



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 05:27 AM EDT

PDB ID : 9P7A / pdb_00009p7a
EMDB ID : EMD-71336
Title : In situ human hibernating class2 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 2.81 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:

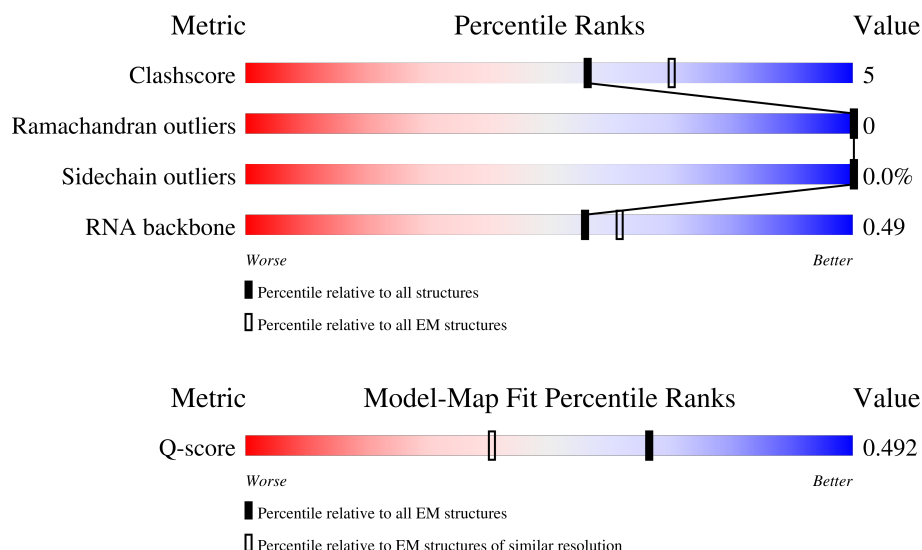
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.81 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.



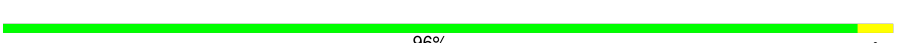
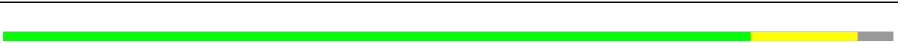
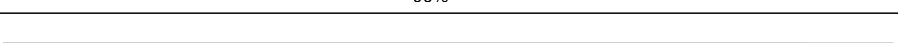
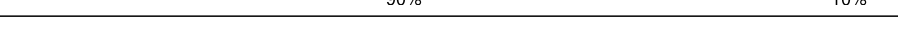
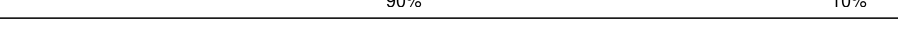
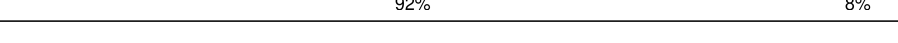
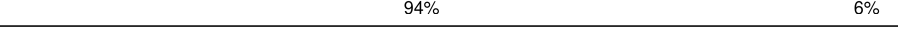
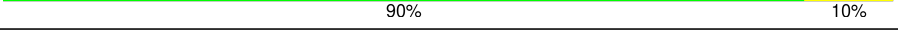
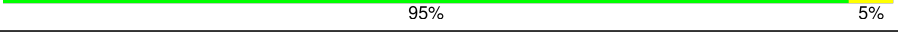
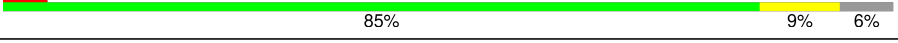
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11740 (2.31 - 3.31)

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	

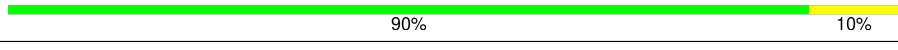
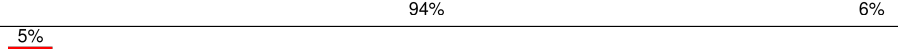
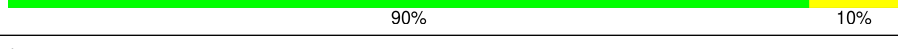
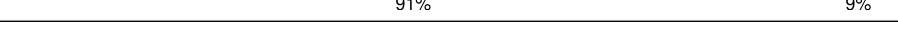
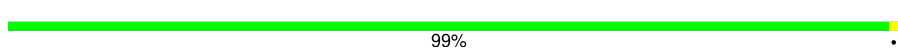
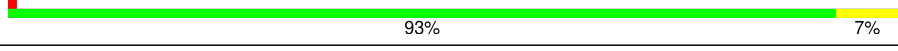
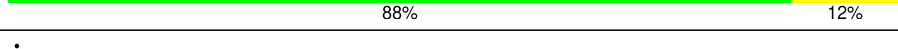
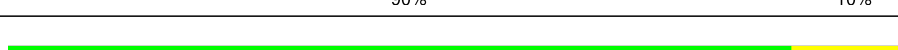
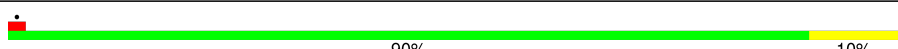
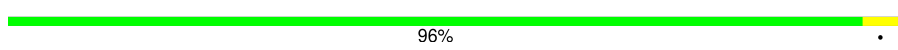
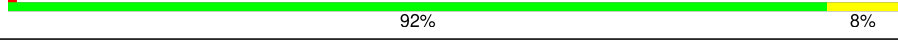
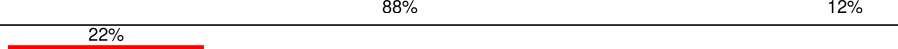
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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	156	
6	LA	248	
7	LB	402	
8	LC	368	
9	LD	293	
10	LE	250	
11	LF	225	
12	LG	241	
13	LH	190	
14	LI	213	
15	LJ	176	
16	LL	210	
17	LM	139	
18	LN	203	
19	LO	201	
20	LP	153	
21	LQ	187	
22	LR	187	
23	LS	175	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

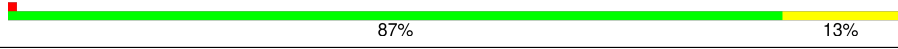
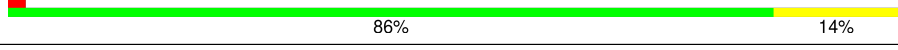
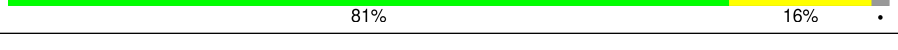
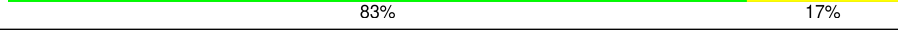
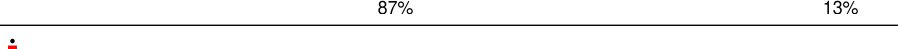
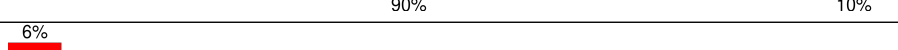
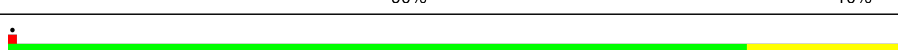
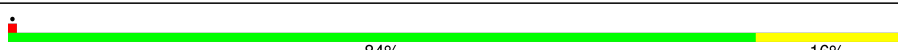
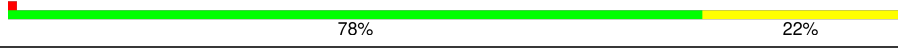
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Mol	Chain	Length	Quality of chain
29	LY	134	
30	LZ	135	
31	La	147	
32	Lb	121	
33	Lc	98	
34	Ld	107	
35	Le	128	
36	Lf	109	
37	Lg	114	
38	Lh	122	
39	Li	102	
40	Lj	86	
41	Lk	69	
42	Ll	50	
43	Lm	52	
44	Ln	24	
45	Lo	105	
46	Lp	91	
47	Lr	125	
48	Ls	196	
49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

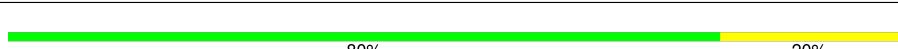
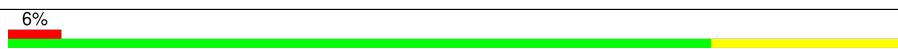
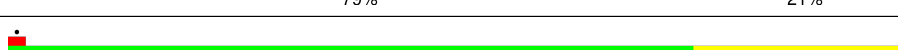
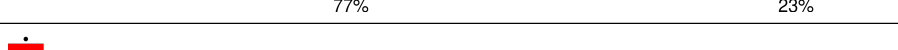
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Mol	Chain	Length	Quality of chain
54	SG	237	
55	SH	189	
56	SI	206	
57	SJ	185	
58	SL	153	
59	SN	150	
60	SO	140	
61	SV	83	
62	SW	129	
63	SX	141	
64	SY	131	
65	Sa	102	
66	Sb	83	
67	Se	58	
68	S2	1740	
69	SR	135	
70	SD	227	
71	SF	189	
72	SK	98	
73	SM	122	
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.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 85 is a protein called Elongation factor 2.

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

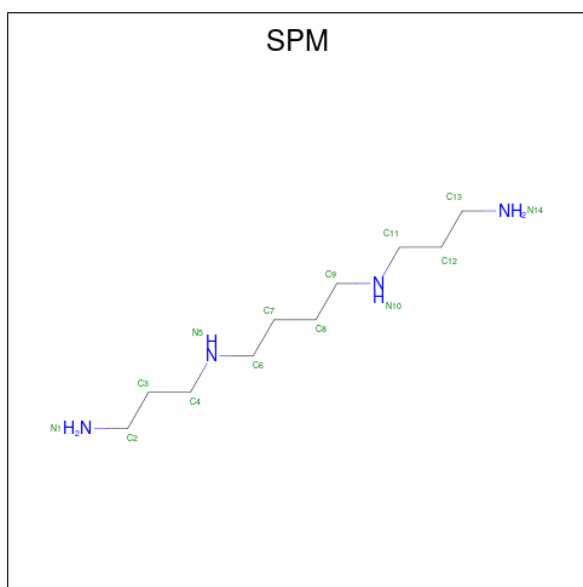
- Molecule 86 is a protein called Proliferation-associated protein 2G4.

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

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

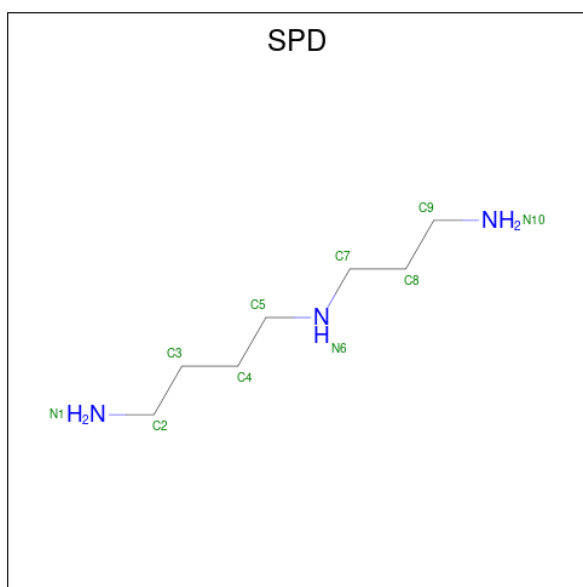
Mol	Chain	Residues	Atoms		AltConf
87	L5	179	Total	Mg	0
			179	179	
87	L7	3	Total	Mg	0
			3	3	
87	L8	5	Total	Mg	0
			5	5	
87	LA	1	Total	Mg	0
			1	1	
87	LP	1	Total	Mg	0
			1	1	
87	LV	1	Total	Mg	0
			1	1	
87	Le	1	Total	Mg	0
			1	1	
87	S2	27	Total	Mg	0
			27	27	

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



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

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



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

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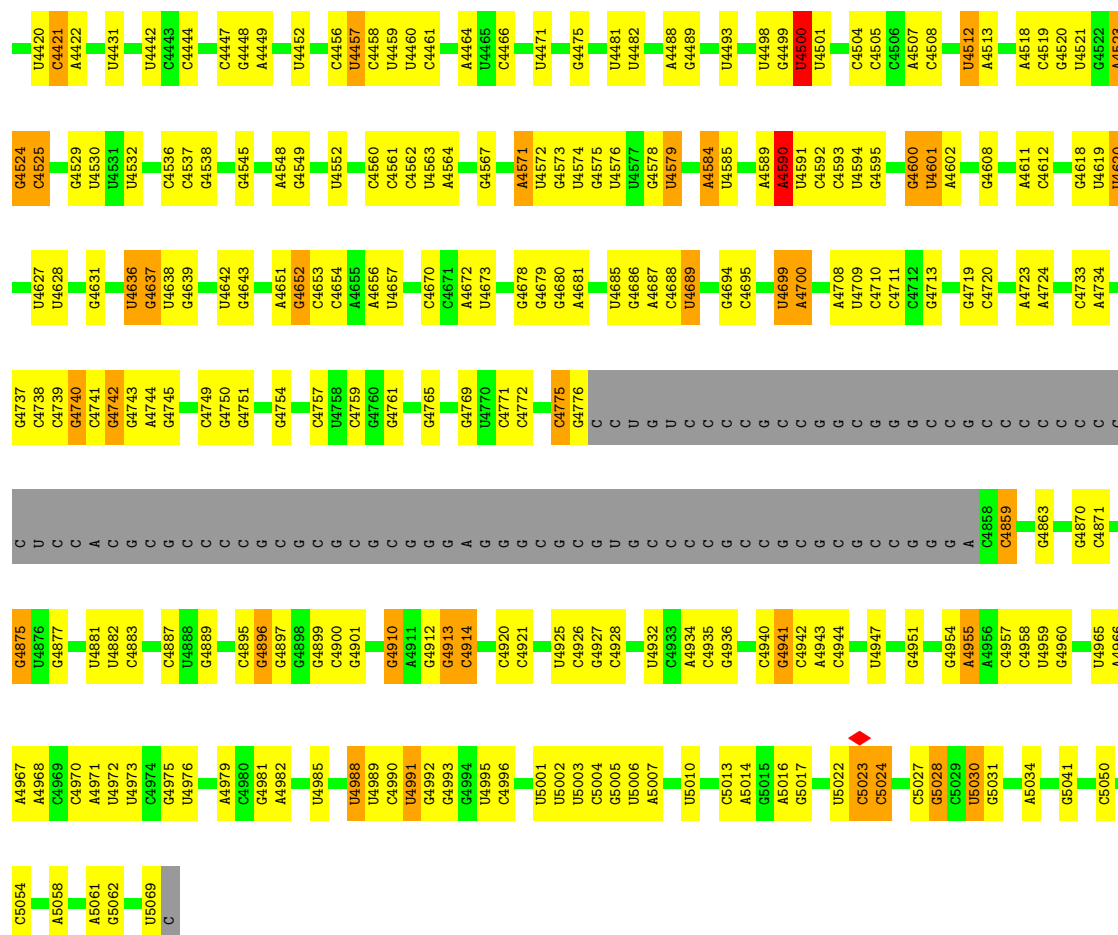
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Mol	Chain	Residues	Atoms		AltConf
90	Lj	1	Total 1	Zn 1	0
90	Lm	1	Total 1	Zn 1	0
90	Lo	1	Total 1	Zn 1	0
90	Lp	1	Total 1	Zn 1	0
90	Sa	1	Total 1	Zn 1	0



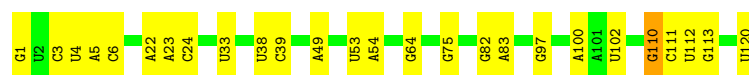






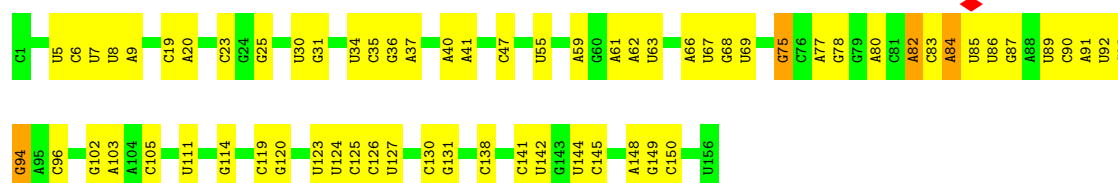
• Molecule 4: 5S rRNA

Chain L7: 78% 21%



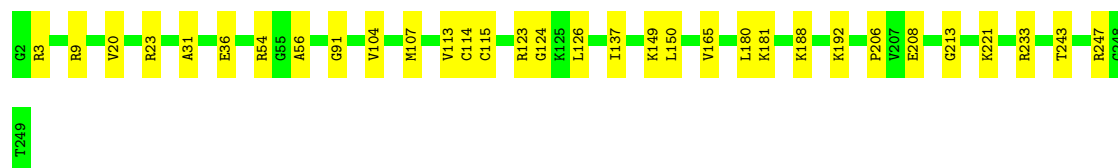
• Molecule 5: 5.8S rRNA

Chain L8: 58% 40%

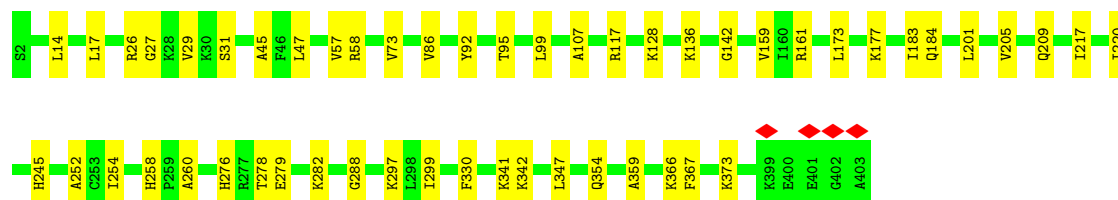


• Molecule 6: 60S ribosomal protein L8

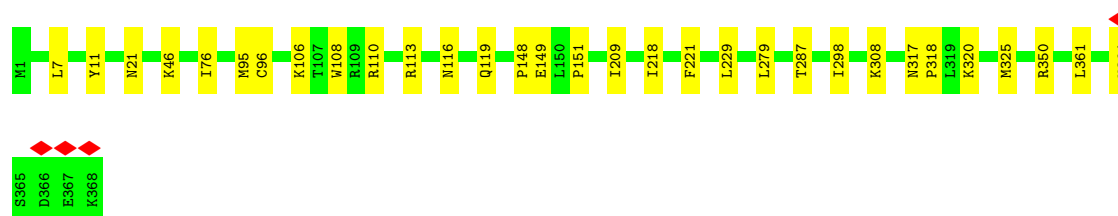
Chain LA: 87% 13%



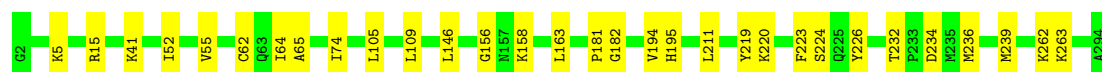
- Molecule 7: Large ribosomal subunit protein uL3



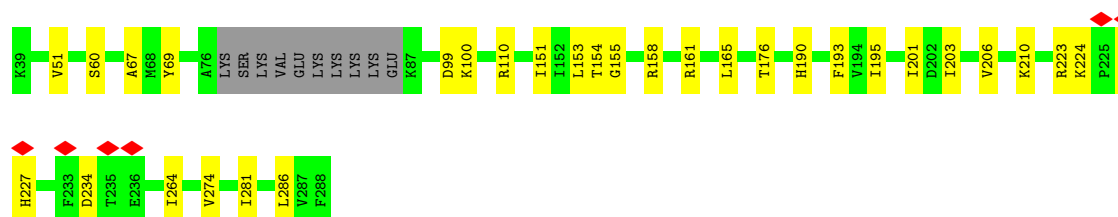
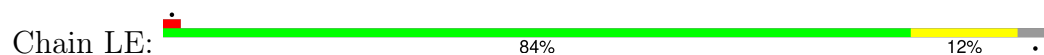
- Molecule 8: 60S ribosomal protein L4



- Molecule 9: Large ribosomal subunit protein uL18



- Molecule 10: Large ribosomal subunit protein eL6

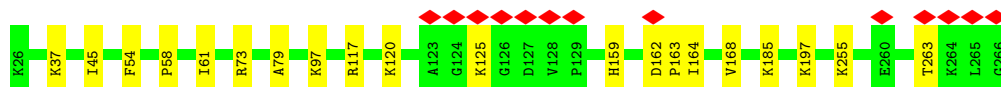


- Molecule 11: 60S ribosomal protein L7

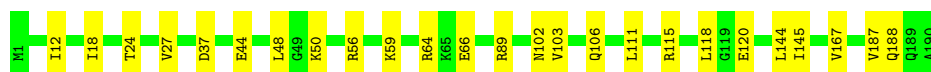
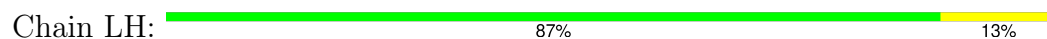




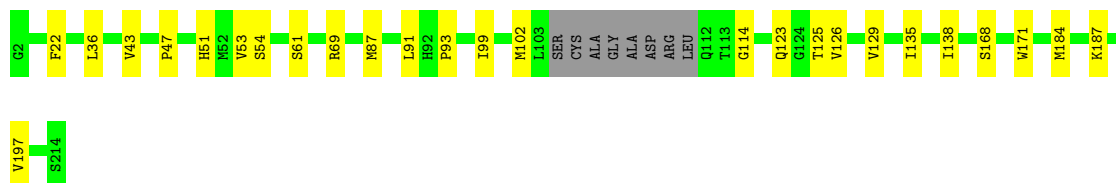
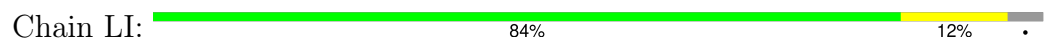
- Molecule 12: 60S ribosomal protein L7a



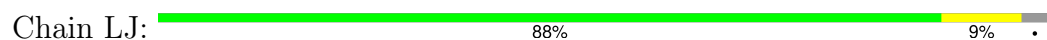
- Molecule 13: 60S ribosomal protein L9



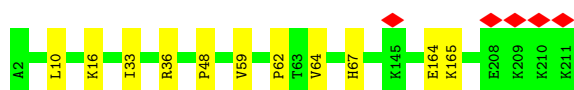
- Molecule 14: Ribosomal protein uL16-like



- Molecule 15: 60S ribosomal protein L11



- Molecule 16: Large ribosomal subunit protein eL13



- Molecule 17: 60S ribosomal protein L14



- Molecule 18: 60S ribosomal protein L15

Chain LN:  90% 10%



- Molecule 19: 60S ribosomal protein L13a

Chain LO:  90% 10%



- Molecule 20: 60S ribosomal protein L17

Chain LP:  92% 8%



- Molecule 21: 60S ribosomal protein L18

Chain LQ:  91% 9%



- Molecule 22: 60S ribosomal protein L19

Chain LR:  94% 6%



- Molecule 23: 60S ribosomal protein L18a

Chain LS:  90% 10%



- Molecule 24: 60S ribosomal protein L21

Chain LT:  95% 5%



- Molecule 25: Heparin-binding protein HBp15

Chain LU:  86% 14%



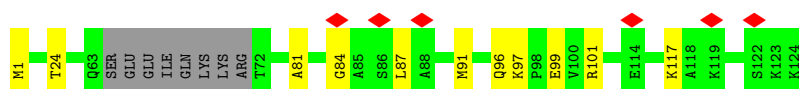
- Molecule 26: 60S ribosomal protein L23

Chain LV:  91% 9%



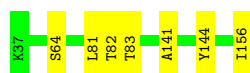
- Molecule 27: Ribosomal protein L24

Chain LW:  5% 85% 9% 6%



- Molecule 28: 60S ribosomal protein L23a

Chain LX:  94% 6%



- Molecule 29: 60S ribosomal protein L26

Chain LY:  90% 10%



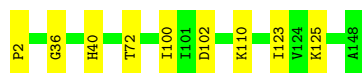
- Molecule 30: 60S ribosomal protein L27

Chain LZ:  90% 10%

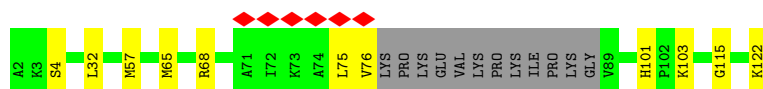
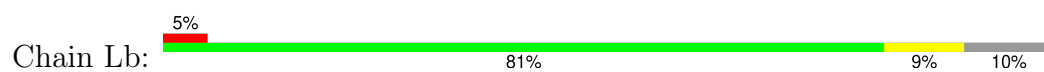


- Molecule 31: 60S ribosomal protein L27a

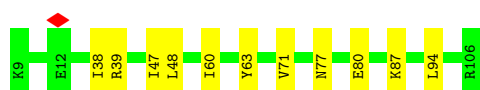
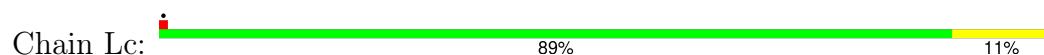
Chain La:  94% 6%



- Molecule 32: Large ribosomal subunit protein eL29



- Molecule 33: 60S ribosomal protein L30



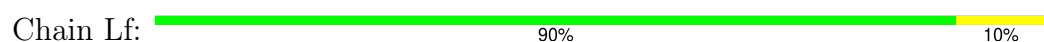
- Molecule 34: 60S ribosomal protein L31



- Molecule 35: 60S ribosomal protein L32



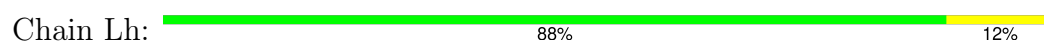
- Molecule 36: 60S ribosomal protein L35a



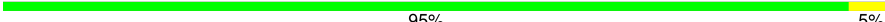
- Molecule 37: 60S ribosomal protein L34



- Molecule 38: 60S ribosomal protein L35

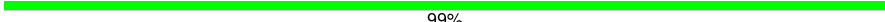


- Molecule 39: 60S ribosomal protein L36

Chain Li:  95% 5%



- Molecule 40: 60S ribosomal protein L37

Chain Lj:  99% .



- Molecule 41: 60S ribosomal protein L38

Chain Lk:  93% 7%



- Molecule 42: 60S ribosomal protein L39

Chain Ll:  88% 12%



- Molecule 43: Large ribosomal subunit protein eL40

Chain Lm:  90% 10%



- Molecule 44: 60S ribosomal protein L41

Chain Ln:  88% 12%

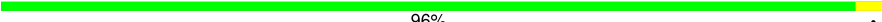


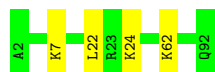
- Molecule 45: 60S ribosomal protein L36a

Chain Lo:  90% 10%



- Molecule 46: 60S ribosomal protein L37a

Chain Lp:  96%



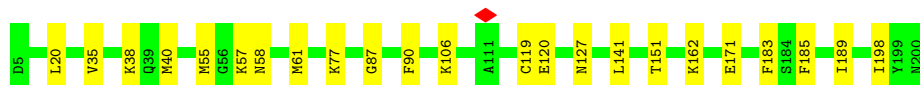
- Molecule 47: 60S ribosomal protein L28

Chain Lr:  92%



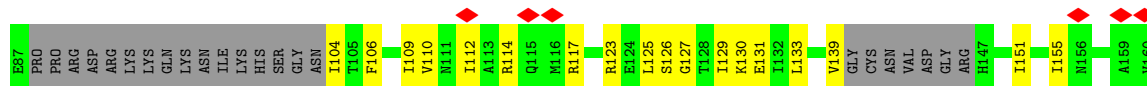
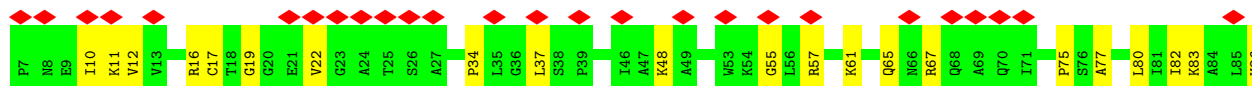
- Molecule 48: 60S acidic ribosomal protein P0

Chain Ls:  88%



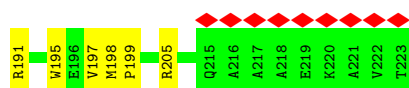
- Molecule 49: Large ribosomal subunit protein uL11

Chain Lt:  22% 60% 25% 15%



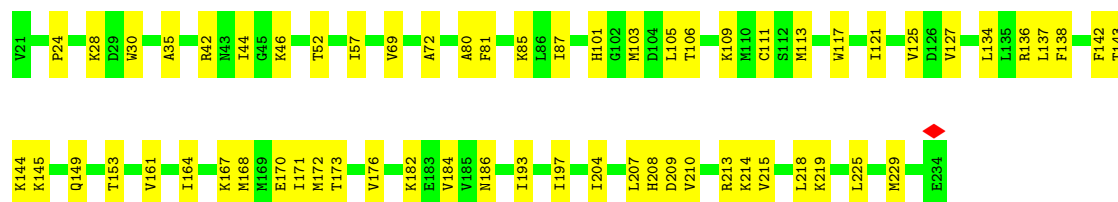
- Molecule 50: 40S ribosomal protein SA

Chain SA:  5% 82% 18%

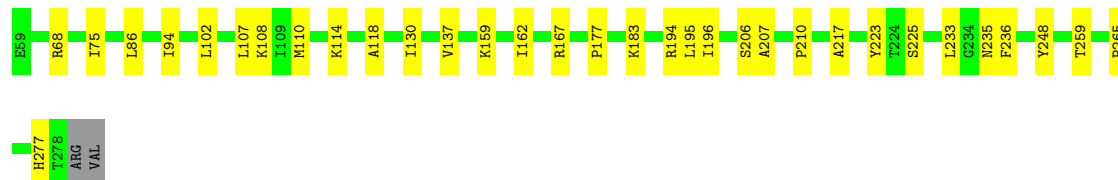
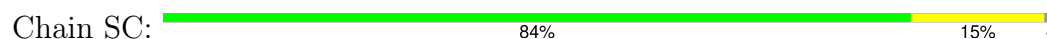


- Molecule 51: 40S ribosomal protein S3a

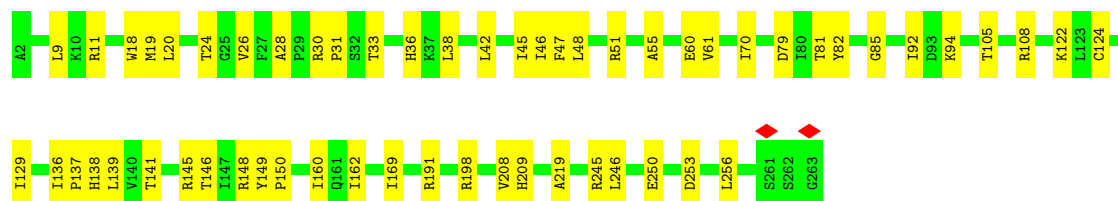
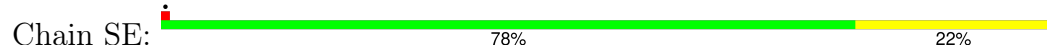
Chain SB:  71% 29%



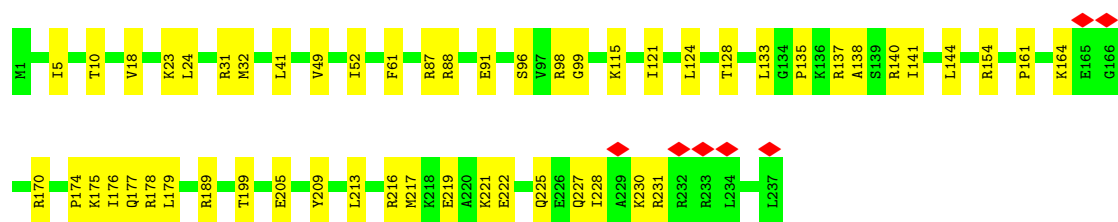
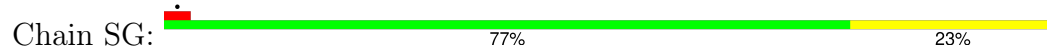
• Molecule 52: 40S ribosomal protein S2



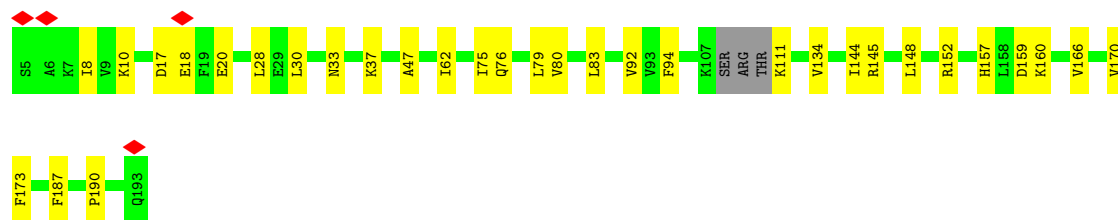
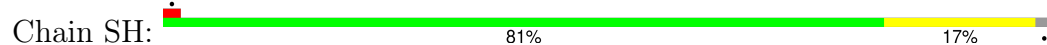
• Molecule 53: Small ribosomal subunit protein eS4, X isoform



• Molecule 54: 40S ribosomal protein S6

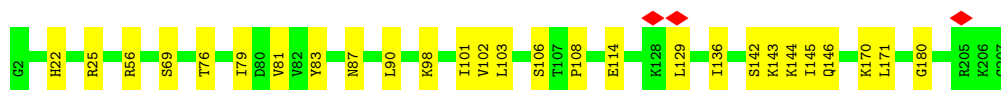


• Molecule 55: Small ribosomal subunit protein eS7



- Molecule 56: 40S ribosomal protein S8

Chain SI:  87% 13%



- Molecule 57: 40S ribosomal protein S9

Chain SJ:  86% 14%



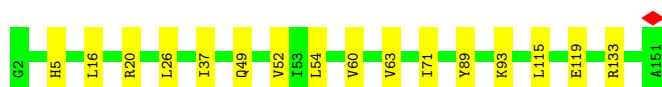
- Molecule 58: 40S ribosomal protein S11

Chain SL:  89% 11%



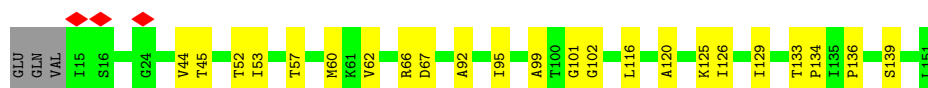
- Molecule 59: 40S ribosomal protein S13

Chain SN:  89% 11%



- Molecule 60: Small ribosomal subunit protein uS11

Chain SO:  81% 16%



- Molecule 61: Small ribosomal subunit protein eS21

Chain SV:  83% 17%

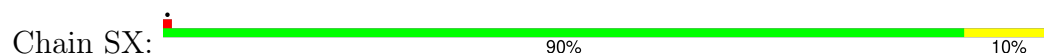


- Molecule 62: 40S ribosomal protein S15a

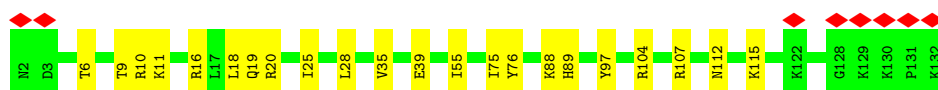
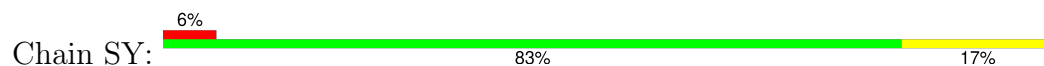
Chain SW:  87% 13%



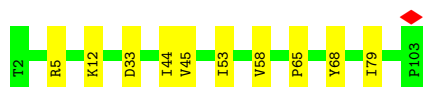
- Molecule 63: 40S ribosomal protein S23



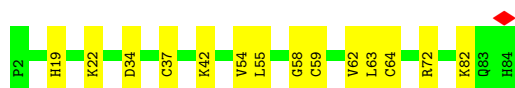
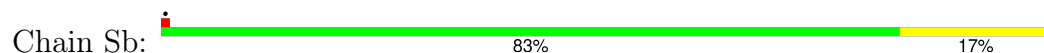
- Molecule 64: 40S ribosomal protein S24



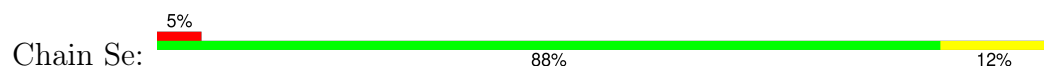
- Molecule 65: 40S ribosomal protein S26



- Molecule 66: Small ribosomal subunit protein eS27

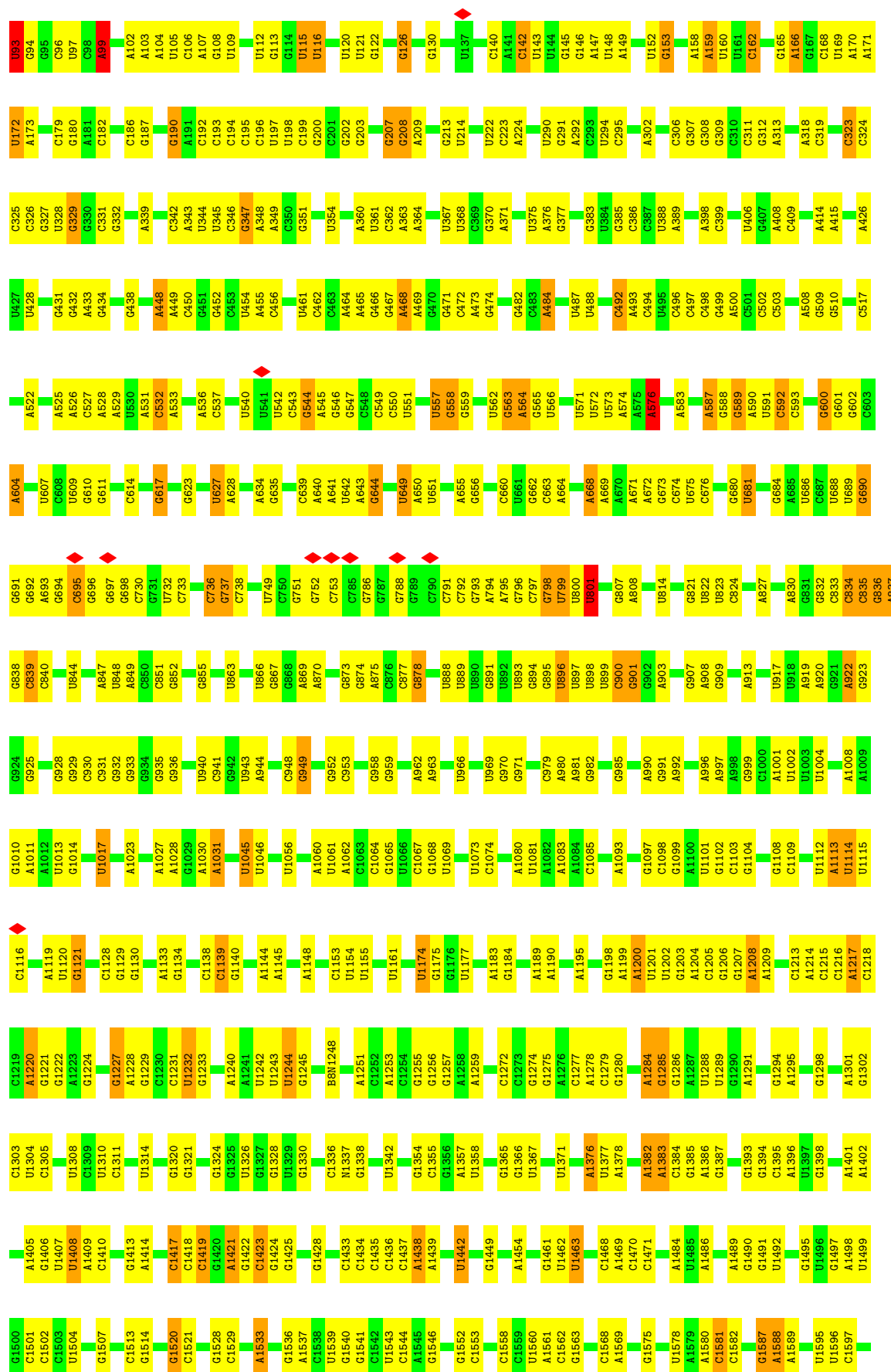


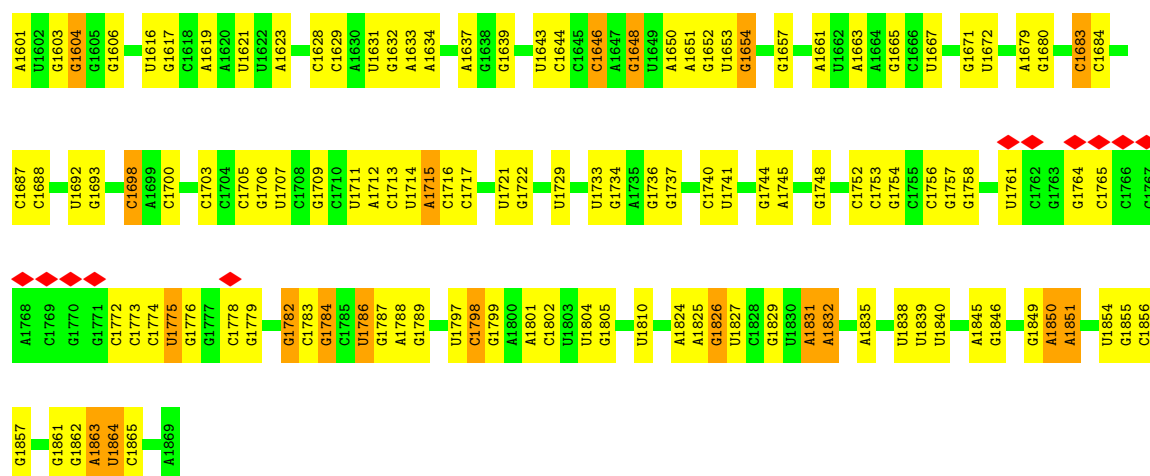
- Molecule 67: Small ribosomal subunit protein eS30



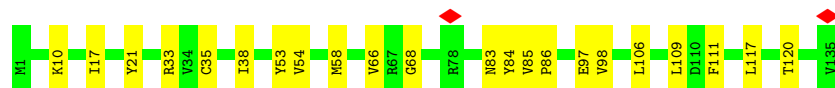
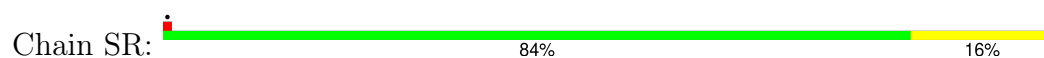
- Molecule 68: 18S rRNA







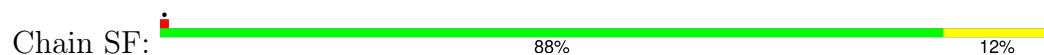
- Molecule 69: Small ribosomal subunit protein eS17



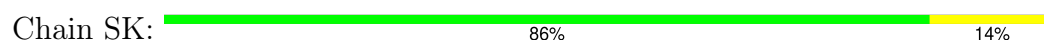
- Molecule 70: Small ribosomal subunit protein uS3



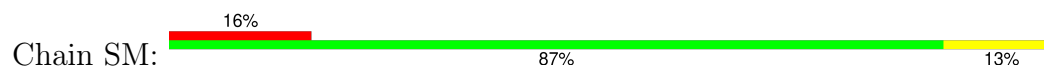
- Molecule 71: 40S ribosomal protein S5

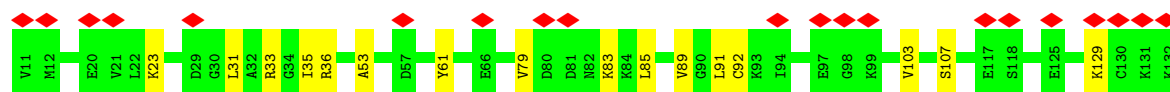


- Molecule 72: 40S ribosomal protein S10

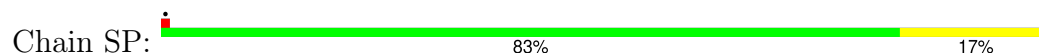


- Molecule 73: Small ribosomal subunit protein eS12

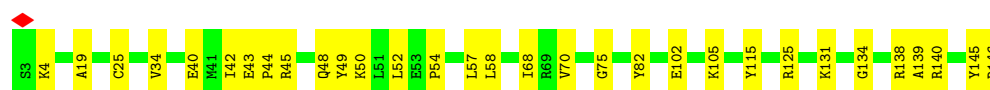
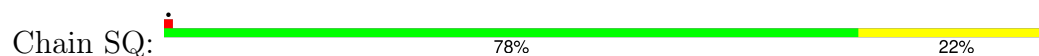




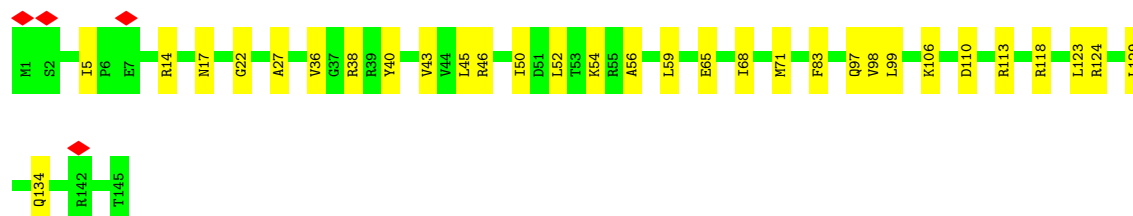
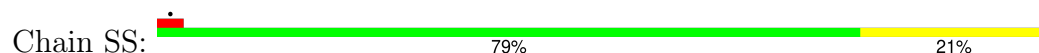
- Molecule 74: Small ribosomal subunit protein uS19



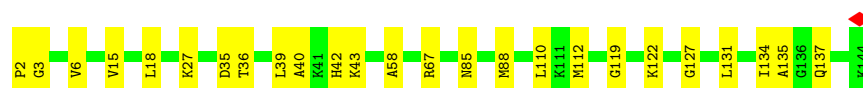
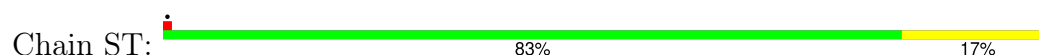
- Molecule 75: Small ribosomal subunit protein uS9



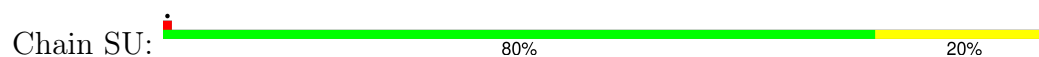
- Molecule 76: 40S ribosomal protein S18



- Molecule 77: 40S ribosomal protein S19

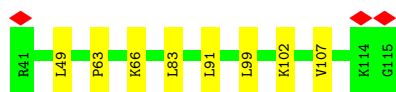


- Molecule 78: 40S ribosomal protein S20

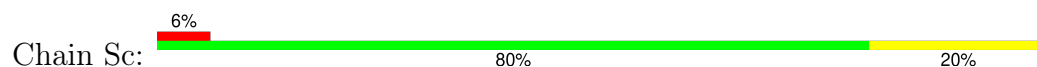


- Molecule 79: Small ribosomal subunit protein eS25

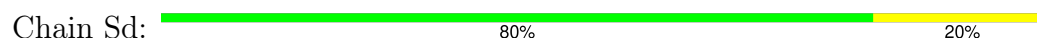




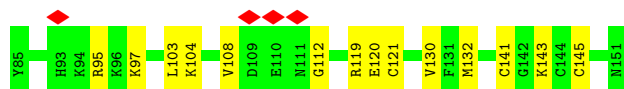
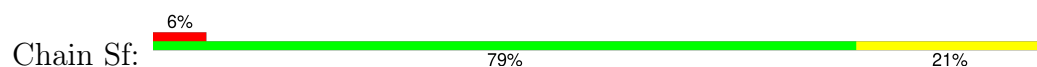
- Molecule 80: 40S ribosomal protein S28



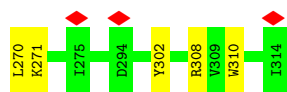
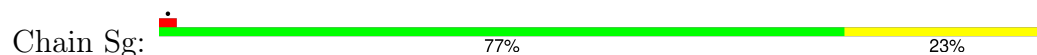
- Molecule 81: 40S ribosomal protein S29



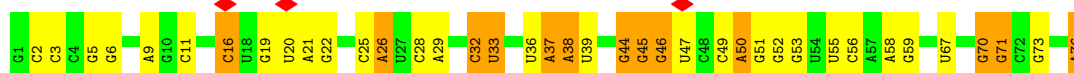
- Molecule 82: Ubiquitin-40S ribosomal protein S27a



- Molecule 83: Receptor of activated protein C kinase 1

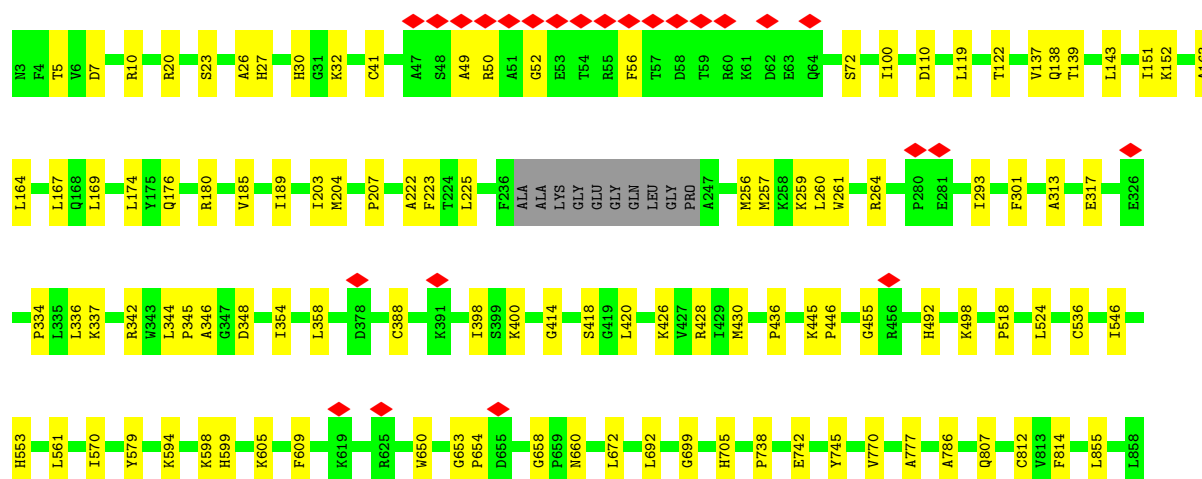


- Molecule 84: E site tRNA



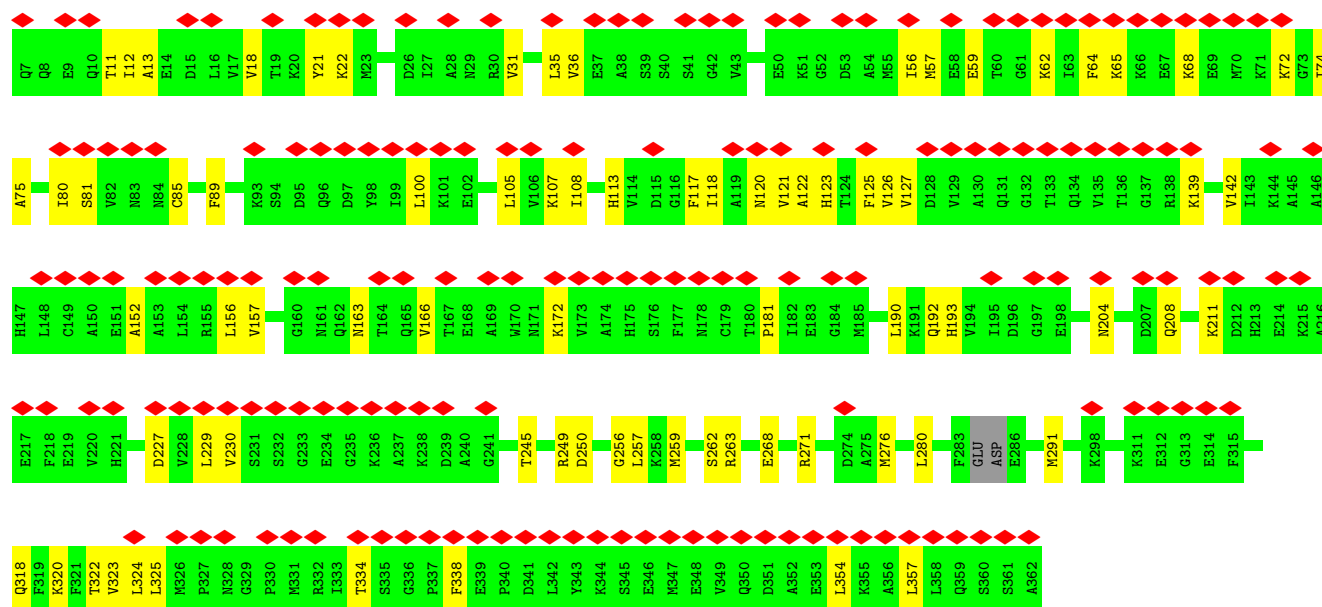
- Molecule 85: Elongation factor 2

Chain CB:  86% 12%



• Molecule 86: Proliferation-associated protein 2G4

Chain CA:  49% 78% 22%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59299	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	0.176	Depositor
Minimum map value	-0.051	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.016	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CD	0.10	0/447	0.27	0/592
2	CI	0.09	0/247	0.25	0/323
3	L5	0.21	0/85098	0.30	0/132762
4	L7	0.18	0/2861	0.25	0/4459
5	L8	0.19	0/3631	0.28	0/5657
6	LA	0.20	0/1936	0.34	0/2596
7	LB	0.18	0/3306	0.33	0/4424
8	LC	0.18	0/2981	0.30	0/4002
9	LD	0.15	0/2428	0.30	0/3252
10	LE	0.16	0/1973	0.32	0/2645
11	LF	0.18	0/1905	0.27	0/2539
12	LG	0.16	0/1960	0.31	0/2637
13	LH	0.17	0/1537	0.31	0/2066
14	LI	0.16	0/1697	0.25	0/2266
15	LJ	0.14	0/1385	0.29	0/1852
16	LL	0.16	0/1732	0.29	0/2315
17	LM	0.18	0/1161	0.33	0/1554
18	LN	0.19	0/1746	0.29	0/2338
19	LO	0.18	0/1682	0.29	0/2250
20	LP	0.18	0/1268	0.32	0/1701
21	LQ	0.19	0/1537	0.32	0/2052
22	LR	0.15	0/1582	0.26	0/2091
23	LS	0.18	0/1493	0.30	0/2003
24	LT	0.17	0/1326	0.27	0/1770
25	LU	0.15	0/839	0.32	0/1126
26	LV	0.18	0/993	0.32	0/1332
27	LW	0.14	0/959	0.28	0/1270
28	LX	0.16	0/1002	0.26	0/1345
29	LY	0.18	0/1132	0.30	0/1504
30	LZ	0.15	0/1130	0.35	0/1507
31	La	0.18	0/1191	0.27	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.15	0/889	0.35	0/1175
33	Lc	0.16	0/774	0.34	0/1038
34	Ld	0.17	0/903	0.31	0/1216
35	Le	0.18	0/1071	0.28	0/1429
36	Lf	0.20	0/895	0.33	0/1198
37	Lg	0.15	0/916	0.27	0/1220
38	Lh	0.14	0/1023	0.31	0/1351
39	Li	0.13	0/843	0.26	0/1115
40	Lj	0.20	0/720	0.41	0/952
41	Lk	0.14	0/575	0.25	0/761
42	Ll	0.17	0/454	0.26	0/599
43	Lm	0.16	0/435	0.32	0/575
44	Ln	0.14	0/231	0.24	0/294
45	Lo	0.17	0/876	0.31	0/1156
46	Lp	0.17	0/718	0.27	0/953
47	Lr	0.18	0/1017	0.34	0/1364
48	Ls	0.12	0/1519	0.32	0/2052
49	Lt	0.16	0/1009	0.46	0/1363
50	SA	0.15	0/1778	0.36	0/2416
51	SB	0.13	0/1765	0.32	0/2362
52	SC	0.14	0/1744	0.33	0/2357
53	SE	0.13	0/2118	0.29	0/2849
54	SG	0.13	0/1946	0.34	0/2590
55	SH	0.15	0/1519	0.40	0/2033
56	SI	0.14	0/1715	0.33	0/2287
57	SJ	0.13	0/1550	0.32	0/2069
58	SL	0.13	0/1268	0.28	0/1696
59	SN	0.13	0/1232	0.29	0/1656
60	SO	0.14	0/1037	0.32	0/1391
61	SV	0.12	0/643	0.28	0/860
62	SW	0.13	0/1051	0.29	0/1406
63	SX	0.14	0/1116	0.36	0/1490
64	SY	0.14	0/1083	0.32	0/1438
65	Sa	0.16	0/836	0.33	0/1121
66	Sb	0.14	0/665	0.30	0/891
67	Se	0.13	0/465	0.30	0/612
68	S2	0.18	0/39756	0.27	0/61939
69	SR	0.13	0/1105	0.37	0/1484
70	SD	0.12	0/1793	0.29	0/2414
71	SF	0.11	0/1516	0.32	0/2037
72	SK	0.14	0/851	0.35	0/1147
73	SM	0.15	0/950	0.41	0/1275
74	SP	0.12	0/1003	0.30	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SQ	0.14	0/1160	0.35	0/1553
76	SS	0.12	0/1216	0.29	0/1628
77	ST	0.12	0/1131	0.32	0/1515
78	SU	0.14	0/831	0.34	0/1115
79	SZ	0.14	0/604	0.36	0/810
80	Sc	0.11	0/508	0.28	0/680
81	Sd	0.13	0/470	0.31	0/623
82	Sf	0.15	0/560	0.43	0/745
83	Sg	0.12	0/2493	0.33	0/3394
84	Et	0.15	0/1778	0.36	0/2767
85	CB	0.13	0/6734	0.32	1/9094 (0.0%)
86	CA	0.12	0/2810	0.34	0/3780
All	All	0.18	0/239833	0.30	1/350498 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
50	SA	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	CB	777	ALA	CB-CA-C	-5.59	110.11	116.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	SA	147	LEU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CD	440	0	402	4	0
2	CI	247	0	283	1	0
3	L5	78444	0	39719	596	0
4	L7	2561	0	1295	13	0
5	L8	3315	0	1685	33	0
6	LA	1898	0	1993	22	0
7	LB	3238	0	3376	34	0
8	LC	2927	0	3104	23	0
9	LD	2382	0	2410	20	0
10	LE	1935	0	2096	19	0
11	LF	1870	0	1996	6	0
12	LG	1927	0	2074	16	0
13	LH	1518	0	1601	16	0
14	LI	1658	0	1697	15	0
15	LJ	1362	0	1399	9	0
16	LL	1701	0	1818	11	0
17	LM	1138	0	1204	4	0
18	LN	1701	0	1749	17	0
19	LO	1650	0	1794	13	0
20	LP	1242	0	1269	9	0
21	LQ	1513	0	1628	12	0
22	LR	1566	0	1729	8	0
23	LS	1453	0	1490	10	0
24	LT	1298	0	1366	7	0
25	LU	825	0	850	7	0
26	LV	979	0	1039	7	0
27	LW	945	0	1003	8	0
28	LX	985	0	1066	5	0
29	LY	1115	0	1205	8	0
30	LZ	1107	0	1182	10	0
31	La	1162	0	1213	6	0
32	Lb	876	0	948	8	0
33	Lc	764	0	804	7	0
34	Ld	888	0	930	7	0
35	Le	1053	0	1147	8	0
36	Lf	876	0	912	6	0
37	Lg	906	0	998	8	0
38	Lh	1015	0	1148	13	0
39	Li	832	0	917	5	0
40	Lj	705	0	737	1	0
41	Lk	569	0	637	3	0
42	Ll	444	0	483	4	0
43	Lm	429	0	465	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Ln	230	0	276	2	0
45	Lo	862	0	929	6	0
46	Lp	708	0	756	4	0
47	Lr	1002	0	1068	8	0
48	Ls	1496	0	1540	13	0
49	Lt	998	0	1032	28	0
50	SA	1741	0	1744	29	0
51	SB	1738	0	1809	39	0
52	SC	1707	0	1791	21	0
53	SE	2076	0	2177	41	0
54	SG	1923	0	2089	42	0
55	SH	1497	0	1590	21	0
56	SI	1686	0	1772	19	0
57	SJ	1525	0	1640	20	0
58	SL	1247	0	1323	10	0
59	SN	1208	0	1294	11	0
60	SO	1024	0	1050	19	0
61	SV	636	0	637	12	0
62	SW	1034	0	1080	12	0
63	SX	1098	0	1167	9	0
64	SY	1065	0	1142	17	0
65	Sa	821	0	870	11	0
66	Sb	651	0	669	9	0
67	Se	459	0	503	9	0
68	S2	36952	0	18678	399	0
69	SR	1090	0	1149	16	0
70	SD	1765	0	1865	19	0
71	SF	1495	0	1549	18	0
72	SK	827	0	854	9	0
73	SM	940	0	965	14	0
74	SP	985	0	1031	14	0
75	SQ	1142	0	1213	28	0
76	SS	1198	0	1261	21	0
77	ST	1112	0	1146	19	0
78	SU	821	0	883	14	0
79	SZ	598	0	656	7	0
80	Sc	506	0	536	9	0
81	Sd	459	0	449	11	0
82	Sf	548	0	551	14	0
83	Sg	2436	0	2391	44	0
84	Et	1593	0	810	20	0
85	CB	6605	0	6679	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	CA	2764	0	2779	55	0
87	L5	179	0	0	0	0
87	L7	3	0	0	0	0
87	L8	5	0	0	0	0
87	LA	1	0	0	0	0
87	LP	1	0	0	0	0
87	LV	1	0	0	0	0
87	Le	1	0	0	0	0
87	S2	27	0	0	0	0
88	L5	98	0	182	4	0
89	L5	100	0	190	4	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	172626	1979	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 (1979) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1417:C:H42	68:S2:1422:G:H22	1.07	0.98
67:Se:39:ASN:HD21	68:S2:551:U:H4'	1.30	0.96
84:Et:26:A:H62	84:Et:44:G:N2	1.63	0.95
3:L5:3946:G:H1	3:L5:4067:U:H3	1.17	0.92
84:Et:26:A:N6	84:Et:44:G:H21	1.68	0.92
84:Et:26:A:H62	84:Et:44:G:H21	1.02	0.91
56:SI:98:LYS:HB3	68:S2:377:G:H5'	1.60	0.84
49:Lt:65:GLN:HG3	49:Lt:67:ARG:H	1.47	0.79
68:S2:1417:C:H42	68:S2:1422:G:N2	1.82	0.78
68:S2:1417:C:N4	68:S2:1422:G:H22	1.80	0.78
3:L5:4887:C:H42	3:L5:4932:U:H3	1.32	0.78
60:SO:52:THR:HG21	68:S2:952:G:H21	1.49	0.77
55:SH:145:ARG:HE	62:SW:51:GLU:HB3	1.48	0.77
3:L5:4775:C:H41	3:L5:4859:C:H42	1.33	0.76
85:CB:10:ARG:HH22	85:CB:420:LEU:HD11	1.51	0.76
85:CB:110:ASP:HB3	85:CB:553:HIS:HB2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1748:G:H1	68:S2:1786:U:H3	1.32	0.75
86:CA:157:VAL:HG22	86:CA:325:LEU:HD21	1.68	0.75
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.69	0.74
3:L5:964:A:H2'	3:L5:965:G:H4'	1.70	0.73
57:SJ:162:ARG:HH21	57:SJ:169:ARG:HG2	1.53	0.73
78:SU:24:LEU:HB3	78:SU:32:LEU:HD11	1.69	0.73
83:Sg:127:LYS:HG2	83:Sg:150:TRP:H	1.53	0.73
3:L5:4618:OMG:H5'	26:LV:15:ARG:HB2	1.69	0.72
49:Lt:114:ARG:HD3	49:Lt:129:ILE:HG22	1.69	0.72
60:SO:99:ALA:H	60:SO:133:THR:HG22	1.55	0.72
76:SS:50:ILE:HD12	76:SS:54:LYS:HZ1	1.55	0.71
63:SX:50:ILE:HG13	85:CB:518:PRO:HB3	1.70	0.71
86:CA:80:ILE:HG12	86:CA:108:ILE:HG12	1.72	0.71
68:S2:851:C:H5''	68:S2:852:G:H5'	1.72	0.71
6:LA:104:VAL:HA	6:LA:107:MET:HE2	1.71	0.71
86:CA:21:TYR:HE1	86:CA:117:PHE:HB3	1.55	0.71
42:Ll:23:ILE:HD11	42:Ll:28:ARG:HE	1.55	0.71
49:Lt:12:VAL:HG11	49:Lt:65:GLN:H	1.55	0.71
3:L5:1366:G:H5''	16:LL:36:ARG:HH12	1.56	0.70
85:CB:164:LEU:HD21	85:CB:174:LEU:HD22	1.72	0.70
68:S2:70:G:H21	68:S2:79:A:H62	1.39	0.70
3:L5:1270:A:H8	3:L5:2106:G:H21	1.40	0.70
48:Ls:55:MET:HG2	48:Ls:87:GLY:HA3	1.74	0.69
3:L5:1976:G:H21	49:Lt:139:VAL:HG12	1.56	0.69
76:SS:36:VAL:HG23	76:SS:40:TYR:HB3	1.73	0.69
6:LA:114:CYS:HB3	6:LA:165:VAL:HB	1.75	0.69
7:LB:205:VAL:HG13	7:LB:209:GLN:HE21	1.58	0.69
38:Lh:73:TYR:HA	38:Lh:76:LYS:HD2	1.74	0.69
60:SO:95:ILE:HD13	60:SO:116:LEU:HD11	1.74	0.69
3:L5:158:A:H5''	3:L5:159:C:H2'	1.73	0.68
3:L5:1404:G:N7	3:L5:1408:G:N2	2.41	0.68
59:SN:20:ARG:HH21	62:SW:56:HIS:HB3	1.59	0.68
68:S2:1854:U:H2'	68:S2:1855:G:H8	1.59	0.68
85:CB:692:LEU:HD11	85:CB:738:PRO:HB2	1.76	0.68
68:S2:140:C:H42	68:S2:313:A:H61	1.40	0.68
12:LG:58:PRO:HD2	12:LG:61:ILE:HD12	1.77	0.67
53:SE:139:LEU:HD22	53:SE:150:PRO:HB3	1.76	0.67
83:Sg:247:TRP:HB3	83:Sg:258:ILE:HD11	1.76	0.67
60:SO:101:GLY:HA3	60:SO:134:PRO:HD2	1.77	0.67
85:CB:594:LYS:HE2	85:CB:598:LYS:HD2	1.77	0.67
57:SJ:38:ARG:HA	67:Se:31:ARG:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SG:167:LYS:HZ3	54:SG:170:ARG:HH11	1.44	0.66
54:SG:176:ILE:HG23	54:SG:179:LEU:HD11	1.77	0.66
3:L5:2458:C:H5'	18:LN:67:ARG:HD2	1.78	0.66
13:LH:106:GLN:HB2	13:LH:111:LEU:HB3	1.78	0.66
82:Sf:119:ARG:HB3	82:Sf:132:MET:HB2	1.77	0.66
68:S2:1337:4AC:H2'	68:S2:1338:G:H8	1.60	0.66
51:SB:127:VAL:HG11	51:SB:176:VAL:HG13	1.78	0.66
86:CA:31:VAL:HG21	86:CA:56:ILE:HD11	1.77	0.66
68:S2:557:U:H2'	68:S2:558:G:C8	2.32	0.65
68:S2:1291:A:H62	82:Sf:95:ARG:HH12	1.43	0.65
86:CA:122:ALA:HB2	86:CA:320:LYS:HE3	1.79	0.65
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.60	0.65
66:Sb:34:ASP:HB3	66:Sb:82:LYS:HE2	1.77	0.65
68:S2:1228:A:H2'	68:S2:1229:G:C8	2.30	0.65
3:L5:2611:A:H5'	3:L5:2688:G:H4'	1.78	0.65
34:Ld:90:ARG:HD3	34:Ld:102:LEU:HD13	1.79	0.65
3:L5:2351:OMC:HM22	8:LC:95:MET:HG3	1.77	0.65
3:L5:3937:C:H1'	18:LN:125:SER:HB3	1.79	0.65
56:SI:87:ASN:HB3	56:SI:90:LEU:HD13	1.77	0.65
67:Se:39:ASN:ND2	68:S2:551:U:H4'	2.09	0.65
55:SH:83:LEU:HB3	55:SH:92:VAL:HG11	1.77	0.64
68:S2:1030:A:H2'	68:S2:1031:A2M:H8	1.79	0.64
68:S2:1277:C:H2'	68:S2:1278:A:H8	1.62	0.64
68:S2:1324:G:H1	68:S2:1504:U:H3	1.42	0.64
48:Ls:77:LYS:HB3	48:Ls:198:ILE:HD11	1.79	0.64
12:LG:263:THR:HB	51:SB:225:LEU:HD23	1.78	0.64
73:SM:92:CYS:HB3	73:SM:103:VAL:HG12	1.79	0.64
85:CB:137:VAL:HG22	85:CB:807:GLN:HE21	1.62	0.64
3:L5:3868:G:H22	3:L5:3900:G:H1'	1.61	0.64
42:Ll:38:ASN:HB3	42:Ll:41:ARG:HG2	1.79	0.64
83:Sg:107:ASP:HB2	83:Sg:125:ARG:HD2	1.79	0.64
88:L5:5294:SPM:H112	19:LO:91:LYS:HD3	1.80	0.64
9:LD:223:PHE:HB3	9:LD:226:TYR:HB2	1.80	0.64
3:L5:1095:A:H2	3:L5:1200:G:H1	1.43	0.63
68:S2:943:U:H2'	68:S2:944:A:H8	1.63	0.63
3:L5:502:C:H3'	3:L5:503:C:H3'	1.80	0.63
50:SA:80:ARG:HH21	50:SA:126:ASP:HB2	1.63	0.63
53:SE:45:ILE:HG13	53:SE:61:VAL:HG11	1.79	0.63
16:LL:64:VAL:HA	16:LL:67:HIS:CD2	2.33	0.63
3:L5:1095:A:C2	3:L5:1200:G:N1	2.66	0.63
79:SZ:63:PRO:HG3	79:SZ:91:LEU:HD21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LF:182:TYR:HB3	11:LF:200:ARG:HG3	1.80	0.63
21:LQ:39:THR:HG22	21:LQ:41:SER:H	1.63	0.63
68:S2:834:C:H42	68:S2:839:C:H42	1.46	0.63
77:ST:18:LEU:HD11	77:ST:131:LEU:HD22	1.80	0.63
1:CD:183:ASP:HB2	85:CB:599:HIS:HE2	1.64	0.63
10:LE:224:LYS:HG3	10:LE:227:HIS:HB3	1.81	0.63
3:L5:5030:U:H2'	3:L5:5031:G:H8	1.62	0.63
20:LP:107:LEU:HD12	20:LP:152:GLU:HG3	1.80	0.62
70:SD:137:VAL:HG22	70:SD:151:LYS:HG3	1.81	0.62
85:CB:334:PRO:HA	85:CB:337:LYS:HD2	1.81	0.62
7:LB:107:ALA:HB2	7:LB:201:LEU:HD22	1.81	0.62
14:LI:91:LEU:HD21	14:LI:129:VAL:HB	1.80	0.62
51:SB:145:LYS:HB2	51:SB:149:GLN:HG2	1.80	0.62
68:S2:1423:C:H41	75:SQ:4:LYS:HG3	1.64	0.62
68:S2:1536:G:H2'	68:S2:1537:A:H8	1.63	0.62
68:S2:1729:U:H3	68:S2:1805:G:H1	1.45	0.62
86:CA:181:PRO:HB2	86:CA:204:ASN:HB2	1.80	0.62
3:L5:1095:A:N1	3:L5:1200:G:O6	2.32	0.62
3:L5:2517:A:H5'	37:Lg:62:LYS:HD3	1.81	0.62
3:L5:4611:A:H2	13:LH:120:GLU:HB3	1.63	0.62
68:S2:600:G:H2'	68:S2:601:OMG:H8	1.65	0.62
3:L5:691:C:H2'	3:L5:692:A:C8	2.34	0.62
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.35	0.62
3:L5:2557:G:H1	3:L5:2570:U:H3	1.45	0.62
16:LL:64:VAL:HA	16:LL:67:HIS:HD2	1.65	0.62
51:SB:87:ILE:H	51:SB:101:HIS:HB2	1.65	0.62
85:CB:20:ARG:HB3	85:CB:100:ILE:HD13	1.82	0.62
3:L5:2303:C:H5''	35:Le:104:SER:HB3	1.81	0.62
27:LW:97:LYS:HG3	27:LW:99:GLU:H	1.64	0.62
83:Sg:87:LEU:HB2	83:Sg:101:PHE:HB2	1.82	0.62
56:SI:76:THR:HG22	56:SI:108:PRO:HG2	1.81	0.61
57:SJ:164:PRO:HB3	57:SJ:170:PRO:HA	1.81	0.61
63:SX:123:VAL:HG12	63:SX:124:LYS:HG3	1.82	0.61
49:Lt:10:ILE:HG21	49:Lt:65:GLN:HB3	1.81	0.61
50:SA:190:SER:HA	61:SV:45:ARG:HH22	1.65	0.61
3:L5:138:G:H2'	3:L5:139:G:H8	1.66	0.61
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.65	0.61
3:L5:1629:G:H1	6:LA:208:GLU:HG2	1.65	0.61
68:S2:1129:G:H3'	68:S2:1130:G:H21	1.65	0.61
75:SQ:34:VAL:HG12	75:SQ:70:VAL:HB	1.82	0.61
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SI:79:ILE:HG21	56:SI:170:LYS:HE3	1.81	0.61
64:SY:6:THR:HG23	64:SY:28:LEU:HD13	1.83	0.61
64:SY:104:ARG:HH12	68:S2:492:C:H5	1.49	0.61
68:S2:5:U:H2'	68:S2:6:G:H8	1.65	0.61
34:Ld:64:ILE:HG23	34:Ld:68:LEU:HD23	1.83	0.61
56:SI:22:HIS:HB3	68:S2:433:A:H5''	1.82	0.60
71:SF:49:LEU:HD12	75:SQ:50:LYS:HG3	1.82	0.60
3:L5:1994:C:H2'	3:L5:1995:G:C8	2.36	0.60
6:LA:31:ALA:HB2	6:LA:123:ARG:HH21	1.66	0.60
14:LI:91:LEU:HD13	14:LI:135:ILE:HA	1.82	0.60
59:SN:26:LEU:HD11	59:SN:60:VAL:HG12	1.83	0.60
68:S2:1382:A:H2'	68:S2:1383:A2M:H8	1.82	0.60
68:S2:1562:C:H2'	68:S2:1563:G:H8	1.64	0.60
27:LW:87:LEU:HG	27:LW:91:MET:HE1	1.82	0.60
68:S2:508:A:H3'	68:S2:509:OMG:H8	1.66	0.60
68:S2:1764:G:H5''	68:S2:1765:C:H5''	1.83	0.60
3:L5:2362:U:H2'	3:L5:2363:A2M:H8	1.84	0.60
30:LZ:95:VAL:HG11	30:LZ:113:GLU:HG3	1.83	0.60
68:S2:928:G:H2'	68:S2:929:G:C8	2.37	0.60
73:SM:35:ILE:HD11	73:SM:61:TYR:HE1	1.66	0.60
83:Sg:246:TYR:HB3	83:Sg:261:LEU:HG	1.83	0.60
19:LO:125:LYS:HG3	19:LO:129:LEU:HD12	1.84	0.60
53:SE:19:MET:HB2	53:SE:51:ARG:HH22	1.66	0.60
18:LN:146:PRO:HB2	38:Lh:104:THR:HG23	1.84	0.60
68:S2:1203:G:H2'	68:S2:1204:A:C8	2.37	0.60
5:L8:67:U:H2'	5:L8:68:G:H8	1.66	0.60
68:S2:874:G:H2'	68:S2:875:A:H8	1.65	0.60
64:SY:10:ARG:HA	68:S2:839:C:H41	1.67	0.59
68:S2:1101:U:H2'	68:S2:1102:G:H8	1.67	0.59
86:CA:57:MET:HE2	86:CA:74:ILE:HD12	1.83	0.59
53:SE:38:LEU:HD22	68:S2:346:C:H5''	1.83	0.59
68:S2:1417:C:O2	68:S2:1422:G:O6	2.20	0.59
83:Sg:7:LEU:HA	83:Sg:310:TRP:HD1	1.66	0.59
53:SE:191:ARG:HD2	53:SE:245:ARG:HH11	1.67	0.59
58:SL:111:VAL:HG12	58:SL:140:PHE:HB2	1.84	0.59
61:SV:22:ARG:HH22	61:SV:59:ILE:HG23	1.66	0.59
68:S2:165:G:H2'	68:S2:166:A2M:H8	1.84	0.59
12:LG:120:LYS:HE3	12:LG:125:LYS:HG3	1.84	0.59
70:SD:135:GLU:HB2	70:SD:153:VAL:HG23	1.84	0.59
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.83	0.59
3:L5:4363:A:H5''	45:Lo:36:GLN:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Lo:69:ARG:HE	45:Lo:80:LYS:HG2	1.68	0.59
68:S2:1228:A:H2'	68:S2:1229:G:H8	1.66	0.59
2:CI:50:MET:HE1	2:CI:58:LEU:HD22	1.84	0.59
3:L5:2411:C:H2'	3:L5:2412:A:H8	1.68	0.59
3:L5:2903:G:H1'	3:L5:2904:U:H5	1.68	0.59
54:SG:10:THR:HG23	54:SG:128:THR:HA	1.82	0.59
86:CA:172:LYS:HG2	86:CA:354:LEU:HD11	1.84	0.59
3:L5:1414:C:H2'	3:L5:1415:G:H8	1.68	0.59
85:CB:27:HIS:HB2	85:CB:139:THR:HG23	1.84	0.59
3:L5:4910:G:H4'	7:LB:95:THR:HG22	1.84	0.59
23:LS:15:ARG:HB3	23:LS:27:LEU:HD23	1.85	0.59
49:Lt:12:VAL:HG21	49:Lt:65:GLN:HB2	1.85	0.59
83:Sg:152:SER:HG	83:Sg:170:TRP:CD1	2.20	0.59
3:L5:268:G:H2'	3:L5:269:G:H8	1.67	0.58
3:L5:4992:G:H2'	3:L5:4993:G:C8	2.38	0.58
51:SB:105:LEU:HD13	51:SB:213:ARG:HA	1.85	0.58
51:SB:134:LEU:HG	51:SB:218:LEU:HD12	1.84	0.58
52:SC:118:ALA:HB2	68:S2:1486:A:H4'	1.85	0.58
68:S2:106:C:H2'	68:S2:107:A:H8	1.68	0.58
68:S2:116:OMU:HN3	68:S2:347:G:H1	1.50	0.58
68:S2:414:A:H2'	68:S2:415:A:H8	1.69	0.58
71:SF:103:LEU:HD11	71:SF:178:ILE:HD13	1.83	0.58
3:L5:3950:U:H3'	3:L5:3951:G:C8	2.39	0.58
68:S2:649:PSU:H2'	68:S2:650:A:H8	1.68	0.58
49:Lt:19:GLY:HA2	49:Lt:48:LYS:HZ3	1.67	0.58
68:S2:948:C:H2'	68:S2:949:G:H8	1.68	0.58
83:Sg:24:THR:HB	83:Sg:71:ILE:HG21	1.85	0.58
3:L5:4302:U:H4'	24:LT:5:LYS:HD2	1.84	0.58
50:SA:52:LYS:HB2	69:SR:109:LEU:HD13	1.85	0.58
68:S2:1284:A:C6	73:SM:91:LEU:HD11	2.39	0.58
68:S2:1661:A:H8	81:Sd:14:PHE:HB2	1.68	0.58
74:SP:22:LEU:HA	74:SP:25:LEU:HB2	1.85	0.58
81:Sd:23:VAL:HG21	81:Sd:38:MET:HE3	1.84	0.58
3:L5:2554:U:O2	3:L5:2764:A:N7	2.37	0.58
50:SA:42:LYS:HE3	50:SA:48:ILE:HD11	1.84	0.58
55:SH:10:LYS:HE3	55:SH:20:GLU:HG2	1.85	0.58
68:S2:1461:G:H3'	68:S2:1463:U:H3	1.68	0.58
3:L5:2745:A:H2'	3:L5:2746:A:H8	1.69	0.58
6:LA:188:LYS:HZ2	6:LA:192:LYS:HE3	1.69	0.58
11:LF:105:VAL:HG13	11:LF:136:VAL:HG12	1.85	0.58
49:Lt:57:ARG:HD2	49:Lt:83:LYS:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SA:176:TRP:HE1	50:SA:197:VAL:HG12	1.68	0.58
83:Sg:256:ILE:HB	83:Sg:270:LEU:HB2	1.86	0.58
60:SO:57:THR:HG22	60:SO:60:MET:HE3	1.86	0.58
68:S2:925:G:H1	68:S2:1017:U:H3	1.52	0.58
68:S2:1438:A:H2'	68:S2:1439:A:C8	2.39	0.58
86:CA:64:PHE:HD2	86:CA:72:LYS:HE2	1.69	0.58
51:SB:85:LYS:HB2	51:SB:101:HIS:HB3	1.86	0.57
55:SH:10:LYS:HE2	55:SH:47:ALA:HA	1.85	0.57
10:LE:165:LEU:HD11	10:LE:176:THR:HB	1.85	0.57
50:SA:198:MET:HE1	69:SR:86:PRO:HD2	1.86	0.57
53:SE:79:ASP:HB3	53:SE:82:TYR:HB2	1.86	0.57
53:SE:145:ARG:HD2	53:SE:162:ILE:HD13	1.84	0.57
78:SU:59:LYS:HB2	78:SU:84:ILE:HB	1.86	0.57
85:CB:745:TYR:HB2	85:CB:814:PHE:HA	1.85	0.57
3:L5:4220:6MZ:O5'	3:L5:4220:6MZ:H8	2.04	0.57
63:SX:107:ARG:HG3	63:SX:110:HIS:HB3	1.85	0.57
68:S2:640:A:H2'	68:S2:641:A:C8	2.39	0.57
85:CB:650:TRP:HZ2	85:CB:672:LEU:HD21	1.69	0.57
3:L5:1352:C:H3'	21:LQ:104:ARG:HH22	1.70	0.57
68:S2:940:U:H3	68:S2:1002:U:H3	1.52	0.57
13:LH:12:ILE:HG12	13:LH:18:ILE:HD12	1.86	0.57
38:Lh:80:PRO:HD2	38:Lh:83:LEU:HD12	1.86	0.57
52:SC:259:THR:HG21	61:SV:16:LYS:H	1.70	0.57
77:ST:27:LYS:HE3	77:ST:110:LEU:HG	1.87	0.57
82:Sf:132:MET:HA	82:Sf:141:CYS:HA	1.87	0.57
68:S2:1679:A:H2'	71:SF:60:ARG:HD2	1.85	0.57
85:CB:354:ILE:HG23	85:CB:358:LEU:HD12	1.86	0.57
86:CA:75:ALA:HB2	86:CA:113:HIS:HB3	1.87	0.57
3:L5:3604:A:H5'	22:LR:71:ARG:HH21	1.70	0.57
8:LC:287:THR:HG21	47:Lr:5:LEU:HD12	1.86	0.57
19:LO:34:VAL:HG22	19:LO:103:LYS:HB2	1.85	0.57
52:SC:207:ALA:HB2	68:S2:4:C:H4'	1.87	0.57
71:SF:103:LEU:HA	79:SZ:66:LYS:HD2	1.86	0.57
3:L5:3732:A:H2'	3:L5:3733:A:H8	1.70	0.57
3:L5:4940:C:H5'	3:L5:4941:G:H5''	1.87	0.57
14:LI:53:VAL:HG11	24:LT:158:PHE:HZ	1.70	0.57
50:SA:124:VAL:HG13	50:SA:130:ASP:HB2	1.86	0.57
68:S2:28:U:H2'	68:S2:29:G:H8	1.70	0.57
3:L5:4887:C:N4	3:L5:4932:U:H3	2.02	0.57
68:S2:532:C:H2'	68:S2:533:A:H8	1.70	0.57
83:Sg:87:LEU:HD11	83:Sg:108:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:SP:37:TYR:HB3	74:SP:41:GLN:HB2	1.86	0.56
82:Sf:108:VAL:HB	82:Sf:112:GLY:HA2	1.85	0.56
83:Sg:68:ASP:HB3	83:Sg:111:VAL:HG22	1.86	0.56
86:CA:105:LEU:HD23	86:CA:139:LYS:HD3	1.87	0.56
60:SO:62:VAL:HG21	60:SO:67:ASP:HB2	1.87	0.56
18:LN:138:PHE:HA	18:LN:143:ARG:HD2	1.86	0.56
54:SG:135:PRO:HA	68:S2:169:U:H5''	1.86	0.56
83:Sg:166:VAL:HG22	83:Sg:176:VAL:HG22	1.88	0.56
51:SB:197:ILE:HB	51:SB:210:VAL:HG11	1.86	0.56
50:SA:10:MET:HE3	50:SA:55:TRP:HB2	1.87	0.56
55:SH:8:ILE:HD11	55:SH:28:LEU:HD13	1.88	0.56
3:L5:4571:A2M:H2'	3:L5:4572:U:H6	1.70	0.56
22:LR:172:ARG:HH22	68:S2:908:A:H5''	1.70	0.56
49:Lt:106:PHE:HB2	49:Lt:109:ILE:HG12	1.88	0.56
66:Sb:22:LYS:HE3	68:S2:1129:G:H5''	1.88	0.56
68:S2:1417:C:N3	68:S2:1422:G:N1	2.46	0.56
3:L5:4139:G:H21	3:L5:4140:C:H41	1.52	0.56
7:LB:92:TYR:HB2	7:LB:159:VAL:HB	1.88	0.56
78:SU:56:MET:HB2	78:SU:86:LYS:HB3	1.87	0.56
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.35	0.56
18:LN:159:ARG:HB3	18:LN:164:LEU:HB2	1.87	0.56
60:SO:95:ILE:HD11	60:SO:126:ILE:HD12	1.88	0.56
9:LD:232:THR:HG22	9:LD:234:ASP:H	1.71	0.56
10:LE:190:HIS:HB3	10:LE:193:PHE:HD2	1.70	0.56
10:LE:274:VAL:HG21	36:Lf:2:SER:HB3	1.86	0.56
63:SX:68:LYS:HB3	63:SX:91:LEU:HD13	1.86	0.56
3:L5:257:C:H2'	3:L5:258:G:C8	2.41	0.56
3:L5:2020:U:H2'	3:L5:2021:G:H8	1.71	0.56
3:L5:4274:A:H2'	3:L5:4275:G:H8	1.71	0.56
3:L5:4991:U:H2'	3:L5:4992:G:C8	2.41	0.56
8:LC:361:LEU:HA	8:LC:364:LYS:HE2	1.87	0.56
3:L5:2845:A:H61	3:L5:3843:C:H42	1.52	0.55
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.40	0.55
8:LC:116:ASN:HB2	8:LC:119:GLN:HG3	1.88	0.55
54:SG:189:ARG:HH21	68:S2:331:C:H5''	1.72	0.55
86:CA:100:LEU:HD21	86:CA:127:VAL:HG11	1.88	0.55
3:L5:4353:PSU:H5'	3:L5:4354:U:H5'	1.88	0.55
75:SQ:45:ARG:HA	75:SQ:48:GLN:HB2	1.87	0.55
3:L5:1175:A:H2	3:L5:1185:G:H1	1.53	0.55
88:L5:5289:SPM:H82	88:L5:5289:SPM:H22	1.87	0.55
5:L8:96:C:H5''	38:Lh:66:LYS:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LI:54:SER:HB3	14:LI:135:ILE:HD11	1.87	0.55
56:SI:25:ARG:HA	68:S2:448:A:H5'	1.89	0.55
64:SY:55:ILE:HD13	64:SY:75:ILE:HD13	1.89	0.55
68:S2:1536:G:H2'	68:S2:1537:A:C8	2.41	0.55
68:S2:1562:C:H2'	68:S2:1563:G:C8	2.42	0.55
85:CB:56:PHE:HB3	85:CB:455:GLY:HA3	1.87	0.55
86:CA:18:VAL:HG12	86:CA:22:LYS:HE2	1.88	0.55
53:SE:136:ILE:HD12	53:SE:149:TYR:HE1	1.71	0.55
68:S2:159:A2M:O5'	68:S2:159:A2M:H8	2.07	0.55
68:S2:1217:A:H2'	68:S2:1218:C:C6	2.42	0.55
68:S2:1398:G:H1'	83:Sg:63:SER:HB2	1.89	0.55
3:L5:300:A:H2'	3:L5:301:G:H8	1.71	0.55
3:L5:433:A:C2	3:L5:3867:A2M:H4'	2.41	0.55
3:L5:1464:C:H5'	32:Lb:32:LEU:HD12	1.88	0.55
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.41	0.55
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.41	0.55
9:LD:62:CYS:HB3	9:LD:105:LEU:HD22	1.88	0.55
11:LF:127:LYS:HB2	24:LT:133:ALA:HB3	1.87	0.55
20:LP:131:ARG:HG3	20:LP:137:ASN:OD1	2.07	0.55
68:S2:12:U:H2'	68:S2:13:C:C6	2.42	0.55
68:S2:1581:C:H5'	68:S2:1582:C:H5	1.71	0.55
45:Lo:33:LEU:HA	45:Lo:38:LYS:HG2	1.88	0.55
50:SA:205:ARG:HH22	69:SR:84:TYR:H	1.54	0.55
60:SO:136:PRO:HG2	60:SO:139:SER:HB3	1.89	0.55
86:CA:118:ILE:HD11	86:CA:190:LEU:HG	1.89	0.55
3:L5:3848:U:H2'	3:L5:3849:A:H8	1.72	0.55
3:L5:4070:U:H2'	3:L5:4071:U:H6	1.72	0.55
85:CB:654:PRO:HD2	85:CB:658:GLY:HA3	1.87	0.55
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.41	0.55
3:L5:5024:C:H41	3:L5:5028:G:H21	1.54	0.55
12:LG:79:ALA:HB3	18:LN:18:VAL:HG11	1.89	0.55
23:LS:11:LYS:HE3	23:LS:29:ARG:HD3	1.88	0.55
56:SI:103:LEU:HD22	56:SI:170:LYS:HB3	1.89	0.55
57:SJ:63:LEU:HD23	57:SJ:70:ARG:HB2	1.87	0.55
68:S2:1588:A:H2'	68:S2:1589:A:C8	2.42	0.55
85:CB:561:LEU:HD22	85:CB:570:ILE:HD13	1.88	0.55
3:L5:1972:G:H5'	48:Ls:38:LYS:HE2	1.89	0.55
54:SG:175:LYS:HG3	68:S2:77:A:H2	1.72	0.55
68:S2:1298:G:H5'	74:SP:77:LYS:HB2	1.89	0.55
78:SU:91:LEU:HB3	78:SU:97:ILE:HD11	1.89	0.55
3:L5:1514:U:H2'	3:L5:1515:A:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:SQ:19:ALA:HB2	75:SQ:75:GLY:HA3	1.88	0.54
85:CB:345:PRO:HG2	85:CB:348:ASP:HB2	1.90	0.54
3:L5:135:G:H5''	38:Lh:97:LYS:H	1.73	0.54
3:L5:2708:U:H3	86:CA:257:LEU:HD23	1.72	0.54
3:L5:4139:G:N2	3:L5:4140:C:H41	2.05	0.54
53:SE:26:VAL:HG22	57:SJ:4:ALA:HB2	1.89	0.54
56:SI:81:VAL:HG22	56:SI:102:VAL:HG12	1.89	0.54
68:S2:639:C:H2'	68:S2:640:A:H8	1.71	0.54
68:S2:1603:G:H4'	76:SS:38:ARG:HH22	1.71	0.54
3:L5:182:G:H2'	3:L5:183:C:H4'	1.88	0.54
3:L5:1538:U:H2'	3:L5:1539:G:H8	1.72	0.54
3:L5:4281:A:H2'	3:L5:4282:A:H2'	1.89	0.54
53:SE:18:TRP:HB3	53:SE:20:LEU:HD13	1.89	0.54
64:SY:9:THR:H	68:S2:837:A:H61	1.56	0.54
3:L5:3848:U:H2'	3:L5:3849:A:C8	2.43	0.54
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.43	0.54
61:SV:15:ARG:HH21	61:SV:24:ILE:HG21	1.73	0.54
83:Sg:206:LEU:HD11	83:Sg:218:LEU:HD23	1.89	0.54
85:CB:260:LEU:HD12	85:CB:293:ILE:HD11	1.87	0.54
68:S2:1692:U:H2'	68:S2:1693:G:C8	2.42	0.54
72:SK:27:VAL:HB	72:SK:43:LEU:HD12	1.89	0.54
78:SU:27:ARG:HD2	78:SU:82:MET:HE2	1.89	0.54
6:LA:54:ARG:HG2	6:LA:56:ALA:H	1.73	0.54
8:LC:110:ARG:HB2	18:LN:204:ARG:HH21	1.72	0.54
54:SG:87:ARG:HH22	68:S2:162:C:H5''	1.71	0.54
69:SR:84:TYR:HD2	69:SR:86:PRO:HG3	1.73	0.54
85:CB:152:LYS:HA	85:CB:203:ILE:HD11	1.90	0.54
3:L5:907:C:H2'	3:L5:908:G:H8	1.73	0.54
3:L5:2745:A:H2'	3:L5:2746:A:C8	2.43	0.54
3:L5:3870:C:H2'	3:L5:3871:A:H8	1.72	0.54
55:SH:75:ILE:HG23	55:SH:79:LEU:HD23	1.89	0.54
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.42	0.54
9:LD:156:GLY:HA2	9:LD:181:PRO:HG3	1.90	0.54
26:LV:13:LYS:HD2	26:LV:128:LEU:HD11	1.89	0.54
31:La:36:GLY:HA3	31:La:40:HIS:CE1	2.43	0.54
66:Sb:54:VAL:HG23	66:Sb:63:LEU:HB2	1.89	0.54
68:S2:690:G:H5''	68:S2:691:G:H21	1.72	0.54
3:L5:4260:U:H2'	3:L5:4261:C:C6	2.43	0.54
6:LA:247:ARG:HB3	68:S2:1069:U:H4'	1.90	0.54
15:LJ:146:ARG:HG2	15:LJ:147:ARG:HG3	1.90	0.54
32:Lb:65:MET:HG3	32:Lb:68:ARG:HH12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SA:145:ILE:HG12	50:SA:159:ILE:HD13	1.90	0.54
52:SC:94:ILE:HD11	52:SC:159:LYS:HG2	1.90	0.54
68:S2:1205:C:H2'	68:S2:1206:G:H8	1.73	0.54
83:Sg:223:GLU:HB3	83:Sg:225:LYS:HE3	1.90	0.54
3:L5:1509:C:H5''	31:La:2:PRO:HD3	1.89	0.53
14:LI:184:MET:HA	14:LI:187:LYS:HE2	1.90	0.53
27:LW:96:GLN:HB2	27:LW:101:ARG:HH21	1.72	0.53
79:SZ:99:LEU:HD11	79:SZ:102:LYS:HB2	1.90	0.53
81:Sd:6:LEU:HA	81:Sd:9:SER:HB3	1.89	0.53
85:CB:225:LEU:HD12	85:CB:260:LEU:HB3	1.89	0.53
8:LC:218:ILE:HA	8:LC:229:LEU:HD13	1.89	0.53
52:SC:167:ARG:HB3	52:SC:177:PRO:HB2	1.91	0.53
54:SG:23:LYS:HE2	54:SG:41:LEU:HA	1.90	0.53
3:L5:701:G:H2'	3:L5:702:U:C6	2.43	0.53
3:L5:4967:A:H2'	3:L5:4968:A:H8	1.73	0.53
51:SB:137:LEU:HG	51:SB:215:VAL:HG12	1.91	0.53
54:SG:32:MET:HA	54:SG:52:ILE:HB	1.91	0.53
57:SJ:127:ARG:HD3	67:Se:31:ARG:HD3	1.91	0.53
3:L5:187:U:H2'	3:L5:245:C:H1'	1.90	0.53
59:SN:16:LEU:HD22	68:S2:919:A:H5''	1.90	0.53
68:S2:543:C:H3'	68:S2:544:G:H8	1.74	0.53
68:S2:980:A:H2'	68:S2:981:A:C8	2.43	0.53
77:ST:40:ALA:HB3	77:ST:43:LYS:HG2	1.90	0.53
83:Sg:236:ILE:HG13	83:Sg:252:THR:HG22	1.91	0.53
13:LH:103:VAL:HG11	13:LH:144:LEU:HD21	1.89	0.53
54:SG:227:GLN:HB3	54:SG:231:ARG:HH21	1.74	0.53
3:L5:4642:U:H2'	3:L5:4643:G:H8	1.74	0.53
6:LA:137:ILE:HD11	6:LA:149:LYS:HB2	1.90	0.53
68:S2:1337:4AC:H2'	68:S2:1338:G:C8	2.42	0.53
68:S2:1856:C:H2'	68:S2:1857:G:C8	2.43	0.53
70:SD:141:LYS:HE2	70:SD:179:GLN:HB3	1.89	0.53
3:L5:137:G:H2'	3:L5:138:G:H8	1.74	0.53
3:L5:3932:U:H2'	3:L5:3933:G:C8	2.44	0.53
7:LB:92:TYR:HB3	7:LB:99:LEU:HD22	1.91	0.53
7:LB:258:HIS:HA	7:LB:260:ALA:H	1.74	0.53
68:S2:527:C:H2'	68:S2:528:A:H8	1.74	0.53
68:S2:1098:C:H2'	68:S2:1099:G:C8	2.43	0.53
86:CA:229:LEU:HG	86:CA:318:GLN:HG3	1.89	0.53
3:L5:93:G:H2'	3:L5:94:A:C8	2.44	0.53
3:L5:1177:U:H3	3:L5:1183:C:H42	1.56	0.53
3:L5:1683:PSU:H2'	3:L5:1684:A:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2521:G:H4'	37:Lg:26:PRO:HD2	1.90	0.53
3:L5:4489:G:H4'	89:L5:5290:SPD:H91	1.91	0.53
86:CA:268:GLU:HG2	86:CA:271:ARG:HH22	1.73	0.53
3:L5:138:G:H2'	3:L5:139:G:C8	2.44	0.53
15:LJ:52:LYS:HB3	15:LJ:65:ASN:HA	1.91	0.53
62:SW:79:PHE:H	62:SW:125:ILE:HG22	1.74	0.53
84:Et:22:G:N7	84:Et:46:G:O6	2.42	0.53
85:CB:163:ALA:HB1	85:CB:169:LEU:HD12	1.90	0.53
3:L5:1500:A:H5''	3:L5:1501:C:H5''	1.90	0.53
68:S2:152:U:H2'	68:S2:153:G:C8	2.44	0.53
68:S2:1421:A:H61	77:ST:3:GLY:H	1.56	0.53
75:SQ:146:ARG:HH11	84:Et:32:C:H5''	1.74	0.53
3:L5:2543:A:H2	3:L5:2773:G:H22	1.56	0.52
7:LB:258:HIS:HA	7:LB:260:ALA:N	2.23	0.52
52:SC:68:ARG:HG2	52:SC:277:HIS:HB2	1.91	0.52
70:SD:136:VAL:HG12	70:SD:186:VAL:HG22	1.91	0.52
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.44	0.52
34:Ld:50:ARG:HG2	34:Ld:54:MET:HE3	1.90	0.52
49:Lt:126:SER:HB3	49:Lt:163:PRO:HD3	1.91	0.52
3:L5:3641:U:H5	3:L5:3646:A:N7	2.07	0.52
14:LI:43:VAL:HG21	14:LI:197:VAL:HG13	1.91	0.52
50:SA:38:ILE:HD12	50:SA:47:TYR:HB3	1.91	0.52
67:Se:32:ALA:HB2	68:S2:525:A:H5''	1.92	0.52
68:S2:562:U:H2'	68:S2:563:G:C8	2.45	0.52
75:SQ:102:GLU:HA	75:SQ:105:LYS:HB3	1.91	0.52
86:CA:122:ALA:HB3	86:CA:320:LYS:HG3	1.92	0.52
3:L5:132:G:H2'	3:L5:133:C:H4'	1.92	0.52
3:L5:4238:G:H2'	3:L5:4239:A:H8	1.75	0.52
68:S2:544:G:H2'	68:S2:545:A:C8	2.44	0.52
68:S2:1845:A:H2'	68:S2:1846:G:C8	2.44	0.52
73:SM:36:ARG:HH22	82:Sf:130:VAL:HA	1.74	0.52
74:SP:34:MET:HB3	74:SP:42:ARG:HG3	1.89	0.52
82:Sf:119:ARG:HG3	82:Sf:120:GLU:H	1.74	0.52
3:L5:381:U:H4'	3:L5:415:G:H5'	1.90	0.52
3:L5:1645:C:H2'	3:L5:1646:A:C8	2.44	0.52
3:L5:1914:C:H4'	19:LO:89:PRO:HD3	1.91	0.52
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.41	0.52
62:SW:36:ARG:HG2	62:SW:110:ILE:HB	1.91	0.52
68:S2:367:U:H4'	68:S2:371:A:C8	2.45	0.52
68:S2:1336:C:H2'	68:S2:1337:4AC:H6	1.91	0.52
3:L5:1405:C:H2'	3:L5:1406:G:H8	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LD:65:ALA:HB2	9:LD:74:ILE:HD13	1.92	0.52
54:SG:213:LEU:HA	54:SG:216:ARG:HB3	1.90	0.52
64:SY:104:ARG:HA	64:SY:107:ARG:HE	1.75	0.52
68:S2:1711:U:H2'	68:S2:1712:A:H8	1.74	0.52
75:SQ:146:ARG:NH1	84:Et:32:C:H5''	2.24	0.52
80:Sc:17:VAL:HA	80:Sc:30:VAL:HG23	1.91	0.52
85:CB:524:LEU:HD12	85:CB:536:CYS:HB3	1.91	0.52
3:L5:2095:A:H1'	3:L5:2096:G:N2	2.25	0.52
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.45	0.52
3:L5:2520:C:H2'	3:L5:2521:G:H8	1.74	0.52
33:Lc:38:ILE:HG21	33:Lc:63:TYR:HB3	1.91	0.52
44:Ln:1:MET:HB2	68:S2:1706:G:H5'	1.91	0.52
45:Lo:75:PRO:HA	45:Lo:78:ARG:HE	1.73	0.52
50:SA:184:ARG:HE	50:SA:191:ARG:HD3	1.74	0.52
51:SB:164:ILE:HD11	51:SB:204:ILE:HB	1.91	0.52
53:SE:42:LEU:HG	53:SE:46:ILE:HD11	1.92	0.52
68:S2:1651:A:H2'	68:S2:1652:G:H8	1.74	0.52
83:Sg:302:TYR:HE2	83:Sg:308:ARG:HD2	1.75	0.52
3:L5:2495:U:H2'	3:L5:2496:G:C8	2.45	0.52
3:L5:5030:U:H2'	3:L5:5031:G:C8	2.43	0.52
43:Lm:99:CYS:HB2	43:Lm:114:LYS:HE3	1.91	0.52
68:S2:51:U:H2'	68:S2:52:G:H8	1.75	0.52
86:CA:156:LEU:HD11	86:CA:166:VAL:HG22	1.92	0.52
3:L5:3599:A:H2'	3:L5:3600:G:C8	2.45	0.52
60:SO:45:THR:HG22	60:SO:52:THR:HG22	1.92	0.52
68:S2:1801:A:H2'	68:S2:1802:C:H6	1.75	0.52
85:CB:745:TYR:HE2	85:CB:812:CYS:HB2	1.74	0.52
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.10	0.52
3:L5:2016:C:H2'	3:L5:2017:A:H8	1.74	0.52
8:LC:110:ARG:HG3	18:LN:204:ARG:HE	1.75	0.52
60:SO:120:ALA:HB2	65:Sa:53:ILE:HD13	1.91	0.52
62:SW:3:ARG:HH12	62:SW:28:ARG:HH21	1.58	0.52
68:S2:5:U:H2'	68:S2:6:G:C8	2.44	0.52
68:S2:388:U:H2'	68:S2:389:A:H8	1.75	0.52
68:S2:929:G:H2'	68:S2:930:C:O4'	2.10	0.52
68:S2:1201:U:H2'	68:S2:1202:U:C6	2.45	0.52
68:S2:1424:G:H2'	68:S2:1425:G:H8	1.75	0.52
3:L5:3910:C:H2'	3:L5:3911:C:C6	2.46	0.51
3:L5:4750:G:H2'	3:L5:4751:G:H8	1.75	0.51
9:LD:211:LEU:HB3	9:LD:219:TYR:HB2	1.92	0.51
31:La:72:THR:HG22	31:La:110:LYS:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SB:103:MET:HB3	51:SB:215:VAL:HG22	1.91	0.51
68:S2:388:U:H2'	68:S2:389:A:C8	2.45	0.51
68:S2:543:C:H3'	68:S2:544:G:C8	2.46	0.51
85:CB:653:GLY:HA2	85:CB:660:ASN:HB2	1.92	0.51
3:L5:1761:G:H1'	3:L5:1764:G:H22	1.76	0.51
25:LU:100:LEU:HD13	25:LU:112:LEU:HD23	1.93	0.51
3:L5:2295:C:H2'	3:L5:2296:G:H8	1.75	0.51
3:L5:2539:C:H2'	3:L5:2540:C:C6	2.46	0.51
13:LH:102:ASN:HB2	13:LH:115:ARG:HB2	1.91	0.51
34:Ld:19:GLU:HA	34:Ld:90:ARG:HH11	1.75	0.51
54:SG:228:ILE:HA	54:SG:231:ARG:HG2	1.91	0.51
57:SJ:26:ASP:HB2	67:Se:42:PHE:HZ	1.75	0.51
59:SN:49:GLN:HA	59:SN:52:VAL:HG22	1.92	0.51
3:L5:1508:A:H5''	8:LC:113:ARG:HD2	1.92	0.51
3:L5:2570:U:H2'	3:L5:2571:C:C6	2.46	0.51
3:L5:2709:C:H42	86:CA:256:GLY:HA2	1.75	0.51
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.45	0.51
3:L5:3911:C:H2'	3:L5:3912:U:H6	1.74	0.51
86:CA:65:LYS:HA	86:CA:68:LYS:HD3	1.92	0.51
3:L5:1669:A:H4'	3:L5:1685:G:N2	2.25	0.51
3:L5:2335:C:H2'	3:L5:2336:G:H8	1.75	0.51
3:L5:2495:U:H2'	3:L5:2496:G:H8	1.76	0.51
6:LA:115:CYS:SG	6:LA:124:GLY:HA3	2.50	0.51
51:SB:30:TRP:HB3	51:SB:46:LYS:HD3	1.92	0.51
68:S2:112:U:H3	68:S2:349:A:H61	1.57	0.51
68:S2:639:C:H2'	68:S2:640:A:C8	2.45	0.51
72:SK:41:PRO:HD2	72:SK:44:HIS:HD2	1.76	0.51
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.46	0.51
28:LX:141:ALA:HB3	28:LX:144:TYR:HD1	1.75	0.51
3:L5:947:C:H5''	10:LE:51:VAL:HG21	1.93	0.51
3:L5:4174:U:H2'	3:L5:4175:G:H8	1.76	0.51
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.91	0.51
5:L8:6:C:H2'	5:L8:7:U:H6	1.75	0.51
48:Ls:127:ASN:HD21	48:Ls:151:THR:HG23	1.76	0.51
53:SE:124:CYS:HB3	53:SE:141:THR:HB	1.92	0.51
55:SH:170:VAL:HG13	55:SH:187:PHE:HB2	1.92	0.51
68:S2:1422:G:H4'	68:S2:1423:C:H3'	1.91	0.51
68:S2:1650:A:H5''	75:SQ:139:ALA:HB2	1.93	0.51
69:SR:35:CYS:HA	69:SR:38:ILE:HG12	1.91	0.51
78:SU:81:GLN:HB2	81:Sd:55:LEU:HD23	1.93	0.51
3:L5:1199:G:H2'	3:L5:1200:G:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.46	0.51
29:LY:33:PRO:HG2	29:LY:105:VAL:HG12	1.93	0.51
59:SN:37:ILE:HG12	59:SN:54:LEU:HD11	1.93	0.51
68:S2:656:G:H21	68:S2:663:C:H5''	1.76	0.51
68:S2:1221:G:H2'	68:S2:1222:G:C8	2.46	0.51
68:S2:1648:G:H5''	75:SQ:125:ARG:HB2	1.92	0.51
77:ST:6:VAL:HG12	77:ST:135:ALA:HB2	1.93	0.51
77:ST:85:ASN:HB3	77:ST:88:MET:HB2	1.93	0.51
1:CD:220:THR:HG23	1:CD:222:LYS:H	1.76	0.51
3:L5:2765:A:H2'	3:L5:2766:A:C8	2.45	0.51
3:L5:3870:C:H2'	3:L5:3871:A:C8	2.46	0.51
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.46	0.51
5:L8:130:C:H2'	5:L8:131:G:H8	1.75	0.51
51:SB:117:TRP:HB3	51:SB:153:THR:HG22	1.93	0.51
54:SG:10:THR:HA	54:SG:128:THR:HG23	1.92	0.51
64:SY:9:THR:HG22	64:SY:25:ILE:HG22	1.92	0.51
68:S2:1222:G:H5''	71:SF:78:MET:HE1	1.92	0.51
3:L5:318:A:H2'	3:L5:319:A:C8	2.47	0.51
5:L8:47:C:H1'	5:L8:61:A:H2'	1.92	0.51
49:Lt:104:ILE:HG13	49:Lt:106:PHE:HD1	1.76	0.51
55:SH:17:ASP:HB2	55:SH:20:GLU:HB3	1.92	0.51
60:SO:134:PRO:HB3	68:S2:944:A:H5''	1.93	0.51
71:SF:122:ARG:HE	80:Sc:59:LEU:HD21	1.76	0.51
85:CB:745:TYR:CE2	85:CB:812:CYS:HB2	2.45	0.51
3:L5:256:G:H2'	3:L5:257:C:C6	2.46	0.50
3:L5:1725:U:H2'	3:L5:1726:U:H6	1.77	0.50
8:LC:221:PHE:HB2	8:LC:229:LEU:HD11	1.92	0.50
68:S2:1405:A:H2'	68:S2:1406:G:O4'	2.11	0.50
71:SF:145:ARG:HB2	80:Sc:48:GLY:HA3	1.93	0.50
3:L5:1333:A:H2'	3:L5:1334:A:C8	2.46	0.50
3:L5:4459:U:H2'	3:L5:4460:U:C6	2.46	0.50
22:LR:169:ALA:HA	22:LR:172:ARG:HE	1.76	0.50
51:SB:72:ALA:HB2	51:SB:80:ALA:HA	1.92	0.50
60:SO:136:PRO:HB3	68:S2:944:A:H1'	1.92	0.50
68:S2:1010:G:H2'	68:S2:1011:A:C8	2.46	0.50
85:CB:207:PRO:HG2	85:CB:261:TRP:CE2	2.45	0.50
3:L5:1820:C:H2'	3:L5:1822:U:H5'	1.94	0.50
3:L5:3718:A2M:H2'	3:L5:3719:A:O4'	2.11	0.50
13:LH:44:GLU:HG3	17:LM:2:VAL:HG12	1.93	0.50
25:LU:45:GLU:HG3	25:LU:46:ARG:HG2	1.93	0.50
51:SB:138:PHE:HD2	51:SB:214:LYS:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SI:143:LYS:HD3	56:SI:146:GLN:HB2	1.92	0.50
68:S2:1845:A:H2'	68:S2:1846:G:H8	1.76	0.50
71:SF:62:ARG:HD2	71:SF:65:GLN:HE22	1.75	0.50
75:SQ:50:LYS:HE2	75:SQ:82:TYR:CZ	2.47	0.50
3:L5:153:G:H2'	3:L5:154:G:H8	1.77	0.50
3:L5:908:G:H2'	3:L5:909:A:H8	1.76	0.50
3:L5:1095:A:H2	3:L5:1200:G:N1	2.07	0.50
57:SJ:145:PRO:HD2	68:S2:522:A:H5''	1.93	0.50
68:S2:145:G:H2'	68:S2:146:G:C8	2.47	0.50
68:S2:736:C:H2'	68:S2:737:G:C4	2.47	0.50
68:S2:1221:G:H2'	68:S2:1222:G:H8	1.77	0.50
72:SK:16:PHE:HE2	72:SK:89:ILE:HG22	1.75	0.50
3:L5:710:G:H2'	3:L5:711:A:H8	1.76	0.50
3:L5:1461:C:H2'	3:L5:1462:A:C8	2.47	0.50
3:L5:2638:G:N1	3:L5:2718:U:H2'	2.27	0.50
8:LC:149:GLU:HG2	8:LC:151:PRO:HD2	1.94	0.50
59:SN:63:VAL:HG11	59:SN:71:ILE:HD11	1.92	0.50
76:SS:46:ARG:HG2	77:ST:35:ASP:HB2	1.92	0.50
79:SZ:102:LYS:HA	79:SZ:107:VAL:HG12	1.94	0.50
3:L5:2484:A:H62	3:L5:2494:U:H3	1.60	0.50
3:L5:4371:G:H5'	84:Et:76:A:H62	1.76	0.50
12:LG:162:ASP:HB2	12:LG:163:PRO:HD3	1.93	0.50
52:SC:196:ILE:HB	52:SC:223:TYR:HB2	1.93	0.50
53:SE:31:PRO:HG2	53:SE:38:LEU:HB2	1.94	0.50
68:S2:24:C:HO2'	68:S2:25:A:H8	1.59	0.50
68:S2:525:A:H2'	68:S2:526:A:H8	1.75	0.50
75:SQ:145:TYR:C	75:SQ:146:ARG:HD2	2.37	0.50
3:L5:4279:A:H5'	3:L5:4281:A:H1'	1.92	0.50
3:L5:4591:U:H2'	3:L5:4592:C:C6	2.47	0.50
53:SE:11:ARG:HH12	53:SE:24:THR:HG22	1.76	0.50
68:S2:70:G:N2	68:S2:79:A:H62	2.06	0.50
61:SV:60:ARG:HG2	61:SV:65:SER:HB3	1.94	0.50
70:SD:80:PRO:HD2	70:SD:83:SER:HB2	1.94	0.50
4:L7:49:A:H5''	9:LD:224:SER:HB3	1.94	0.50
5:L8:67:U:H2'	5:L8:68:G:C8	2.45	0.50
53:SE:11:ARG:HA	53:SE:28:ALA:HB2	1.92	0.50
68:S2:1128:C:H2'	68:S2:1129:G:C8	2.47	0.50
69:SR:17:ILE:HD11	69:SR:54:VAL:HA	1.94	0.50
3:L5:229:G:H5''	29:LY:11:ARG:HG3	1.93	0.49
49:Lt:16:ARG:HE	49:Lt:17:CYS:H	1.60	0.49
68:S2:414:A:H2'	68:S2:415:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SR:98:VAL:HG21	69:SR:117:LEU:HB2	1.94	0.49
85:CB:20:ARG:HD2	85:CB:358:LEU:HB3	1.94	0.49
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.27	0.49
3:L5:4088:C:H2'	3:L5:4089:G:H8	1.77	0.49
48:Ls:106:LYS:HD2	48:Ls:185:PHE:HA	1.93	0.49
56:SI:83:TYR:HB3	56:SI:101:ILE:HD12	1.94	0.49
86:CA:208:GLN:HA	86:CA:211:LYS:HE3	1.94	0.49
15:LJ:141:ILE:HA	15:LJ:144:LYS:HD2	1.93	0.49
22:LR:32:ILE:HD13	22:LR:44:LEU:HD13	1.94	0.49
31:La:100:ILE:HG12	31:La:123:ILE:HB	1.94	0.49
68:S2:107:A:H2'	68:S2:108:G:C8	2.47	0.49
3:L5:162:A:H2'	3:L5:163:A:C8	2.48	0.49
3:L5:184:U:H3'	3:L5:185:C:O4'	2.12	0.49
3:L5:3610:A:H2'	3:L5:3611:A:C8	2.47	0.49
3:L5:4067:U:H2'	3:L5:4068:U:C6	2.46	0.49
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.48	0.49
3:L5:4238:G:H2'	3:L5:4239:A:C8	2.47	0.49
7:LB:29:VAL:HG12	7:LB:31:SER:H	1.77	0.49
51:SB:121:ILE:HG12	51:SB:161:VAL:HG13	1.94	0.49
55:SH:157:HIS:HB3	55:SH:190:PRO:HG3	1.94	0.49
66:Sb:42:LYS:HE3	66:Sb:58:GLY:H	1.76	0.49
84:Et:37:A:H3'	84:Et:38:A:C8	2.48	0.49
3:L5:3732:A:H2'	3:L5:3733:A:C8	2.47	0.49
3:L5:4743:G:H2'	3:L5:4744:A:C8	2.48	0.49
13:LH:118:LEU:HD11	13:LH:167:VAL:HG22	1.95	0.49
30:LZ:50:PRO:HD3	30:LZ:68:ILE:HG12	1.94	0.49
61:SV:59:ILE:HA	61:SV:62:MET:HG2	1.95	0.49
68:S2:494:C:N4	68:S2:509:OMG:HN22	2.10	0.49
3:L5:3607:U:H2'	3:L5:3608:A:C8	2.48	0.49
3:L5:3610:A:H2'	3:L5:3611:A:H8	1.77	0.49
3:L5:3664:G:H2'	3:L5:3665:G:H8	1.77	0.49
3:L5:3722:G:H2'	3:L5:3723:A:H8	1.77	0.49
4:L7:120:U:H5''	9:LD:262:LYS:HE2	1.95	0.49
26:LV:99:GLU:HB3	27:LW:24:THR:HG23	1.94	0.49
49:Lt:110:VAL:O	49:Lt:114:ARG:HG2	2.12	0.49
58:SL:150:GLY:HA2	59:SN:133:ARG:HH22	1.77	0.49
3:L5:1326:A2M:H2'	3:L5:1327:C:C6	2.48	0.49
3:L5:2611:A:H2'	3:L5:2612:G:C8	2.47	0.49
68:S2:26:U:H2'	68:S2:27:A2M:H8	1.93	0.49
68:S2:948:C:H2'	68:S2:949:G:C8	2.46	0.49
3:L5:1468:C:H2'	3:L5:1469:C:H6	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LA:20:VAL:HA	6:LA:23:ARG:HG3	1.93	0.49
49:Lt:61:LYS:HA	49:Lt:75:PRO:HD2	1.94	0.49
53:SE:19:MET:HE3	53:SE:108:ARG:HD3	1.94	0.49
68:S2:656:G:H5'	68:S2:662:G:N2	2.27	0.49
68:S2:1144:A:H2'	68:S2:1145:A:C8	2.47	0.49
3:L5:179:G:H2'	3:L5:180:C:C6	2.48	0.49
3:L5:1306:C:H2'	3:L5:1307:A:H8	1.78	0.49
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.48	0.49
3:L5:1494:U:H2'	3:L5:1495:G:H8	1.78	0.49
3:L5:2709:C:H42	86:CA:257:LEU:H	1.61	0.49
3:L5:4507:A:H2'	3:L5:4508:C:C6	2.48	0.49
3:L5:4590:A2M:HM'3	3:L5:4590:A2M:H1'	1.63	0.49
51:SB:170:GLU:HA	51:SB:173:THR:HG22	1.94	0.49
53:SE:149:TYR:CD2	54:SG:205:GLU:HG3	2.47	0.49
68:S2:931:C:H2'	68:S2:932:G:C8	2.48	0.49
68:S2:1174:PSU:H2'	68:S2:1175:G:H8	1.78	0.49
75:SQ:146:ARG:HH22	84:Et:33:U:H3'	1.78	0.49
3:L5:325:U:H2'	3:L5:326:C:C6	2.47	0.49
3:L5:1251:C:H2'	3:L5:1252:C:C6	2.48	0.49
3:L5:1994:C:H2'	3:L5:1995:G:H8	1.76	0.49
3:L5:4162:C:H5	12:LG:73:ARG:HH12	1.61	0.49
3:L5:4627:U:H5''	7:LB:373:LYS:HG2	1.95	0.49
3:L5:4991:U:H2'	3:L5:4992:G:H8	1.78	0.49
7:LB:367:PHE:HB2	27:LW:1:MET:HG3	1.94	0.49
35:Le:78:LEU:HB3	47:Lr:20:ARG:HD2	1.95	0.49
50:SA:141:ASN:HD22	52:SC:86:LEU:HD23	1.78	0.49
53:SE:136:ILE:HD12	53:SE:149:TYR:CE1	2.48	0.49
54:SG:5:ILE:HD12	54:SG:124:LEU:HD22	1.95	0.49
83:Sg:149:GLU:HB2	83:Sg:171:ASP:HB3	1.95	0.49
3:L5:10:A:H2'	3:L5:11:G:C8	2.48	0.48
3:L5:1730:U:H4'	24:LT:100:LYS:HB2	1.95	0.48
3:L5:3736:A:H2'	3:L5:3737:A:H8	1.78	0.48
3:L5:4563:U:H2'	3:L5:4564:A:H8	1.78	0.48
7:LB:86:VAL:HG12	7:LB:201:LEU:HD23	1.94	0.48
56:SI:114:GLU:HB3	56:SI:136:ILE:HD12	1.95	0.48
57:SJ:169:ARG:HH12	57:SJ:175:ARG:NH1	2.10	0.48
60:SO:102:GLY:H	60:SO:134:PRO:HB2	1.78	0.48
68:S2:15:U:H2'	68:S2:16:G:O4'	2.13	0.48
68:S2:454:U:H2'	68:S2:455:A:C8	2.48	0.48
68:S2:1010:G:H2'	68:S2:1011:A:H8	1.78	0.48
68:S2:1501:C:H2'	68:S2:1502:C:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:SF:18:LYS:HD3	71:SF:22:LYS:HA	1.95	0.48
84:Et:6:G:H22	84:Et:67:U:H3	1.61	0.48
84:Et:25:C:H3'	84:Et:26:A:H5''	1.94	0.48
3:L5:1779:U:H2'	3:L5:1780:A:C8	2.49	0.48
3:L5:2777:G:H5''	3:L5:2778:G:H5'	1.96	0.48
3:L5:4688:C:H2'	3:L5:4689:PSU:C6	2.48	0.48
52:SC:183:LYS:HA	52:SC:195:LEU:O	2.13	0.48
68:S2:1279:C:H2'	68:S2:1280:G:H8	1.77	0.48
68:S2:1850:MA6:H8	68:S2:1850:MA6:O5'	2.13	0.48
3:L5:233:U:O2'	3:L5:234:G:H2'	2.13	0.48
3:L5:717:U:H2'	3:L5:718:C:C6	2.48	0.48
3:L5:1095:A:N1	3:L5:1200:G:C6	2.81	0.48
3:L5:4723:A:H2'	3:L5:4724:A:C8	2.49	0.48
20:LP:40:HIS:HE2	20:LP:111:SER:HA	1.78	0.48
56:SI:56:ARG:HA	56:SI:180:GLY:HA2	1.94	0.48
60:SO:129:ILE:HG21	65:Sa:44:ILE:HG21	1.95	0.48
64:SY:10:ARG:HG2	64:SY:11:LYS:HG3	1.94	0.48
68:S2:1284:A:H4'	68:S2:1285:G:H5''	1.96	0.48
74:SP:28:MET:HE1	74:SP:36:LEU:HG	1.94	0.48
77:ST:42:HIS:CD2	77:ST:43:LYS:HE3	2.48	0.48
86:CA:11:THR:HG23	86:CA:13:ALA:H	1.78	0.48
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.48	0.48
3:L5:4184:G:H5'	6:LA:233:ARG:HB2	1.96	0.48
53:SE:146:THR:HG21	68:S2:122:G:H21	1.78	0.48
68:S2:895:G:H3'	68:S2:896:U:H4'	1.94	0.48
68:S2:1314:U:H2'	72:SK:2:LEU:HD12	1.95	0.48
69:SR:10:LYS:HG2	69:SR:53:TYR:CZ	2.49	0.48
74:SP:29:SER:H	74:SP:32:GLN:NE2	2.10	0.48
3:L5:7:C:H2'	3:L5:8:U:C6	2.49	0.48
3:L5:968:C:H5'	10:LE:110:ARG:NE	2.29	0.48
3:L5:2528:G:H4'	3:L5:2783:A:H4'	1.95	0.48
3:L5:2870:A:H2'	3:L5:2871:A:H8	1.78	0.48
52:SC:206:SER:HB2	52:SC:210:PRO:HG2	1.96	0.48
68:S2:508:A:H3'	68:S2:509:OMG:C8	2.48	0.48
78:SU:80:PHE:HB3	81:Sd:52:PHE:HB3	1.96	0.48
3:L5:1478:C:H2'	3:L5:1479:G:H8	1.79	0.48
3:L5:2706:G:H22	3:L5:2709:C:H5''	1.78	0.48
5:L8:141:C:H2'	5:L8:142:U:C6	2.49	0.48
53:SE:246:LEU:HD22	53:SE:250:GLU:HG3	1.96	0.48
68:S2:1244:PSU:H2'	68:S2:1245:G:H8	1.79	0.48
74:SP:133:ILE:HG22	74:SP:134:GLY:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Sg:79:LEU:HD12	83:Sg:89:LEU:HD12	1.95	0.48
3:L5:1992:U:H4'	3:L5:1993:C:H5''	1.94	0.48
3:L5:2749:C:H2'	3:L5:2750:G:C8	2.49	0.48
3:L5:3770:U:H2'	3:L5:3771:C:C6	2.49	0.48
7:LB:217:ILE:HD12	7:LB:347:LEU:HB3	1.95	0.48
17:LM:25:VAL:HB	17:LM:38:VAL:HG22	1.96	0.48
25:LU:27:HIS:HB3	25:LU:114:TYR:HE1	1.79	0.48
43:Lm:98:LYS:HG3	43:Lm:118:THR:HG21	1.96	0.48
49:Lt:114:ARG:NE	49:Lt:133:LEU:HD12	2.28	0.48
57:SJ:115:PHE:HZ	57:SJ:122:SER:C	2.22	0.48
68:S2:807:G:H2'	68:S2:808:A:H8	1.79	0.48
71:SF:127:ARG:HA	71:SF:136:ARG:HD2	1.96	0.48
3:L5:710:G:H2'	3:L5:711:A:C8	2.49	0.48
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.48	0.48
3:L5:4347:G:H2'	3:L5:4348:A:C8	2.49	0.48
56:SI:145:ILE:HD13	68:S2:190:G:H5'	1.95	0.48
59:SN:63:VAL:HG21	59:SN:71:ILE:HG12	1.96	0.48
68:S2:1203:G:H2'	68:S2:1204:A:H8	1.79	0.48
70:SD:60:GLY:HA3	70:SD:65:ARG:H	1.78	0.48
3:L5:1702:C:H4'	8:LC:308:LYS:HD2	1.95	0.48
3:L5:1978:C:H2'	3:L5:1979:A:O4'	2.14	0.48
14:LI:93:PRO:HB2	14:LI:125:THR:HB	1.95	0.48
51:SB:81:PHE:CG	51:SB:109:LYS:HE3	2.49	0.48
52:SC:114:LYS:HE2	68:S2:1202:U:H4'	1.95	0.48
71:SF:144:LEU:HD23	80:Sc:49:PRO:HB2	1.96	0.48
75:SQ:131:LYS:HB2	75:SQ:140:ARG:HH22	1.78	0.48
86:CA:105:LEU:HB3	86:CA:126:VAL:HG22	1.95	0.48
3:L5:978:G:H2'	3:L5:979:C:C6	2.49	0.48
42:LI:12:PHE:CE2	42:LI:51:LEU:HD22	2.49	0.48
50:SA:158:ASP:HB2	50:SA:159:ILE:HD12	1.95	0.48
53:SE:105:THR:HG23	53:SE:245:ARG:HA	1.95	0.48
61:SV:22:ARG:NH2	61:SV:58:ALA:HB3	2.29	0.48
68:S2:66:G:H2'	68:S2:67:C:H4'	1.95	0.48
68:S2:808:A:H2	68:S2:855:G:H22	1.61	0.48
68:S2:1616:U:H2'	68:S2:1617:G:C8	2.48	0.48
68:S2:1740:C:H2'	68:S2:1741:U:C6	2.48	0.48
83:Sg:31:ILE:HG12	83:Sg:45:LEU:HD21	1.96	0.48
3:L5:162:A:H2'	3:L5:163:A:H8	1.78	0.47
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.96	0.47
51:SB:125:VAL:HG13	51:SB:172:MET:HE3	1.95	0.47
51:SB:176:VAL:HG23	51:SB:184:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SG:230:LYS:HG3	68:S2:786:G:H5'	1.94	0.47
68:S2:981:A:H2'	68:S2:982:G:C8	2.49	0.47
3:L5:268:G:H2'	3:L5:269:G:C8	2.47	0.47
3:L5:711:A:H2'	3:L5:712:C:C6	2.49	0.47
3:L5:1942:A:H2'	3:L5:1943:A:H8	1.78	0.47
3:L5:4067:U:H2'	3:L5:4068:U:H6	1.79	0.47
3:L5:4389:C:H2'	3:L5:4390:A:C8	2.49	0.47
7:LB:14:LEU:HD22	7:LB:17:LEU:HD11	1.97	0.47
23:LS:96:GLU:HG3	23:LS:139:ARG:HG2	1.96	0.47
30:LZ:77:TYR:HD2	33:Lc:39:ARG:HD3	1.77	0.47
53:SE:149:TYR:HD2	54:SG:205:GLU:HG3	1.78	0.47
54:SG:121:ILE:HG23	54:SG:124:LEU:HB3	1.96	0.47
68:S2:342:C:H2'	68:S2:343:A:H8	1.80	0.47
68:S2:1213:C:H2'	68:S2:1214:A:C8	2.49	0.47
71:SF:47:LYS:HD2	75:SQ:115:TYR:OH	2.14	0.47
71:SF:82:ASN:HD22	71:SF:88:MET:HE1	1.78	0.47
85:CB:770:VAL:HA	85:CB:786:ALA:HA	1.96	0.47
3:L5:1084:C:H2'	3:L5:1085:C:C6	2.49	0.47
3:L5:1733:G:N3	3:L5:4214:A:H2'	2.29	0.47
3:L5:1764:G:H4'	3:L5:1769:G:C6	2.49	0.47
3:L5:4232:U:H5'	45:Lo:3:ASN:HB3	1.97	0.47
3:L5:4578:G:H2'	3:L5:4579:PSU:C6	2.49	0.47
3:L5:4954:G:H2'	3:L5:4955:A:C8	2.50	0.47
5:L8:148:A:H2'	5:L8:149:G:C8	2.49	0.47
14:LI:36:LEU:HD21	14:LI:69:ARG:NH1	2.30	0.47
38:Lh:95:LEU:HB3	38:Lh:99:GLU:HG3	1.96	0.47
48:Ls:141:LEU:HD21	48:Ls:171:GLU:HA	1.97	0.47
60:SO:92:ALA:HA	60:SO:125:LYS:HB2	1.96	0.47
84:Et:6:G:H1	84:Et:67:U:H3	1.61	0.47
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.15	0.47
3:L5:4642:U:H2'	3:L5:4643:G:C8	2.49	0.47
5:L8:19:C:H2'	5:L8:20:A:C8	2.49	0.47
68:S2:27:A2M:H2'	68:S2:28:U:O4'	2.15	0.47
68:S2:344:U:H2'	68:S2:345:U:H6	1.79	0.47
83:Sg:34:ALA:HB1	83:Sg:66:VAL:HG13	1.97	0.47
3:L5:253:G:H2'	3:L5:254:G:C8	2.50	0.47
3:L5:1188:C:H2'	3:L5:1189:G:C8	2.50	0.47
3:L5:1751:A:H2'	3:L5:1752:G:H8	1.80	0.47
3:L5:2743:A:H2'	3:L5:2744:A:C8	2.50	0.47
3:L5:3867:A2M:H2'	3:L5:3868:G:O4'	2.14	0.47
3:L5:4619:U:H2'	3:L5:4620:OMU:H6	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:LH:48:LEU:HD21	13:LH:56:ARG:HD2	1.97	0.47
51:SB:109:LYS:O	51:SB:113:MET:HG2	2.14	0.47
65:Sa:5:ARG:HH21	68:S2:1864:U:H3'	1.79	0.47
68:S2:526:A:H2'	68:S2:527:C:C6	2.50	0.47
3:L5:261:G:H2'	3:L5:262:G:C8	2.50	0.47
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.49	0.47
3:L5:4098:A:H2'	3:L5:4099:G:H4'	1.96	0.47
3:L5:4146:G:H2'	3:L5:4147:G:C8	2.50	0.47
3:L5:4524:G:N3	7:LB:252:ALA:HB1	2.29	0.47
3:L5:4612:C:C2	13:LH:120:GLU:HB2	2.49	0.47
4:L7:110:G:H2'	4:L7:111:C:C6	2.50	0.47
15:LJ:78:LYS:HE3	15:LJ:82:ILE:HD11	1.96	0.47
29:LY:67:ILE:HD12	29:LY:107:THR:HG21	1.96	0.47
54:SG:137:ARG:HD2	54:SG:140:ARG:HG2	1.97	0.47
58:SL:113:LEU:HD21	58:SL:120:VAL:HG11	1.96	0.47
60:SO:44:VAL:HG13	60:SO:53:ILE:HB	1.97	0.47
68:S2:93:PSU:H2'	68:S2:94:G:O4'	2.14	0.47
68:S2:323:C:H2'	68:S2:327:G:H1	1.79	0.47
68:S2:558:G:H1'	68:S2:559:G:C8	2.49	0.47
68:S2:1284:A:C8	73:SM:33:ARG:HG3	2.49	0.47
68:S2:1320:G:H2'	68:S2:1321:G:O4'	2.15	0.47
86:CA:157:VAL:HG11	86:CA:323:VAL:HG21	1.97	0.47
3:L5:481:G:H2'	3:L5:482:G:C8	2.50	0.47
3:L5:491:G:H2'	3:L5:492:U:C6	2.49	0.47
3:L5:3598:C:H2'	3:L5:3599:A:C8	2.49	0.47
3:L5:3619:G:H22	3:L5:3624:A:H1'	1.78	0.47
3:L5:3760:A:H4'	3:L5:3761:C:H5''	1.97	0.47
3:L5:3910:C:H2'	3:L5:3911:C:H6	1.80	0.47
3:L5:3952:A:H2'	3:L5:3953:G:C4	2.49	0.47
13:LH:187:VAL:HG12	13:LH:188:GLN:HG3	1.96	0.47
14:LI:61:SER:HA	14:LI:126:VAL:HG12	1.96	0.47
28:LX:82:THR:HG21	38:Lh:37:THR:HG22	1.96	0.47
50:SA:121:LEU:HD11	50:SA:145:ILE:HG13	1.96	0.47
68:S2:573:U:O2	68:S2:576:A2M:H8	2.14	0.47
68:S2:1240:A:C6	74:SP:100:LYS:HB2	2.50	0.47
68:S2:1277:C:H2'	68:S2:1278:A:C8	2.46	0.47
68:S2:1407:U:H2'	68:S2:1408:U:C6	2.50	0.47
68:S2:1687:C:H2'	68:S2:1688:C:H6	1.80	0.47
79:SZ:49:LEU:HD23	79:SZ:83:LEU:HD13	1.97	0.47
83:Sg:32:LEU:HD21	83:Sg:71:ILE:HD11	1.97	0.47
86:CA:113:HIS:CD2	86:CA:276:MET:HE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1504:G:H2'	3:L5:1505:C:C6	2.50	0.47
3:L5:3917:A:H2'	3:L5:3918:G:H8	1.80	0.47
3:L5:4457:PSU:H1'	7:LB:252:ALA:HB3	1.97	0.47
88:L5:5294:SPM:H132	19:LO:91:LYS:HB3	1.96	0.47
28:LX:156:ILE:HD11	86:CA:291:MET:HB2	1.96	0.47
63:SX:129:SER:HB2	68:S2:29:G:H4'	1.96	0.47
66:Sb:19:HIS:HB3	66:Sb:22:LYS:HG3	1.96	0.47
69:SR:97:GLU:HG2	69:SR:120:THR:HG21	1.96	0.47
3:L5:1174:G:H1	3:L5:1186:U:H3	1.63	0.47
3:L5:1974:U:OP1	49:Lt:77:ALA:HA	2.15	0.47
3:L5:1993:C:H2'	3:L5:1994:C:H6	1.80	0.47
3:L5:4523:A2M:HM'3	3:L5:4523:A2M:H1'	1.75	0.47
41:Lk:26:LYS:HB2	41:Lk:69:LEU:HD12	1.97	0.47
47:Lr:45:HIS:CG	47:Lr:103:ARG:HH22	2.33	0.47
63:SX:9:THR:HG22	68:S2:681:PSU:H4'	1.97	0.47
68:S2:1513:C:H2'	68:S2:1514:G:H8	1.78	0.47
83:Sg:110:SER:HB2	83:Sg:154:VAL:HG12	1.97	0.47
3:L5:208:A:H2	3:L5:233:U:H5''	1.80	0.47
3:L5:2765:A:H2'	3:L5:2766:A:H8	1.80	0.47
9:LD:64:ILE:HD13	9:LD:109:LEU:HD22	1.96	0.47
54:SG:154:ARG:HD2	68:S2:77:A:N7	2.30	0.47
58:SL:23:VAL:HG23	58:SL:25:LEU:HG	1.97	0.47
68:S2:484:A2M:H8	68:S2:484:A2M:O5'	2.15	0.47
68:S2:527:C:H2'	68:S2:528:A:C8	2.49	0.47
68:S2:1587:G:C5	77:ST:67:ARG:HD2	2.50	0.47
68:S2:1595:U:H2'	68:S2:1596:U:C6	2.51	0.47
68:S2:1775:U:H2'	68:S2:1776:G:C8	2.50	0.47
3:L5:163:A:H2'	3:L5:164:G:H8	1.80	0.46
3:L5:223:G:H4'	3:L5:225:G:N7	2.30	0.46
3:L5:2400:G:H21	37:Lg:6:THR:HG22	1.80	0.46
3:L5:4088:C:H2'	3:L5:4089:G:C8	2.50	0.46
7:LB:58:ARG:HA	7:LB:366:LYS:HG3	1.97	0.46
11:LF:199:LYS:HG3	11:LF:200:ARG:HG2	1.96	0.46
51:SB:106:THR:HG23	51:SB:109:LYS:H	1.79	0.46
53:SE:122:LYS:NZ	53:SE:145:ARG:HH12	2.13	0.46
54:SG:88:ARG:HB3	54:SG:91:GLU:HB2	1.96	0.46
62:SW:11:LEU:HD12	62:SW:74:VAL:HB	1.96	0.46
64:SY:112:ASN:HA	64:SY:115:LYS:HE2	1.96	0.46
68:S2:694:G:H5''	68:S2:730:C:H5	1.79	0.46
68:S2:1189:A:H2'	68:S2:1190:A:H8	1.81	0.46
68:S2:1856:C:H2'	68:S2:1857:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:CB:426:LYS:HD2	85:CB:446:PRO:HB3	1.97	0.46
3:L5:318:A:H2'	3:L5:319:A:H8	1.78	0.46
3:L5:3607:U:H2'	3:L5:3608:A:H8	1.80	0.46
5:L8:93:C:HO2'	5:L8:94:G:H8	1.62	0.46
5:L8:102:G:H5''	40:Lj:39:TYR:HE1	1.79	0.46
6:LA:107:MET:HE1	6:LA:113:VAL:HG11	1.97	0.46
10:LE:226:ARG:HD3	10:LE:226:ARG:H	1.80	0.46
26:LV:42:VAL:HB	26:LV:45:ILE:HG13	1.96	0.46
50:SA:31:ASP:HB3	50:SA:34:MET:HB2	1.98	0.46
51:SB:225:LEU:HD11	51:SB:229:MET:HE3	1.97	0.46
55:SH:144:ILE:HG21	55:SH:152:ARG:HE	1.79	0.46
68:S2:179:C:H3'	68:S2:180:G:H8	1.80	0.46
68:S2:600:G:H2'	68:S2:601:OMG:C8	2.49	0.46
68:S2:835:C:H4'	68:S2:836:G:C8	2.50	0.46
68:S2:1499:U:H4'	70:SD:176:LEU:HD11	1.97	0.46
73:SM:31:LEU:HD21	73:SM:89:VAL:HG22	1.98	0.46
3:L5:462:G:H2'	3:L5:463:A:C8	2.50	0.46
3:L5:1307:A:H2'	3:L5:1308:C:C6	2.49	0.46
3:L5:2676:A:OP2	3:L5:2676:A:H8	1.97	0.46
3:L5:2870:A:H2'	3:L5:2871:A:C8	2.49	0.46
3:L5:3722:G:H2'	3:L5:3723:A:C8	2.50	0.46
68:S2:1826:G:H2'	68:S2:1827:U:H6	1.80	0.46
86:CA:113:HIS:CG	86:CA:276:MET:HE1	2.50	0.46
3:L5:1751:A:H2'	3:L5:1752:G:C8	2.51	0.46
10:LE:201:ILE:HG22	10:LE:264:ILE:HD12	1.98	0.46
51:SB:52:THR:HG23	51:SB:57:ILE:HA	1.96	0.46
52:SC:94:ILE:HD13	52:SC:162:ILE:HG13	1.96	0.46
52:SC:210:PRO:HD3	52:SC:236:PHE:CE2	2.50	0.46
55:SH:159:ASP:O	55:SH:160:LYS:HG2	2.15	0.46
68:S2:1073:U:H2'	68:S2:1074:C:H6	1.81	0.46
70:SD:16:ILE:HG21	81:Sd:22:ARG:HH11	1.80	0.46
3:L5:260:C:H2'	3:L5:261:G:C8	2.51	0.46
3:L5:1949:U:H5''	13:LH:64:ARG:HD3	1.96	0.46
3:L5:4896:G:H2'	3:L5:4897:G:H8	1.80	0.46
5:L8:144:U:H2'	5:L8:145:C:C6	2.51	0.46
16:LL:164:GLU:HB3	31:La:100:ILE:HD12	1.98	0.46
68:S2:27:A2M:HM'3	68:S2:27:A2M:H1'	1.59	0.46
68:S2:526:A:H2'	68:S2:527:C:H6	1.81	0.46
68:S2:1139:C:H2'	68:S2:1140:G:O4'	2.15	0.46
69:SR:109:LEU:HG	69:SR:111:PHE:HD1	1.80	0.46
83:Sg:259:TRP:HB3	83:Sg:266:ILE:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:CB:27:HIS:ND1	85:CB:138:GLN:HB2	2.29	0.46
3:L5:5006:U:H4'	3:L5:5007:A:H5'	1.96	0.46
38:Lh:52:LYS:HA	38:Lh:52:LYS:HD3	1.67	0.46
54:SG:18:VAL:HG23	54:SG:24:LEU:HD11	1.97	0.46
58:SL:126:VAL:HG12	58:SL:145:VAL:HG22	1.97	0.46
66:Sb:72:ARG:HH22	68:S2:1120:U:H5'	1.81	0.46
68:S2:1468:C:H2'	68:S2:1469:A:H8	1.80	0.46
76:SS:22:GLY:HA2	76:SS:56:ALA:HB3	1.97	0.46
3:L5:1693:U:H2'	3:L5:1694:C:O4'	2.15	0.46
3:L5:2421:G:OP2	3:L5:2828:U:H1'	2.16	0.46
3:L5:3619:G:H4'	22:LR:79:GLY:O	2.16	0.46
3:L5:3720:G:H22	3:L5:3733:A:H2	1.62	0.46
3:L5:4913:G:H4'	3:L5:4914:C:O5'	2.15	0.46
9:LD:182:GLY:HA2	9:LD:194:VAL:HG23	1.97	0.46
36:Lf:41:PHE:HE1	36:Lf:110:ILE:HD13	1.79	0.46
54:SG:31:ARG:NH2	68:S2:1745:A:H4'	2.31	0.46
57:SJ:46:VAL:HA	57:SJ:49:THR:HG22	1.98	0.46
62:SW:36:ARG:HA	62:SW:39:THR:HG22	1.98	0.46
62:SW:50:PHE:HB3	62:SW:63:VAL:HG13	1.98	0.46
68:S2:432:G:H2'	68:S2:433:A:C8	2.51	0.46
68:S2:1220:A:H2'	68:S2:1221:G:O4'	2.16	0.46
70:SD:219:PRO:HB2	83:Sg:192:THR:HG22	1.98	0.46
83:Sg:5:MET:HG3	83:Sg:310:TRP:HB3	1.98	0.46
83:Sg:79:LEU:HD21	83:Sg:87:LEU:HD23	1.96	0.46
83:Sg:153:CYS:SG	83:Sg:198:VAL:HG12	2.56	0.46
83:Sg:212:LYS:HD2	83:Sg:235:ILE:HG12	1.98	0.46
85:CB:445:LYS:HE3	85:CB:446:PRO:HD2	1.98	0.46
85:CB:524:LEU:HD22	85:CB:561:LEU:HD11	1.98	0.46
86:CA:59:GLU:HA	86:CA:62:LYS:HE3	1.96	0.46
86:CA:105:LEU:HA	86:CA:126:VAL:HA	1.98	0.46
3:L5:423:G:H5'	20:LP:26:PHE:HZ	1.79	0.46
3:L5:1317:U:H2'	3:L5:1318:C:C6	2.51	0.46
3:L5:4536:OMC:HM22	3:L5:4537:C:O4'	2.15	0.46
3:L5:4680:G:H2'	3:L5:4681:A:C8	2.50	0.46
3:L5:4965:U:H4'	3:L5:4966:A:H5'	1.98	0.46
32:Lb:75:LEU:HD23	32:Lb:76:VAL:HG22	1.98	0.46
51:SB:46:LYS:HE2	51:SB:46:LYS:HB2	1.66	0.46
57:SJ:46:VAL:HG13	57:SJ:102:ILE:HD11	1.98	0.46
68:S2:375:U:H2'	68:S2:376:A:C8	2.51	0.46
68:S2:848:U:H2'	68:S2:849:A:H8	1.81	0.46
68:S2:1365:G:H2'	68:S2:1366:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1705:C:H2'	68:S2:1706:G:C8	2.51	0.46
70:SD:158:ILE:HG23	70:SD:189:MET:HE1	1.98	0.46
75:SQ:48:GLN:NE2	75:SQ:52:LEU:HD23	2.31	0.46
3:L5:424:U:H2'	3:L5:425:U:C6	2.50	0.46
19:LO:43:ILE:HD11	19:LO:138:LEU:HD13	1.98	0.46
25:LU:18:VAL:HG13	25:LU:73:THR:HG23	1.96	0.46
25:LU:28:PRO:HB2	25:LU:34:MET:HB3	1.98	0.46
68:S2:996:A:H2'	68:S2:997:A:C8	2.51	0.46
68:S2:1657:G:H1	68:S2:1667:U:H3	1.64	0.46
68:S2:1713:C:H2'	68:S2:1714:U:C6	2.51	0.46
83:Sg:249:CYS:SG	83:Sg:258:ILE:HD13	2.56	0.46
85:CB:23:SER:HB3	85:CB:122:THR:HG21	1.98	0.46
3:L5:137:G:H2'	3:L5:138:G:C8	2.50	0.46
3:L5:1278:C:H2'	3:L5:1279:A:O4'	2.16	0.46
3:L5:4239:A:H2'	3:L5:4240:G:C8	2.51	0.46
3:L5:4336:A:H5''	3:L5:4337:C:H5'	1.98	0.46
3:L5:4957:C:H2'	3:L5:4958:C:C6	2.51	0.46
3:L5:4996:C:H4'	34:Ld:26:THR:HG23	1.98	0.46
4:L7:4:U:H2'	4:L7:5:A:H8	1.80	0.46
7:LB:161:ARG:HG2	7:LB:184:GLN:HA	1.98	0.46
68:S2:29:G:H2'	68:S2:30:C:C6	2.50	0.46
68:S2:1031:A2M:HM'3	68:S2:1031:A2M:H1'	1.59	0.46
68:S2:1189:A:H2'	68:S2:1190:A:C8	2.50	0.46
68:S2:1661:A:C8	81:Sd:14:PHE:HB2	2.51	0.46
75:SQ:40:GLU:HA	75:SQ:48:GLN:NE2	2.31	0.46
76:SS:124:ARG:HE	76:SS:129:LEU:HB2	1.81	0.46
85:CB:50:ARG:HG2	85:CB:52:GLY:H	1.79	0.46
3:L5:10:A:H2'	3:L5:11:G:H8	1.81	0.45
3:L5:2448:G:H2'	3:L5:2449:A:C8	2.52	0.45
3:L5:3932:U:H2'	3:L5:3933:G:H8	1.79	0.45
3:L5:4070:U:H2'	3:L5:4071:U:C6	2.49	0.45
4:L7:1:G:H5'	9:LD:263:LYS:HE2	1.98	0.45
8:LC:318:PRO:HB2	8:LC:325:MET:HE2	1.97	0.45
13:LH:89:ARG:HG3	13:LH:145:ILE:HG23	1.96	0.45
53:SE:55:ALA:HB1	53:SE:60:GLU:HB2	1.97	0.45
53:SE:129:ILE:HG22	53:SE:139:LEU:HB2	1.98	0.45
53:SE:136:ILE:HG23	53:SE:149:TYR:CE1	2.51	0.45
54:SG:221:LYS:O	54:SG:225:GLN:HG2	2.15	0.45
68:S2:17:C:H2'	68:S2:18:C:C6	2.52	0.45
68:S2:1438:A:H2'	68:S2:1439:A:H8	1.79	0.45
86:CA:36:VAL:HG12	86:CA:125:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:276:C:H2'	39:Li:29:ARG:HH22	1.82	0.45
3:L5:1494:U:H2'	3:L5:1495:G:C8	2.51	0.45
3:L5:4066:U:H2'	3:L5:4067:U:C6	2.51	0.45
3:L5:4742:G:H2'	3:L5:4743:G:C8	2.50	0.45
3:L5:5004:C:H2'	3:L5:5005:G:O4'	2.15	0.45
3:L5:5023:C:H3'	3:L5:5024:C:H4'	1.98	0.45
4:L7:23:A:H2'	4:L7:24:C:C6	2.52	0.45
5:L8:119:C:H2'	5:L8:120:G:H8	1.79	0.45
7:LB:45:ALA:HB3	7:LB:183:ILE:HG23	1.99	0.45
21:LQ:43:PHE:CD2	21:LQ:133:GLY:HA3	2.51	0.45
68:S2:694:G:H5''	68:S2:730:C:C5	2.51	0.45
76:SS:45:LEU:HD12	76:SS:50:ILE:HD11	1.98	0.45
82:Sf:132:MET:HG2	82:Sf:141:CYS:HB2	1.97	0.45
85:CB:189:ILE:HD11	85:CB:204:MET:HA	1.99	0.45
3:L5:460:C:H2'	3:L5:461:G:H8	1.80	0.45
3:L5:1419:G:H5''	21:LQ:71:LYS:NZ	2.31	0.45
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.50	0.45
3:L5:4196:OMG:HM23	3:L5:4196:OMG:H1'	1.68	0.45
18:LN:200:LEU:HD13	18:LN:204:ARG:HH12	1.79	0.45
46:Lp:62:LYS:HE2	46:Lp:62:LYS:HB2	1.80	0.45
71:SF:51:HIS:HA	71:SF:86:LYS:HE3	1.97	0.45
3:L5:422:C:H2'	3:L5:423:G:H8	1.82	0.45
3:L5:1503:A:H1'	3:L5:1504:G:C8	2.51	0.45
3:L5:2056:G:H4'	19:LO:18:ARG:HH22	1.81	0.45
3:L5:3925:OMU:HM23	3:L5:3925:OMU:H1'	1.77	0.45
8:LC:209:ILE:HB	8:LC:229:LEU:HD23	1.98	0.45
23:LS:76:LYS:HB2	23:LS:131:GLU:OE1	2.17	0.45
25:LU:79:SER:HB2	25:LU:82:TYR:HB2	1.97	0.45
26:LV:111:GLU:HG3	26:LV:131:ARG:HD3	1.98	0.45
56:SI:144:LYS:HG3	56:SI:145:ILE:HG23	1.99	0.45
68:S2:194:C:H2'	68:S2:195:C:H6	1.82	0.45
68:S2:1128:C:H2'	68:S2:1129:G:H8	1.81	0.45
68:S2:1406:G:H2'	68:S2:1407:U:C6	2.52	0.45
68:S2:1643:U:H2'	68:S2:1644:C:C6	2.51	0.45
70:SD:131:ALA:HA	70:SD:191:PRO:HD3	1.98	0.45
85:CB:609:PHE:CD2	85:CB:699:GLY:HA2	2.52	0.45
3:L5:425:U:H4'	20:LP:6:LEU:HD21	1.99	0.45
3:L5:691:C:H2'	3:L5:692:A:H8	1.78	0.45
3:L5:965:G:N2	3:L5:2092:G:H1'	2.32	0.45
3:L5:1092:G:H2'	3:L5:1093:C:C6	2.52	0.45
3:L5:4392:OMG:HM21	3:L5:4394:A:H2'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LA:206:PRO:HG3	6:LA:213:GLY:HA3	1.99	0.45
17:LM:33:GLN:O	17:LM:33:GLN:HG2	2.16	0.45
51:SB:167:LYS:O	51:SB:171:ILE:HG12	2.17	0.45
53:SE:198:ARG:HG2	53:SE:208:VAL:HG22	1.99	0.45
60:SO:66:ARG:HG3	68:S2:962:A:H5''	1.98	0.45
68:S2:674:C:H2'	68:S2:675:U:C6	2.51	0.45
68:S2:1383:A2M:HM'3	68:S2:1383:A2M:H1'	1.69	0.45
73:SM:35:ILE:H	73:SM:35:ILE:HD12	1.81	0.45
3:L5:270:U:H2'	3:L5:271:C:C6	2.52	0.45
3:L5:1778:C:H5''	9:LD:5:LYS:HG3	1.98	0.45
6:LA:221:LYS:HE3	6:LA:221:LYS:HB3	1.81	0.45
15:LJ:35:ARG:HD2	15:LJ:123:ILE:H	1.81	0.45
50:SA:76:VAL:HG12	50:SA:123:VAL:HB	1.99	0.45
58:SL:17:PHE:CD2	68:S2:222:U:H5''	2.52	0.45
68:S2:1129:G:H2'	68:S2:1130:G:N3	2.32	0.45
68:S2:1714:U:H2'	68:S2:1715:A:C8	2.52	0.45
69:SR:83:ASN:HB3	69:SR:85:VAL:HG13	1.99	0.45
76:SS:14:ARG:HH21	76:SS:17:ASN:HA	1.81	0.45
76:SS:27:ALA:HB2	76:SS:52:LEU:HD11	1.99	0.45
82:Sf:141:CYS:HB3	82:Sf:145:CYS:HB2	1.39	0.45
3:L5:1414:C:H2'	3:L5:1415:G:C8	2.51	0.45
3:L5:2844:A:O2'	3:L5:4631:G:H4'	2.16	0.45
4:L7:112:U:H2'	4:L7:113:G:H8	1.82	0.45
7:LB:220:ILE:HG12	7:LB:278:THR:HG23	1.98	0.45
8:LC:7:LEU:HG	8:LC:21:ASN:HB3	1.98	0.45
9:LD:146:LEU:HB2	9:LD:163:LEU:HD12	1.98	0.45
23:LS:161:ARG:HE	23:LS:164:LYS:HB2	1.82	0.45
64:SY:35:VAL:HG13	64:SY:39:GLU:HB3	1.99	0.45
65:Sa:44:ILE:HD12	65:Sa:65:PRO:HD2	1.99	0.45
68:S2:96:C:H2'	68:S2:97:U:C6	2.52	0.45
68:S2:468:A2M:HM'3	68:S2:468:A2M:H1'	1.61	0.45
68:S2:468:A2M:H2'	68:S2:469:A:O4'	2.16	0.45
68:S2:587:A:H5'	68:S2:592:C:H41	1.82	0.45
68:S2:1298:G:C8	74:SP:79:HIS:CE1	3.04	0.45
82:Sf:121:CYS:HB3	82:Sf:141:CYS:HB2	1.57	0.45
86:CA:123:HIS:HE1	86:CA:338:PHE:HB2	1.82	0.45
3:L5:702:U:H2'	3:L5:703:G:O4'	2.17	0.45
3:L5:1847:C:H2'	3:L5:1848:C:C6	2.52	0.45
3:L5:2709:C:H2'	86:CA:263:ARG:NE	2.32	0.45
3:L5:4309:G:H5'	3:L5:4338:G:H5''	1.99	0.45
3:L5:4742:G:H2'	3:L5:4743:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LB:341:LYS:O	7:LB:342:LYS:HG2	2.17	0.45
14:LI:87:MET:HG2	14:LI:138:ILE:HG12	1.99	0.45
65:Sa:45:VAL:HG11	65:Sa:53:ILE:HG13	1.99	0.45
68:S2:609:U:H2'	68:S2:610:G:H8	1.80	0.45
68:S2:656:G:N2	68:S2:663:C:H5''	2.31	0.45
68:S2:1199:A:H2'	68:S2:1200:A:C8	2.51	0.45
81:Sd:22:ARG:HH21	81:Sd:37:ASN:HB2	1.82	0.45
3:L5:518:G:N1	3:L5:643:C:H2'	2.32	0.45
3:L5:1338:G:H4'	3:L5:1339:U:H6	1.81	0.45
3:L5:1593:A:H5''	3:L5:2839:PSU:H5'	1.98	0.45
3:L5:4601:U:H2'	3:L5:4602:A:H8	1.81	0.45
3:L5:4737:G:H2'	3:L5:4738:C:C6	2.52	0.45
19:LO:81:TRP:HB2	19:LO:104:VAL:HG21	1.98	0.45
28:LX:64:SER:HB2	38:Lh:69:LEU:HD13	1.99	0.45
32:Lb:101:HIS:CE1	32:Lb:103:LYS:HG2	2.52	0.45
33:Lc:87:LYS:HA	33:Lc:87:LYS:HD3	1.80	0.45
52:SC:235:ASN:HD21	68:S2:1355:C:H6	1.64	0.45
68:S2:1801:A:H2'	68:S2:1802:C:C6	2.52	0.45
76:SS:65:GLU:HA	76:SS:68:ILE:HG12	1.98	0.45
78:SU:49:LYS:HG3	78:SU:92:HIS:HB2	1.99	0.45
3:L5:4458:C:H2'	3:L5:4459:U:C6	2.52	0.45
10:LE:210:LYS:HD3	10:LE:210:LYS:HA	1.78	0.45
12:LG:120:LYS:HB3	12:LG:125:LYS:HG3	1.99	0.45
27:LW:81:ALA:HB2	27:LW:87:LEU:HB2	1.99	0.45
29:LY:47:MET:HG2	29:LY:115:ARG:HH21	1.82	0.45
35:Le:35:TRP:CZ2	35:Le:56:PRO:HD2	2.51	0.45
68:S2:461:U:H2'	68:S2:462:OMC:H6	1.82	0.45
68:S2:1628:C:H2'	68:S2:1629:C:C6	2.51	0.45
68:S2:1736:G:H2'	68:S2:1737:G:C8	2.52	0.45
83:Sg:129:ILE:HD11	83:Sg:151:VAL:HG11	1.98	0.45
3:L5:6:C:H5''	12:LG:197:LYS:HB3	1.99	0.44
3:L5:499:G:H2'	3:L5:499:G:N3	2.31	0.44
3:L5:690:C:H4'	47:Lr:85:ASN:ND2	2.32	0.44
3:L5:907:C:H2'	3:L5:908:G:C8	2.51	0.44
3:L5:1244:G:H2'	3:L5:1245:C:H6	1.81	0.44
3:L5:2478:C:H2'	3:L5:2479:G:H5'	1.99	0.44
3:L5:2749:C:H2'	3:L5:2750:G:H8	1.80	0.44
3:L5:3611:A:H2	3:L5:5016:A:H8	1.65	0.44
3:L5:3690:U:H2'	3:L5:3691:G:O4'	2.17	0.44
3:L5:4113:U:H4'	3:L5:4115:G:C4	2.52	0.44
7:LB:354:GLN:HB3	7:LB:359:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LP:54:GLN:HA	20:LP:83:TRP:CD1	2.52	0.44
30:LZ:73:LYS:HE3	30:LZ:73:LYS:HB3	1.76	0.44
34:Ld:92:ARG:HA	34:Ld:102:LEU:HD23	1.98	0.44
55:SH:148:LEU:HD22	62:SW:49:GLU:OE1	2.17	0.44
56:SI:129:LEU:HD12	56:SI:129:LEU:HA	1.88	0.44
66:Sb:37:CYS:HB3	66:Sb:59:CYS:HB3	1.51	0.44
68:S2:142:C:N4	68:S2:329:G:H5''	2.32	0.44
68:S2:342:C:H2'	68:S2:343:A:C8	2.52	0.44
68:S2:496:C:H2'	68:S2:497:C:C6	2.52	0.44
68:S2:1788:A:H2'	68:S2:1789:G:O4'	2.17	0.44
3:L5:434:A:H3'	3:L5:435:A:H8	1.81	0.44
3:L5:1084:C:H2'	3:L5:1085:C:H6	1.81	0.44
3:L5:1239:C:H5	10:LE:60:SER:HB2	1.82	0.44
3:L5:1628:C:OP2	6:LA:9:ARG:HD2	2.17	0.44
3:L5:1998:A:H2'	3:L5:1999:A:C8	2.52	0.44
3:L5:3697:U:H5''	3:L5:3698:G:H5'	1.99	0.44
5:L8:77:A:H2'	5:L8:78:G:C8	2.51	0.44
5:L8:130:C:H2'	5:L8:131:G:C8	2.52	0.44
19:LO:61:ARG:HA	19:LO:70:PRO:HD2	1.98	0.44
19:LO:126:VAL:HG13	19:LO:127:VAL:HG13	1.98	0.44
52:SC:107:LEU:HD23	52:SC:233:LEU:HD21	2.00	0.44
68:S2:433:A:H2'	68:S2:434:G:C8	2.52	0.44
68:S2:793:G:H2'	68:S2:794:A:H8	1.82	0.44
68:S2:1213:C:H2'	68:S2:1214:A:H8	1.81	0.44
68:S2:1711:U:H2'	68:S2:1712:A:C8	2.53	0.44
76:SS:43:VAL:HG21	77:ST:36:THR:HG23	1.98	0.44
83:Sg:157:SER:HB3	83:Sg:164:ILE:HG12	1.99	0.44
3:L5:190:G:H2'	3:L5:191:G:H8	1.83	0.44
3:L5:1340:OMC:HM23	3:L5:1340:OMC:H1'	1.73	0.44
3:L5:1359:G:H4'	18:LN:203:TYR:HB2	2.00	0.44
3:L5:1514:U:H2'	3:L5:1515:A:H8	1.80	0.44
3:L5:2542:G:H2'	3:L5:2543:A:C8	2.52	0.44
3:L5:4524:G:C2	7:LB:252:ALA:HB1	2.52	0.44
89:L5:5288:SPD:HN11	89:L5:5288:SPD:H42	1.54	0.44
5:L8:8:U:H2'	5:L8:9:A:C8	2.52	0.44
8:LC:298:ILE:HD13	21:LQ:131:PRO:HB3	1.98	0.44
9:LD:181:PRO:HD2	9:LD:195:HIS:CD2	2.52	0.44
54:SG:219:GLU:HA	54:SG:222:GLU:HB2	1.98	0.44
59:SN:115:LEU:O	59:SN:119:GLU:HG2	2.17	0.44
68:S2:348:A:H2'	68:S2:349:A:C8	2.52	0.44
68:S2:1311:C:H5'	82:Sf:143:LYS:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1468:C:H2'	68:S2:1469:A:C8	2.52	0.44
68:S2:1831:A:H2'	68:S2:1832:6MZ:H8	1.99	0.44
70:SD:109:LEU:HD13	70:SD:182:LEU:HD23	1.99	0.44
84:Et:70:G:H2'	84:Et:71:G:C8	2.53	0.44
86:CA:142[A]:VAL:HG23	86:CA:230:VAL:HG12	2.00	0.44
3:L5:208:A:C2	3:L5:233:U:H5''	2.53	0.44
3:L5:455:C:O2'	3:L5:456:C:H5'	2.17	0.44
3:L5:1326:A2M:HM'3	3:L5:1326:A2M:H1'	1.62	0.44
3:L5:1345:A:H2'	3:L5:1346:C:C6	2.52	0.44
3:L5:1431:C:H2'	3:L5:1432:G:O4'	2.18	0.44
3:L5:1458:C:H5''	21:LQ:69:LYS:HD2	1.99	0.44
3:L5:4637:OMG:HM23	3:L5:4637:OMG:H1'	1.72	0.44
3:L5:4651:A:H2'	3:L5:4652:G:O4'	2.17	0.44
68:S2:462:OMC:HM23	68:S2:462:OMC:H1'	1.81	0.44
68:S2:1775:U:H2'	68:S2:1776:G:H8	1.83	0.44
69:SR:106:LEU:HD13	69:SR:109:LEU:HD23	1.99	0.44
3:L5:35:U:H4'	3:L5:1525:A:C2	2.53	0.44
3:L5:280:G:H5''	18:LN:14:LYS:HE2	1.99	0.44
3:L5:1980:U:O2'	3:L5:1981:G:H5''	2.18	0.44
3:L5:2845:A:H61	3:L5:3843:C:N4	2.16	0.44
3:L5:3684:G:H2'	3:L5:3685:C:C6	2.52	0.44
3:L5:4420:U:H5''	3:L5:4421:C:H5	1.82	0.44
49:Lt:34:PRO:HA	49:Lt:37:LEU:HG	1.99	0.44
51:SB:143:THR:HA	51:SB:207:LEU:HD23	1.98	0.44
53:SE:36:HIS:CG	53:SE:85:GLY:HA3	2.53	0.44
55:SH:30:LEU:HG	55:SH:33:ASN:HD22	1.83	0.44
60:SO:116:LEU:HD23	65:Sa:45:VAL:HG22	1.99	0.44
64:SY:88:LYS:HD2	64:SY:97:TYR:CZ	2.52	0.44
68:S2:588:G:H4'	68:S2:589:G:H5'	2.00	0.44
69:SR:21:TYR:HD1	69:SR:58:MET:HE1	1.82	0.44
76:SS:59:LEU:HD12	76:SS:59:LEU:HA	1.76	0.44
85:CB:27:HIS:HB3	85:CB:30:HIS:CD2	2.53	0.44
3:L5:1468:C:H2'	3:L5:1469:C:C6	2.52	0.44
3:L5:2654:C:H2'	3:L5:2655:C:H6	1.83	0.44
3:L5:3748:A:H5''	6:LA:243:THR:HB	2.00	0.44
3:L5:4246:G:H2'	3:L5:4247:G:H8	1.83	0.44
3:L5:5002:U:H2'	3:L5:5003:U:C6	2.52	0.44
6:LA:180:LEU:HD21	46:Lp:22:LEU:HB3	1.99	0.44
10:LE:155:GLY:O	10:LE:158:ARG:HG3	2.17	0.44
18:LN:169:ARG:HG3	18:LN:174:LEU:HD12	1.99	0.44
39:Li:76:ARG:HA	39:Li:76:ARG:HD3	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:SW:3:ARG:HD3	62:SW:6:VAL:HG12	1.99	0.44
68:S2:12:U:H2'	68:S2:13:C:H6	1.83	0.44
68:S2:1804:U:H2'	68:S2:1805:G:C8	2.52	0.44
70:SD:39:VAL:HG12	70:SD:48:ILE:HG12	1.98	0.44
86:CA:107:LYS:HD2	86:CA:318:GLN:OE1	2.17	0.44
3:L5:1217:G:H2'	3:L5:1218:G:H8	1.83	0.44
3:L5:2351:OMC:HM23	3:L5:2351:OMC:H1'	1.69	0.44
3:L5:3598:C:H2'	3:L5:3599:A:H8	1.83	0.44
3:L5:4578:G:H2'	3:L5:4579:PSU:H6	1.82	0.44
3:L5:4685:U:H2'	3:L5:4686:G:C8	2.53	0.44
51:SB:35:ALA:HB3	51:SB:42:ARG:HA	2.00	0.44
62:SW:69:LEU:HD21	62:SW:72:CYS:HB3	1.98	0.44
70:SD:40:ARG:HB2	78:SU:108:PRO:HG3	1.99	0.44
72:SK:3:MET:HE3	72:SK:48:ALA:HB2	1.99	0.44
73:SM:36:ARG:NH2	82:Sf:130:VAL:HA	2.32	0.44
86:CA:245:THR:HG23	86:CA:280:LEU:HB2	1.99	0.44
3:L5:429:A:H2'	3:L5:430:G:C8	2.53	0.44
3:L5:4935:C:H2'	3:L5:4936:G:C8	2.52	0.44
5:L8:75:OMG:HM23	5:L8:75:OMG:H1'	1.79	0.44
21:LQ:3:VAL:HG13	21:LQ:5:ILE:HG12	2.00	0.44
22:LR:36:ASN:HD21	86:CA:256:GLY:H	1.65	0.44
30:LZ:14:LEU:HB3	37:Lg:88:ARG:HG3	1.99	0.44
45:Lo:4:VAL:HG23	45:Lo:93:LEU:HD12	2.00	0.44
49:Lt:123:ARG:HE	49:Lt:125:LEU:C	2.25	0.44
57:SJ:46:VAL:HG11	57:SJ:106:LEU:HD21	2.00	0.44
57:SJ:131:ARG:HA	57:SJ:131:ARG:HD2	1.78	0.44
72:SK:64:TRP:HB3	81:Sd:23:VAL:HA	2.00	0.44
80:Sc:12:ALA:HB1	80:Sc:32:VAL:HB	1.99	0.44
86:CA:64:PHE:CD2	86:CA:72:LYS:HE2	2.52	0.44
3:L5:2079:G:H2'	3:L5:2080:U:C6	2.53	0.44
3:L5:2256:C:H2'	3:L5:2257:C:O4'	2.17	0.44
3:L5:2568:C:H2'	3:L5:2569:G:H8	1.83	0.44
3:L5:3721:U:H2'	3:L5:3722:G:H8	1.82	0.44
3:L5:4364:G:H2'	3:L5:4365:C:H6	1.82	0.44
26:LV:69:LYS:HB2	26:LV:72:LEU:HD12	2.00	0.44
35:Le:91:CYS:HB3	35:Le:95:TYR:HD2	1.82	0.44
50:SA:205:ARG:HH22	69:SR:84:TYR:N	2.15	0.44
55:SH:111:LYS:HB3	68:S2:798:G:C8	2.53	0.44
68:S2:900:C:H5'	68:S2:901:G:N7	2.33	0.44
68:S2:1533:A:H2	68:S2:1536:G:N3	2.16	0.44
68:S2:1782:G:H2'	68:S2:1784:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:CB:342:ARG:HA	85:CB:342:ARG:HD3	1.79	0.44
3:L5:287:U:H2'	3:L5:288:G:C8	2.53	0.43
3:L5:497:G:N2	3:L5:498:C:H41	2.16	0.43
3:L5:4291:G:H5'	3:L5:4293:PSU:C6	2.53	0.43
3:L5:4920:C:H2'	3:L5:4921:C:C6	2.53	0.43
7:LB:128:LYS:HA	7:LB:128:LYS:HD2	1.87	0.43
8:LC:76:ILE:HG12	8:LC:96:CYS:SG	2.58	0.43
48:Ls:57:LYS:O	48:Ls:61:MET:HG2	2.18	0.43
68:S2:223:C:H2'	68:S2:224:A:C8	2.53	0.43
68:S2:571:U:H2'	68:S2:572:U:H6	1.83	0.43
68:S2:1064:C:H2'	68:S2:1065:G:H8	1.83	0.43
68:S2:1101:U:H2'	68:S2:1102:G:C8	2.49	0.43
70:SD:202:LYS:HA	70:SD:202:LYS:HD2	1.73	0.43
83:Sg:234:ASP:H	83:Sg:252:THR:HB	1.83	0.43
85:CB:41:CYS:HA	85:CB:49:ALA:HA	2.00	0.43
86:CA:21:TYR:CE1	86:CA:117:PHE:HB3	2.44	0.43
3:L5:215:C:H5''	3:L5:216:C:H5''	2.00	0.43
3:L5:398:A2M:O5'	3:L5:398:A2M:H8	2.18	0.43
3:L5:457:G:H2'	3:L5:458:C:C6	2.54	0.43
3:L5:518:G:H1	3:L5:643:C:H2'	1.83	0.43
3:L5:1356:U:H2'	3:L5:1357:C:C6	2.53	0.43
3:L5:3825:A2M:H2'	3:L5:3826:C:O4'	2.17	0.43
3:L5:3916:G:H2'	3:L5:3917:A:C8	2.53	0.43
3:L5:4710:C:H2'	3:L5:4711:C:C6	2.53	0.43
5:L8:75:OMG:H8	5:L8:75:OMG:OP1	2.01	0.43
5:L8:82:A:N7	5:L8:84:A:H3'	2.33	0.43
36:Lf:15:LYS:HB3	36:Lf:25:THR:HG23	1.99	0.43
49:Lt:109:ILE:HA	49:Lt:112:ILE:HG12	1.99	0.43
50:SA:8:LEU:HD12	50:SA:191:ARG:HH12	1.83	0.43
64:SY:10:ARG:HA	68:S2:839:C:N4	2.33	0.43
68:S2:115:U:H2'	68:S2:116:OMU:C6	2.48	0.43
68:S2:1198:G:H2'	68:S2:1199:A:C8	2.53	0.43
68:S2:1328:OMG:HM23	68:S2:1328:OMG:H1'	1.78	0.43
83:Sg:106:LYS:HD2	83:Sg:126:ASP:HA	2.01	0.43
85:CB:222:ALA:HB3	85:CB:346:ALA:HA	2.00	0.43
3:L5:1327:C:H2'	3:L5:1328:G:C8	2.53	0.43
3:L5:1428:U:H5''	21:LQ:42:THR:HB	1.99	0.43
3:L5:1995:G:H2'	3:L5:1996:C:C6	2.53	0.43
3:L5:3856:A:H5''	20:LP:83:TRP:O	2.19	0.43
27:LW:117:LYS:HA	27:LW:117:LYS:HD3	1.87	0.43
34:Ld:24:GLU:HB2	34:Ld:120:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SE:137:PRO:HG2	53:SE:150:PRO:HD2	1.99	0.43
68:S2:24:C:O2'	68:S2:25:A:H8	2.01	0.43
68:S2:51:U:H2'	68:S2:52:G:C8	2.51	0.43
68:S2:549:C:H2'	68:S2:550:C:C6	2.53	0.43
68:S2:919:A:H8	68:S2:919:A:OP2	2.02	0.43
68:S2:1748:G:O6	68:S2:1786:U:O4	2.37	0.43
83:Sg:120:ILE:HB	83:Sg:132:TRP:HB2	1.99	0.43
3:L5:500:G:O2'	3:L5:504:G:H3'	2.18	0.43
3:L5:1588:U:H2'	3:L5:1589:C:C6	2.54	0.43
3:L5:1700:G:H5'	3:L5:1702:C:OP2	2.19	0.43
3:L5:2275:G:H2'	3:L5:2276:A:C8	2.53	0.43
9:LD:41:LYS:HG3	24:LT:93:ILE:HG21	2.00	0.43
9:LD:55:VAL:HG11	9:LD:158:LYS:HE3	2.00	0.43
20:LP:140:MET:HE3	20:LP:140:MET:HB3	1.95	0.43
23:LS:83:ARG:HG3	23:LS:125:GLN:HB3	2.01	0.43
43:Lm:106:ARG:HE	43:Lm:106:ARG:HB3	1.64	0.43
49:Lt:127:GLY:O	49:Lt:131:GLU:HG2	2.18	0.43
51:SB:144:LYS:HD3	51:SB:208:HIS:CG	2.53	0.43
53:SE:160:ILE:HD12	53:SE:169:ILE:HD12	2.00	0.43
54:SG:222:GLU:HA	54:SG:225:GLN:HB2	2.00	0.43
56:SI:69:SER:HB2	58:SL:21:LYS:HB2	2.00	0.43
68:S2:1112:U:O2	68:S2:1121:G:O6	2.35	0.43
68:S2:1244:PSU:H2'	68:S2:1245:G:C8	2.53	0.43
68:S2:1588:A:H2'	68:S2:1589:A:H8	1.82	0.43
3:L5:1741:G:N3	3:L5:1781:PSU:H5''	2.33	0.43
3:L5:2884:G:H2'	3:L5:2885:A:H8	1.84	0.43
3:L5:4740:G:O6	3:L5:4959:U:O2	2.36	0.43
3:L5:4769:G:H5''	19:LO:176:ARG:HD3	1.99	0.43
9:LD:220:LYS:HE2	9:LD:220:LYS:HB3	1.79	0.43
13:LH:18:ILE:HG12	13:LH:27:VAL:HG22	1.99	0.43
30:LZ:11:VAL:HG12	30:LZ:82:PRO:HA	2.00	0.43
53:SE:70:ILE:HG22	53:SE:92:ILE:HG13	2.00	0.43
55:SH:10:LYS:HA	55:SH:10:LYS:HD2	1.83	0.43
68:S2:604:A:H1'	68:S2:639:C:O2'	2.19	0.43
68:S2:943:U:H2'	68:S2:944:A:C8	2.49	0.43
68:S2:1736:G:H2'	68:S2:1737:G:H8	1.83	0.43
76:SS:40:TYR:CZ	76:SS:97:GLN:HG2	2.54	0.43
78:SU:22:ILE:HD11	78:SU:112:VAL:HB	2.01	0.43
84:Et:5:G:H2'	84:Et:6:G:H8	1.84	0.43
85:CB:498:LYS:HE3	85:CB:498:LYS:HB3	1.91	0.43
86:CA:121:VAL:HB	86:CA:334:THR:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:71:C:H1'	16:LL:62:PRO:O	2.19	0.43
3:L5:683:C:H2'	3:L5:684:G:O4'	2.18	0.43
3:L5:4186:A:H2'	3:L5:4187:G:C8	2.54	0.43
3:L5:4242:U:H3	3:L5:4281:A:H2	1.63	0.43
5:L8:30:U:H2'	5:L8:31:G:C8	2.53	0.43
6:LA:126:LEU:HD13	6:LA:150:LEU:HD21	2.00	0.43
10:LE:203:ILE:O	10:LE:206:VAL:HG22	2.19	0.43
10:LE:223:ARG:HH11	10:LE:234:ASP:HB3	1.83	0.43
42:Ll:41:ARG:HA	42:Ll:41:ARG:HD2	1.72	0.43
52:SC:102:LEU:HD12	52:SC:130:ILE:HG12	2.01	0.43
53:SE:138:HIS:CD2	53:SE:148:ARG:HG3	2.53	0.43
53:SE:149:TYR:HB3	54:SG:209:TYR:CD1	2.54	0.43
54:SG:61:PHE:CE2	54:SG:96:SER:HB2	2.53	0.43
54:SG:135:PRO:HG3	54:SG:144:LEU:HD13	2.00	0.43
54:SG:164:LYS:HD3	54:SG:164:LYS:HA	1.88	0.43
62:SW:28:ARG:HH22	68:S2:1093:A:H5''	1.83	0.43
64:SY:89:HIS:HB2	68:S2:574:A:H4'	2.01	0.43
68:S2:399:C:H5	68:S2:680:G:H5''	1.84	0.43
68:S2:690:G:H5''	68:S2:691:G:N2	2.34	0.43
72:SK:14:LEU:HD22	72:SK:35:LEU:HD23	2.01	0.43
82:Sf:103:LEU:HG	82:Sf:104:LYS:H	1.83	0.43
85:CB:72:SER:HB3	85:CB:400:LYS:NZ	2.33	0.43
85:CB:259:LYS:HD2	85:CB:264:ARG:CZ	2.48	0.43
85:CB:855:LEU:HD12	85:CB:855:LEU:HA	1.83	0.43
86:CA:35:LEU:HD13	86:CA:108:ILE:HG21	2.00	0.43
86:CA:192:GLN:HG2	86:CA:193:HIS:ND1	2.33	0.43
3:L5:64:A:H1'	3:L5:76:A:H1'	2.00	0.43
3:L5:729:G:H5''	11:LF:76:ARG:HD2	2.01	0.43
3:L5:1298:C:H2'	3:L5:1299:G:C8	2.53	0.43
3:L5:1307:A:H2'	3:L5:1308:C:H6	1.84	0.43
3:L5:1332:C:H5''	35:Le:29:VAL:HB	2.01	0.43
3:L5:3920:PSU:H2'	3:L5:3921:U:C6	2.54	0.43
3:L5:4525:C:H5''	7:LB:245:HIS:HB3	2.01	0.43
3:L5:4750:G:H2'	3:L5:4751:G:C8	2.53	0.43
4:L7:75:G:H5''	23:LS:49:SER:O	2.19	0.43
7:LB:173:LEU:HD22	7:LB:342:LYS:HD2	2.01	0.43
29:LY:72:GLN:HB3	29:LY:81:TYR:HB2	2.01	0.43
54:SG:133:LEU:HB3	68:S2:65:C:N3	2.34	0.43
57:SJ:136:ARG:HD3	57:SJ:160:SER:HA	2.01	0.43
68:S2:601:OMG:HM23	68:S2:601:OMG:H1'	1.82	0.43
68:S2:1395:C:H2'	68:S2:1396:A:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1839:U:H2'	68:S2:1840:U:C6	2.54	0.43
73:SM:83:LYS:HB2	73:SM:83:LYS:HE3	1.77	0.43
74:SP:41:GLN:H	74:SP:41:GLN:HG2	1.69	0.43
74:SP:60:LEU:HD12	74:SP:89:MET:HG2	2.01	0.43
3:L5:99:A:H5''	18:LN:184:ILE:HD12	1.99	0.43
3:L5:724:C:OP1	8:LC:350:ARG:HD2	2.17	0.43
3:L5:1344:C:H1'	16:LL:10:LEU:HD11	2.00	0.43
3:L5:1461:C:H2'	3:L5:1462:A:H8	1.82	0.43
3:L5:1878:G:H2'	3:L5:1879:C:C6	2.54	0.43
3:L5:3652:A:H2'	3:L5:3653:A:C5	2.53	0.43
3:L5:3911:C:H2'	3:L5:3912:U:C6	2.52	0.43
3:L5:4345:C:H2'	3:L5:4346:U:C6	2.54	0.43
14:LI:51:HIS:CD2	14:LI:168:SER:HB3	2.54	0.43
44:Ln:11:ARG:O	44:Ln:15:ARG:HG3	2.18	0.43
47:Lr:45:HIS:HB2	47:Lr:48:THR:HG22	2.00	0.43
54:SG:138:ALA:HA	54:SG:176:ILE:HD11	2.01	0.43
54:SG:199:THR:HG21	68:S2:126:G:C8	2.53	0.43
68:S2:152:U:H2'	68:S2:153:G:H8	1.83	0.43
68:S2:641:A:H2'	68:S2:642:U:O4'	2.19	0.43
68:S2:1103:C:H2'	68:S2:1104:G:C8	2.53	0.43
77:ST:18:LEU:HD22	77:ST:58:ALA:HA	2.00	0.43
85:CB:257:MET:HA	85:CB:260:LEU:HB2	2.01	0.43
3:L5:2568:C:H2'	3:L5:2569:G:C8	2.53	0.43
3:L5:2730:U:H2'	3:L5:2731:C:C6	2.54	0.43
5:L8:36:G:C5	38:Lh:89:ARG:HD3	2.54	0.43
13:LH:59:LYS:HE2	13:LH:66:GLU:HG3	2.00	0.43
14:LI:99:ILE:HG22	14:LI:123:GLN:HB2	2.01	0.43
47:Lr:88:ALA:HA	47:Lr:91:SER:HB3	2.01	0.43
48:Ls:35:VAL:HG21	48:Ls:40:MET:HE3	2.01	0.43
54:SG:177:GLN:HG3	54:SG:178:ARG:N	2.34	0.43
67:Se:52:LYS:HD3	67:Se:52:LYS:HA	1.76	0.43
68:S2:877:C:H2'	68:S2:878:G:C8	2.54	0.43
68:S2:1183:A:H2'	68:S2:1184:G:H8	1.84	0.43
68:S2:1217:A:H2'	68:S2:1218:C:H6	1.84	0.43
68:S2:1709:G:H1	68:S2:1824:A:H61	1.67	0.43
70:SD:217:ILE:HD12	70:SD:219:PRO:HG3	2.00	0.43
86:CA:152:ALA:HA	86:CA:357:LEU:HD13	2.01	0.43
3:L5:74:G:H1'	16:LL:62:PRO:HG3	2.01	0.43
3:L5:99:A:H2'	3:L5:100:C:O2	2.19	0.43
3:L5:662:C:H2'	3:L5:663:G:C8	2.54	0.43
3:L5:2656:U:H5''	30:LZ:38:TYR:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3726:A:H2'	3:L5:3727:A:C8	2.53	0.43
3:L5:5002:U:H2'	3:L5:5003:U:H6	1.84	0.43
88:L5:5267:SPM:H32	18:LN:81:TYR:CE2	2.54	0.43
10:LE:281:ILE:HG23	10:LE:286:LEU:HD21	2.00	0.43
18:LN:75:VAL:HG11	18:LN:80:THR:HG22	2.00	0.43
33:Lc:48:LEU:HD11	33:Lc:60:ILE:HG21	2.01	0.43
49:Lt:12:VAL:HG11	49:Lt:65:GLN:N	2.29	0.43
63:SX:46:HIS:CD2	63:SX:103:ALA:HB2	2.54	0.43
68:S2:99:A2M:H1'	68:S2:99:A2M:HM'3	1.62	0.43
68:S2:207:G:H3'	68:S2:208:G:H8	1.84	0.43
68:S2:1528:G:H2'	68:S2:1529:C:C6	2.54	0.43
68:S2:1706:G:H2'	68:S2:1707:U:H6	1.83	0.43
71:SF:100:ILE:HG22	71:SF:178:ILE:HD11	2.00	0.43
72:SK:64:TRP:CE3	81:Sd:23:VAL:HG22	2.53	0.43
85:CB:176:GLN:O	85:CB:180:ARG:HG2	2.18	0.43
86:CA:249:ARG:HD2	86:CA:250:ASP:C	2.44	0.43
3:L5:1097:C:H2'	3:L5:1098:G:C8	2.54	0.42
3:L5:2385:U:H2'	3:L5:2386:U:C6	2.54	0.42
3:L5:2696:A:H5'	41:Lk:70:LYS:HE2	2.00	0.42
12:LG:37:LYS:HE2	12:LG:37:LYS:HB3	1.89	0.42
29:LY:31:SER:HA	29:LY:48:PRO:HA	2.00	0.42
49:Lt:82:ILE:HG22	49:Lt:86:LYS:HE2	2.01	0.42
51:SB:44:ILE:HG23	51:SB:69:VAL:HG21	2.00	0.42
53:SE:31:PRO:HA	53:SE:81:THR:HB	2.01	0.42
54:SG:49:VAL:HB	54:SG:115:LYS:HB3	2.01	0.42
54:SG:135:PRO:HG2	54:SG:141:ILE:HG22	2.00	0.42
55:SH:134:VAL:HG12	55:SH:173:PHE:CD2	2.54	0.42
68:S2:1671:G:H2'	68:S2:1672:U:H6	1.84	0.42
71:SF:49:LEU:HD11	75:SQ:49:TYR:HB2	2.00	0.42
73:SM:79:VAL:HG11	73:SM:85:LEU:HB3	2.00	0.42
85:CB:143:LEU:HD21	85:CB:185:VAL:HG13	2.00	0.42
3:L5:1241:C:O2	32:Lb:115:GLY:HA2	2.20	0.42
3:L5:2021:G:H5''	48:Ls:58:ASN:ND2	2.33	0.42
3:L5:2648:G:H2'	3:L5:2649:G:H8	1.84	0.42
3:L5:2904:U:O2	3:L5:3591:C:H2'	2.19	0.42
3:L5:4344:U:H2'	3:L5:4345:C:C6	2.54	0.42
3:L5:4500:PSU:H2'	3:L5:4501:U:C6	2.54	0.42
5:L8:5:U:H2'	5:L8:6:C:C6	2.55	0.42
12:LG:255:LYS:HB3	12:LG:255:LYS:HE3	1.81	0.42
31:La:102:ASP:HA	31:La:125:LYS:HB2	2.01	0.42
50:SA:176:TRP:CD1	50:SA:199:PRO:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SE:209:HIS:CD2	53:SE:219:ALA:HB2	2.54	0.42
58:SL:18:GLN:HG3	58:SL:33:LEU:HD11	2.00	0.42
68:S2:1304:U:H2'	68:S2:1305:C:C6	2.54	0.42
83:Sg:129:ILE:HB	83:Sg:142:VAL:HB	2.00	0.42
85:CB:26:ALA:HB3	85:CB:32:LYS:HE2	2.01	0.42
85:CB:119:LEU:HD22	85:CB:151:ILE:HG13	2.02	0.42
3:L5:492:U:H2'	3:L5:493:G:C8	2.54	0.42
3:L5:1092:G:H2'	3:L5:1093:C:H6	1.85	0.42
3:L5:4573:G:H2'	3:L5:4574:U:C6	2.53	0.42
4:L7:4:U:H2'	4:L7:5:A:C8	2.54	0.42
5:L8:6:C:H2'	5:L8:7:U:C6	2.53	0.42
7:LB:57:VAL:HG22	7:LB:73:VAL:HG22	2.00	0.42
37:Lg:33:LEU:HD23	37:Lg:33:LEU:HA	1.83	0.42
47:Lr:16:PHE:HB3	47:Lr:27:THR:H	1.84	0.42
48:Ls:189:ILE:HD13	48:Ls:189:ILE:HA	1.91	0.42
68:S2:16:G:H2'	68:S2:17:C:C6	2.54	0.42
68:S2:532:C:H2'	68:S2:533:A:C8	2.53	0.42
68:S2:800:U:H2'	68:S2:801:PSU:O4'	2.19	0.42
68:S2:1384:C:C2	68:S2:1385:G:C8	3.08	0.42
68:S2:1560:U:H2'	68:S2:1561:A:H8	1.83	0.42
68:S2:1797:U:H2'	68:S2:1798:C:C6	2.53	0.42
80:Sc:58:LEU:HD23	80:Sc:58:LEU:HA	1.87	0.42
83:Sg:101:PHE:CE2	83:Sg:136:GLY:HA2	2.54	0.42
83:Sg:149:GLU:O	83:Sg:170:TRP:HB2	2.18	0.42
84:Et:44:G:H2'	84:Et:45:G:C8	2.54	0.42
3:L5:1333:A:H2'	3:L5:1334:A:H8	1.82	0.42
3:L5:1867:A:H2'	3:L5:1868:A:C8	2.55	0.42
3:L5:2683:C:H2'	3:L5:2684:C:C6	2.55	0.42
3:L5:2815:A2M:H2'	3:L5:2816:G:C8	2.53	0.42
3:L5:4988:U:H4'	3:L5:4989:U:H5	1.84	0.42
30:LZ:91:LEU:HD23	30:LZ:91:LEU:HA	1.88	0.42
35:Le:38:PRO:HB2	35:Le:46:ARG:HB2	2.01	0.42
57:SJ:124:HIS:NE2	67:Se:35:ARG:HB2	2.34	0.42
58:SL:68:ILE:HG21	58:SL:143:LEU:HD11	2.02	0.42
68:S2:166:A2M:HM'3	68:S2:166:A2M:H1'	1.53	0.42
68:S2:795:A:H2'	68:S2:796:G:C8	2.53	0.42
68:S2:1232:PSU:H2'	68:S2:1233:G:C8	2.54	0.42
73:SM:91:LEU:HA	73:SM:91:LEU:HD12	1.89	0.42
76:SS:71:MET:HE2	76:SS:99:LEU:HG	2.00	0.42
77:ST:134:ILE:HA	77:ST:137:GLN:HG2	2.01	0.42
78:SU:51:LYS:HD3	78:SU:51:LYS:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Sg:7:LEU:HA	83:Sg:310:TRP:CD1	2.49	0.42
83:Sg:271:LYS:HD2	83:Sg:271:LYS:HA	1.91	0.42
85:CB:436:PRO:HG3	85:CB:492:HIS:HA	2.01	0.42
3:L5:460:C:H2'	3:L5:461:G:C8	2.54	0.42
3:L5:1589:C:H2'	3:L5:1590:C:C6	2.54	0.42
3:L5:1773:U:H2'	3:L5:1774:C:C6	2.55	0.42
3:L5:2611:A:H2'	3:L5:2612:G:H8	1.84	0.42
3:L5:2634:C:H2'	3:L5:2635:U:H6	1.85	0.42
3:L5:4638:U:H2'	3:L5:4639:G:N3	2.34	0.42
3:L5:4981:G:H3'	3:L5:4982:A:H8	1.83	0.42
5:L8:92:U:H2'	5:L8:93:C:O4'	2.19	0.42
13:LH:50:LYS:HB3	13:LH:50:LYS:HE3	1.88	0.42
17:LM:96:GLU:O	17:LM:100:ARG:HG2	2.20	0.42
18:LN:140:LYS:HD3	18:LN:140:LYS:HA	1.72	0.42
48:Ls:120:GLU:HG2	48:Ls:162:LYS:HA	2.02	0.42
51:SB:219:LYS:HE3	51:SB:219:LYS:HB3	1.90	0.42
52:SC:137:VAL:HB	52:SC:217:ALA:HA	2.01	0.42
61:SV:15:ARG:HE	61:SV:15:ARG:HB2	1.59	0.42
63:SX:140:ARG:HA	63:SX:141:PRO:HD3	1.93	0.42
68:S2:736:C:H2'	68:S2:737:G:C5	2.54	0.42
68:S2:1337:4AC:H5''	78:SU:67:LYS:HE3	2.00	0.42
3:L5:444:G:H2'	3:L5:445:U:C6	2.54	0.42
3:L5:475:G:H2'	3:L5:476:G:H8	1.84	0.42
3:L5:1973:G:H4'	49:Lt:117:ARG:HH22	1.83	0.42
3:L5:1993:C:H2'	3:L5:1994:C:C6	2.55	0.42
3:L5:2293:U:H2'	3:L5:2294:G:C8	2.55	0.42
3:L5:2385:U:H2'	3:L5:2386:U:H6	1.85	0.42
3:L5:2610:G:H2'	3:L5:2611:A:C8	2.55	0.42
3:L5:2787:A2M:H1'	3:L5:2787:A2M:HM'2	1.79	0.42
3:L5:3861:A:H2'	3:L5:3862:A:H8	1.84	0.42
3:L5:4942:C:H4'	10:LE:154:THR:HG22	1.99	0.42
35:Le:100:ALA:HB3	35:Le:103:VAL:HG23	2.00	0.42
55:SH:166:VAL:O	55:SH:170:VAL:HG23	2.18	0.42
57:SJ:30:LYS:HD2	67:Se:38:TYR:HE1	1.85	0.42
61:SV:22:ARG:NH2	61:SV:59:ILE:HG23	2.33	0.42
61:SV:70:LEU:HD21	61:SV:83:PHE:HE2	1.84	0.42
66:Sb:55:LEU:HD11	66:Sb:62:VAL:HG12	2.00	0.42
68:S2:28:U:H2'	68:S2:29:G:C8	2.51	0.42
68:S2:59:U:H5''	68:S2:503:C:N4	2.34	0.42
68:S2:1393:G:H2'	68:S2:1394:G:C8	2.54	0.42
68:S2:1646:C:H5''	75:SQ:138:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:SQ:25:CYS:HA	75:SQ:68:ILE:HG22	2.02	0.42
75:SQ:43:GLU:HB2	75:SQ:44:PRO:HD3	2.01	0.42
85:CB:313:ALA:O	85:CB:317:GLU:HG2	2.20	0.42
3:L5:1076:C:H2'	3:L5:1077:C:C6	2.54	0.42
3:L5:1309:C:H2'	3:L5:1310:C:C6	2.54	0.42
3:L5:1824:G:H2'	3:L5:1825:A:C8	2.55	0.42
3:L5:4460:U:H2'	3:L5:4461:C:C6	2.54	0.42
3:L5:4499:OMG:N2	3:L5:4529:G:H1'	2.35	0.42
7:LB:279:GLU:HB3	7:LB:282:LYS:HZ3	1.84	0.42
27:LW:84:GLY:HA3	54:SG:161:PRO:HD2	2.02	0.42
28:LX:81:LEU:HG	28:LX:83:THR:HG23	2.00	0.42
37:Lg:64:LEU:HD23	37:Lg:67:LEU:HD12	2.02	0.42
38:Lh:89:ARG:O	38:Lh:93:ARG:HG2	2.20	0.42
49:Lt:151:ILE:O	49:Lt:155:ILE:HB	2.19	0.42
68:S2:1540:G:H5''	77:ST:39:LEU:HD12	2.02	0.42
68:S2:1541:G:H4'	77:ST:15:VAL:HG11	2.01	0.42
68:S2:1798:C:H2'	68:S2:1799:G:O4'	2.19	0.42
85:CB:256:MET:O	85:CB:260:LEU:HD23	2.19	0.42
3:L5:1725:U:H2'	3:L5:1726:U:C6	2.54	0.42
3:L5:1875:C:H2'	3:L5:1876:U:C6	2.55	0.42
3:L5:4344:U:H2'	3:L5:4345:C:H6	1.85	0.42
3:L5:4739:C:H2'	3:L5:4740:G:H5'	2.02	0.42
7:LB:136:LYS:HB2	7:LB:142:GLY:HA3	2.02	0.42
21:LQ:39:THR:HG21	21:LQ:132:LYS:HG2	2.02	0.42
33:Lc:47:ILE:HB	33:Lc:94:LEU:HG	2.01	0.42
57:SJ:49:THR:O	57:SJ:53:ILE:HD12	2.20	0.42
57:SJ:121:LYS:HD3	68:S2:527:C:H4'	2.01	0.42
68:S2:13:C:H4'	68:S2:1355:C:C5	2.54	0.42
68:S2:13:C:H4'	68:S2:1355:C:H5	1.85	0.42
68:S2:106:C:H5''	68:S2:431:G:O2'	2.20	0.42
68:S2:564:A:H2'	68:S2:565:G:O4'	2.19	0.42
68:S2:991:G:N1	68:S2:1134:G:H4'	2.34	0.42
68:S2:1067:C:H2'	68:S2:1068:G:O4'	2.20	0.42
68:S2:1683:C:H2'	68:S2:1684:C:H6	1.85	0.42
75:SQ:54:PRO:O	75:SQ:58:LEU:HD23	2.20	0.42
84:Et:28:C:H2'	84:Et:29:A:H8	1.85	0.42
85:CB:388:CYS:HB2	85:CB:418:SER:HA	2.01	0.42
3:L5:288:G:H2'	3:L5:289:C:C6	2.55	0.42
3:L5:347:A:H2'	3:L5:348:G:C8	2.54	0.42
3:L5:742:G:H2'	3:L5:743:G:H8	1.85	0.42
3:L5:950:G:H2'	3:L5:951:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2341:A:H5''	8:LC:46:LYS:HE2	2.02	0.42
3:L5:2439:G:H5'	3:L5:2778:G:OP2	2.20	0.42
3:L5:3661:G:H4'	3:L5:3662:A:H5'	2.02	0.42
3:L5:4146:G:H2'	3:L5:4147:G:H8	1.85	0.42
3:L5:4392:OMG:N3	3:L5:4447:5MC:HM52	2.34	0.42
3:L5:4481:U:H2'	3:L5:4482:U:H6	1.84	0.42
30:LZ:135:ARG:HD2	30:LZ:135:ARG:HA	1.90	0.42
35:Le:7:LEU:HB2	35:Le:93:LYS:HB3	2.01	0.42
48:Ls:20:LEU:HD23	48:Ls:90:PHE:CE1	2.55	0.42
50:SA:111:GLN:HA	50:SA:116:PHE:CG	2.55	0.42
65:Sa:79:ILE:HD13	68:S2:1863:A:H1'	2.02	0.42
68:S2:102:A:H4'	68:S2:104:A:C8	2.55	0.42
68:S2:461:U:H2'	68:S2:462:OMC:C6	2.55	0.42
68:S2:1232:PSU:H2'	68:S2:1233:G:H8	1.85	0.42
68:S2:1330:G:N7	68:S2:1492:U:H3'	2.34	0.42
73:SM:53:ALA:HB3	73:SM:107:SER:HB2	2.02	0.42
75:SQ:48:GLN:HE22	75:SQ:52:LEU:HD23	1.85	0.42
76:SS:98:VAL:HG11	76:SS:106:LYS:HG3	2.01	0.42
77:ST:18:LEU:HB3	77:ST:58:ALA:HB1	2.02	0.42
80:Sc:35:MET:HE3	80:Sc:35:MET:HB3	1.98	0.42
83:Sg:147:HIS:CD2	83:Sg:169:GLY:HA3	2.55	0.42
3:L5:716:C:OP1	8:LC:317:ASN:HB2	2.20	0.42
3:L5:1811:G:H2'	3:L5:1812:C:C6	2.54	0.42
3:L5:1895:G:H2'	3:L5:1896:A:O4'	2.20	0.42
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.55	0.42
3:L5:4518:A:O5'	3:L5:4520:G:H4'	2.20	0.42
3:L5:4653:C:H2'	3:L5:4654:C:C6	2.55	0.42
4:L7:82:G:H2'	4:L7:83:A:C8	2.54	0.42
7:LB:26:ARG:HD2	7:LB:47:LEU:HD11	2.02	0.42
8:LC:318:PRO:C	8:LC:320:LYS:H	2.27	0.42
23:LS:28:TYR:HD2	23:LS:54:MET:HE1	1.85	0.42
36:Lf:33:VAL:HG13	36:Lf:38:GLU:HB2	2.02	0.42
51:SB:24:PRO:O	51:SB:28:LYS:HG2	2.20	0.42
51:SB:193:ILE:O	51:SB:197:ILE:HG12	2.19	0.42
53:SE:105:THR:HG23	53:SE:245:ARG:HD2	2.02	0.42
54:SG:174:PRO:HB3	68:S2:65:C:C6	2.55	0.42
59:SN:89:TYR:CE2	59:SN:93:LYS:HD2	2.55	0.42
68:S2:922:A:H2'	68:S2:923:G:O4'	2.19	0.42
68:S2:1114:U:O2'	68:S2:1115:U:H2'	2.20	0.42
68:S2:1227:G:C2	68:S2:1228:A:C8	3.08	0.42
68:S2:1568:C:H2'	68:S2:1569:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SR:66:VAL:HG23	69:SR:68:GLY:H	1.85	0.42
72:SK:21:MET:HB3	72:SK:49:MET:HE1	2.02	0.42
3:L5:46:U:H5''	16:LL:16:LYS:HG3	2.02	0.41
3:L5:52:G:H4'	3:L5:1529:G:H4'	2.03	0.41
3:L5:272:U:H2'	3:L5:273:U:C6	2.55	0.41
3:L5:426:A:H2'	3:L5:427:A:C8	2.55	0.41
3:L5:454:U:H2'	3:L5:455:C:O4'	2.19	0.41
3:L5:2610:G:H2'	3:L5:2611:A:H8	1.85	0.41
89:L5:5287:SPD:H92	5:L8:138:C:OP1	2.21	0.41
4:L7:6:C:H4'	9:LD:52:ILE:HD13	2.01	0.41
6:LA:3:ARG:HD2	6:LA:208:GLU:HG3	2.00	0.41
16:LL:48:PRO:HG3	38:Lh:118:LYS:HE2	2.01	0.41
50:SA:195:TRP:CD2	50:SA:197:VAL:HB	2.55	0.41
52:SC:108:LYS:HE2	52:SC:110:MET:HB3	2.02	0.41
53:SE:9:LEU:HB2	53:SE:30:ARG:HB2	2.01	0.41
55:SH:18:GLU:C	55:SH:20:GLU:H	2.28	0.41
63:SX:88:ASP:HA	68:S2:617:G:H4'	2.01	0.41
68:S2:1279:C:H2'	68:S2:1280:G:C8	2.53	0.41
73:SM:129:LYS:HE3	73:SM:129:LYS:HB3	1.92	0.41
74:SP:45:LEU:HD23	74:SP:49:LEU:HD21	2.01	0.41
86:CA:227:ASP:HA	86:CA:320:LYS:HB3	2.01	0.41
86:CA:259:MET:HB2	86:CA:262:SER:HB2	2.02	0.41
3:L5:270:U:H2'	3:L5:271:C:H6	1.85	0.41
3:L5:2090:U:H4'	3:L5:2091:C:H3'	2.02	0.41
3:L5:2109:G:H2'	3:L5:2110:C:C6	2.54	0.41
3:L5:2648:G:H2'	3:L5:2649:G:C8	2.56	0.41
3:L5:3787:G:H1'	3:L5:3789:C:N4	2.35	0.41
3:L5:4174:U:H2'	3:L5:4175:G:C8	2.54	0.41
3:L5:4389:C:H2'	3:L5:4390:A:H8	1.85	0.41
3:L5:4600:G:H4'	3:L5:4601:U:O5'	2.20	0.41
5:L8:66:A:H2'	5:L8:67:U:C6	2.54	0.41
8:LC:106:LYS:HD3	8:LC:108:TRP:CZ2	2.55	0.41
12:LG:164:ILE:O	12:LG:168:VAL:HG13	2.20	0.41
29:LY:59:ARG:HB2	29:LY:103:LYS:HD2	2.01	0.41
46:Lp:7:LYS:HB3	46:Lp:7:LYS:HE2	1.76	0.41
50:SA:41:ARG:HD2	50:SA:47:TYR:CZ	2.54	0.41
53:SE:94:LYS:HG3	64:SY:16:ARG:HG3	2.02	0.41
58:SL:128:VAL:HG12	58:SL:142:VAL:HA	2.01	0.41
68:S2:528:A:H2'	68:S2:529:A:C8	2.55	0.41
68:S2:694:G:H2'	68:S2:695:C:O4'	2.20	0.41
68:S2:1653:U:H2'	68:S2:1654:G:C8	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1826:G:H2'	68:S2:1827:U:C6	2.55	0.41
77:ST:112:MET:HB2	77:ST:127:GLY:HA2	2.02	0.41
85:CB:163:ALA:HA	85:CB:167:LEU:HB2	2.02	0.41
3:L5:258:G:H2'	3:L5:259:C:O4'	2.19	0.41
3:L5:469:C:H2'	3:L5:470:A:H8	1.85	0.41
3:L5:1217:G:H2'	3:L5:1218:G:C8	2.55	0.41
3:L5:1504:G:H2'	3:L5:1505:C:H6	1.84	0.41
3:L5:1876:U:H2'	3:L5:1877:G:C8	2.55	0.41
3:L5:2273:G:H2'	3:L5:2274:C:C6	2.56	0.41
3:L5:4103:C:H4'	3:L5:4104:G:N7	2.35	0.41
3:L5:4306:OMU:H1'	3:L5:4306:OMU:HM23	1.82	0.41
5:L8:89:U:H2'	5:L8:90:C:C6	2.55	0.41
15:LJ:163:MET:HE3	15:LJ:174:ILE:HG21	2.02	0.41
36:Lf:45:LYS:NZ	36:Lf:108:SER:HA	2.34	0.41
37:Lg:61:PRO:HA	37:Lg:64:LEU:HD12	2.01	0.41
51:SB:111:CYS:HB3	65:Sa:68:TYR:HB2	2.01	0.41
54:SG:154:ARG:HD2	68:S2:77:A:C8	2.55	0.41
54:SG:213:LEU:HD22	54:SG:217:MET:HE3	2.03	0.41
59:SN:5:HIS:HD2	68:S2:676:C:H5''	1.85	0.41
68:S2:186:C:H2'	68:S2:187:G:C8	2.55	0.41
68:S2:1520:G:H21	74:SP:126:VAL:HG11	1.85	0.41
73:SM:23:LYS:HD3	73:SM:23:LYS:HA	1.89	0.41
76:SS:5:ILE:HG12	79:SZ:49:LEU:HB2	2.02	0.41
77:ST:122:LYS:HB2	77:ST:122:LYS:HE2	1.85	0.41
82:Sf:121:CYS:HB2	82:Sf:145:CYS:HB3	1.71	0.41
84:Et:16:C:H5''	84:Et:59:G:H1	1.86	0.41
85:CB:398:ILE:HD13	85:CB:414:GLY:HA3	2.01	0.41
86:CA:81:SER:OG	86:CA:107:LYS:HE3	2.21	0.41
3:L5:276:C:OP1	39:Li:36:HIS:HB3	2.20	0.41
3:L5:457:G:H2'	3:L5:458:C:H6	1.86	0.41
3:L5:956:A:H1'	3:L5:2076:G:H5''	2.03	0.41
3:L5:1503:A:H62	21:LQ:87:THR:HG21	1.86	0.41
3:L5:1812:C:H1'	32:Lb:57:MET:HE2	2.02	0.41
3:L5:4260:U:H2'	3:L5:4261:C:H6	1.84	0.41
3:L5:5003:U:H2'	3:L5:5004:C:C6	2.55	0.41
5:L8:90:C:H2'	5:L8:91:A:C8	2.55	0.41
12:LG:117:ARG:HD2	12:LG:117:ARG:HA	1.74	0.41
18:LN:5:LYS:HD2	18:LN:5:LYS:HA	1.87	0.41
68:S2:1113:A:O2'	68:S2:1114:U:H5'	2.20	0.41
68:S2:1310:U:H2'	68:S2:1311:C:C6	2.55	0.41
68:S2:1386:A:H2'	68:S2:1387:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1543:U:H4'	75:SQ:43:GLU:CD	2.44	0.41
70:SD:109:LEU:HD12	70:SD:184:ILE:HD11	2.03	0.41
80:Sc:10:LYS:HE3	80:Sc:61:SER:HB2	2.02	0.41
83:Sg:227:LEU:HD23	83:Sg:228:TYR:HB2	2.02	0.41
86:CA:120:ASN:H	86:CA:322:THR:HG23	1.84	0.41
3:L5:106:A:H2'	3:L5:107:G:O4'	2.20	0.41
3:L5:159:C:H5''	39:Li:25:ARG:NH2	2.35	0.41
3:L5:511:C:H5'	16:LL:165:LYS:HG3	2.03	0.41
3:L5:1577:G:H5'	3:L5:1578:U:H5''	2.02	0.41
3:L5:1701:A:C6	3:L5:1702:C:C5	3.08	0.41
3:L5:1855:G:OP1	32:Lb:4:SER:HB3	2.20	0.41
3:L5:2671:C:H2'	3:L5:2672:C:C6	2.55	0.41
7:LB:297:LYS:HG3	7:LB:299:ILE:HG23	2.03	0.41
14:LI:47:PRO:HB3	14:LI:171:TRP:CZ2	2.55	0.41
22:LR:10:LEU:HD22	22:LR:38:ARG:HG2	2.02	0.41
23:LS:133:ALA:HB3	23:LS:136:LYS:HG2	2.03	0.41
50:SA:41:ARG:HE	50:SA:45:GLY:HA2	1.86	0.41
53:SE:33:THR:O	68:S2:120:U:H1'	2.20	0.41
64:SY:16:ARG:HA	64:SY:19:GLN:HA	2.03	0.41
65:Sa:12:LYS:HB2	65:Sa:33:ASP:OD2	2.21	0.41
68:S2:194:C:H2'	68:S2:195:C:C6	2.55	0.41
68:S2:1687:C:H2'	68:S2:1688:C:C6	2.56	0.41
75:SQ:134:GLY:HA3	75:SQ:140:ARG:HA	2.01	0.41
1:CD:190:LYS:HB3	1:CD:190:LYS:HE2	1.72	0.41
3:L5:475:G:H2'	3:L5:476:G:C8	2.56	0.41
3:L5:1662:C:H2'	3:L5:1663:C:H6	1.86	0.41
3:L5:1701:A:C8	3:L5:2096:G:C6	3.08	0.41
3:L5:2323:C:H2'	3:L5:2324:C:C6	2.55	0.41
3:L5:2521:G:H2'	3:L5:2522:G:C8	2.56	0.41
3:L5:3898:G:H5'	7:LB:254:ILE:HG13	2.01	0.41
3:L5:4125:C:H5'	12:LG:45:ILE:HD12	2.03	0.41
10:LE:151:ILE:HG12	10:LE:161:ARG:HG2	2.02	0.41
25:LU:36:ALA:HB1	25:LU:65:ARG:HD2	2.01	0.41
26:LV:19:GLY:O	26:LV:21:PRO:HD3	2.20	0.41
33:Lc:48:LEU:HD13	33:Lc:71:VAL:HG13	2.02	0.41
36:Lf:29:LYS:HG3	36:Lf:83:MET:HE1	2.01	0.41
47:Lr:45:HIS:HB3	47:Lr:103:ARG:HH22	1.85	0.41
51:SB:136:ARG:NH1	68:S2:941:C:H5''	2.35	0.41
51:SB:168:MET:HG3	51:SB:197:ILE:HD12	2.03	0.41
52:SC:75:ILE:HD11	52:SC:265:PRO:HB3	2.02	0.41
55:SH:76:GLN:O	55:SH:80:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:958:G:H2'	68:S2:959:G:C8	2.55	0.41
68:S2:1619:A:OP1	74:SP:47:ARG:HD3	2.20	0.41
68:S2:1652:G:H1	68:S2:1672:U:H3	1.67	0.41
75:SQ:57:LEU:HD23	75:SQ:57:LEU:HA	1.90	0.41
76:SS:110:ASP:HA	76:SS:113:ARG:HG2	2.03	0.41
76:SS:118:ARG:HE	76:SS:123:LEU:HD21	1.85	0.41
84:Et:52:G:H2'	84:Et:53:G:H8	1.85	0.41
3:L5:260:C:H2'	3:L5:261:G:H8	1.85	0.41
3:L5:2496:G:H2'	3:L5:2497:C:H6	1.86	0.41
3:L5:4460:U:H2'	3:L5:4461:C:H6	1.85	0.41
8:LC:279:LEU:HD23	8:LC:279:LEU:HA	1.92	0.41
9:LD:236:MET:O	9:LD:239:MET:HG3	2.20	0.41
12:LG:97:LYS:HE2	12:LG:97:LYS:HB3	1.77	0.41
21:LQ:177:ALA:O	21:LQ:184:ARG:HB2	2.19	0.41
46:Lp:24:LYS:HE3	46:Lp:24:LYS:HB3	1.93	0.41
48:Ls:119:CYS:HB3	48:Ls:183:PHE:HB3	2.03	0.41
54:SG:98:ARG:HH11	54:SG:99:GLY:H	1.68	0.41
60:SO:125:LYS:HB3	65:Sa:58:VAL:HG13	2.03	0.41
68:S2:498:C:H2'	68:S2:499:G:C8	2.56	0.41
68:S2:1013:U:H2'	68:S2:1014:G:H8	1.86	0.41
68:S2:1174:PSU:H2'	68:S2:1175:G:C8	2.55	0.41
68:S2:1716:C:H2'	68:S2:1717:C:H6	1.86	0.41
69:SR:33:ARG:HD3	69:SR:33:ARG:HA	1.76	0.41
78:SU:32:LEU:HD12	78:SU:32:LEU:HA	1.82	0.41
80:Sc:21:THR:HG21	80:Sc:29:GLN:HG2	2.03	0.41
83:Sg:67:SER:HB3	83:Sg:83:TRP:CD1	2.55	0.41
85:CB:5:THR:HG23	85:CB:7:ASP:H	1.85	0.41
85:CB:428:ARG:NH1	85:CB:430:MET:HE1	2.35	0.41
3:L5:163:A:H2'	3:L5:164:G:C8	2.56	0.41
3:L5:261:G:H2'	3:L5:262:G:H8	1.85	0.41
3:L5:674:G:H2'	3:L5:675:C:C6	2.55	0.41
3:L5:1199:G:H2'	3:L5:1200:G:H8	1.85	0.41
3:L5:1647:U:OP1	89:L5:5291:SPD:H51	2.19	0.41
3:L5:2496:G:H2'	3:L5:2497:C:C6	2.55	0.41
3:L5:3588:C:H2'	3:L5:3589:G:O4'	2.21	0.41
3:L5:4098:A:N7	3:L5:4099:G:H1'	2.35	0.41
10:LE:67:ALA:HA	10:LE:69:TYR:CE2	2.56	0.41
30:LZ:30:ASP:HA	30:LZ:39:SER:OG	2.21	0.41
49:Lt:55:GLY:HA3	49:Lt:80:LEU:HD11	2.03	0.41
49:Lt:114:ARG:HG3	49:Lt:130:LYS:HB3	2.03	0.41
50:SA:126:ASP:HB3	50:SA:129:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1289:U:C5	82:Sf:97:LYS:HE2	2.55	0.41
68:S2:1491:G:H2'	68:S2:1492:U:C6	2.56	0.41
68:S2:1733:U:H2'	68:S2:1734:G:O4'	2.21	0.41
68:S2:1778:C:H2'	68:S2:1779:G:O4'	2.21	0.41
75:SQ:145:TYR:O	75:SQ:146:ARG:HD2	2.21	0.41
76:SS:40:TYR:HA	76:SS:83:PHE:HE2	1.86	0.41
85:CB:524:LEU:HD11	85:CB:546:ILE:HD11	2.03	0.41
85:CB:605:LYS:HD3	85:CB:705:HIS:CE1	2.56	0.41
86:CA:85:CYS:SG	86:CA:89:PHE:HB2	2.60	0.41
3:L5:161:G:H2'	3:L5:162:A:H8	1.85	0.41
3:L5:734:G:C2	3:L5:735:G:C8	3.09	0.41
3:L5:1300:G:H2'	3:L5:1301:C:C6	2.56	0.41
3:L5:1577:G:C8	6:LA:181:LYS:HE3	2.56	0.41
3:L5:2364:OMG:HM23	3:L5:2364:OMG:H1'	1.79	0.41
3:L5:3825:A2M:HM'3	3:L5:3825:A2M:H1'	1.75	0.41
3:L5:3861:A:H2'	3:L5:3862:A:C8	2.56	0.41
3:L5:4080:C:H2'	3:L5:4081:G:H8	1.85	0.41
3:L5:4164:C:H2'	3:L5:4165:C:C6	2.56	0.41
3:L5:4244:A:H2'	3:L5:4245:G:O4'	2.21	0.41
3:L5:4383:U:H2'	3:L5:4384:U:C6	2.56	0.41
3:L5:4593:C:H2'	3:L5:4594:U:H6	1.86	0.41
4:L7:3:C:H2'	4:L7:4:U:H6	1.86	0.41
5:L8:40:A:H2'	5:L8:41:A:C8	2.55	0.41
5:L8:90:C:H1'	29:LY:24:HIS:HB3	2.02	0.41
5:L8:93:C:O2'	5:L8:94:G:H8	2.03	0.41
6:LA:36:GLU:HG3	6:LA:91:GLY:HA2	2.03	0.41
7:LB:288:GLY:HA3	7:LB:330:PHE:CE1	2.56	0.41
8:LC:11:TYR:CZ	8:LC:148:PRO:HB2	2.56	0.41
11:LF:34:ARG:HE	11:LF:34:ARG:HB3	1.69	0.41
12:LG:159:HIS:ND1	12:LG:185:LYS:HA	2.35	0.41
15:LJ:15:LEU:HD12	15:LJ:165:TRP:HB2	2.01	0.41
19:LO:47:PHE:HA	19:LO:136:ALA:HB2	2.02	0.41
19:LO:181:ALA:O	19:LO:185:VAL:HG22	2.21	0.41
24:LT:146:LYS:HB2	24:LT:146:LYS:HE2	1.94	0.41
39:Li:16:LYS:HD3	39:Li:16:LYS:HA	1.78	0.41
41:Lk:61:PRO:HA	41:Lk:62:PRO:HD3	1.94	0.41
50:SA:32:PHE:CD1	68:S2:1097:G:H4'	2.55	0.41
52:SC:194:ARG:HG2	52:SC:225:SER:HB3	2.03	0.41
55:SH:62:ILE:HB	55:SH:94:PHE:CD1	2.56	0.41
64:SY:18:LEU:HD22	64:SY:20:ARG:HH21	1.85	0.41
68:S2:192:C:H2'	68:S2:193:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:497:C:H2'	68:S2:498:C:C6	2.56	0.41
68:S2:610:G:H2'	68:S2:611:G:H8	1.85	0.41
68:S2:832:G:H2'	68:S2:833:C:C6	2.55	0.41
68:S2:979:C:H2'	68:S2:980:A:C8	2.56	0.41
68:S2:1365:G:H2'	68:S2:1366:G:C8	2.56	0.41
68:S2:1376:A:H3'	68:S2:1377:U:H6	1.86	0.41
68:S2:1533:A:N7	68:S2:1604:G:H1'	2.36	0.41
68:S2:1562:C:H4'	77:ST:119:GLY:HA3	2.02	0.41
68:S2:1597:C:H4'	68:S2:1603:G:O6	2.21	0.41
68:S2:1631:U:H2'	68:S2:1632:G:O4'	2.20	0.41
71:SF:175:ASP:HA	71:SF:178:ILE:HD12	2.02	0.41
78:SU:36:CYS:SG	78:SU:87:ARG:HD3	2.61	0.41
81:Sd:3:HIS:CD2	81:Sd:5:GLN:HB2	2.56	0.41
84:Et:50:A:H2'	84:Et:51:G:H8	1.86	0.41
86:CA:12:ILE:HD13	86:CA:21:TYR:CE2	2.56	0.41
3:L5:257:C:H2'	3:L5:258:G:H8	1.82	0.41
3:L5:1788:A:H2'	14:LI:22:PHE:CZ	2.56	0.41
3:L5:3867:A2M:HM'3	3:L5:3867:A2M:H1'	1.54	0.41
3:L5:4088:C:C5	12:LG:54:PHE:HZ	2.39	0.41
3:L5:4113:U:H4'	3:L5:4115:G:C5	2.56	0.41
3:L5:4523:A2M:H5''	3:L5:4524:G:H5'	2.03	0.41
10:LE:153:LEU:HD11	10:LE:195:ILE:HG13	2.03	0.41
14:LI:102:MET:HE1	14:LI:114:GLY:H	1.85	0.41
49:Lt:11:LYS:HA	49:Lt:11:LYS:HD2	1.65	0.41
53:SE:253:ASP:HA	53:SE:256:LEU:HB2	2.02	0.41
54:SG:98:ARG:HH11	54:SG:99:GLY:N	2.19	0.41
56:SI:106:SER:HB3	56:SI:171:LEU:HG	2.02	0.41
65:Sa:79:ILE:HD11	68:S2:1864:U:H5'	2.03	0.41
66:Sb:54:VAL:HG22	66:Sb:64:CYS:HB2	2.03	0.41
68:S2:935:G:H2'	68:S2:936:G:H8	1.85	0.41
68:S2:1419:C:H42	77:ST:2:PRO:HG2	1.86	0.41
79:SZ:99:LEU:HD21	79:SZ:102:LYS:HB2	2.03	0.41
1:CD:205:LYS:HG3	68:S2:1698:C:H5'	2.02	0.40
3:L5:1366:G:N2	16:LL:33:ILE:HD13	2.36	0.40
3:L5:2540:C:H2'	3:L5:2541:G:H8	1.85	0.40
3:L5:2633:U:H2'	3:L5:2634:C:H6	1.86	0.40
3:L5:4593:C:H2'	3:L5:4594:U:C6	2.56	0.40
3:L5:4749:C:H2'	3:L5:4750:G:O4'	2.21	0.40
3:L5:4875:G:H5''	23:LS:170:LYS:HE3	2.03	0.40
3:L5:4896:G:H2'	3:L5:4897:G:C8	2.57	0.40
4:L7:3:C:H2'	4:L7:4:U:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LB:27:GLY:HA2	7:LB:276:HIS:CD2	2.56	0.40
7:LB:117:ARG:HA	7:LB:177:LYS:HD2	2.02	0.40
20:LP:94:MET:HE1	20:LP:146:ILE:HB	2.02	0.40
24:LT:44:GLY:HA2	24:LT:95:HIS:HB3	2.04	0.40
56:SI:142:SER:O	56:SI:146:GLN:HG2	2.22	0.40
68:S2:1208:A:H2'	68:S2:1209:A:C8	2.56	0.40
68:S2:1231:C:OP1	76:SS:134:GLN:HB2	2.21	0.40
68:S2:1470:C:H2'	68:S2:1471:C:H6	1.86	0.40
70:SD:142:LEU:HD23	70:SD:142:LEU:HA	1.94	0.40
86:CA:21:TYR:CE2	86:CA:324:LEU:HD11	2.56	0.40
86:CA:118:ILE:HG13	86:CA:190:LEU:HD23	2.03	0.40
3:L5:214:G:H2'	3:L5:215:C:C6	2.55	0.40
3:L5:2375:A:H2'	3:L5:2376:A:H8	1.86	0.40
3:L5:3718:A2M:HM'3	3:L5:3718:A2M:H1'	1.94	0.40
10:LE:99:ASP:O	10:LE:100:LYS:HG2	2.21	0.40
13:LH:24:THR:HA	13:LH:37:ASP:HA	2.02	0.40
15:LJ:147:ARG:HE	15:LJ:147:ARG:HB3	1.73	0.40
37:Lg:57:ARG:HG2	37:Lg:59:VAL:HG13	2.02	0.40
50:SA:10:MET:HE1	50:SA:51:LEU:HG	2.03	0.40
68:S2:171:A:C4	68:S2:173:A:C8	3.09	0.40
68:S2:1073:U:H2'	68:S2:1074:C:C6	2.56	0.40
76:SS:40:TYR:HA	76:SS:83:PHE:CE2	2.57	0.40
3:L5:922:C:H2'	3:L5:923:C:O4'	2.20	0.40
3:L5:1405:C:H41	3:L5:1408:G:N2	2.20	0.40
3:L5:1629:G:N1	6:LA:208:GLU:HG2	2.33	0.40
3:L5:3841:OMC:HM23	3:L5:3841:OMC:H1'	1.87	0.40
3:L5:4508:C:N3	3:L5:4512:U:H5	2.18	0.40
3:L5:4561:C:H2'	3:L5:4562:C:C6	2.57	0.40
22:LR:139:MET:HG2	22:LR:143:HIS:CE1	2.57	0.40
51:SB:142:PHE:HB2	51:SB:209:ASP:HB3	2.03	0.40
51:SB:182:LYS:NZ	51:SB:186:ASN:HD22	2.19	0.40
52:SC:248:TYR:O	61:SV:23:ILE:HG21	2.22	0.40
53:SE:47:PHE:HD2	53:SE:48:LEU:HD12	1.85	0.40
55:SH:37:LYS:HD2	55:SH:37:LYS:HA	1.88	0.40
56:SI:144:LYS:HE2	68:S2:192:C:H41	1.87	0.40
68:S2:5:U:O2'	68:S2:602:G:H4'	2.21	0.40
68:S2:14:C:H2'	68:S2:15:U:C6	2.55	0.40
70:SD:59:LEU:HD23	70:SD:66:ILE:HG13	2.04	0.40
75:SQ:42:ILE:HG13	75:SQ:43:GLU:H	1.86	0.40
85:CB:223:PHE:HB3	85:CB:344:LEU:HD13	2.03	0.40
3:L5:982:U:H2'	3:L5:983:C:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1557:C:H2'	3:L5:1558:A:C8	2.57	0.40
3:L5:1743:A:O4'	9:LD:15:ARG:HD2	2.22	0.40
3:L5:3595:U:H5''	3:L5:3597:G:OP2	2.21	0.40
3:L5:3923:A:H2'	3:L5:3924:C:C6	2.57	0.40
3:L5:4572:U:H1'	3:L5:4720:C:C4	2.56	0.40
3:L5:4970:C:C2	3:L5:4971:A:C8	3.09	0.40
5:L8:37:A:OP2	38:Lh:89:ARG:HD2	2.22	0.40
5:L8:119:C:H2'	5:L8:120:G:C8	2.56	0.40
21:LQ:105:VAL:HB	21:LQ:110:ARG:NH2	2.37	0.40
50:SA:33:GLN:HE22	61:SV:63:GLY:HA3	1.86	0.40
50:SA:85:ARG:NH1	50:SA:205:ARG:HH21	2.19	0.40
64:SY:20:ARG:HD3	64:SY:76:TYR:CZ	2.57	0.40
68:S2:455:A:H2'	68:S2:456:C:C6	2.56	0.40
68:S2:509:OMG:HM22	68:S2:510:G:O4'	2.22	0.40
68:S2:1539:U:H2'	68:S2:1540:G:C8	2.56	0.40
71:SF:155:CYS:HB3	71:SF:159:ARG:NH2	2.36	0.40
85:CB:301:PHE:HD1	85:CB:336:LEU:HD11	1.86	0.40
85:CB:579:TYR:HD2	85:CB:742:GLU:HA	1.86	0.40
3:L5:2709:C:N4	86:CA:256:GLY:HA2	2.36	0.40
3:L5:4153:C:H2'	3:L5:4154:G:H8	1.86	0.40
3:L5:4227:OMU:HM21	3:L5:4336:A:H1'	2.03	0.40
3:L5:4251:A:H5''	15:LJ:108:GLY:HA3	2.03	0.40
3:L5:4504:C:H2'	3:L5:4505:C:C6	2.56	0.40
3:L5:4678:G:N2	3:L5:4713:G:H1'	2.36	0.40
32:Lb:122:LYS:HE2	32:Lb:122:LYS:HB2	1.89	0.40
33:Lc:77:ASN:OD1	33:Lc:80:GLU:HG2	2.21	0.40
49:Lt:22:VAL:HA	49:Lt:48:LYS:HG2	2.03	0.40
51:SB:164:ILE:HD13	51:SB:164:ILE:HA	1.92	0.40
57:SJ:136:ARG:HA	57:SJ:141:VAL:HA	2.04	0.40
68:S2:39:A:H2'	68:S2:40:A:O4'	2.22	0.40
68:S2:634:A:H2'	68:S2:635:G:H8	1.86	0.40
68:S2:644:OMG:H1'	68:S2:644:OMG:HM23	1.78	0.40
68:S2:1409:A:H2'	68:S2:1410:C:C6	2.57	0.40
83:Sg:98:THR:HG22	83:Sg:99:ARG:HG2	2.02	0.40
84:Et:2:C:H2'	84:Et:3:C:C6	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%)	50 (98%)	1 (2%)	0	100	100
2	CI	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
6	LA	246/248 (99%)	239 (97%)	7 (3%)	0	100	100
7	LB	400/402 (100%)	386 (96%)	14 (4%)	0	100	100
8	LC	366/368 (100%)	355 (97%)	11 (3%)	0	100	100
9	LD	291/293 (99%)	283 (97%)	8 (3%)	0	100	100
10	LE	236/250 (94%)	222 (94%)	14 (6%)	0	100	100
11	LF	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
12	LG	239/241 (99%)	230 (96%)	9 (4%)	0	100	100
13	LH	188/190 (99%)	183 (97%)	5 (3%)	0	100	100
14	LI	201/213 (94%)	199 (99%)	2 (1%)	0	100	100
15	LJ	168/176 (96%)	164 (98%)	4 (2%)	0	100	100
16	LL	208/210 (99%)	201 (97%)	7 (3%)	0	100	100
17	LM	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
18	LN	201/203 (99%)	196 (98%)	5 (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%)	169 (98%)	4 (2%)	0	100	100
24	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
25	LU	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
26	LV	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
27	LW	112/124 (90%)	110 (98%)	2 (2%)	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%)	130 (98%)	2 (2%)	0	100	100
30	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
31	La	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
32	Lb	105/121 (87%)	98 (93%)	7 (7%)	0	100	100
33	Lc	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
34	Ld	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
35	Le	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
36	Lf	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
37	Lg	112/114 (98%)	112 (100%)	0	0	100	100
38	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
39	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
40	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
41	Lk	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
42	Ll	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
43	Lm	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
44	Ln	22/24 (92%)	22 (100%)	0	0	100	100
45	Lo	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
46	Lp	89/91 (98%)	87 (98%)	2 (2%)	0	100	100
47	Lr	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
48	Ls	194/196 (99%)	182 (94%)	12 (6%)	0	100	100
49	Lt	128/157 (82%)	109 (85%)	19 (15%)	0	100	100
50	SA	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
51	SB	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
52	SC	218/222 (98%)	210 (96%)	8 (4%)	0	100	100
53	SE	260/262 (99%)	251 (96%)	9 (4%)	0	100	100
54	SG	235/237 (99%)	221 (94%)	14 (6%)	0	100	100
55	SH	182/189 (96%)	168 (92%)	14 (8%)	0	100	100
56	SI	204/206 (99%)	198 (97%)	6 (3%)	0	100	100
57	SJ	183/185 (99%)	172 (94%)	11 (6%)	0	100	100
58	SL	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
59	SN	148/150 (99%)	144 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	SO	135/140 (96%)	130 (96%)	5 (4%)	0	100	100
61	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
62	SW	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
63	SX	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
64	SY	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
65	Sa	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
66	Sb	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
67	Se	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
69	SR	133/135 (98%)	131 (98%)	2 (2%)	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%)	90 (94%)	6 (6%)	0	100	100
73	SM	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
74	SP	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
75	SQ	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
76	SS	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
77	ST	141/143 (99%)	140 (99%)	1 (1%)	0	100	100
78	SU	102/104 (98%)	97 (95%)	5 (5%)	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%)	53 (100%)	0	0	100	100
82	Sf	65/67 (97%)	59 (91%)	6 (9%)	0	100	100
83	Sg	311/313 (99%)	291 (94%)	20 (6%)	0	100	100
85	CB	842/856 (98%)	820 (97%)	22 (3%)	0	100	100
86	CA	350/356 (98%)	336 (96%)	14 (4%)	0	100	100
All	All	12905/13527 (95%)	12457 (96%)	448 (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	92
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%)	74 (100%)	0	100	100
47	Lr	109/109 (100%)	109 (100%)	0	100	100
48	Ls	162/164 (99%)	162 (100%)	0	100	100
49	Lt	107/130 (82%)	107 (100%)	0	100	100
50	SA	183/183 (100%)	183 (100%)	0	100	100
51	SB	195/195 (100%)	195 (100%)	0	100	100
52	SC	186/188 (99%)	186 (100%)	0	100	100
53	SE	224/224 (100%)	224 (100%)	0	100	100
54	SG	207/207 (100%)	207 (100%)	0	100	100
55	SH	166/169 (98%)	166 (100%)	0	100	100
56	SI	178/178 (100%)	178 (100%)	0	100	100
57	SJ	161/161 (100%)	161 (100%)	0	100	100
58	SL	137/137 (100%)	137 (100%)	0	100	100
59	SN	130/130 (100%)	130 (100%)	0	100	100
60	SO	107/110 (97%)	107 (100%)	0	100	100
61	SV	67/67 (100%)	67 (100%)	0	100	100
62	SW	112/112 (100%)	112 (100%)	0	100	100
63	SX	113/113 (100%)	113 (100%)	0	100	100

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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%)	11212 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	LL	59	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
6	LA	97	ASN
6	LA	140	ASN
7	LB	68	ASN

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Mol	Chain	Res	Type
7	LB	121	ASN
7	LB	145	GLN
7	LB	184	GLN
7	LB	209	GLN
7	LB	289	GLN
8	LC	43	ASN
8	LC	329	ASN
8	LC	362	GLN
9	LD	202	GLN
10	LE	266	GLN
11	LF	80	ASN
12	LG	43	GLN
13	LH	98	HIS
13	LH	102	ASN
13	LH	188	GLN
14	LI	73	ASN
14	LI	144	ASN
15	LJ	65	ASN
15	LJ	98	ASN
17	LM	34	ASN
19	LO	180	GLN
20	LP	10	ASN
20	LP	133	HIS
21	LQ	57	ASN
21	LQ	162	HIS
23	LS	108	GLN
27	LW	17	HIS
28	LX	57	GLN
29	LY	61	HIS
29	LY	96	HIS
30	LZ	78	ASN
31	La	34	ASN
32	Lb	11	ASN
34	Ld	100	ASN
36	Lf	20	ASN
36	Lf	21	GLN
36	Lf	99	HIS
38	Lh	62	ASN
39	Li	92	ASN
40	Lj	66	HIS
44	Ln	22	GLN
48	Ls	58	ASN

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Mol	Chain	Res	Type
48	Ls	68	HIS
48	Ls	71	ASN
49	Lt	68	GLN
49	Lt	115	GLN
49	Lt	137	GLN
49	Lt	149	HIS
50	SA	111	GLN
51	SB	75	GLN
51	SB	186	ASN
51	SB	208	HIS
52	SC	277	HIS
53	SE	17	HIS
53	SE	98	ASN
53	SE	209	HIS
53	SE	214	ASN
54	SG	81	HIS
54	SG	105	ASN
55	SH	25	GLN
56	SI	35	ASN
56	SI	52	ASN
56	SI	146	GLN
57	SJ	111	GLN
59	SN	13	GLN
59	SN	36	GLN
61	SV	49	GLN
62	SW	56	HIS
62	SW	120	HIS
63	SX	31	HIS
65	Sa	72	HIS
66	Sb	51	GLN
67	Se	37	GLN
67	Se	39	ASN
70	SD	145	GLN
71	SF	118	ASN
73	SM	55	ASN
74	SP	41	GLN
75	SQ	48	GLN
77	ST	85	ASN
77	ST	105	GLN
83	Sg	196	ASN
85	CB	168	GLN
85	CB	565	HIS

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Mol	Chain	Res	Type
85	CB	705	HIS
85	CB	715	HIS
85	CB	803	ASN
85	CB	807	GLN
85	CB	816	HIS
86	CA	306	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3643/5070 (71%)	744 (20%)	17 (0%)
4	L7	119/120 (99%)	11 (9%)	0
5	L8	155/156 (99%)	26 (16%)	0
68	S2	1715/1740 (98%)	385 (22%)	4 (0%)
84	Et	73/75 (97%)	26 (35%)	0
All	All	5705/7161 (79%)	1192 (20%)	21 (0%)

All (1192) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L5	5	A
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	73	A
3	L5	91	G
3	L5	104	G
3	L5	108	A
3	L5	109	G
3	L5	110	C
3	L5	119	G
3	L5	120	A
3	L5	132	G
3	L5	133	C
3	L5	135	G

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Mol	Chain	Res	Type
3	L5	136	C
3	L5	139	G
3	L5	159	C
3	L5	165	A
3	L5	181	C
3	L5	182	G
3	L5	183	C
3	L5	184	U
3	L5	185	C
3	L5	186	G
3	L5	188	G
3	L5	189	G
3	L5	200	U
3	L5	209	U
3	L5	210	C
3	L5	216	C
3	L5	218	A
3	L5	237	G
3	L5	255	C
3	L5	256	G
3	L5	261	G
3	L5	263	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	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
3	L5	412	G
3	L5	413	G

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Mol	Chain	Res	Type
3	L5	415	G
3	L5	449	C
3	L5	452	A
3	L5	453	G
3	L5	456	C
3	L5	457	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	493	G
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	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	654	C
3	L5	655	C
3	L5	657	C
3	L5	659	G
3	L5	667	A
3	L5	668	C
3	L5	669	C
3	L5	673	C
3	L5	686	A
3	L5	687	U
3	L5	696	C
3	L5	704	C

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Mol	Chain	Res	Type
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	750	U
3	L5	758	G
3	L5	759	G
3	L5	904	C
3	L5	905	C
3	L5	906	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	943	A
3	L5	945	U
3	L5	946	C
3	L5	956	A
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
3	L5	966	A
3	L5	967	C
3	L5	970	G
3	L5	977	C
3	L5	979	C
3	L5	982	U

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Mol	Chain	Res	Type
3	L5	985	C
3	L5	989	U
3	L5	1070	G
3	L5	1072	C
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	1178	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	1210	C
3	L5	1211	G
3	L5	1214	C
3	L5	1215	C
3	L5	1216	C
3	L5	1218	G
3	L5	1219	G
3	L5	1222	A
3	L5	1245	C
3	L5	1246	G
3	L5	1253	G
3	L5	1254	A
3	L5	1257	A
3	L5	1258	G
3	L5	1266	G
3	L5	1267	C
3	L5	1269	G
3	L5	1270	A
3	L5	1271	G

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Mol	Chain	Res	Type
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	1326	A2M
3	L5	1354	A
3	L5	1359	G
3	L5	1365	C
3	L5	1366	G
3	L5	1379	C
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	1409	C
3	L5	1410	U
3	L5	1415	G
3	L5	1417	C
3	L5	1420	A
3	L5	1437	C
3	L5	1439	C
3	L5	1442	C
3	L5	1443	A
3	L5	1444	G
3	L5	1446	C
3	L5	1447	C
3	L5	1448	G
3	L5	1480	C
3	L5	1482	G
3	L5	1483	C
3	L5	1497	A
3	L5	1498	G

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Mol	Chain	Res	Type
3	L5	1502	G
3	L5	1504	G
3	L5	1516	G
3	L5	1517	G
3	L5	1524	A2M
3	L5	1534	A2M
3	L5	1535	C
3	L5	1537	A
3	L5	1547	A
3	L5	1552	G
3	L5	1566	C
3	L5	1574	G
3	L5	1578	U
3	L5	1591	U
3	L5	1596	U
3	L5	1612	G
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	1694	C
3	L5	1697	G
3	L5	1699	A
3	L5	1700	G
3	L5	1701	A
3	L5	1704	C
3	L5	1705	G
3	L5	1717	C
3	L5	1718	C

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Mol	Chain	Res	Type
3	L5	1719	A
3	L5	1721	G
3	L5	1731	C
3	L5	1733	G
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	1787	A
3	L5	1803	G
3	L5	1804	A
3	L5	1806	G
3	L5	1810	G
3	L5	1815	G
3	L5	1821	G
3	L5	1833	G
3	L5	1834	U
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1855	G
3	L5	1869	G
3	L5	1882	U
3	L5	1888	A
3	L5	1892	A
3	L5	1893	C
3	L5	1897	A
3	L5	1917	A
3	L5	1918	U

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Mol	Chain	Res	Type
3	L5	1919	G
3	L5	1920	C
3	L5	1921	C
3	L5	1922	G
3	L5	1925	G
3	L5	1930	U
3	L5	1931	C
3	L5	1932	A
3	L5	1936	C
3	L5	1940	G
3	L5	1948	G
3	L5	1951	G
3	L5	1961	G
3	L5	1962	A
3	L5	1971	C
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	1998	A
3	L5	1999	A
3	L5	2001	G
3	L5	2002	A
3	L5	2003	G
3	L5	2005	G
3	L5	2011	C
3	L5	2024	G
3	L5	2025	A
3	L5	2026	A
3	L5	2046	G
3	L5	2048	U
3	L5	2055	G
3	L5	2056	G
3	L5	2069	A

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Mol	Chain	Res	Type
3	L5	2084	C
3	L5	2092	G
3	L5	2093	A
3	L5	2095	A
3	L5	2097	U
3	L5	2098	G
3	L5	2099	G
3	L5	2102	G
3	L5	2103	G
3	L5	2107	C
3	L5	2112	G
3	L5	2252	G
3	L5	2253	A
3	L5	2256	C
3	L5	2259	G
3	L5	2269	C
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2306	G
3	L5	2313	A
3	L5	2331	G
3	L5	2333	G
3	L5	2348	G
3	L5	2351	OMC
3	L5	2360	A
3	L5	2364	OMG
3	L5	2383	C
3	L5	2389	A
3	L5	2395	A
3	L5	2397	G
3	L5	2398	U
3	L5	2401	A2M
3	L5	2411	C
3	L5	2412	A
3	L5	2417	A
3	L5	2425	U
3	L5	2450	G
3	L5	2453	A
3	L5	2464	C
3	L5	2465	C
3	L5	2469	C

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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	2480	G
3	L5	2483	G
3	L5	2484	A
3	L5	2485	U
3	L5	2487	G
3	L5	2488	C
3	L5	2489	C
3	L5	2490	U
3	L5	2504	C
3	L5	2513	A
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	2606	G
3	L5	2627	C
3	L5	2638	G
3	L5	2653	C
3	L5	2658	G
3	L5	2662	G
3	L5	2669	C
3	L5	2675	G
3	L5	2676	A
3	L5	2687	U
3	L5	2694	G

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Mol	Chain	Res	Type
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	2719	C
3	L5	2721	G
3	L5	2724	G
3	L5	2726	G
3	L5	2739	C
3	L5	2742	G
3	L5	2743	A
3	L5	2746	A
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	2812	A
3	L5	2815	A2M
3	L5	2826	U
3	L5	2827	G
3	L5	2828	U
3	L5	2848	G
3	L5	2855	G
3	L5	2867	C
3	L5	2877	G
3	L5	2900	U
3	L5	2902	G
3	L5	2903	G
3	L5	2904	U
3	L5	2905	C
3	L5	2906	G
3	L5	2907	G

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Mol	Chain	Res	Type
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	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	3701	OMC
3	L5	3706	C
3	L5	3710	G
3	L5	3711	A
3	L5	3713	U
3	L5	3727	A
3	L5	3748	A
3	L5	3760	A
3	L5	3764	U
3	L5	3774	A
3	L5	3775	A
3	L5	3776	G
3	L5	3777	G
3	L5	3785	A2M
3	L5	3786	U
3	L5	3792	OMG
3	L5	3811	G
3	L5	3814	U
3	L5	3817	A
3	L5	3819	G

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Mol	Chain	Res	Type
3	L5	3824	A
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3843	C
3	L5	3867	A2M
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3880	G
3	L5	3885	G
3	L5	3890	A
3	L5	3892	U
3	L5	3897	G
3	L5	3901	A
3	L5	3906	A
3	L5	3907	G
3	L5	3908	A
3	L5	3915	U
3	L5	3938	G
3	L5	3942	A
3	L5	3943	A
3	L5	3944	G
3	L5	3947	A
3	L5	3948	C
3	L5	3949	A
3	L5	3950	U
3	L5	3951	G
3	L5	3952	A
3	L5	3953	G
3	L5	4057	C
3	L5	4058	U
3	L5	4059	C
3	L5	4060	U
3	L5	4061	G
3	L5	4062	A
3	L5	4063	U
3	L5	4064	C
3	L5	4069	U
3	L5	4076	G
3	L5	4095	G
3	L5	4097	G

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Mol	Chain	Res	Type
3	L5	4099	G
3	L5	4101	C
3	L5	4104	G
3	L5	4107	G
3	L5	4108	G
3	L5	4111	U
3	L5	4114	C
3	L5	4115	G
3	L5	4116	C
3	L5	4122	G
3	L5	4127	A
3	L5	4140	C
3	L5	4141	G
3	L5	4142	C
3	L5	4143	G
3	L5	4144	C
3	L5	4146	G
3	L5	4150	G
3	L5	4162	C
3	L5	4163	U
3	L5	4170	A
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4203	A
3	L5	4222	G
3	L5	4225	G
3	L5	4228	OMG
3	L5	4229	U
3	L5	4232	U
3	L5	4233	A
3	L5	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

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Mol	Chain	Res	Type
3	L5	4291	G
3	L5	4295	U
3	L5	4304	A
3	L5	4305	G
3	L5	4319	C
3	L5	4329	G
3	L5	4330	G
3	L5	4332	C
3	L5	4338	G
3	L5	4349	C
3	L5	4350	C
3	L5	4354	U
3	L5	4373	G
3	L5	4376	A
3	L5	4377	G
3	L5	4378	A
3	L5	4379	A
3	L5	4386	C
3	L5	4387	C
3	L5	4391	G
3	L5	4394	A
3	L5	4405	G
3	L5	4421	C
3	L5	4422	A
3	L5	4444	C
3	L5	4448	G
3	L5	4449	A
3	L5	4452	U
3	L5	4464	A
3	L5	4466	C
3	L5	4475	G
3	L5	4488	A
3	L5	4500	PSU
3	L5	4512	U
3	L5	4513	A
3	L5	4519	C
3	L5	4524	G
3	L5	4525	C
3	L5	4545	G
3	L5	4548	A
3	L5	4549	G
3	L5	4560	C

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Mol	Chain	Res	Type
3	L5	4567	G
3	L5	4575	G
3	L5	4584	A
3	L5	4589	A
3	L5	4590	A2M
3	L5	4600	G
3	L5	4601	U
3	L5	4608	G
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
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	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

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Mol	Chain	Res	Type
3	L5	4875	G
3	L5	4877	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	4899	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	4926	C
3	L5	4927	G
3	L5	4928	C
3	L5	4934	A
3	L5	4941	G
3	L5	4943	A
3	L5	4944	C
3	L5	4947	U
3	L5	4951	G
3	L5	4955	A
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	4990	C
3	L5	4991	U
3	L5	4995	U
3	L5	5013	C
3	L5	5014	A
3	L5	5017	G
3	L5	5022	U
3	L5	5023	C
3	L5	5024	C
3	L5	5027	C
3	L5	5028	G

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Mol	Chain	Res	Type
3	L5	5030	U
3	L5	5034	A
3	L5	5041	G
3	L5	5050	C
3	L5	5054	C
3	L5	5058	A
3	L5	5061	A
3	L5	5062	G
3	L5	5069	U
4	L7	22	A
4	L7	33	U
4	L7	38	U
4	L7	39	C
4	L7	53	U
4	L7	54	A
4	L7	64	G
4	L7	97	G
4	L7	100	A
4	L7	102	U
4	L7	110	G
5	L8	23	C
5	L8	25	G
5	L8	34	U
5	L8	35	C
5	L8	59	A
5	L8	62	A
5	L8	63	U
5	L8	75	OMG
5	L8	80	A
5	L8	82	A
5	L8	83	C
5	L8	84	A
5	L8	85	U
5	L8	86	U
5	L8	87	G
5	L8	94	G
5	L8	103	A
5	L8	105	C
5	L8	111	U
5	L8	114	G
5	L8	123	U
5	L8	124	U

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Mol	Chain	Res	Type
5	L8	125	C
5	L8	126	C
5	L8	127	U
5	L8	150	C
68	S2	4	C
68	S2	25	A
68	S2	33	G
68	S2	41	G
68	S2	42	A
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	65	C
68	S2	67	C
68	S2	68	A
68	S2	72	C
68	S2	73	C
68	S2	74	G
68	S2	76	U
68	S2	92	A
68	S2	93	PSU
68	S2	99	A2M
68	S2	103	A
68	S2	113	G
68	S2	115	U
68	S2	126	G
68	S2	130	G
68	S2	142	C
68	S2	143	U
68	S2	147	A
68	S2	148	U
68	S2	149	A
68	S2	153	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

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Mol	Chain	Res	Type
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	202	G
68	S2	203	G
68	S2	207	G
68	S2	208	G
68	S2	209	A
68	S2	213	G
68	S2	214	U
68	S2	290	U
68	S2	291	G
68	S2	292	A
68	S2	294	U
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
68	S2	312	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	347	G
68	S2	351	G
68	S2	360	A
68	S2	361	U
68	S2	362	C
68	S2	363	A

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Mol	Chain	Res	Type
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	466	G
68	S2	467	G
68	S2	471	G
68	S2	472	C
68	S2	473	A
68	S2	474	G
68	S2	482	G
68	S2	487	U
68	S2	488	U
68	S2	492	C
68	S2	493	A
68	S2	500	A
68	S2	502	C
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

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Mol	Chain	Res	Type
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	600	G
68	S2	604	A
68	S2	607	U
68	S2	614	C
68	S2	617	G
68	S2	623	G
68	S2	627	OMU
68	S2	628	A
68	S2	643	A
68	S2	644	OMG
68	S2	655	A
68	S2	660	C
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	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

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Mol	Chain	Res	Type
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	797	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
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	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

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Mol	Chain	Res	Type
68	S2	901	G
68	S2	903	A
68	S2	907	G
68	S2	909	G
68	S2	913	A
68	S2	917	U
68	S2	920	A
68	S2	922	A
68	S2	933	G
68	S2	949	G
68	S2	953	C
68	S2	963	A
68	S2	969	U
68	S2	970	G
68	S2	971	G
68	S2	985	G
68	S2	990	A
68	S2	992	A
68	S2	999	G
68	S2	1001	A
68	S2	1008	A
68	S2	1017	U
68	S2	1023	A
68	S2	1027	A
68	S2	1028	A
68	S2	1045	PSU
68	S2	1060	A
68	S2	1061	U
68	S2	1062	A
68	S2	1080	A
68	S2	1083	A
68	S2	1085	C
68	S2	1108	G
68	S2	1109	C
68	S2	1113	A
68	S2	1114	U
68	S2	1116	C
68	S2	1119	A
68	S2	1121	G
68	S2	1133	A
68	S2	1138	C
68	S2	1139	C

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Mol	Chain	Res	Type
68	S2	1148	A
68	S2	1153	C
68	S2	1154	U
68	S2	1155	U
68	S2	1161	U
68	S2	1195	A
68	S2	1200	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	1251	A
68	S2	1253	A
68	S2	1255	G
68	S2	1256	G
68	S2	1257	G
68	S2	1259	A
68	S2	1274	G
68	S2	1275	G
68	S2	1284	A
68	S2	1285	G
68	S2	1286	G
68	S2	1294	G
68	S2	1295	A
68	S2	1301	A
68	S2	1302	G
68	S2	1303	C
68	S2	1308	U
68	S2	1342	U
68	S2	1354	G
68	S2	1357	A
68	S2	1358	U
68	S2	1371	U
68	S2	1376	A
68	S2	1378	A
68	S2	1382	A

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Mol	Chain	Res	Type
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	1419	C
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
68	S2	1454	A
68	S2	1462	U
68	S2	1463	U
68	S2	1484	A
68	S2	1489	A
68	S2	1490	OMG
68	S2	1495	G
68	S2	1497	G
68	S2	1498	A
68	S2	1507	G
68	S2	1520	G
68	S2	1521	C
68	S2	1533	A
68	S2	1544	C
68	S2	1546	G
68	S2	1552	G
68	S2	1553	C
68	S2	1558	C
68	S2	1575	G
68	S2	1578	U
68	S2	1580	A
68	S2	1581	C
68	S2	1587	G

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Mol	Chain	Res	Type
68	S2	1588	A
68	S2	1601	A
68	S2	1604	G
68	S2	1606	G
68	S2	1621	U
68	S2	1623	A
68	S2	1633	A
68	S2	1634	A
68	S2	1637	A
68	S2	1646	C
68	S2	1648	G
68	S2	1654	G
68	S2	1663	A
68	S2	1665	G
68	S2	1680	G
68	S2	1683	C
68	S2	1698	C
68	S2	1700	C
68	S2	1715	A
68	S2	1721	U
68	S2	1722	G
68	S2	1744	G
68	S2	1752	C
68	S2	1753	C
68	S2	1754	G
68	S2	1756	C
68	S2	1757	G
68	S2	1758	G
68	S2	1761	U
68	S2	1772	C
68	S2	1773	C
68	S2	1774	C
68	S2	1775	U
68	S2	1782	G
68	S2	1783	C
68	S2	1784	G
68	S2	1786	U
68	S2	1787	G
68	S2	1798	C
68	S2	1810	U
68	S2	1825	A
68	S2	1826	G

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Mol	Chain	Res	Type
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	1864	U
68	S2	1865	C
84	Et	9	A
84	Et	11	C
84	Et	16	C
84	Et	19	G
84	Et	20	U
84	Et	21	A
84	Et	26	A
84	Et	32	C
84	Et	33	U
84	Et	36	U
84	Et	37	A
84	Et	38	A
84	Et	39	U
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	70	G
84	Et	71	G
84	Et	73	G
84	Et	76	A

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	406	C

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Mol	Chain	Res	Type
3	L5	914	U
3	L5	1071	C
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
3	L5	3673	C
3	L5	4600	G
3	L5	4699	U
3	L5	4913	G
68	S2	291	G
68	S2	531	A
68	S2	563	G
68	S2	688	U

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	$\# Z > 2$
5	OMG	L8	75	5	23,26,27	0.50	0	32,38,41	0.50	0
3	A2M	L5	2787	3	22,25,26	1.18	1 (4%)	30,36,39	1.51	8 (26%)
3	OMC	L5	2861	3	19,22,23	0.55	0	25,31,34	0.87	2 (8%)
68	OMU	S2	627	68	19,22,23	3.37	7 (36%)	25,31,34	1.82	5 (20%)
68	PSU	S2	105	68	18,21,22	1.09	1 (5%)	21,30,33	1.92	4 (19%)
3	OMG	L5	2364	87,3	23,26,27	0.52	0	32,38,41	0.45	0
3	PSU	L5	3695	3	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	3718	3	22,25,26	1.15	1 (4%)	30,36,39	1.48	5 (16%)
3	PSU	L5	4471	3	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
68	A2M	S2	668	68,87	22,25,26	1.30	2 (9%)	30,36,39	1.60	6 (20%)
68	OMC	S2	1703	68	19,22,23	0.51	0	25,31,34	0.70	1 (4%)
68	A2M	S2	159	68	22,25,26	1.22	2 (9%)	30,36,39	1.51	7 (23%)
3	PSU	L5	1744	87,3	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
3	OMC	L5	4456	3	19,22,23	0.61	0	25,31,34	0.76	1 (4%)
68	PSU	S2	109	68	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
68	PSU	S2	1081	68	18,21,22	1.09	1 (5%)	21,30,33	1.90	5 (23%)
3	PSU	L5	4457	3	18,21,22	1.07	1 (5%)	21,30,33	1.98	6 (28%)
3	PSU	L5	4403	3	18,21,22	1.08	1 (5%)	21,30,33	1.95	6 (28%)
68	PSU	S2	1244	68	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
68	A2M	S2	1383	68	22,25,26	1.21	1 (4%)	30,36,39	1.59	6 (20%)
3	PSU	L5	4973	3	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)
3	PSU	L5	4579	3	18,21,22	1.04	1 (5%)	21,30,33	1.85	4 (19%)
68	OMU	S2	1288	68	19,22,23	3.41	7 (36%)	25,31,34	1.64	5 (20%)
3	PSU	L5	3637	3	18,21,22	1.09	1 (5%)	21,30,33	1.99	5 (23%)
68	OMC	S2	1272	68	19,22,23	0.52	0	25,31,34	0.76	1 (4%)
68	OMU	S2	116	68	19,22,23	3.34	7 (36%)	25,31,34	1.67	4 (16%)
68	PSU	S2	1177	68	18,21,22	1.08	1 (5%)	21,30,33	1.93	4 (19%)
68	PSU	S2	649	68	18,21,22	1.14	1 (5%)	21,30,33	1.81	4 (19%)
68	6MZ	S2	1832	68,87	22,25,26	3.02	4 (18%)	29,36,39	2.26	10 (34%)
3	A2M	L5	1871	87,3	22,25,26	1.24	1 (4%)	30,36,39	1.59	7 (23%)
3	PSU	L5	4552	3	18,21,22	1.13	1 (5%)	21,30,33	1.92	4 (19%)
3	PSU	L5	5001	3	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
3	5MC	L5	3782	87,3	19,22,23	0.60	0	26,32,35	0.72	0
3	PSU	L5	4576	3	18,21,22	1.10	1 (5%)	21,30,33	1.88	5 (23%)
68	MA6	S2	1851	68	23,26,27	1.27	2 (8%)	33,38,41	3.41	12 (36%)
68	OMU	S2	354	68	19,22,23	3.33	7 (36%)	25,31,34	1.79	5 (20%)
3	OMG	L5	4637	3	23,26,27	0.49	0	32,38,41	0.48	0
3	A2M	L5	3830	3	22,25,26	1.20	1 (4%)	30,36,39	1.57	5 (16%)
68	4AC	S2	1842	68	21,24,25	0.40	0	28,34,37	0.47	0
3	OMG	L5	4228	3	23,26,27	0.55	0	32,38,41	0.69	0
3	UY1	L5	3818	3	19,22,23	4.90	10 (52%)	21,31,34	2.01	5 (23%)
3	PSU	L5	3920	87,3	18,21,22	1.08	1 (5%)	21,30,33	1.92	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	A2M	S2	99	68,87	22,25,26	1.19	1 (4%)	30,36,39	1.53	8 (26%)
3	OMG	L5	4392	3	23,26,27	0.51	0	32,38,41	0.51	0
3	OMU	L5	4227	3	19,22,23	3.33	7 (36%)	25,31,34	1.82	4 (16%)
3	OMG	L5	4370	3	23,26,27	0.50	0	32,38,41	0.48	0
3	OMU	L5	2837	3	19,22,23	3.34	7 (36%)	25,31,34	1.86	5 (20%)
3	OMG	L5	2876	3	23,26,27	0.52	0	32,38,41	0.49	0
3	OMC	L5	3841	3	19,22,23	0.54	0	25,31,34	0.56	0
3	OMG	L5	1625	3	23,26,27	0.51	0	32,38,41	0.47	0
3	OMG	L5	4494	3	23,26,27	0.50	0	32,38,41	0.52	0
3	PSU	L5	4532	3	18,21,22	1.08	1 (5%)	21,30,33	1.93	4 (19%)
68	PSU	S2	651	68	18,21,22	1.13	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	3851	3	18,21,22	1.07	1 (5%)	21,30,33	1.83	4 (19%)
68	B8N	S2	1248	68	25,29,30	3.28	6 (24%)	28,42,45	1.98	7 (25%)
68	PSU	S2	1045	68	18,21,22	1.10	1 (5%)	21,30,33	1.85	4 (19%)
3	PSU	L5	1683	3	18,21,22	1.12	1 (5%)	21,30,33	1.88	4 (19%)
3	OMU	L5	4620	3	19,22,23	3.25	7 (36%)	25,31,34	1.75	4 (16%)
68	OMC	S2	174	68	19,22,23	0.51	0	25,31,34	0.68	0
3	A2M	L5	4523	87,3	22,25,26	1.23	1 (4%)	30,36,39	1.56	8 (26%)
3	PSU	L5	1782	3	18,21,22	1.06	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L5	4293	3	18,21,22	1.08	1 (5%)	21,30,33	1.98	4 (19%)
3	OMG	L5	4623	3	23,26,27	0.52	0	32,38,41	0.56	0
3	OMG	L5	1522	3	23,26,27	0.54	0	32,38,41	0.60	0
68	OMG	S2	644	68	23,26,27	0.46	0	32,38,41	0.49	0
68	OMG	S2	1328	68	23,26,27	0.46	0	32,38,41	0.44	0
3	OMC	L5	2804	3	19,22,23	0.54	0	25,31,34	0.61	0
68	PSU	S2	1046	68	18,21,22	1.08	1 (5%)	21,30,33	1.83	4 (19%)
3	PSU	L5	3844	3	18,21,22	1.10	1 (5%)	21,30,33	1.80	4 (19%)
3	OMG	L5	4618	3	23,26,27	0.53	0	32,38,41	0.51	0
3	PSU	L5	2839	3	18,21,22	1.06	1 (5%)	21,30,33	1.78	4 (19%)
3	PSU	L5	4673	87,3	18,21,22	1.10	1 (5%)	21,30,33	1.84	4 (19%)
3	PSU	L5	5010	3	18,21,22	1.13	1 (5%)	21,30,33	1.86	4 (19%)
3	A2M	L5	1323	3	22,25,26	1.27	2 (9%)	30,36,39	1.59	8 (26%)
3	OMG	L5	4196	3	23,26,27	0.48	0	32,38,41	0.48	0
68	G7M	S2	1639	68,84	23,26,27	2.66	8 (34%)	34,39,42	2.63	11 (32%)
68	PSU	S2	863	68	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
3	A2M	L5	3785	87,3	22,25,26	1.12	1 (4%)	30,36,39	1.54	8 (26%)
3	PSU	L5	4431	3	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
3	OMC	L5	1340	3	19,22,23	0.57	0	25,31,34	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L5	2365	3	19,22,23	0.55	0	25,31,34	0.58	0
3	PSU	L5	3853	87,3	18,21,22	1.07	1 (5%)	21,30,33	1.83	4 (19%)
68	OMU	S2	799	68	19,22,23	3.48	7 (36%)	25,31,34	1.86	5 (20%)
68	A2M	S2	1031	68	22,25,26	1.20	1 (4%)	30,36,39	1.53	7 (23%)
3	OMG	L5	3627	3	23,26,27	0.50	0	32,38,41	0.60	0
3	OMU	L5	4498	3	19,22,23	3.32	7 (36%)	25,31,34	1.86	5 (20%)
3	OMC	L5	3869	3	19,22,23	0.56	0	25,31,34	0.63	0
68	OMU	S2	121	68	19,22,23	3.34	7 (36%)	25,31,34	1.73	5 (20%)
68	OMU	S2	1442	68	19,22,23	3.40	7 (36%)	25,31,34	1.81	5 (20%)
68	PSU	S2	1367	68	18,21,22	1.11	1 (5%)	21,30,33	1.92	5 (23%)
3	OMC	L5	3808	3	19,22,23	0.61	0	25,31,34	0.87	2 (8%)
3	A2M	L5	2363	87,3	22,25,26	1.19	2 (9%)	30,36,39	1.53	9 (30%)
68	PSU	S2	1004	68	18,21,22	1.14	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	3639	3	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
3	OMG	L5	4499	3	23,26,27	0.49	0	32,38,41	0.52	0
68	A2M	S2	484	68	22,25,26	1.19	1 (4%)	30,36,39	1.48	7 (23%)
3	A2M	L5	1326	3	22,25,26	1.18	2 (9%)	30,36,39	1.55	8 (26%)
3	OMG	L5	2424	3	23,26,27	0.50	0	32,38,41	0.46	0
3	A2M	L5	2815	3	22,25,26	1.21	1 (4%)	30,36,39	1.52	9 (30%)
68	OMG	S2	601	68	23,26,27	0.48	0	32,38,41	0.52	0
68	OMG	S2	436	68	23,26,27	0.48	0	32,38,41	0.51	0
3	PSU	L5	3822	3	18,21,22	1.07	1 (5%)	21,30,33	1.89	5 (23%)
68	PSU	S2	686	68	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
68	PSU	S2	93	68	18,21,22	1.05	1 (5%)	21,30,33	1.84	4 (19%)
3	A2M	L5	1534	87,3	22,25,26	1.18	1 (4%)	30,36,39	1.45	7 (23%)
68	A2M	S2	468	68	22,25,26	1.23	1 (4%)	30,36,39	1.56	7 (23%)
68	OMU	S2	172	68	19,22,23	3.35	7 (36%)	25,31,34	1.77	5 (20%)
3	A2M	L5	400	3	22,25,26	1.24	1 (4%)	30,36,39	1.55	7 (23%)
3	OMC	L5	2351	87,3	19,22,23	0.58	0	25,31,34	0.80	1 (4%)
3	A2M	L5	2401	3	22,25,26	1.19	1 (4%)	30,36,39	1.55	5 (16%)
3	PSU	L5	1536	3	18,21,22	1.07	1 (5%)	21,30,33	1.87	4 (19%)
3	PSU	L5	4689	3	18,21,22	1.09	2 (11%)	21,30,33	1.83	4 (19%)
3	PSU	L5	4353	3	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
3	PSU	L5	4636	3	18,21,22	1.09	1 (5%)	21,30,33	2.04	6 (28%)
3	PSU	L5	4521	87,3	18,21,22	1.10	1 (5%)	21,30,33	1.98	5 (23%)
68	OMG	S2	683	68	23,26,27	0.49	0	32,38,41	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	3867	3	22,25,26	1.23	2 (9%)	30,36,39	1.51	8 (26%)
68	4AC	S2	1337	68	21,24,25	0.38	0	28,34,37	0.57	0
68	PSU	S2	1174	68	18,21,22	1.11	1 (5%)	21,30,33	1.87	4 (19%)
3	PSU	L5	4299	3	18,21,22	1.07	1 (5%)	21,30,33	1.79	4 (19%)
3	A2M	L5	398	3	22,25,26	1.19	1 (4%)	30,36,39	1.58	6 (20%)
3	PSU	L5	4442	3	18,21,22	1.09	1 (5%)	21,30,33	1.94	5 (23%)
3	OMG	L5	3792	3	23,26,27	0.50	0	32,38,41	0.50	0
3	PSU	L5	2632	3	18,21,22	1.08	1 (5%)	21,30,33	1.92	5 (23%)
3	PSU	L5	4500	3	18,21,22	1.10	1 (5%)	21,30,33	1.99	5 (23%)
3	OMU	L5	3925	3	19,22,23	3.28	7 (36%)	25,31,34	1.80	5 (20%)
3	PSU	L5	1860	3	18,21,22	1.12	1 (5%)	21,30,33	1.86	4 (19%)
3	OMU	L5	4306	3	19,22,23	3.28	7 (36%)	25,31,34	1.70	4 (16%)
68	A2M	S2	576	68	22,25,26	1.22	2 (9%)	30,36,39	1.51	4 (13%)
68	OMG	S2	509	68	23,26,27	0.47	0	32,38,41	0.50	0
3	PSU	L5	4296	3	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
68	PSU	S2	966	68,87	18,21,22	1.12	1 (5%)	21,30,33	1.90	5 (23%)
3	PSU	L5	4493	3	18,21,22	1.06	1 (5%)	21,30,33	1.79	3 (14%)
68	PSU	S2	1232	68	18,21,22	1.11	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L5	1781	3	18,21,22	1.08	1 (5%)	21,30,33	1.81	4 (19%)
68	OMC	S2	1391	68	19,22,23	0.51	0	25,31,34	0.65	0
3	OMG	L5	3744	3	23,26,27	0.50	0	32,38,41	0.50	0
68	PSU	S2	801	68	18,21,22	1.15	1 (5%)	21,30,33	1.78	4 (19%)
3	OMC	L5	3701	3	19,22,23	0.55	0	25,31,34	0.59	0
68	PSU	S2	1056	68	18,21,22	1.11	1 (5%)	21,30,33	1.87	5 (23%)
68	PSU	S2	681	68	18,21,22	1.07	1 (5%)	21,30,33	1.87	4 (19%)
3	PSU	L5	4972	3	18,21,22	1.09	1 (5%)	21,30,33	1.84	4 (19%)
3	A2M	L5	4571	3	22,25,26	1.28	2 (9%)	30,36,39	1.57	7 (23%)
68	OMC	S2	462	68	19,22,23	0.53	0	25,31,34	0.74	0
68	OMG	S2	867	68	23,26,27	0.47	0	32,38,41	0.45	0
5	PSU	L8	69	5	18,21,22	1.11	1 (5%)	21,30,33	1.90	5 (23%)
3	PSU	L5	1862	3	18,21,22	1.07	1 (5%)	21,30,33	1.91	4 (19%)
68	OMG	S2	1490	68	23,26,27	0.47	0	32,38,41	0.46	0
68	PSU	S2	866	68	18,21,22	1.12	1 (5%)	21,30,33	1.89	4 (19%)
68	A2M	S2	166	68	22,25,26	1.25	1 (4%)	30,36,39	1.60	7 (23%)
3	5MC	L5	4447	3	19,22,23	0.74	0	26,32,35	0.65	0
68	OMC	S2	517	68	19,22,23	0.54	0	25,31,34	0.78	1 (4%)
3	OMC	L5	2824	3	19,22,23	0.57	0	25,31,34	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4312	3	18,21,22	1.08	1 (5%)	21,30,33	1.85	4 (19%)
68	PSU	S2	814	68	18,21,22	1.12	1 (5%)	21,30,33	1.86	4 (19%)
3	OMC	L5	3887	3	19,22,23	0.55	0	25,31,34	0.68	0
3	1MA	L5	1322	87,3	21,25,26	0.55	0	30,37,40	0.78	1 (3%)
3	OMC	L5	2422	87,3	19,22,23	0.58	0	25,31,34	0.73	1 (4%)
68	A2M	S2	27	68	22,25,26	1.23	1 (4%)	30,36,39	1.51	7 (23%)
3	UR3	L5	4530	3	19,22,23	2.73	7 (36%)	26,32,35	1.59	3 (11%)
3	OMG	L5	1316	3	23,26,27	0.56	0	32,38,41	0.59	0
68	OMU	S2	428	68	19,22,23	3.38	7 (36%)	25,31,34	1.82	5 (20%)
3	PSU	L5	1677	3	18,21,22	1.15	1 (5%)	21,30,33	1.95	6 (28%)
3	6MZ	L5	4220	3	22,25,26	2.97	5 (22%)	29,36,39	2.34	10 (34%)
3	PSU	L5	4361	3	18,21,22	1.05	1 (5%)	21,30,33	1.81	4 (19%)
3	OMC	L5	4536	3	19,22,23	0.56	0	25,31,34	0.64	0
3	A2M	L5	4590	3	22,25,26	1.17	1 (4%)	30,36,39	1.55	6 (20%)
68	MA6	S2	1850	68	23,26,27	1.27	2 (8%)	33,38,41	3.28	12 (36%)
3	PSU	L5	4628	3	18,21,22	1.03	1 (5%)	21,30,33	1.82	4 (19%)
3	PSU	L5	3884	3	18,21,22	1.10	2 (11%)	21,30,33	1.88	4 (19%)
3	OMG	L5	3899	3	23,26,27	0.54	0	32,38,41	0.50	0
68	PSU	S2	406	68	18,21,22	1.12	1 (5%)	21,30,33	1.88	4 (19%)
5	PSU	L8	55	5	18,21,22	1.09	1 (5%)	21,30,33	1.84	4 (19%)
3	PSU	L5	1582	3	18,21,22	1.11	1 (5%)	21,30,33	1.84	4 (19%)
68	OMU	S2	1326	68	19,22,23	3.36	7 (36%)	25,31,34	1.84	5 (20%)
3	PSU	L5	1792	3	18,21,22	1.05	1 (5%)	21,30,33	1.82	4 (19%)
3	A2M	L5	3825	3	22,25,26	1.20	1 (4%)	30,36,39	1.56	7 (23%)
3	A2M	L5	1524	3	22,25,26	1.27	2 (9%)	30,36,39	1.52	6 (20%)

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
5	OMG	L8	75	5	-	2/9/27/28	0/3/3/3
3	A2M	L5	2787	3	-	5/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
68	OMU	S2	627	68	-	2/9/27/28	0/2/2/2
68	PSU	S2	105	68	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	2364	87,3	-	3/9/27/28	0/3/3/3
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	668	68,87	-	2/9/27/28	0/3/3/3
68	OMC	S2	1703	68	-	2/9/27/28	0/2/2/2
68	A2M	S2	159	68	-	1/9/27/28	0/3/3/3
3	PSU	L5	1744	87,3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	109	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	1081	68	-	1/7/25/26	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1244	68	-	1/7/25/26	0/2/2/2
68	A2M	S2	1383	68	-	3/9/27/28	0/3/3/3
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	1288	68	-	0/9/27/28	0/2/2/2
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
68	OMC	S2	1272	68	-	0/9/27/28	0/2/2/2
68	OMU	S2	116	68	-	0/9/27/28	0/2/2/2
68	PSU	S2	1177	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	649	68	-	0/7/25/26	0/2/2/2
68	6MZ	S2	1832	68,87	-	2/9/27/28	0/3/3/3
3	A2M	L5	1871	87,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	3782	87,3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
68	MA6	S2	1851	68	-	1/11/29/30	0/3/3/3
68	OMU	S2	354	68	-	0/9/27/28	0/2/2/2
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
68	4AC	S2	1842	68	-	0/11/29/30	0/2/2/2
3	OMG	L5	4228	3	-	2/9/27/28	0/3/3/3
3	UY1	L5	3818	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	3920	87,3	-	0/7/25/26	0/2/2/2
68	A2M	S2	99	68,87	-	3/9/27/28	0/3/3/3
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	4370	3	-	1/9/27/28	0/3/3/3
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	1625	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	651	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	0/7/25/26	0/2/2/2
68	B8N	S2	1248	68	-	3/16/34/35	0/2/2/2
68	PSU	S2	1045	68	-	2/7/25/26	0/2/2/2
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
68	OMC	S2	174	68	-	0/9/27/28	0/2/2/2
3	A2M	L5	4523	87,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
68	OMG	S2	644	68	-	4/9/27/28	0/3/3/3
68	OMG	S2	1328	68	-	1/9/27/28	0/3/3/3
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	1046	68	-	1/7/25/26	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	OMG	L5	4618	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	2839	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4673	87,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1323	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	4196	3	-	1/9/27/28	0/3/3/3
68	G7M	S2	1639	68,84	-	1/7/25/26	0/3/3/3
68	PSU	S2	863	68	-	0/7/25/26	0/2/2/2
3	A2M	L5	3785	87,3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
3	OMC	L5	2365	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3853	87,3	-	0/7/25/26	0/2/2/2
68	OMU	S2	799	68	-	2/9/27/28	0/2/2/2
68	A2M	S2	1031	68	-	1/9/27/28	0/3/3/3
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
68	OMU	S2	121	68	-	0/9/27/28	0/2/2/2
68	OMU	S2	1442	68	-	2/9/27/28	0/2/2/2
68	PSU	S2	1367	68	-	0/7/25/26	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	2363	87,3	-	0/9/27/28	0/3/3/3
68	PSU	S2	1004	68	-	0/7/25/26	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	A2M	S2	484	68	-	0/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	4/9/27/28	0/3/3/3
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2815	3	-	2/9/27/28	0/3/3/3
68	OMG	S2	601	68	-	0/9/27/28	0/3/3/3
68	OMG	S2	436	68	-	0/9/27/28	0/3/3/3
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	686	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	93	68	-	2/7/25/26	0/2/2/2
3	A2M	L5	1534	87,3	-	1/9/27/28	0/3/3/3
68	A2M	S2	468	68	-	1/9/27/28	0/3/3/3
68	OMU	S2	172	68	-	2/9/27/28	0/2/2/2
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	2351	87,3	-	1/9/27/28	0/2/2/2
3	A2M	L5	2401	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4636	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4521	87,3	-	0/7/25/26	0/2/2/2
68	OMG	S2	683	68	-	0/9/27/28	0/3/3/3
3	A2M	L5	3867	3	-	3/9/27/28	0/3/3/3
68	4AC	S2	1337	68	-	0/11/29/30	0/2/2/2
68	PSU	S2	1174	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4500	3	-	5/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
68	A2M	S2	576	68	-	3/9/27/28	0/3/3/3
68	OMG	S2	509	68	-	0/9/27/28	0/3/3/3
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	966	68,87	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1232	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	0/7/25/26	0/2/2/2
68	OMC	S2	1391	68	-	0/9/27/28	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
68	PSU	S2	801	68	-	2/7/25/26	0/2/2/2
3	OMC	L5	3701	3	-	6/9/27/28	0/2/2/2
68	PSU	S2	1056	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	681	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
68	OMC	S2	462	68	-	0/9/27/28	0/2/2/2
68	OMG	S2	867	68	-	1/9/27/28	0/3/3/3
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
68	OMG	S2	1490	68	-	1/9/27/28	0/3/3/3
68	PSU	S2	866	68	-	0/7/25/26	0/2/2/2
68	A2M	S2	166	68	-	1/9/27/28	0/3/3/3
3	5MC	L5	4447	3	-	3/7/25/26	0/2/2/2
68	OMC	S2	517	68	-	0/9/27/28	0/2/2/2
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	814	68	-	0/7/25/26	0/2/2/2
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
3	1MA	L5	1322	87,3	-	2/7/25/26	0/3/3/3
3	OMC	L5	2422	87,3	-	2/9/27/28	0/2/2/2
68	A2M	S2	27	68	-	1/9/27/28	0/3/3/3
3	UR3	L5	4530	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	-	2/9/27/28	0/2/2/2
3	PSU	L5	1677	3	-	1/7/25/26	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
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	4590	3	-	4/9/27/28	0/3/3/3
68	MA6	S2	1850	68	-	0/11/29/30	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	2/9/27/28	0/3/3/3
68	PSU	S2	406	68	-	0/7/25/26	0/2/2/2
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	1326	68	-	0/9/27/28	0/2/2/2
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	3/9/27/28	0/3/3/3

All (268) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	C6-C5	12.74	1.49	1.35
68	S2	1832	6MZ	C6-N6	12.71	1.48	1.34
3	L5	4220	6MZ	C6-N6	12.17	1.48	1.34
3	L5	3818	UY1	C2-N1	11.67	1.51	1.36
68	S2	799	OMU	C2-N1	8.98	1.52	1.38
68	S2	1288	OMU	C2-N1	8.46	1.51	1.38
68	S2	1442	OMU	C2-N1	8.41	1.51	1.38
68	S2	428	OMU	C2-N1	8.29	1.51	1.38
3	L5	2837	OMU	C2-N1	8.23	1.51	1.38
68	S2	627	OMU	C2-N1	8.21	1.51	1.38
3	L5	4227	OMU	C2-N1	8.20	1.51	1.38
68	S2	121	OMU	C2-N1	8.20	1.51	1.38
68	S2	172	OMU	C2-N1	8.18	1.51	1.38
68	S2	116	OMU	C2-N1	8.15	1.51	1.38
68	S2	1326	OMU	C2-N1	8.15	1.51	1.38
68	S2	354	OMU	C2-N1	8.12	1.51	1.38
3	L5	4498	OMU	C2-N1	8.06	1.51	1.38
3	L5	4306	OMU	C2-N1	8.03	1.51	1.38
3	L5	3925	OMU	C2-N1	8.00	1.51	1.38
68	S2	1248	B8N	C6-N1	7.93	1.55	1.36
3	L5	3818	UY1	C2-N3	7.92	1.50	1.37
3	L5	4620	OMU	C2-N1	7.86	1.50	1.38
68	S2	1248	B8N	C4-N3	-7.73	1.26	1.40
68	S2	1248	B8N	C4-C5	7.10	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	1442	OMU	C2-N3	7.01	1.50	1.38
68	S2	172	OMU	C2-N3	7.00	1.50	1.38
68	S2	799	OMU	C2-N3	6.99	1.50	1.38
68	S2	1288	OMU	C2-N3	6.96	1.50	1.38
68	S2	1326	OMU	C2-N3	6.95	1.50	1.38
68	S2	428	OMU	C2-N3	6.94	1.50	1.38
68	S2	116	OMU	C2-N3	6.89	1.50	1.38
68	S2	627	OMU	C2-N3	6.88	1.50	1.38
3	L5	2837	OMU	C2-N3	6.86	1.49	1.38
3	L5	4498	OMU	C2-N3	6.83	1.49	1.38
68	S2	121	OMU	C2-N3	6.83	1.49	1.38
68	S2	354	OMU	C2-N3	6.81	1.49	1.38
3	L5	4227	OMU	C2-N3	6.73	1.49	1.38
3	L5	4306	OMU	C2-N3	6.72	1.49	1.38
68	S2	1639	G7M	C4-N3	6.71	1.49	1.34
3	L5	3925	OMU	C2-N3	6.69	1.49	1.38
3	L5	4620	OMU	C2-N3	6.61	1.49	1.38
3	L5	4530	UR3	C2-N1	6.43	1.47	1.38
3	L5	4530	UR3	C6-C5	6.25	1.49	1.35
68	S2	1248	B8N	C2-N1	5.96	1.56	1.39
68	S2	1288	OMU	C6-C5	5.90	1.48	1.35
68	S2	799	OMU	C6-C5	5.87	1.48	1.35
68	S2	627	OMU	C6-C5	5.87	1.48	1.35
68	S2	121	OMU	C6-C5	5.86	1.48	1.35
68	S2	428	OMU	C6-C5	5.85	1.48	1.35
68	S2	1442	OMU	C6-C5	5.84	1.48	1.35
68	S2	172	OMU	C6-C5	5.83	1.48	1.35
68	S2	1326	OMU	C6-C5	5.82	1.48	1.35
68	S2	116	OMU	C6-C5	5.82	1.48	1.35
68	S2	354	OMU	C6-C5	5.80	1.48	1.35
3	L5	4227	OMU	C6-C5	5.80	1.48	1.35
3	L5	4498	OMU	C6-C5	5.80	1.48	1.35
3	L5	2837	OMU	C6-C5	5.79	1.48	1.35
3	L5	4530	UR3	C2-N3	5.79	1.50	1.39
3	L5	3925	OMU	C6-C5	5.77	1.48	1.35
3	L5	4620	OMU	C6-C5	5.70	1.48	1.35
3	L5	4306	OMU	C6-C5	5.70	1.48	1.35
3	L5	4620	OMU	O4-C4	-5.56	1.13	1.24
68	S2	1326	OMU	O4-C4	-5.50	1.13	1.24
3	L5	4306	OMU	O4-C4	-5.50	1.13	1.24
3	L5	2837	OMU	O4-C4	-5.50	1.13	1.24
68	S2	799	OMU	O4-C4	-5.48	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3925	OMU	O4-C4	-5.48	1.13	1.24
68	S2	1248	B8N	C6-C5	5.47	1.42	1.35
68	S2	1639	G7M	C2-N3	5.47	1.46	1.33
68	S2	354	OMU	O4-C4	-5.46	1.13	1.24
3	L5	4227	OMU	O4-C4	-5.46	1.13	1.24
3	L5	4498	OMU	O4-C4	-5.46	1.13	1.24
68	S2	428	OMU	O4-C4	-5.46	1.13	1.24
68	S2	627	OMU	O4-C4	-5.43	1.13	1.24
68	S2	172	OMU	O4-C4	-5.42	1.13	1.24
68	S2	1288	OMU	O4-C4	-5.40	1.14	1.24
68	S2	116	OMU	O4-C4	-5.40	1.14	1.24
68	S2	1442	OMU	O4-C4	-5.39	1.14	1.24
68	S2	121	OMU	O4-C4	-5.38	1.14	1.24
3	L5	3818	UY1	C6-N1	5.32	1.45	1.36
68	S2	1639	G7M	C2-N2	4.95	1.45	1.34
68	S2	1639	G7M	C5-N7	-4.60	1.33	1.39
3	L5	3818	UY1	C4-N3	4.54	1.47	1.38
68	S2	627	OMU	C4-N3	4.47	1.46	1.38
68	S2	428	OMU	C4-N3	4.45	1.46	1.38
68	S2	1442	OMU	C4-N3	4.42	1.46	1.38
68	S2	799	OMU	C4-N3	4.39	1.46	1.38
68	S2	1288	OMU	C4-N3	4.38	1.46	1.38
68	S2	1326	OMU	C4-N3	4.38	1.46	1.38
68	S2	116	OMU	C4-N3	4.34	1.46	1.38
68	S2	172	OMU	C4-N3	4.32	1.46	1.38
68	S2	354	OMU	C4-N3	4.29	1.46	1.38
3	L5	4227	OMU	C4-N3	4.26	1.45	1.38
68	S2	121	OMU	C4-N3	4.26	1.45	1.38
3	L5	2837	OMU	C4-N3	4.25	1.45	1.38
3	L5	4498	OMU	C4-N3	4.23	1.45	1.38
3	L5	4306	OMU	C4-N3	4.09	1.45	1.38
3	L5	3925	OMU	C4-N3	4.06	1.45	1.38
3	L5	4620	OMU	C4-N3	4.04	1.45	1.38
68	S2	1639	G7M	C5-C6	3.86	1.54	1.43
68	S2	801	PSU	C6-C5	3.80	1.39	1.35
68	S2	1004	PSU	C6-C5	3.77	1.39	1.35
68	S2	1248	B8N	C1'-C5	3.76	1.58	1.50
68	S2	649	PSU	C6-C5	3.74	1.39	1.35
68	S2	966	PSU	C6-C5	3.72	1.39	1.35
68	S2	814	PSU	C6-C5	3.72	1.39	1.35
68	S2	651	PSU	C6-C5	3.72	1.39	1.35
68	S2	1244	PSU	C6-C5	3.71	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	866	PSU	C6-C5	3.71	1.39	1.35
3	L5	5010	PSU	C6-C5	3.70	1.39	1.35
3	L5	1677	PSU	C6-C5	3.67	1.39	1.35
68	S2	863	PSU	C6-C5	3.67	1.39	1.35
3	L5	1683	PSU	C6-C5	3.65	1.39	1.35
68	S2	686	PSU	C6-C5	3.64	1.39	1.35
68	S2	109	PSU	C6-C5	3.63	1.39	1.35
3	L5	1860	PSU	C6-C5	3.63	1.39	1.35
68	S2	1232	PSU	C6-C5	3.62	1.39	1.35
68	S2	105	PSU	C6-C5	3.60	1.39	1.35
3	L5	4552	PSU	C6-C5	3.60	1.39	1.35
3	L5	3818	UY1	O4-C4	-3.60	1.16	1.23
68	S2	1045	PSU	C6-C5	3.60	1.39	1.35
68	S2	1174	PSU	C6-C5	3.59	1.39	1.35
68	S2	1367	PSU	C6-C5	3.59	1.39	1.35
68	S2	1056	PSU	C6-C5	3.57	1.39	1.35
3	L5	1744	PSU	C6-C5	3.57	1.39	1.35
5	L8	55	PSU	C6-C5	3.56	1.39	1.35
5	L8	69	PSU	C6-C5	3.56	1.39	1.35
68	S2	406	PSU	C6-C5	3.56	1.39	1.35
3	L5	4576	PSU	C6-C5	3.54	1.39	1.35
68	S2	1046	PSU	C6-C5	3.54	1.39	1.35
3	L5	1781	PSU	C6-C5	3.54	1.39	1.35
3	L5	3844	PSU	C6-C5	3.53	1.39	1.35
3	L5	4312	PSU	C6-C5	3.52	1.39	1.35
3	L5	4471	PSU	C6-C5	3.52	1.39	1.35
3	L5	3695	PSU	C6-C5	3.51	1.39	1.35
3	L5	1582	PSU	C6-C5	3.51	1.39	1.35
3	L5	4431	PSU	C6-C5	3.50	1.39	1.35
3	L5	4972	PSU	C6-C5	3.49	1.39	1.35
3	L5	2632	PSU	C6-C5	3.49	1.39	1.35
3	L5	4673	PSU	C6-C5	3.49	1.39	1.35
3	L5	1862	PSU	C6-C5	3.49	1.39	1.35
68	S2	1177	PSU	C6-C5	3.49	1.39	1.35
3	L5	4296	PSU	C6-C5	3.48	1.39	1.35
3	L5	3853	PSU	C6-C5	3.48	1.39	1.35
3	L5	5001	PSU	C6-C5	3.48	1.39	1.35
3	L5	4353	PSU	C6-C5	3.48	1.39	1.35
3	L5	4493	PSU	C6-C5	3.47	1.39	1.35
3	L5	4532	PSU	C6-C5	3.47	1.39	1.35
68	S2	1081	PSU	C6-C5	3.46	1.39	1.35
3	L5	3851	PSU	C6-C5	3.46	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4293	PSU	C6-C5	3.46	1.39	1.35
3	L5	4299	PSU	C6-C5	3.45	1.39	1.35
3	L5	400	A2M	O5'-C5'	-3.44	1.34	1.44
3	L5	3637	PSU	C6-C5	3.44	1.39	1.35
68	S2	576	A2M	O5'-C5'	-3.44	1.34	1.44
3	L5	4442	PSU	C6-C5	3.44	1.39	1.35
68	S2	668	A2M	O5'-C5'	-3.43	1.34	1.44
3	L5	3884	PSU	C6-C5	3.43	1.39	1.35
3	L5	4521	PSU	C6-C5	3.42	1.39	1.35
3	L5	3822	PSU	C6-C5	3.42	1.39	1.35
3	L5	1782	PSU	C6-C5	3.42	1.39	1.35
3	L5	4973	PSU	C6-C5	3.41	1.39	1.35
68	S2	93	PSU	C6-C5	3.41	1.39	1.35
3	L5	1524	A2M	O5'-C5'	-3.40	1.34	1.44
3	L5	3830	A2M	O5'-C5'	-3.40	1.34	1.44
3	L5	1536	PSU	C6-C5	3.39	1.39	1.35
3	L5	1792	PSU	C6-C5	3.39	1.39	1.35
3	L5	3920	PSU	C6-C5	3.38	1.39	1.35
68	S2	681	PSU	C6-C5	3.38	1.39	1.35
3	L5	4361	PSU	C6-C5	3.38	1.39	1.35
3	L5	1871	A2M	O5'-C5'	-3.37	1.34	1.44
3	L5	4500	PSU	C6-C5	3.37	1.39	1.35
3	L5	1323	A2M	O5'-C5'	-3.36	1.34	1.44
3	L5	3639	PSU	C6-C5	3.36	1.39	1.35
3	L5	4220	6MZ	C5-N7	-3.36	1.33	1.39
3	L5	3825	A2M	O5'-C5'	-3.36	1.34	1.44
3	L5	2401	A2M	O5'-C5'	-3.35	1.34	1.44
3	L5	2815	A2M	O5'-C5'	-3.35	1.34	1.44
68	S2	27	A2M	O5'-C5'	-3.34	1.34	1.44
3	L5	2787	A2M	O5'-C5'	-3.34	1.34	1.44
3	L5	4689	PSU	C6-C5	3.34	1.39	1.35
68	S2	468	A2M	O5'-C5'	-3.32	1.34	1.44
3	L5	4571	A2M	O5'-C5'	-3.32	1.34	1.44
3	L5	4636	PSU	C6-C5	3.31	1.39	1.35
3	L5	2363	A2M	O5'-C5'	-3.31	1.34	1.44
68	S2	99	A2M	O5'-C5'	-3.29	1.34	1.44
3	L5	3785	A2M	O5'-C5'	-3.29	1.34	1.44
3	L5	4403	PSU	C6-C5	3.28	1.38	1.35
3	L5	3718	A2M	O5'-C5'	-3.28	1.34	1.44
3	L5	3867	A2M	O5'-C5'	-3.27	1.34	1.44
68	S2	1383	A2M	O5'-C5'	-3.26	1.34	1.44
3	L5	2839	PSU	C6-C5	3.25	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	166	A2M	O5'-C5'	-3.24	1.34	1.44
68	S2	1031	A2M	O5'-C5'	-3.24	1.34	1.44
3	L5	4523	A2M	O5'-C5'	-3.23	1.34	1.44
3	L5	4457	PSU	C6-C5	3.23	1.38	1.35
68	S2	484	A2M	O5'-C5'	-3.22	1.34	1.44
3	L5	3818	UY1	O2-C2	-3.22	1.16	1.23
3	L5	398	A2M	O5'-C5'	-3.22	1.34	1.44
3	L5	1326	A2M	O5'-C5'	-3.21	1.34	1.44
3	L5	4579	PSU	C6-C5	3.21	1.38	1.35
3	L5	4220	6MZ	C5-C4	-3.20	1.33	1.39
68	S2	1850	MA6	C6-N6	3.19	1.45	1.36
68	S2	1851	MA6	C6-N6	3.16	1.45	1.36
3	L5	4628	PSU	C6-C5	3.16	1.38	1.35
3	L5	4590	A2M	O5'-C5'	-3.15	1.35	1.44
3	L5	1534	A2M	O5'-C5'	-3.13	1.35	1.44
3	L5	3818	UY1	C1'-C5	3.11	1.57	1.50
68	S2	1832	6MZ	C5-N7	-3.06	1.33	1.39
68	S2	159	A2M	O5'-C5'	-3.01	1.35	1.44
68	S2	627	OMU	C5-C4	2.91	1.50	1.43
3	L5	4220	6MZ	C8-N9	-2.87	1.32	1.37
68	S2	1832	6MZ	C5-C4	-2.87	1.34	1.39
68	S2	1442	OMU	C5-C4	2.84	1.49	1.43
68	S2	1288	OMU	C5-C4	2.82	1.49	1.43
68	S2	1639	G7M	C2-N1	2.82	1.44	1.37
68	S2	1326	OMU	C5-C4	2.80	1.49	1.43
68	S2	428	OMU	C5-C4	2.80	1.49	1.43
3	L5	4498	OMU	C5-C4	2.80	1.49	1.43
68	S2	1288	OMU	C6-N1	2.79	1.44	1.38
68	S2	799	OMU	C5-C4	2.79	1.49	1.43
68	S2	121	OMU	C5-C4	2.78	1.49	1.43
68	S2	116	OMU	C5-C4	2.78	1.49	1.43
68	S2	799	OMU	C6-N1	2.77	1.44	1.38
3	L5	4227	OMU	C5-C4	2.76	1.49	1.43
68	S2	354	OMU	C5-C4	2.76	1.49	1.43
68	S2	1832	6MZ	C8-N9	-2.72	1.32	1.37
68	S2	172	OMU	C5-C4	2.71	1.49	1.43
68	S2	1442	OMU	C6-N1	2.70	1.44	1.38
3	L5	2837	OMU	C5-C4	2.69	1.49	1.43
68	S2	121	OMU	C6-N1	2.69	1.44	1.38
68	S2	354	OMU	C6-N1	2.67	1.44	1.38
3	L5	3925	OMU	C5-C4	2.66	1.49	1.43
68	S2	428	OMU	C6-N1	2.65	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	627	OMU	C6-N1	2.65	1.44	1.38
68	S2	1326	OMU	C6-N1	2.64	1.44	1.38
68	S2	116	OMU	C6-N1	2.63	1.44	1.38
3	L5	4498	OMU	C6-N1	2.63	1.44	1.38
3	L5	4530	UR3	O2-C2	-2.62	1.17	1.22
3	L5	4306	OMU	C5-C4	2.62	1.49	1.43
3	L5	4306	OMU	C6-N1	2.59	1.44	1.38
3	L5	4620	OMU	C5-C4	2.59	1.49	1.43
3	L5	2837	OMU	C6-N1	2.58	1.44	1.38
3	L5	4620	OMU	C6-N1	2.56	1.44	1.38
3	L5	4227	OMU	C6-N1	2.55	1.44	1.38
3	L5	4530	UR3	C6-N1	2.54	1.44	1.38
3	L5	3925	OMU	C6-N1	2.54	1.44	1.38
68	S2	172	OMU	C6-N1	2.53	1.44	1.38
68	S2	1639	G7M	C6-N1	2.49	1.43	1.38
3	L5	1524	A2M	O4'-C4'	-2.48	1.39	1.45
68	S2	1639	G7M	O6-C6	-2.47	1.18	1.23
3	L5	1323	A2M	O4'-C4'	-2.42	1.39	1.45
68	S2	668	A2M	O4'-C4'	-2.42	1.39	1.45
3	L5	3818	UY1	O4'-C1'	-2.42	1.40	1.43
68	S2	1851	MA6	C5-C4	-2.40	1.34	1.39
68	S2	1850	MA6	C5-C4	-2.31	1.35	1.39
3	L5	4571	A2M	O4'-C4'	-2.30	1.39	1.45
3	L5	4530	UR3	C5-C4	2.28	1.49	1.43
3	L5	2363	A2M	O4'-C4'	-2.23	1.40	1.45
3	L5	4220	6MZ	C6-N1	-2.23	1.31	1.35
3	L5	4530	UR3	C3U-N3	2.19	1.50	1.47
3	L5	3818	UY1	C4-C5	2.10	1.50	1.44
68	S2	576	A2M	C5-C4	2.08	1.42	1.39
3	L5	3884	PSU	C4-C5	-2.08	1.38	1.44
3	L5	1326	A2M	O4'-C4'	-2.06	1.40	1.45
3	L5	3867	A2M	O4'-C4'	-2.06	1.40	1.45
68	S2	159	A2M	C5-C4	2.03	1.42	1.39
3	L5	4689	PSU	C4-C5	-2.00	1.38	1.44

All (668) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1851	MA6	N1-C6-N6	-12.04	102.18	116.86
68	S2	1850	MA6	N1-C6-N6	-11.32	103.06	116.86
68	S2	1851	MA6	C5-C6-N6	7.86	137.78	125.33
68	S2	1639	G7M	C1'-N9-C4	7.62	149.00	126.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1639	G7M	C1'-N9-C8	-7.49	101.45	126.74
68	S2	1850	MA6	C5-C6-N6	7.43	137.09	125.33
3	L5	4220	6MZ	N1-C2-N3	-5.78	119.83	128.58
3	L5	4498	OMU	C4-N3-C2	-5.78	119.44	126.61
68	S2	1851	MA6	N1-C2-N3	-5.78	119.84	128.58
68	S2	627	OMU	C4-N3-C2	-5.74	119.48	126.61
3	L5	4227	OMU	C4-N3-C2	-5.73	119.50	126.61
68	S2	1832	6MZ	N1-C2-N3	-5.68	119.98	128.58
68	S2	428	OMU	C4-N3-C2	-5.64	119.61	126.61
68	S2	1326	OMU	C4-N3-C2	-5.64	119.61	126.61
3	L5	2837	OMU	C4-N3-C2	-5.62	119.64	126.61
68	S2	1442	OMU	C4-N3-C2	-5.57	119.70	126.61
3	L5	3925	OMU	C4-N3-C2	-5.53	119.75	126.61
3	L5	4530	UR3	C4-N3-C2	-5.50	120.15	124.58
68	S2	1850	MA6	N1-C2-N3	-5.44	120.34	128.58
68	S2	172	OMU	C4-N3-C2	-5.43	119.87	126.61
68	S2	354	OMU	C4-N3-C2	-5.37	119.94	126.61
68	S2	1851	MA6	N9-C8-N7	-5.37	106.32	113.94
3	L5	3637	PSU	N1-C2-N3	5.28	120.73	115.17
68	S2	1248	B8N	C5-C4-N3	5.27	125.72	116.15
68	S2	799	OMU	C4-N3-C2	-5.23	120.12	126.61
68	S2	121	OMU	C4-N3-C2	-5.23	120.12	126.61
68	S2	1850	MA6	N9-C8-N7	-5.19	106.57	113.94
3	L5	4306	OMU	C4-N3-C2	-5.10	120.28	126.61
3	L5	4620	OMU	C4-N3-C2	-5.09	120.30	126.61
3	L5	4636	PSU	C4-N3-C2	-5.04	119.42	126.37
3	L5	4636	PSU	N1-C2-N3	5.03	120.48	115.17
68	S2	116	OMU	C4-N3-C2	-5.01	120.39	126.61
3	L5	4293	PSU	C4-N3-C2	-5.01	119.47	126.37
3	L5	4293	PSU	N1-C2-N3	5.01	120.45	115.17
3	L5	4353	PSU	N1-C2-N3	4.97	120.41	115.17
68	S2	105	PSU	N1-C2-N3	4.95	120.39	115.17
3	L5	4532	PSU	N1-C2-N3	4.94	120.38	115.17
3	L5	4500	PSU	C4-N3-C2	-4.94	119.57	126.37
3	L5	4521	PSU	N1-C2-N3	4.93	120.37	115.17
3	L5	1582	PSU	C4-N3-C2	-4.93	119.58	126.37
3	L5	4457	PSU	C4-N3-C2	-4.93	119.59	126.37
3	L5	4353	PSU	C4-N3-C2	-4.92	119.59	126.37
3	L5	4457	PSU	N1-C2-N3	4.91	120.35	115.17
3	L5	1677	PSU	C4-N3-C2	-4.90	119.63	126.37
3	L5	4973	PSU	C4-N3-C2	-4.90	119.63	126.37
3	L5	5001	PSU	N1-C2-N3	4.89	120.33	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4500	PSU	N1-C2-N3	4.89	120.32	115.17
68	S2	1081	PSU	C4-N3-C2	-4.89	119.64	126.37
68	S2	1177	PSU	C4-N3-C2	-4.88	119.65	126.37
3	L5	3920	PSU	N1-C2-N3	4.86	120.29	115.17
3	L5	4442	PSU	N1-C2-N3	4.85	120.28	115.17
3	L5	1862	PSU	C4-N3-C2	-4.85	119.70	126.37
3	L5	4403	PSU	N1-C2-N3	4.84	120.28	115.17
3	L5	3637	PSU	C4-N3-C2	-4.84	119.70	126.37
68	S2	686	PSU	C4-N3-C2	-4.84	119.70	126.37
3	L5	4521	PSU	C4-N3-C2	-4.83	119.71	126.37
3	L5	4552	PSU	C4-N3-C2	-4.83	119.71	126.37
3	L5	4442	PSU	C4-N3-C2	-4.83	119.72	126.37
5	L8	69	PSU	N1-C2-N3	4.83	120.26	115.17
3	L5	1862	PSU	N1-C2-N3	4.82	120.25	115.17
68	S2	1177	PSU	N1-C2-N3	4.81	120.25	115.17
3	L5	2632	PSU	N1-C2-N3	4.81	120.24	115.17
3	L5	4973	PSU	N1-C2-N3	4.81	120.24	115.17
3	L5	4296	PSU	C4-N3-C2	-4.81	119.75	126.37
3	L5	4403	PSU	C4-N3-C2	-4.81	119.75	126.37
68	S2	1288	OMU	C4-N3-C2	-4.80	120.65	126.61
3	L5	3818	UY1	C4-N3-C2	-4.80	119.76	126.37
68	S2	866	PSU	C4-N3-C2	-4.79	119.77	126.37
68	S2	1367	PSU	N1-C2-N3	4.79	120.22	115.17
3	L5	4532	PSU	C4-N3-C2	-4.79	119.78	126.37
68	S2	1081	PSU	N1-C2-N3	4.78	120.21	115.17
68	S2	1244	PSU	N1-C2-N3	4.78	120.21	115.17
3	L5	1782	PSU	C4-N3-C2	-4.78	119.78	126.37
3	L5	1744	PSU	N1-C2-N3	4.78	120.21	115.17
3	L5	4552	PSU	N1-C2-N3	4.78	120.21	115.17
3	L5	3822	PSU	N1-C2-N3	4.78	120.21	115.17
68	S2	966	PSU	N1-C2-N3	4.78	120.21	115.17
68	S2	1832	6MZ	C5-C4-N3	-4.78	120.14	126.72
68	S2	109	PSU	C4-N3-C2	-4.78	119.79	126.37
68	S2	1174	PSU	C4-N3-C2	-4.77	119.79	126.37
68	S2	1244	PSU	C4-N3-C2	-4.77	119.80	126.37
3	L5	1677	PSU	N1-C2-N3	4.77	120.20	115.17
3	L5	4576	PSU	N1-C2-N3	4.77	120.20	115.17
68	S2	1232	PSU	C4-N3-C2	-4.77	119.81	126.37
3	L5	3920	PSU	C4-N3-C2	-4.76	119.81	126.37
68	S2	814	PSU	C4-N3-C2	-4.76	119.81	126.37
68	S2	1850	MA6	C5-C4-N3	-4.76	120.17	126.72
68	S2	1851	MA6	C5-C4-N3	-4.76	120.17	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1367	PSU	C4-N3-C2	-4.76	119.82	126.37
3	L5	3695	PSU	N1-C2-N3	4.75	120.18	115.17
3	L5	3695	PSU	C4-N3-C2	-4.75	119.83	126.37
68	S2	105	PSU	C4-N3-C2	-4.75	119.83	126.37
3	L5	1782	PSU	N1-C2-N3	4.75	120.18	115.17
3	L5	1683	PSU	N1-C2-N3	4.75	120.17	115.17
68	S2	681	PSU	C4-N3-C2	-4.74	119.84	126.37
68	S2	1832	6MZ	N9-C8-N7	-4.73	107.22	113.94
3	L5	4431	PSU	N1-C2-N3	4.73	120.16	115.17
3	L5	2632	PSU	C4-N3-C2	-4.73	119.86	126.37
3	L5	4471	PSU	N1-C2-N3	4.73	120.15	115.17
3	L5	4431	PSU	C4-N3-C2	-4.72	119.87	126.37
68	S2	686	PSU	N1-C2-N3	4.72	120.15	115.17
68	S2	93	PSU	C4-N3-C2	-4.72	119.87	126.37
3	L5	4296	PSU	N1-C2-N3	4.72	120.14	115.17
3	L5	1536	PSU	N1-C2-N3	4.71	120.14	115.17
3	L5	3884	PSU	N1-C2-N3	4.71	120.14	115.17
3	L5	1683	PSU	C4-N3-C2	-4.71	119.88	126.37
68	S2	651	PSU	N1-C2-N3	4.71	120.14	115.17
3	L5	3851	PSU	C4-N3-C2	-4.71	119.88	126.37
3	L5	1860	PSU	N1-C2-N3	4.71	120.14	115.17
3	L5	5001	PSU	C4-N3-C2	-4.71	119.89	126.37
68	S2	966	PSU	C4-N3-C2	-4.71	119.89	126.37
5	L8	69	PSU	C4-N3-C2	-4.70	119.89	126.37
68	S2	866	PSU	N1-C2-N3	4.70	120.13	115.17
68	S2	1232	PSU	N1-C2-N3	4.70	120.13	115.17
68	S2	814	PSU	N1-C2-N3	4.69	120.12	115.17
3	L5	3851	PSU	N1-C2-N3	4.69	120.11	115.17
3	L5	5010	PSU	C4-N3-C2	-4.69	119.92	126.37
68	S2	109	PSU	N1-C2-N3	4.69	120.11	115.17
68	S2	1056	PSU	N1-C2-N3	4.69	120.11	115.17
3	L5	4493	PSU	C4-N3-C2	-4.68	119.92	126.37
3	L5	1744	PSU	C4-N3-C2	-4.68	119.93	126.37
3	L5	4972	PSU	C4-N3-C2	-4.67	119.93	126.37
68	S2	406	PSU	N1-C2-N3	4.67	120.10	115.17
3	L5	3822	PSU	C4-N3-C2	-4.67	119.94	126.37
3	L5	4576	PSU	C4-N3-C2	-4.67	119.94	126.37
3	L5	4312	PSU	C4-N3-C2	-4.67	119.94	126.37
3	L5	4689	PSU	N1-C2-N3	4.67	120.09	115.17
3	L5	4673	PSU	N1-C2-N3	4.67	120.09	115.17
68	S2	681	PSU	N1-C2-N3	4.66	120.09	115.17
3	L5	1781	PSU	N1-C2-N3	4.66	120.08	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	5010	PSU	N1-C2-N3	4.66	120.08	115.17
68	S2	863	PSU	N1-C2-N3	4.66	120.08	115.17
3	L5	3639	PSU	N1-C2-N3	4.66	120.08	115.17
3	L5	3853	PSU	N1-C2-N3	4.65	120.08	115.17
3	L5	4471	PSU	C4-N3-C2	-4.65	119.96	126.37
68	S2	651	PSU	C4-N3-C2	-4.65	119.96	126.37
3	L5	4312	PSU	N1-C2-N3	4.65	120.07	115.17
3	L5	4220	6MZ	C9-N6-C6	-4.65	118.54	122.85
68	S2	1004	PSU	N1-C2-N3	4.64	120.06	115.17
68	S2	1045	PSU	N1-C2-N3	4.64	120.06	115.17
68	S2	1174	PSU	N1-C2-N3	4.64	120.06	115.17
3	L5	1792	PSU	C4-N3-C2	-4.64	119.98	126.37
68	S2	863	PSU	C4-N3-C2	-4.64	119.98	126.37
68	S2	1248	B8N	C4-N3-C2	-4.64	119.91	125.62
5	L8	55	PSU	N1-C2-N3	4.64	120.06	115.17
3	L5	1536	PSU	C4-N3-C2	-4.63	119.99	126.37
68	S2	1056	PSU	C4-N3-C2	-4.63	119.99	126.37
68	S2	1046	PSU	N1-C2-N3	4.63	120.05	115.17
3	L5	4220	6MZ	C5-C4-N3	-4.63	120.34	126.72
68	S2	801	PSU	N1-C2-N3	4.63	120.05	115.17
68	S2	1045	PSU	C4-N3-C2	-4.62	120.00	126.37
3	L5	4579	PSU	N1-C2-N3	4.62	120.04	115.17
3	L5	1582	PSU	N1-C2-N3	4.61	120.03	115.17
68	S2	649	PSU	N1-C2-N3	4.61	120.03	115.17
3	L5	3884	PSU	C4-N3-C2	-4.60	120.03	126.37
68	S2	406	PSU	C4-N3-C2	-4.60	120.03	126.37
68	S2	93	PSU	N1-C2-N3	4.60	120.02	115.17
3	L5	4361	PSU	C4-N3-C2	-4.59	120.04	126.37
3	L5	1792	PSU	N1-C2-N3	4.59	120.01	115.17
3	L5	4972	PSU	N1-C2-N3	4.59	120.01	115.17
3	L5	4673	PSU	C4-N3-C2	-4.59	120.05	126.37
68	S2	1004	PSU	C4-N3-C2	-4.58	120.06	126.37
3	L5	3844	PSU	N1-C2-N3	4.58	120.00	115.17
5	L8	55	PSU	C4-N3-C2	-4.58	120.06	126.37
3	L5	4579	PSU	C4-N3-C2	-4.58	120.07	126.37
3	L5	4628	PSU	N1-C2-N3	4.57	119.99	115.17
3	L5	4628	PSU	C4-N3-C2	-4.57	120.08	126.37
3	L5	4299	PSU	N1-C2-N3	4.56	119.98	115.17
3	L5	3853	PSU	C4-N3-C2	-4.56	120.09	126.37
3	L5	4361	PSU	N1-C2-N3	4.56	119.98	115.17
68	S2	1639	G7M	C2-N3-C4	4.56	120.15	112.30
3	L5	3639	PSU	C4-N3-C2	-4.55	120.11	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1860	PSU	C4-N3-C2	-4.51	120.16	126.37
3	L5	4220	6MZ	N9-C8-N7	-4.50	107.55	113.94
3	L5	1781	PSU	C4-N3-C2	-4.50	120.18	126.37
3	L5	4493	PSU	N1-C2-N3	4.49	119.91	115.17
3	L5	4299	PSU	C4-N3-C2	-4.48	120.19	126.37
68	S2	1046	PSU	C4-N3-C2	-4.48	120.20	126.37
3	L5	3818	UY1	N1-C2-N3	4.45	119.86	115.17
3	L5	2839	PSU	N1-C2-N3	4.43	119.84	115.17
68	S2	649	PSU	C4-N3-C2	-4.36	120.37	126.37
3	L5	3844	PSU	C4-N3-C2	-4.35	120.39	126.37
3	L5	2839	PSU	C4-N3-C2	-4.31	120.43	126.37
68	S2	801	PSU	C4-N3-C2	-4.23	120.55	126.37
3	L5	4689	PSU	C4-N3-C2	-4.18	120.62	126.37
68	S2	1639	G7M	C5-C4-N3	-4.09	120.42	128.15
68	S2	1851	MA6	C4-N9-C8	4.06	110.00	105.74
68	S2	1850	MA6	C4-N9-C8	4.05	110.00	105.74
3	L5	4498	OMU	N3-C2-N1	4.05	120.17	114.89
68	S2	1639	G7M	C5-C6-N1	3.99	120.10	111.84
3	L5	3830	A2M	C3'-C2'-C1'	-3.99	95.17	102.81
3	L5	1871	A2M	C3'-C2'-C1'	-3.94	95.26	102.81
3	L5	2837	OMU	N3-C2-N1	3.92	120.00	114.89
68	S2	1383	A2M	C3'-C2'-C1'	-3.92	95.29	102.81
3	L5	3925	OMU	N3-C2-N1	3.92	119.99	114.89
68	S2	1850	MA6	C4-C5-C6	3.91	119.95	115.91
3	L5	4227	OMU	N3-C2-N1	3.88	119.94	114.89
68	S2	354	OMU	N3-C2-N1	3.80	119.84	114.89
3	L5	4620	OMU	N3-C2-N1	3.77	119.81	114.89
68	S2	1326	OMU	N3-C2-N1	3.74	119.76	114.89
68	S2	1442	OMU	N3-C2-N1	3.74	119.76	114.89
68	S2	627	OMU	C5-C4-N3	3.73	120.02	114.80
68	S2	121	OMU	N3-C2-N1	3.72	119.74	114.89
68	S2	1326	OMU	C5-C4-N3	3.72	120.00	114.80
68	S2	428	OMU	N3-C2-N1	3.71	119.72	114.89
68	S2	627	OMU	N3-C2-N1	3.71	119.72	114.89
3	L5	3818	UY1	C6-C5-C4	3.70	120.67	118.17
68	S2	1442	OMU	C5-C4-N3	3.68	119.95	114.80
68	S2	428	OMU	C5-C4-N3	3.67	119.94	114.80
68	S2	799	OMU	N3-C2-N1	3.66	119.65	114.89
3	L5	4227	OMU	C5-C4-N3	3.66	119.92	114.80
3	L5	4498	OMU	C5-C4-N3	3.65	119.91	114.80
68	S2	172	OMU	N3-C2-N1	3.64	119.63	114.89
3	L5	4530	UR3	C5-C4-N3	3.62	119.81	115.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	398	A2M	C3'-C2'-C1'	-3.62	95.87	102.81
68	S2	1248	B8N	C1'-C5-C4	3.62	123.10	117.61
68	S2	1850	MA6	N3-C4-N9	3.61	133.31	127.17
68	S2	468	A2M	C3'-C2'-C1'	-3.60	95.90	102.81
3	L5	4306	OMU	N3-C2-N1	3.59	119.56	114.89
3	L5	398	A2M	O3'-C3'-C2'	3.58	121.22	111.19
3	L5	2837	OMU	C5-C4-N3	3.57	119.80	114.80
68	S2	1851	MA6	C4-C5-C6	3.57	119.60	115.91
68	S2	799	OMU	C5-C4-N3	3.57	119.80	114.80
68	S2	116	OMU	N3-C2-N1	3.56	119.53	114.89
3	L5	3825	A2M	C3'-C2'-C1'	-3.56	95.99	102.81
3	L5	3925	OMU	C5-C4-N3	3.55	119.78	114.80
68	S2	354	OMU	C5-C4-N3	3.54	119.76	114.80
3	L5	4571	A2M	O3'-C3'-C2'	3.53	121.06	111.19
68	S2	576	A2M	O3'-C3'-C2'	3.51	121.02	111.19
68	S2	1383	A2M	O3'-C3'-C2'	3.51	121.01	111.19
68	S2	166	A2M	O3'-C3'-C2'	3.50	120.97	111.19
68	S2	1851	MA6	N3-C4-N9	3.47	133.08	127.17
68	S2	1851	MA6	C2-N1-C6	3.46	120.28	111.83
68	S2	1832	6MZ	C2-N3-C4	3.46	120.27	111.83
3	L5	4523	A2M	C3'-C2'-C1'	-3.45	96.20	102.81
68	S2	1639	G7M	CN7-N7-C5	3.44	131.09	126.80
3	L5	2787	A2M	O3'-C3'-C2'	3.44	120.81	111.19
68	S2	121	OMU	C5-C4-N3	3.44	119.61	114.80
68	S2	1248	B8N	N3-C2-N1	3.43	120.91	116.72
68	S2	166	A2M	C3'-C2'-C1'	-3.40	96.29	102.81
68	S2	1288	OMU	N3-C2-N1	3.40	119.32	114.89
3	L5	4689	PSU	C6-N1-C2	-3.40	119.54	122.69
68	S2	172	OMU	C5-C4-N3	3.39	119.55	114.80
68	S2	99	A2M	C3'-C2'-C1'	-3.39	96.32	102.81
68	S2	1851	MA6	C2-N3-C4	3.38	120.08	111.83
68	S2	799	OMU	C1'-N1-C2	3.38	123.66	117.59
3	L5	4620	OMU	C5-C4-N3	3.38	119.53	114.80
68	S2	116	OMU	C5-C4-N3	3.37	119.53	114.80
3	L5	4220	6MZ	C2-N3-C4	3.37	120.06	111.83
68	S2	1850	MA6	C2-N1-C6	3.37	120.06	111.83
68	S2	1639	G7M	O6-C6-C5	-3.35	120.53	128.01
3	L5	1323	A2M	C2'-C1'-N9	3.33	119.24	113.75
3	L5	4306	OMU	C5-C4-N3	3.32	119.45	114.80
68	S2	576	A2M	C3'-C2'-C1'	-3.31	96.47	102.81
3	L5	3830	A2M	O3'-C3'-C2'	3.30	120.42	111.19
68	S2	1288	OMU	C5-C4-N3	3.29	119.41	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1639	G7M	N9-C4-N3	3.29	132.53	125.95
3	L5	4590	A2M	C3'-C2'-C1'	-3.25	96.59	102.81
68	S2	1031	A2M	C3'-C2'-C1'	-3.24	96.61	102.81
68	S2	1832	6MZ	C5-N7-C8	3.23	108.53	103.45
68	S2	1851	MA6	C5-N7-C8	3.22	108.51	103.45
3	L5	3718	A2M	O3'-C3'-C2'	3.21	120.17	111.19
3	L5	1871	A2M	O3'-C3'-C2'	3.20	120.14	111.19
3	L5	1524	A2M	O3'-C3'-C2'	3.19	120.13	111.19
68	S2	1850	MA6	C2-N3-C4	3.19	119.63	111.83
3	L5	2401	A2M	O3'-C3'-C2'	3.19	120.12	111.19
3	L5	3825	A2M	O3'-C3'-C2'	3.18	120.08	111.19
68	S2	99	A2M	O3'-C3'-C2'	3.18	120.08	111.19
68	S2	159	A2M	O3'-C3'-C2'	3.18	120.08	111.19
68	S2	468	A2M	O3'-C3'-C2'	3.17	120.06	111.19
3	L5	4220	6MZ	N3-C4-N9	3.17	132.56	127.17
68	S2	1832	6MZ	N3-C4-N9	3.17	132.56	127.17
3	L5	4523	A2M	O3'-C3'-C2'	3.17	120.05	111.19
3	L5	2401	A2M	C3'-C2'-C1'	-3.16	96.76	102.81
3	L5	400	A2M	C3'-C2'-C1'	-3.15	96.77	102.81
68	S2	668	A2M	C4-N9-C1'	-3.15	119.27	126.63
68	S2	1850	MA6	C5-N7-C8	3.13	108.37	103.45
3	L5	3718	A2M	C3'-C2'-C1'	-3.12	96.84	102.81
3	L5	3785	A2M	O3'-C3'-C2'	3.12	119.91	111.19
68	S2	1046	PSU	O2-C2-N1	-3.11	119.58	122.79
3	L5	4457	PSU	O2-C2-N1	-3.10	119.59	122.79
3	L5	3818	UY1	C6-N1-C2	-3.09	119.82	122.69
3	L5	400	A2M	O3'-C3'-C2'	3.08	119.81	111.19
3	L5	4532	PSU	O2-C2-N1	-3.08	119.61	122.79
3	L5	1536	PSU	O2-C2-N1	-3.08	119.61	122.79
68	S2	428	OMU	O4-C4-C5	-3.08	119.86	125.16
68	S2	1031	A2M	O3'-C3'-C2'	3.07	119.79	111.19
68	S2	27	A2M	O3'-C3'-C2'	3.06	119.74	111.19
68	S2	1832	6MZ	C4-C5-C6	3.05	119.31	116.78
68	S2	1326	OMU	O4-C4-C5	-3.05	119.91	125.16
3	L5	1326	A2M	O3'-C3'-C2'	3.04	119.70	111.19
3	L5	4590	A2M	C4-N9-C1'	-3.04	119.52	126.63
3	L5	2837	OMU	O4-C4-C5	-3.04	119.92	125.16
68	S2	1832	6MZ	C4-N9-C8	3.04	108.93	105.74
68	S2	484	A2M	O3'-C3'-C2'	3.03	119.67	111.19
68	S2	1442	OMU	O4-C4-C5	-3.03	119.94	125.16
3	L5	4571	A2M	C3'-C2'-C1'	-3.03	97.01	102.81
3	L5	1323	A2M	O3'-C3'-C2'	3.02	119.63	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3867	A2M	C2'-C1'-N9	3.02	118.72	113.75
3	L5	2815	A2M	O3'-C3'-C2'	2.98	119.54	111.19
3	L5	4498	OMU	O4-C4-C5	-2.98	120.03	125.16
68	S2	27	A2M	C3'-C2'-C1'	-2.97	97.12	102.81
68	S2	627	OMU	O4-C4-C5	-2.97	120.05	125.16
3	L5	1534	A2M	C3'-C2'-C1'	-2.97	97.13	102.81
3	L5	1871	A2M	C4-N9-C1'	-2.96	119.71	126.63
3	L5	4579	PSU	O2-C2-N1	-2.95	119.75	122.79
68	S2	1639	G7M	C2-N1-C6	-2.94	119.79	125.11
3	L5	1677	PSU	O2-C2-N1	-2.93	119.76	122.79
68	S2	799	OMU	O4-C4-C5	-2.93	120.11	125.16
3	L5	4220	6MZ	C4-C5-C6	2.93	119.22	116.78
3	L5	4220	6MZ	C4-N9-C8	2.93	108.82	105.74
68	S2	354	OMU	O4-C4-C5	-2.93	120.11	125.16
3	L5	1683	PSU	O2-C2-N1	-2.92	119.77	122.79
3	L5	4523	A2M	C4-N9-C1'	-2.92	119.80	126.63
68	S2	1177	PSU	O2-C2-N1	-2.92	119.78	122.79
3	L5	2401	A2M	C4-N9-C1'	-2.92	119.81	126.63
3	L5	2632	PSU	O2-C2-N1	-2.91	119.78	122.79
68	S2	166	A2M	C4-N9-C1'	-2.91	119.83	126.63
68	S2	668	A2M	C1'-N9-C8	2.90	133.52	127.09
68	S2	172	OMU	O4-C4-C5	-2.89	120.18	125.16
3	L5	4590	A2M	O3'-C3'-C2'	2.88	119.26	111.19
3	L5	3925	OMU	O4-C4-C5	-2.88	120.20	125.16
68	S2	801	PSU	C6-N1-C2	-2.88	120.02	122.69
3	L5	1323	A2M	C3'-C2'-C1'	-2.87	97.30	102.81
3	L5	3818	UY1	O2-C2-N1	-2.87	119.83	122.79
68	S2	121	OMU	O4-C4-C5	-2.87	120.22	125.16
3	L5	4227	OMU	O4-C4-C5	-2.86	120.23	125.16
3	L5	3822	PSU	O2-C2-N1	-2.86	119.84	122.79
68	S2	1639	G7M	CN7-N7-C8	-2.85	120.48	124.79
68	S2	468	A2M	C4-N9-C1'	-2.85	119.97	126.63
3	L5	4500	PSU	O2-C2-N1	-2.84	119.86	122.79
3	L5	4220	6MZ	C5-N7-C8	2.84	107.92	103.45
68	S2	116	OMU	O4-C4-C5	-2.84	120.26	125.16
68	S2	966	PSU	O2-C2-N1	-2.84	119.86	122.79
3	L5	4628	PSU	O2-C2-N1	-2.83	119.87	122.79
68	S2	1031	A2M	C4-N9-C1'	-2.83	120.02	126.63
68	S2	668	A2M	O3'-C3'-C2'	2.83	119.09	111.19
3	L5	4306	OMU	O4-C4-C5	-2.82	120.29	125.16
68	S2	863	PSU	O2-C2-N1	-2.82	119.88	122.79
3	L5	4293	PSU	O2-C2-N1	-2.82	119.88	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1046	PSU	C6-N1-C2	-2.82	120.08	122.69
3	L5	4590	A2M	C1'-N9-C8	2.82	133.34	127.09
3	L5	4442	PSU	O2-C2-N1	-2.82	119.89	122.79
3	L5	4353	PSU	O2-C2-N1	-2.81	119.89	122.79
68	S2	99	A2M	C4-N9-C1'	-2.81	120.06	126.63
68	S2	105	PSU	O2-C2-N1	-2.80	119.90	122.79
3	L5	2839	PSU	C6-N1-C2	-2.80	120.10	122.69
68	S2	1045	PSU	O2-C2-N1	-2.79	119.91	122.79
3	L5	398	A2M	C4-N9-C1'	-2.79	120.10	126.63
3	L5	2363	A2M	C2'-C1'-N9	2.79	118.35	113.75
3	L5	1862	PSU	O2-C2-N1	-2.79	119.91	122.79
68	S2	649	PSU	C6-N1-C2	-2.79	120.11	122.69
3	L5	1781	PSU	O2-C2-N1	-2.78	119.92	122.79
3	L5	1860	PSU	C6-N1-C2	-2.78	120.11	122.69
3	L5	4620	OMU	O4-C4-C5	-2.77	120.38	125.16
5	L8	69	PSU	O2-C2-N1	-2.77	119.93	122.79
68	S2	1244	PSU	O2-C2-N1	-2.77	119.93	122.79
68	S2	1248	B8N	O4-C4-N3	-2.77	115.49	119.99
68	S2	1004	PSU	O2-C2-N1	-2.76	119.94	122.79
68	S2	668	A2M	O4'-C1'-C2'	2.75	111.33	106.59
3	L5	3853	PSU	O2-C2-N1	-2.75	119.95	122.79
68	S2	1288	OMU	O4-C4-C5	-2.75	120.41	125.16
3	L5	3844	PSU	C6-N1-C2	-2.75	120.14	122.69
3	L5	2787	A2M	O4'-C1'-C2'	2.75	111.32	106.59
3	L5	4973	PSU	O2-C2-N1	-2.75	119.95	122.79
3	L5	2815	A2M	C2'-C1'-N9	2.75	118.27	113.75
3	L5	4552	PSU	O2-C2-N1	-2.74	119.96	122.79
3	L5	1871	A2M	C1'-N9-C8	2.74	133.18	127.09
68	S2	27	A2M	C4-N9-C1'	-2.74	120.22	126.63
3	L5	3830	A2M	C4-N9-C1'	-2.74	120.23	126.63
3	L5	3884	PSU	C6-N1-C2	-2.74	120.15	122.69
3	L5	4521	PSU	O2-C2-N1	-2.73	119.97	122.79
68	S2	1383	A2M	C4-N9-C1'	-2.73	120.24	126.63
68	S2	1367	PSU	O2-C2-N1	-2.73	119.97	122.79
3	L5	4636	PSU	C6-C5-C4	2.73	120.01	118.17
3	L5	4579	PSU	C6-N1-C2	-2.73	120.16	122.69
3	L5	3884	PSU	O2-C2-N1	-2.72	119.98	122.79
3	L5	2401	A2M	C1'-N9-C8	2.71	133.11	127.09
68	S2	166	A2M	C1'-N9-C8	2.71	133.11	127.09
3	L5	4576	PSU	O2-C2-N1	-2.71	120.00	122.79
3	L5	4296	PSU	O2-C2-N1	-2.70	120.00	122.79
3	L5	5010	PSU	O2-C2-N1	-2.70	120.00	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	93	PSU	O2-C2-N1	-2.70	120.00	122.79
3	L5	3808	OMC	C1'-N1-C2	2.70	124.40	118.44
3	L5	3825	A2M	C4-N9-C1'	-2.70	120.33	126.63
3	L5	2363	A2M	O3'-C3'-C2'	2.70	118.73	111.19
3	L5	4431	PSU	O2-C2-N1	-2.69	120.02	122.79
3	L5	400	A2M	C4-N9-C1'	-2.69	120.34	126.63
3	L5	1792	PSU	O2-C2-N1	-2.69	120.02	122.79
3	L5	4636	PSU	O2-C2-N1	-2.69	120.02	122.79
3	L5	4471	PSU	O2-C2-N1	-2.68	120.02	122.79
3	L5	3695	PSU	O2-C2-N1	-2.67	120.03	122.79
3	L5	2861	OMC	C1'-N1-C2	2.67	124.34	118.44
3	L5	1323	A2M	O4'-C1'-C2'	2.67	111.18	106.59
3	L5	3639	PSU	O2-C2-N1	-2.67	120.04	122.79
3	L5	1744	PSU	C6-N1-C2	-2.67	120.22	122.69
68	S2	686	PSU	O2-C2-N1	-2.67	120.04	122.79
68	S2	109	PSU	O2-C2-N1	-2.66	120.04	122.79
68	S2	1232	PSU	O2-C2-N1	-2.66	120.04	122.79
3	L5	3639	PSU	C6-N1-C2	-2.66	120.22	122.69
68	S2	681	PSU	O2-C2-N1	-2.66	120.04	122.79
3	L5	1524	A2M	O4'-C1'-C2'	2.66	111.17	106.59
68	S2	406	PSU	O2-C2-N1	-2.66	120.04	122.79
68	S2	1174	PSU	O2-C2-N1	-2.66	120.04	122.79
3	L5	5001	PSU	O2-C2-N1	-2.66	120.05	122.79
3	L5	2363	A2M	C3'-C2'-C1'	-2.66	97.72	102.81
68	S2	468	A2M	C1'-N9-C8	2.66	132.99	127.09
3	L5	1524	A2M	C4'-O4'-C1'	-2.65	103.61	109.47
3	L5	4571	A2M	C4-N9-C1'	-2.65	120.44	126.63
68	S2	866	PSU	O2-C2-N1	-2.64	120.06	122.79
3	L5	3920	PSU	O2-C2-N1	-2.64	120.07	122.79
68	S2	863	PSU	C6-N1-C2	-2.64	120.24	122.69
3	L5	1860	PSU	O2-C2-N1	-2.64	120.07	122.79
3	L5	3637	PSU	C6-N1-C2	-2.63	120.25	122.69
3	L5	1326	A2M	C4-N9-C1'	-2.63	120.48	126.63
68	S2	99	A2M	C1'-N9-C8	2.63	132.94	127.09
68	S2	651	PSU	O2-C2-N1	-2.63	120.08	122.79
5	L8	69	PSU	C6-N1-C2	-2.63	120.25	122.69
3	L5	1536	PSU	C6-N1-C2	-2.63	120.25	122.69
68	S2	1056	PSU	O2-C2-N1	-2.63	120.08	122.79
3	L5	5001	PSU	C6-N1-C2	-2.63	120.25	122.69
68	S2	1031	A2M	C1'-N9-C8	2.62	132.92	127.09
3	L5	3844	PSU	O2-C2-N1	-2.62	120.08	122.79
3	L5	398	A2M	C1'-N9-C8	2.62	132.90	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	814	PSU	O2-C2-N1	-2.62	120.09	122.79
68	S2	406	PSU	C6-N1-C2	-2.61	120.27	122.69
3	L5	3785	A2M	C4-N9-C1'	-2.60	120.54	126.63
3	L5	1782	PSU	O2-C2-N1	-2.60	120.11	122.79
3	L5	4312	PSU	O2-C2-N1	-2.60	120.11	122.79
3	L5	1744	PSU	O2-C2-N1	-2.59	120.11	122.79
68	S2	801	PSU	O2-C2-N1	-2.59	120.12	122.79
3	L5	1683	PSU	C6-N1-C2	-2.59	120.29	122.69
3	L5	4523	A2M	C1'-N9-C8	2.59	132.84	127.09
3	L5	3830	A2M	C1'-N9-C8	2.58	132.83	127.09
3	L5	4673	PSU	C6-N1-C2	-2.58	120.30	122.69
68	S2	1004	PSU	C6-N1-C2	-2.58	120.30	122.69
3	L5	4361	PSU	O2-C2-N1	-2.57	120.13	122.79
68	S2	105	PSU	C6-N1-C2	-2.57	120.31	122.69
3	L5	3695	PSU	C6-N1-C2	-2.56	120.31	122.69
3	L5	1326	A2M	C3'-C2'-C1'	-2.56	97.90	102.81
3	L5	3825	A2M	C1'-N9-C8	2.56	132.78	127.09
3	L5	4530	UR3	C6-N1-C2	-2.56	119.71	121.80
3	L5	4972	PSU	O2-C2-N1	-2.56	120.15	122.79
68	S2	159	A2M	C1'-N9-C8	2.56	132.77	127.09
3	L5	4689	PSU	O2-C2-N1	-2.56	120.15	122.79
68	S2	159	A2M	C4-N9-C1'	-2.55	120.66	126.63
3	L5	4471	PSU	C6-N1-C2	-2.55	120.32	122.69
3	L5	1326	A2M	C2'-C1'-N9	2.55	117.94	113.75
3	L5	2363	A2M	C4-N9-C1'	-2.55	120.67	126.63
68	S2	27	A2M	C1'-N9-C8	2.55	132.75	127.09
3	L5	4403	PSU	O2-C2-N1	-2.55	120.16	122.79
3	L5	2363	A2M	O4'-C1'-C2'	2.55	110.97	106.59
68	S2	1056	PSU	C6-N1-C2	-2.55	120.33	122.69
3	L5	2839	PSU	O2-C2-N1	-2.54	120.17	122.79
3	L5	5010	PSU	C6-N1-C2	-2.54	120.33	122.69
3	L5	3867	A2M	C4-N9-C1'	-2.54	120.69	126.63
3	L5	2632	PSU	C6-N1-C2	-2.54	120.33	122.69
3	L5	4576	PSU	C6-N1-C2	-2.54	120.33	122.69
3	L5	4532	PSU	C6-N1-C2	-2.54	120.33	122.69
3	L5	3867	A2M	O3'-C3'-C2'	2.53	118.27	111.19
68	S2	651	PSU	C6-N1-C2	-2.53	120.34	122.69
3	L5	4628	PSU	C6-N1-C2	-2.53	120.35	122.69
3	L5	3822	PSU	C6-N1-C2	-2.52	120.36	122.69
3	L5	4521	PSU	C6-N1-C2	-2.52	120.36	122.69
3	L5	4673	PSU	O2-C2-N1	-2.51	120.20	122.79
68	S2	649	PSU	O2-C2-N1	-2.51	120.20	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1781	PSU	C6-N1-C2	-2.51	120.36	122.69
3	L5	4353	PSU	C6-N1-C2	-2.51	120.36	122.69
68	S2	1383	A2M	C1'-N9-C8	2.51	132.67	127.09
3	L5	3851	PSU	O2-C2-N1	-2.51	120.20	122.79
68	S2	1851	MA6	C1'-N9-C8	-2.51	121.53	127.09
3	L5	3920	PSU	C6-N1-C2	-2.51	120.37	122.69
68	S2	93	PSU	C6-N1-C2	-2.50	120.37	122.69
3	L5	400	A2M	C1'-N9-C8	2.50	132.65	127.09
3	L5	4431	PSU	C6-N1-C2	-2.48	120.39	122.69
3	L5	4403	PSU	C6-N1-C2	-2.48	120.39	122.69
68	S2	1850	MA6	C1'-N9-C8	-2.48	121.59	127.09
3	L5	4500	PSU	C6-N1-C2	-2.48	120.39	122.69
68	S2	1367	PSU	C6-N1-C2	-2.47	120.39	122.69
68	S2	484	A2M	C4-N9-C1'	-2.47	120.85	126.63
68	S2	681	PSU	C6-N1-C2	-2.47	120.40	122.69
68	S2	1177	PSU	C6-N1-C2	-2.47	120.40	122.69
5	L8	55	PSU	C6-N1-C2	-2.47	120.40	122.69
3	L5	4500	PSU	C6-C5-C4	2.46	119.84	118.17
68	S2	484	A2M	C1'-N9-C8	2.46	132.56	127.09
3	L5	4552	PSU	C6-N1-C2	-2.46	120.41	122.69
3	L5	4442	PSU	C6-N1-C2	-2.46	120.41	122.69
3	L5	4457	PSU	C6-N1-C2	-2.46	120.41	122.69
3	L5	1534	A2M	C4-N9-C1'	-2.46	120.88	126.63
68	S2	966	PSU	C6-N1-C2	-2.45	120.41	122.69
3	L5	1534	A2M	C1'-N9-C8	2.45	132.53	127.09
3	L5	1323	A2M	C4-N9-C1'	-2.45	120.90	126.63
3	L5	1326	A2M	C1'-N9-C8	2.44	132.51	127.09
5	L8	55	PSU	O2-C2-N1	-2.44	120.28	122.79
3	L5	4571	A2M	C1'-N9-C8	2.44	132.50	127.09
3	L5	2787	A2M	C4-N9-C1'	-2.44	120.94	126.63
3	L5	3718	A2M	C1'-N9-C8	2.43	132.49	127.09
3	L5	1677	PSU	C6-N1-C2	-2.43	120.44	122.69
68	S2	1045	PSU	C6-N1-C2	-2.43	120.44	122.69
3	L5	1524	A2M	C4-N9-C1'	-2.43	120.96	126.63
68	S2	668	A2M	C2'-C1'-N9	2.42	117.74	113.75
3	L5	4299	PSU	C6-N1-C2	-2.42	120.45	122.69
3	L5	4493	PSU	O2-C2-N1	-2.42	120.29	122.79
3	L5	4361	PSU	C6-N1-C2	-2.42	120.45	122.69
3	L5	4299	PSU	O2-C2-N1	-2.41	120.30	122.79
3	L5	1782	PSU	C6-N1-C2	-2.41	120.46	122.69
3	L5	4312	PSU	C6-N1-C2	-2.41	120.46	122.69
68	S2	484	A2M	O4'-C1'-C2'	2.41	110.73	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2363	A2M	C1'-N9-C8	2.40	132.43	127.09
3	L5	4972	PSU	C6-N1-C2	-2.40	120.46	122.69
3	L5	4293	PSU	C6-N1-C2	-2.40	120.46	122.69
68	S2	1232	PSU	C6-N1-C2	-2.40	120.46	122.69
3	L5	4973	PSU	C6-N1-C2	-2.40	120.47	122.69
3	L5	3867	A2M	C1'-N9-C8	2.40	132.42	127.09
3	L5	3785	A2M	C1'-N9-C8	2.40	132.41	127.09
68	S2	1174	PSU	C6-N1-C2	-2.39	120.47	122.69
3	L5	3718	A2M	C4-N9-C1'	-2.39	121.04	126.63
3	L5	1862	PSU	C6-N1-C2	-2.39	120.48	122.69
68	S2	1244	PSU	C6-N1-C2	-2.38	120.48	122.69
3	L5	4521	PSU	C6-C5-C4	2.38	119.78	118.17
3	L5	1534	A2M	O3'-C3'-C2'	2.38	117.84	111.19
68	S2	814	PSU	C6-N1-C2	-2.37	120.49	122.69
68	S2	576	A2M	C4-N9-C1'	-2.37	121.09	126.63
3	L5	4296	PSU	C6-N1-C2	-2.36	120.50	122.69
3	L5	1582	PSU	O2-C2-N1	-2.36	120.35	122.79
3	L5	2815	A2M	O4'-C1'-C2'	2.36	110.65	106.59
3	L5	3637	PSU	C6-C5-C4	2.35	119.76	118.17
3	L5	4636	PSU	C6-N1-C2	-2.35	120.51	122.69
3	L5	3785	A2M	O4'-C4'-C3'	2.35	109.81	105.15
68	S2	686	PSU	C6-N1-C2	-2.34	120.52	122.69
3	L5	4220	6MZ	C5-C6-N1	2.34	120.66	118.15
3	L5	4590	A2M	C6-C5-C4	-2.33	113.99	117.18
3	L5	2815	A2M	C4-N9-C1'	-2.33	121.19	126.63
68	S2	109	PSU	C6-N1-C2	-2.32	120.53	122.69
3	L5	1322	1MA	N1-C6-N6	2.32	125.54	119.71
3	L5	3853	PSU	C6-N1-C2	-2.32	120.54	122.69
3	L5	1323	A2M	C1'-N9-C8	2.31	132.22	127.09
68	S2	159	A2M	C2'-C1'-N9	2.31	117.55	113.75
3	L5	4403	PSU	O4'-C1'-C2'	2.31	108.34	105.15
68	S2	668	A2M	C6-C5-C4	-2.29	114.05	117.18
3	L5	3785	A2M	C3'-C2'-C1'	-2.29	98.42	102.81
3	L5	3851	PSU	C6-N1-C2	-2.29	120.57	122.69
68	S2	576	A2M	C1'-N9-C8	2.29	132.18	127.09
3	L5	1792	PSU	C6-N1-C2	-2.29	120.57	122.69
68	S2	866	PSU	C6-N1-C2	-2.28	120.57	122.69
68	S2	166	A2M	O4'-C1'-C2'	2.28	110.52	106.59
68	S2	1081	PSU	O2-C2-N1	-2.28	120.44	122.79
3	L5	2351	OMC	C1'-N1-C2	2.28	123.47	118.44
3	L5	1524	A2M	C1'-N9-C8	2.28	132.15	127.09
3	L5	2787	A2M	C1'-N9-C8	2.28	132.15	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2815	A2M	C3'-C2'-C1'	-2.25	98.51	102.81
68	S2	1832	6MZ	C4-C5-N7	-2.25	108.01	110.58
68	S2	484	A2M	O4'-C4'-C3'	2.24	109.61	105.15
3	L5	1326	A2M	O4'-C1'-C2'	2.24	110.45	106.59
68	S2	1288	OMU	C1'-N1-C2	2.24	121.61	117.59
3	L5	3867	A2M	O4'-C1'-C2'	2.24	110.44	106.59
68	S2	1639	G7M	N9-C8-N7	-2.24	107.05	112.48
68	S2	166	A2M	C6-C5-C4	-2.23	114.13	117.18
3	L5	4353	PSU	C6-C5-C4	2.23	119.68	118.17
3	L5	4498	OMU	O2-C2-N1	-2.23	119.90	122.80
3	L5	2815	A2M	C1'-N9-C8	2.22	132.03	127.09
3	L5	2787	A2M	O4'-C4'-C3'	2.22	109.57	105.15
3	L5	1871	A2M	C6-C5-C4	-2.21	114.17	117.18
3	L5	2401	A2M	C6-C5-C4	-2.21	114.17	117.18
68	S2	27	A2M	O4'-C1'-C2'	2.20	110.38	106.59
3	L5	4590	A2M	O4'-C1'-C2'	2.20	110.38	106.59
68	S2	1272	OMC	C1'-N1-C2	2.20	123.30	118.44
68	S2	1248	B8N	O4'-C1'-C2'	2.20	108.19	105.15
68	S2	1248	B8N	O4-C4-C5	-2.19	118.79	122.58
68	S2	1367	PSU	C6-C5-C4	2.19	119.65	118.17
5	L8	69	PSU	O4'-C1'-C2'	2.18	108.16	105.15
3	L5	4442	PSU	O4'-C1'-C2'	2.17	108.16	105.15
3	L5	2837	OMU	O2-C2-N1	-2.17	119.97	122.80
68	S2	159	A2M	C3'-C2'-C1'	-2.17	98.65	102.81
3	L5	4523	A2M	C6-C5-C4	-2.17	114.22	117.18
68	S2	468	A2M	C6-C5-C4	-2.16	114.22	117.18
3	L5	4523	A2M	O4'-C1'-C2'	2.16	110.31	106.59
3	L5	4636	PSU	O4'-C1'-C2'	2.16	108.14	105.15
3	L5	3785	A2M	C2-N1-C6	-2.16	115.19	118.73
3	L5	3822	PSU	O4'-C1'-C2'	2.15	108.13	105.15
68	S2	172	OMU	O2-C2-N1	-2.15	120.00	122.80
68	S2	627	OMU	O2-C2-N1	-2.14	120.00	122.80
68	S2	1081	PSU	C6-N1-C2	-2.14	120.71	122.69
3	L5	3867	A2M	C3'-C2'-C1'	-2.14	98.71	102.81
3	L5	3785	A2M	C5-C6-N1	2.14	122.94	117.51
3	L5	1326	A2M	C6-C5-C4	-2.13	114.26	117.18
3	L5	1582	PSU	C6-N1-C2	-2.13	120.71	122.69
3	L5	4403	PSU	C6-C5-C4	2.13	119.61	118.17
3	L5	3867	A2M	C2-N1-C6	-2.13	115.23	118.73
3	L5	4571	A2M	O4'-C1'-C2'	2.13	110.26	106.59
68	S2	1031	A2M	C6-C5-C4	-2.12	114.28	117.18
68	S2	27	A2M	C6-C5-C4	-2.12	114.28	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3830	A2M	C6-C5-C4	-2.12	114.29	117.18
3	L5	400	A2M	C6-C5-C4	-2.12	114.29	117.18
68	S2	1081	PSU	O4'-C1'-C2'	2.12	108.08	105.15
3	L5	3808	OMC	C1'-N1-C6	-2.12	116.26	120.78
3	L5	398	A2M	C6-C5-C4	-2.11	114.29	117.18
3	L5	3637	PSU	O2-C2-N1	-2.11	120.61	122.79
3	L5	3925	OMU	O2-C2-N1	-2.11	120.06	122.80
3	L5	4973	PSU	C6-C5-C4	2.10	119.59	118.17
3	L5	4571	A2M	C6-C5-C4	-2.10	114.31	117.18
68	S2	354	OMU	O2-C2-N1	-2.10	120.06	122.80
68	S2	159	A2M	O4'-C1'-C2'	2.10	110.20	106.59
3	L5	1323	A2M	C6-C5-C4	-2.10	114.32	117.18
3	L5	1871	A2M	O4'-C1'-C2'	2.09	110.19	106.59
68	S2	428	OMU	O2-C2-N1	-2.08	120.08	122.80
3	L5	4456	OMC	C1'-N1-C2	2.08	123.03	118.44
68	S2	484	A2M	C2'-C1'-N9	2.08	117.18	113.75
68	S2	1832	6MZ	C5-C6-N1	2.08	120.38	118.15
68	S2	1383	A2M	C6-C5-C4	-2.08	114.34	117.18
3	L5	2363	A2M	C6-C5-C4	-2.08	114.34	117.18
3	L5	3867	A2M	C6-C5-C4	-2.07	114.35	117.18
3	L5	4457	PSU	O4'-C1'-C2'	2.07	108.01	105.15
3	L5	2861	OMC	C1'-N1-C6	-2.07	116.36	120.78
68	S2	1031	A2M	O4'-C1'-C2'	2.07	110.15	106.59
3	L5	3785	A2M	C6-C5-C4	-2.07	114.36	117.18
3	L5	3825	A2M	C6-C5-C4	-2.07	114.36	117.18
3	L5	1534	A2M	O4'-C1'-C2'	2.06	110.14	106.59
3	L5	2787	A2M	C6-C5-C4	-2.06	114.36	117.18
3	L5	400	A2M	O4'-C1'-C2'	2.06	110.14	106.59
68	S2	99	A2M	C5-C6-N1	2.06	122.74	117.51
3	L5	3718	A2M	C2-N1-C6	-2.06	115.35	118.73
3	L5	2787	A2M	C5-C6-N1	2.06	122.74	117.51
3	L5	4576	PSU	O4'-C1'-C2'	2.06	108.00	105.15
3	L5	2815	A2M	C6-C5-C4	-2.06	114.37	117.18
68	S2	1326	OMU	O2-C2-N1	-2.06	120.12	122.80
68	S2	99	A2M	O4'-C1'-C2'	2.05	110.12	106.59
68	S2	159	A2M	C2-N1-C6	-2.05	115.36	118.73
68	S2	966	PSU	C6-C5-C4	2.05	119.56	118.17
3	L5	4457	PSU	C6-C5-C4	2.05	119.56	118.17
3	L5	1677	PSU	O4'-C1'-C2'	2.05	107.99	105.15
3	L5	4523	A2M	C5-C6-N1	2.04	122.70	117.51
68	S2	166	A2M	C5-C6-N1	2.04	122.70	117.51
68	S2	1442	OMU	C1'-N1-C2	2.04	121.26	117.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	99	A2M	C6-C5-C4	-2.04	114.39	117.18
3	L5	2815	A2M	C5-C6-N1	2.04	122.69	117.51
3	L5	3920	PSU	O4'-C1'-C2'	2.04	107.97	105.15
68	S2	99	A2M	C2-N1-C6	-2.04	115.38	118.73
68	S2	121	OMU	O2-C2-N1	-2.04	120.14	122.80
3	L5	2787	A2M	C2-N1-C6	-2.04	115.38	118.73
3	L5	398	A2M	O4'-C1'-C2'	2.04	110.09	106.59
3	L5	1534	A2M	C2-N1-C6	-2.04	115.39	118.73
68	S2	1031	A2M	C5-C6-N1	2.03	122.68	117.51
3	L5	1326	A2M	C5-C6-N1	2.03	122.67	117.51
3	L5	2632	PSU	C6-C5-C4	2.03	119.55	118.17
3	L5	2422	OMC	C1'-N1-C2	2.03	122.92	118.44
3	L5	4523	A2M	C2-N1-C6	-2.03	115.40	118.73
3	L5	3825	A2M	C2-N1-C6	-2.03	115.40	118.73
3	L5	1677	PSU	C6-C5-C4	2.03	119.54	118.17
68	S2	1383	A2M	C5-C6-N1	2.03	122.66	117.51
3	L5	1871	A2M	C4'-O4'-C1'	-2.03	105.00	109.47
3	L5	2815	A2M	C2-N1-C6	-2.02	115.41	118.73
68	S2	484	A2M	C5-C6-N1	2.02	122.64	117.51
3	L5	2363	A2M	C5-C6-N1	2.02	122.63	117.51
3	L5	400	A2M	C5-C6-N1	2.02	122.63	117.51
3	L5	4571	A2M	C5-C6-N1	2.02	122.63	117.51
3	L5	1534	A2M	C6-C5-C4	-2.01	114.43	117.18
3	L5	1524	A2M	C6-C5-C4	-2.01	114.43	117.18
68	S2	27	A2M	C5-C6-N1	2.01	122.62	117.51
3	L5	2363	A2M	C2-N1-C6	-2.01	115.43	118.73
3	L5	1323	A2M	C5-C6-N1	2.01	122.61	117.51
68	S2	1703	OMC	C1'-N1-C2	2.01	122.88	118.44
68	S2	468	A2M	C5-C6-N1	2.01	122.61	117.51
68	S2	1056	PSU	C6-C5-C4	2.01	119.53	118.17
68	S2	517	OMC	C1'-N1-C2	2.01	122.87	118.44
68	S2	468	A2M	O4'-C1'-C2'	2.00	110.04	106.59
68	S2	1244	PSU	C6-C5-C4	2.00	119.52	118.17
3	L5	3825	A2M	C5-C6-N1	2.00	122.59	117.51

There are no chirality outliers.

All (135) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L5	1326	A2M	O4'-C4'-C5'-O5'
3	L5	1326	A2M	C3'-C4'-C5'-O5'
3	L5	1340	OMC	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
3	L5	1625	OMG	O4'-C4'-C5'-O5'
3	L5	2351	OMC	C1'-C2'-O2'-CM2
3	L5	2364	OMG	O4'-C4'-C5'-O5'
3	L5	2364	OMG	C1'-C2'-O2'-CM2
3	L5	2787	A2M	C1'-C2'-O2'-CM'
3	L5	3701	OMC	C2'-C1'-N1-C6
3	L5	3701	OMC	O4'-C4'-C5'-O5'
3	L5	3785	A2M	O4'-C4'-C5'-O5'
3	L5	3792	OMG	O4'-C4'-C5'-O5'
3	L5	3867	A2M	C1'-C2'-O2'-CM'
3	L5	4196	OMG	C1'-C2'-O2'-CM2
3	L5	4590	A2M	C1'-C2'-O2'-CM'
3	L5	4636	PSU	C2'-C1'-C5-C4
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	99	A2M	C1'-C2'-O2'-CM'
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	468	A2M	C1'-C2'-O2'-CM'
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	644	OMG	C1'-C2'-O2'-CM2
68	S2	801	PSU	C3'-C4'-C5'-O5'
68	S2	801	PSU	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	1832	6MZ	C5-C6-N6-C9
68	S2	1832	6MZ	N1-C6-N6-C9
3	L5	3701	OMC	C2'-C1'-N1-C2
3	L5	1323	A2M	O4'-C4'-C5'-O5'
3	L5	1536	PSU	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	3785	A2M	C3'-C4'-C5'-O5'
3	L5	3867	A2M	C3'-C4'-C5'-O5'
3	L5	4500	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	L5	4590	A2M	O4'-C4'-C5'-O5'
3	L5	4590	A2M	C3'-C4'-C5'-O5'
68	S2	99	A2M	O4'-C4'-C5'-O5'
68	S2	172	OMU	C3'-C4'-C5'-O5'
68	S2	644	OMG	C3'-C4'-C5'-O5'
68	S2	1442	OMU	C3'-C4'-C5'-O5'
68	S2	1442	OMU	O4'-C4'-C5'-O5'
3	L5	2401	A2M	O4'-C4'-C5'-O5'
3	L5	3701	OMC	C3'-C4'-C5'-O5'
3	L5	4228	OMG	O4'-C4'-C5'-O5'
3	L5	4228	OMG	C3'-C4'-C5'-O5'
3	L5	4500	PSU	C3'-C4'-C5'-O5'
68	S2	576	A2M	O4'-C4'-C5'-O5'
68	S2	1045	PSU	C3'-C4'-C5'-O5'
68	S2	1045	PSU	O4'-C4'-C5'-O5'
68	S2	1703	OMC	O4'-C4'-C5'-O5'
3	L5	2364	OMG	C3'-C4'-C5'-O5'
3	L5	3782	5MC	O4'-C4'-C5'-O5'
3	L5	3792	OMG	C3'-C4'-C5'-O5'
3	L5	4637	OMG	C3'-C4'-C5'-O5'
68	S2	576	A2M	C3'-C4'-C5'-O5'
68	S2	668	A2M	O4'-C4'-C5'-O5'
68	S2	668	A2M	C3'-C4'-C5'-O5'
3	L5	1323	A2M	C3'-C4'-C5'-O5'
3	L5	1524	A2M	O4'-C4'-C5'-O5'
3	L5	2815	A2M	C3'-C4'-C5'-O5'
68	S2	93	PSU	O4'-C4'-C5'-O5'
68	S2	99	A2M	C3'-C4'-C5'-O5'
3	L5	1524	A2M	C3'-C4'-C5'-O5'
3	L5	3867	A2M	O4'-C4'-C5'-O5'
68	S2	1248	B8N	N34-C33-C34-O36
3	L5	2787	A2M	C2'-C1'-N9-C8
3	L5	2422	OMC	O4'-C4'-C5'-O5'
68	S2	93	PSU	C3'-C4'-C5'-O5'
3	L5	4590	A2M	C4'-C5'-O5'-P
3	L5	2422	OMC	C3'-C4'-C5'-O5'
3	L5	1326	A2M	C1'-C2'-O2'-CM'
3	L5	3925	OMU	C1'-C2'-O2'-CM2
3	L5	3818	UY1	C4'-C5'-O5'-P
3	L5	398	A2M	O4'-C4'-C5'-O5'
3	L5	3899	OMG	C3'-C4'-C5'-O5'
68	S2	428	OMU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	L5	4447	5MC	C2'-C1'-N1-C6
68	S2	576	A2M	C4'-C5'-O5'-P
68	S2	1244	PSU	O4'-C4'-C5'-O5'
3	L5	2787	A2M	C3'-C4'-C5'-O5'
68	S2	1383	A2M	O4'-C4'-C5'-O5'
3	L5	1322	1MA	C2'-C1'-N9-C8
3	L5	4447	5MC	O4'-C1'-N1-C6
3	L5	1524	A2M	C3'-C2'-O2'-CM'
5	L8	75	OMG	C4'-C5'-O5'-P
68	S2	644	OMG	C4'-C5'-O5'-P
3	L5	4500	PSU	O4'-C1'-C5-C4
3	L5	4636	PSU	O4'-C1'-C5-C4
68	S2	1248	B8N	O4'-C1'-C5-C4
3	L5	2787	A2M	C2'-C1'-N9-C4
68	S2	428	OMU	C3'-C4'-C5'-O5'
68	S2	867	OMG	C3'-C4'-C5'-O5'
68	S2	1383	A2M	C3'-C4'-C5'-O5'
68	S2	1703	OMC	C3'-C4'-C5'-O5'
68	S2	1490	OMG	C4'-C5'-O5'-P
3	L5	3701	OMC	O4'-C1'-N1-C6
3	L5	4370	OMG	C3'-C2'-O2'-CM2
3	L5	1322	1MA	C2'-C1'-N9-C4
3	L5	1326	A2M	C4'-C5'-O5'-P
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	3844	PSU	C4'-C5'-O5'-P
3	L5	3782	5MC	C3'-C4'-C5'-O5'
3	L5	3701	OMC	O4'-C1'-N1-C2
3	L5	3887	OMC	C4'-C5'-O5'-P
3	L5	4500	PSU	C4'-C5'-O5'-P
68	S2	1851	MA6	C4'-C5'-O5'-P
68	S2	1046	PSU	O4'-C4'-C5'-O5'
5	L8	75	OMG	C1'-C2'-O2'-CM2
68	S2	1081	PSU	C4'-C5'-O5'-P
3	L5	2839	PSU	C3'-C4'-C5'-O5'
3	L5	4623	OMG	C3'-C4'-C5'-O5'
68	S2	1639	G7M	C3'-C4'-C5'-O5'
3	L5	1677	PSU	O4'-C1'-C5-C6
3	L5	4500	PSU	O4'-C1'-C5-C6
68	S2	1248	B8N	O4'-C1'-C5-C6
3	L5	4447	5MC	O4'-C1'-N1-C2
3	L5	3899	OMG	O4'-C4'-C5'-O5'
3	L5	4618	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	L5	2787	A2M	O4'-C1'-N9-C8
3	L5	3785	A2M	C4'-C5'-O5'-P
68	S2	799	OMU	C2'-C1'-N1-C6
3	L5	2839	PSU	O4'-C4'-C5'-O5'
3	L5	398	A2M	C3'-C4'-C5'-O5'
68	S2	799	OMU	C2'-C1'-N1-C2

There are no ring outliers.

64 monomers are involved in 96 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L8	75	OMG	2	0
3	L5	2787	A2M	1	0
3	L5	2364	OMG	1	0
3	L5	3718	A2M	4	0
68	S2	159	A2M	1	0
3	L5	4457	PSU	1	0
68	S2	1244	PSU	2	0
68	S2	1383	A2M	2	0
3	L5	4579	PSU	2	0
68	S2	116	OMU	2	0
68	S2	649	PSU	1	0
68	S2	1832	6MZ	1	0
3	L5	1871	A2M	1	0
3	L5	4637	OMG	1	0
3	L5	3920	PSU	1	0
68	S2	99	A2M	1	0
3	L5	4392	OMG	2	0
3	L5	4227	OMU	1	0
3	L5	3841	OMC	1	0
3	L5	1683	PSU	1	0
3	L5	4620	OMU	1	0
3	L5	4523	A2M	2	0
3	L5	4293	PSU	1	0
68	S2	644	OMG	1	0
68	S2	1328	OMG	1	0
3	L5	4618	OMG	1	0
3	L5	2839	PSU	1	0
3	L5	4196	OMG	1	0
3	L5	1340	OMC	2	0
68	S2	1031	A2M	2	0
3	L5	2363	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4499	OMG	1	0
68	S2	484	A2M	1	0
3	L5	1326	A2M	2	0
3	L5	2815	A2M	1	0
68	S2	601	OMG	3	0
68	S2	93	PSU	1	0
68	S2	468	A2M	2	0
3	L5	2351	OMC	2	0
3	L5	4689	PSU	1	0
3	L5	4353	PSU	1	0
3	L5	3867	A2M	3	0
68	S2	1337	4AC	4	0
68	S2	1174	PSU	2	0
3	L5	398	A2M	1	0
3	L5	4500	PSU	1	0
3	L5	3925	OMU	1	0
3	L5	4306	OMU	1	0
68	S2	576	A2M	1	0
68	S2	509	OMG	4	0
68	S2	1232	PSU	2	0
3	L5	1781	PSU	1	0
68	S2	801	PSU	1	0
68	S2	681	PSU	1	0
3	L5	4571	A2M	1	0
68	S2	462	OMC	3	0
68	S2	166	A2M	2	0
3	L5	4447	5MC	1	0
68	S2	27	A2M	3	0
3	L5	4220	6MZ	1	0
3	L5	4536	OMC	1	0
3	L5	4590	A2M	1	0
68	S2	1850	MA6	1	0
3	L5	3825	A2M	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	5287	-	9,9,9	0.32	0	8,8,8	0.82	0
89	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.90	0
89	SPD	L5	5288	-	9,9,9	0.32	0	8,8,8	0.79	0
89	SPD	L5	5283	-	9,9,9	0.32	0	8,8,8	0.81	0
88	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.92	0
89	SPD	L5	5290	-	9,9,9	0.32	0	8,8,8	0.88	0
89	SPD	L5	5286	-	9,9,9	0.33	0	8,8,8	0.88	0
89	SPD	L5	5261	-	9,9,9	0.32	0	8,8,8	1.00	0
89	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.89	0
88	SPM	L5	5294	-	13,13,13	0.35	0	12,12,12	0.89	0
88	SPM	L5	5267	-	13,13,13	0.36	0	12,12,12	0.89	0
88	SPM	L5	5259	-	13,13,13	0.35	0	12,12,12	1.00	0
88	SPM	L5	5289	-	13,13,13	0.37	0	12,12,12	0.93	0
89	SPD	L5	5291	-	9,9,9	0.33	0	8,8,8	0.80	0
88	SPM	L5	5264	-	13,13,13	0.35	0	12,12,12	1.02	0
88	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	1.01	0
89	SPD	L5	5293	-	9,9,9	0.33	0	8,8,8	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
89	SPD	L5	5287	-	-	2/7/7/7	-
89	SPD	L5	5285	-	-	1/7/7/7	-
89	SPD	L5	5288	-	-	3/7/7/7	-
89	SPD	L5	5283	-	-	1/7/7/7	-
88	SPM	L5	5292	-	-	3/11/11/11	-
89	SPD	L5	5290	-	-	0/7/7/7	-
89	SPD	L5	5286	-	-	1/7/7/7	-
89	SPD	L5	5261	-	-	1/7/7/7	-
89	SPD	L5	5284	-	-	3/7/7/7	-
88	SPM	L5	5294	-	-	4/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SPM	L5	5267	-	-	3/11/11/11	-
88	SPM	L5	5259	-	-	3/11/11/11	-
88	SPM	L5	5289	-	-	6/11/11/11	-
89	SPD	L5	5291	-	-	2/7/7/7	-
88	SPM	L5	5264	-	-	3/11/11/11	-
88	SPM	L5	5263	-	-	4/11/11/11	-
89	SPD	L5	5293	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (41) torsion outliers are listed below:

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

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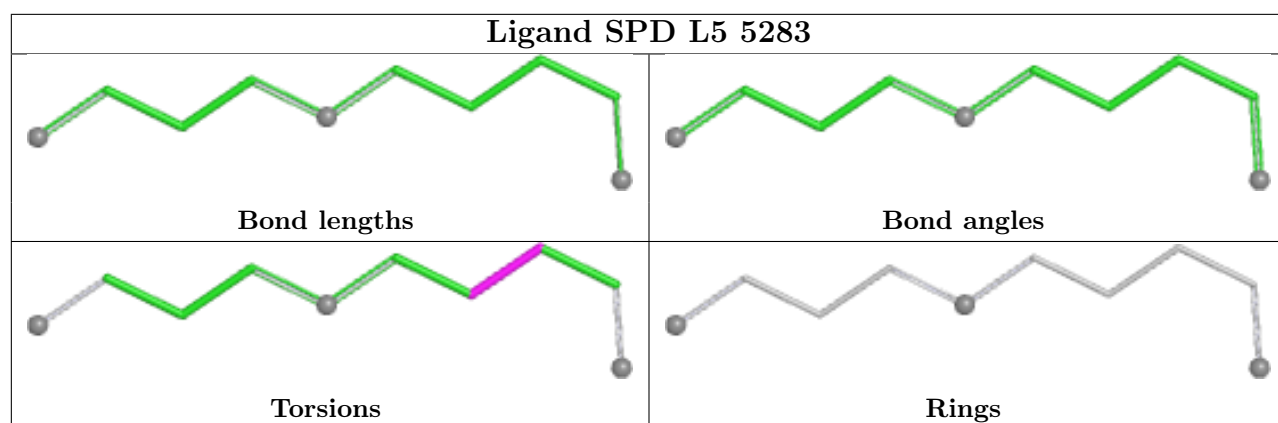
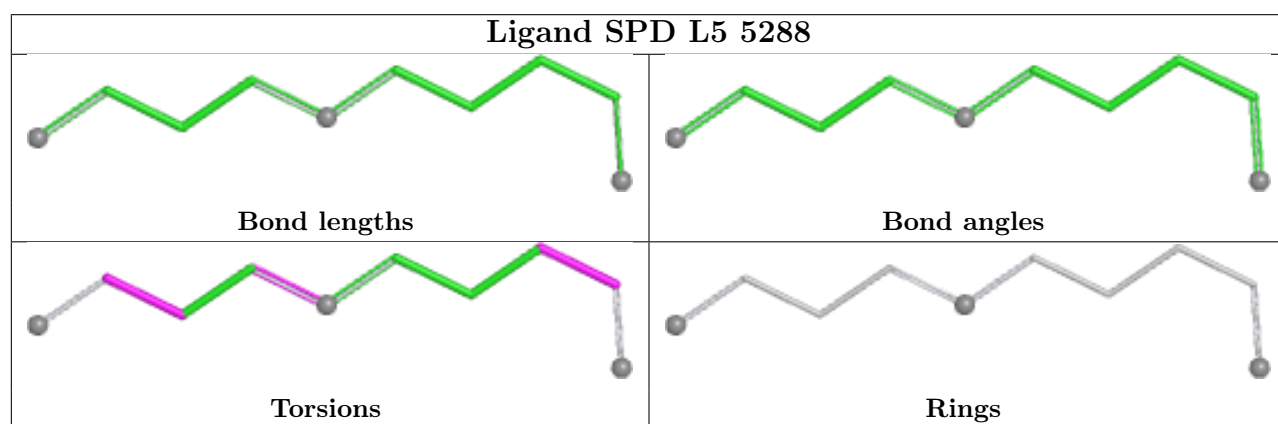
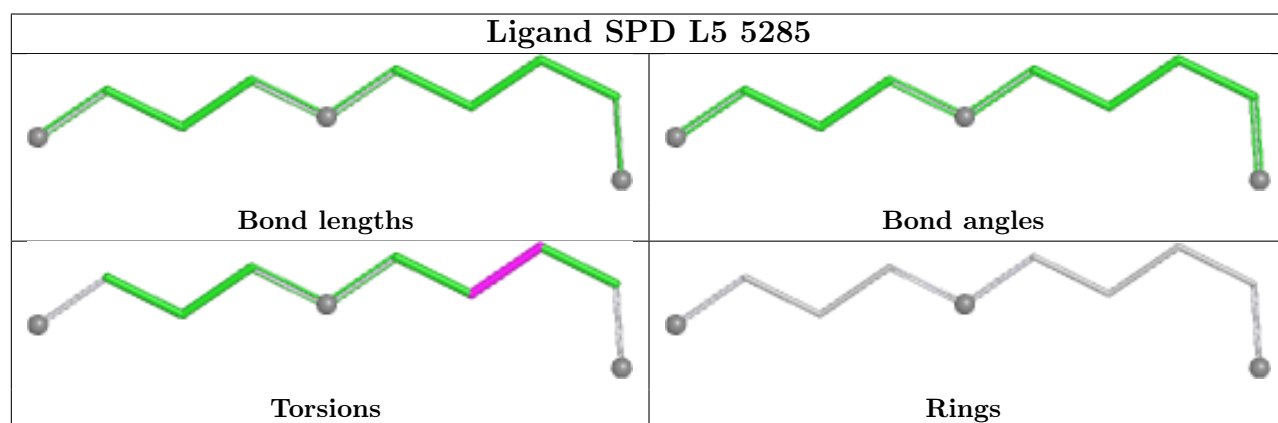
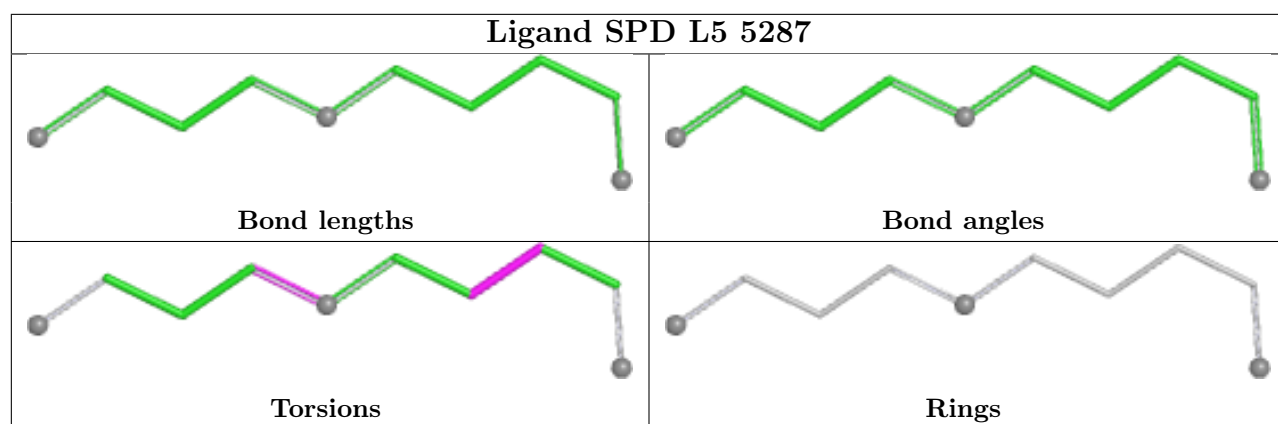
Mol	Chain	Res	Type	Atoms
88	L5	5292	SPM	N10-C11-C12-C13
88	L5	5267	SPM	C8-C9-N10-C11
89	L5	5291	SPD	C8-C7-N6-C5
89	L5	5283	SPD	C2-C3-C4-C5
89	L5	5288	SPD	C8-C7-N6-C5
89	L5	5293	SPD	C8-C7-N6-C5
89	L5	5291	SPD	N6-C7-C8-C9
88	L5	5259	SPM	C3-C4-N5-C6
89	L5	5261	SPD	C8-C7-N6-C5
88	L5	5294	SPM	N10-C11-C12-C13
89	L5	5284	SPD	C3-C4-C5-N6
88	L5	5289	SPM	N1-C2-C3-C4
88	L5	5292	SPM	C11-C12-C13-N14
88	L5	5294	SPM	C11-C12-C13-N14
89	L5	5288	SPD	C7-C8-C9-N10
89	L5	5285	SPD	C2-C3-C4-C5

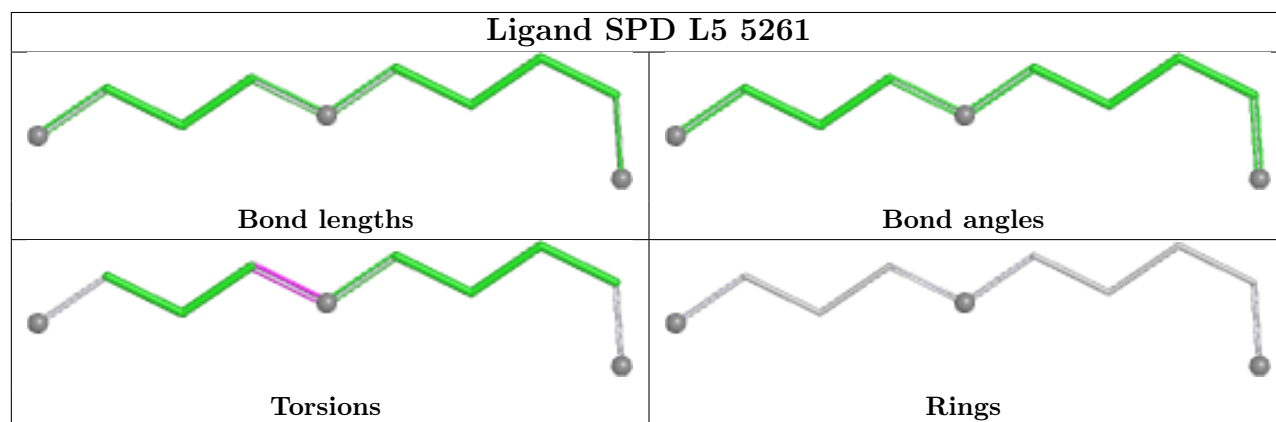
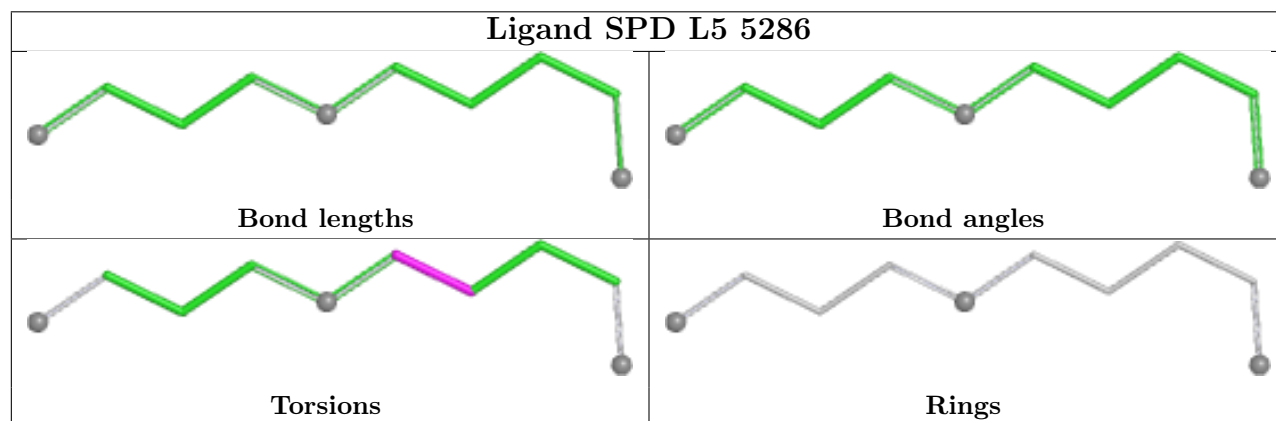
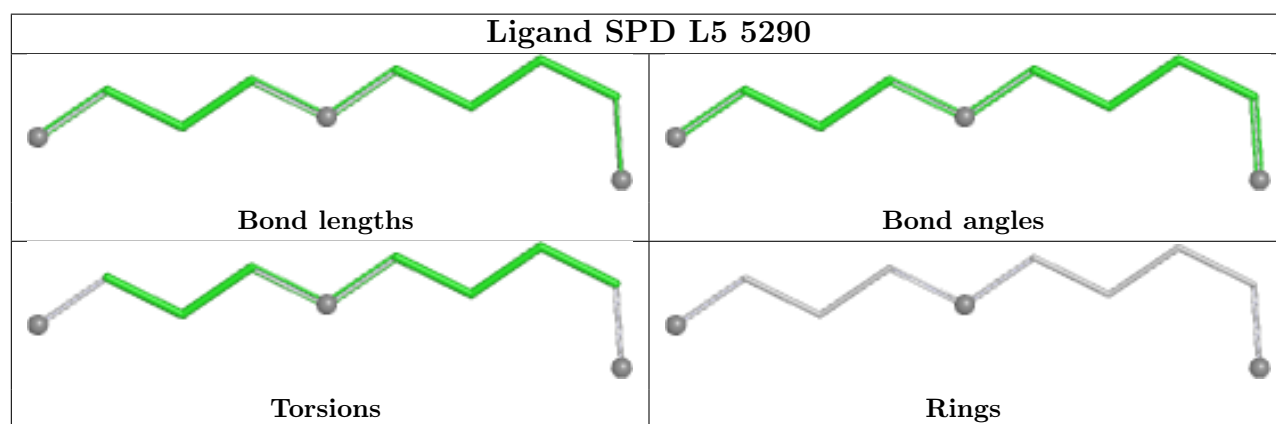
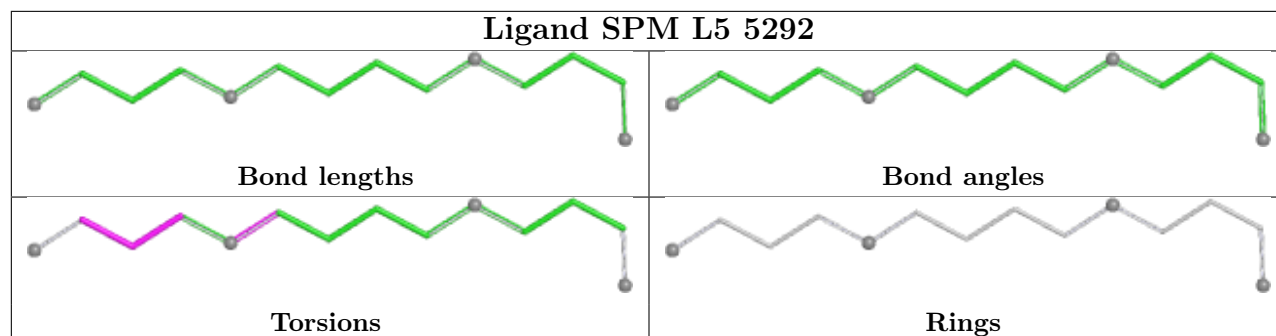
There are no ring outliers.

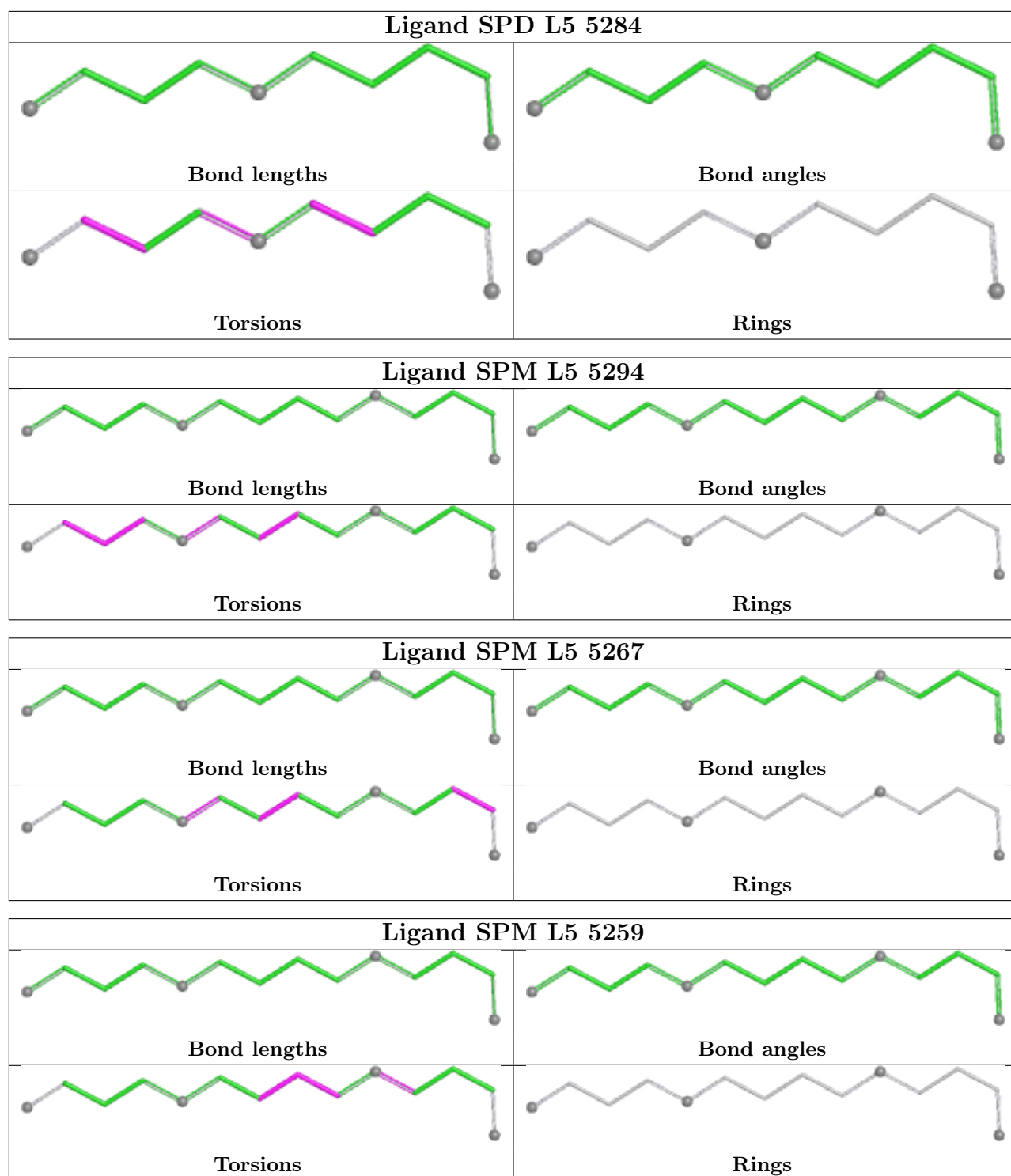
7 monomers are involved in 8 short contacts:

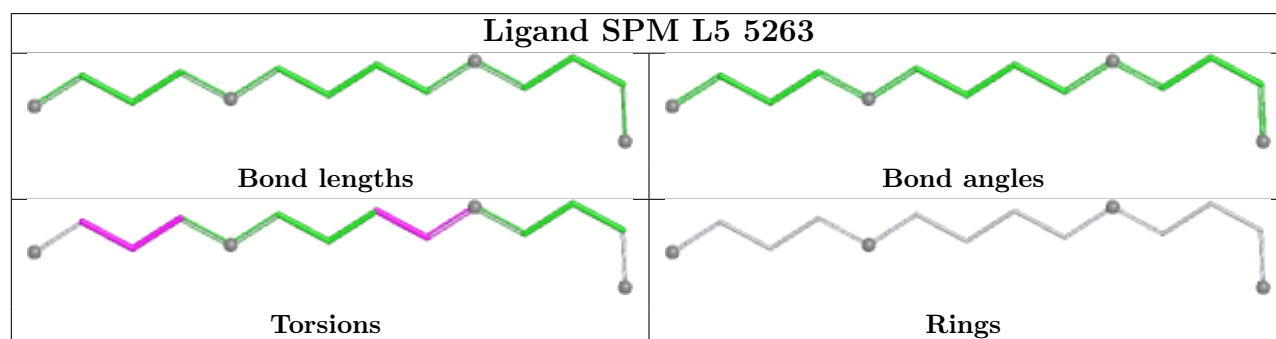
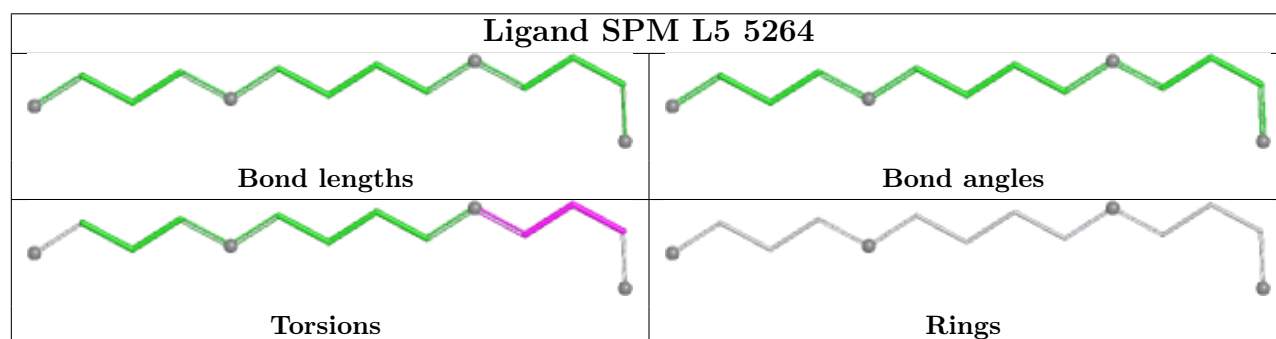
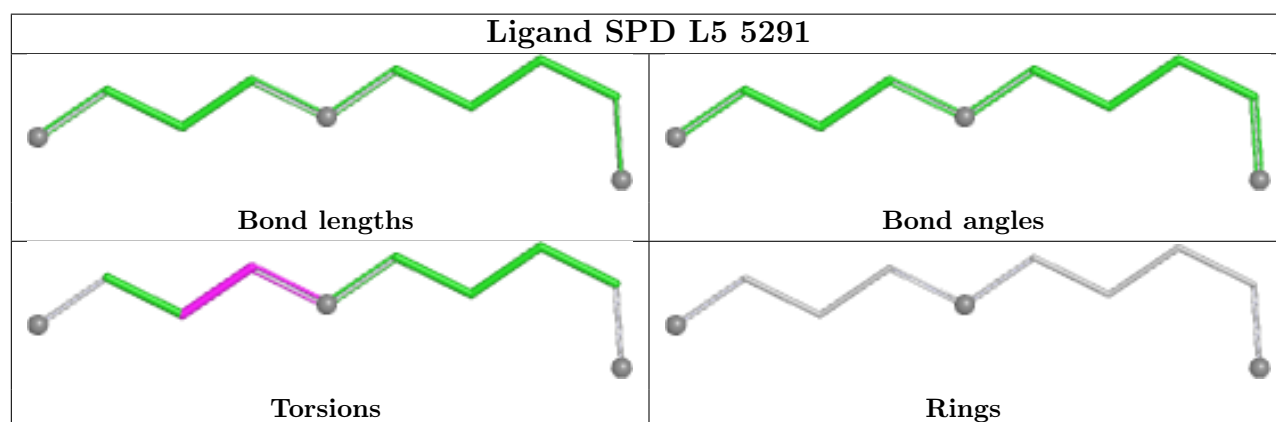
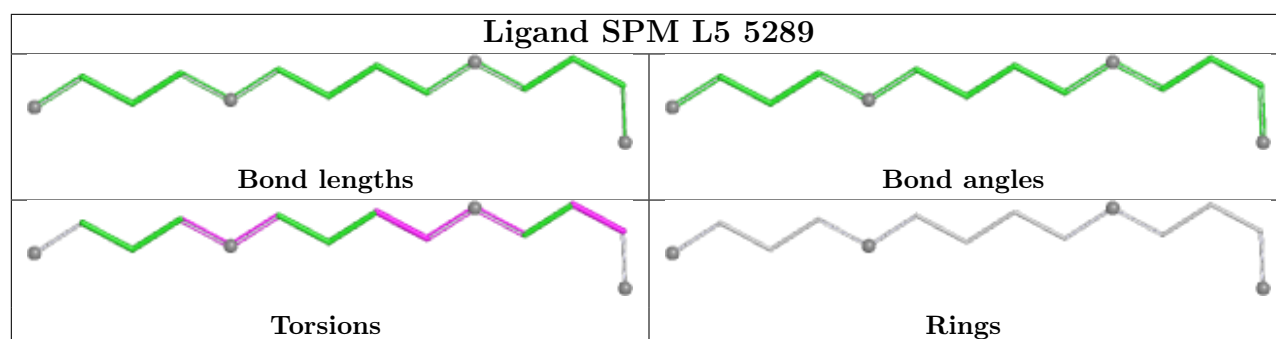
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	L5	5287	SPD	1	0
89	L5	5288	SPD	1	0
89	L5	5290	SPD	1	0
88	L5	5294	SPM	2	0
88	L5	5267	SPM	1	0
88	L5	5289	SPM	1	0
89	L5	5291	SPD	1	0

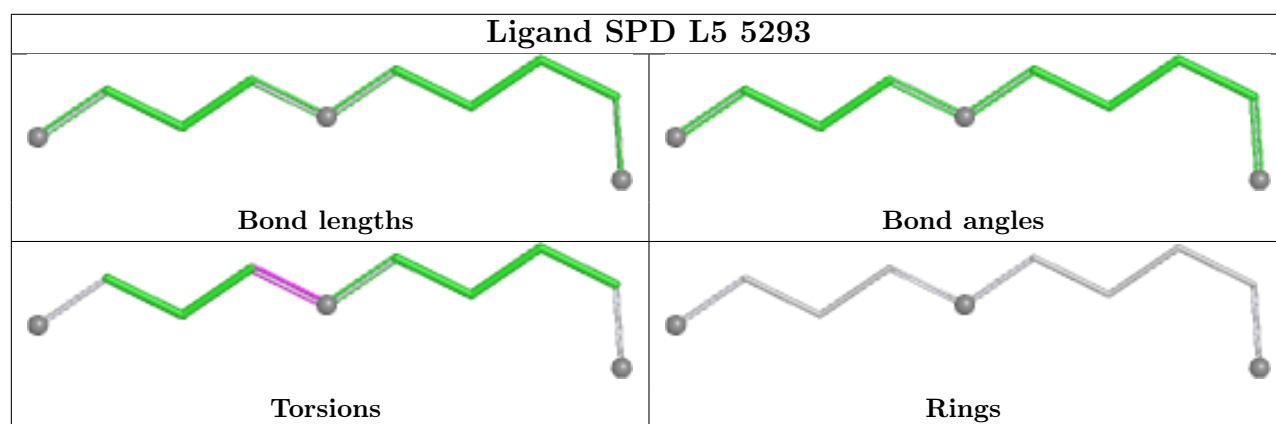
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
68	S2	4
84	Et	1
3	L5	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	29.69
1	S2	698:G	O3'	730:C	P	14.25
1	S2	739:C	O3'	746:C	P	12.73
1	Et	16:C	O3'	18:U	P	7.17
1	S2	225:G	O3'	287:U	P	6.94
1	L5	3818:UY1	O3'	3819:G	P	3.42

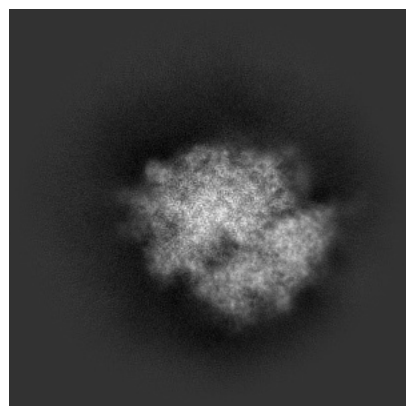
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71336. These allow visual inspection of the internal detail of the map and identification of artifacts.

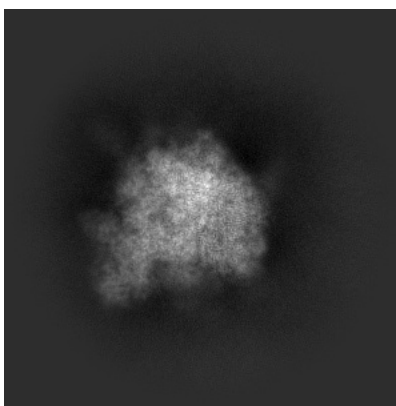
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

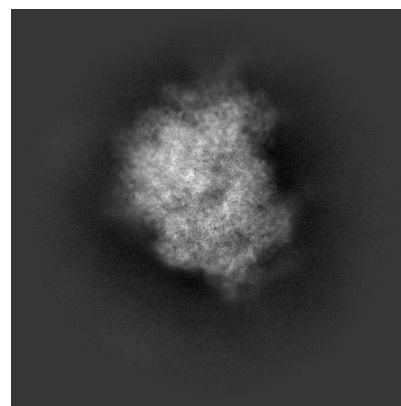
6.1.1 Primary map



X

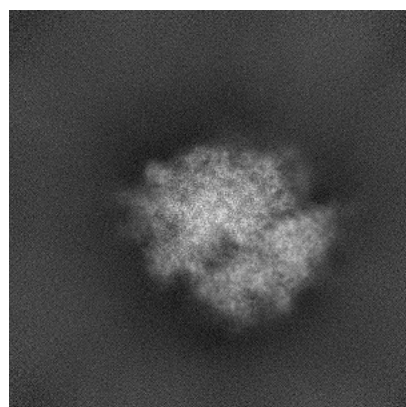


Y

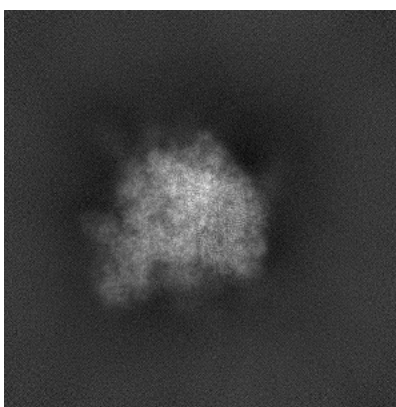


Z

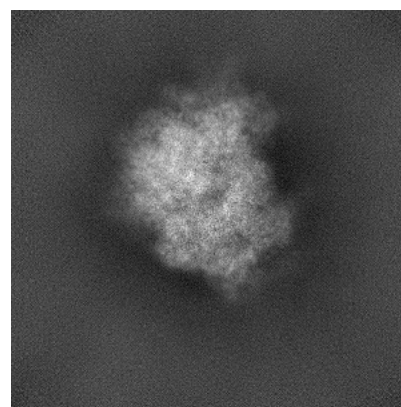
6.1.2 Raw map



X



Y

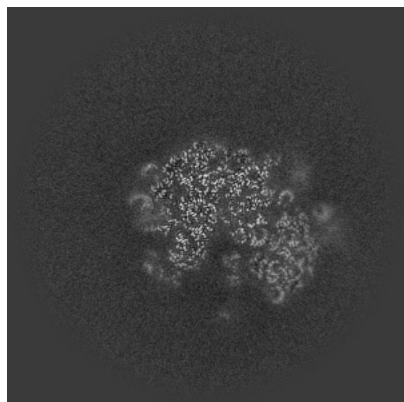


Z

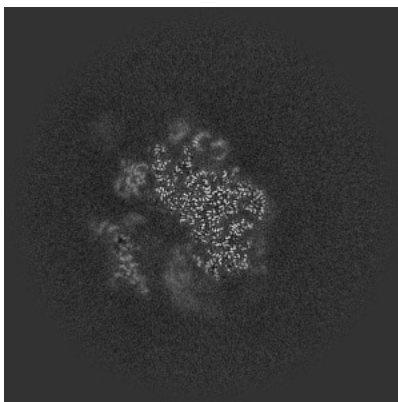
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

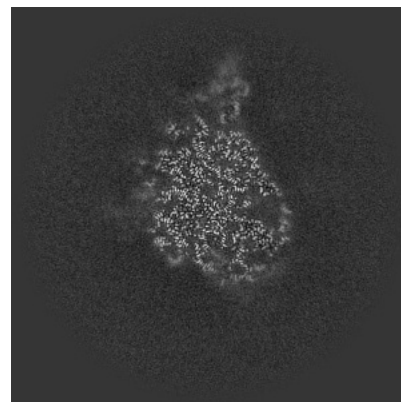
6.2.1 Primary map



X Index: 256

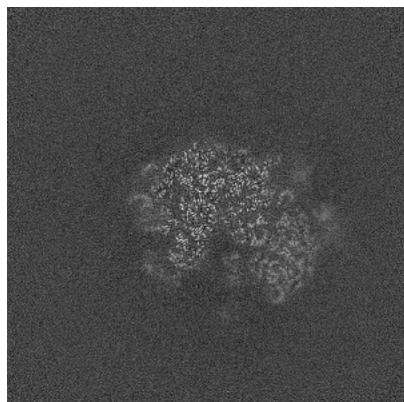


Y Index: 256

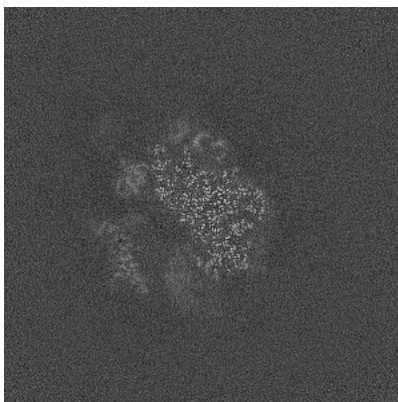


Z Index: 256

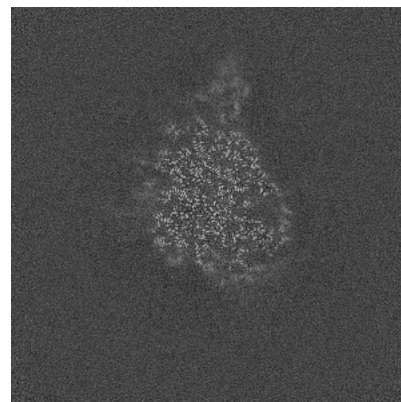
6.2.2 Raw map



X Index: 256



Y Index: 256

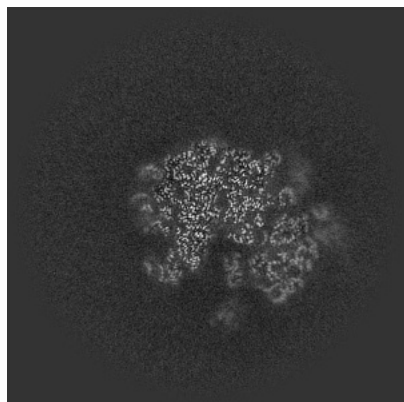


Z Index: 256

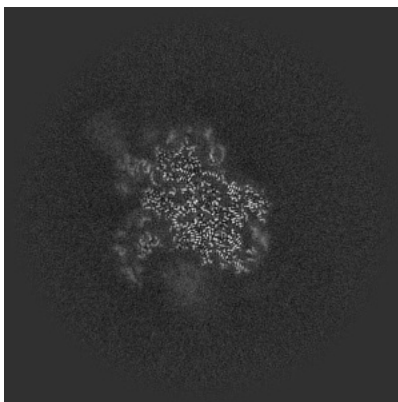
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

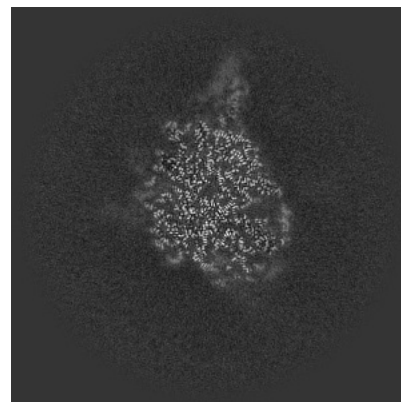
6.3.1 Primary map



X Index: 253

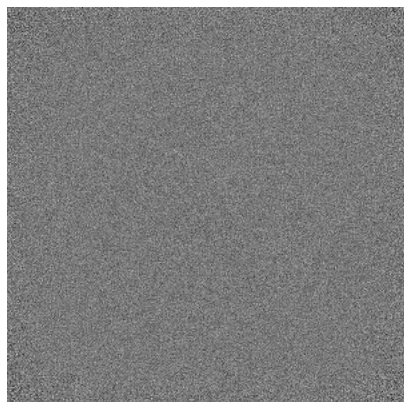


Y Index: 243

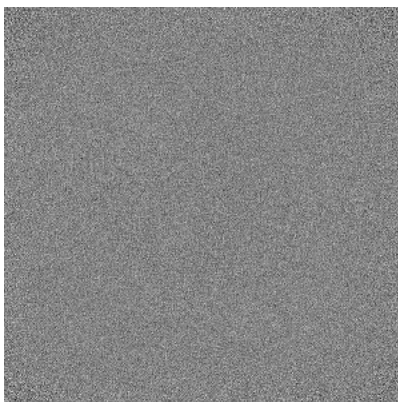


Z Index: 258

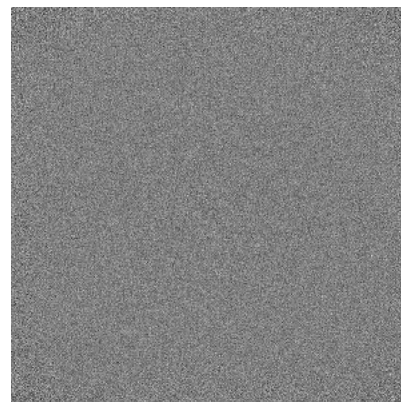
6.3.2 Raw map



X Index: 0



Y Index: 0

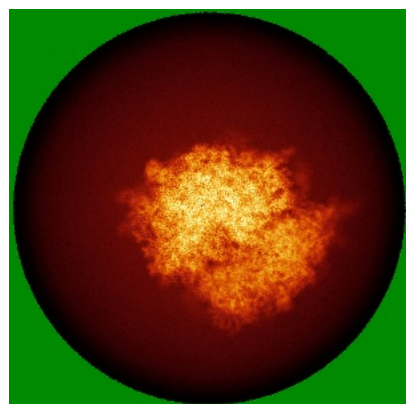


Z Index: 0

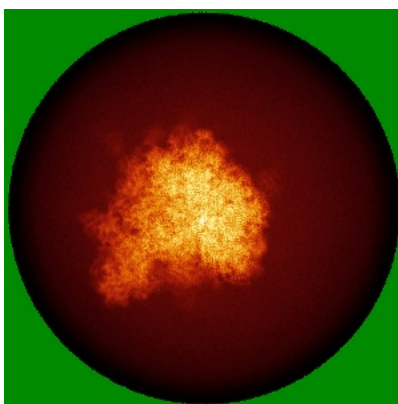
The images above show the largest variance slices of the map in three orthogonal directions.

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

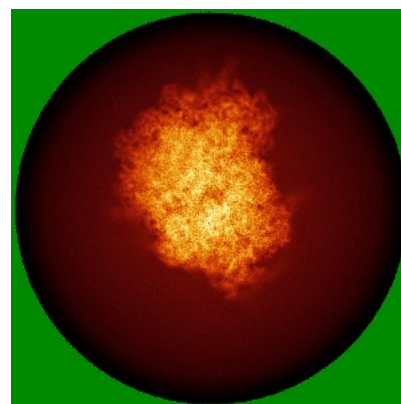
6.4.1 Primary map



X

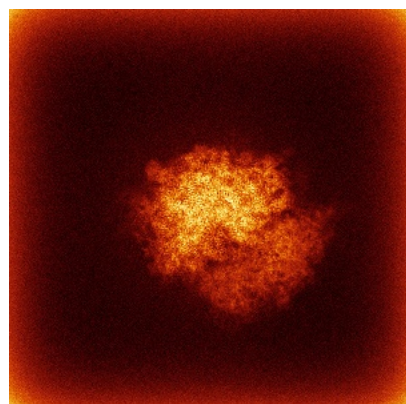


Y

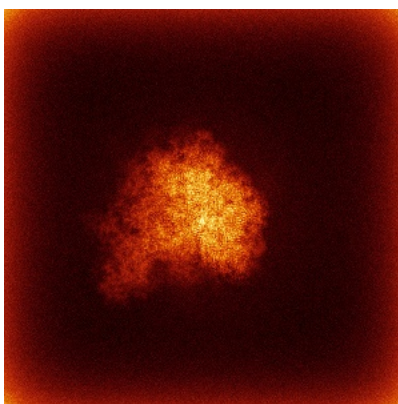


Z

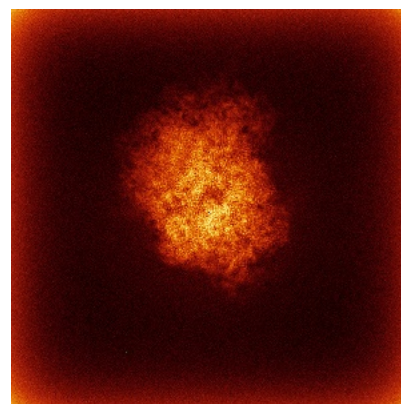
6.4.2 Raw map



X



Y

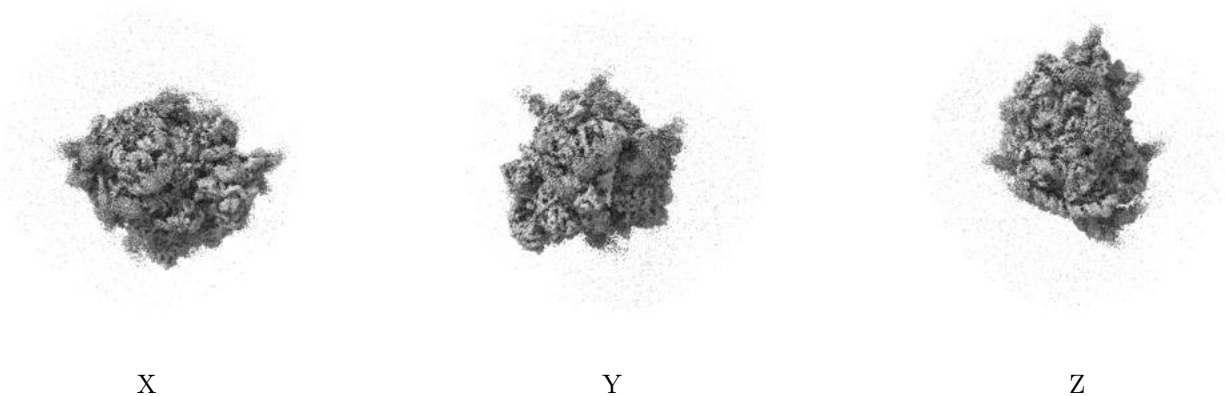


Z

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.

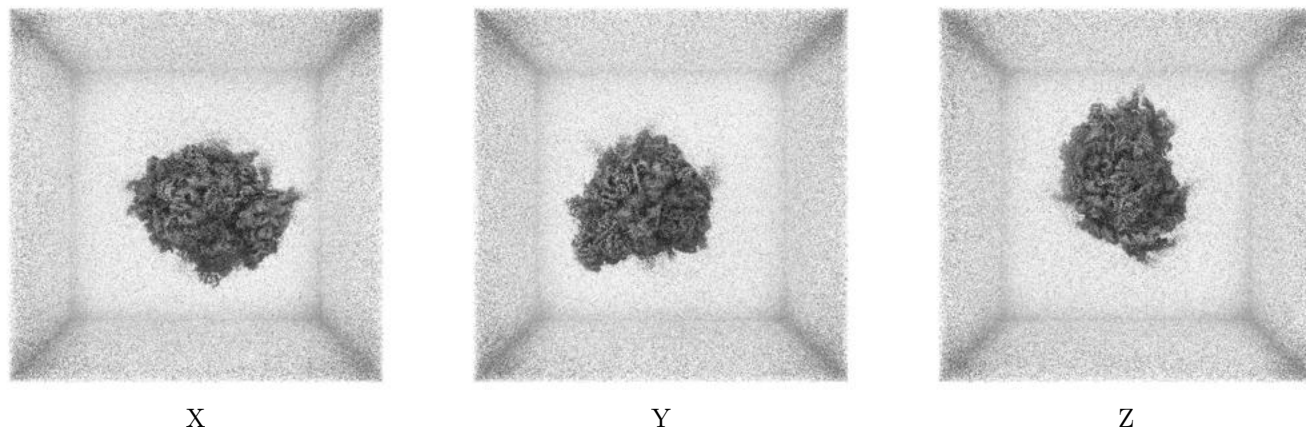
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. 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.

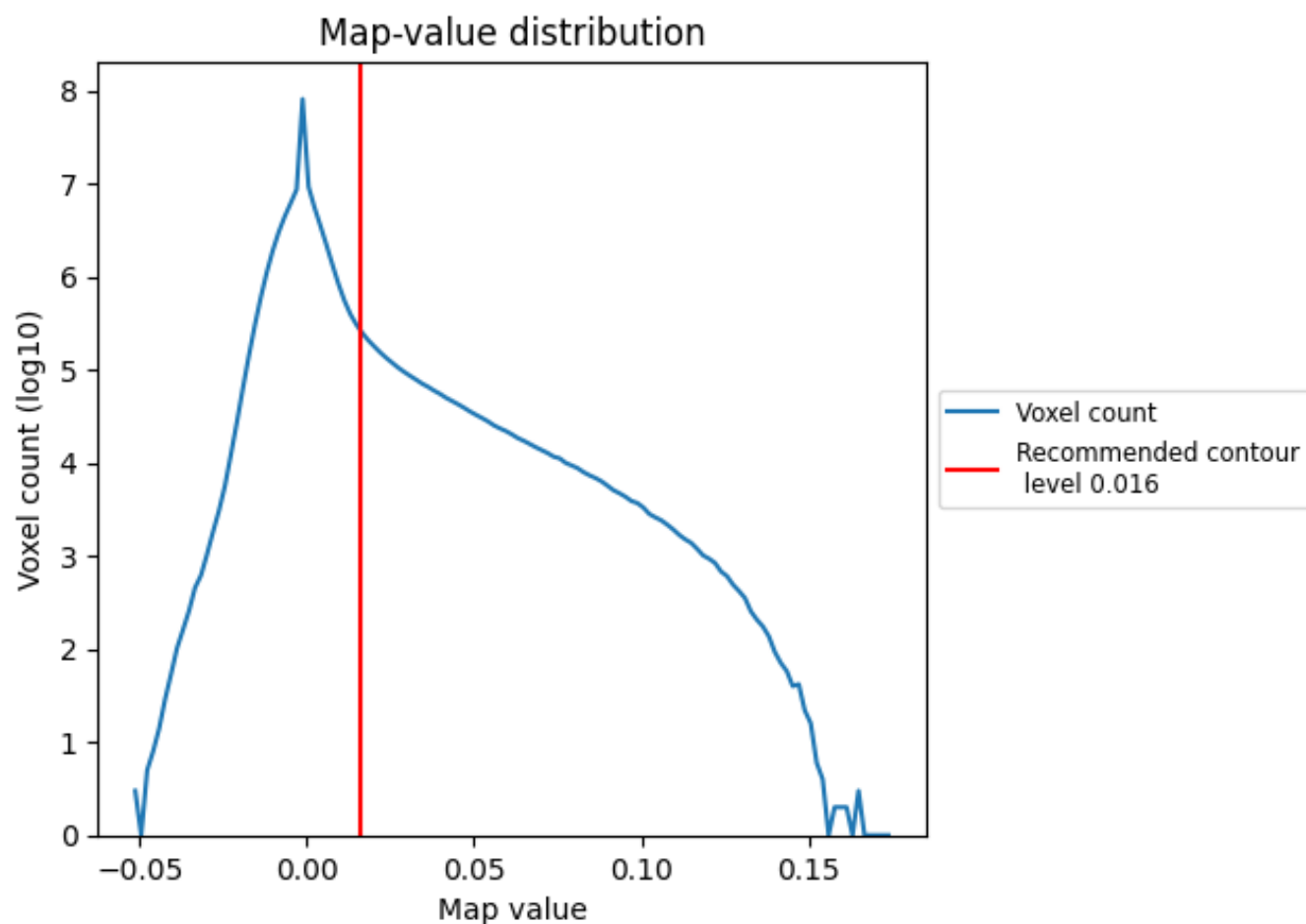
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

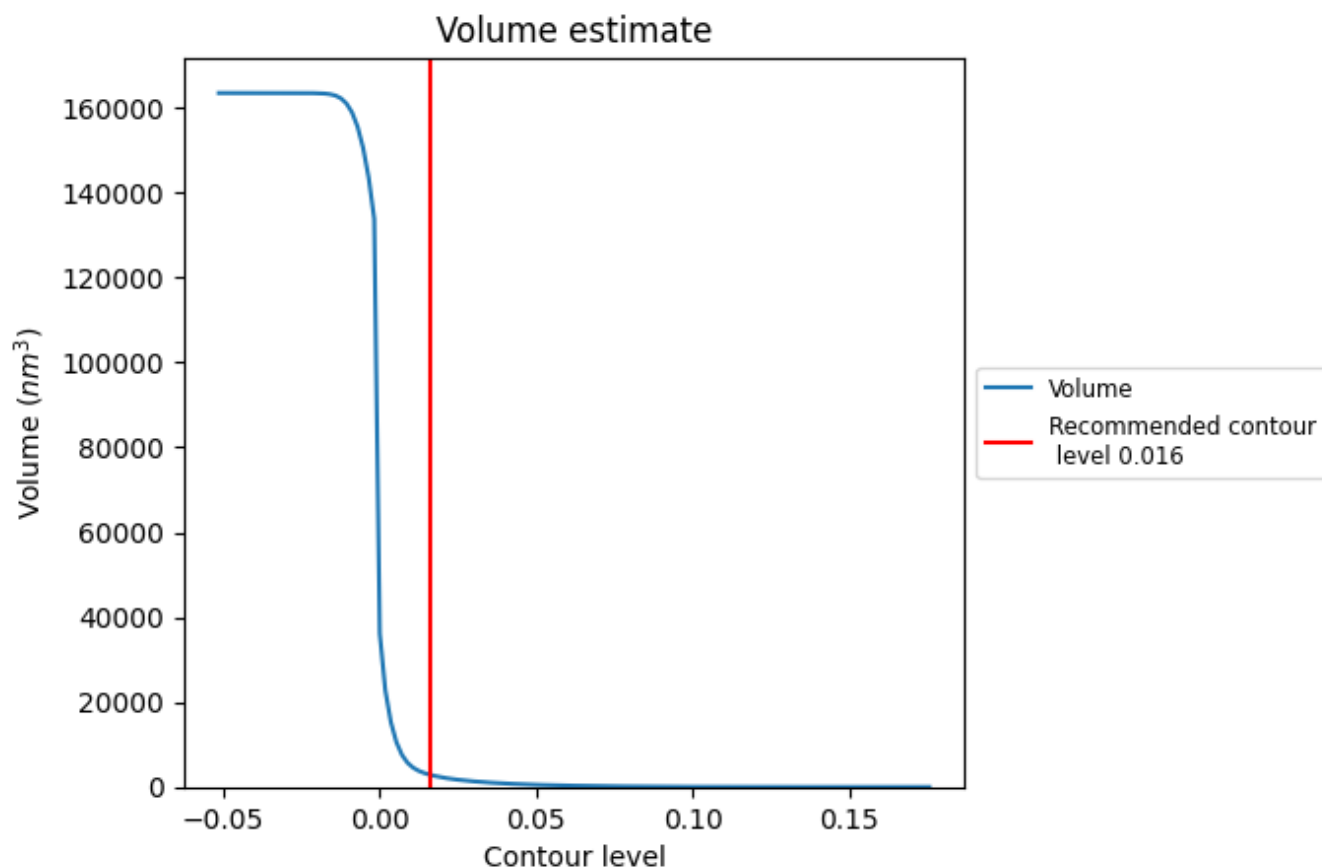
This section contains the results of statistical analysis of the map.

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.

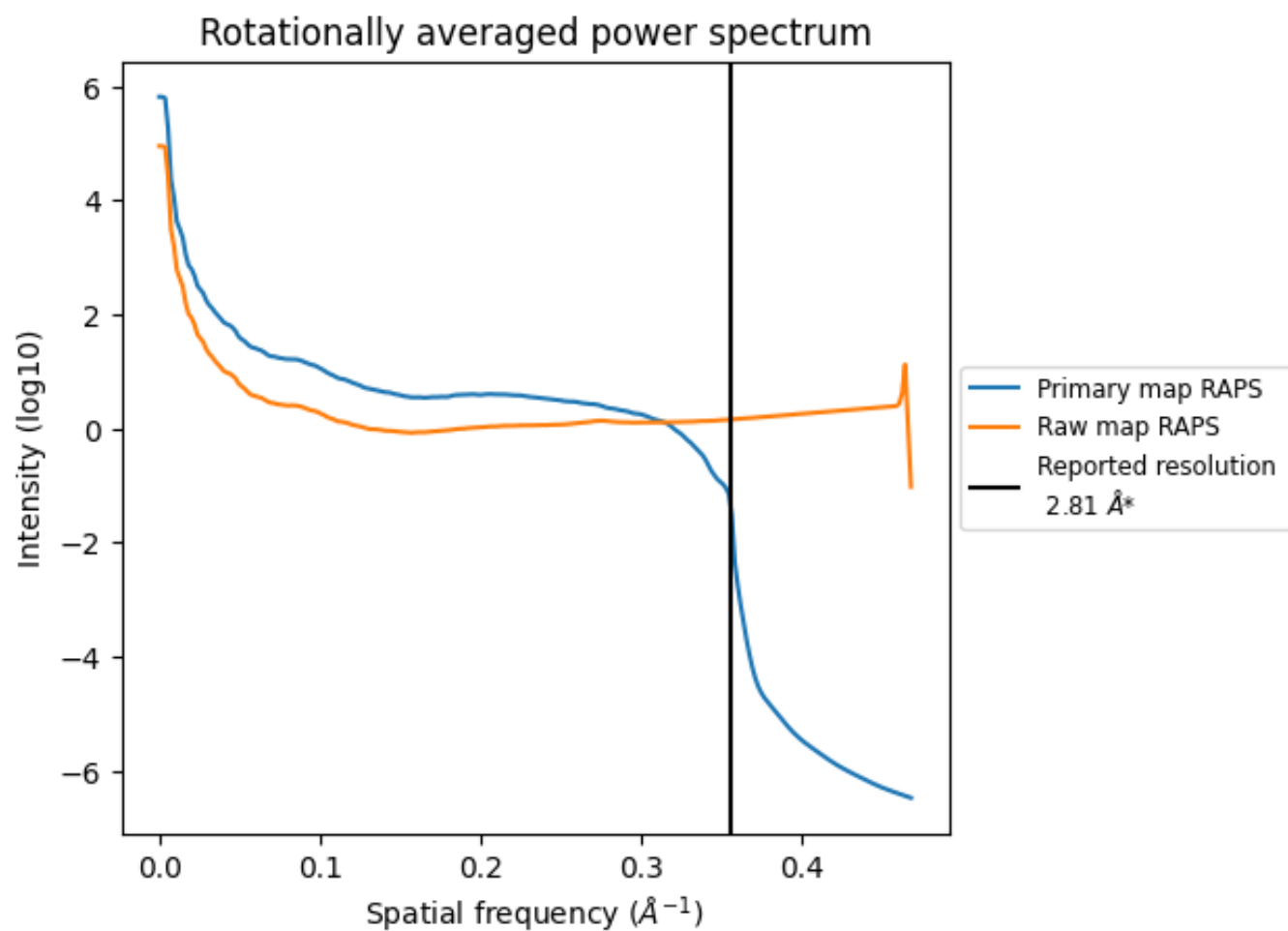
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2911 nm^3 ; this corresponds to an approximate mass of 2629 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 ⓘ

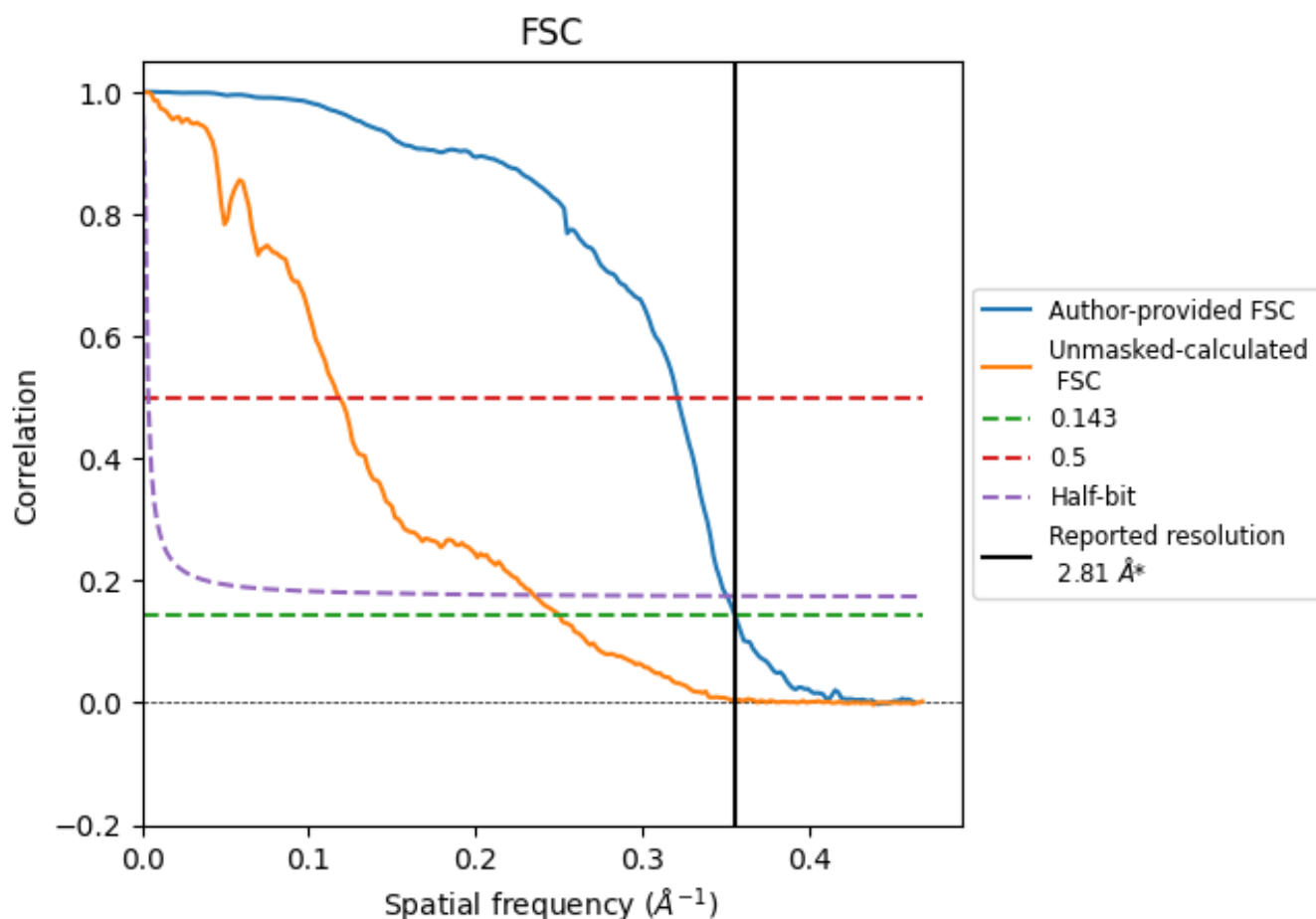


*Reported resolution corresponds to spatial frequency of 0.356 $\text{\AA}^{-1}$

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 0.356 Å⁻¹

8.2 Resolution estimates [i](#)

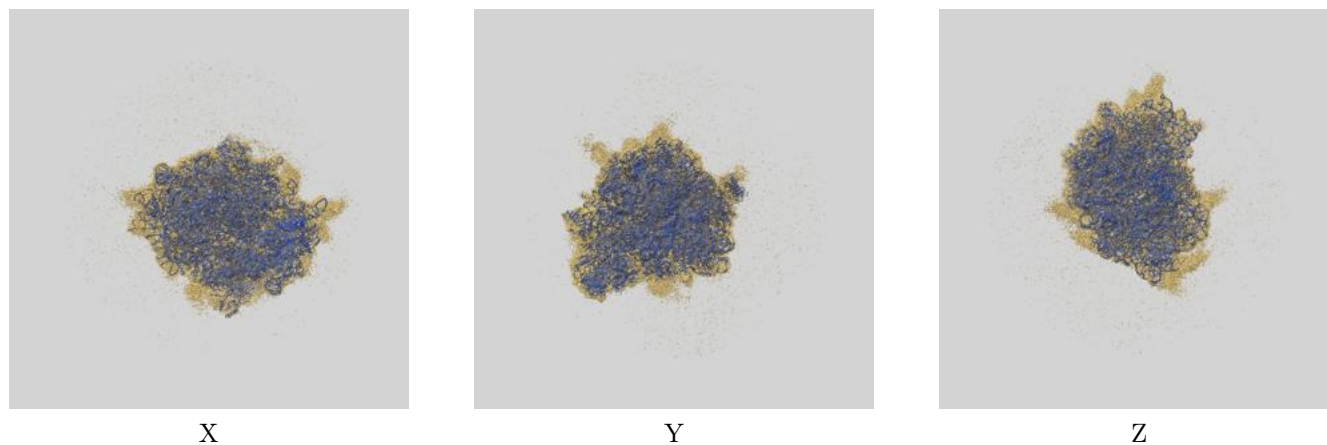
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.81	3.11	2.85
Unmasked-calculated*	4.00	8.46	4.26

*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 4.00 differs from the reported value 2.81 by more than 10 %

9 Map-model fit [i](#)

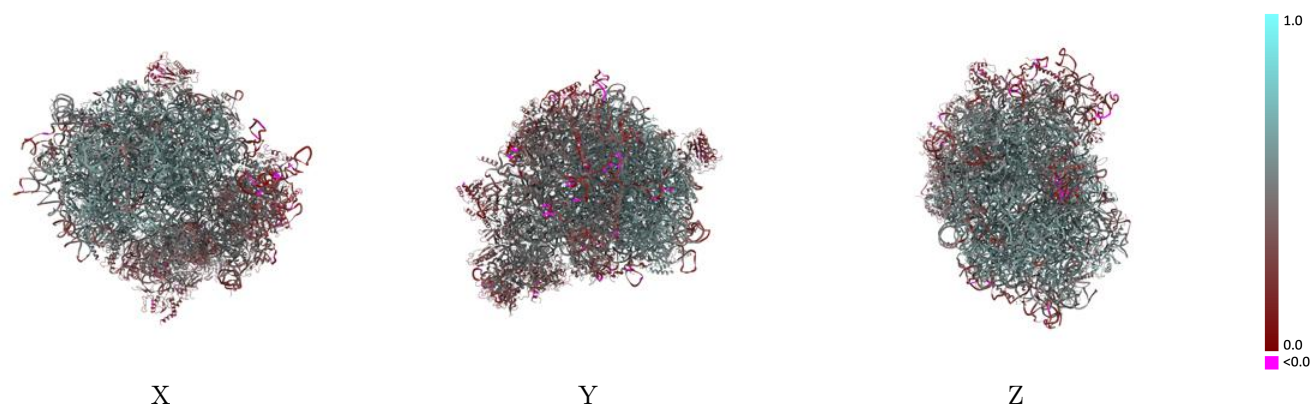
This section contains information regarding the fit between EMDB map EMD-71336 and PDB model 9P7A. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



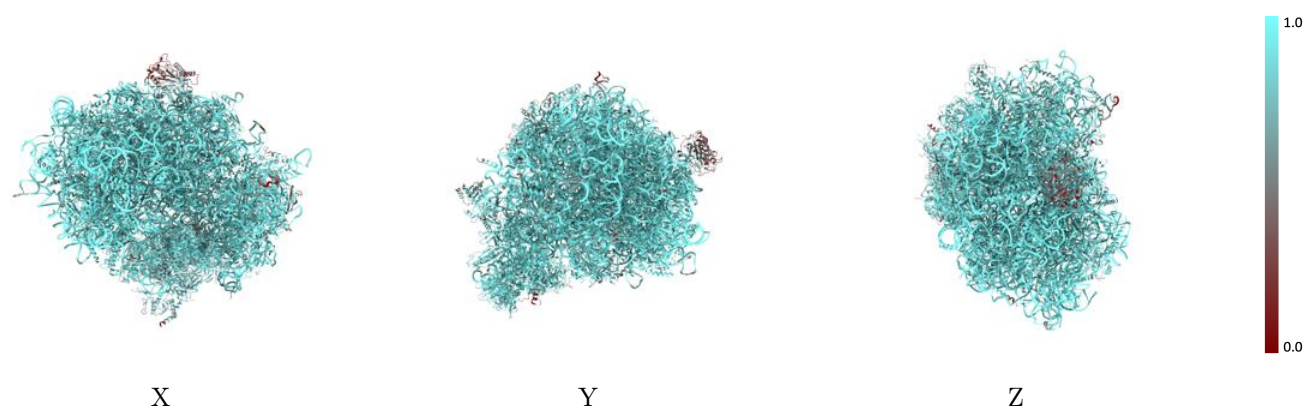
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



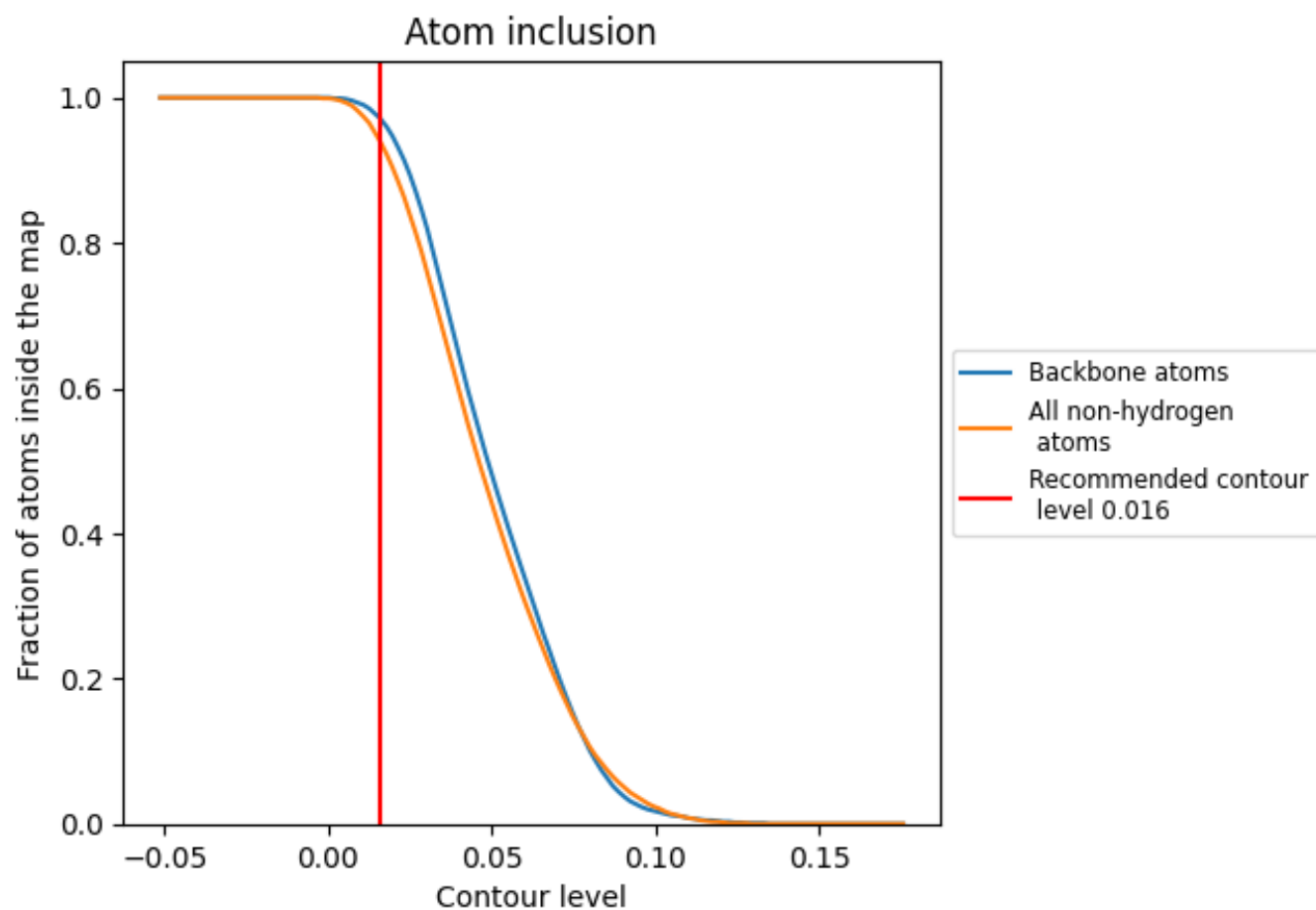
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9390	 0.4920
CA	 0.4460	 0.2670
CB	 0.8160	 0.4020
CD	 0.8760	 0.3980
CI	 0.7240	 0.4170
Et	 0.7620	 0.3260
L5	 0.9810	 0.5340
L7	 0.9970	 0.5760
L8	 0.9840	 0.5580
LA	 0.9880	 0.5970
LB	 0.9540	 0.5750
LC	 0.9610	 0.5780
LD	 0.9430	 0.5390
LE	 0.9250	 0.5220
LF	 0.9670	 0.5760
LG	 0.9070	 0.5260
LH	 0.9540	 0.5640
LI	 0.9580	 0.5780
LJ	 0.9170	 0.5090
LL	 0.9300	 0.5470
LM	 0.9700	 0.5630
LN	 0.9930	 0.6050
LO	 0.9680	 0.5790
LP	 0.9620	 0.5890
LQ	 0.9780	 0.5940
LR	 0.9270	 0.5190
LS	 0.9770	 0.5880
LT	 0.9490	 0.5650
LU	 0.8980	 0.4830
LV	 0.9730	 0.5820
LW	 0.8470	 0.3990
LX	 0.9510	 0.5550
LY	 0.9490	 0.5530
LZ	 0.9590	 0.5470
La	 0.9780	 0.5980



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Chain	Atom inclusion	Q-score
Lb	 0.9020	 0.5080
Lc	 0.9380	 0.5330
Ld	 0.9560	 0.5650
Le	 0.9750	 0.5960
Lf	 0.9860	 0.6000
Lg	 0.9590	 0.5740
Lh	 0.9420	 0.5590
Li	 0.9520	 0.5440
Lj	 0.9880	 0.5930
Lk	 0.8940	 0.5050
Ll	 0.9760	 0.5730
Lm	 0.9470	 0.5750
Ln	 0.9520	 0.5480
Lo	 0.9520	 0.5750
Lp	 0.9590	 0.5750
Lr	 0.9740	 0.5800
Ls	 0.8220	 0.3560
Lt	 0.5940	 0.2040
S2	 0.9750	 0.4470
SA	 0.8670	 0.4170
SB	 0.8570	 0.3890
SC	 0.9420	 0.4790
SD	 0.8680	 0.4090
SE	 0.9230	 0.4270
SF	 0.8680	 0.3960
SG	 0.8370	 0.2970
SH	 0.8170	 0.3340
SI	 0.8940	 0.4370
SJ	 0.9030	 0.4330
SK	 0.8700	 0.3960
SL	 0.8940	 0.4700
SM	 0.6620	 0.2170
SN	 0.9110	 0.4550
SO	 0.9000	 0.4220
SP	 0.8770	 0.4320
SQ	 0.8980	 0.3890
SR	 0.8550	 0.3760
SS	 0.8440	 0.3910
ST	 0.9060	 0.3950
SU	 0.8680	 0.3830
SV	 0.9150	 0.4400
SW	 0.9500	 0.4830

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Chain	Atom inclusion	Q-score
SX	 0.9100	 0.4940
SY	 0.8470	 0.3530
SZ	 0.7840	 0.3410
Sa	 0.9330	 0.4680
Sb	 0.8780	 0.4030
Sc	 0.8170	 0.3650
Sd	 0.9460	 0.4770
Se	 0.8360	 0.4060
Sf	 0.7770	 0.2710
Sg	 0.8470	 0.3220