2.19	0.43
1:CD:195:ARG:HA	1:CD:195:ARG:HD2	1.81	0.43
3:L5:729:G:H5''	11:LF:76:ARG:HD2	2.00	0.43
3:L5:1080:C:H2'	3:L5:1081:C:H6	1.84	0.43
3:L5:1084:C:H2'	3:L5:1085:C:H6	1.82	0.43
3:L5:3732:A:H2'	3:L5:3733:A:C8	2.54	0.43
3:L5:4571:A2M:H2'	3:L5:4572:U:C6	2.48	0.43
3:L5:4749:C:H2'	3:L5:4750:G:O4'	2.18	0.43
5:L8:144:U:H2'	5:L8:145:C:C6	2.53	0.43
19:LO:9:LEU:HD23	19:LO:118:MET:HB2	2.00	0.43
28:LX:82:THR:HG21	38:Lh:37:THR:HG22	2.00	0.43
31:La:93:ASN:HD21	31:La:97:ALA:HB3	1.83	0.43
51:SB:71:LEU:HD12	51:SB:84:PHE:CE1	2.53	0.43
53:SE:146:THR:HG21	68:S2:122:G:H21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Sd:21:CYS:HB2	81:Sd:39:CYS:HB3	1.81	0.43
85:CB:5:THR:O	85:CB:9:ILE:HG12	2.18	0.43
3:L5:190:G:H2'	3:L5:191:G:C8	2.54	0.43
3:L5:253:G:H2'	3:L5:254:G:C8	2.54	0.43
3:L5:1304:C:H2'	3:L5:1305:C:C6	2.53	0.43
3:L5:1431:C:H2'	3:L5:1432:G:O4'	2.18	0.43
3:L5:1662:C:H2'	3:L5:1663:C:H6	1.84	0.43
3:L5:4069:U:H2'	3:L5:4070:U:C6	2.54	0.43
4:L7:4:U:H2'	4:L7:5:A:H8	1.83	0.43
8:LC:150:LEU:HA	8:LC:150:LEU:HD12	1.78	0.43
9:LD:236:MET:O	9:LD:239:MET:HG3	2.19	0.43
17:LM:104:MET:HE2	17:LM:109:ARG:HG2	1.99	0.43
22:LR:162:ARG:HE	68:S2:873:G:H1'	1.82	0.43
36:Lf:78:HIS:O	36:Lf:83:MET:HB2	2.18	0.43
49:Lt:62:LEU:HB3	49:Lt:73:VAL:HG23	2.01	0.43
57:SJ:111:GLN:HE22	57:SJ:127:ARG:HD2	1.83	0.43
60:SO:95:ILE:HD11	60:SO:126:ILE:HD12	2.00	0.43
62:SW:111:MET:HE2	62:SW:111:MET:HB3	1.84	0.43
68:S2:556:U:H3'	68:S2:557:U:H4'	2.01	0.43
68:S2:1651:A:H2'	68:S2:1652:G:H8	1.84	0.43
3:L5:400:A2M:HM'3	3:L5:400:A2M:H1'	1.62	0.43
3:L5:1095:A:H2	3:L5:1200:G:H1	1.54	0.43
3:L5:1307:A:H2'	3:L5:1308:C:H6	1.84	0.43
3:L5:1577:G:H5'	3:L5:1578:U:H5''	2.00	0.43
3:L5:1914:C:H4'	19:LO:89:PRO:HD3	2.00	0.43
3:L5:2424:OMG:H1'	3:L5:2424:OMG:HM23	1.77	0.43
3:L5:2495:U:H2'	3:L5:2496:G:H8	1.84	0.43
3:L5:2844:A:O2'	3:L5:4631:G:H4'	2.18	0.43
10:LE:108:LYS:HE3	10:LE:111:LYS:HA	2.01	0.43
12:LG:117:ARG:HD2	12:LG:117:ARG:HA	1.69	0.43
20:LP:61:ARG:NH2	20:LP:76:TRP:HB3	2.34	0.43
23:LS:16:CYS:SG	23:LS:54:MET:HG2	2.58	0.43
46:Lp:62:LYS:HE2	46:Lp:62:LYS:HB2	1.79	0.43
52:SC:210:PRO:HD3	52:SC:236:PHE:CE2	2.54	0.43
57:SJ:7:TRP:HE1	68:S2:39:A:H5'	1.84	0.43
66:Sb:51:GLN:NE2	68:S2:1014:G:H21	2.17	0.43
68:S2:328:U:HO2'	68:S2:329:G:H8	1.66	0.43
68:S2:517:OMC:HM23	68:S2:517:OMC:H1'	1.73	0.43
68:S2:1671:G:H2'	68:S2:1672:U:H6	1.84	0.43
68:S2:1804:U:H2'	68:S2:1805:G:H8	1.84	0.43
68:S2:1850:MA6:H8	68:S2:1850:MA6:O5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SR:9:VAL:HG23	69:SR:50:ILE:HA	2.01	0.43
74:SP:43:ARG:NH1	74:SP:47:ARG:HE	2.17	0.43
3:L5:159:C:H5''	39:Li:25:ARG:NH2	2.34	0.43
3:L5:1096:C:H2'	3:L5:1097:C:H6	1.84	0.43
3:L5:1895:G:H2'	3:L5:1896:A:O4'	2.19	0.43
3:L5:2484:A:H3'	3:L5:2486:G:N2	2.33	0.43
3:L5:3606:U:H2'	3:L5:3607:U:H6	1.84	0.43
3:L5:3867:A2M:HM'3	3:L5:3867:A2M:H1'	1.59	0.43
3:L5:4935:C:H2'	3:L5:4936:G:H8	1.84	0.43
4:L7:75:G:H5''	23:LS:49:SER:O	2.18	0.43
7:LB:50:LYS:HB2	7:LB:345:LEU:HD11	1.99	0.43
10:LE:226:ARG:HD3	10:LE:226:ARG:H	1.84	0.43
17:LM:25:VAL:HB	17:LM:38:VAL:HG13	2.01	0.43
39:Li:16:LYS:HD3	39:Li:16:LYS:HA	1.69	0.43
48:Ls:18:ILE:HD11	48:Ls:68:HIS:CG	2.54	0.43
49:Lt:127:GLY:O	49:Lt:131:GLU:HG2	2.19	0.43
67:Se:34:ARG:HA	67:Se:34:ARG:HD3	1.83	0.43
68:S2:66:G:H2'	68:S2:67:C:H4'	2.01	0.43
68:S2:155:G:H2'	68:S2:156:G:C8	2.52	0.43
74:SP:43:ARG:HH12	74:SP:47:ARG:HE	1.67	0.43
83:Sg:173:LEU:HD21	83:Sg:187:ASN:HD21	1.82	0.43
84:Et:62:C:H2'	84:Et:63:C:C6	2.54	0.43
85:CB:364:ALA:HA	85:CB:367:TYR:CZ	2.54	0.43
85:CB:373:TYR:CZ	85:CB:492:HIS:HB2	2.54	0.43
3:L5:423:G:H5'	20:LP:26:PHE:HZ	1.84	0.43
3:L5:1250:C:H2'	3:L5:1251:C:C6	2.53	0.43
3:L5:2326:G:H5''	35:Le:127:ALA:HB1	2.00	0.43
3:L5:3848:U:H2'	3:L5:3849:A:C8	2.54	0.43
3:L5:4771:C:H2'	3:L5:4772:C:C6	2.53	0.43
5:L8:19:C:H2'	5:L8:20:A:C8	2.53	0.43
7:LB:128:LYS:HA	7:LB:128:LYS:HD2	1.87	0.43
8:LC:159:GLU:HA	8:LC:217:ILE:HB	2.01	0.43
30:LZ:91:LEU:HD23	30:LZ:91:LEU:HA	1.81	0.43
68:S2:12:U:H2'	68:S2:13:C:H6	1.83	0.43
68:S2:80:G:H2'	68:S2:81:U:C6	2.54	0.43
68:S2:159:A2M:HM'3	68:S2:159:A2M:H1'	1.51	0.43
68:S2:878:G:H22	68:S2:908:A:H2	1.67	0.43
69:SR:10:LYS:HE2	69:SR:10:LYS:HB2	1.83	0.43
72:SK:24:LYS:HB2	72:SK:66:HIS:CE1	2.54	0.43
83:Sg:32:LEU:HA	83:Sg:42:MET:HA	2.01	0.43
83:Sg:125:ARG:HG2	83:Sg:150:TRP:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:Et:36:U:H5''	84:Et:37:A:C2	2.52	0.43
85:CB:45:ILE:HD11	85:CB:454:MET:HE2	2.01	0.43
85:CB:66:ARG:HH22	85:CB:552:LEU:HD11	1.84	0.43
3:L5:223:G:H4'	3:L5:225:G:C8	2.54	0.42
3:L5:1449:C:H2'	3:L5:1450:C:H6	1.83	0.42
3:L5:1588:U:H2'	3:L5:1589:C:C6	2.54	0.42
3:L5:2107:C:H2'	3:L5:2108:G:H8	1.84	0.42
3:L5:3664:G:H2'	3:L5:3665:G:H8	1.84	0.42
3:L5:3928:A:H2'	3:L5:3929:G:O4'	2.18	0.42
3:L5:4192:A:H2'	3:L5:4193:C:H6	1.83	0.42
4:L7:112:U:H2'	4:L7:113:G:H8	1.84	0.42
8:LC:252:TRP:CH2	8:LC:260:LEU:HD11	2.55	0.42
11:LF:93:ILE:HD12	11:LF:243:LEU:HD23	2.00	0.42
13:LH:92:MET:HE2	13:LH:179:ILE:HG22	2.01	0.42
20:LP:94:MET:HE1	20:LP:146:ILE:HB	2.00	0.42
24:LT:44:GLY:HA2	24:LT:95:HIS:HB3	2.00	0.42
53:SE:123:LEU:HD23	53:SE:161:GLN:HA	2.01	0.42
54:SG:21:GLU:HA	54:SG:24:LEU:HB2	2.01	0.42
54:SG:219:GLU:HA	54:SG:222:GLU:HB2	2.01	0.42
56:SI:122:GLY:HA2	56:SI:167:GLN:HG2	2.00	0.42
68:S2:1630:A:H5'	76:SS:37:GLY:N	2.34	0.42
71:SF:186:ASN:HA	71:SF:191:LYS:HE2	2.01	0.42
78:SU:116:ILE:HG22	78:SU:118:ASP:H	1.83	0.42
86:CA:72:LYS:HD2	86:CA:114:VAL:HA	2.01	0.42
3:L5:270:U:H2'	3:L5:271:C:C6	2.54	0.42
3:L5:347:A:H2'	3:L5:348:G:C8	2.53	0.42
3:L5:426:A:H2'	3:L5:427:A:C8	2.54	0.42
3:L5:1248:C:H2'	3:L5:1249:C:C6	2.54	0.42
3:L5:4113:U:H3'	3:L5:4114:C:H4'	2.01	0.42
3:L5:5023:C:H3'	3:L5:5024:C:H4'	2.00	0.42
5:L8:102:G:H4'	40:Lj:21:ARG:HB2	2.02	0.42
12:LG:83:PHE:HA	12:LG:183:ILE:HD13	2.01	0.42
17:LM:117:LYS:O	17:LM:121:ARG:HG2	2.19	0.42
54:SG:217:MET:HG3	54:SG:221:LYS:HZ3	1.83	0.42
56:SI:114:GLU:HB3	56:SI:136:ILE:HD12	2.01	0.42
68:S2:388:U:H2'	68:S2:389:A:C8	2.54	0.42
68:S2:448:A:H4'	68:S2:449:A:H5''	2.01	0.42
68:S2:864:A:H2'	68:S2:865:A:H8	1.84	0.42
68:S2:893:U:H3'	68:S2:894:G:C8	2.54	0.42
68:S2:1217:A:H2'	68:S2:1218:C:H6	1.83	0.42
68:S2:1736:G:H2'	68:S2:1737:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:SU:67:LYS:HG2	78:SU:78:ASP:HB2	2.00	0.42
85:CB:72:SER:HB3	85:CB:400:LYS:NZ	2.34	0.42
85:CB:152:LYS:HA	85:CB:203:ILE:HD11	2.01	0.42
3:L5:2654:C:H2'	3:L5:2655:C:C6	2.55	0.42
3:L5:3870:C:H2'	3:L5:3871:A:H8	1.84	0.42
3:L5:3951:G:H2'	3:L5:3952:A:C4	2.54	0.42
3:L5:5002:U:H2'	3:L5:5003:U:H6	1.84	0.42
3:L5:5003:U:H2'	3:L5:5004:C:C6	2.54	0.42
9:LD:89:LYS:HB2	9:LD:89:LYS:HE2	1.85	0.42
20:LP:8:PRO:HD3	20:LP:149:ILE:HD13	2.01	0.42
32:Lb:73:LYS:HA	32:Lb:73:LYS:HD3	1.78	0.42
54:SG:199:THR:HG21	68:S2:126:G:C8	2.54	0.42
54:SG:222:GLU:HA	54:SG:225:GLN:HB2	2.01	0.42
64:SY:10:ARG:HH21	64:SY:70:THR:HG21	1.84	0.42
66:Sb:20:LYS:HA	66:Sb:23:ARG:NH1	2.34	0.42
68:S2:1396:A:C5	68:S2:1449:G:O6	2.71	0.42
68:S2:1687:C:H2'	68:S2:1688:C:H6	1.83	0.42
68:S2:1756:C:H3'	68:S2:1757:G:H21	1.83	0.42
72:SK:46:MET:HE1	72:SK:67:PHE:CD1	2.54	0.42
86:CA:32:LEU:HA	86:CA:35:LEU:HD12	2.02	0.42
3:L5:966:A:H5''	3:L5:2092:G:H22	1.84	0.42
3:L5:3619:G:H22	3:L5:3624:A:H1'	1.83	0.42
3:L5:4236:G:H4'	3:L5:4328:G:O2'	2.19	0.42
3:L5:4461:C:OP1	88:L5:5287:SPM:H92	2.19	0.42
3:L5:4651:A:H2'	3:L5:4652:G:O4'	2.18	0.42
11:LF:216:PRO:HD3	11:LF:247:MET:HE2	2.01	0.42
14:LI:48:LEU:O	14:LI:139:ARG:HA	2.18	0.42
48:Ls:52:VAL:HG23	48:Ls:90:PHE:HB2	2.02	0.42
48:Ls:106:LYS:HD2	48:Ls:185:PHE:HA	2.01	0.42
50:SA:137:ALA:HB1	50:SA:142:LEU:HB3	2.00	0.42
52:SC:171:GLY:HA2	62:SW:98:GLN:HE22	1.84	0.42
53:SE:55:ALA:HB1	53:SE:60:GLU:HB2	2.01	0.42
54:SG:190:ARG:NH1	68:S2:334:C:H5	2.17	0.42
61:SV:70:LEU:HD21	61:SV:83:PHE:HE2	1.85	0.42
62:SW:28:ARG:HH22	68:S2:1093:A:H5''	1.84	0.42
66:Sb:34:ASP:HB2	66:Sb:43:ILE:HG23	2.00	0.42
67:Se:39:ASN:ND2	68:S2:551:U:H4'	2.34	0.42
68:S2:76:U:O2'	68:S2:77:A:H5''	2.19	0.42
68:S2:900:C:H5'	68:S2:901:G:N7	2.33	0.42
68:S2:1291:A:H62	82:Sf:95:ARG:HH12	1.65	0.42
68:S2:1692:U:H2'	68:S2:1693:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1702:G:H2'	68:S2:1703:OMC:O4'	2.19	0.42
71:SF:42:LYS:HD3	71:SF:42:LYS:HA	1.80	0.42
83:Sg:149:GLU:O	83:Sg:170:TRP:HB2	2.19	0.42
83:Sg:236:ILE:HG13	83:Sg:252:THR:HG22	2.01	0.42
3:L5:182:G:H8	3:L5:182:G:O5'	2.02	0.42
3:L5:2409:U:H5	3:L5:2783:A:N1	2.18	0.42
3:L5:2730:U:H2'	3:L5:2731:C:C6	2.54	0.42
3:L5:4153:C:H2'	3:L5:4154:G:H8	1.84	0.42
3:L5:4301:U:H4'	24:LT:54:HIS:CD2	2.55	0.42
3:L5:4364:G:H2'	3:L5:4365:C:H6	1.84	0.42
3:L5:4775:C:H2'	3:L5:4776:G:O4'	2.18	0.42
5:L8:5:U:H2'	5:L8:6:C:C6	2.53	0.42
5:L8:96:C:H5''	38:Lh:66:LYS:HG2	2.01	0.42
14:LI:76:MET:HE2	14:LI:138:ILE:HG21	2.01	0.42
21:LQ:85:THR:HG23	21:LQ:104:ARG:HG2	2.01	0.42
28:LX:141:ALA:HB3	28:LX:144:TYR:HD1	1.85	0.42
42:Ll:12:PHE:CE2	42:Ll:51:LEU:HD22	2.54	0.42
51:SB:111:CYS:HB3	65:Sa:68:TYR:HB2	2.01	0.42
54:SG:14:LYS:HA	54:SG:14:LYS:HD3	1.86	0.42
54:SG:121:ILE:HG23	54:SG:124:LEU:HB3	2.00	0.42
56:SI:192:GLY:HA3	58:SL:19:ASN:ND2	2.34	0.42
63:SX:17:ARG:NH1	68:S2:658:U:H1'	2.35	0.42
68:S2:323:C:H5'	68:S2:324:C:OP1	2.20	0.42
68:S2:348:A:H2'	68:S2:349:A:C8	2.53	0.42
3:L5:679:C:H2'	3:L5:680:G:C8	2.54	0.42
3:L5:2079:G:H2'	3:L5:2080:U:C6	2.55	0.42
3:L5:2372:U:H2'	3:L5:2373:C:C6	2.55	0.42
3:L5:2654:C:H2'	3:L5:2655:C:H6	1.84	0.42
3:L5:4113:U:H4'	3:L5:4115:G:C5	2.54	0.42
5:L8:8:U:H2'	5:L8:9:A:C8	2.54	0.42
5:L8:140:C:H2'	5:L8:141:C:C6	2.55	0.42
16:LL:179:PHE:CD2	31:La:131:ARG:HG3	2.54	0.42
51:SB:81:PHE:CG	51:SB:109:LYS:HE3	2.54	0.42
54:SG:133:LEU:HB3	68:S2:65:C:N4	2.33	0.42
60:SO:66:ARG:HG3	68:S2:962:A:H5''	2.02	0.42
60:SO:98:ARG:HB2	60:SO:132:VAL:HG23	2.00	0.42
68:S2:120:U:H2'	68:S2:121:OMU:C6	2.50	0.42
68:S2:381:C:H2'	68:S2:382:C:C6	2.55	0.42
68:S2:495:U:H2'	68:S2:496:C:O4'	2.19	0.42
68:S2:634:A:H2'	68:S2:635:G:H8	1.84	0.42
68:S2:1308:U:H2'	68:S2:1309:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Sg:223:GLU:HB3	83:Sg:225:LYS:HG2	2.00	0.42
83:Sg:294:ASP:OD2	83:Sg:296:GLN:HB2	2.20	0.42
85:CB:45:ILE:HG13	85:CB:46:ILE:N	2.34	0.42
86:CA:342:LEU:HD23	86:CA:342:LEU:H	1.84	0.42
3:L5:71:C:H1'	16:LL:62:PRO:O	2.19	0.42
3:L5:135:G:H3'	38:Lh:96:ASN:HB2	2.00	0.42
3:L5:455:C:C4	3:L5:456:C:N4	2.88	0.42
3:L5:1751:A:H2'	3:L5:1752:G:H8	1.85	0.42
3:L5:2267:U:OP1	47:Lr:37:SER:HB2	2.20	0.42
3:L5:2487:G:C4	3:L5:2489:C:H5''	2.54	0.42
8:LC:116:ASN:HB2	8:LC:119:GLN:HG3	2.02	0.42
16:LL:42:LYS:HB3	16:LL:42:LYS:HE2	1.79	0.42
26:LV:45:ILE:HG21	26:LV:53:PRO:HB3	2.01	0.42
40:Lj:8:PHE:O	40:Lj:11:ARG:HG2	2.19	0.42
53:SE:64:ILE:HD13	64:SY:17:LEU:HD23	2.00	0.42
54:SG:217:MET:O	54:SG:221:LYS:HG2	2.20	0.42
55:SH:76:GLN:O	55:SH:80:VAL:HG13	2.19	0.42
64:SY:8:ARG:HB3	68:S2:835:C:N4	2.34	0.42
65:Sa:12:LYS:HB2	65:Sa:33:ASP:OD2	2.19	0.42
68:S2:207:G:H3'	68:S2:208:G:C8	2.52	0.42
68:S2:389:A:H2'	68:S2:390:C:C6	2.54	0.42
68:S2:1284:A:C4	73:SM:91:LEU:HD11	2.55	0.42
68:S2:1409:A:H2'	68:S2:1410:C:C6	2.54	0.42
68:S2:1435:C:H41	78:SU:19:ARG:HD2	1.85	0.42
68:S2:1587:G:C5	77:ST:67:ARG:HD2	2.55	0.42
73:SM:42:LEU:HD21	73:SM:68:LEU:HD13	2.00	0.42
83:Sg:157:SER:HB3	83:Sg:164:ILE:HG12	2.00	0.42
3:L5:113:A:H2'	3:L5:114:G:O4'	2.19	0.42
3:L5:2864:A:H2'	3:L5:2865:U:C6	2.54	0.42
3:L5:2870:A:H2'	3:L5:2871:A:C8	2.54	0.42
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.20	0.42
9:LD:107:ARG:HH12	9:LD:120:GLU:HA	1.84	0.42
10:LE:155:GLY:O	10:LE:158:ARG:HG3	2.18	0.42
12:LG:87:LEU:HD12	12:LG:184:ILE:HD11	2.01	0.42
33:Lc:80:GLU:H	33:Lc:80:GLU:HG2	1.73	0.42
47:Lr:47:LYS:HB2	47:Lr:102:TYR:CZ	2.55	0.42
48:Ls:95:LEU:HD12	48:Ls:192:VAL:HG21	2.00	0.42
51:SB:59:SER:O	51:SB:63:LYS:HG2	2.19	0.42
52:SC:194:ARG:HH11	68:S2:1154:U:H1'	1.84	0.42
56:SI:56:ARG:HA	56:SI:180:GLY:HA2	2.01	0.42
59:SN:32:ASP:O	59:SN:35:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1223:A:H2'	68:S2:1224:G:O4'	2.20	0.42
73:SM:23:LYS:HD3	73:SM:23:LYS:HA	1.80	0.42
73:SM:35:ILE:H	73:SM:35:ILE:HD12	1.85	0.42
83:Sg:245:ARG:HD2	83:Sg:247:TRP:CD2	2.55	0.42
86:CA:192:GLN:HG2	86:CA:193:HIS:ND1	2.35	0.42
3:L5:173:C:OP1	16:LL:129:ARG:HG2	2.19	0.42
3:L5:1356:U:H2'	3:L5:1357:C:C6	2.55	0.42
3:L5:2669:C:H2'	3:L5:2670:C:O4'	2.20	0.42
3:L5:4069:U:H2'	3:L5:4070:U:H6	1.85	0.42
3:L5:4578:G:H2'	3:L5:4579:PSU:C6	2.55	0.42
7:LB:161:ARG:HG2	7:LB:184:GLN:HA	2.01	0.42
9:LD:232:THR:HG22	9:LD:234:ASP:H	1.85	0.42
14:LI:4:ARG:NH1	14:LI:99:ILE:HG13	2.35	0.42
50:SA:13:GLU:HA	50:SA:16:LEU:HD12	2.02	0.42
51:SB:46:LYS:HE2	51:SB:46:LYS:HB2	1.93	0.42
51:SB:220:LYS:HE3	51:SB:220:LYS:HB3	1.88	0.42
55:SH:69:LEU:HD12	55:SH:96:ALA:HB2	2.02	0.42
58:SL:126:VAL:HG12	58:SL:145:VAL:HG22	2.02	0.42
68:S2:71:G:H2'	68:S2:72:C:H4'	2.02	0.42
71:SF:188:TYR:CZ	71:SF:192:LYS:HE2	2.55	0.42
73:SM:81:ASP:HB3	73:SM:84:LYS:HB3	2.02	0.42
75:SQ:90:LYS:HE2	75:SQ:90:LYS:HB3	1.92	0.42
79:SZ:102:LYS:HA	79:SZ:107:VAL:HG12	2.00	0.42
3:L5:690:C:H2'	3:L5:691:C:C6	2.55	0.42
3:L5:1190:C:H2'	3:L5:1191:C:C6	2.55	0.42
3:L5:1701:A:C6	3:L5:1702:C:C5	3.08	0.42
3:L5:2500:U:H2'	3:L5:2501:C:C6	2.55	0.42
3:L5:3732:A:H2'	3:L5:3733:A:H8	1.84	0.42
3:L5:4967:A:H2'	3:L5:4968:A:H8	1.80	0.42
5:L8:37:A:OP2	38:Lh:89:ARG:HD2	2.19	0.42
7:LB:378:ARG:HE	27:LW:32:LEU:HD21	1.84	0.42
8:LC:25:PRO:HB2	8:LC:27:VAL:HG12	2.01	0.42
9:LD:205:ALA:HB1	9:LD:233:PRO:HB3	2.01	0.42
14:LI:184:MET:HG2	14:LI:189:CYS:HB2	2.01	0.42
22:LR:172:ARG:HH22	68:S2:908:A:P	2.43	0.42
23:LS:161:ARG:HE	23:LS:164:LYS:HB2	1.85	0.42
50:SA:176:TRP:HE1	50:SA:197:VAL:HG12	1.85	0.42
51:SB:38:MET:HG3	51:SB:186:ASN:HB3	2.02	0.42
52:SC:145:LYS:HA	52:SC:145:LYS:HD2	1.89	0.42
54:SG:65:GLN:HE21	54:SG:65:GLN:HB3	1.68	0.42
57:SJ:5:ARG:HB3	68:S2:38:A:H5''	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SY:8:ARG:HB2	64:SY:26:ASP:OD1	2.20	0.42
68:S2:146:G:H2'	68:S2:147:A:O4'	2.19	0.42
68:S2:944:A:H2'	68:S2:945:U:C6	2.55	0.42
68:S2:1433:C:H42	78:SU:92:HIS:CD2	2.38	0.42
84:Et:39:U:H2'	84:Et:40:C:H6	1.84	0.42
3:L5:186:G:H4'	3:L5:187:U:O4'	2.20	0.41
3:L5:959:G:C8	10:LE:123:ARG:HG2	2.55	0.41
3:L5:1773:U:H2'	3:L5:1774:C:H6	1.85	0.41
3:L5:1824:G:H2'	3:L5:1825:A:C8	2.55	0.41
3:L5:4960:G:H2'	3:L5:4961:G:C8	2.55	0.41
3:L5:5001:PSU:H2'	3:L5:5002:U:O4'	2.20	0.41
12:LG:151:LYS:HE2	12:LG:151:LYS:HB3	1.62	0.41
19:LO:181:ALA:O	19:LO:185:VAL:HG22	2.20	0.41
20:LP:16:LYS:HG2	20:LP:149:ILE:HG12	2.01	0.41
35:Le:78:LEU:HB3	47:Lr:20:ARG:HD2	2.01	0.41
52:SC:191:VAL:HG11	52:SC:236:PHE:HD1	1.85	0.41
57:SJ:94:LEU:HD12	57:SJ:97:ILE:HD13	2.02	0.41
63:SX:88:ASP:HA	68:S2:617:G:H4'	2.02	0.41
68:S2:1098:C:H2'	68:S2:1099:G:C8	2.55	0.41
68:S2:1792:G:H2'	68:S2:1793:A:H8	1.86	0.41
76:SS:27:ALA:HB2	76:SS:52:LEU:HD11	2.02	0.41
85:CB:533:MET:HE3	85:CB:533:MET:HB3	1.95	0.41
3:L5:1534:A2M:N3	40:Lj:11:ARG:HB2	2.35	0.41
3:L5:2297:G:H4'	8:LC:242:PRO:HB2	2.01	0.41
3:L5:2377:C:H2'	3:L5:2378:G:O4'	2.20	0.41
3:L5:3898:G:H5'	7:LB:254:ILE:HG13	2.02	0.41
3:L5:4088:C:C5	12:LG:54:PHE:HZ	2.38	0.41
3:L5:4257:A:C2	15:LJ:60:PHE:HB3	2.54	0.41
9:LD:68:ARG:HD3	9:LD:68:ARG:HA	1.85	0.41
11:LF:220:MET:HB3	11:LF:232:ASP:OD2	2.20	0.41
20:LP:113:VAL:HG11	20:LP:153:LYS:HE2	2.02	0.41
25:LU:23:LEU:HD13	25:LU:39:PHE:HE2	1.85	0.41
48:Ls:20:LEU:HB3	48:Ls:90:PHE:CE2	2.55	0.41
49:Lt:19:GLY:HA3	49:Lt:57:ARG:O	2.20	0.41
49:Lt:150:ASP:HA	49:Lt:153:ASP:HB3	2.02	0.41
50:SA:188:THR:OG1	50:SA:189:ILE:HG13	2.20	0.41
68:S2:155:G:C6	68:S2:164:A:C6	3.09	0.41
68:S2:352:U:H2'	68:S2:353:C:C6	2.55	0.41
68:S2:455:A:H2'	68:S2:456:C:H6	1.85	0.41
68:S2:1199:A:H2'	68:S2:1200:A:C8	2.55	0.41
83:Sg:302:TYR:CE2	83:Sg:308:ARG:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:Et:43:A:C6	84:Et:44:G:C6	3.09	0.41
86:CA:245:THR:HG22	86:CA:280:LEU:H	1.85	0.41
3:L5:271:C:H2'	3:L5:272:U:H6	1.86	0.41
3:L5:460:C:H2'	3:L5:461:G:H8	1.85	0.41
3:L5:967:C:H5'	3:L5:969:C:H5	1.85	0.41
3:L5:2004:U:C2	3:L5:2016:C:H1'	2.56	0.41
3:L5:2335:C:H2'	3:L5:2336:G:H8	1.85	0.41
3:L5:2904:U:O2	3:L5:3591:C:H2'	2.20	0.41
3:L5:3951:G:H8	3:L5:3951:G:OP2	2.03	0.41
3:L5:4699:U:H1'	3:L5:4700:A:H5''	2.01	0.41
3:L5:4981:G:H3'	3:L5:4982:A:H8	1.85	0.41
7:LB:47:LEU:HD23	7:LB:47:LEU:HA	1.83	0.41
7:LB:206:PRO:HD2	7:LB:209:GLN:NE2	2.28	0.41
9:LD:156:GLY:HA2	9:LD:181:PRO:HG3	2.01	0.41
11:LF:34:ARG:HE	11:LF:34:ARG:HB3	1.60	0.41
22:LR:19:LYS:HB2	22:LR:19:LYS:HE2	1.82	0.41
45:Lo:32:SER:C	45:Lo:34:TYR:H	2.27	0.41
50:SA:37:TYR:HA	50:SA:53:ARG:HD3	2.02	0.41
54:SG:7:PHE:HB3	54:SG:10:THR:HG22	2.01	0.41
54:SG:190:ARG:HH12	68:S2:334:C:H5	1.68	0.41
57:SJ:18:ARG:HH12	68:S2:20:G:H22	1.67	0.41
58:SL:93:LEU:HB3	58:SL:102:PHE:HB3	2.03	0.41
68:S2:29:G:H2'	68:S2:30:C:C6	2.55	0.41
68:S2:107:A:H2'	68:S2:108:G:C8	2.55	0.41
68:S2:942:G:H2'	68:S2:943:U:C6	2.54	0.41
71:SF:82:ASN:HD22	71:SF:88:MET:HE1	1.85	0.41
83:Sg:34:ALA:HB1	83:Sg:66:VAL:HG13	2.01	0.41
85:CB:70:ILE:HG21	85:CB:556:ILE:HG21	2.02	0.41
3:L5:120:A:H2'	3:L5:149:A:H61	1.85	0.41
3:L5:381:U:H4'	3:L5:415:G:H5'	2.01	0.41
3:L5:497:G:H4'	3:L5:498:C:OP1	2.21	0.41
3:L5:922:C:H2'	3:L5:923:C:O4'	2.20	0.41
3:L5:1194:G:H2'	3:L5:1195:G:C8	2.49	0.41
3:L5:1234:G:H2'	3:L5:1235:G:C8	2.55	0.41
3:L5:1458:C:H5''	21:LQ:69:LYS:HD2	2.02	0.41
3:L5:2909:C:H4'	3:L5:3586:G:N1	2.36	0.41
3:L5:4089:G:H2'	3:L5:4090:G:C8	2.55	0.41
13:LH:89:ARG:HG3	13:LH:145:ILE:HG23	2.01	0.41
15:LJ:95:ARG:HD3	15:LJ:175:LEU:HB2	2.02	0.41
20:LP:107:LEU:HB2	20:LP:152:GLU:OE2	2.20	0.41
21:LQ:39:THR:HG21	21:LQ:132:LYS:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SB:164:ILE:HG23	51:SB:201:CYS:SG	2.60	0.41
54:SG:32:MET:SD	54:SG:63:MET:HE3	2.60	0.41
56:SI:143:LYS:HD3	56:SI:146:GLN:HB2	2.02	0.41
68:S2:1181:A:H2'	68:S2:1182:A:C8	2.56	0.41
68:S2:1776:G:H2'	68:S2:1777:G:O4'	2.20	0.41
80:Sc:13:ARG:HA	80:Sc:55:VAL:HG12	2.01	0.41
84:Et:46:G:H4'	84:Et:47:U:OP2	2.20	0.41
85:CB:486:THR:HG21	85:CB:491:ALA:HB3	2.02	0.41
86:CA:18:VAL:HG13	86:CA:331:MET:HE1	2.03	0.41
86:CA:154:LEU:HD11	86:CA:332:ARG:HD2	2.02	0.41
3:L5:21:G:H1'	5:L8:103:A:N3	2.36	0.41
3:L5:375:G:OP1	8:LC:62:THR:HG23	2.21	0.41
3:L5:1978:C:H2'	3:L5:1979:A:O4'	2.21	0.41
3:L5:2568:C:H2'	3:L5:2569:G:H8	1.85	0.41
3:L5:2777:G:H5''	3:L5:2778:G:H5'	2.03	0.41
3:L5:3652:A:H2'	3:L5:3653:A:C5	2.55	0.41
3:L5:3947:A:H3'	3:L5:3948:C:C6	2.55	0.41
3:L5:4174:U:H2'	3:L5:4175:G:C8	2.55	0.41
3:L5:4488:A:H3'	88:L5:5287:SPM:H131	2.02	0.41
3:L5:4642:U:H2'	3:L5:4643:G:C8	2.56	0.41
12:LG:177:MET:HE2	39:Li:39:PHE:CZ	2.55	0.41
18:LN:200:LEU:HD23	18:LN:200:LEU:HA	1.89	0.41
35:Le:3:ALA:HB1	35:Le:121:ARG:HH12	1.85	0.41
49:Lt:120:SER:O	49:Lt:123:ARG:HG2	2.20	0.41
50:SA:128:ARG:NH1	50:SA:153:PRO:HD3	2.34	0.41
53:SE:18:TRP:HB3	53:SE:20:LEU:HD13	2.01	0.41
56:SI:23:LYS:HB3	56:SI:23:LYS:HE2	1.79	0.41
59:SN:88:LEU:HD22	59:SN:129:TYR:HD2	1.85	0.41
61:SV:55:ILE:HD13	61:SV:55:ILE:HA	1.86	0.41
64:SY:13:MET:HB3	64:SY:22:GLN:NE2	2.35	0.41
64:SY:20:ARG:NH1	64:SY:22:GLN:HB3	2.35	0.41
68:S2:96:C:H2'	68:S2:97:U:C6	2.56	0.41
68:S2:1528:G:H2'	68:S2:1529:C:C6	2.56	0.41
73:SM:58:GLU:HB3	73:SM:61:TYR:HB2	2.02	0.41
3:L5:1693:U:H2'	3:L5:1694:C:O4'	2.21	0.41
3:L5:1831:G:H2'	3:L5:1832:C:O4'	2.20	0.41
3:L5:3910:C:H2'	3:L5:3911:C:H6	1.81	0.41
3:L5:4246:G:H2'	3:L5:4247:G:H8	1.86	0.41
3:L5:4344:U:H2'	3:L5:4345:C:C6	2.55	0.41
6:LA:54:ARG:HG2	6:LA:56:ALA:H	1.85	0.41
7:LB:397:ILE:HG13	7:LB:398:ALA:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LC:138:MET:HE3	8:LC:138:MET:HB3	1.93	0.41
19:LO:47:PHE:HA	19:LO:136:ALA:HB2	2.01	0.41
24:LT:2:THR:HB	24:LT:3:ASN:H	1.66	0.41
26:LV:19:GLY:O	26:LV:21:PRO:HD3	2.21	0.41
58:SL:22:ARG:NH1	58:SL:22:ARG:HA	2.36	0.41
68:S2:1330:G:N7	68:S2:1492:U:H3'	2.35	0.41
68:S2:1595:U:H2'	68:S2:1596:U:H6	1.84	0.41
72:SK:14:LEU:HD23	72:SK:21:MET:SD	2.61	0.41
77:ST:69:GLY:HA2	77:ST:116:ASP:OD2	2.20	0.41
82:Sf:103:LEU:HB2	82:Sf:105:TYR:CE2	2.56	0.41
83:Sg:168:CYS:HB2	83:Sg:195:LEU:HD13	2.02	0.41
85:CB:35:LEU:HD23	85:CB:35:LEU:HA	1.90	0.41
85:CB:635:LEU:HD23	85:CB:641:TRP:CE3	2.55	0.41
85:CB:749:ILE:HG12	85:CB:810:PRO:HB3	2.03	0.41
86:CA:325:LEU:HD23	86:CA:325:LEU:HA	1.93	0.41
3:L5:10:A:H2'	3:L5:11:G:C8	2.56	0.41
3:L5:173:C:H5''	16:LL:129:ARG:HH12	1.85	0.41
3:L5:907:C:H2'	3:L5:908:G:C8	2.55	0.41
3:L5:1811:G:H2'	3:L5:1812:C:H6	1.85	0.41
3:L5:3870:C:H2'	3:L5:3871:A:C8	2.55	0.41
3:L5:4500:PSU:H2'	3:L5:4501:U:C6	2.56	0.41
3:L5:4991:U:H2'	3:L5:4992:G:C8	2.55	0.41
88:L5:5292:SPM:H31	88:L5:5292:SPM:H62	1.76	0.41
9:LD:122:GLN:HG2	9:LD:124:GLU:O	2.21	0.41
16:LL:103:ARG:H	16:LL:103:ARG:HD3	1.86	0.41
17:LM:96:GLU:O	17:LM:100:ARG:HG2	2.21	0.41
21:LQ:177:ALA:O	21:LQ:184:ARG:HB2	2.21	0.41
28:LX:110:LYS:HE3	28:LX:121:VAL:HG13	2.02	0.41
33:Lc:87:LYS:HA	33:Lc:87:LYS:HD3	1.90	0.41
50:SA:205:ARG:HB2	50:SA:209:GLU:OE2	2.21	0.41
51:SB:227:LYS:HA	51:SB:227:LYS:HD3	1.85	0.41
53:SE:29:PRO:HG3	68:S2:496:C:OP1	2.21	0.41
56:SI:172:LEU:HD23	56:SI:172:LEU:HA	1.85	0.41
60:SO:120:ALA:HB2	65:Sa:53:ILE:HD13	2.03	0.41
64:SY:8:ARG:HA	68:S2:837:A:N6	2.35	0.41
68:S2:656:G:H5'	68:S2:662:G:N2	2.36	0.41
68:S2:1139:C:H2'	68:S2:1140:G:O4'	2.20	0.41
68:S2:1667:U:H2'	68:S2:1668:U:C6	2.56	0.41
81:Sd:6:LEU:HA	81:Sd:9:SER:HB3	2.01	0.41
83:Sg:24:THR:HG23	83:Sg:27:PHE:H	1.85	0.41
85:CB:85:ASP:HA	85:CB:88:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:CB:143:LEU:HD21	85:CB:185:VAL:HG13	2.02	0.41
3:L5:659:G:H2'	3:L5:660:A:C8	2.53	0.41
3:L5:690:C:H2'	3:L5:691:C:H6	1.85	0.41
3:L5:1883:G:O6	3:L5:1896:A:H2	2.04	0.41
3:L5:1995:G:H2'	3:L5:1996:C:C6	2.55	0.41
3:L5:3722:G:H2'	3:L5:3723:A:H8	1.85	0.41
3:L5:4159:C:H2'	3:L5:4160:C:C6	2.56	0.41
3:L5:5024:C:N4	3:L5:5028:G:H21	2.18	0.41
5:L8:40:A:H2'	5:L8:41:A:C8	2.55	0.41
5:L8:65:A:H2'	5:L8:66:A:H8	1.84	0.41
5:L8:88:A:H2'	5:L8:89:U:O4'	2.20	0.41
6:LA:163:ARG:HE	6:LA:163:ARG:HB2	1.44	0.41
16:LL:105:LYS:HE2	16:LL:105:LYS:HB3	1.91	0.41
19:LO:193:THR:HG22	19:LO:197:LYS:HD2	2.02	0.41
27:LW:80:ARG:NH1	68:S2:167:G:H4'	2.35	0.41
45:Lo:35:ALA:O	45:Lo:39:ARG:HG3	2.21	0.41
51:SB:68:GLU:OE2	51:SB:83:LYS:HD2	2.21	0.41
59:SN:18:TYR:HE1	62:SW:55:ASP:HA	1.86	0.41
62:SW:28:ARG:HD2	68:S2:921:G:C5	2.56	0.41
66:Sb:69:GLY:HA3	68:S2:1105:G:O3'	2.21	0.41
68:S2:160:U:O2'	68:S2:161:U:H3'	2.20	0.41
80:Sc:58:LEU:HD23	80:Sc:58:LEU:HA	1.84	0.41
81:Sd:3:HIS:CD2	81:Sd:5:GLN:HB2	2.56	0.41
83:Sg:139:LYS:HD3	83:Sg:140:TYR:HB2	2.02	0.41
85:CB:653:GLY:HA2	85:CB:660:ASN:HB2	2.03	0.41
3:L5:457:G:H2'	3:L5:458:C:C6	2.56	0.41
3:L5:674:G:H2'	3:L5:675:C:C6	2.56	0.41
3:L5:684:G:H5''	10:LE:100:LYS:HG3	2.03	0.41
3:L5:1076:C:H2'	3:L5:1077:C:C6	2.56	0.41
3:L5:1317:U:H2'	3:L5:1318:C:C6	2.56	0.41
3:L5:1705:G:H2'	3:L5:1706:A:O4'	2.21	0.41
3:L5:1807:C:H2'	3:L5:1808:C:C6	2.56	0.41
3:L5:1858:A:H2'	3:L5:1859:C:H6	1.86	0.41
3:L5:1866:U:H2'	3:L5:1867:A:O4'	2.21	0.41
3:L5:2720:C:H2'	3:L5:2721:G:O4'	2.20	0.41
3:L5:2864:A:H2'	3:L5:2865:U:H6	1.86	0.41
3:L5:3851:PSU:H2'	3:L5:3852:A:O4'	2.21	0.41
3:L5:4620:OMU:HM23	3:L5:4620:OMU:H1'	1.88	0.41
3:L5:4732:G:H2'	3:L5:4733:C:O4'	2.20	0.41
7:LB:258:HIS:HA	7:LB:260:ALA:H	1.85	0.41
14:LI:140:THR:HG23	14:LI:141:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LM:47:ARG:HB3	23:LS:73:LEU:HD13	2.03	0.41
25:LU:56:LEU:HD11	25:LU:63:ILE:HD11	2.02	0.41
27:LW:97:LYS:HB3	27:LW:100:VAL:HG23	2.03	0.41
29:LY:22:PRO:HG2	29:LY:25:ILE:HG12	2.03	0.41
30:LZ:41:ALA:HB2	30:LZ:77:TYR:HE1	1.86	0.41
31:La:7:LYS:HB3	31:La:7:LYS:HE2	1.81	0.41
48:Ls:15:LEU:HA	48:Ls:18:ILE:HG22	2.02	0.41
50:SA:161:ILE:HG22	50:SA:163:CYS:SG	2.61	0.41
51:SB:149:GLN:OE1	51:SB:151:ARG:HB3	2.21	0.41
52:SC:83:LEU:HD12	52:SC:83:LEU:HA	1.89	0.41
52:SC:194:ARG:NH1	68:S2:1154:U:H1'	2.35	0.41
54:SG:65:GLN:HE22	68:S2:1745:A:H2	1.67	0.41
56:SI:144:LYS:HA	56:SI:147:LYS:HE3	2.02	0.41
62:SW:11:LEU:HB3	62:SW:72:CYS:O	2.20	0.41
65:Sa:37:LYS:HE3	65:Sa:37:LYS:HB2	1.85	0.41
68:S2:15:U:H2'	68:S2:16:G:O4'	2.21	0.41
68:S2:1313:A:OP1	72:SK:5:LYS:HE2	2.21	0.41
68:S2:1328:OMG:H1'	68:S2:1328:OMG:HM23	1.74	0.41
68:S2:1687:C:H2'	68:S2:1688:C:C6	2.56	0.41
68:S2:1803:U:H2'	68:S2:1804:U:C6	2.56	0.41
70:SD:51:LEU:HB3	70:SD:91:VAL:HG22	2.03	0.41
71:SF:127:ARG:HG3	71:SF:136:ARG:HH11	1.86	0.41
71:SF:145:ARG:HB2	80:Sc:48:GLY:HA3	2.03	0.41
72:SK:71:LEU:HD12	72:SK:71:LEU:HA	1.88	0.41
73:SM:23:LYS:O	73:SM:27:ILE:HG12	2.21	0.41
79:SZ:57:LYS:HA	79:SZ:60:LYS:HG2	2.03	0.41
80:Sc:33:GLU:HB3	80:Sc:41:SER:HB3	2.02	0.41
81:Sd:24:CYS:SG	81:Sd:26:ASN:HB2	2.61	0.41
85:CB:50:ARG:HG2	85:CB:52:GLY:H	1.86	0.41
85:CB:452:LEU:HD23	85:CB:459:GLU:O	2.21	0.41
86:CA:249:ARG:HD2	86:CA:250:ASP:C	2.46	0.41
3:L5:92:C:C2	31:La:55:LYS:HE2	2.55	0.41
3:L5:454:U:H2'	3:L5:455:C:O4'	2.21	0.41
3:L5:702:U:H2'	3:L5:703:G:O4'	2.21	0.41
3:L5:1092:G:H2'	3:L5:1093:C:C6	2.55	0.41
3:L5:1316:OMG:HM23	3:L5:1316:OMG:H1'	1.91	0.41
3:L5:1504:G:H2'	3:L5:1505:C:C6	2.56	0.41
3:L5:2351:OMC:HM23	3:L5:2351:OMC:H1'	1.93	0.41
3:L5:4685:U:H2'	3:L5:4686:G:C8	2.56	0.41
3:L5:4859:C:H2'	3:L5:4860:G:C8	2.56	0.41
7:LB:117:ARG:NH2	7:LB:177:LYS:HG2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LC:205:ARG:HD3	8:LC:205:ARG:HA	1.92	0.41
10:LE:115:TYR:CD2	47:Lr:115:SER:HB3	2.56	0.41
13:LH:100:PRO:O	13:LH:116:ASN:HB3	2.21	0.41
25:LU:47:ILE:HD12	25:LU:63:ILE:HD11	2.03	0.41
29:LY:49:ILE:HD12	29:LY:49:ILE:HA	1.98	0.41
33:Lc:47:ILE:HD12	33:Lc:94:LEU:HD11	2.03	0.41
49:Lt:29:ALA:HA	49:Lt:32:ILE:HG22	2.03	0.41
52:SC:69:LEU:HD23	52:SC:69:LEU:HA	1.95	0.41
52:SC:165:VAL:HG21	52:SC:217:ALA:HB1	2.03	0.41
55:SH:31:GLU:HG3	55:SH:32:MET:H	1.86	0.41
68:S2:671:A:H4'	68:S2:672:A:H5''	2.03	0.41
68:S2:1043:G:H2'	68:S2:1044:G:O4'	2.21	0.41
68:S2:1310:U:H2'	68:S2:1311:C:C6	2.56	0.41
74:SP:56:LEU:O	74:SP:60:LEU:HG	2.21	0.41
84:Et:6:G:H2'	84:Et:7:A:C8	2.56	0.41
85:CB:398:ILE:HD13	85:CB:398:ILE:HA	1.96	0.41
3:L5:718:C:OP1	11:LF:217:ARG:HD3	2.21	0.40
3:L5:1695:U:H2'	3:L5:1696:C:C6	2.56	0.40
3:L5:4244:A:H2'	3:L5:4245:G:O4'	2.21	0.40
7:LB:302:ASN:HB2	7:LB:313:SER:HA	2.02	0.40
8:LC:106:LYS:HD3	8:LC:108:TRP:CZ2	2.56	0.40
18:LN:126:THR:HG23	18:LN:127:TYR:CD2	2.57	0.40
41:Lk:29:LYS:HE2	41:Lk:29:LYS:HB2	1.92	0.40
48:Ls:37:SER:O	48:Ls:41:GLN:HG2	2.21	0.40
50:SA:141:ASN:HD22	52:SC:86:LEU:HD23	1.86	0.40
50:SA:155:ARG:HG2	50:SA:156:TYR:CD2	2.55	0.40
68:S2:62:G:H4'	68:S2:172:OMU:H5	2.01	0.40
68:S2:99:A2M:O5'	68:S2:99:A2M:H8	2.21	0.40
68:S2:159:A2M:H2	68:S2:467:G:N2	2.25	0.40
68:S2:386:C:H2'	68:S2:387:C:C6	2.57	0.40
68:S2:1227:G:C2	68:S2:1228:A:C8	3.10	0.40
68:S2:1407:U:H2'	68:S2:1408:U:H6	1.84	0.40
68:S2:1474:A:H2'	68:S2:1475:G:C8	2.56	0.40
68:S2:1716:C:H2'	68:S2:1717:C:H6	1.86	0.40
70:SD:67:ARG:HD3	72:SK:96:ARG:HE	1.85	0.40
80:Sc:10:LYS:HE2	80:Sc:34:PHE:CE1	2.56	0.40
85:CB:531:ASP:HB3	85:CB:534:VAL:HG12	2.02	0.40
1:CD:218:TRP:NE1	70:SD:142:LEU:HB2	2.36	0.40
3:L5:650:C:H2'	3:L5:651:C:C6	2.56	0.40
3:L5:1534:A2M:HM'2	3:L5:1535:C:H5'	2.03	0.40
3:L5:1697:G:H2'	3:L5:1698:C:C5	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2749:C:H2'	3:L5:2750:G:C8	2.56	0.40
3:L5:3723:A:H2'	3:L5:3724:A:C8	2.57	0.40
3:L5:4219:A:H2'	3:L5:4220:6MZ:C8	2.51	0.40
5:L8:127:U:C2	5:L8:128:C:H5	2.39	0.40
8:LC:62:THR:HG22	8:LC:64:ALA:H	1.85	0.40
15:LJ:53:ALA:HB2	15:LJ:68:ILE:HG13	2.03	0.40
38:Lh:9:LEU:HD23	38:Lh:9:LEU:HA	1.92	0.40
51:SB:184:VAL:O	51:SB:187:LYS:HG2	2.21	0.40
54:SG:20:ASP:HB2	54:SG:23:LYS:HD2	2.03	0.40
57:SJ:170:PRO:HG2	57:SJ:175:ARG:HG2	2.03	0.40
58:SL:21:LYS:HA	58:SL:21:LYS:HD3	1.81	0.40
68:S2:221:A:H2'	68:S2:222:U:H6	1.87	0.40
68:S2:1274:G:C5	72:SK:43:LEU:HD11	2.55	0.40
68:S2:1442:OMU:HM21	75:SQ:13:PHE:N	2.36	0.40
68:S2:1490:OMG:HM23	68:S2:1490:OMG:H1'	1.92	0.40
83:Sg:244:ASN:OD1	83:Sg:295:GLY:HA3	2.21	0.40
84:Et:28:C:H2'	84:Et:29:A:C8	2.56	0.40
1:CD:217:ASN:ND2	70:SD:143:ARG:HD2	2.36	0.40
3:L5:2016:C:C2	3:L5:2017:A:C8	3.10	0.40
3:L5:2376:A:H2'	3:L5:2377:C:C6	2.57	0.40
3:L5:4092:G:H2'	3:L5:4093:G:O4'	2.21	0.40
3:L5:4220:6MZ:H2'	3:L5:4222:G:H5''	2.02	0.40
3:L5:4239:A:H2'	3:L5:4240:G:H8	1.85	0.40
3:L5:4536:OMC:HM22	3:L5:4537:C:O4'	2.21	0.40
3:L5:4642:U:H2'	3:L5:4643:G:H8	1.85	0.40
3:L5:4773:C:N4	3:L5:4774:C:N4	2.69	0.40
6:LA:80:GLU:HB2	6:LA:170:ALA:HA	2.04	0.40
7:LB:92:TYR:HB3	7:LB:99:LEU:HD22	2.04	0.40
8:LC:76:ILE:HG12	8:LC:96:CYS:SG	2.61	0.40
10:LE:91:THR:HG22	10:LE:108:LYS:HA	2.03	0.40
22:LR:135:LYS:HE2	22:LR:135:LYS:HB3	1.89	0.40
52:SC:72:ASP:OD1	52:SC:74:LYS:HG2	2.22	0.40
53:SE:26:VAL:HG22	57:SJ:4:ALA:HB2	2.04	0.40
53:SE:104:ASP:OD1	53:SE:108:ARG:HG2	2.21	0.40
53:SE:127:ARG:HB2	53:SE:140:VAL:HG23	2.02	0.40
55:SH:66:VAL:HG11	68:S2:913:A:N3	2.36	0.40
55:SH:99:ARG:HD3	68:S2:913:A:OP1	2.21	0.40
86:CA:92:LEU:HD21	86:CA:280:LEU:HB2	2.03	0.40
3:L5:497:G:N2	3:L5:498:C:H41	2.20	0.40
3:L5:1188:C:H2'	3:L5:1189:G:C8	2.56	0.40
3:L5:2611:A:H2'	3:L5:2612:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2743:A:H2'	3:L5:2744:A:C8	2.56	0.40
3:L5:4625:C:O2'	3:L5:4626:A:H5'	2.21	0.40
3:L5:4960:G:H2'	3:L5:4961:G:H8	1.86	0.40
4:L7:22:A:H2'	4:L7:23:A:C8	2.56	0.40
5:L8:6:C:H2'	5:L8:7:U:H6	1.86	0.40
11:LF:54:ALA:HB2	11:LF:188:GLU:HG3	2.03	0.40
52:SC:253:PRO:HA	52:SC:256:TRP:CD2	2.56	0.40
53:SE:21:ASP:HB2	68:S2:829:C:OP1	2.21	0.40
54:SG:4:ASN:HB3	54:SG:110:ASN:HA	2.02	0.40
55:SH:107:LYS:HE2	55:SH:107:LYS:HB2	1.94	0.40
59:SN:33:VAL:HG21	59:SN:66:VAL:HG11	2.04	0.40
63:SX:55:VAL:HG21	63:SX:71:ARG:HG2	2.04	0.40
68:S2:1164:G:O2'	68:S2:1165:G:H5'	2.21	0.40
76:SS:86:ARG:NH1	76:SS:106:LYS:HB3	2.36	0.40
83:Sg:155:ARG:HD2	83:Sg:199:THR:HA	2.03	0.40
85:CB:609:PHE:CD2	85:CB:699:GLY:HA2	2.57	0.40
3:L5:978:G:H2'	3:L5:979:C:H6	1.86	0.40
3:L5:1081:C:O2'	3:L5:1082:C:H5'	2.22	0.40
3:L5:1392:A:H2'	3:L5:1393:G:C8	2.56	0.40
3:L5:2683:C:H2'	3:L5:2684:C:C6	2.57	0.40
3:L5:3684:G:H2'	3:L5:3685:C:C6	2.57	0.40
3:L5:3916:G:H2'	3:L5:3917:A:C8	2.57	0.40
15:LJ:161:GLU:HG2	15:LJ:164:ARG:NH2	2.36	0.40
16:LL:46:ILE:HB	16:LL:49:ARG:HB2	2.04	0.40
52:SC:82:TYR:OH	52:SC:162:ILE:HG22	2.21	0.40
55:SH:70:LYS:HG3	55:SH:74:LYS:NZ	2.36	0.40
55:SH:100:ILE:HD12	55:SH:122:LEU:HA	2.02	0.40
68:S2:24:C:O2'	68:S2:25:A:H8	2.03	0.40
68:S2:458:A:H2'	68:S2:459:C:C6	2.56	0.40
68:S2:696:G:H21	68:S2:737:G:N2	2.19	0.40
68:S2:996:A:H2'	68:S2:997:A:H8	1.86	0.40
68:S2:1239:U:H4'	74:SP:124:LYS:HB2	2.04	0.40
68:S2:1665:G:C6	77:ST:88:MET:HE1	2.56	0.40
80:Sc:31:ARG:HD2	80:Sc:41:SER:HB2	2.02	0.40
83:Sg:302:TYR:HB2	83:Sg:304:ASP:OD1	2.21	0.40
85:CB:88:PHE:HE1	85:CB:250:ALA:HA	1.86	0.40
85:CB:251:LYS:HD2	85:CB:251:LYS:HA	1.83	0.40
85:CB:436:PRO:HG2	85:CB:492:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CD	51/408 (12%)	49 (96%)	2 (4%)	0	100	100
2	CI	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
6	LA	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
7	LB	400/402 (100%)	387 (97%)	13 (3%)	0	100	100
8	LC	366/368 (100%)	354 (97%)	12 (3%)	0	100	100
9	LD	291/293 (99%)	281 (97%)	10 (3%)	0	100	100
10	LE	236/250 (94%)	224 (95%)	12 (5%)	0	100	100
11	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
12	LG	239/241 (99%)	229 (96%)	10 (4%)	0	100	100
13	LH	188/190 (99%)	181 (96%)	7 (4%)	0	100	100
14	LI	201/213 (94%)	197 (98%)	4 (2%)	0	100	100
15	LJ	168/176 (96%)	164 (98%)	4 (2%)	0	100	100
16	LL	208/210 (99%)	200 (96%)	8 (4%)	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%)	196 (98%)	3 (2%)	0	100	100
20	LP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
21	LQ	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
22	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
23	LS	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
24	LT	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
25	LU	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
26	LV	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
27	LW	112/124 (90%)	111 (99%)	1 (1%)	0	100	100
28	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	LY	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
30	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
31	La	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
32	Lb	105/121 (87%)	101 (96%)	4 (4%)	0	100	100
33	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
34	Ld	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
35	Le	126/128 (98%)	124 (98%)	2 (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%)	117 (98%)	3 (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%)	45 (94%)	3 (6%)	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%)	95 (92%)	8 (8%)	0	100	100
46	Lp	89/91 (98%)	87 (98%)	2 (2%)	0	100	100
47	Lr	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
48	Ls	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
49	Lt	128/157 (82%)	105 (82%)	23 (18%)	0	100	100
50	SA	219/221 (99%)	210 (96%)	9 (4%)	0	100	100
51	SB	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
52	SC	218/222 (98%)	211 (97%)	7 (3%)	0	100	100
53	SE	260/262 (99%)	248 (95%)	12 (5%)	0	100	100
54	SG	235/237 (99%)	218 (93%)	17 (7%)	0	100	100
55	SH	182/189 (96%)	163 (90%)	19 (10%)	0	100	100
56	SI	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
57	SJ	183/185 (99%)	171 (93%)	12 (7%)	0	100	100
58	SL	151/153 (99%)	141 (93%)	10 (7%)	0	100	100
59	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	SO	135/140 (96%)	127 (94%)	8 (6%)	0	100	100
61	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
62	SW	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
63	SX	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
64	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
65	Sa	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
66	Sb	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
67	Se	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
69	SR	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
70	SD	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
71	SF	187/189 (99%)	177 (95%)	10 (5%)	0	100	100
72	SK	96/98 (98%)	91 (95%)	5 (5%)	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%)	137 (96%)	5 (4%)	0	100	100
76	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
77	ST	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
78	SU	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
79	SZ	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
80	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
81	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
82	Sf	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
83	Sg	311/313 (99%)	285 (92%)	26 (8%)	0	100	100
85	CB	842/856 (98%)	814 (97%)	28 (3%)	0	100	100
86	CA	350/356 (98%)	335 (96%)	15 (4%)	0	100	100
All	All	12905/13527 (95%)	12389 (96%)	516 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CD	46/328 (14%)	46 (100%)	0	100	100
2	CI	25/25 (100%)	25 (100%)	0	100	100
6	LA	190/190 (100%)	190 (100%)	0	100	100
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%)	175 (99%)	1 (1%)	78	91
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	73 (99%)	1 (1%)	59	82
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
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%)	160 (99%)	1 (1%)	78	91
58	SL	137/137 (100%)	137 (100%)	0	100	100
59	SN	130/130 (100%)	129 (99%)	1 (1%)	73	89
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	122 (100%)	0	100	100
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
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%)	11209 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	LL	59	VAL
46	Lp	83	ILE
57	SJ	53	ILE
59	SN	49	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
6	LA	38	HIS
7	LB	68	ASN
7	LB	121	ASN
7	LB	145	GLN
7	LB	184	GLN
7	LB	209	GLN
8	LC	38	ASN
8	LC	41	HIS
8	LC	187	GLN
8	LC	347	HIS
9	LD	195	HIS
10	LE	266	GLN
12	LG	195	HIS
14	LI	59	GLN
14	LI	73	ASN
14	LI	144	ASN
16	LL	111	GLN
17	LM	34	ASN
18	LN	199	GLN
20	LP	21	ASN
20	LP	75	GLN
22	LR	143	HIS
23	LS	23	HIS
23	LS	108	GLN
24	LT	131	GLN
25	LU	50	ASN
25	LU	94	ASN
27	LW	17	HIS
27	LW	50	ASN
28	LX	108	GLN
29	LY	72	GLN
30	LZ	78	ASN
30	LZ	132	GLN
31	La	34	ASN
36	Lf	20	ASN
37	Lg	100	GLN
37	Lg	114	GLN
38	Lh	62	ASN
38	Lh	107	GLN
39	Li	15	HIS
43	Lm	109	ASN
43	Lm	117	HIS
43	Lm	120	ASN

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Mol	Chain	Res	Type
44	Ln	22	GLN
47	Lr	83	ASN
48	Ls	42	GLN
48	Ls	68	HIS
48	Ls	190	GLN
49	Lt	65	GLN
50	SA	50	ASN
51	SB	76	ASN
51	SB	149	GLN
51	SB	159	GLN
53	SE	112	HIS
54	SG	65	GLN
54	SG	81	HIS
55	SH	25	GLN
55	SH	76	GLN
56	SI	52	ASN
56	SI	87	ASN
56	SI	146	GLN
56	SI	181	GLN
57	SJ	111	GLN
58	SL	11	GLN
58	SL	19	ASN
59	SN	49	GLN
63	SX	16	HIS
63	SX	127	ASN
67	Se	22	GLN
67	Se	37	GLN
67	Se	39	ASN
67	Se	58	ASN
70	SD	22	ASN
71	SF	79	HIS
71	SF	110	GLN
71	SF	114	ASN
71	SF	118	ASN
72	SK	66	HIS
73	SM	15	ASN
76	SS	19	ASN
77	ST	85	ASN
77	ST	126	GLN
81	Sd	3	HIS
83	Sg	76	GLN
83	Sg	296	GLN

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Mol	Chain	Res	Type
85	CB	357	HIS
85	CB	490	HIS
85	CB	493	ASN
85	CB	660	ASN
85	CB	705	HIS
85	CB	803	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3643/5070 (71%)	765 (20%)	17 (0%)
4	L7	119/120 (99%)	11 (9%)	0
5	L8	155/156 (99%)	27 (17%)	0
68	S2	1715/1740 (98%)	390 (22%)	3 (0%)
84	Et	73/75 (97%)	29 (39%)	0
All	All	5705/7161 (79%)	1222 (21%)	20 (0%)

All (1222) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L5	2	G
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

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Mol	Chain	Res	Type
3	L5	135	G
3	L5	136	C
3	L5	139	G
3	L5	144	G
3	L5	159	C
3	L5	165	A
3	L5	166	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
3	L5	209	U
3	L5	210	C
3	L5	216	C
3	L5	218	A
3	L5	234	G
3	L5	237	G
3	L5	255	C
3	L5	256	G
3	L5	265	C
3	L5	266	C
3	L5	267	G
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	396	A
3	L5	407	A
3	L5	409	G
3	L5	410	A
3	L5	411	G

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Mol	Chain	Res	Type
3	L5	412	G
3	L5	413	G
3	L5	415	G
3	L5	432	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	464	G
3	L5	467	U
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	495	C
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	507	G
3	L5	509	A
3	L5	510	U
3	L5	512	U
3	L5	513	U
3	L5	514	U
3	L5	518	G
3	L5	643	C
3	L5	645	G
3	L5	654	C
3	L5	655	C
3	L5	657	C
3	L5	659	G
3	L5	666	G
3	L5	667	A

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Mol	Chain	Res	Type
3	L5	668	C
3	L5	669	C
3	L5	672	C
3	L5	673	C
3	L5	686	A
3	L5	696	C
3	L5	704	C
3	L5	708	G
3	L5	730	G
3	L5	731	G
3	L5	738	C
3	L5	739	G
3	L5	742	G
3	L5	746	A
3	L5	747	A
3	L5	750	U
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	934	C
3	L5	935	A
3	L5	936	C
3	L5	944	A
3	L5	945	U
3	L5	946	C
3	L5	957	G
3	L5	958	G
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	964	A
3	L5	965	G

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Mol	Chain	Res	Type
3	L5	966	A
3	L5	967	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	1075	G
3	L5	1082	C
3	L5	1083	U
3	L5	1094	G
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	1184	A
3	L5	1187	G
3	L5	1202	C
3	L5	1203	G
3	L5	1205	G
3	L5	1210	C
3	L5	1211	G
3	L5	1214	C
3	L5	1215	C
3	L5	1219	G
3	L5	1222	A
3	L5	1253	G
3	L5	1254	A
3	L5	1255	A
3	L5	1257	A
3	L5	1258	G
3	L5	1266	G
3	L5	1267	C

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Mol	Chain	Res	Type
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	1280	C
3	L5	1284	G
3	L5	1285	U
3	L5	1287	G
3	L5	1293	G
3	L5	1294	A
3	L5	1295	C
3	L5	1296	G
3	L5	1301	C
3	L5	1312	A
3	L5	1314	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	1370	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	1411	C
3	L5	1415	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

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Mol	Chain	Res	Type
3	L5	1443	A
3	L5	1444	G
3	L5	1446	C
3	L5	1447	C
3	L5	1480	C
3	L5	1482	G
3	L5	1483	C
3	L5	1497	A
3	L5	1498	G
3	L5	1502	G
3	L5	1504	G
3	L5	1516	G
3	L5	1517	G
3	L5	1534	A2M
3	L5	1535	C
3	L5	1537	A
3	L5	1547	A
3	L5	1552	G
3	L5	1564	A
3	L5	1566	C
3	L5	1574	G
3	L5	1578	U
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	1680	G
3	L5	1697	G

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Mol	Chain	Res	Type
3	L5	1699	A
3	L5	1700	G
3	L5	1701	A
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	1750	G
3	L5	1757	U
3	L5	1758	G
3	L5	1760	G
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	1785	C
3	L5	1787	A
3	L5	1797	G
3	L5	1803	G
3	L5	1804	A
3	L5	1806	G
3	L5	1810	G
3	L5	1821	G
3	L5	1822	U
3	L5	1834	U
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1855	G

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Mol	Chain	Res	Type
3	L5	1869	G
3	L5	1882	U
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	1931	C
3	L5	1932	A
3	L5	1940	G
3	L5	1948	G
3	L5	1961	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
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	2052	G
3	L5	2055	G
3	L5	2056	G
3	L5	2069	A

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Mol	Chain	Res	Type
3	L5	2084	C
3	L5	2092	G
3	L5	2093	A
3	L5	2094	G
3	L5	2095	A
3	L5	2096	G
3	L5	2097	U
3	L5	2098	G
3	L5	2099	G
3	L5	2102	G
3	L5	2107	C
3	L5	2112	G
3	L5	2252	G
3	L5	2253	A
3	L5	2256	C
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2306	G
3	L5	2313	A
3	L5	2331	G
3	L5	2333	G
3	L5	2344	U
3	L5	2345	G
3	L5	2348	G
3	L5	2351	OMC
3	L5	2360	A
3	L5	2364	OMG
3	L5	2382	A
3	L5	2383	C
3	L5	2389	A
3	L5	2395	A
3	L5	2397	G
3	L5	2401	A2M
3	L5	2411	C
3	L5	2412	A
3	L5	2417	A
3	L5	2425	U
3	L5	2453	A
3	L5	2464	C
3	L5	2465	C
3	L5	2469	C

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Mol	Chain	Res	Type
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	2486	G
3	L5	2487	G
3	L5	2488	C
3	L5	2489	C
3	L5	2490	U
3	L5	2504	C
3	L5	2513	A
3	L5	2515	G
3	L5	2518	G
3	L5	2519	U
3	L5	2520	C
3	L5	2537	A
3	L5	2544	G
3	L5	2546	G
3	L5	2547	G
3	L5	2554	U
3	L5	2555	G
3	L5	2560	C
3	L5	2565	A
3	L5	2573	A
3	L5	2583	C
3	L5	2586	G
3	L5	2587	A
3	L5	2589	C
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	2673	G
3	L5	2675	G
3	L5	2676	A
3	L5	2687	U

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Mol	Chain	Res	Type
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	2719	C
3	L5	2721	G
3	L5	2724	G
3	L5	2726	G
3	L5	2738	C
3	L5	2739	C
3	L5	2742	G
3	L5	2743	A
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	2814	C
3	L5	2815	A2M
3	L5	2826	U
3	L5	2827	G
3	L5	2834	C
3	L5	2835	A
3	L5	2848	G
3	L5	2855	G
3	L5	2867	C
3	L5	2876	OMG
3	L5	2877	G
3	L5	2892	C
3	L5	2900	U
3	L5	2902	G

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Mol	Chain	Res	Type
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	3588	C
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
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	3691	G
3	L5	3701	OMC
3	L5	3710	G
3	L5	3711	A
3	L5	3713	U
3	L5	3726	A
3	L5	3727	A
3	L5	3736	A
3	L5	3748	A
3	L5	3757	G
3	L5	3774	A
3	L5	3775	A
3	L5	3776	G
3	L5	3777	G

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Mol	Chain	Res	Type
3	L5	3785	A2M
3	L5	3786	U
3	L5	3792	OMG
3	L5	3810	C
3	L5	3811	G
3	L5	3814	U
3	L5	3817	A
3	L5	3819	G
3	L5	3824	A
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3843	C
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
3	L5	3915	U
3	L5	3930	U
3	L5	3938	G
3	L5	3942	A
3	L5	3943	A
3	L5	3947	A
3	L5	3948	C
3	L5	3949	A
3	L5	3950	U
3	L5	3951	G
3	L5	3952	A
3	L5	3953	G
3	L5	3954	A
3	L5	4057	C
3	L5	4058	U
3	L5	4059	C
3	L5	4060	U

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Mol	Chain	Res	Type
3	L5	4061	G
3	L5	4062	A
3	L5	4063	U
3	L5	4064	C
3	L5	4069	U
3	L5	4076	G
3	L5	4093	G
3	L5	4095	G
3	L5	4097	G
3	L5	4099	G
3	L5	4101	C
3	L5	4104	G
3	L5	4105	A
3	L5	4106	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	4121	G
3	L5	4122	G
3	L5	4127	A
3	L5	4133	C
3	L5	4138	C
3	L5	4140	C
3	L5	4141	G
3	L5	4142	C
3	L5	4143	G
3	L5	4146	G
3	L5	4150	G
3	L5	4162	C
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	4222	G
3	L5	4225	G
3	L5	4228	OMG

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Mol	Chain	Res	Type
3	L5	4229	U
3	L5	4232	U
3	L5	4233	A
3	L5	4234	A
3	L5	4238	G
3	L5	4243	C
3	L5	4251	A
3	L5	4254	G
3	L5	4256	A
3	L5	4257	A
3	L5	4258	C
3	L5	4265	U
3	L5	4268	A
3	L5	4273	A
3	L5	4291	G
3	L5	4295	U
3	L5	4305	G
3	L5	4306	OMU
3	L5	4314	C
3	L5	4319	C
3	L5	4326	G
3	L5	4329	G
3	L5	4330	G
3	L5	4332	C
3	L5	4338	G
3	L5	4339	A
3	L5	4349	C
3	L5	4350	C
3	L5	4373	G
3	L5	4376	A
3	L5	4377	G
3	L5	4378	A
3	L5	4379	A
3	L5	4387	C
3	L5	4391	G
3	L5	4394	A
3	L5	4405	G
3	L5	4415	A
3	L5	4421	C
3	L5	4422	A
3	L5	4427	G
3	L5	4430	G

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Mol	Chain	Res	Type
3	L5	4438	U
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	4528	G
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	4575	G
3	L5	4583	C
3	L5	4584	A
3	L5	4589	A
3	L5	4590	A2M
3	L5	4600	G
3	L5	4601	U
3	L5	4635	A
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4652	G
3	L5	4656	A
3	L5	4657	U
3	L5	4670	C
3	L5	4672	A
3	L5	4679	G
3	L5	4687	A
3	L5	4694	G
3	L5	4695	C
3	L5	4700	A

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Mol	Chain	Res	Type
3	L5	4708	A
3	L5	4709	U
3	L5	4719	G
3	L5	4733	C
3	L5	4734	A
3	L5	4740	G
3	L5	4741	C
3	L5	4742	G
3	L5	4745	G
3	L5	4750	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4765	G
3	L5	4771	C
3	L5	4772	C
3	L5	4775	C
3	L5	4776	G
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	4925	U
3	L5	4927	G
3	L5	4928	C
3	L5	4934	A
3	L5	4937	C
3	L5	4940	C
3	L5	4941	G

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Mol	Chain	Res	Type
3	L5	4943	A
3	L5	4951	G
3	L5	4960	G
3	L5	4975	G
3	L5	4976	U
3	L5	4979	A
3	L5	4985	U
3	L5	4988	U
3	L5	4989	U
3	L5	4990	C
3	L5	4991	U
3	L5	5006	U
3	L5	5007	A
3	L5	5013	C
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	5055	G
3	L5	5061	A
3	L5	5062	G
3	L5	5063	G
3	L5	5069	U
4	L7	7	G
4	L7	22	A
4	L7	33	U
4	L7	38	U
4	L7	49	A
4	L7	53	U
4	L7	54	A
4	L7	64	G
4	L7	100	A
4	L7	102	U
4	L7	110	G
5	L8	23	C

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Mol	Chain	Res	Type
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
5	L8	150	C
68	S2	2	A
68	S2	4	C
68	S2	17	C
68	S2	25	A
68	S2	33	G
68	S2	44	U
68	S2	45	A
68	S2	46	A
68	S2	56	G
68	S2	58	C
68	S2	62	G
68	S2	67	C
68	S2	68	A
68	S2	72	C
68	S2	73	C
68	S2	74	G

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Mol	Chain	Res	Type
68	S2	76	U
68	S2	79	A
68	S2	92	A
68	S2	93	PSU
68	S2	103	A
68	S2	105	PSU
68	S2	113	G
68	S2	115	U
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	153	G
68	S2	155	G
68	S2	158	A
68	S2	160	U
68	S2	162	C
68	S2	168	C
68	S2	170	A
68	S2	172	OMU
68	S2	182	C
68	S2	190	G
68	S2	196	C
68	S2	197	U
68	S2	198	U
68	S2	199	C
68	S2	200	G
68	S2	203	G
68	S2	207	G
68	S2	208	G
68	S2	214	U
68	S2	291	G
68	S2	292	A
68	S2	295	C
68	S2	302	A
68	S2	306	C
68	S2	307	G
68	S2	308	G
68	S2	309	G
68	S2	311	C

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Mol	Chain	Res	Type
68	S2	312	G
68	S2	316	G
68	S2	318	A
68	S2	319	C
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	340	C
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	383	G
68	S2	385	G
68	S2	386	C
68	S2	398	A
68	S2	408	A
68	S2	409	C
68	S2	426	A
68	S2	438	G
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	471	G
68	S2	472	C
68	S2	473	A
68	S2	474	G
68	S2	478	G
68	S2	482	G
68	S2	487	U

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Mol	Chain	Res	Type
68	S2	488	U
68	S2	492	C
68	S2	493	A
68	S2	500	A
68	S2	502	C
68	S2	516	A
68	S2	525	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	566	U
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	594	A
68	S2	604	A
68	S2	607	U
68	S2	613	G
68	S2	614	C
68	S2	623	G
68	S2	627	OMU
68	S2	628	A
68	S2	631	U
68	S2	643	A
68	S2	644	OMG
68	S2	655	A
68	S2	660	C

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Mol	Chain	Res	Type
68	S2	664	A
68	S2	668	A2M
68	S2	669	A
68	S2	671	A
68	S2	672	A
68	S2	673	G
68	S2	678	U
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	737	G
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	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
68	S2	836	G
68	S2	837	A

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Mol	Chain	Res	Type
68	S2	838	G
68	S2	839	C
68	S2	840	C
68	S2	844	U
68	S2	847	A
68	S2	867	OMG
68	S2	869	A
68	S2	870	A
68	S2	873	G
68	S2	878	G
68	S2	886	A
68	S2	888	U
68	S2	889	U
68	S2	891	G
68	S2	893	U
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	906	U
68	S2	907	G
68	S2	909	G
68	S2	913	A
68	S2	920	A
68	S2	922	A
68	S2	933	G
68	S2	949	G
68	S2	953	C
68	S2	954	U
68	S2	963	A
68	S2	969	U
68	S2	970	G
68	S2	971	G
68	S2	979	C
68	S2	985	G
68	S2	990	A
68	S2	992	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	1056	PSU
68	S2	1060	A
68	S2	1061	U
68	S2	1062	A
68	S2	1078	C
68	S2	1083	A
68	S2	1085	C
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	1133	A
68	S2	1138	C
68	S2	1148	A
68	S2	1150	A
68	S2	1153	C
68	S2	1154	U
68	S2	1155	U
68	S2	1195	A
68	S2	1207	G
68	S2	1208	A
68	S2	1215	C
68	S2	1216	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	1248	B8N
68	S2	1251	A
68	S2	1253	A
68	S2	1256	G

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Mol	Chain	Res	Type
68	S2	1257	G
68	S2	1259	A
68	S2	1274	G
68	S2	1275	G
68	S2	1285	G
68	S2	1286	G
68	S2	1293	A
68	S2	1294	G
68	S2	1295	A
68	S2	1301	A
68	S2	1302	G
68	S2	1303	C
68	S2	1308	U
68	S2	1313	A
68	S2	1327	G
68	S2	1342	U
68	S2	1354	G
68	S2	1357	A
68	S2	1358	U
68	S2	1371	U
68	S2	1372	U
68	S2	1376	A
68	S2	1378	A
68	S2	1401	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	1420	G
68	S2	1421	A
68	S2	1423	C
68	S2	1428	G
68	S2	1433	C
68	S2	1434	C
68	S2	1435	C
68	S2	1436	C
68	S2	1437	C
68	S2	1438	A
68	S2	1442	OMU
68	S2	1449	G

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Mol	Chain	Res	Type
68	S2	1454	A
68	S2	1462	U
68	S2	1463	U
68	S2	1480	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	1520	G
68	S2	1521	C
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	1557	C
68	S2	1558	C
68	S2	1573	G
68	S2	1575	G
68	S2	1579	A
68	S2	1580	A
68	S2	1581	C
68	S2	1582	C
68	S2	1585	U
68	S2	1587	G
68	S2	1588	A
68	S2	1600	G
68	S2	1601	A
68	S2	1604	G
68	S2	1621	U
68	S2	1623	A
68	S2	1633	A
68	S2	1634	A
68	S2	1637	A
68	S2	1648	G
68	S2	1654	G
68	S2	1663	A
68	S2	1665	G

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Mol	Chain	Res	Type
68	S2	1680	G
68	S2	1683	C
68	S2	1698	C
68	S2	1700	C
68	S2	1701	C
68	S2	1712	A
68	S2	1715	A
68	S2	1721	U
68	S2	1722	G
68	S2	1744	G
68	S2	1745	A
68	S2	1752	C
68	S2	1753	C
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	1825	A
68	S2	1826	G
68	S2	1829	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	4	C
84	Et	9	A
84	Et	11	C
84	Et	19	G

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Mol	Chain	Res	Type
84	Et	20	U
84	Et	21	A
84	Et	22	G
84	Et	26	A
84	Et	33	U
84	Et	36	U
84	Et	37	A
84	Et	38	A
84	Et	39	U
84	Et	43	A
84	Et	44	G
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	59	G
84	Et	61	C
84	Et	63	C
84	Et	70	G
84	Et	73	G
84	Et	76	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	134	G
3	L5	406	C
3	L5	914	U
3	L5	1082	C
3	L5	1590	C
3	L5	1633	G
3	L5	1698	C
3	L5	1703	C
3	L5	1977	C
3	L5	2416	G
3	L5	2675	G
3	L5	2760	G
3	L5	2763	U

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Mol	Chain	Res	Type
3	L5	3673	C
3	L5	4600	G
3	L5	4699	U
3	L5	4913	G
68	S2	291	G
68	S2	563	G
68	S2	688	U

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	OMC	L5	4456	3	19,22,23	0.74	0	25,31,34	0.65	0
68	OMG	S2	1490	68	23,26,27	0.53	0	32,38,41	0.44	0
3	A2M	L5	2787	3	22,25,26	1.16	1 (4%)	30,36,39	1.50	7 (23%)
3	OMC	L5	2861	3	19,22,23	0.67	0	25,31,34	0.80	1 (4%)
3	OMG	L5	3627	3	23,26,27	0.62	0	32,38,41	0.61	0
3	PSU	L5	1782	3	18,21,22	1.10	1 (5%)	21,30,33	1.93	4 (19%)
3	OMG	L5	4494	3	23,26,27	0.59	0	32,38,41	0.49	0
68	PSU	S2	649	68	18,21,22	1.10	2 (11%)	21,30,33	1.88	4 (19%)
3	OMG	L5	4196	3	23,26,27	0.56	0	32,38,41	0.47	0
3	OMC	L5	4536	3	19,22,23	0.70	0	25,31,34	0.71	0
3	OMC	L5	3869	3	19,22,23	0.71	0	25,31,34	0.63	0
3	A2M	L5	4523	87,3	22,25,26	1.28	2 (9%)	30,36,39	1.57	8 (26%)
3	PSU	L5	4628	3	18,21,22	1.08	2 (11%)	21,30,33	1.98	4 (19%)
3	OMG	L5	4618	3	23,26,27	0.64	0	32,38,41	0.51	0
68	PSU	S2	866	68	18,21,22	1.14	1 (5%)	21,30,33	2.01	5 (23%)
68	OMC	S2	1391	68	19,22,23	0.59	0	25,31,34	0.69	0
68	PSU	S2	1174	68	18,21,22	1.06	2 (11%)	21,30,33	1.91	4 (19%)
68	PSU	S2	863	68	18,21,22	1.12	1 (5%)	21,30,33	1.96	4 (19%)
3	OMC	L5	2365	3	19,22,23	0.66	0	25,31,34	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	PSU	S2	93	68	18,21,22	1.05	1 (5%)	21,30,33	1.78	4 (19%)
3	OMG	L5	4370	3	23,26,27	0.60	0	32,38,41	0.47	0
3	A2M	L5	2363	87,3	22,25,26	1.27	3 (13%)	30,36,39	1.56	9 (30%)
3	PSU	L5	4973	3	18,21,22	1.05	2 (11%)	21,30,33	1.93	4 (19%)
68	A2M	S2	166	68	22,25,26	1.25	1 (4%)	30,36,39	1.60	7 (23%)
68	OMC	S2	1703	68	19,22,23	0.57	0	25,31,34	0.63	0
3	A2M	L5	398	3	22,25,26	1.21	2 (9%)	30,36,39	1.58	7 (23%)
3	OMG	L5	3744	3	23,26,27	0.60	0	32,38,41	0.49	0
3	1MA	L5	1322	87,3	21,25,26	0.66	0	30,37,40	0.82	2 (6%)
3	PSU	L5	4296	3	18,21,22	1.10	2 (11%)	21,30,33	2.06	5 (23%)
3	OMG	L5	2424	3	23,26,27	0.58	0	32,38,41	0.43	0
3	OMG	L5	1625	3	23,26,27	0.58	0	32,38,41	0.49	0
68	A2M	S2	27	68	22,25,26	1.23	1 (4%)	30,36,39	1.50	8 (26%)
68	OMG	S2	601	68	23,26,27	0.55	0	32,38,41	0.44	0
68	OMU	S2	1442	68	19,22,23	3.32	7 (36%)	25,31,34	1.80	5 (20%)
3	OMU	L5	4306	3	19,22,23	3.18	7 (36%)	25,31,34	1.76	4 (16%)
3	PSU	L5	4579	3	18,21,22	1.05	2 (11%)	21,30,33	1.99	4 (19%)
3	PSU	L5	4353	3	18,21,22	1.10	2 (11%)	21,30,33	1.94	4 (19%)
3	OMC	L5	2422	87,3	19,22,23	0.70	0	25,31,34	0.75	1 (4%)
3	PSU	L5	4532	3	18,21,22	1.09	1 (5%)	21,30,33	1.98	4 (19%)
68	PSU	S2	1046	68	18,21,22	1.07	1 (5%)	21,30,33	1.85	4 (19%)
3	PSU	L5	4293	3	18,21,22	1.08	2 (11%)	21,30,33	1.92	4 (19%)
3	PSU	L5	3822	3	18,21,22	1.08	2 (11%)	21,30,33	2.01	6 (28%)
68	OMU	S2	172	68	19,22,23	3.32	7 (36%)	25,31,34	1.74	5 (20%)
3	PSU	L5	4431	3	18,21,22	1.08	2 (11%)	21,30,33	1.93	4 (19%)
68	PSU	S2	1081	68	18,21,22	1.04	1 (5%)	21,30,33	1.89	4 (19%)
3	A2M	L5	3867	3	22,25,26	1.36	2 (9%)	30,36,39	1.53	9 (30%)
68	PSU	S2	109	68	18,21,22	1.09	1 (5%)	21,30,33	1.92	4 (19%)
68	PSU	S2	681	68	18,21,22	1.00	2 (11%)	21,30,33	1.89	4 (19%)
68	PSU	S2	1367	68	18,21,22	1.10	2 (11%)	21,30,33	1.95	5 (23%)
3	OMG	L5	3899	3	23,26,27	0.67	0	32,38,41	0.49	0
3	PSU	L5	4299	3	18,21,22	1.04	2 (11%)	21,30,33	1.82	4 (19%)
3	PSU	L5	3920	87,3	18,21,22	1.08	2 (11%)	21,30,33	1.99	6 (28%)
3	UR3	L5	4530	3	19,22,23	2.64	7 (36%)	26,32,35	1.64	4 (15%)
68	OMU	S2	354	68	19,22,23	3.25	7 (36%)	25,31,34	1.81	5 (20%)
3	PSU	L5	2632	3	18,21,22	1.04	1 (5%)	21,30,33	1.91	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	B8N	S2	1248	68	25,29,30	3.21	6 (24%)	28,42,45	1.96	8 (28%)
68	OMU	S2	1288	68	19,22,23	3.32	7 (36%)	25,31,34	1.73	5 (20%)
3	6MZ	L5	4220	3	22,25,26	2.94	6 (27%)	29,36,39	2.39	10 (34%)
68	OMC	S2	462	68	19,22,23	0.52	0	25,31,34	0.64	0
3	A2M	L5	1524	3	22,25,26	1.33	3 (13%)	30,36,39	1.51	8 (26%)
68	OMC	S2	517	68	19,22,23	0.59	0	25,31,34	0.74	0
3	OMC	L5	2804	3	19,22,23	0.67	0	25,31,34	0.61	0
68	OMG	S2	1328	68	23,26,27	0.52	0	32,38,41	0.44	0
3	OMC	L5	2824	3	19,22,23	0.66	0	25,31,34	0.80	1 (4%)
68	OMG	S2	644	68	23,26,27	0.52	0	32,38,41	0.49	0
68	PSU	S2	406	68	18,21,22	1.11	2 (11%)	21,30,33	1.92	4 (19%)
68	PSU	S2	814	68	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
3	OMC	L5	3701	3	19,22,23	0.62	0	25,31,34	0.58	0
3	PSU	L5	4521	87,3	18,21,22	1.08	2 (11%)	21,30,33	2.07	5 (23%)
3	PSU	L5	1536	3	18,21,22	1.07	2 (11%)	21,30,33	1.91	4 (19%)
3	PSU	L5	4552	3	18,21,22	1.12	2 (11%)	21,30,33	2.00	4 (19%)
3	PSU	L5	1862	3	18,21,22	1.04	1 (5%)	21,30,33	1.92	4 (19%)
3	OMG	L5	1316	3	23,26,27	0.75	0	32,38,41	0.60	0
68	OMU	S2	428	68	19,22,23	3.31	7 (36%)	25,31,34	1.80	5 (20%)
3	A2M	L5	3785	87,3	22,25,26	1.20	1 (4%)	30,36,39	1.57	9 (30%)
3	A2M	L5	1326	3	22,25,26	1.24	2 (9%)	30,36,39	1.48	8 (26%)
3	PSU	L5	4636	3	18,21,22	1.09	2 (11%)	21,30,33	2.09	6 (28%)
3	PSU	L5	5001	3	18,21,22	1.08	1 (5%)	21,30,33	1.97	5 (23%)
3	OMC	L5	3841	3	19,22,23	0.70	0	25,31,34	0.52	0
3	PSU	L5	4689	3	18,21,22	1.06	2 (11%)	21,30,33	1.91	4 (19%)
68	PSU	S2	686	68	18,21,22	1.09	1 (5%)	21,30,33	1.93	4 (19%)
3	PSU	L5	4442	3	18,21,22	1.06	1 (5%)	21,30,33	1.96	5 (23%)
68	PSU	S2	1244	68	18,21,22	1.08	1 (5%)	21,30,33	1.94	4 (19%)
3	OMG	L5	2876	3	23,26,27	0.57	0	32,38,41	0.53	0
3	A2M	L5	1323	3	22,25,26	1.31	3 (13%)	30,36,39	1.61	9 (30%)
3	PSU	L5	1683	3	18,21,22	1.04	2 (11%)	21,30,33	2.00	4 (19%)
3	PSU	L5	3851	3	18,21,22	1.05	2 (11%)	21,30,33	1.92	4 (19%)
3	PSU	L5	4500	3	18,21,22	1.10	2 (11%)	21,30,33	2.08	5 (23%)
3	OMU	L5	4227	3	19,22,23	3.15	7 (36%)	25,31,34	1.84	4 (16%)
3	PSU	L5	3853	87,3	18,21,22	1.03	1 (5%)	21,30,33	1.87	4 (19%)
3	A2M	L5	3718	3	22,25,26	1.19	2 (9%)	30,36,39	1.59	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	2401	3	22,25,26	1.21	2 (9%)	30,36,39	1.54	7 (23%)
3	OMC	L5	3808	87,3	19,22,23	0.73	1 (5%)	25,31,34	0.88	2 (8%)
3	PSU	L5	3884	3	18,21,22	1.09	2 (11%)	21,30,33	1.96	4 (19%)
3	PSU	L5	3695	3	18,21,22	1.05	2 (11%)	21,30,33	1.97	4 (19%)
68	4AC	S2	1337	68	21,24,25	0.41	0	28,34,37	0.58	0
3	PSU	L5	4361	3	18,21,22	1.00	1 (5%)	21,30,33	1.89	4 (19%)
68	PSU	S2	1056	68	18,21,22	1.10	1 (5%)	21,30,33	1.93	4 (19%)
3	PSU	L5	4403	3	18,21,22	1.09	2 (11%)	21,30,33	1.99	6 (28%)
3	5MC	L5	4447	3	19,22,23	1.03	2 (10%)	26,32,35	0.80	0
3	OMC	L5	2351	87,3	19,22,23	0.73	1 (5%)	25,31,34	0.86	1 (4%)
68	OMC	S2	174	68	19,22,23	0.55	0	25,31,34	0.68	0
68	PSU	S2	1004	68	18,21,22	1.07	1 (5%)	21,30,33	1.91	4 (19%)
3	PSU	L5	3844	3	18,21,22	1.14	1 (5%)	21,30,33	1.88	4 (19%)
68	OMG	S2	867	68	23,26,27	0.54	0	32,38,41	0.48	0
3	PSU	L5	1582	3	18,21,22	1.09	2 (11%)	21,30,33	2.02	4 (19%)
68	A2M	S2	1031	68	22,25,26	1.16	1 (4%)	30,36,39	1.55	7 (23%)
3	A2M	L5	4571	3	22,25,26	1.42	3 (13%)	30,36,39	1.66	8 (26%)
68	A2M	S2	159	68	22,25,26	1.25	1 (4%)	30,36,39	1.61	7 (23%)
68	PSU	S2	1045	68	18,21,22	1.15	1 (5%)	21,30,33	1.89	4 (19%)
68	PSU	S2	1232	68	18,21,22	1.06	1 (5%)	21,30,33	1.98	5 (23%)
3	OMC	L5	3887	3	19,22,23	0.62	0	25,31,34	0.66	0
68	PSU	S2	1177	68	18,21,22	1.10	2 (11%)	21,30,33	1.99	4 (19%)
3	OMG	L5	2364	87,3	23,26,27	0.62	0	32,38,41	0.44	0
68	MA6	S2	1851	68	23,26,27	1.29	3 (13%)	33,38,41	3.38	12 (36%)
3	A2M	L5	3825	3	22,25,26	1.25	2 (9%)	30,36,39	1.56	7 (23%)
3	PSU	L5	1744	87,3	18,21,22	1.05	2 (11%)	21,30,33	1.95	4 (19%)
5	OMG	L8	75	5	23,26,27	0.58	0	32,38,41	0.46	0
3	OMG	L5	1522	3	23,26,27	0.62	0	32,38,41	0.62	0
5	PSU	L8	55	5	18,21,22	1.09	2 (11%)	21,30,33	1.85	4 (19%)
3	OMG	L5	4637	3	23,26,27	0.59	0	32,38,41	0.48	0
3	OMU	L5	2837	3	19,22,23	3.21	7 (36%)	25,31,34	1.92	5 (20%)
68	PSU	S2	801	68	18,21,22	1.16	1 (5%)	21,30,33	1.78	4 (19%)
3	A2M	L5	1871	87,3	22,25,26	1.36	3 (13%)	30,36,39	1.64	8 (26%)
68	G7M	S2	1639	84,68	23,26,27	2.66	9 (39%)	34,39,42	2.58	11 (32%)
3	PSU	L5	4972	3	18,21,22	1.06	1 (5%)	21,30,33	1.94	4 (19%)
68	OMG	S2	683	68	23,26,27	0.54	0	32,38,41	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	1860	3	18,21,22	1.07	2 (11%)	21,30,33	1.88	4 (19%)
3	A2M	L5	400	3	22,25,26	1.26	2 (9%)	30,36,39	1.56	9 (30%)
68	PSU	S2	105	68	18,21,22	1.03	1 (5%)	21,30,33	1.98	5 (23%)
68	6MZ	S2	1832	87,68	22,25,26	3.04	5 (22%)	29,36,39	2.21	10 (34%)
3	PSU	L5	4312	3	18,21,22	1.08	2 (11%)	21,30,33	1.81	4 (19%)
68	OMU	S2	627	68	19,22,23	3.30	7 (36%)	25,31,34	1.84	5 (20%)
3	A2M	L5	3830	3	22,25,26	1.23	1 (4%)	30,36,39	1.57	6 (20%)
3	PSU	L5	4673	3	18,21,22	1.04	2 (11%)	21,30,33	1.86	4 (19%)
3	PSU	L5	4493	3	18,21,22	1.07	1 (5%)	21,30,33	1.87	4 (19%)
3	A2M	L5	4590	3	22,25,26	1.27	3 (13%)	30,36,39	1.57	6 (20%)
68	A2M	S2	576	68	22,25,26	1.19	1 (4%)	30,36,39	1.53	5 (16%)
3	PSU	L5	2839	3	18,21,22	1.06	2 (11%)	21,30,33	1.93	4 (19%)
3	PSU	L5	1792	3	18,21,22	1.01	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L5	3639	3	18,21,22	1.09	2 (11%)	21,30,33	1.97	4 (19%)
3	OMG	L5	4499	3	23,26,27	0.60	0	32,38,41	0.50	0
68	OMU	S2	799	68	19,22,23	3.40	7 (36%)	25,31,34	1.89	5 (20%)
3	OMG	L5	4623	3	23,26,27	0.64	0	32,38,41	0.58	0
3	OMU	L5	4620	3	19,22,23	3.10	7 (36%)	25,31,34	1.78	5 (20%)
68	4AC	S2	1842	68	21,24,25	0.41	0	28,34,37	0.46	0
3	5MC	L5	3782	87,3	19,22,23	0.79	0	26,32,35	0.83	1 (3%)
3	OMG	L5	4228	3	23,26,27	0.61	0	32,38,41	0.61	0
68	OMU	S2	1326	68	19,22,23	3.26	7 (36%)	25,31,34	1.85	5 (20%)
68	OMU	S2	121	68	19,22,23	3.22	7 (36%)	25,31,34	1.59	4 (16%)
3	PSU	L5	1677	3	18,21,22	1.15	2 (11%)	21,30,33	2.12	6 (28%)
68	A2M	S2	468	68	22,25,26	1.21	1 (4%)	30,36,39	1.57	8 (26%)
3	OMG	L5	4392	3	23,26,27	0.65	0	32,38,41	0.49	0
68	A2M	S2	484	68	22,25,26	1.20	2 (9%)	30,36,39	1.46	7 (23%)
68	PSU	S2	966	87,68	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
68	A2M	S2	1383	68	22,25,26	1.16	1 (4%)	30,36,39	1.58	7 (23%)
68	PSU	S2	651	68	18,21,22	1.10	1 (5%)	21,30,33	1.96	4 (19%)
3	A2M	L5	1534	87,3	22,25,26	1.21	2 (9%)	30,36,39	1.42	7 (23%)
3	OMU	L5	4498	3	19,22,23	3.18	7 (36%)	25,31,34	1.96	5 (20%)
3	OMC	L5	1340	3	19,22,23	0.72	0	25,31,34	0.76	0
3	A2M	L5	2815	3	22,25,26	1.21	2 (9%)	30,36,39	1.51	9 (30%)
68	OMU	S2	116	68	19,22,23	3.31	7 (36%)	25,31,34	1.74	5 (20%)
3	UY1	L5	3818	3	19,22,23	4.76	9 (47%)	21,31,34	1.94	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	OMG	S2	436	68	23,26,27	0.54	0	32,38,41	0.53	0
68	OMC	S2	1272	68	19,22,23	0.57	0	25,31,34	0.78	1 (4%)
68	A2M	S2	99	87,68	22,25,26	1.19	1 (4%)	30,36,39	1.64	8 (26%)
3	PSU	L5	4471	3	18,21,22	1.11	2 (11%)	21,30,33	1.94	4 (19%)
68	A2M	S2	668	87,68	22,25,26	1.37	2 (9%)	30,36,39	1.64	8 (26%)
3	PSU	L5	4457	3	18,21,22	1.09	3 (16%)	21,30,33	2.06	4 (19%)
3	PSU	L5	3637	3	18,21,22	1.08	1 (5%)	21,30,33	2.06	5 (23%)
68	OMG	S2	509	68	23,26,27	0.52	0	32,38,41	0.49	0
5	PSU	L8	69	5	18,21,22	1.08	1 (5%)	21,30,33	1.99	5 (23%)
3	OMG	L5	3792	3	23,26,27	0.60	0	32,38,41	0.53	0
3	OMU	L5	3925	3	19,22,23	3.13	7 (36%)	25,31,34	1.84	5 (20%)
3	PSU	L5	1781	3	18,21,22	1.06	2 (11%)	21,30,33	1.88	4 (19%)
3	PSU	L5	4576	3	18,21,22	1.09	2 (11%)	21,30,33	1.88	4 (19%)
3	PSU	L5	5010	3	18,21,22	1.08	2 (11%)	21,30,33	1.89	4 (19%)
68	MA6	S2	1850	68	23,26,27	1.27	2 (8%)	33,38,41	3.38	11 (33%)

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	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
68	OMG	S2	1490	68	-	1/9/27/28	0/3/3/3
3	A2M	L5	2787	3	-	5/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
68	PSU	S2	649	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	4196	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	3869	3	-	1/9/27/28	0/2/2/2
3	A2M	L5	4523	87,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4618	3	-	0/9/27/28	0/3/3/3
68	PSU	S2	866	68	-	0/7/25/26	0/2/2/2
68	OMC	S2	1391	68	-	0/9/27/28	0/2/2/2
68	PSU	S2	1174	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	863	68	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L5	2365	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	93	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2363	87,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	166	68	-	1/9/27/28	0/3/3/3
68	OMC	S2	1703	68	-	1/9/27/28	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	1MA	L5	1322	87,3	-	2/7/25/26	0/3/3/3
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	1625	3	-	2/9/27/28	0/3/3/3
68	A2M	S2	27	68	-	1/9/27/28	0/3/3/3
68	OMG	S2	601	68	-	1/9/27/28	0/3/3/3
68	OMU	S2	1442	68	-	3/9/27/28	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2422	87,3	-	2/9/27/28	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1046	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	172	68	-	6/9/27/28	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1081	68	-	1/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	2/9/27/28	0/3/3/3
68	PSU	S2	109	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	681	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	1367	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	87,3	-	0/7/25/26	0/2/2/2
3	UR3	L5	4530	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	2632	3	-	2/7/25/26	0/2/2/2
68	B8N	S2	1248	68	-	6/16/34/35	0/2/2/2
68	OMU	S2	1288	68	-	1/9/27/28	0/2/2/2
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	OMC	S2	462	68	-	0/9/27/28	0/2/2/2
3	A2M	L5	1524	3	-	2/9/27/28	0/3/3/3
68	OMC	S2	517	68	-	1/9/27/28	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
68	OMG	S2	1328	68	-	1/9/27/28	0/3/3/3
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
68	OMG	S2	644	68	-	3/9/27/28	0/3/3/3
68	PSU	S2	406	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	814	68	-	0/7/25/26	0/2/2/2
3	OMC	L5	3701	3	-	6/9/27/28	0/2/2/2
3	PSU	L5	4521	87,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
68	OMU	S2	428	68	-	6/9/27/28	0/2/2/2
3	A2M	L5	3785	87,3	-	2/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4636	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	686	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1244	68	-	1/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	1323	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3853	87,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2401	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	3808	87,3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
68	4AC	S2	1337	68	-	0/11/29/30	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	PSU	S2	1056	68	-	2/7/25/26	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
3	OMC	L5	2351	87,3	-	1/9/27/28	0/2/2/2
68	OMC	S2	174	68	-	0/9/27/28	0/2/2/2
68	PSU	S2	1004	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
68	OMG	S2	867	68	-	2/9/27/28	0/3/3/3
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	1031	68	-	1/9/27/28	0/3/3/3
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
68	A2M	S2	159	68	-	1/9/27/28	0/3/3/3
68	PSU	S2	1045	68	-	2/7/25/26	0/2/2/2
68	PSU	S2	1232	68	-	0/7/25/26	0/2/2/2
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
68	PSU	S2	1177	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	2364	87,3	-	2/9/27/28	0/3/3/3
68	MA6	S2	1851	68	-	1/11/29/30	0/3/3/3
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1744	87,3	-	0/7/25/26	0/2/2/2
5	OMG	L8	75	5	-	1/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
5	PSU	L8	55	5	-	0/7/25/26	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
68	PSU	S2	801	68	-	2/7/25/26	0/2/2/2
3	A2M	L5	1871	87,3	-	0/9/27/28	0/3/3/3
68	G7M	S2	1639	84,68	-	0/7/25/26	0/3/3/3
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
68	OMG	S2	683	68	-	0/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3
68	PSU	S2	105	68	-	1/7/25/26	0/2/2/2
68	6MZ	S2	1832	87,68	-	2/9/27/28	0/3/3/3
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	627	68	-	2/9/27/28	0/2/2/2
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4590	3	-	4/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	A2M	S2	576	68	-	3/9/27/28	0/3/3/3
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1792	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
68	OMU	S2	799	68	-	2/9/27/28	0/2/2/2
3	OMG	L5	4623	3	-	2/9/27/28	0/3/3/3
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
68	4AC	S2	1842	68	-	0/11/29/30	0/2/2/2
3	5MC	L5	3782	87,3	-	1/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	2/9/27/28	0/3/3/3
68	OMU	S2	1326	68	-	0/9/27/28	0/2/2/2
68	OMU	S2	121	68	-	1/9/27/28	0/2/2/2
3	PSU	L5	1677	3	-	1/7/25/26	0/2/2/2
68	A2M	S2	468	68	-	0/9/27/28	0/3/3/3
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
68	PSU	S2	966	87,68	-	0/7/25/26	0/2/2/2
68	A2M	S2	1383	68	-	1/9/27/28	0/3/3/3
68	PSU	S2	651	68	-	0/7/25/26	0/2/2/2
3	A2M	L5	1534	87,3	-	1/9/27/28	0/3/3/3
3	OMU	L5	4498	3	-	1/9/27/28	0/2/2/2
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
3	A2M	L5	2815	3	-	2/9/27/28	0/3/3/3
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
68	OMG	S2	436	68	-	0/9/27/28	0/3/3/3
68	OMC	S2	1272	68	-	0/9/27/28	0/2/2/2
68	A2M	S2	99	87,68	-	2/9/27/28	0/3/3/3
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	668	87,68	-	2/9/27/28	0/3/3/3
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
68	OMG	S2	509	68	-	0/9/27/28	0/3/3/3
5	PSU	L8	69	5	-	1/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1781	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	MA6	S2	1850	68	-	0/11/29/30	0/3/3/3

All (330) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	1832	6MZ	C6-N6	12.63	1.48	1.34
3	L5	3818	UY1	C6-C5	12.21	1.48	1.35
3	L5	4220	6MZ	C6-N6	11.80	1.47	1.34
3	L5	3818	UY1	C2-N1	11.47	1.51	1.36
68	S2	799	OMU	C2-N1	8.70	1.52	1.38
68	S2	1288	OMU	C2-N1	8.23	1.51	1.38
68	S2	172	OMU	C2-N1	8.12	1.51	1.38
68	S2	116	OMU	C2-N1	8.07	1.51	1.38
68	S2	1248	B8N	C4-N3	-7.95	1.26	1.40
68	S2	627	OMU	C2-N1	7.93	1.50	1.38
68	S2	1442	OMU	C2-N1	7.91	1.50	1.38
68	S2	428	OMU	C2-N1	7.88	1.50	1.38
68	S2	1326	OMU	C2-N1	7.86	1.50	1.38
68	S2	121	OMU	C2-N1	7.75	1.50	1.38
68	S2	354	OMU	C2-N1	7.74	1.50	1.38
3	L5	2837	OMU	C2-N1	7.70	1.50	1.38
68	S2	1248	B8N	C6-N1	7.67	1.55	1.36
3	L5	4306	OMU	C2-N1	7.59	1.50	1.38
3	L5	3818	UY1	C2-N3	7.57	1.49	1.37
3	L5	4227	OMU	C2-N1	7.56	1.50	1.38
3	L5	4498	OMU	C2-N1	7.54	1.50	1.38
3	L5	3925	OMU	C2-N1	7.53	1.50	1.38
3	L5	4620	OMU	C2-N1	7.33	1.49	1.38
68	S2	116	OMU	C2-N3	6.89	1.50	1.38
68	S2	1442	OMU	C2-N3	6.88	1.49	1.38
68	S2	1248	B8N	C4-C5	6.87	1.63	1.47
68	S2	428	OMU	C2-N3	6.87	1.49	1.38
68	S2	172	OMU	C2-N3	6.85	1.49	1.38
68	S2	1288	OMU	C2-N3	6.81	1.49	1.38
68	S2	799	OMU	C2-N3	6.77	1.49	1.38
68	S2	627	OMU	C2-N3	6.73	1.49	1.38
68	S2	1326	OMU	C2-N3	6.61	1.49	1.38
68	S2	354	OMU	C2-N3	6.60	1.49	1.38
3	L5	2837	OMU	C2-N3	6.53	1.49	1.38
68	S2	121	OMU	C2-N3	6.51	1.49	1.38
68	S2	1639	G7M	C4-N3	6.49	1.49	1.34
3	L5	4306	OMU	C2-N3	6.40	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4498	OMU	C2-N3	6.38	1.49	1.38
3	L5	4620	OMU	C2-N3	6.33	1.49	1.38
3	L5	4227	OMU	C2-N3	6.27	1.48	1.38
3	L5	3925	OMU	C2-N3	6.26	1.48	1.38
3	L5	4530	UR3	C2-N1	6.17	1.47	1.38
3	L5	4530	UR3	C6-C5	6.09	1.49	1.35
68	S2	627	OMU	C6-C5	5.84	1.48	1.35
68	S2	799	OMU	C6-C5	5.84	1.48	1.35
68	S2	172	OMU	C6-C5	5.84	1.48	1.35
68	S2	428	OMU	C6-C5	5.83	1.48	1.35
68	S2	1248	B8N	C2-N1	5.81	1.56	1.39
3	L5	3925	OMU	O4-C4	-5.78	1.13	1.24
3	L5	4306	OMU	O4-C4	-5.77	1.13	1.24
68	S2	354	OMU	C6-C5	5.77	1.48	1.35
68	S2	1442	OMU	C6-C5	5.75	1.48	1.35
68	S2	121	OMU	C6-C5	5.74	1.48	1.35
68	S2	1326	OMU	C6-C5	5.73	1.48	1.35
68	S2	116	OMU	C6-C5	5.71	1.48	1.35
3	L5	4620	OMU	O4-C4	-5.70	1.13	1.24
3	L5	2837	OMU	C6-C5	5.67	1.48	1.35
68	S2	1288	OMU	C6-C5	5.66	1.48	1.35
3	L5	4227	OMU	O4-C4	-5.66	1.13	1.24
68	S2	1326	OMU	O4-C4	-5.59	1.13	1.24
3	L5	4498	OMU	O4-C4	-5.58	1.13	1.24
3	L5	4498	OMU	C6-C5	5.58	1.48	1.35
3	L5	4306	OMU	C6-C5	5.57	1.48	1.35
68	S2	799	OMU	O4-C4	-5.55	1.13	1.24
68	S2	354	OMU	O4-C4	-5.55	1.13	1.24
3	L5	4530	UR3	C2-N3	5.55	1.49	1.39
3	L5	2837	OMU	O4-C4	-5.54	1.13	1.24
68	S2	1442	OMU	O4-C4	-5.54	1.13	1.24
68	S2	121	OMU	O4-C4	-5.53	1.13	1.24
68	S2	116	OMU	O4-C4	-5.52	1.13	1.24
3	L5	4227	OMU	C6-C5	5.49	1.47	1.35
3	L5	3925	OMU	C6-C5	5.49	1.47	1.35
3	L5	4620	OMU	C6-C5	5.46	1.47	1.35
68	S2	172	OMU	O4-C4	-5.41	1.14	1.24
68	S2	1288	OMU	O4-C4	-5.41	1.14	1.24
68	S2	428	OMU	O4-C4	-5.41	1.14	1.24
68	S2	1639	G7M	C2-N3	5.35	1.46	1.33
68	S2	627	OMU	O4-C4	-5.35	1.14	1.24
3	L5	3818	UY1	C6-N1	5.27	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	1248	B8N	C6-C5	5.05	1.42	1.35
68	S2	1639	G7M	C5-N7	-4.99	1.33	1.39
68	S2	1639	G7M	C2-N2	4.96	1.45	1.34
68	S2	627	OMU	C4-N3	4.39	1.46	1.38
68	S2	1442	OMU	C4-N3	4.39	1.46	1.38
68	S2	428	OMU	C4-N3	4.37	1.46	1.38
68	S2	116	OMU	C4-N3	4.32	1.46	1.38
68	S2	1288	OMU	C4-N3	4.32	1.46	1.38
3	L5	3818	UY1	C4-N3	4.31	1.46	1.38
68	S2	172	OMU	C4-N3	4.18	1.45	1.38
68	S2	354	OMU	C4-N3	4.15	1.45	1.38
68	S2	799	OMU	C4-N3	4.13	1.45	1.38
68	S2	1326	OMU	C4-N3	4.11	1.45	1.38
68	S2	121	OMU	C4-N3	4.03	1.45	1.38
3	L5	2837	OMU	C4-N3	3.97	1.45	1.38
3	L5	4498	OMU	C4-N3	3.95	1.45	1.38
3	L5	4227	OMU	C4-N3	3.92	1.45	1.38
3	L5	3818	UY1	O4-C4	-3.80	1.16	1.23
3	L5	4306	OMU	C4-N3	3.78	1.45	1.38
68	S2	1045	PSU	C6-C5	3.76	1.39	1.35
68	S2	1639	G7M	C5-C6	3.73	1.53	1.43
3	L5	3825	A2M	O5'-C5'	-3.73	1.33	1.44
3	L5	3830	A2M	O5'-C5'	-3.69	1.33	1.44
3	L5	3925	OMU	C4-N3	3.69	1.44	1.38
68	S2	801	PSU	C6-C5	3.67	1.39	1.35
3	L5	3785	A2M	O5'-C5'	-3.66	1.33	1.44
68	S2	866	PSU	C6-C5	3.63	1.39	1.35
3	L5	1871	A2M	O5'-C5'	-3.59	1.33	1.44
3	L5	400	A2M	O5'-C5'	-3.58	1.33	1.44
68	S2	27	A2M	O5'-C5'	-3.58	1.33	1.44
3	L5	4523	A2M	O5'-C5'	-3.58	1.33	1.44
3	L5	4620	OMU	C4-N3	3.57	1.44	1.38
3	L5	4571	A2M	O5'-C5'	-3.57	1.33	1.44
68	S2	668	A2M	O5'-C5'	-3.53	1.33	1.44
3	L5	2363	A2M	O5'-C5'	-3.52	1.33	1.44
68	S2	863	PSU	C6-C5	3.51	1.39	1.35
68	S2	1031	A2M	O5'-C5'	-3.51	1.34	1.44
68	S2	1248	B8N	C1'-C5	3.50	1.58	1.50
68	S2	966	PSU	C6-C5	3.50	1.39	1.35
3	L5	1524	A2M	O5'-C5'	-3.49	1.34	1.44
3	L5	2815	A2M	O5'-C5'	-3.49	1.34	1.44
3	L5	1323	A2M	O5'-C5'	-3.48	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	1056	PSU	C6-C5	3.47	1.39	1.35
3	L5	4220	6MZ	C5-N7	-3.46	1.32	1.39
3	L5	3867	A2M	O5'-C5'	-3.45	1.34	1.44
68	S2	99	A2M	O5'-C5'	-3.45	1.34	1.44
3	L5	4220	6MZ	C5-C4	-3.45	1.32	1.39
68	S2	484	A2M	O5'-C5'	-3.44	1.34	1.44
68	S2	93	PSU	C6-C5	3.42	1.39	1.35
68	S2	686	PSU	C6-C5	3.41	1.39	1.35
3	L5	3844	PSU	C6-C5	3.40	1.39	1.35
68	S2	468	A2M	O5'-C5'	-3.40	1.34	1.44
3	L5	2787	A2M	O5'-C5'	-3.40	1.34	1.44
3	L5	1326	A2M	O5'-C5'	-3.40	1.34	1.44
3	L5	398	A2M	O5'-C5'	-3.39	1.34	1.44
68	S2	651	PSU	C6-C5	3.38	1.39	1.35
68	S2	814	PSU	C6-C5	3.37	1.39	1.35
3	L5	1677	PSU	C6-C5	3.37	1.39	1.35
3	L5	2401	A2M	O5'-C5'	-3.36	1.34	1.44
3	L5	3718	A2M	O5'-C5'	-3.36	1.34	1.44
68	S2	406	PSU	C6-C5	3.36	1.39	1.35
68	S2	668	A2M	O4'-C4'	-3.35	1.37	1.45
68	S2	1383	A2M	O5'-C5'	-3.35	1.34	1.44
68	S2	1244	PSU	C6-C5	3.34	1.39	1.35
3	L5	4590	A2M	O5'-C5'	-3.33	1.34	1.44
68	S2	166	A2M	O5'-C5'	-3.33	1.34	1.44
68	S2	1046	PSU	C6-C5	3.32	1.39	1.35
68	S2	1367	PSU	C6-C5	3.32	1.39	1.35
3	L5	1782	PSU	C6-C5	3.31	1.39	1.35
68	S2	649	PSU	C6-C5	3.31	1.39	1.35
68	S2	1177	PSU	C6-C5	3.30	1.38	1.35
68	S2	109	PSU	C6-C5	3.30	1.38	1.35
3	L5	5010	PSU	C6-C5	3.30	1.38	1.35
68	S2	1004	PSU	C6-C5	3.29	1.38	1.35
3	L5	3818	UY1	O2-C2	-3.27	1.16	1.23
68	S2	1832	6MZ	C5-N7	-3.26	1.33	1.39
68	S2	576	A2M	O5'-C5'	-3.26	1.34	1.44
5	L8	55	PSU	C6-C5	3.24	1.38	1.35
3	L5	4552	PSU	C6-C5	3.24	1.38	1.35
3	L5	4493	PSU	C6-C5	3.23	1.38	1.35
3	L5	4312	PSU	C6-C5	3.22	1.38	1.35
3	L5	4532	PSU	C6-C5	3.21	1.38	1.35
3	L5	1860	PSU	C6-C5	3.21	1.38	1.35
68	S2	1081	PSU	C6-C5	3.19	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4431	PSU	C6-C5	3.19	1.38	1.35
3	L5	4576	PSU	C6-C5	3.19	1.38	1.35
3	L5	4353	PSU	C6-C5	3.17	1.38	1.35
3	L5	2632	PSU	C6-C5	3.16	1.38	1.35
3	L5	4296	PSU	C6-C5	3.16	1.38	1.35
3	L5	4972	PSU	C6-C5	3.16	1.38	1.35
68	S2	1851	MA6	C6-N6	3.15	1.45	1.36
3	L5	4571	A2M	O4'-C4'	-3.14	1.38	1.45
68	S2	105	PSU	C6-C5	3.13	1.38	1.35
68	S2	1232	PSU	C6-C5	3.13	1.38	1.35
3	L5	3637	PSU	C6-C5	3.12	1.38	1.35
3	L5	4471	PSU	C6-C5	3.11	1.38	1.35
3	L5	3818	UY1	C1'-C5	3.11	1.57	1.50
3	L5	1534	A2M	O5'-C5'	-3.11	1.35	1.44
5	L8	69	PSU	C6-C5	3.11	1.38	1.35
68	S2	1174	PSU	C6-C5	3.10	1.38	1.35
3	L5	1781	PSU	C6-C5	3.09	1.38	1.35
68	S2	1850	MA6	C6-N6	3.08	1.45	1.36
3	L5	5001	PSU	C6-C5	3.06	1.38	1.35
3	L5	1862	PSU	C6-C5	3.05	1.38	1.35
68	S2	1832	6MZ	C5-C4	-3.05	1.33	1.39
3	L5	3822	PSU	C6-C5	3.05	1.38	1.35
3	L5	4442	PSU	C6-C5	3.05	1.38	1.35
3	L5	4973	PSU	C6-C5	3.04	1.38	1.35
3	L5	4293	PSU	C6-C5	3.03	1.38	1.35
3	L5	4220	6MZ	C8-N9	-3.03	1.32	1.37
3	L5	3853	PSU	C6-C5	3.02	1.38	1.35
68	S2	159	A2M	O5'-C5'	-3.02	1.35	1.44
3	L5	4636	PSU	C6-C5	3.01	1.38	1.35
3	L5	4500	PSU	C6-C5	3.01	1.38	1.35
3	L5	3695	PSU	C6-C5	3.00	1.38	1.35
3	L5	1323	A2M	O4'-C4'	-2.98	1.38	1.45
3	L5	1582	PSU	C6-C5	2.96	1.38	1.35
3	L5	4521	PSU	C6-C5	2.94	1.38	1.35
68	S2	627	OMU	C5-C4	2.94	1.50	1.43
68	S2	1832	6MZ	C8-N9	-2.93	1.32	1.37
3	L5	4579	PSU	C6-C5	2.92	1.38	1.35
3	L5	1524	A2M	O4'-C4'	-2.92	1.38	1.45
3	L5	1536	PSU	C6-C5	2.92	1.38	1.35
3	L5	4673	PSU	C6-C5	2.91	1.38	1.35
3	L5	4628	PSU	C6-C5	2.91	1.38	1.35
3	L5	4403	PSU	C6-C5	2.89	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2839	PSU	C6-C5	2.89	1.38	1.35
3	L5	4689	PSU	C6-C5	2.86	1.38	1.35
3	L5	3639	PSU	C6-C5	2.85	1.38	1.35
3	L5	3920	PSU	C6-C5	2.85	1.38	1.35
3	L5	3884	PSU	C6-C5	2.84	1.38	1.35
3	L5	4299	PSU	C6-C5	2.84	1.38	1.35
3	L5	1744	PSU	C6-C5	2.83	1.38	1.35
3	L5	1792	PSU	C6-C5	2.80	1.38	1.35
68	S2	1639	G7M	C2-N1	2.80	1.44	1.37
68	S2	428	OMU	C5-C4	2.79	1.49	1.43
3	L5	1683	PSU	C6-C5	2.79	1.38	1.35
68	S2	1442	OMU	C5-C4	2.77	1.49	1.43
3	L5	3851	PSU	C6-C5	2.77	1.38	1.35
3	L5	4457	PSU	C6-C5	2.76	1.38	1.35
3	L5	4530	UR3	O2-C2	-2.75	1.17	1.22
68	S2	172	OMU	C5-C4	2.73	1.49	1.43
68	S2	799	OMU	C5-C4	2.73	1.49	1.43
3	L5	4361	PSU	C6-C5	2.73	1.38	1.35
3	L5	4498	OMU	C5-C4	2.69	1.49	1.43
68	S2	1326	OMU	C5-C4	2.69	1.49	1.43
68	S2	1288	OMU	C5-C4	2.68	1.49	1.43
68	S2	354	OMU	C5-C4	2.68	1.49	1.43
68	S2	1639	G7M	O6-C6	-2.64	1.18	1.23
3	L5	2363	A2M	O4'-C4'	-2.63	1.39	1.45
68	S2	681	PSU	C6-C5	2.61	1.38	1.35
3	L5	3867	A2M	O4'-C4'	-2.61	1.39	1.45
3	L5	2837	OMU	C5-C4	2.59	1.49	1.43
3	L5	4220	6MZ	C6-N1	-2.59	1.30	1.35
68	S2	428	OMU	C6-N1	2.58	1.44	1.38
68	S2	121	OMU	C5-C4	2.58	1.49	1.43
68	S2	1288	OMU	C6-N1	2.57	1.44	1.38
3	L5	1871	A2M	O4'-C4'	-2.56	1.39	1.45
68	S2	1442	OMU	C6-N1	2.55	1.44	1.38
68	S2	799	OMU	C6-N1	2.55	1.44	1.38
68	S2	116	OMU	C5-C4	2.53	1.49	1.43
3	L5	4227	OMU	C5-C4	2.52	1.49	1.43
68	S2	172	OMU	C6-N1	2.52	1.44	1.38
3	L5	4523	A2M	O4'-C4'	-2.52	1.39	1.45
68	S2	354	OMU	C6-N1	2.51	1.44	1.38
3	L5	4306	OMU	C6-N1	2.49	1.44	1.38
68	S2	627	OMU	C6-N1	2.49	1.44	1.38
68	S2	1326	OMU	C6-N1	2.48	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	1639	G7M	C6-N1	2.48	1.43	1.38
3	L5	1534	A2M	O4'-C4'	-2.47	1.39	1.45
3	L5	400	A2M	O4'-C4'	-2.46	1.39	1.45
3	L5	4498	OMU	C6-N1	2.46	1.44	1.38
3	L5	2837	OMU	C6-N1	2.45	1.43	1.38
3	L5	1326	A2M	O4'-C4'	-2.45	1.39	1.45
68	S2	1851	MA6	C5-C4	-2.43	1.34	1.39
68	S2	121	OMU	C6-N1	2.43	1.43	1.38
3	L5	3925	OMU	C5-C4	2.41	1.48	1.43
3	L5	1871	A2M	O3'-C3'	-2.41	1.37	1.43
3	L5	1323	A2M	O3'-C3'	-2.40	1.37	1.43
68	S2	1850	MA6	C5-C4	-2.40	1.34	1.39
3	L5	4447	5MC	C5-C4	-2.38	1.42	1.44
68	S2	116	OMU	C6-N1	2.37	1.43	1.38
3	L5	3884	PSU	C4-C5	-2.37	1.37	1.44
3	L5	4447	5MC	C4-N3	-2.33	1.30	1.34
3	L5	4620	OMU	C5-C4	2.33	1.48	1.43
3	L5	4306	OMU	C5-C4	2.32	1.48	1.43
3	L5	4227	OMU	C6-N1	2.30	1.43	1.38
3	L5	4620	OMU	C6-N1	2.29	1.43	1.38
3	L5	4571	A2M	O3'-C3'	-2.28	1.37	1.43
3	L5	4530	UR3	C6-N1	2.28	1.43	1.38
3	L5	3825	A2M	O4'-C4'	-2.27	1.39	1.45
3	L5	3925	OMU	C6-N1	2.27	1.43	1.38
68	S2	1832	6MZ	C6-N1	-2.27	1.31	1.35
3	L5	4590	A2M	O3'-C3'	-2.26	1.37	1.43
3	L5	2815	A2M	O4'-C4'	-2.25	1.40	1.45
3	L5	3639	PSU	C4-C5	-2.23	1.38	1.44
3	L5	2839	PSU	C4-C5	-2.23	1.38	1.44
3	L5	4403	PSU	C4-C5	-2.23	1.38	1.44
3	L5	3920	PSU	C4-C5	-2.23	1.38	1.44
68	S2	1639	G7M	C4-N9	-2.23	1.32	1.38
3	L5	4689	PSU	C4-C5	-2.21	1.38	1.44
3	L5	4353	PSU	C4-C5	-2.21	1.38	1.44
3	L5	3818	UY1	O4'-C1'	-2.20	1.40	1.43
3	L5	4628	PSU	C4-C5	-2.19	1.38	1.44
3	L5	4552	PSU	C4-C5	-2.19	1.38	1.44
3	L5	1524	A2M	O3'-C3'	-2.19	1.37	1.43
3	L5	4590	A2M	O4'-C4'	-2.19	1.40	1.45
3	L5	4521	PSU	C4-C5	-2.18	1.38	1.44
3	L5	3695	PSU	C4-C5	-2.18	1.38	1.44
3	L5	4500	PSU	C4-C5	-2.15	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4293	PSU	C4-C5	-2.15	1.38	1.44
3	L5	4636	PSU	C4-C5	-2.14	1.38	1.44
3	L5	4457	PSU	C4-C5	-2.13	1.38	1.44
68	S2	1177	PSU	C4-C5	-2.13	1.38	1.44
3	L5	4296	PSU	C4-C5	-2.13	1.38	1.44
5	L8	55	PSU	C4-C5	-2.12	1.38	1.44
3	L5	4530	UR3	C5-C4	2.12	1.49	1.43
68	S2	1174	PSU	C4-C5	-2.12	1.38	1.44
3	L5	4530	UR3	C3U-N3	2.12	1.50	1.47
3	L5	1744	PSU	C4-C5	-2.12	1.38	1.44
3	L5	4579	PSU	C4-C5	-2.11	1.38	1.44
3	L5	4457	PSU	O4'-C1'	-2.11	1.40	1.43
3	L5	3851	PSU	C4-C5	-2.11	1.38	1.44
68	S2	406	PSU	C4-C5	-2.10	1.38	1.44
3	L5	4673	PSU	C4-C5	-2.10	1.38	1.44
68	S2	484	A2M	O4'-C4'	-2.09	1.40	1.45
3	L5	1683	PSU	C4-C5	-2.09	1.38	1.44
3	L5	4471	PSU	C4-C5	-2.09	1.38	1.44
3	L5	2351	OMC	C4-N3	-2.09	1.30	1.34
68	S2	649	PSU	C4-C5	-2.09	1.38	1.44
3	L5	1536	PSU	C4-C5	-2.08	1.38	1.44
3	L5	398	A2M	O4'-C4'	-2.07	1.40	1.45
3	L5	2363	A2M	O3'-C3'	-2.07	1.37	1.43
3	L5	3718	A2M	O4'-C4'	-2.07	1.40	1.45
68	S2	681	PSU	C4-C5	-2.07	1.38	1.44
3	L5	2401	A2M	O4'-C4'	-2.06	1.40	1.45
3	L5	4576	PSU	C4-C5	-2.06	1.38	1.44
3	L5	4973	PSU	C4-C5	-2.06	1.38	1.44
68	S2	1367	PSU	C4-C5	-2.06	1.38	1.44
3	L5	4220	6MZ	C4-N9	-2.05	1.33	1.37
3	L5	1582	PSU	C4-C5	-2.05	1.38	1.44
3	L5	4312	PSU	C4-C5	-2.05	1.38	1.44
3	L5	3808	OMC	C4-N3	-2.04	1.30	1.34
3	L5	4299	PSU	C4-C5	-2.04	1.38	1.44
3	L5	1860	PSU	C4-C5	-2.03	1.38	1.44
3	L5	1677	PSU	O4'-C1'	-2.02	1.41	1.43
3	L5	3822	PSU	C4-C5	-2.02	1.38	1.44
3	L5	5010	PSU	C4-C5	-2.02	1.38	1.44
3	L5	1781	PSU	C4-C5	-2.01	1.38	1.44
68	S2	1851	MA6	C5-N7	-2.01	1.35	1.39
3	L5	4431	PSU	C4-C5	-2.00	1.38	1.44

All (688) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1850	MA6	N1-C6-N6	-12.18	102.02	116.86
68	S2	1851	MA6	N1-C6-N6	-11.97	102.27	116.86
68	S2	1850	MA6	C5-C6-N6	8.04	138.05	125.33
68	S2	1851	MA6	C5-C6-N6	7.98	137.97	125.33
68	S2	1639	G7M	C1'-N9-C4	7.40	148.35	126.49
68	S2	1639	G7M	C1'-N9-C8	-7.28	102.16	126.74
3	L5	4498	OMU	C4-N3-C2	-6.21	118.90	126.61
3	L5	2837	OMU	C4-N3-C2	-5.86	119.33	126.61
3	L5	4220	6MZ	N1-C2-N3	-5.83	119.75	128.58
68	S2	1326	OMU	C4-N3-C2	-5.81	119.39	126.61
3	L5	4227	OMU	C4-N3-C2	-5.79	119.42	126.61
68	S2	627	OMU	C4-N3-C2	-5.79	119.43	126.61
3	L5	3925	OMU	C4-N3-C2	-5.71	119.53	126.61
3	L5	4530	UR3	C4-N3-C2	-5.71	119.99	124.58
68	S2	1832	6MZ	N1-C2-N3	-5.70	119.95	128.58
68	S2	1850	MA6	N1-C2-N3	-5.65	120.03	128.58
68	S2	1442	OMU	C4-N3-C2	-5.58	119.69	126.61
68	S2	1851	MA6	N1-C2-N3	-5.57	120.15	128.58
68	S2	428	OMU	C4-N3-C2	-5.57	119.70	126.61
68	S2	799	OMU	C4-N3-C2	-5.56	119.70	126.61
3	L5	3637	PSU	N1-C2-N3	5.53	121.00	115.17
68	S2	354	OMU	C4-N3-C2	-5.53	119.75	126.61
68	S2	172	OMU	C4-N3-C2	-5.41	119.90	126.61
3	L5	4220	6MZ	C9-N6-C6	-5.40	117.84	122.85
3	L5	4636	PSU	C4-N3-C2	-5.39	118.95	126.37
3	L5	1582	PSU	C4-N3-C2	-5.32	119.05	126.37
68	S2	1850	MA6	N9-C8-N7	-5.30	106.41	113.94
3	L5	4306	OMU	C4-N3-C2	-5.27	120.07	126.61
3	L5	4457	PSU	N1-C2-N3	5.27	120.73	115.17
3	L5	1677	PSU	N1-C2-N3	5.23	120.69	115.17
3	L5	1677	PSU	C4-N3-C2	-5.23	119.16	126.37
3	L5	4457	PSU	C4-N3-C2	-5.23	119.17	126.37
3	L5	4620	OMU	C4-N3-C2	-5.23	120.12	126.61
3	L5	4296	PSU	N1-C2-N3	5.19	120.65	115.17
3	L5	4521	PSU	N1-C2-N3	5.16	120.61	115.17
68	S2	1851	MA6	N9-C8-N7	-5.15	106.62	113.94
3	L5	1582	PSU	N1-C2-N3	5.13	120.58	115.17
3	L5	4636	PSU	N1-C2-N3	5.13	120.58	115.17
68	S2	1248	B8N	C5-C4-N3	5.13	125.46	116.15
3	L5	3695	PSU	C4-N3-C2	-5.12	119.32	126.37
3	L5	4500	PSU	N1-C2-N3	5.12	120.57	115.17
3	L5	4628	PSU	C4-N3-C2	-5.11	119.34	126.37
3	L5	4532	PSU	N1-C2-N3	5.11	120.55	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1288	OMU	C4-N3-C2	-5.10	120.28	126.61
3	L5	4500	PSU	C4-N3-C2	-5.10	119.35	126.37
3	L5	3822	PSU	N1-C2-N3	5.08	120.52	115.17
68	S2	105	PSU	N1-C2-N3	5.08	120.52	115.17
3	L5	4552	PSU	C4-N3-C2	-5.07	119.38	126.37
68	S2	866	PSU	N1-C2-N3	5.07	120.52	115.17
3	L5	4521	PSU	C4-N3-C2	-5.07	119.39	126.37
3	L5	1683	PSU	N1-C2-N3	5.06	120.51	115.17
68	S2	116	OMU	C4-N3-C2	-5.06	120.33	126.61
68	S2	1232	PSU	C4-N3-C2	-5.05	119.41	126.37
68	S2	1177	PSU	N1-C2-N3	5.05	120.50	115.17
3	L5	4296	PSU	C4-N3-C2	-5.05	119.42	126.37
68	S2	814	PSU	C4-N3-C2	-5.05	119.42	126.37
3	L5	3920	PSU	N1-C2-N3	5.04	120.49	115.17
3	L5	3637	PSU	C4-N3-C2	-5.04	119.43	126.37
3	L5	4579	PSU	N1-C2-N3	5.03	120.47	115.17
68	S2	866	PSU	C4-N3-C2	-5.02	119.45	126.37
3	L5	1683	PSU	C4-N3-C2	-5.01	119.47	126.37
3	L5	4552	PSU	N1-C2-N3	5.00	120.45	115.17
3	L5	4442	PSU	N1-C2-N3	5.00	120.44	115.17
68	S2	1177	PSU	C4-N3-C2	-5.00	119.49	126.37
3	L5	4972	PSU	C4-N3-C2	-4.99	119.50	126.37
3	L5	4353	PSU	N1-C2-N3	4.97	120.41	115.17
3	L5	5001	PSU	N1-C2-N3	4.97	120.41	115.17
68	S2	863	PSU	N1-C2-N3	4.97	120.41	115.17
68	S2	1232	PSU	N1-C2-N3	4.95	120.39	115.17
5	L8	69	PSU	N1-C2-N3	4.95	120.39	115.17
68	S2	109	PSU	C4-N3-C2	-4.95	119.56	126.37
68	S2	1056	PSU	C4-N3-C2	-4.94	119.56	126.37
3	L5	3884	PSU	N1-C2-N3	4.94	120.38	115.17
68	S2	651	PSU	C4-N3-C2	-4.94	119.57	126.37
3	L5	4403	PSU	N1-C2-N3	4.93	120.37	115.17
3	L5	3851	PSU	C4-N3-C2	-4.93	119.58	126.37
3	L5	4972	PSU	N1-C2-N3	4.93	120.37	115.17
3	L5	4442	PSU	C4-N3-C2	-4.93	119.58	126.37
3	L5	3639	PSU	N1-C2-N3	4.93	120.36	115.17
3	L5	4431	PSU	C4-N3-C2	-4.93	119.59	126.37
3	L5	3822	PSU	C4-N3-C2	-4.92	119.59	126.37
68	S2	1081	PSU	C4-N3-C2	-4.92	119.59	126.37
68	S2	105	PSU	C4-N3-C2	-4.92	119.59	126.37
3	L5	4293	PSU	C4-N3-C2	-4.92	119.60	126.37
3	L5	4471	PSU	N1-C2-N3	4.91	120.35	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	651	PSU	N1-C2-N3	4.91	120.34	115.17
3	L5	5001	PSU	C4-N3-C2	-4.90	119.62	126.37
3	L5	3844	PSU	N1-C2-N3	4.90	120.34	115.17
3	L5	3818	UY1	C4-N3-C2	-4.90	119.62	126.37
3	L5	1782	PSU	N1-C2-N3	4.90	120.33	115.17
3	L5	4628	PSU	N1-C2-N3	4.90	120.33	115.17
3	L5	2632	PSU	N1-C2-N3	4.90	120.33	115.17
3	L5	3695	PSU	N1-C2-N3	4.90	120.33	115.17
3	L5	3920	PSU	C4-N3-C2	-4.90	119.63	126.37
68	S2	1244	PSU	C4-N3-C2	-4.88	119.64	126.37
68	S2	1056	PSU	N1-C2-N3	4.88	120.32	115.17
68	S2	1244	PSU	N1-C2-N3	4.88	120.31	115.17
3	L5	4403	PSU	C4-N3-C2	-4.87	119.66	126.37
3	L5	3853	PSU	N1-C2-N3	4.87	120.31	115.17
3	L5	4689	PSU	N1-C2-N3	4.87	120.31	115.17
3	L5	1744	PSU	N1-C2-N3	4.87	120.30	115.17
68	S2	1045	PSU	N1-C2-N3	4.87	120.30	115.17
3	L5	4973	PSU	N1-C2-N3	4.87	120.30	115.17
5	L8	69	PSU	C4-N3-C2	-4.87	119.67	126.37
3	L5	1792	PSU	C4-N3-C2	-4.86	119.68	126.37
3	L5	1862	PSU	C4-N3-C2	-4.86	119.68	126.37
3	L5	1782	PSU	C4-N3-C2	-4.86	119.68	126.37
3	L5	4431	PSU	N1-C2-N3	4.86	120.29	115.17
68	S2	1004	PSU	N1-C2-N3	4.86	120.29	115.17
68	S2	1367	PSU	N1-C2-N3	4.85	120.28	115.17
3	L5	4361	PSU	C4-N3-C2	-4.84	119.70	126.37
3	L5	4579	PSU	C4-N3-C2	-4.84	119.71	126.37
3	L5	3884	PSU	C4-N3-C2	-4.84	119.71	126.37
3	L5	4532	PSU	C4-N3-C2	-4.84	119.71	126.37
3	L5	1536	PSU	N1-C2-N3	4.84	120.27	115.17
68	S2	686	PSU	C4-N3-C2	-4.82	119.72	126.37
68	S2	686	PSU	N1-C2-N3	4.82	120.25	115.17
68	S2	1367	PSU	C4-N3-C2	-4.82	119.74	126.37
68	S2	1174	PSU	C4-N3-C2	-4.81	119.74	126.37
3	L5	2839	PSU	N1-C2-N3	4.80	120.23	115.17
3	L5	4361	PSU	N1-C2-N3	4.80	120.23	115.17
3	L5	4493	PSU	C4-N3-C2	-4.80	119.76	126.37
68	S2	1851	MA6	C5-C4-N3	-4.79	120.12	126.72
3	L5	1536	PSU	C4-N3-C2	-4.79	119.78	126.37
3	L5	3851	PSU	N1-C2-N3	4.79	120.22	115.17
68	S2	406	PSU	C4-N3-C2	-4.79	119.78	126.37
3	L5	5010	PSU	N1-C2-N3	4.78	120.21	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1860	PSU	N1-C2-N3	4.78	120.20	115.17
68	S2	863	PSU	C4-N3-C2	-4.77	119.79	126.37
3	L5	2632	PSU	C4-N3-C2	-4.77	119.80	126.37
3	L5	4973	PSU	C4-N3-C2	-4.77	119.80	126.37
68	S2	1174	PSU	N1-C2-N3	4.76	120.19	115.17
3	L5	3639	PSU	C4-N3-C2	-4.75	119.83	126.37
3	L5	1862	PSU	N1-C2-N3	4.75	120.18	115.17
3	L5	4673	PSU	N1-C2-N3	4.75	120.18	115.17
3	L5	4293	PSU	N1-C2-N3	4.75	120.18	115.17
3	L5	1792	PSU	N1-C2-N3	4.74	120.17	115.17
3	L5	1781	PSU	N1-C2-N3	4.74	120.17	115.17
68	S2	1832	6MZ	N9-C8-N7	-4.74	107.22	113.94
68	S2	1081	PSU	N1-C2-N3	4.73	120.16	115.17
3	L5	2839	PSU	C4-N3-C2	-4.73	119.85	126.37
68	S2	814	PSU	N1-C2-N3	4.73	120.15	115.17
3	L5	4299	PSU	C4-N3-C2	-4.72	119.86	126.37
3	L5	4471	PSU	C4-N3-C2	-4.72	119.87	126.37
3	L5	1744	PSU	C4-N3-C2	-4.72	119.88	126.37
68	S2	681	PSU	C4-N3-C2	-4.71	119.88	126.37
68	S2	649	PSU	N1-C2-N3	4.71	120.14	115.17
68	S2	109	PSU	N1-C2-N3	4.71	120.14	115.17
68	S2	406	PSU	N1-C2-N3	4.71	120.13	115.17
3	L5	1781	PSU	C4-N3-C2	-4.70	119.90	126.37
68	S2	121	OMU	C4-N3-C2	-4.70	120.78	126.61
3	L5	4493	PSU	N1-C2-N3	4.69	120.12	115.17
68	S2	681	PSU	N1-C2-N3	4.68	120.11	115.17
3	L5	4673	PSU	C4-N3-C2	-4.68	119.92	126.37
68	S2	1046	PSU	N1-C2-N3	4.68	120.10	115.17
3	L5	4353	PSU	C4-N3-C2	-4.68	119.93	126.37
3	L5	5010	PSU	C4-N3-C2	-4.66	119.95	126.37
3	L5	4576	PSU	C4-N3-C2	-4.66	119.95	126.37
68	S2	1639	G7M	C2-N3-C4	4.66	120.33	112.30
5	L8	55	PSU	N1-C2-N3	4.65	120.07	115.17
3	L5	4576	PSU	N1-C2-N3	4.65	120.07	115.17
3	L5	1860	PSU	C4-N3-C2	-4.62	120.01	126.37
3	L5	3844	PSU	C4-N3-C2	-4.62	120.01	126.37
3	L5	4312	PSU	C4-N3-C2	-4.61	120.02	126.37
68	S2	966	PSU	N1-C2-N3	4.61	120.03	115.17
3	L5	3853	PSU	C4-N3-C2	-4.60	120.03	126.37
68	S2	1045	PSU	C4-N3-C2	-4.59	120.04	126.37
68	S2	93	PSU	C4-N3-C2	-4.59	120.05	126.37
3	L5	4220	6MZ	C5-C4-N3	-4.59	120.40	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1004	PSU	C4-N3-C2	-4.56	120.09	126.37
68	S2	801	PSU	N1-C2-N3	4.55	119.97	115.17
3	L5	4220	6MZ	N9-C8-N7	-4.55	107.48	113.94
3	L5	4312	PSU	N1-C2-N3	4.54	119.95	115.17
68	S2	649	PSU	C4-N3-C2	-4.54	120.12	126.37
68	S2	1832	6MZ	C5-C4-N3	-4.53	120.47	126.72
5	L8	55	PSU	C4-N3-C2	-4.53	120.13	126.37
3	L5	4299	PSU	N1-C2-N3	4.52	119.94	115.17
68	S2	966	PSU	C4-N3-C2	-4.51	120.16	126.37
68	S2	93	PSU	N1-C2-N3	4.48	119.89	115.17
68	S2	1046	PSU	C4-N3-C2	-4.47	120.21	126.37
3	L5	4689	PSU	C4-N3-C2	-4.44	120.25	126.37
68	S2	1850	MA6	C5-C4-N3	-4.43	120.62	126.72
3	L5	4498	OMU	N3-C2-N1	4.29	120.47	114.89
68	S2	801	PSU	C4-N3-C2	-4.20	120.58	126.37
68	S2	1248	B8N	C4-N3-C2	-4.20	120.46	125.62
68	S2	1850	MA6	C4-N9-C8	4.11	110.05	105.74
68	S2	1639	G7M	C5-C6-N1	4.10	120.32	111.84
3	L5	1871	A2M	C3'-C2'-C1'	-4.10	94.96	102.81
68	S2	1248	B8N	C1'-C5-C4	4.09	123.81	117.61
3	L5	3818	UY1	N1-C2-N3	4.09	119.48	115.17
68	S2	799	OMU	N3-C2-N1	4.03	120.14	114.89
68	S2	1639	G7M	C5-C4-N3	-4.03	120.54	128.15
3	L5	2837	OMU	N3-C2-N1	3.97	120.06	114.89
3	L5	3830	A2M	C3'-C2'-C1'	-3.95	95.25	102.81
3	L5	4498	OMU	C5-C4-N3	3.94	120.31	114.80
3	L5	3718	A2M	C3'-C2'-C1'	-3.90	95.33	102.81
3	L5	4523	A2M	C3'-C2'-C1'	-3.90	95.34	102.81
3	L5	4227	OMU	C5-C4-N3	3.87	120.22	114.80
3	L5	4620	OMU	N3-C2-N1	3.86	119.92	114.89
68	S2	1326	OMU	N3-C2-N1	3.86	119.91	114.89
3	L5	3925	OMU	N3-C2-N1	3.84	119.89	114.89
68	S2	1851	MA6	C4-C5-C6	3.83	119.87	115.91
68	S2	1326	OMU	C5-C4-N3	3.83	120.17	114.80
68	S2	1442	OMU	N3-C2-N1	3.83	119.88	114.89
68	S2	428	OMU	N3-C2-N1	3.82	119.86	114.89
68	S2	627	OMU	N3-C2-N1	3.81	119.85	114.89
3	L5	3925	OMU	C5-C4-N3	3.81	120.14	114.80
3	L5	4227	OMU	N3-C2-N1	3.78	119.81	114.89
3	L5	2837	OMU	C5-C4-N3	3.77	120.08	114.80
68	S2	354	OMU	N3-C2-N1	3.75	119.77	114.89
3	L5	398	A2M	C3'-C2'-C1'	-3.74	95.64	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1851	MA6	C4-N9-C8	3.74	109.67	105.74
3	L5	4530	UR3	C5-C4-N3	3.73	119.95	115.04
3	L5	4306	OMU	C5-C4-N3	3.72	120.02	114.80
68	S2	99	A2M	C3'-C2'-C1'	-3.72	95.68	102.81
3	L5	4571	A2M	C3'-C2'-C1'	-3.72	95.68	102.81
3	L5	4590	A2M	C3'-C2'-C1'	-3.67	95.78	102.81
3	L5	4306	OMU	N3-C2-N1	3.64	119.63	114.89
68	S2	627	OMU	C5-C4-N3	3.64	119.90	114.80
68	S2	354	OMU	C5-C4-N3	3.63	119.89	114.80
68	S2	116	OMU	N3-C2-N1	3.62	119.60	114.89
68	S2	172	OMU	N3-C2-N1	3.60	119.58	114.89
68	S2	1288	OMU	C5-C4-N3	3.60	119.84	114.80
68	S2	1442	OMU	C5-C4-N3	3.59	119.83	114.80
3	L5	3825	A2M	C3'-C2'-C1'	-3.57	95.97	102.81
68	S2	1850	MA6	C2-N1-C6	3.53	120.46	111.83
68	S2	799	OMU	C5-C4-N3	3.53	119.75	114.80
68	S2	428	OMU	C5-C4-N3	3.53	119.75	114.80
68	S2	1639	G7M	O6-C6-C5	-3.49	120.21	128.01
68	S2	1851	MA6	C2-N1-C6	3.48	120.33	111.83
68	S2	121	OMU	C5-C4-N3	3.47	119.65	114.80
3	L5	398	A2M	O3'-C3'-C2'	3.46	120.87	111.19
3	L5	4620	OMU	C5-C4-N3	3.43	119.61	114.80
3	L5	4689	PSU	C6-N1-C2	-3.43	119.51	122.69
68	S2	1851	MA6	N3-C4-N9	3.43	133.00	127.17
68	S2	1031	A2M	C3'-C2'-C1'	-3.42	96.25	102.81
68	S2	1832	6MZ	C2-N3-C4	3.41	120.16	111.83
68	S2	116	OMU	C5-C4-N3	3.39	119.55	114.80
3	L5	4220	6MZ	C2-N3-C4	3.39	120.11	111.83
68	S2	1832	6MZ	C5-N7-C8	3.38	108.76	103.45
68	S2	99	A2M	O3'-C3'-C2'	3.38	120.64	111.19
68	S2	166	A2M	C3'-C2'-C1'	-3.37	96.36	102.81
3	L5	4571	A2M	O3'-C3'-C2'	3.36	120.58	111.19
68	S2	1383	A2M	O3'-C3'-C2'	3.35	120.57	111.19
68	S2	172	OMU	C5-C4-N3	3.34	119.48	114.80
68	S2	1383	A2M	C3'-C2'-C1'	-3.34	96.41	102.81
3	L5	1683	PSU	O2-C2-N1	-3.33	119.35	122.79
68	S2	1850	MA6	C4-C5-C6	3.32	119.35	115.91
68	S2	159	A2M	O3'-C3'-C2'	3.32	120.49	111.19
68	S2	576	A2M	O3'-C3'-C2'	3.32	120.47	111.19
3	L5	4579	PSU	O2-C2-N1	-3.29	119.40	122.79
3	L5	4296	PSU	O2-C2-N1	-3.28	119.40	122.79
68	S2	166	A2M	O3'-C3'-C2'	3.28	120.36	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3818	UY1	C6-C5-C4	3.27	120.38	118.17
3	L5	4532	PSU	O2-C2-N1	-3.27	119.42	122.79
3	L5	1323	A2M	C2'-C1'-N9	3.26	119.12	113.75
68	S2	668	A2M	C4-N9-C1'	-3.26	119.01	126.63
3	L5	2401	A2M	C3'-C2'-C1'	-3.25	96.58	102.81
68	S2	1288	OMU	N3-C2-N1	3.25	119.12	114.89
68	S2	1851	MA6	C2-N3-C4	3.25	119.76	111.83
68	S2	1046	PSU	O2-C2-N1	-3.24	119.44	122.79
68	S2	863	PSU	O2-C2-N1	-3.24	119.45	122.79
68	S2	1248	B8N	N3-C2-N1	3.24	120.67	116.72
3	L5	1744	PSU	O2-C2-N1	-3.21	119.47	122.79
68	S2	1850	MA6	N3-C4-N9	3.20	132.61	127.17
68	S2	468	A2M	O3'-C3'-C2'	3.19	120.13	111.19
3	L5	2787	A2M	O3'-C3'-C2'	3.19	120.12	111.19
3	L5	4590	A2M	C4-N9-C1'	-3.19	119.17	126.63
68	S2	1851	MA6	C5-N7-C8	3.19	108.46	103.45
68	S2	1639	G7M	N9-C4-N3	3.18	132.32	125.95
68	S2	1850	MA6	C2-N3-C4	3.18	119.60	111.83
3	L5	3825	A2M	O3'-C3'-C2'	3.17	120.06	111.19
3	L5	2363	A2M	C2'-C1'-N9	3.16	118.95	113.75
68	S2	1639	G7M	CN7-N7-C5	3.15	130.72	126.80
68	S2	468	A2M	C3'-C2'-C1'	-3.15	96.78	102.81
68	S2	159	A2M	C4-N9-C1'	-3.15	119.27	126.63
68	S2	121	OMU	N3-C2-N1	3.14	118.97	114.89
68	S2	1850	MA6	C5-N7-C8	3.13	108.38	103.45
3	L5	4220	6MZ	N3-C4-N9	3.13	132.49	127.17
3	L5	3830	A2M	O3'-C3'-C2'	3.12	119.91	111.19
3	L5	1871	A2M	O3'-C3'-C2'	3.11	119.90	111.19
68	S2	686	PSU	O2-C2-N1	-3.11	119.58	122.79
5	L8	69	PSU	O2-C2-N1	-3.10	119.59	122.79
68	S2	966	PSU	O2-C2-N1	-3.09	119.60	122.79
3	L5	4293	PSU	O2-C2-N1	-3.09	119.60	122.79
68	S2	576	A2M	C3'-C2'-C1'	-3.09	96.89	102.81
3	L5	1534	A2M	C3'-C2'-C1'	-3.09	96.89	102.81
68	S2	166	A2M	C4-N9-C1'	-3.09	119.41	126.63
68	S2	109	PSU	O2-C2-N1	-3.08	119.61	122.79
3	L5	1871	A2M	C4-N9-C1'	-3.08	119.43	126.63
3	L5	1323	A2M	O3'-C3'-C2'	3.08	119.79	111.19
68	S2	99	A2M	C4-N9-C1'	-3.06	119.47	126.63
68	S2	1639	G7M	C2-N1-C6	-3.06	119.56	125.11
3	L5	1536	PSU	O2-C2-N1	-3.06	119.63	122.79
3	L5	2837	OMU	O4-C4-C5	-3.06	119.89	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1288	OMU	O4-C4-C5	-3.05	119.90	125.16
3	L5	400	A2M	O3'-C3'-C2'	3.05	119.72	111.19
3	L5	4552	PSU	O2-C2-N1	-3.05	119.65	122.79
3	L5	3639	PSU	O2-C2-N1	-3.04	119.65	122.79
3	L5	2401	A2M	O3'-C3'-C2'	3.04	119.69	111.19
3	L5	4220	6MZ	C4-N9-C8	3.03	108.92	105.74
3	L5	3718	A2M	O3'-C3'-C2'	3.03	119.66	111.19
3	L5	1862	PSU	O2-C2-N1	-3.02	119.68	122.79
3	L5	4521	PSU	O2-C2-N1	-3.01	119.68	122.79
68	S2	1442	OMU	O4-C4-C5	-3.01	119.97	125.16
68	S2	116	OMU	O4-C4-C5	-3.00	119.99	125.16
68	S2	1244	PSU	O2-C2-N1	-3.00	119.70	122.79
3	L5	4227	OMU	O4-C4-C5	-2.99	120.01	125.16
3	L5	4571	A2M	C4-N9-C1'	-2.99	119.65	126.63
68	S2	863	PSU	C6-N1-C2	-2.98	119.93	122.69
3	L5	3925	OMU	O4-C4-C5	-2.98	120.03	125.16
68	S2	1046	PSU	C6-N1-C2	-2.98	119.93	122.69
3	L5	2839	PSU	O2-C2-N1	-2.98	119.72	122.79
3	L5	4306	OMU	O4-C4-C5	-2.98	120.03	125.16
68	S2	1004	PSU	C6-N1-C2	-2.97	119.93	122.69
68	S2	668	A2M	C1'-N9-C8	2.97	133.69	127.09
68	S2	1031	A2M	O3'-C3'-C2'	2.97	119.50	111.19
3	L5	4973	PSU	O2-C2-N1	-2.97	119.73	122.79
3	L5	1744	PSU	C6-N1-C2	-2.96	119.95	122.69
68	S2	27	A2M	C3'-C2'-C1'	-2.95	97.15	102.81
3	L5	4353	PSU	C6-N1-C2	-2.94	119.96	122.69
3	L5	4457	PSU	O2-C2-N1	-2.94	119.76	122.79
68	S2	801	PSU	C6-N1-C2	-2.94	119.97	122.69
68	S2	1004	PSU	O2-C2-N1	-2.92	119.77	122.79
68	S2	799	OMU	O4-C4-C5	-2.92	120.12	125.16
3	L5	1524	A2M	O3'-C3'-C2'	2.92	119.36	111.19
3	L5	4523	A2M	O3'-C3'-C2'	2.91	119.33	111.19
3	L5	4498	OMU	O4-C4-C5	-2.91	120.14	125.16
3	L5	4590	A2M	C1'-N9-C8	2.91	133.55	127.09
3	L5	5010	PSU	O2-C2-N1	-2.91	119.79	122.79
3	L5	4579	PSU	C6-N1-C2	-2.91	119.99	122.69
68	S2	159	A2M	C1'-N9-C8	2.90	133.54	127.09
68	S2	1326	OMU	O4-C4-C5	-2.90	120.16	125.16
3	L5	3884	PSU	C6-N1-C2	-2.90	120.00	122.69
3	L5	1677	PSU	O2-C2-N1	-2.90	119.80	122.79
68	S2	484	A2M	O3'-C3'-C2'	2.90	119.30	111.19
3	L5	3853	PSU	O2-C2-N1	-2.89	119.80	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	649	PSU	C6-N1-C2	-2.89	120.01	122.69
3	L5	1326	A2M	O3'-C3'-C2'	2.89	119.27	111.19
3	L5	400	A2M	C3'-C2'-C1'	-2.89	97.28	102.81
68	S2	428	OMU	O4-C4-C5	-2.88	120.20	125.16
3	L5	2839	PSU	C6-N1-C2	-2.88	120.02	122.69
3	L5	4576	PSU	O2-C2-N1	-2.87	119.82	122.79
3	L5	5001	PSU	O2-C2-N1	-2.87	119.83	122.79
68	S2	1045	PSU	O2-C2-N1	-2.87	119.83	122.79
3	L5	1323	A2M	C3'-C2'-C1'	-2.87	97.31	102.81
68	S2	1174	PSU	O2-C2-N1	-2.87	119.83	122.79
68	S2	651	PSU	O2-C2-N1	-2.87	119.83	122.79
68	S2	1383	A2M	C4-N9-C1'	-2.87	119.93	126.63
3	L5	3639	PSU	C6-N1-C2	-2.86	120.03	122.69
3	L5	1871	A2M	C1'-N9-C8	2.86	133.44	127.09
3	L5	4500	PSU	O2-C2-N1	-2.85	119.84	122.79
3	L5	5010	PSU	C6-N1-C2	-2.85	120.05	122.69
3	L5	4471	PSU	O2-C2-N1	-2.85	119.85	122.79
3	L5	4689	PSU	O2-C2-N1	-2.85	119.85	122.79
68	S2	406	PSU	O2-C2-N1	-2.84	119.86	122.79
3	L5	3867	A2M	C4-N9-C1'	-2.84	119.98	126.63
3	L5	2401	A2M	C4-N9-C1'	-2.83	120.01	126.63
68	S2	354	OMU	O4-C4-C5	-2.83	120.28	125.16
68	S2	27	A2M	C4-N9-C1'	-2.83	120.02	126.63
3	L5	2815	A2M	C2'-C1'-N9	2.83	118.41	113.75
68	S2	99	A2M	C1'-N9-C8	2.83	133.37	127.09
3	L5	4628	PSU	O2-C2-N1	-2.83	119.87	122.79
3	L5	3808	OMC	C1'-N1-C2	2.82	124.68	118.44
68	S2	166	A2M	C1'-N9-C8	2.82	133.36	127.09
3	L5	3884	PSU	O2-C2-N1	-2.81	119.89	122.79
68	S2	649	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L5	4532	PSU	C6-N1-C2	-2.80	120.09	122.69
68	S2	681	PSU	O2-C2-N1	-2.80	119.90	122.79
3	L5	1860	PSU	C6-N1-C2	-2.80	120.09	122.69
68	S2	627	OMU	O4-C4-C5	-2.80	120.34	125.16
3	L5	1683	PSU	C6-N1-C2	-2.79	120.10	122.69
68	S2	1232	PSU	O2-C2-N1	-2.78	119.92	122.79
3	L5	1781	PSU	O2-C2-N1	-2.78	119.92	122.79
3	L5	2632	PSU	O2-C2-N1	-2.78	119.92	122.79
68	S2	468	A2M	C4-N9-C1'	-2.78	120.14	126.63
3	L5	3822	PSU	O2-C2-N1	-2.78	119.93	122.79
68	S2	121	OMU	O4-C4-C5	-2.77	120.39	125.16
3	L5	1677	PSU	C6-C5-C4	2.77	120.04	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3637	PSU	C6-N1-C2	-2.77	120.12	122.69
3	L5	4220	6MZ	C5-N7-C8	2.76	107.79	103.45
3	L5	3851	PSU	O2-C2-N1	-2.76	119.94	122.79
3	L5	4471	PSU	C6-N1-C2	-2.76	120.13	122.69
3	L5	2351	OMC	C1'-N1-C2	2.75	124.52	118.44
68	S2	1031	A2M	C4-N9-C1'	-2.75	120.20	126.63
3	L5	4296	PSU	C6-N1-C2	-2.75	120.14	122.69
68	S2	1832	6MZ	C4-N9-C8	2.74	108.62	105.74
3	L5	3785	A2M	O3'-C3'-C2'	2.74	118.86	111.19
3	L5	4620	OMU	O4-C4-C5	-2.74	120.44	125.16
3	L5	4500	PSU	C6-N1-C2	-2.74	120.15	122.69
68	S2	1045	PSU	C6-N1-C2	-2.74	120.15	122.69
3	L5	1326	A2M	C3'-C2'-C1'	-2.73	97.58	102.81
68	S2	172	OMU	O4-C4-C5	-2.73	120.45	125.16
3	L5	2787	A2M	O4'-C1'-C2'	2.73	111.29	106.59
3	L5	3844	PSU	O2-C2-N1	-2.73	119.98	122.79
3	L5	3785	A2M	C4'-O4'-C1'	-2.72	103.45	109.47
3	L5	1323	A2M	O4'-C1'-C2'	2.71	111.26	106.59
68	S2	668	A2M	C2'-C1'-N9	2.71	118.21	113.75
68	S2	799	OMU	C1'-N1-C2	2.71	122.46	117.59
3	L5	4973	PSU	C6-N1-C2	-2.71	120.18	122.69
3	L5	3830	A2M	C4-N9-C1'	-2.70	120.31	126.63
3	L5	4500	PSU	C6-C5-C4	2.70	120.00	118.17
3	L5	3867	A2M	C1'-N9-C8	2.70	133.09	127.09
3	L5	4673	PSU	O2-C2-N1	-2.70	120.00	122.79
68	S2	1056	PSU	O2-C2-N1	-2.70	120.00	122.79
3	L5	3695	PSU	O2-C2-N1	-2.70	120.00	122.79
68	S2	1177	PSU	O2-C2-N1	-2.70	120.00	122.79
68	S2	1832	6MZ	C4-C5-N7	-2.70	107.50	110.58
3	L5	1524	A2M	O4'-C1'-C2'	2.69	111.23	106.59
5	L8	55	PSU	C6-N1-C2	-2.69	120.19	122.69
3	L5	4361	PSU	O2-C2-N1	-2.69	120.02	122.79
3	L5	4403	PSU	O2-C2-N1	-2.68	120.02	122.79
68	S2	105	PSU	O2-C2-N1	-2.68	120.02	122.79
68	S2	1177	PSU	C6-N1-C2	-2.68	120.20	122.69
3	L5	4442	PSU	O2-C2-N1	-2.68	120.03	122.79
3	L5	3718	A2M	C1'-N9-C8	2.67	133.02	127.09
68	S2	1383	A2M	C1'-N9-C8	2.67	133.02	127.09
3	L5	3920	PSU	O2-C2-N1	-2.67	120.03	122.79
68	S2	668	A2M	O4'-C1'-C2'	2.67	111.18	106.59
3	L5	2401	A2M	C1'-N9-C8	2.66	133.01	127.09
3	L5	3844	PSU	C6-N1-C2	-2.66	120.22	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2815	A2M	O3'-C3'-C2'	2.66	118.63	111.19
3	L5	3825	A2M	C4-N9-C1'	-2.66	120.41	126.63
5	L8	55	PSU	O2-C2-N1	-2.66	120.05	122.79
3	L5	3867	A2M	C2'-C1'-N9	2.66	118.12	113.75
3	L5	1536	PSU	C6-N1-C2	-2.66	120.23	122.69
68	S2	668	A2M	O3'-C3'-C2'	2.65	118.61	111.19
68	S2	866	PSU	O2-C2-N1	-2.65	120.05	122.79
3	L5	3853	PSU	C6-N1-C2	-2.65	120.23	122.69
68	S2	93	PSU	O2-C2-N1	-2.65	120.06	122.79
3	L5	4220	6MZ	C4-C5-C6	2.64	118.98	116.78
3	L5	4523	A2M	C4-N9-C1'	-2.64	120.46	126.63
3	L5	2363	A2M	C4-N9-C1'	-2.63	120.47	126.63
68	S2	681	PSU	C6-N1-C2	-2.63	120.25	122.69
3	L5	4431	PSU	O2-C2-N1	-2.63	120.08	122.79
68	S2	686	PSU	C6-N1-C2	-2.63	120.25	122.69
68	S2	406	PSU	C6-N1-C2	-2.63	120.25	122.69
68	S2	966	PSU	C6-N1-C2	-2.63	120.25	122.69
3	L5	4521	PSU	C6-N1-C2	-2.62	120.26	122.69
68	S2	576	A2M	C4-N9-C1'	-2.62	120.50	126.63
68	S2	27	A2M	O3'-C3'-C2'	2.62	118.52	111.19
68	S2	484	A2M	O4'-C1'-C2'	2.62	111.10	106.59
68	S2	1832	6MZ	N3-C4-N9	2.62	131.62	127.17
3	L5	4403	PSU	C6-N1-C2	-2.62	120.26	122.69
3	L5	4571	A2M	C1'-N9-C8	2.61	132.90	127.09
68	S2	801	PSU	O2-C2-N1	-2.61	120.09	122.79
3	L5	3920	PSU	C6-N1-C2	-2.61	120.27	122.69
68	S2	1031	A2M	C1'-N9-C8	2.61	132.88	127.09
3	L5	1792	PSU	O2-C2-N1	-2.61	120.10	122.79
68	S2	27	A2M	C1'-N9-C8	2.61	132.88	127.09
3	L5	4220	6MZ	C5-C6-N1	2.60	120.95	118.15
3	L5	4552	PSU	C6-N1-C2	-2.60	120.28	122.69
68	S2	1174	PSU	C6-N1-C2	-2.59	120.28	122.69
3	L5	2815	A2M	C3'-C2'-C1'	-2.58	97.87	102.81
68	S2	1244	PSU	C6-N1-C2	-2.58	120.30	122.69
5	L8	69	PSU	C6-N1-C2	-2.57	120.30	122.69
3	L5	1782	PSU	C6-N1-C2	-2.57	120.30	122.69
68	S2	159	A2M	C3'-C2'-C1'	-2.57	97.88	102.81
68	S2	651	PSU	C6-N1-C2	-2.57	120.31	122.69
3	L5	4576	PSU	C6-N1-C2	-2.57	120.31	122.69
3	L5	4636	PSU	C6-C5-C4	2.57	119.91	118.17
3	L5	4442	PSU	C6-N1-C2	-2.56	120.31	122.69
3	L5	4673	PSU	C6-N1-C2	-2.56	120.31	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4353	PSU	O2-C2-N1	-2.56	120.15	122.79
68	S2	1832	6MZ	C4-C5-C6	2.56	118.91	116.78
68	S2	105	PSU	C6-N1-C2	-2.56	120.32	122.69
3	L5	3818	UY1	C6-N1-C2	-2.55	120.32	122.69
3	L5	5001	PSU	C6-N1-C2	-2.55	120.32	122.69
3	L5	3825	A2M	C1'-N9-C8	2.55	132.76	127.09
3	L5	3785	A2M	C4-N9-C1'	-2.55	120.67	126.63
68	S2	484	A2M	C4-N9-C1'	-2.55	120.67	126.63
3	L5	1677	PSU	C6-N1-C2	-2.55	120.33	122.69
3	L5	3822	PSU	C6-N1-C2	-2.55	120.33	122.69
68	S2	484	A2M	C1'-N9-C8	2.55	132.75	127.09
3	L5	398	A2M	C4-N9-C1'	-2.54	120.69	126.63
3	L5	398	A2M	C1'-N9-C8	2.54	132.74	127.09
68	S2	468	A2M	C1'-N9-C8	2.54	132.74	127.09
3	L5	2363	A2M	C1'-N9-C8	2.54	132.73	127.09
68	S2	866	PSU	C6-N1-C2	-2.54	120.34	122.69
68	S2	1248	B8N	O4-C4-N3	-2.54	115.87	119.99
3	L5	2632	PSU	C6-N1-C2	-2.53	120.34	122.69
3	L5	3785	A2M	C3'-C2'-C1'	-2.53	97.95	102.81
68	S2	1288	OMU	C1'-N1-C2	2.53	122.14	117.59
3	L5	400	A2M	C4-N9-C1'	-2.53	120.72	126.63
3	L5	3718	A2M	C4-N9-C1'	-2.53	120.73	126.63
3	L5	4457	PSU	C6-N1-C2	-2.52	120.35	122.69
3	L5	1782	PSU	O2-C2-N1	-2.52	120.19	122.79
3	L5	2861	OMC	C1'-N1-C2	2.52	124.00	118.44
3	L5	2363	A2M	O3'-C3'-C2'	2.51	118.22	111.19
3	L5	3830	A2M	C1'-N9-C8	2.51	132.66	127.09
68	S2	576	A2M	C1'-N9-C8	2.50	132.65	127.09
3	L5	1582	PSU	O2-C2-N1	-2.50	120.21	122.79
3	L5	1781	PSU	C6-N1-C2	-2.50	120.37	122.69
3	L5	4498	OMU	O2-C2-N1	-2.50	119.55	122.80
3	L5	2787	A2M	C4-N9-C1'	-2.49	120.81	126.63
3	L5	4312	PSU	O2-C2-N1	-2.49	120.22	122.79
68	S2	1639	G7M	CN7-N7-C8	-2.49	121.03	124.79
3	L5	2363	A2M	C3'-C2'-C1'	-2.49	98.05	102.81
68	S2	814	PSU	O2-C2-N1	-2.48	120.23	122.79
3	L5	4493	PSU	O2-C2-N1	-2.47	120.24	122.79
68	S2	1081	PSU	O2-C2-N1	-2.47	120.25	122.79
3	L5	3818	UY1	O2-C2-N1	-2.46	120.25	122.79
3	L5	4972	PSU	C6-N1-C2	-2.46	120.41	122.69
68	S2	1367	PSU	C6-N1-C2	-2.46	120.41	122.69
3	L5	4972	PSU	O2-C2-N1	-2.45	120.26	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1860	PSU	O2-C2-N1	-2.45	120.27	122.79
3	L5	4431	PSU	C6-N1-C2	-2.43	120.44	122.69
3	L5	400	A2M	C2'-C1'-N9	2.43	117.75	113.75
3	L5	4521	PSU	C6-C5-C4	2.43	119.81	118.17
3	L5	2837	OMU	O2-C2-N1	-2.42	119.64	122.80
3	L5	4590	A2M	O3'-C3'-C2'	2.42	117.96	111.19
3	L5	1322	1MA	CM1-N1-C6	-2.42	116.40	120.15
68	S2	1232	PSU	C6-N1-C2	-2.42	120.45	122.69
68	S2	93	PSU	C6-N1-C2	-2.42	120.45	122.69
3	L5	2363	A2M	O4'-C1'-C2'	2.41	110.74	106.59
3	L5	400	A2M	C1'-N9-C8	2.41	132.44	127.09
3	L5	3867	A2M	C6-C5-C4	-2.41	113.89	117.18
68	S2	116	OMU	C1'-N1-C2	2.40	121.91	117.59
3	L5	1524	A2M	C4-N9-C1'	-2.40	121.02	126.63
3	L5	3718	A2M	C2'-C1'-N9	2.40	117.70	113.75
3	L5	1323	A2M	C4-N9-C1'	-2.39	121.04	126.63
68	S2	1367	PSU	C6-C5-C4	2.39	119.79	118.17
3	L5	4590	A2M	C6-C5-C4	-2.39	113.92	117.18
3	L5	4523	A2M	C1'-N9-C8	2.39	132.40	127.09
3	L5	1524	A2M	C4'-O4'-C1'	-2.38	104.20	109.47
68	S2	428	OMU	O2-C2-N1	-2.38	119.70	122.80
3	L5	4628	PSU	C6-N1-C2	-2.37	120.49	122.69
68	S2	1367	PSU	O2-C2-N1	-2.37	120.34	122.79
3	L5	2787	A2M	C1'-N9-C8	2.37	132.35	127.09
3	L5	2824	OMC	C1'-N1-C2	2.37	123.67	118.44
68	S2	1056	PSU	C6-N1-C2	-2.37	120.50	122.69
3	L5	1326	A2M	C1'-N9-C8	2.36	132.34	127.09
3	L5	1582	PSU	C6-N1-C2	-2.36	120.50	122.69
3	L5	4312	PSU	C6-N1-C2	-2.35	120.51	122.69
68	S2	1851	MA6	C1'-N9-C8	-2.35	121.88	127.09
68	S2	627	OMU	O2-C2-N1	-2.35	119.74	122.80
3	L5	1326	A2M	C4-N9-C1'	-2.33	121.17	126.63
68	S2	109	PSU	C6-N1-C2	-2.32	120.54	122.69
68	S2	166	A2M	C6-C5-C4	-2.32	114.01	117.18
68	S2	484	A2M	O4'-C4'-C3'	2.32	109.75	105.15
3	L5	4493	PSU	C6-N1-C2	-2.32	120.54	122.69
3	L5	3695	PSU	C6-N1-C2	-2.31	120.54	122.69
3	L5	4293	PSU	C6-N1-C2	-2.31	120.55	122.69
3	L5	4636	PSU	O2-C2-N1	-2.31	120.41	122.79
68	S2	1248	B8N	O4'-C1'-C2'	2.30	108.34	105.15
3	L5	1871	A2M	C6-C5-C4	-2.30	114.04	117.18
3	L5	4620	OMU	O2-C2-N1	-2.29	119.81	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	866	PSU	C6-C5-C4	2.29	119.72	118.17
3	L5	3785	A2M	C2-N1-C6	-2.29	114.96	118.73
68	S2	668	A2M	C6-C5-C4	-2.29	114.05	117.18
3	L5	1862	PSU	C6-N1-C2	-2.29	120.57	122.69
3	L5	3785	A2M	C1'-N9-C8	2.28	132.16	127.09
3	L5	4361	PSU	C6-N1-C2	-2.28	120.58	122.69
3	L5	3830	A2M	C6-C5-C4	-2.27	114.08	117.18
3	L5	1534	A2M	C1'-N9-C8	2.27	132.13	127.09
3	L5	2815	A2M	C4-N9-C1'	-2.26	121.34	126.63
68	S2	1248	B8N	O4-C4-C5	-2.26	118.67	122.58
68	S2	99	A2M	C6-C5-C4	-2.26	114.09	117.18
68	S2	354	OMU	O2-C2-N1	-2.26	119.86	122.80
3	L5	3637	PSU	C6-C5-C4	2.25	119.69	118.17
3	L5	400	A2M	O4'-C1'-C2'	2.25	110.46	106.59
3	L5	4299	PSU	O2-C2-N1	-2.25	120.47	122.79
3	L5	2815	A2M	O4'-C1'-C2'	2.25	110.46	106.59
3	L5	1323	A2M	C1'-N9-C8	2.25	132.09	127.09
3	L5	4636	PSU	O4'-C1'-C2'	2.25	108.26	105.15
3	L5	4403	PSU	O4'-C1'-C2'	2.24	108.26	105.15
68	S2	1639	G7M	N9-C8-N7	-2.24	107.03	112.48
3	L5	1524	A2M	C1'-N9-C8	2.24	132.07	127.09
68	S2	159	A2M	O4'-C1'-C2'	2.24	110.44	106.59
3	L5	1326	A2M	C2'-C1'-N9	2.24	117.43	113.75
3	L5	1534	A2M	C4-N9-C1'	-2.23	121.41	126.63
68	S2	1272	OMC	C1'-N1-C2	2.23	123.37	118.44
68	S2	468	A2M	C6-C5-C4	-2.23	114.14	117.18
3	L5	3785	A2M	C5-C6-N1	2.23	123.17	117.51
68	S2	1081	PSU	C6-N1-C2	-2.23	120.62	122.69
3	L5	3822	PSU	O4'-C1'-C2'	2.21	108.22	105.15
68	S2	1031	A2M	C6-C5-C4	-2.21	114.16	117.18
3	L5	2401	A2M	C6-C5-C4	-2.21	114.16	117.18
68	S2	27	A2M	C6-C5-C4	-2.21	114.16	117.18
68	S2	27	A2M	O4'-C1'-C2'	2.21	110.39	106.59
3	L5	4571	A2M	C6-C5-C4	-2.21	114.17	117.18
68	S2	1326	OMU	O2-C2-N1	-2.20	119.93	122.80
3	L5	1792	PSU	C6-N1-C2	-2.20	120.65	122.69
3	L5	3782	5MC	C1'-N1-C6	-2.20	117.53	121.15
3	L5	4530	UR3	C1'-N1-C2	2.19	120.63	117.04
3	L5	3851	PSU	C6-N1-C2	-2.19	120.66	122.69
68	S2	99	A2M	C5-C6-N1	2.19	123.07	117.51
3	L5	3808	OMC	C1'-N1-C6	-2.19	116.10	120.78
68	S2	166	A2M	O4'-C1'-C2'	2.19	110.35	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4299	PSU	C6-N1-C2	-2.19	120.66	122.69
3	L5	2787	A2M	C2-N1-C6	-2.18	115.15	118.73
68	S2	105	PSU	C6-C5-C4	2.18	119.64	118.17
3	L5	3718	A2M	C6-C5-C4	-2.17	114.22	117.18
3	L5	1322	1MA	N1-C6-N6	2.17	125.16	119.71
3	L5	2815	A2M	C1'-N9-C8	2.17	131.90	127.09
3	L5	3920	PSU	C6-C5-C4	2.17	119.64	118.17
68	S2	159	A2M	C6-C5-C4	-2.16	114.22	117.18
3	L5	4571	A2M	O4'-C1'-C2'	2.16	110.31	106.59
5	L8	69	PSU	O4'-C1'-C2'	2.16	108.14	105.15
3	L5	3822	PSU	C6-C5-C4	2.15	119.63	118.17
3	L5	4523	A2M	C2-N1-C6	-2.15	115.19	118.73
3	L5	1326	A2M	O4'-C1'-C2'	2.15	110.29	106.59
3	L5	400	A2M	C2-N1-C6	-2.15	115.20	118.73
3	L5	1534	A2M	O4'-C1'-C2'	2.15	110.28	106.59
3	L5	3867	A2M	C2-N1-C6	-2.14	115.21	118.73
3	L5	4403	PSU	C6-C5-C4	2.14	119.62	118.17
3	L5	4523	A2M	C5-C6-N1	2.14	122.95	117.51
68	S2	468	A2M	O4'-C1'-C2'	2.14	110.27	106.59
68	S2	1442	OMU	O2-C2-N1	-2.14	120.01	122.80
3	L5	1871	A2M	O4'-C1'-C2'	2.14	110.27	106.59
68	S2	172	OMU	O2-C2-N1	-2.14	120.02	122.80
3	L5	2363	A2M	C6-C5-C4	-2.14	114.26	117.18
3	L5	3867	A2M	O3'-C3'-C2'	2.13	117.16	111.19
3	L5	1326	A2M	C2-N1-C6	-2.13	115.23	118.73
3	L5	3825	A2M	C2-N1-C6	-2.13	115.23	118.73
68	S2	576	A2M	C6-C5-C4	-2.13	114.27	117.18
68	S2	1248	B8N	C31-N3-C4	2.13	120.19	117.18
3	L5	4571	A2M	C2-N1-C6	-2.13	115.24	118.73
3	L5	3785	A2M	O4'-C4'-C3'	2.13	109.37	105.15
3	L5	1534	A2M	C2-N1-C6	-2.12	115.24	118.73
68	S2	1031	A2M	C5-C6-N1	2.12	122.90	117.51
3	L5	2815	A2M	C6-C5-C4	-2.12	114.28	117.18
3	L5	3785	A2M	C6-C5-C4	-2.12	114.28	117.18
3	L5	3637	PSU	O2-C2-N3	-2.11	118.11	121.86
3	L5	3825	A2M	C6-C5-C4	-2.11	114.29	117.18
68	S2	99	A2M	O4'-C1'-C2'	2.11	110.22	106.59
3	L5	4523	A2M	C6-C5-C4	-2.11	114.30	117.18
3	L5	1323	A2M	C2-N1-C6	-2.11	115.27	118.73
3	L5	1524	A2M	C6-C5-C4	-2.11	114.30	117.18
68	S2	1383	A2M	C2-N1-C6	-2.10	115.28	118.73
3	L5	2787	A2M	C5-C6-N1	2.10	122.84	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3867	A2M	O4'-C1'-C2'	2.09	110.19	106.59
3	L5	1871	A2M	C4'-O4'-C1'	-2.09	104.84	109.47
3	L5	1677	PSU	O4'-C1'-C2'	2.09	108.05	105.15
68	S2	166	A2M	C5-C6-N1	2.09	122.82	117.51
68	S2	99	A2M	C2-N1-C6	-2.09	115.30	118.73
68	S2	1031	A2M	C2-N1-C6	-2.09	115.30	118.73
3	L5	4296	PSU	C6-C5-C4	2.08	119.58	118.17
3	L5	3718	A2M	C2-N1-C6	-2.08	115.31	118.73
68	S2	668	A2M	O3'-C3'-C4'	-2.08	105.11	111.08
3	L5	3920	PSU	O4'-C1'-C2'	2.08	108.03	105.15
3	L5	3925	OMU	O2-C2-N1	-2.08	120.09	122.80
3	L5	3825	A2M	C5-C6-N1	2.08	122.79	117.51
3	L5	2815	A2M	C5-C6-N1	2.08	122.79	117.51
3	L5	1524	A2M	C2-N1-C6	-2.08	115.32	118.73
68	S2	1383	A2M	C6-C5-C4	-2.08	114.34	117.18
3	L5	4636	PSU	C6-N1-C2	-2.07	120.77	122.69
68	S2	468	A2M	C2-N1-C6	-2.07	115.33	118.73
3	L5	398	A2M	C6-C5-C4	-2.07	114.35	117.18
3	L5	4523	A2M	C4'-O4'-C1'	-2.07	104.90	109.47
3	L5	2363	A2M	C5-C6-N1	2.07	122.76	117.51
3	L5	3867	A2M	C5-C6-N1	2.07	122.76	117.51
3	L5	1326	A2M	C5-C6-N1	2.07	122.76	117.51
3	L5	398	A2M	C5-C6-N1	2.07	122.76	117.51
68	S2	484	A2M	C5-C6-N1	2.06	122.75	117.51
3	L5	4530	UR3	C6-N1-C2	-2.06	120.11	121.80
3	L5	5001	PSU	C6-C5-C4	2.06	119.56	118.17
3	L5	2401	A2M	C5-C6-N1	2.05	122.73	117.51
3	L5	4571	A2M	C5-C6-N1	2.05	122.72	117.51
3	L5	1534	A2M	C5-C6-N1	2.05	122.72	117.51
68	S2	27	A2M	C5-C6-N1	2.05	122.72	117.51
3	L5	398	A2M	C2-N1-C6	-2.05	115.36	118.73
3	L5	400	A2M	C5-C6-N1	2.05	122.72	117.51
68	S2	468	A2M	C5-C6-N1	2.05	122.71	117.51
68	S2	1383	A2M	C5-C6-N1	2.05	122.70	117.51
68	S2	484	A2M	C2-N1-C6	-2.04	115.37	118.73
3	L5	3718	A2M	C5-C6-N1	2.04	122.70	117.51
68	S2	1832	6MZ	C5-C6-N1	2.04	120.34	118.15
3	L5	1323	A2M	C5-C6-N1	2.04	122.69	117.51
68	S2	27	A2M	C2-N1-C6	-2.04	115.38	118.73
3	L5	2815	A2M	C2-N1-C6	-2.04	115.38	118.73
3	L5	2422	OMC	C1'-N1-C2	2.04	122.94	118.44
3	L5	4442	PSU	O4'-C1'-C2'	2.04	107.97	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	159	A2M	C2-N1-C6	-2.03	115.39	118.73
3	L5	1323	A2M	C6-C5-C4	-2.03	114.41	117.18
3	L5	2363	A2M	C2-N1-C6	-2.03	115.40	118.73
68	S2	814	PSU	C6-N1-C2	-2.03	120.81	122.69
68	S2	668	A2M	C4'-O4'-C1'	-2.02	105.00	109.47
3	L5	1534	A2M	O3'-C3'-C4'	-2.02	105.29	111.08
3	L5	3830	A2M	C5-C6-N1	2.02	122.63	117.51
3	L5	2401	A2M	C2-N1-C6	-2.01	115.42	118.73
3	L5	1524	A2M	C5-C6-N1	2.01	122.62	117.51
3	L5	2787	A2M	C6-C5-C4	-2.01	114.43	117.18
3	L5	1871	A2M	C5-C6-N1	2.01	122.61	117.51
68	S2	1232	PSU	C6-C5-C4	2.00	119.52	118.17
3	L5	4590	A2M	O4'-C1'-C2'	2.00	110.03	106.59
3	L5	3867	A2M	O3'-C3'-C4'	-2.00	105.34	111.08
3	L5	400	A2M	C6-C5-C4	-2.00	114.45	117.18

There are no chirality outliers.

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L5	400	A2M	C1'-C2'-O2'-CM'
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	2364	OMG	O4'-C4'-C5'-O5'
3	L5	2424	OMG	C1'-C2'-O2'-CM2
3	L5	2787	A2M	C1'-C2'-O2'-CM'
3	L5	2824	OMC	C1'-C2'-O2'-CM2
3	L5	2861	OMC	C1'-C2'-O2'-CM2
3	L5	2876	OMG	O4'-C4'-C5'-O5'
3	L5	3701	OMC	C2'-C1'-N1-C6
3	L5	3792	OMG	O4'-C4'-C5'-O5'
3	L5	4196	OMG	C1'-C2'-O2'-CM2
3	L5	4637	OMG	O4'-C4'-C5'-O5'
3	L5	4637	OMG	C1'-C2'-O2'-CM2
68	S2	27	A2M	C1'-C2'-O2'-CM'
68	S2	121	OMU	C1'-C2'-O2'-CM2
68	S2	159	A2M	C1'-C2'-O2'-CM'
68	S2	166	A2M	C1'-C2'-O2'-CM'
68	S2	172	OMU	O4'-C4'-C5'-O5'
68	S2	517	OMC	C1'-C2'-O2'-CM2
68	S2	601	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
68	S2	627	OMU	C3'-C4'-C5'-O5'
68	S2	627	OMU	O4'-C4'-C5'-O5'
68	S2	644	OMG	O4'-C4'-C5'-O5'
68	S2	1031	A2M	C1'-C2'-O2'-CM'
68	S2	1328	OMG	C1'-C2'-O2'-CM2
68	S2	1383	A2M	C1'-C2'-O2'-CM'
68	S2	1442	OMU	C1'-C2'-O2'-CM2
68	S2	1832	6MZ	N1-C6-N6-C9
3	L5	3701	OMC	C2'-C1'-N1-C2
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	2401	A2M	C3'-C4'-C5'-O5'
3	L5	2815	A2M	O4'-C4'-C5'-O5'
3	L5	2876	OMG	C3'-C4'-C5'-O5'
3	L5	4590	A2M	O4'-C4'-C5'-O5'
3	L5	4590	A2M	C3'-C4'-C5'-O5'
68	S2	172	OMU	C3'-C4'-C5'-O5'
68	S2	576	A2M	O4'-C4'-C5'-O5'
68	S2	576	A2M	C3'-C4'-C5'-O5'
68	S2	799	OMU	C3'-C4'-C5'-O5'
68	S2	799	OMU	O4'-C4'-C5'-O5'
68	S2	801	PSU	C3'-C4'-C5'-O5'
68	S2	867	OMG	C3'-C4'-C5'-O5'
3	L5	1536	PSU	C3'-C4'-C5'-O5'
3	L5	2364	OMG	C3'-C4'-C5'-O5'
3	L5	2401	A2M	O4'-C4'-C5'-O5'
3	L5	3701	OMC	C3'-C4'-C5'-O5'
3	L5	3701	OMC	O4'-C4'-C5'-O5'
3	L5	3899	OMG	C3'-C4'-C5'-O5'
3	L5	4228	OMG	O4'-C4'-C5'-O5'
3	L5	4228	OMG	C3'-C4'-C5'-O5'
3	L5	4500	PSU	O4'-C4'-C5'-O5'
68	S2	801	PSU	O4'-C4'-C5'-O5'
68	S2	1045	PSU	O4'-C4'-C5'-O5'
68	S2	1248	B8N	C3'-C4'-C5'-O5'
68	S2	1442	OMU	O4'-C4'-C5'-O5'
3	L5	2815	A2M	C3'-C4'-C5'-O5'
3	L5	3792	OMG	C3'-C4'-C5'-O5'
3	L5	4500	PSU	C3'-C4'-C5'-O5'
3	L5	4637	OMG	C3'-C4'-C5'-O5'
68	S2	644	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
68	S2	668	A2M	O4'-C4'-C5'-O5'
68	S2	668	A2M	C3'-C4'-C5'-O5'
68	S2	1442	OMU	C3'-C4'-C5'-O5'
3	L5	1323	A2M	O4'-C4'-C5'-O5'
3	L5	3899	OMG	O4'-C4'-C5'-O5'
68	S2	99	A2M	O4'-C4'-C5'-O5'
68	S2	428	OMU	O4'-C4'-C5'-O5'
68	S2	867	OMG	O4'-C4'-C5'-O5'
68	S2	1248	B8N	O4'-C4'-C5'-O5'
68	S2	172	OMU	C2'-C1'-N1-C6
3	L5	1524	A2M	O4'-C4'-C5'-O5'
3	L5	1524	A2M	C3'-C4'-C5'-O5'
68	S2	428	OMU	C3'-C4'-C5'-O5'
68	S2	1045	PSU	C3'-C4'-C5'-O5'
3	L5	2632	PSU	O4'-C4'-C5'-O5'
3	L5	3867	A2M	C3'-C4'-C5'-O5'
68	S2	1056	PSU	O4'-C4'-C5'-O5'
3	L5	2787	A2M	C2'-C1'-N9-C8
68	S2	1248	B8N	N34-C33-C34-O35
3	L5	2632	PSU	C3'-C4'-C5'-O5'
68	S2	1056	PSU	C3'-C4'-C5'-O5'
68	S2	1244	PSU	O4'-C4'-C5'-O5'
3	L5	3867	A2M	C1'-C2'-O2'-CM'
3	L5	2787	A2M	C3'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C6
68	S2	428	OMU	C2'-C1'-N1-C6
68	S2	1832	6MZ	C5-C6-N6-C9
3	L5	4447	5MC	O4'-C1'-N1-C6
68	S2	172	OMU	O4'-C1'-N1-C6
68	S2	1703	OMC	O4'-C4'-C5'-O5'
3	L5	4590	A2M	C4'-C5'-O5'-P
68	S2	576	A2M	C4'-C5'-O5'-P
3	L5	3785	A2M	O4'-C4'-C5'-O5'
3	L5	3701	OMC	O4'-C1'-N1-C2
68	S2	172	OMU	C2'-C1'-N1-C2
3	L5	3818	UY1	C4'-C5'-O5'-P
68	S2	1288	OMU	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
3	L5	3701	OMC	O4'-C1'-N1-C6
68	S2	644	OMG	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
68	S2	1248	B8N	C4'-C5'-O5'-P
3	L5	4500	PSU	C4'-C5'-O5'-P
68	S2	1490	OMG	C4'-C5'-O5'-P
3	L5	4623	OMG	C3'-C4'-C5'-O5'
68	S2	428	OMU	O4'-C1'-N1-C6
3	L5	3869	OMC	C3'-C2'-O2'-CM2
3	L5	4498	OMU	C3'-C2'-O2'-CM2
3	L5	1326	A2M	C4'-C5'-O5'-P
3	L5	3887	OMC	C4'-C5'-O5'-P
3	L5	398	A2M	O4'-C4'-C5'-O5'
3	L5	3782	5MC	O4'-C4'-C5'-O5'
3	L5	4447	5MC	O4'-C1'-N1-C2
68	S2	172	OMU	O4'-C1'-N1-C2
5	L8	75	OMG	C4'-C5'-O5'-P
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	3844	PSU	C4'-C5'-O5'-P
68	S2	1851	MA6	C4'-C5'-O5'-P
3	L5	2422	OMC	C3'-C4'-C5'-O5'
3	L5	1322	1MA	C2'-C1'-N9-C8
3	L5	3841	OMC	C1'-C2'-O2'-CM2
3	L5	4590	A2M	C1'-C2'-O2'-CM'
3	L5	1322	1MA	C2'-C1'-N9-C4
68	S2	1081	PSU	C4'-C5'-O5'-P
68	S2	1248	B8N	N34-C33-C34-O36
3	L5	1677	PSU	O4'-C1'-C5-C6
3	L5	3818	UY1	O4'-C1'-C5-C6
3	L5	4636	PSU	O4'-C1'-C5-C6
5	L8	69	PSU	O4'-C4'-C5'-O5'
68	S2	99	A2M	C3'-C4'-C5'-O5'
3	L5	2787	A2M	O4'-C1'-N9-C8
3	L5	1323	A2M	C3'-C4'-C5'-O5'
68	S2	105	PSU	C3'-C4'-C5'-O5'
3	L5	1792	PSU	O4'-C4'-C5'-O5'
68	S2	428	OMU	O4'-C1'-N1-C2
3	L5	3785	A2M	C2'-C1'-N9-C8
3	L5	2422	OMC	O4'-C4'-C5'-O5'
3	L5	4623	OMG	O4'-C4'-C5'-O5'
3	L5	2351	OMC	C2'-C1'-N1-C2
3	L5	4447	5MC	C2'-C1'-N1-C2
68	S2	428	OMU	C2'-C1'-N1-C2

There are no ring outliers.

67 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	S2	1490	OMG	1	0
3	L5	2861	OMC	1	0
68	S2	649	PSU	1	0
3	L5	4196	OMG	1	0
3	L5	4536	OMC	1	0
3	L5	4523	A2M	1	0
3	L5	4618	OMG	1	0
68	S2	93	PSU	1	0
3	L5	2363	A2M	1	0
68	S2	166	A2M	3	0
68	S2	1703	OMC	2	0
3	L5	2424	OMG	1	0
3	L5	1625	OMG	1	0
68	S2	27	A2M	1	0
68	S2	601	OMG	2	0
68	S2	1442	OMU	1	0
3	L5	4579	PSU	1	0
68	S2	172	OMU	2	0
3	L5	3867	A2M	3	0
68	S2	681	PSU	1	0
3	L5	3920	PSU	1	0
3	L5	4530	UR3	1	0
68	S2	1288	OMU	2	0
3	L5	4220	6MZ	3	0
68	S2	517	OMC	1	0
68	S2	1328	OMG	1	0
3	L5	2824	OMC	1	0
3	L5	1316	OMG	1	0
3	L5	1326	A2M	1	0
3	L5	5001	PSU	1	0
3	L5	3841	OMC	1	0
3	L5	4689	PSU	1	0
3	L5	1683	PSU	1	0
3	L5	3851	PSU	1	0
3	L5	4500	PSU	1	0
3	L5	4227	OMU	1	0
3	L5	3718	A2M	2	0
68	S2	1337	4AC	2	0
3	L5	4447	5MC	2	0
3	L5	2351	OMC	2	0
68	S2	867	OMG	1	0
68	S2	1031	A2M	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4571	A2M	2	0
68	S2	159	A2M	3	0
68	S2	1232	PSU	2	0
3	L5	4637	OMG	1	0
68	S2	801	PSU	1	0
3	L5	1871	A2M	1	0
3	L5	400	A2M	1	0
3	L5	2839	PSU	1	0
3	L5	4499	OMG	1	0
3	L5	4620	OMU	1	0
68	S2	1842	4AC	1	0
68	S2	121	OMU	2	0
3	L5	4392	OMG	2	0
68	S2	484	A2M	1	0
68	S2	1383	A2M	2	0
68	S2	651	PSU	1	0
3	L5	1534	A2M	2	0
3	L5	4498	OMU	1	0
3	L5	1340	OMC	2	0
68	S2	116	OMU	2	0
68	S2	99	A2M	2	0
3	L5	4457	PSU	1	0
68	S2	509	OMG	2	0
3	L5	1781	PSU	1	0
68	S2	1850	MA6	2	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	5284	-	9,9,9	0.32	0	8,8,8	0.81	0
88	SPM	L5	5258	-	13,13,13	0.37	0	12,12,12	0.96	0
89	SPD	L5	5288	-	9,9,9	0.32	0	8,8,8	0.89	0
88	SPM	L5	5266	-	13,13,13	0.35	0	12,12,12	0.94	0
89	SPD	L5	5289	-	9,9,9	0.34	0	8,8,8	0.80	0
89	SPD	L5	5282	-	9,9,9	0.31	0	8,8,8	0.80	0
89	SPD	L5	5286	-	9,9,9	0.30	0	8,8,8	0.80	0
88	SPM	L5	5290	-	13,13,13	0.36	0	12,12,12	0.84	0
89	SPD	L5	5291	-	9,9,9	0.35	0	8,8,8	0.91	0
88	SPM	L5	5292	-	13,13,13	0.36	0	12,12,12	0.82	0
88	SPM	L5	5262	-	13,13,13	0.35	0	12,12,12	0.99	0
89	SPD	L5	5260	-	9,9,9	0.33	0	8,8,8	1.08	0
89	SPD	L5	5283	-	9,9,9	0.31	0	8,8,8	0.90	0
89	SPD	L5	5285	-	9,9,9	0.34	0	8,8,8	0.87	0
89	SPD	L8	202	-	9,9,9	0.31	0	8,8,8	0.86	0
88	SPM	L5	5263	-	13,13,13	0.38	0	12,12,12	1.13	0
88	SPM	L5	5287	-	13,13,13	0.38	0	12,12,12	0.99	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	5284	-	-	0/7/7/7	-
88	SPM	L5	5258	-	-	5/11/11/11	-
89	SPD	L5	5288	-	-	1/7/7/7	-
88	SPM	L5	5266	-	-	4/11/11/11	-
89	SPD	L5	5289	-	-	5/7/7/7	-
89	SPD	L5	5282	-	-	0/7/7/7	-
89	SPD	L5	5286	-	-	3/7/7/7	-
88	SPM	L5	5290	-	-	4/11/11/11	-
89	SPD	L5	5291	-	-	1/7/7/7	-
88	SPM	L5	5292	-	-	4/11/11/11	-
88	SPM	L5	5262	-	-	3/11/11/11	-
89	SPD	L5	5260	-	-	1/7/7/7	-
89	SPD	L5	5283	-	-	2/7/7/7	-
89	SPD	L5	5285	-	-	2/7/7/7	-
89	SPD	L8	202	-	-	2/7/7/7	-
88	SPM	L5	5263	-	-	2/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SPM	L5	5287	-	-	4/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	L5	5290	SPM	N10-C11-C12-C13
88	L5	5262	SPM	N5-C6-C7-C8
88	L5	5263	SPM	C2-C3-C4-N5
89	L5	5285	SPD	C3-C4-C5-N6
88	L5	5262	SPM	N10-C11-C12-C13
88	L5	5262	SPM	C7-C6-N5-C4
88	L5	5292	SPM	C7-C6-N5-C4
88	L5	5292	SPM	C8-C9-N10-C11
89	L5	5286	SPD	C8-C7-N6-C5
88	L5	5292	SPM	N10-C11-C12-C13
88	L5	5287	SPM	C7-C6-N5-C4
88	L5	5287	SPM	C12-C11-N10-C9
89	L5	5288	SPD	C3-C4-C5-N6
88	L5	5266	SPM	C8-C9-N10-C11
89	L5	5289	SPD	C8-C7-N6-C5
89	L5	5289	SPD	C3-C4-C5-N6
89	L8	202	SPD	C2-C3-C4-C5
89	L5	5289	SPD	C2-C3-C4-C5
88	L5	5258	SPM	C6-C7-C8-C9
88	L5	5287	SPM	C8-C9-N10-C11
89	L5	5285	SPD	C2-C3-C4-C5
88	L5	5292	SPM	C6-C7-C8-C9
88	L5	5266	SPM	C6-C7-C8-C9
89	L5	5283	SPD	C7-C8-C9-N10
88	L5	5266	SPM	N5-C6-C7-C8
89	L5	5286	SPD	N1-C2-C3-C4
88	L5	5266	SPM	C3-C4-N5-C6
88	L5	5287	SPM	C2-C3-C4-N5
89	L5	5283	SPD	C8-C7-N6-C5
88	L5	5263	SPM	N1-C2-C3-C4
88	L5	5290	SPM	N1-C2-C3-C4
88	L5	5258	SPM	N5-C6-C7-C8
89	L5	5289	SPD	N1-C2-C3-C4

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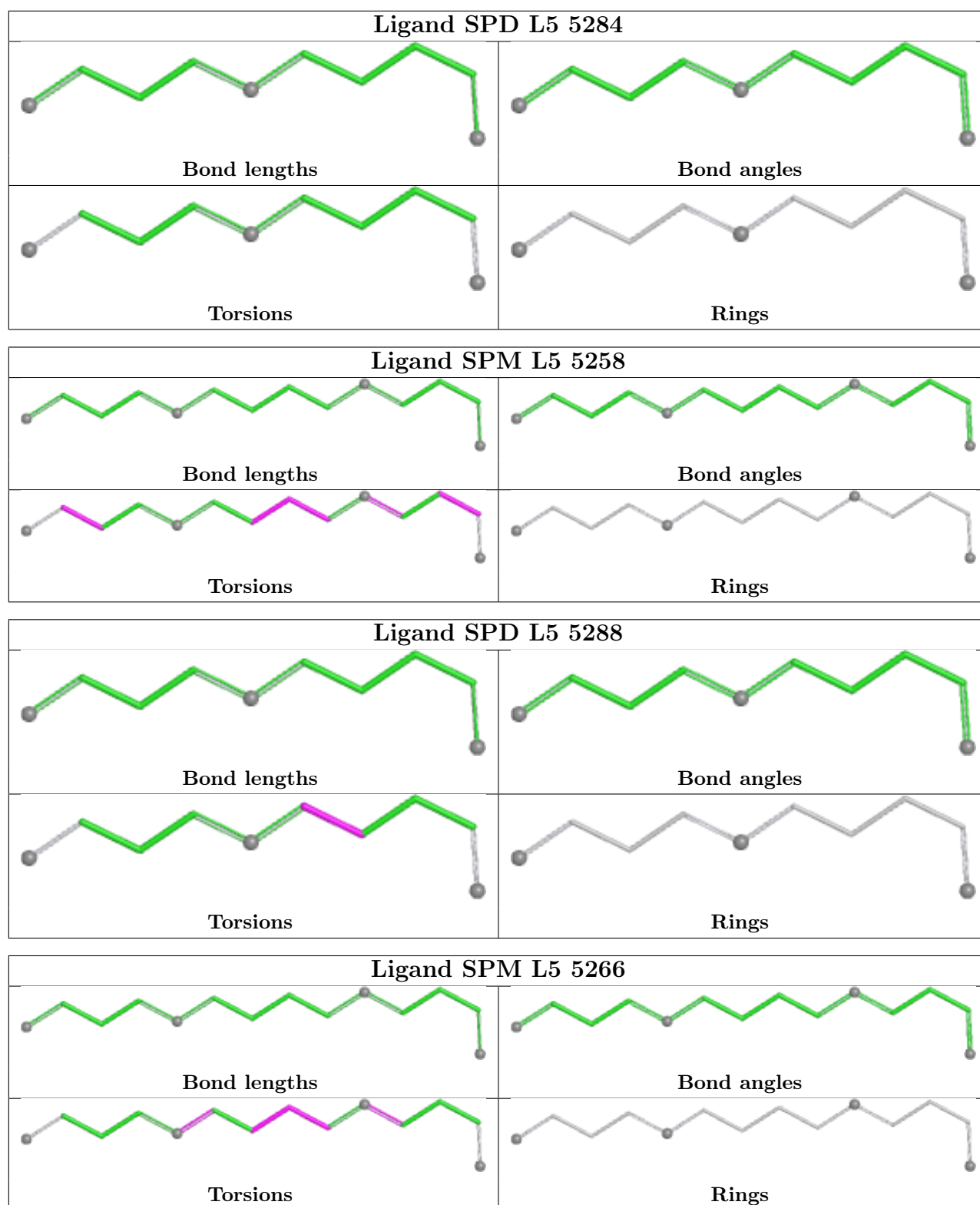
Mol	Chain	Res	Type	Atoms
89	L5	5291	SPD	C8-C7-N6-C5
89	L5	5289	SPD	N6-C7-C8-C9
88	L5	5258	SPM	C3-C4-N5-C6
89	L8	202	SPD	C8-C7-N6-C5
88	L5	5290	SPM	C8-C9-N10-C11
89	L5	5260	SPD	C8-C7-N6-C5
88	L5	5290	SPM	C7-C6-N5-C4
88	L5	5258	SPM	N1-C2-C3-C4
88	L5	5258	SPM	C11-C12-C13-N14
89	L5	5286	SPD	C4-C5-N6-C7

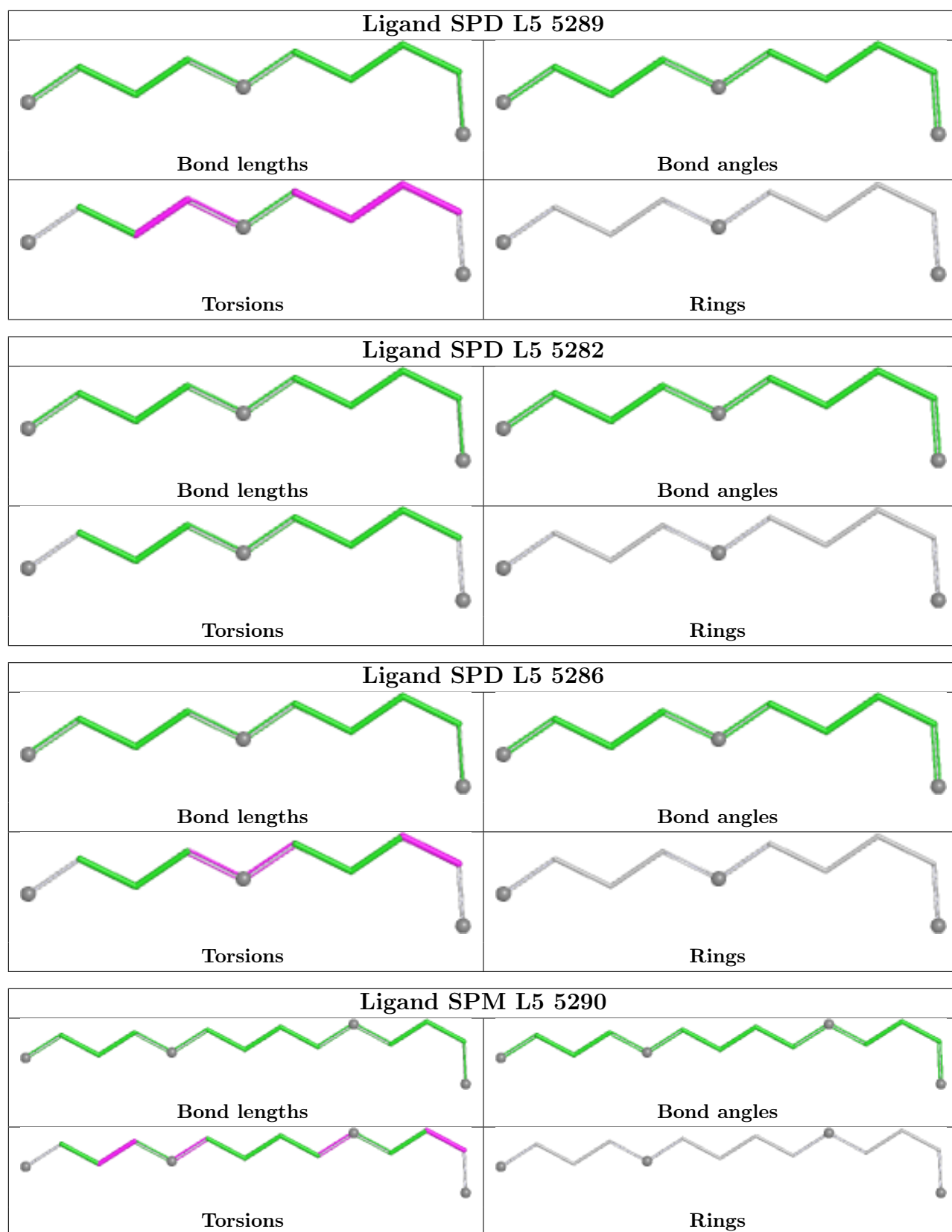
There are no ring outliers.

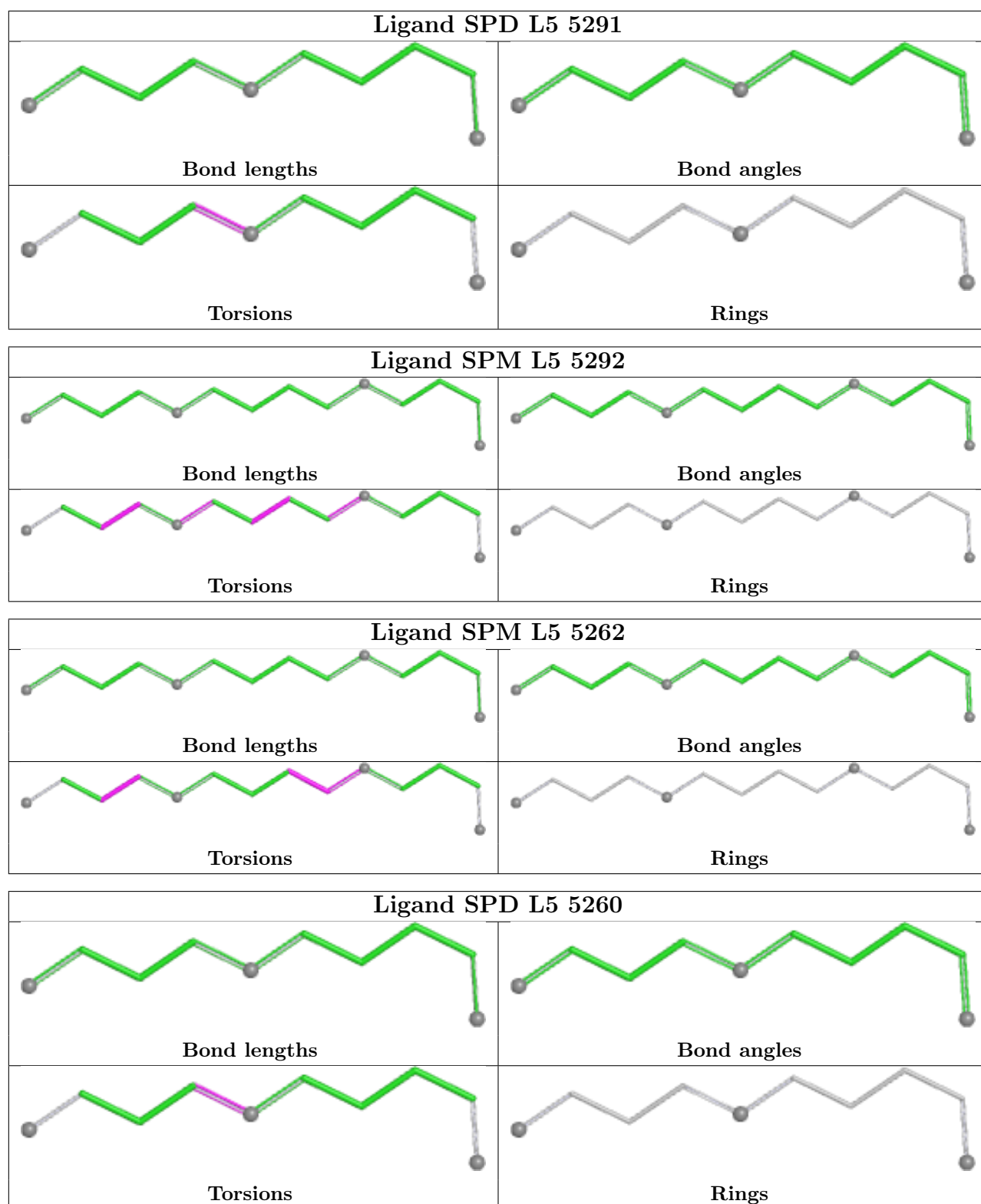
4 monomers are involved in 7 short contacts:

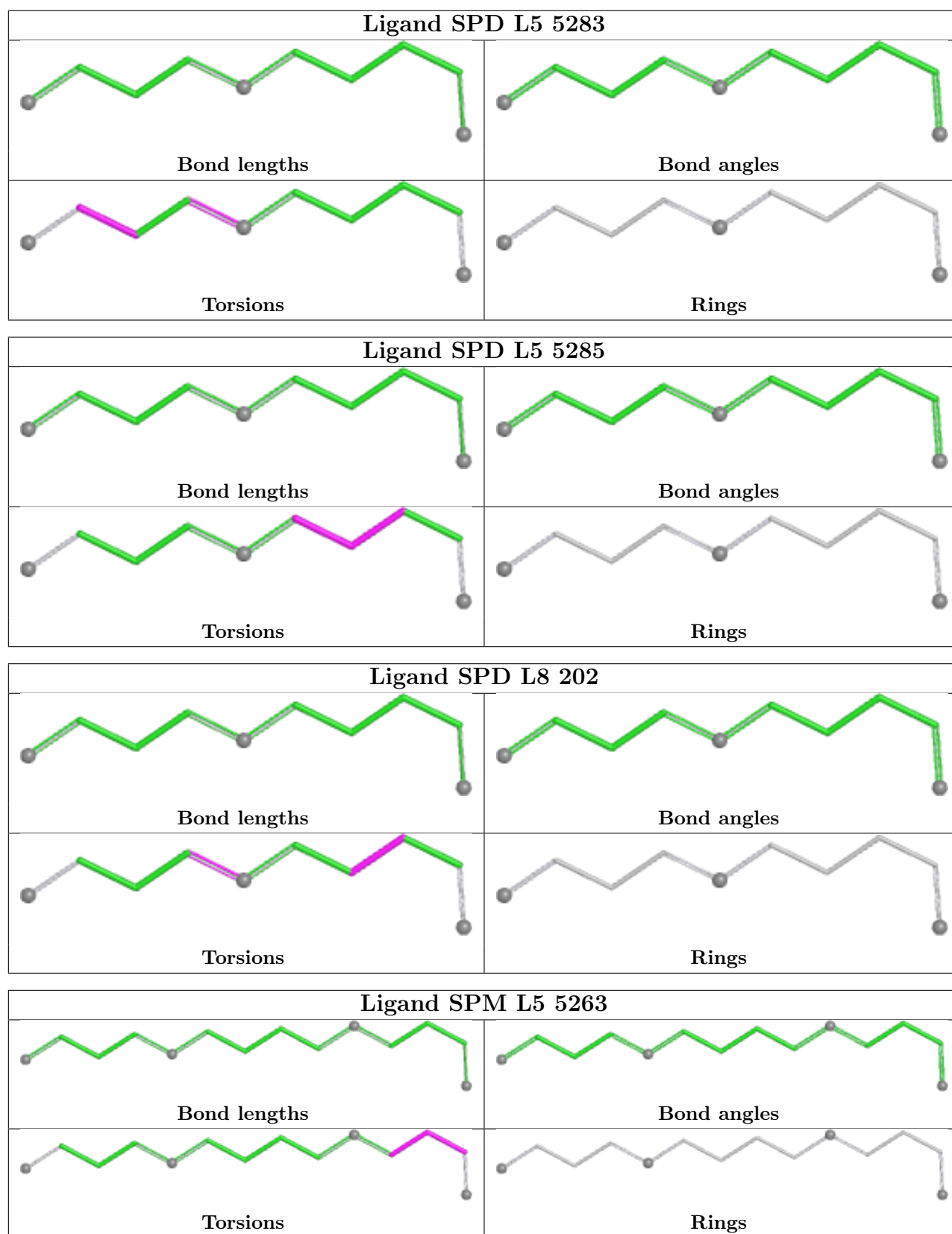
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	L5	5288	SPD	1	0
89	L5	5282	SPD	1	0
88	L5	5292	SPM	3	0
88	L5	5287	SPM	2	0

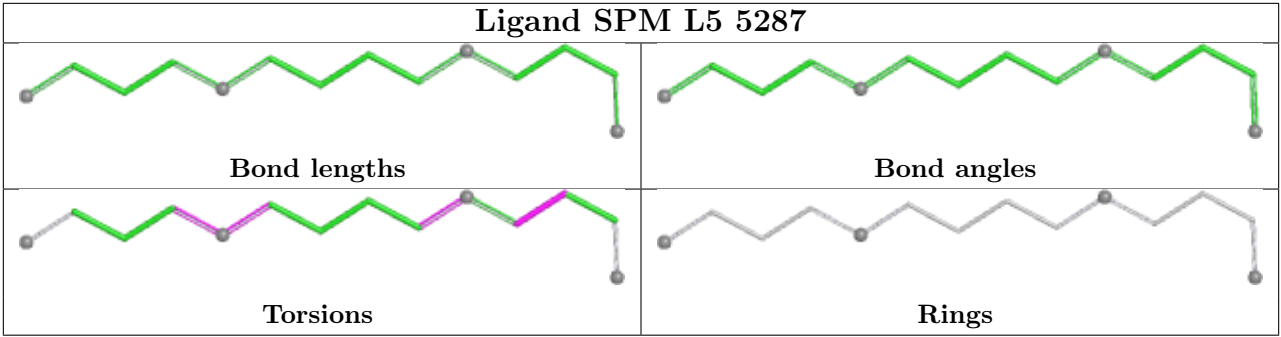
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
68	S2	5
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	28.96
1	S2	698:G	O3'	730:C	P	14.10
1	S2	739:C	O3'	746:C	P	13.38
1	S2	225:G	O3'	287:U	P	7.80
1	Et	16:C	O3'	18:U	P	7.35
1	S2	1247:C	O3'	1248:B8N	P	3.05

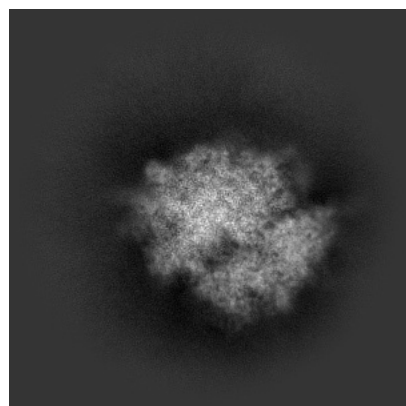
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71337. These allow visual inspection of the internal detail of the map and identification of artifacts.

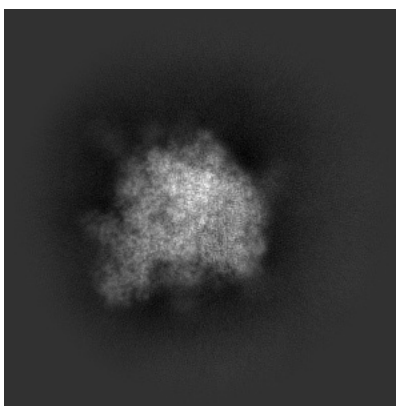
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

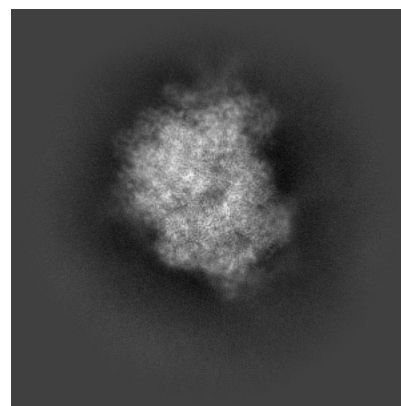
6.1.1 Primary map



X

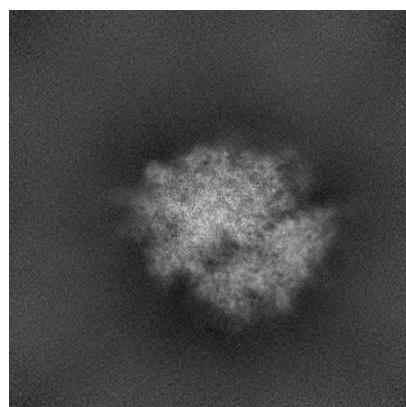


Y

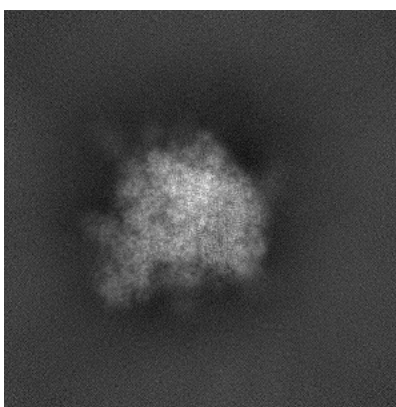


Z

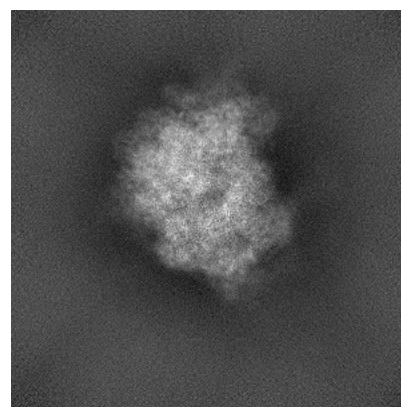
6.1.2 Raw map



X



Y

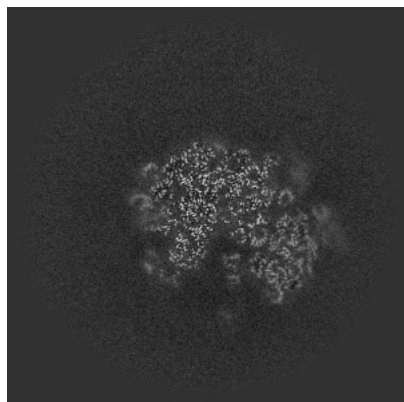


Z

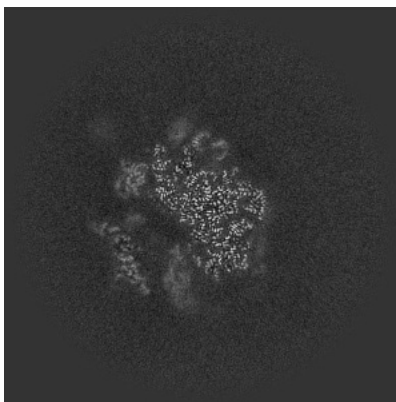
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

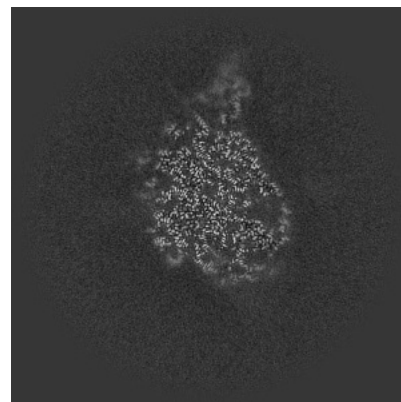
6.2.1 Primary map



X Index: 256

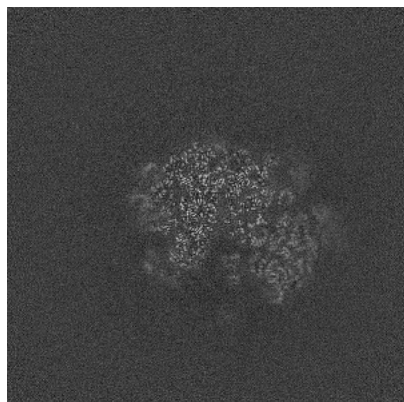


Y Index: 256

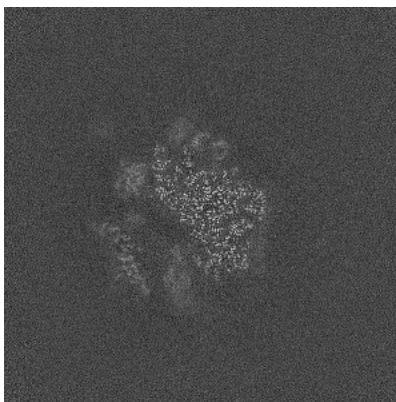


Z Index: 256

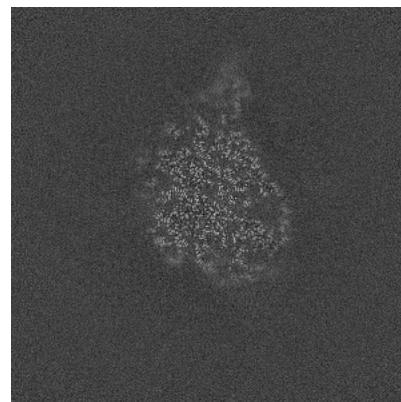
6.2.2 Raw map



X Index: 256



Y Index: 256

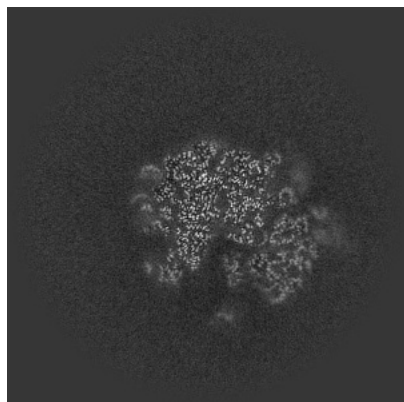


Z Index: 256

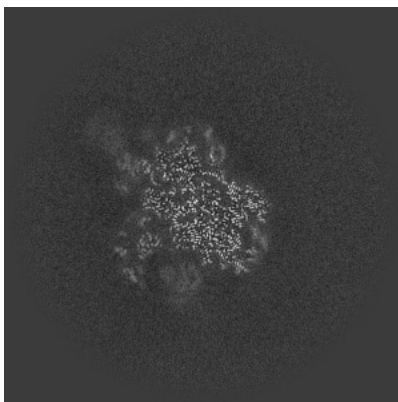
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

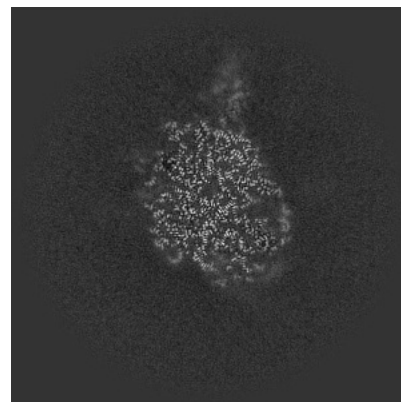
6.3.1 Primary map



X Index: 253

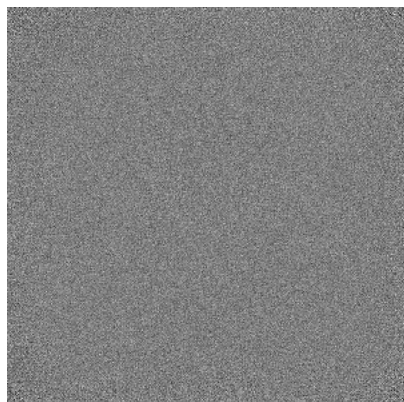


Y Index: 243

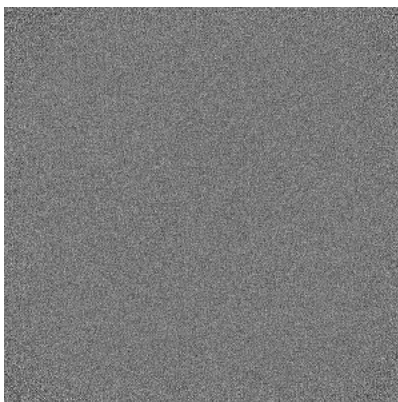


Z Index: 258

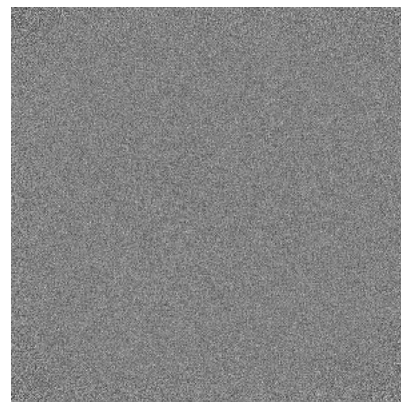
6.3.2 Raw map



X Index: 0



Y Index: 0

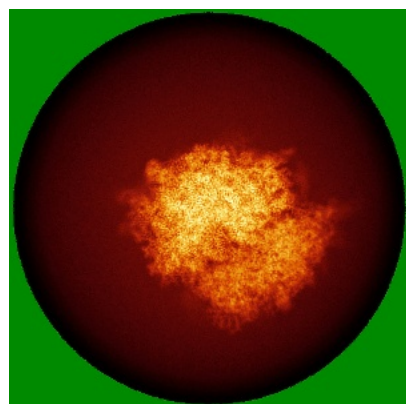


Z Index: 0

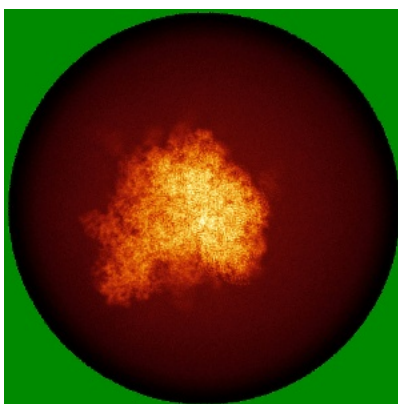
The images above show the largest variance slices of the map in three orthogonal directions.

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

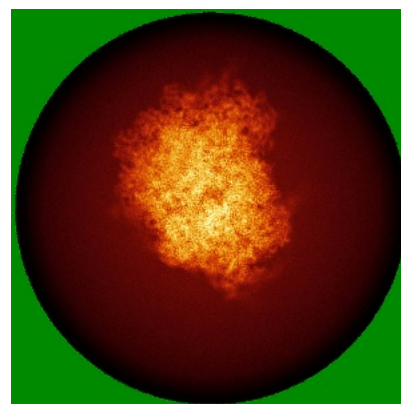
6.4.1 Primary map



X

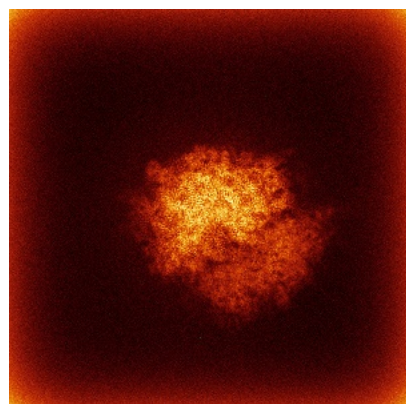


Y

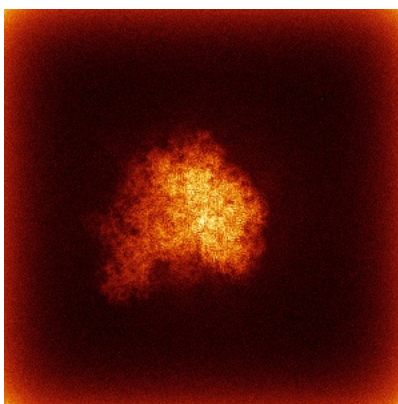


Z

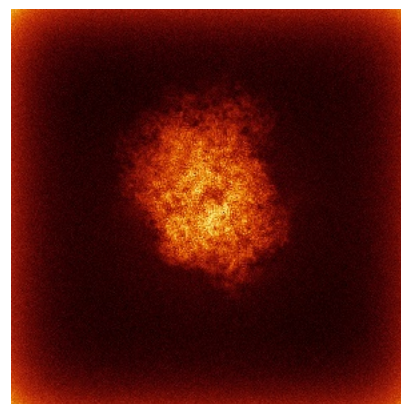
6.4.2 Raw map



X



Y

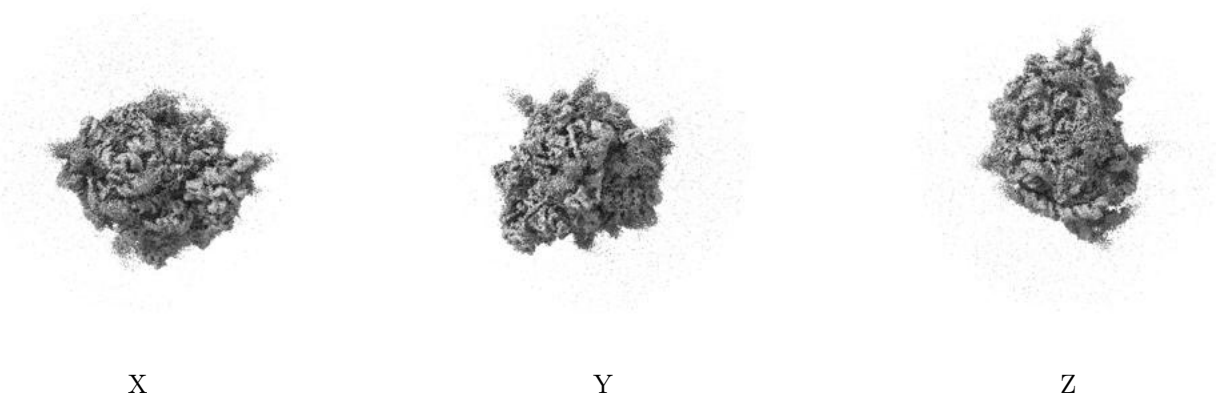


Z

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.

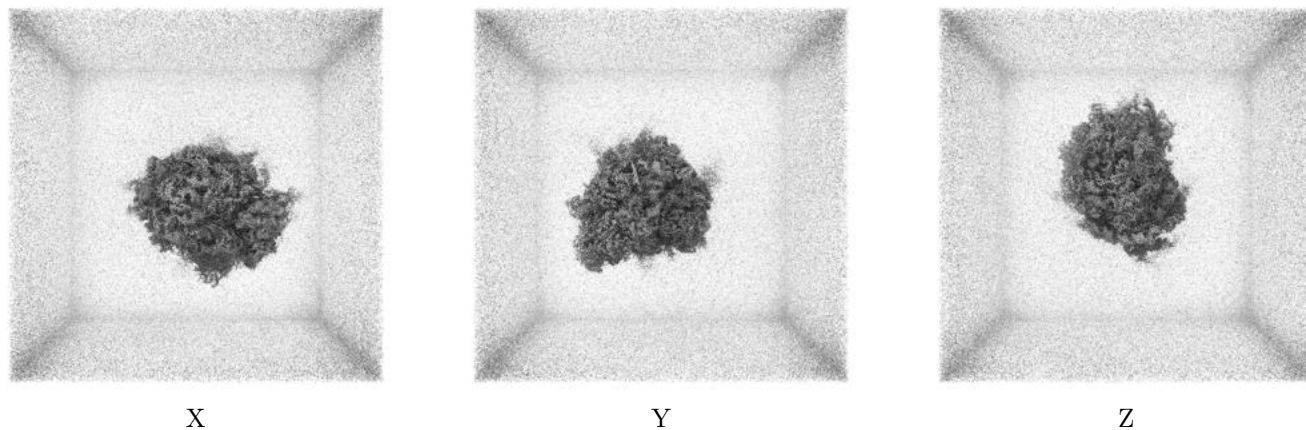
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. 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.

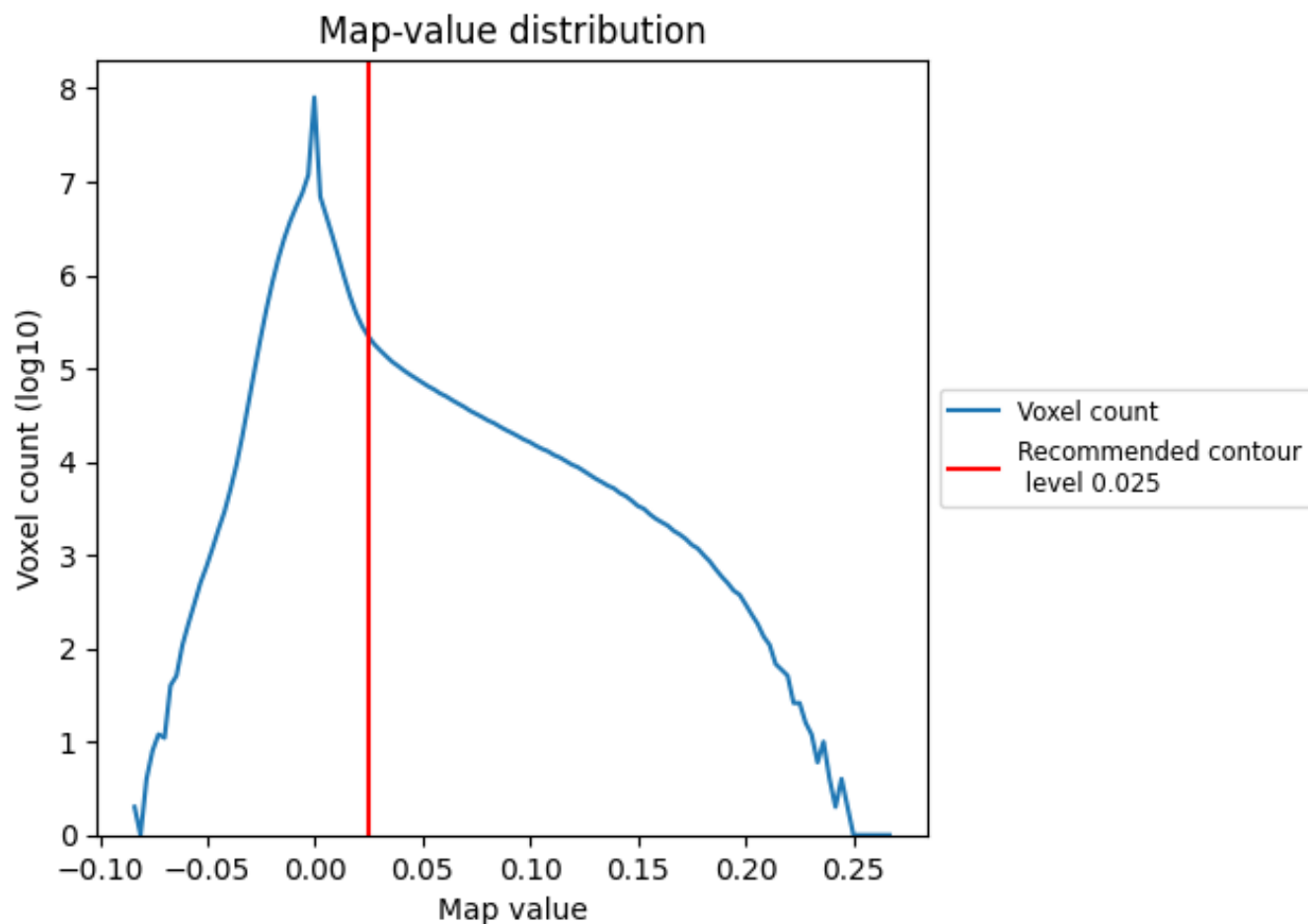
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

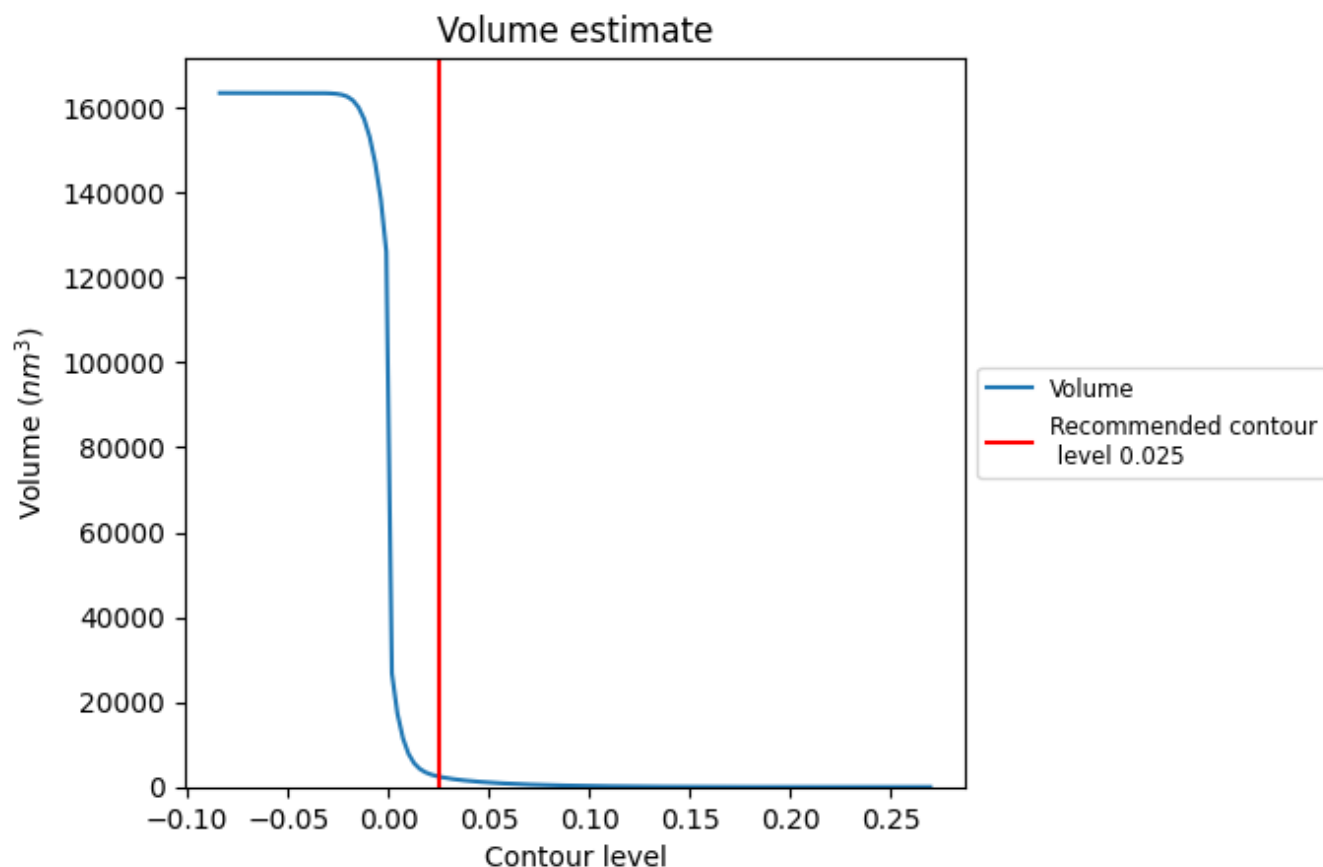
This section contains the results of statistical analysis of the map.

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.

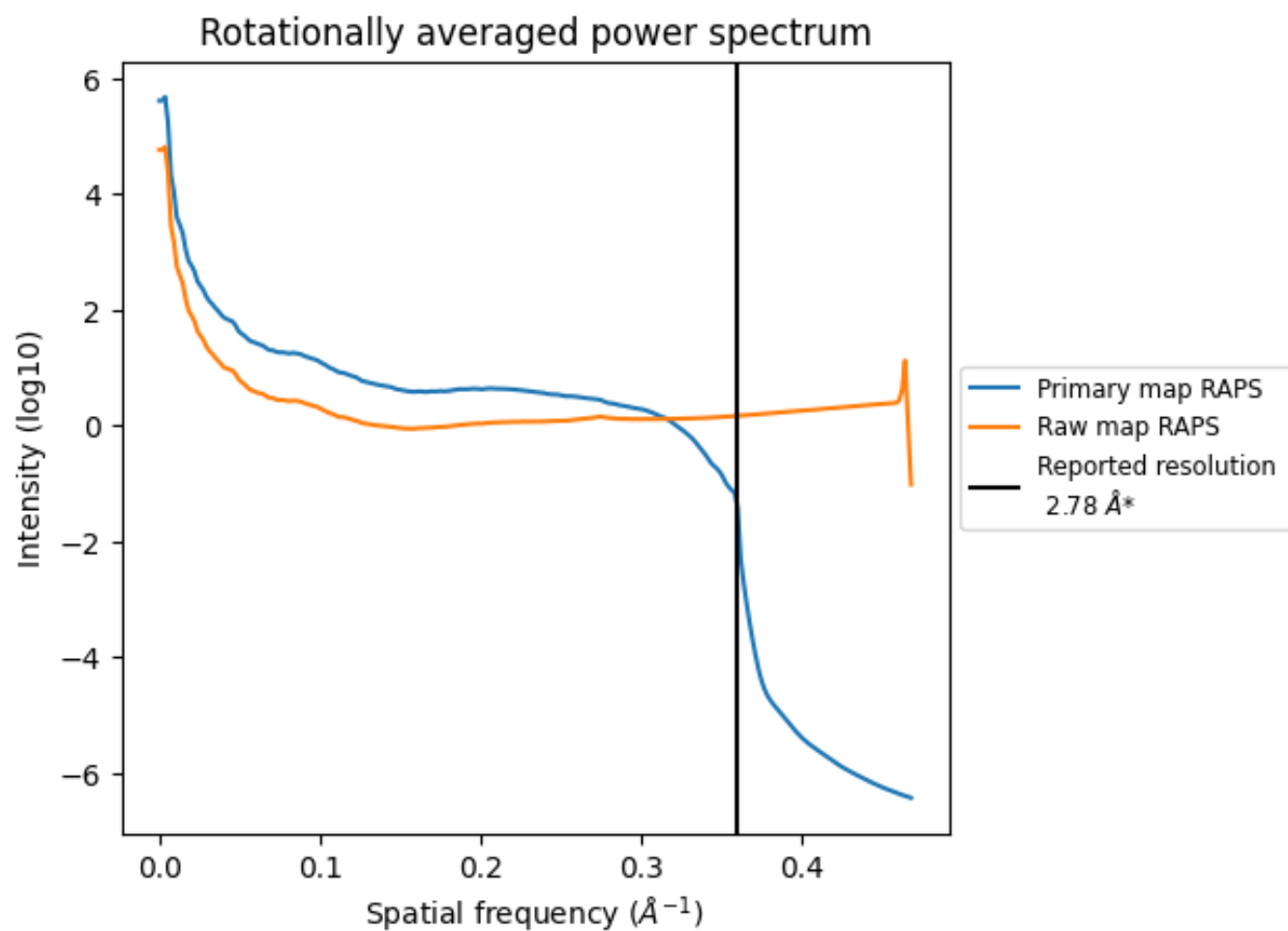
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2467 nm^3 ; this corresponds to an approximate mass of 2229 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 ⓘ

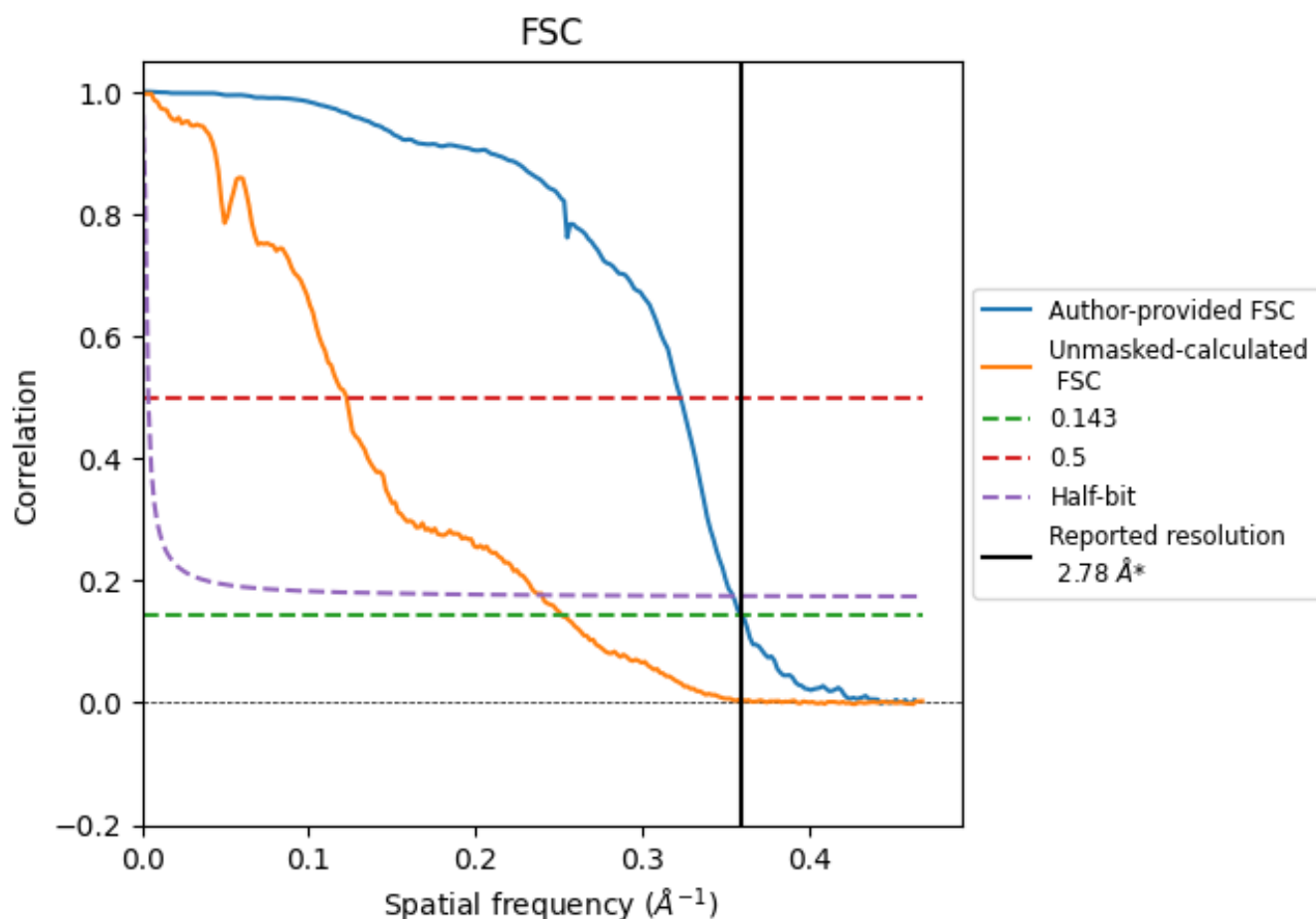


*Reported resolution corresponds to spatial frequency of 0.360 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.360 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

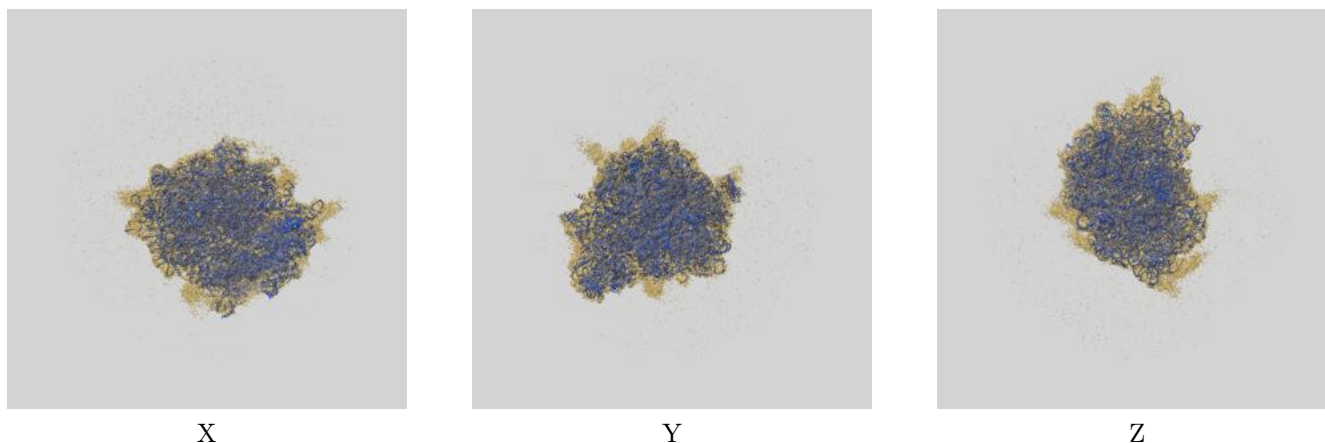
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.78	3.10	2.82
Unmasked-calculated*	3.97	8.16	4.17

*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 3.97 differs from the reported value 2.78 by more than 10 %

9 Map-model fit [i](#)

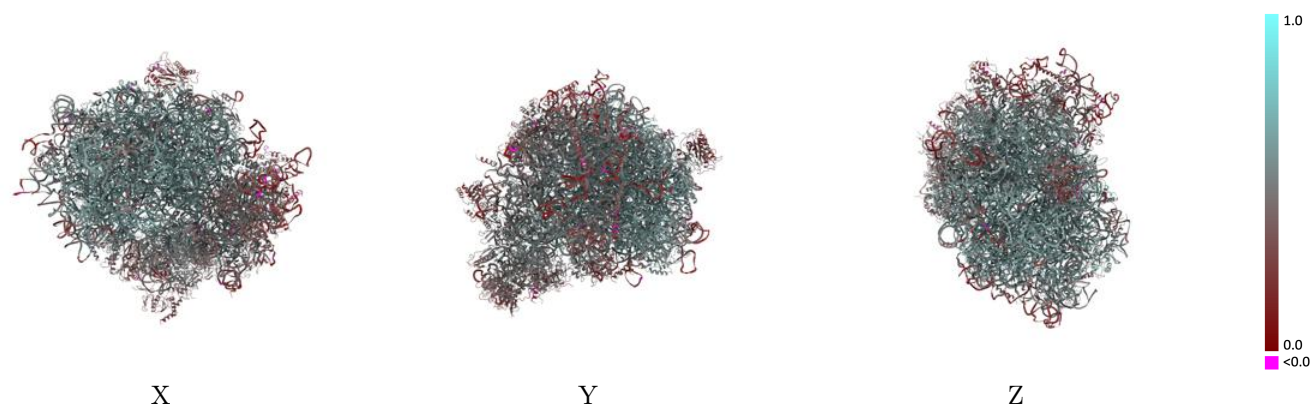
This section contains information regarding the fit between EMDB map EMD-71337 and PDB model 9P7C. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



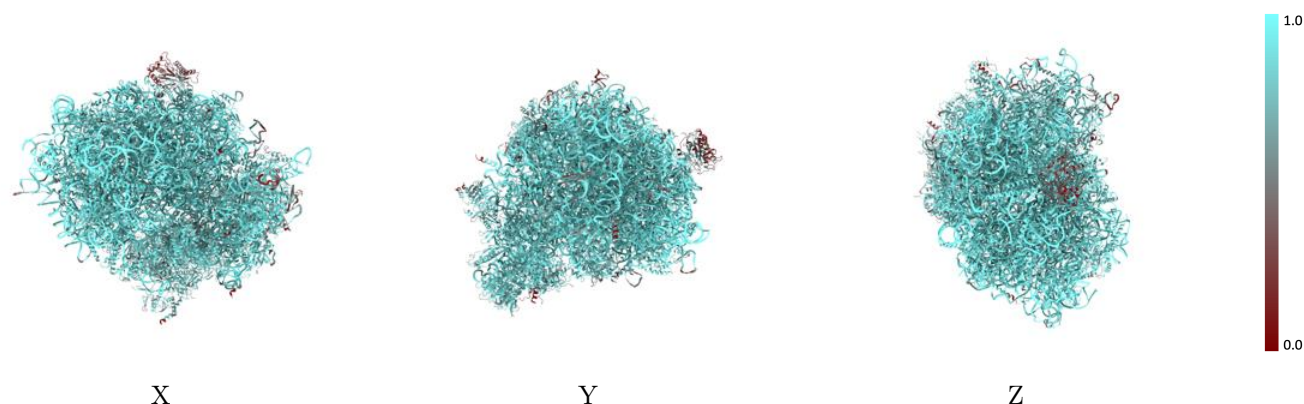
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



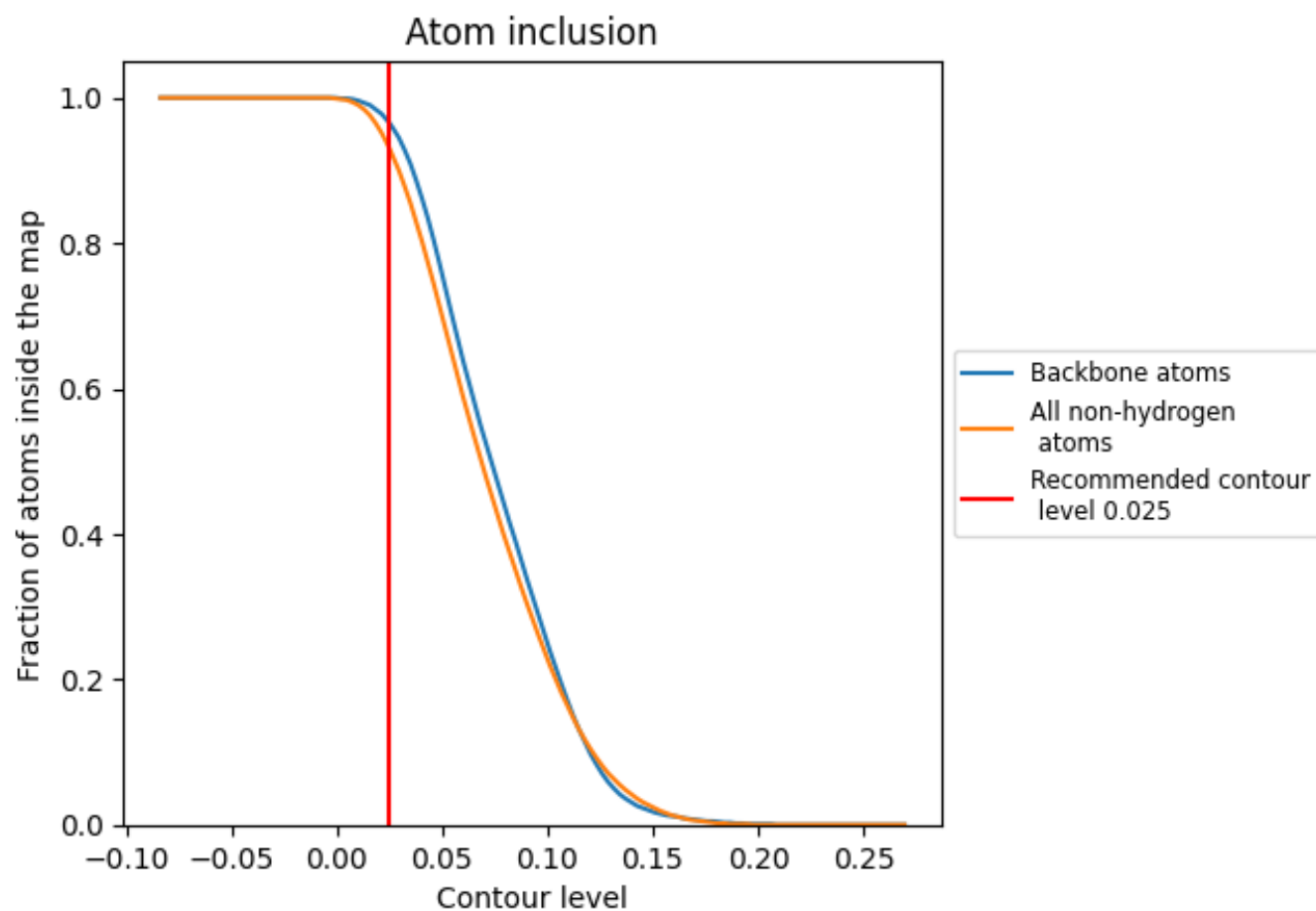
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9300	 0.5130
CA	 0.4220	 0.3300
CB	 0.8160	 0.4580
CD	 0.8530	 0.4530
CI	 0.6570	 0.4460
Et	 0.8780	 0.4030
L5	 0.9760	 0.5450
L7	 0.9960	 0.5850
L8	 0.9880	 0.5690
LA	 0.9850	 0.6080
LB	 0.9510	 0.5890
LC	 0.9600	 0.5880
LD	 0.9490	 0.5600
LE	 0.9190	 0.5430
LF	 0.9730	 0.5890
LG	 0.8970	 0.5410
LH	 0.9470	 0.5780
LI	 0.9580	 0.5920
LJ	 0.8940	 0.5340
LL	 0.9270	 0.5630
LM	 0.9650	 0.5790
LN	 0.9930	 0.6140
LO	 0.9720	 0.5930
LP	 0.9600	 0.5990
LQ	 0.9790	 0.6060
LR	 0.9050	 0.5290
LS	 0.9770	 0.5990
LT	 0.9450	 0.5760
LU	 0.9160	 0.5140
LV	 0.9640	 0.5950
LW	 0.8050	 0.4400
LX	 0.9470	 0.5680
LY	 0.9530	 0.5760
LZ	 0.9620	 0.5640
La	 0.9770	 0.6080



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Chain	Atom inclusion	Q-score
Lb	 0.9040	 0.5290
Lc	 0.9180	 0.5420
Ld	 0.9430	 0.5770
Le	 0.9800	 0.6060
Lf	 0.9830	 0.6070
Lg	 0.9510	 0.5800
Lh	 0.9450	 0.5700
Li	 0.9460	 0.5640
Lj	 0.9900	 0.6020
Lk	 0.9070	 0.5350
Ll	 0.9840	 0.5900
Lm	 0.9520	 0.5910
Ln	 0.9470	 0.5770
Lo	 0.9440	 0.5850
Lp	 0.9520	 0.5890
Lr	 0.9750	 0.5920
Ls	 0.8370	 0.4100
Lt	 0.6050	 0.2490
S2	 0.9630	 0.4660
SA	 0.8410	 0.4470
SB	 0.7970	 0.4050
SC	 0.9250	 0.5140
SD	 0.8510	 0.4630
SE	 0.8970	 0.4650
SF	 0.8230	 0.4320
SG	 0.7700	 0.3180
SH	 0.7780	 0.3650
SI	 0.8620	 0.4530
SJ	 0.8980	 0.4720
SK	 0.8520	 0.4430
SL	 0.8630	 0.4860
SM	 0.6890	 0.3090
SN	 0.8870	 0.4870
SO	 0.8450	 0.4380
SP	 0.8670	 0.4760
SQ	 0.8520	 0.4400
SR	 0.8230	 0.4250
SS	 0.8240	 0.4450
ST	 0.8730	 0.4430
SU	 0.8380	 0.4430
SV	 0.8780	 0.4700
SW	 0.9290	 0.5140

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Chain	Atom inclusion	Q-score
SX	 0.8990	 0.5270
SY	 0.8060	 0.3830
SZ	 0.7560	 0.3900
Sa	 0.8820	 0.4920
Sb	 0.8390	 0.4370
Sc	 0.7980	 0.4310
Sd	 0.9360	 0.5200
Se	 0.8240	 0.4500
Sf	 0.7360	 0.3330
Sg	 0.8030	 0.3750