



Full wwPDB EM Validation Report ⓘ

Jun 26, 2026 – 01:18 AM EDT

PDB ID : 9P7E / pdb_00009p7e
EMDB ID : EMD-71339
Title : In situ human Hibernating class5 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 2.59 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:

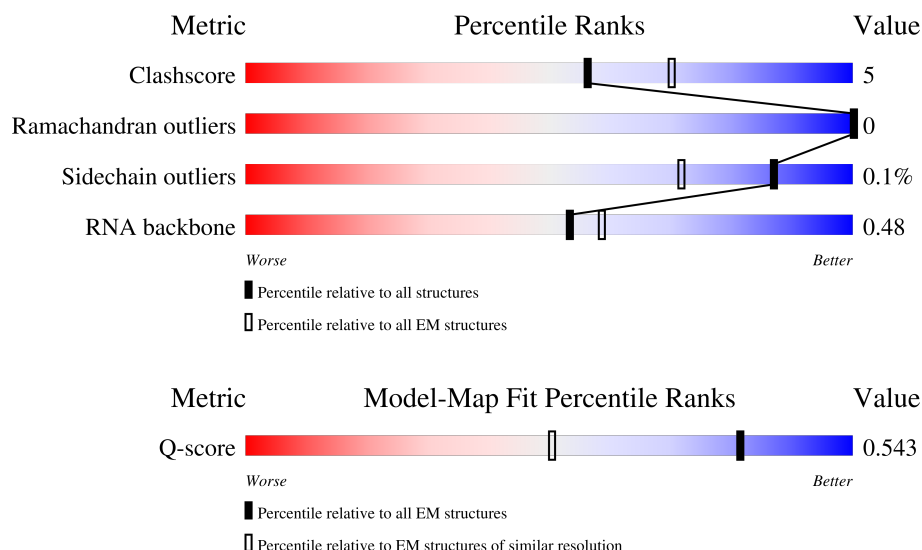
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.59 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.



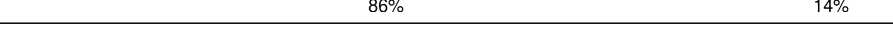
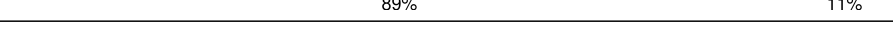
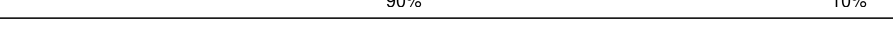
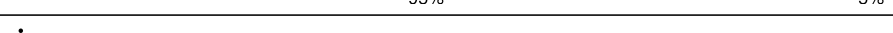
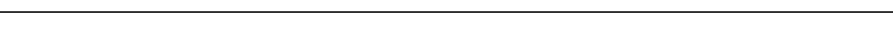
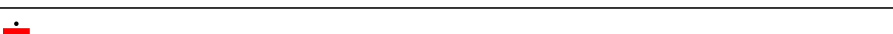
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7741 (2.09 - 3.09)

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	206	
3	L5	5070	

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Mol	Chain	Length	Quality of chain
4	L7	120	 84% 14%
5	L8	156	 68% 29%
6	LA	248	 85% 15%
7	LB	402	 86% 14%
8	LC	368	 91% 9%
9	LD	293	 90% 10%
10	LE	250	 86% 10%
11	LF	225	 90% 10%
12	LG	241	 89% 11%
13	LH	190	 88% 12%
14	LI	213	 85% 11%
15	LJ	176	 84% 13%
16	LL	210	 86% 14%
17	LM	139	 89% 11%
18	LN	203	 86% 14%
19	LO	201	 90% 10%
20	LP	153	 84% 16%
21	LQ	187	 95% 5%
22	LR	187	 87% 13%
23	LS	175	 95% 5%
24	LT	159	 91% 9%
25	LU	101	 86% 14%
26	LV	131	 89% 11%
27	LW	124	 77% 16% 6%
28	LX	120	 92% 8%

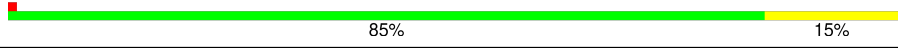
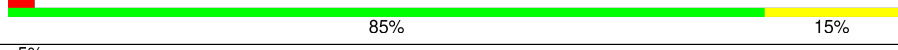
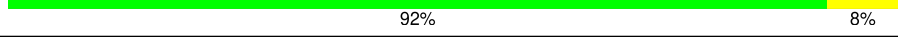
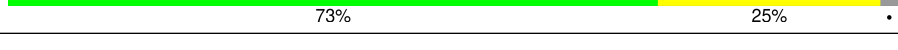
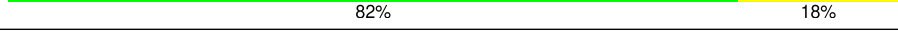
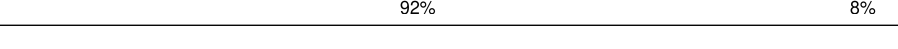
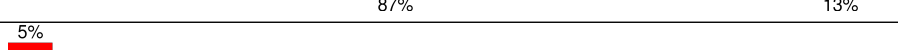
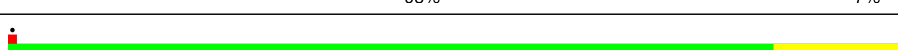
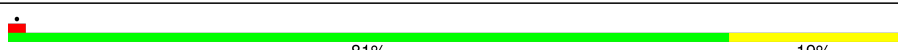
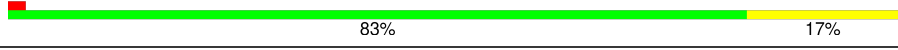
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Mol	Chain	Length	Quality of chain
29	LY	134	
30	LZ	135	
31	La	147	
32	Lb	121	
33	Lc	98	
34	Ld	107	
35	Le	128	
36	Lf	109	
37	Lg	114	
38	Lh	122	
39	Li	102	
40	Lj	86	
41	Lk	69	
42	Ll	50	
43	Lm	52	
44	Ln	24	
45	Lo	105	
46	Lp	91	
47	Lr	125	
48	Ls	196	
49	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 228141 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	204	Total	C	N	O	S	0	0
			1650	1046	317	273	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		

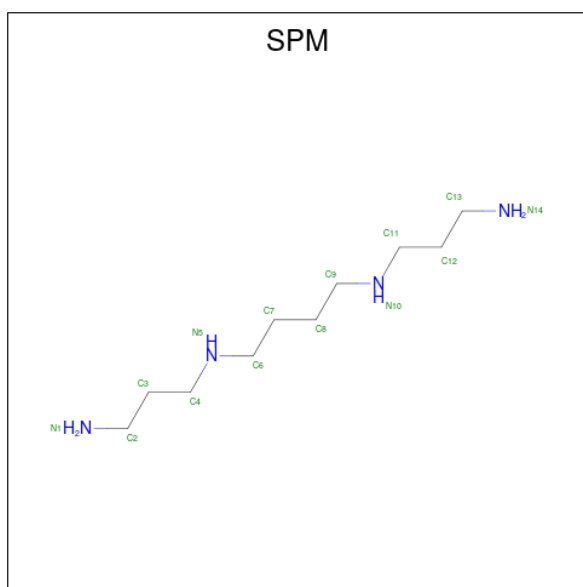
- Molecule 86 is a protein called Proliferation-associated protein 2G4.

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).

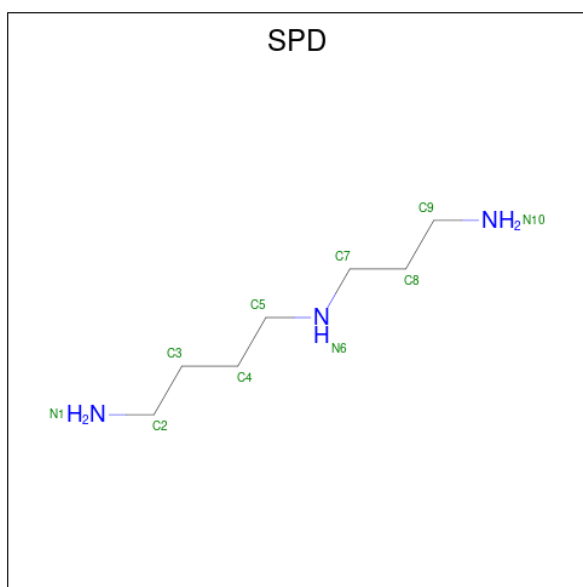
Mol	Chain	Residues	Atoms		AltConf
87	L5	178	Total	Mg	0
			178	178	
87	L7	3	Total	Mg	0
			3	3	
87	L8	5	Total	Mg	0
			5	5	
87	LA	1	Total	Mg	0
			1	1	
87	LI	1	Total	Mg	0
			1	1	
87	LP	1	Total	Mg	0
			1	1	
87	LV	1	Total	Mg	0
			1	1	
87	Le	1	Total	Mg	0
			1	1	
87	SG	1	Total	Mg	0
			1	1	
87	S2	26	Total	Mg	0
			26	26	

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



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

- Molecule 89 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (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	LN	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).

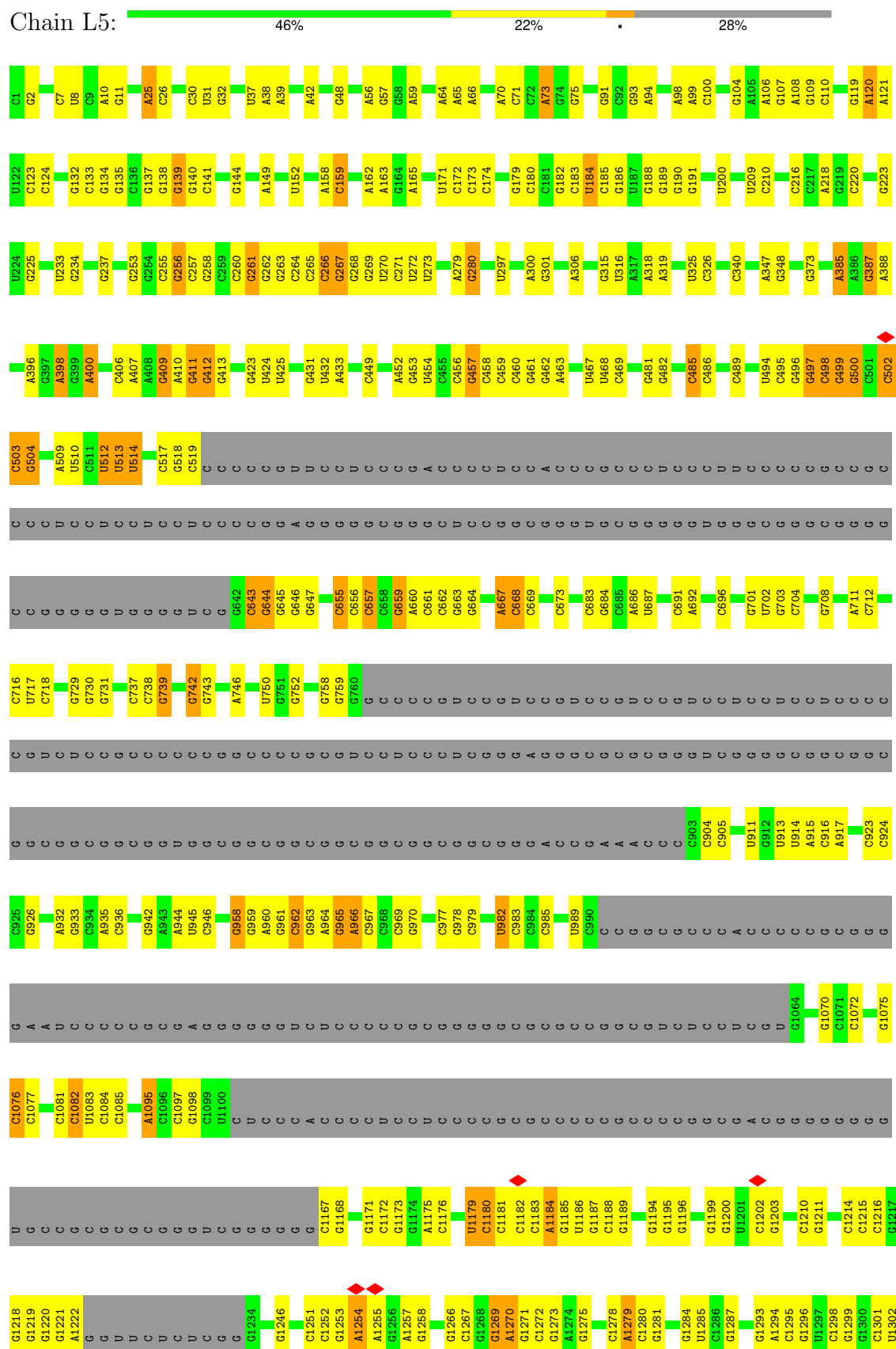
Mol	Chain	Residues	Atoms		AltConf
90	Lg	1	Total	Zn	0
			1	1	

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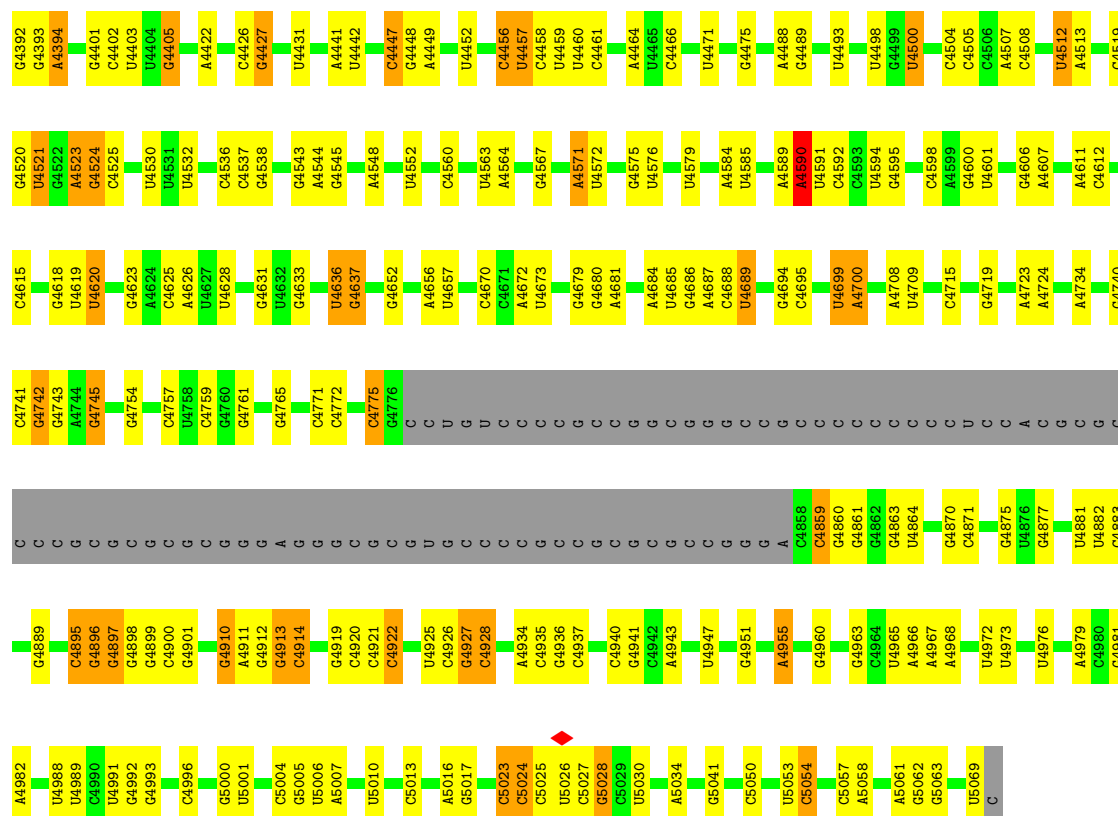
Mol	Chain	Residues	Atoms		AltConf
90	Lj	1	Total 1	Zn 1	0
90	Lm	1	Total 1	Zn 1	0
90	Lo	1	Total 1	Zn 1	0
90	Lp	1	Total 1	Zn 1	0
90	Sa	1	Total 1	Zn 1	0

● Molecule 3: 28S rRNA



U2900	G2754	G2618	C2497	U2372	C	G	G	U1997	C1893	U1781	A1701	U1582	U1428	A1307
G2901	G2760	C2627	C2498	C2373	C	G	G	G2001	A1897	U1782	C1702	U1588	C1437	C1308
G2902	G2761	G2632	G2502	C2383	G	U	G	A2002	G2003	A1787	C1703	U1589	U1438	C1309
G2903	U2761	U2632	C2503	A2396	C	U	G	U2004	A1907	A1788	G1704	C1590	C1439	U1317
G2904	G2762	U2633	C2504	A2396	U	U	G	G2005	A1908	U1792	A1706	U1591	C1442	C1318
G2905	U2763	G2638	C2505	G2397	C	G	G	C2016	C1914	U1797	C	U1596	A1443	A1322
G2906	A2764	U2639	G2506	A2401	C	G	G	A2017	A1917	G1797	G	U1596	A1444	A1323
U2907	U2769	U2640	A2513	G2405	C	G	G	C2018	U1918	A1801	A	U1596	U1445	A1324
U2908	C2770	A2641	C2519	C2411	C	C	C	G2024	G1919	A1802	C	U1596	U1446	A1325
G2910	G2773	C2653	C2520	A2412	C	C	C	A2025	C1920	G1803	C	U1596	C1447	A1326
G	G	G	C2521	G2415	C	U	G	A2026	C1921	A1804	C	U1596	C1327	C1328
C	C	C	G2522	A2416	C	C	C	G2029	G1925	A1805	G1716	A1462	C1332	C1332
C	C	C	A2253	A2417	C	C	C	A2030	G1925	C1807	C1717	A1468	A1333	A1334
C	C	C	C2541	U2425	C	C	C	G2045	C1931	G1810	C1720	C1469	A1337	A1337
C	C	C	G2542	G2428	C	G	U	G2046	A1932	C1820	G1721	C1481	G1338	G1338
C	C	C	A2543	A2448	C	U	G	U2047	G1933	G1821	U1725	C1482	C1339	C1340
C	C	C	G2544	A2449	C	U	G	A2048	A1934	U1822	U1726	C1483	C1340	C1340
C	C	C	U2545	G2450	C	G	G	G2055	C1936	G1823	U1726	A1497	A1345	A1345
C	C	C	G2546	U2567	C	C	C	G2056	A1942	G1824	U1726	G1498	C1346	C1346
C	C	C	G2547	A2268	C	U	G	G2056	A1943	A1825	C1731	G1502	A1354	A1354
C	C	C	U2554	C2269	C	C	C	G2060	G1948	U1834	C1732	G1504	G1359	G1359
C	C	C	C2557	A2276	C	C	C	A2069	G1951	G1836	C1733	C1509	C1365	C1365
C	C	C	G2558	C2277	C	C	C	C2073	A1960	A1842	C1741	G1517	G1366	G1366
C	C	C	U2559	C2289	C	C	C	G2079	G1961	G1846	A1742	G1522	C1367	C1367
C	C	C	C2560	U2298	C	A	C	U2080	A1962	C1847	A1744	A1524	G1380	G1380
C	C	C	G2561	G2299	C	C	G	C2084	G1969	G1855	G1750	A1534	U1381	U1381
C	C	C	C2562	A2300	C	C	C	G2092	U1974	C1856	A1751	C1535	A1387	A1387
C	C	C	G2563	G2301	C	C	C	A2093	G1975	C1857	G1752	U1536	G1394	G1394
C	C	C	C2564	G2302	C	C	C	G2094	C1977	C1858	G1753	A1537	A1397	A1397
C	C	C	A2565	C2302	C	C	C	A2095	C1978	U1860	U1754	U1538	A1398	A1398
C	C	C	G2566	G2303	C	C	C	G2096	A1979	U1861	U1757	G1539	G1404	G1404
C	C	C	G2567	C2306	C	U	C	G2098	U1980	U1862	G1758	A1547	C1407	C1407
C	C	C	U2570	G2326	C	C	C	G2099	G1981	A1867	G1759	A1558	G1408	G1408
C	C	C	C2571	G2333	C	C	C	A2100	G1982	U1867	G1760	U1559	C1409	C1409
C	C	C	G2572	G2345	C	C	C	C2101	A1983	A1868	G1761	A1563	U1410	U1410
C	C	C	U2573	G2348	C	C	C	G2102	A1984	G1869	C1762	C1566	C1411	C1411
C	C	C	C2583	G2348	C	C	C	G2103	G1985	C1870	C1763	U1567	G1415	G1415
C	C	C	G2586	C2351	C	C	C	G2104	U1986	A1871	G1764	C1568	G1416	G1416
C	C	C	U2587	A2360	C	C	C	A2105	G1989	C1875	A1765	G1574	C1417	C1417
C	C	C	C2588	G2362	C	C	C	C2107	U1991	U1876	A1766	U1577	A1420	A1420
C	C	C	A2601	A2363	C	C	C	C2107	U1992	C1882	A1767	G1577	U1578	U1578
C	C	C	G2602	G2364	C	C	C	C2110	C1993	A1888	C1768	C1568	C1417	C1417
C	C	C	C2603	U2362	C	C	C	G2111	U1994	A1888	C1769	G1574	C1417	C1417
C	C	C	A2611	A2364	C	C	C	G2112	G1995	A1888	C1770	G1577	U1578	U1578
C	C	C	G2612	G2364	C	C	C	G	C	A1892	C1774	G1700	U1578	U1578
C	C	C	U2494	G2496	C	C	C	G	C	A1892	C1774	G1700	U1578	U1578
C	C	C	U2495	G2496	C	C	C	G	C	A1892	C1774	G1700	U1578	U1578
C	C	C	G2496	G2496	C	C	C	G	C	A1892	C1774	G1700	U1578	U1578





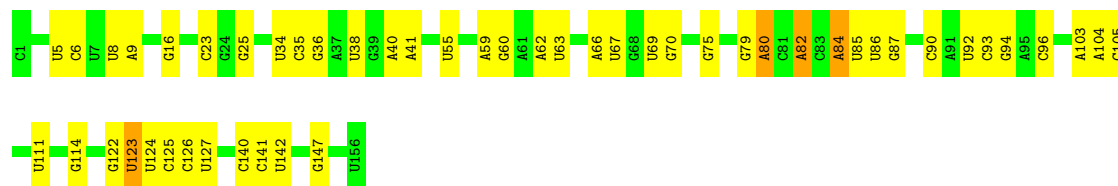
• Molecule 4: 5S rRNA

Chain L7:  84% 14%



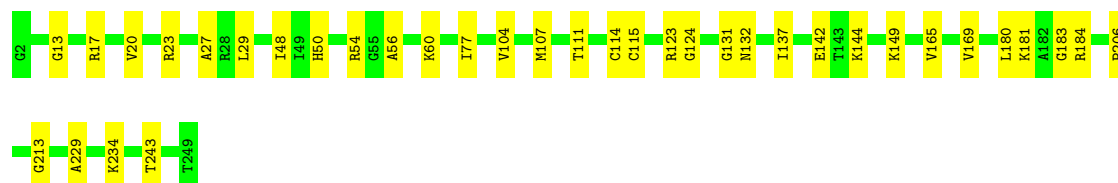
• Molecule 5: 5.8S rRNA

Chain L8:  68% 29%

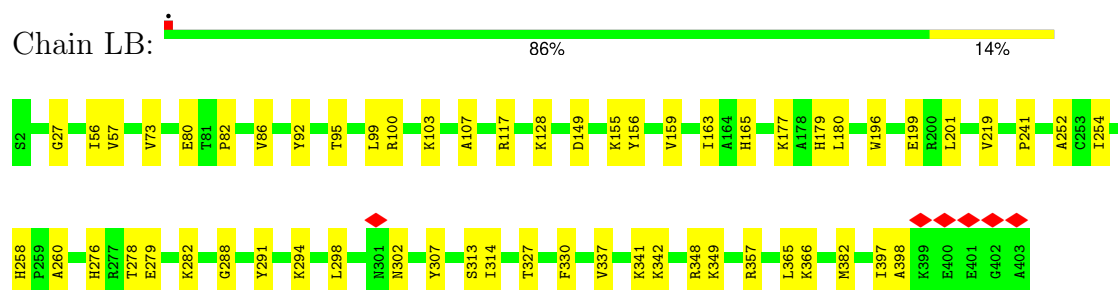


• Molecule 6: 60S ribosomal protein L8

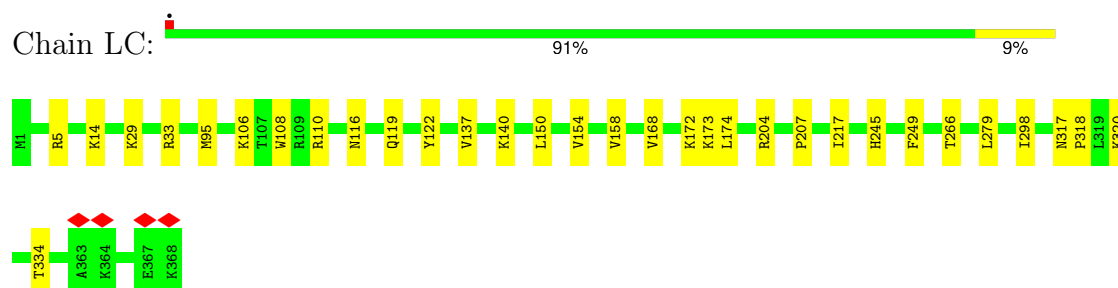
Chain LA:  85% 15%



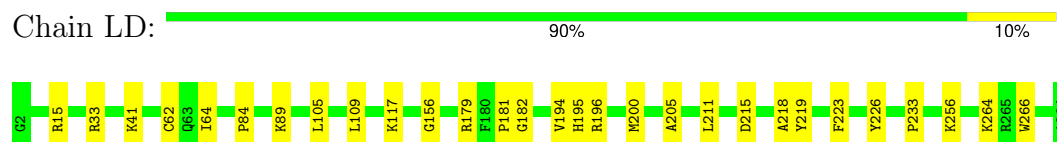
- Molecule 7: Large ribosomal subunit protein uL3



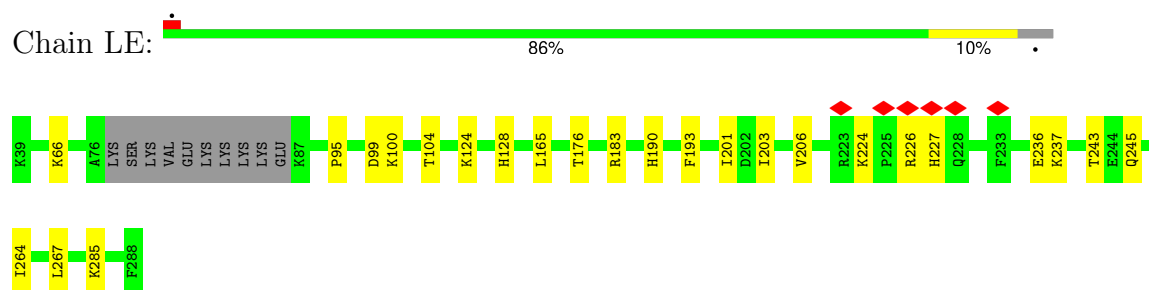
- Molecule 8: 60S ribosomal protein L4



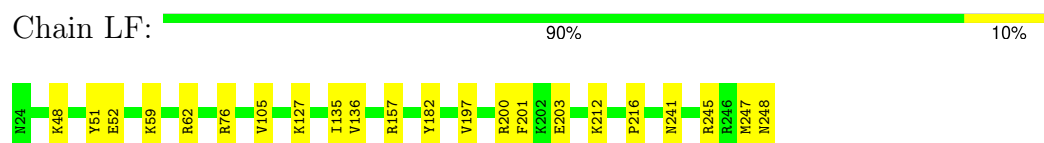
- Molecule 9: Large ribosomal subunit protein uL18



- Molecule 10: Large ribosomal subunit protein eL6

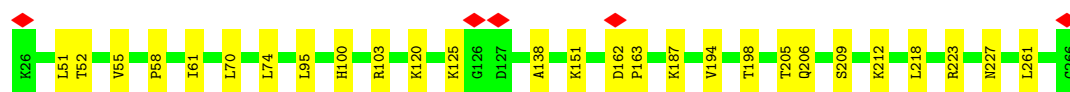


- Molecule 11: 60S ribosomal protein L7



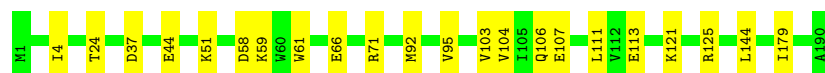
- Molecule 12: 60S ribosomal protein L7a





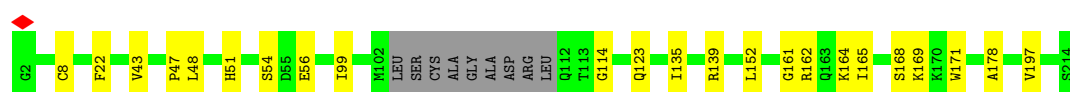
- Molecule 13: 60S ribosomal protein L9

Chain LH: 88% 12%



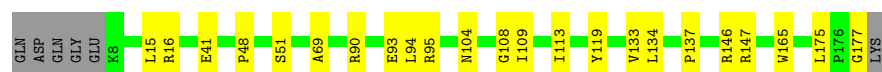
- Molecule 14: Ribosomal protein uL16-like

Chain LI: 85% 11%



- Molecule 15: 60S ribosomal protein L11

Chain LJ: 84% 13%



- Molecule 16: Large ribosomal subunit protein eL13

Chain LL: 86% 14%



- Molecule 17: 60S ribosomal protein L14

Chain LM: 89% 11%



- Molecule 18: 60S ribosomal protein L15

Chain LN: 86% 14%

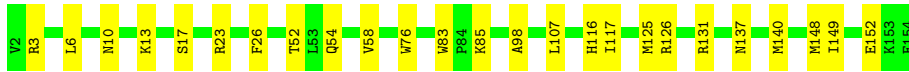
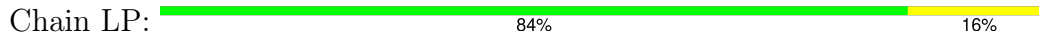


- Molecule 19: 60S ribosomal protein L13a

Chain LO: 90% 10%



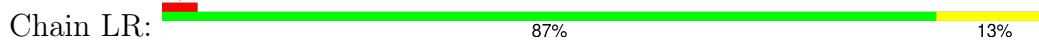
- Molecule 20: 60S ribosomal protein L17



- Molecule 21: 60S ribosomal protein L18



- Molecule 22: 60S ribosomal protein L19



- Molecule 23: 60S ribosomal protein L18a



- Molecule 24: 60S ribosomal protein L21



- Molecule 25: Heparin-binding protein HBp15



- Molecule 26: 60S ribosomal protein L23





- Molecule 27: Ribosomal protein L24

Chain LW: 77% 16% 6%



- Molecule 28: 60S ribosomal protein L23a

Chain LX: 92% 8%



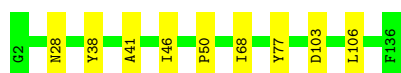
- Molecule 29: 60S ribosomal protein L26

Chain LY: 92% 8%



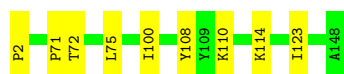
- Molecule 30: 60S ribosomal protein L27

Chain LZ: 93% 7%



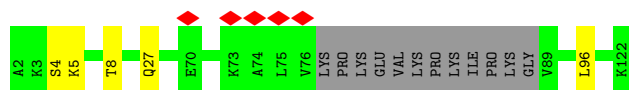
- Molecule 31: 60S ribosomal protein L27a

Chain La: 94% 6%



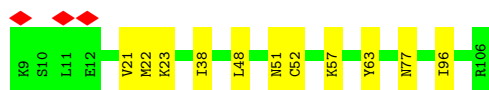
- Molecule 32: Large ribosomal subunit protein eL29

Chain Lb: 86% 10%

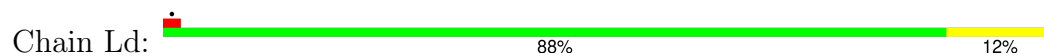


- Molecule 33: 60S ribosomal protein L30

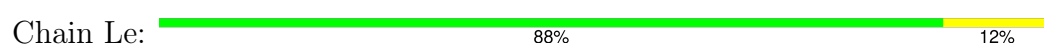
Chain Lc: 89% 11%



- Molecule 34: 60S ribosomal protein L31



- Molecule 35: 60S ribosomal protein L32



- Molecule 36: 60S ribosomal protein L35a



- Molecule 37: 60S ribosomal protein L34



- Molecule 38: 60S ribosomal protein L35



- Molecule 39: 60S ribosomal protein L36

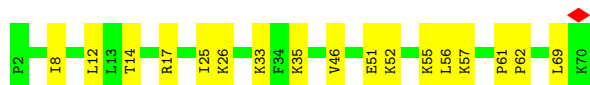
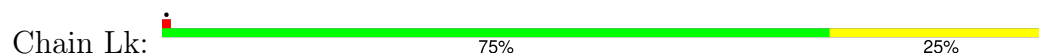


- Molecule 40: 60S ribosomal protein L37

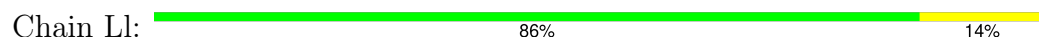




- Molecule 41: 60S ribosomal protein L38



- Molecule 42: 60S ribosomal protein L39



- Molecule 43: Large ribosomal subunit protein eL40



- Molecule 44: 60S ribosomal protein L41



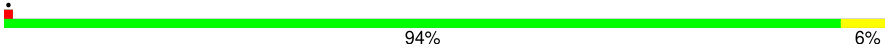
- Molecule 45: 60S ribosomal protein L36a



- Molecule 46: 60S ribosomal protein L37a



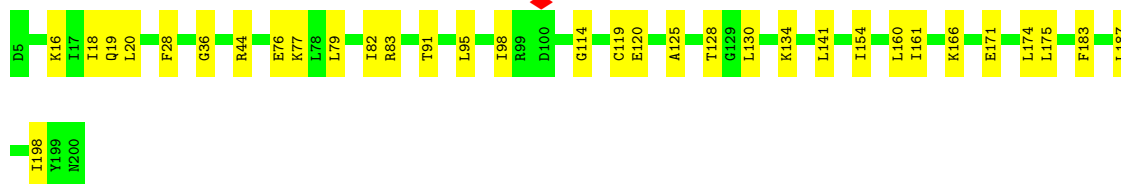
- Molecule 47: 60S ribosomal protein L28

Chain Lr:  94% 6%



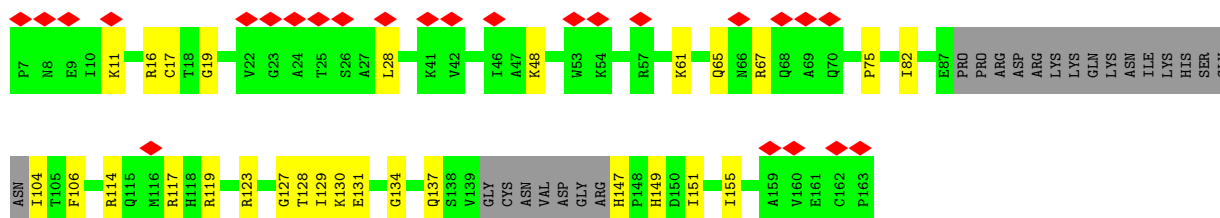
- Molecule 48: 60S acidic ribosomal protein P0

Chain Ls:  83% 17%



- Molecule 49: Large ribosomal subunit protein uL11

Chain Lt:  16% 68% 18% 15%



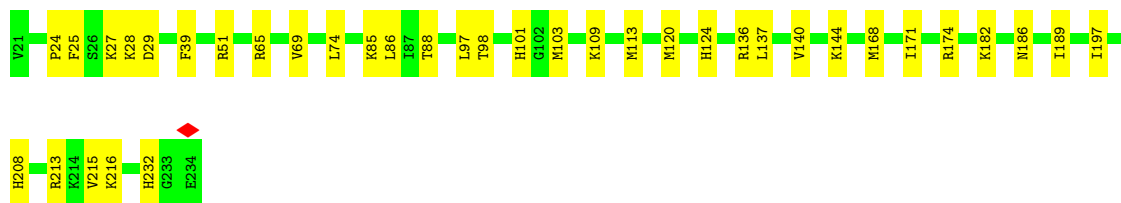
- Molecule 50: 40S ribosomal protein SA

Chain SA:  82% 18%



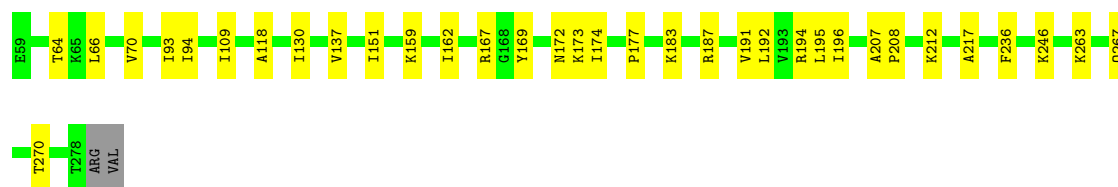
- Molecule 51: 40S ribosomal protein S3a

Chain SB:  83% 17%



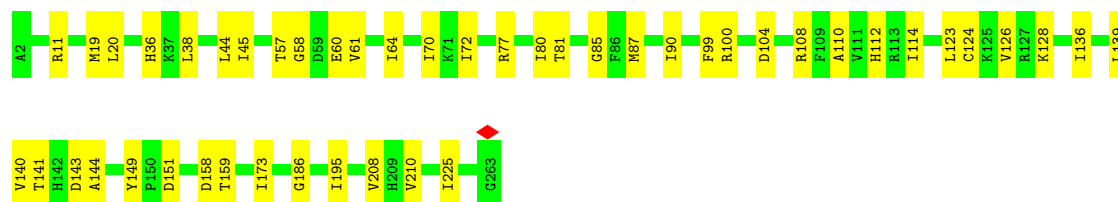
- Molecule 52: 40S ribosomal protein S2

Chain SC:  84% 15%



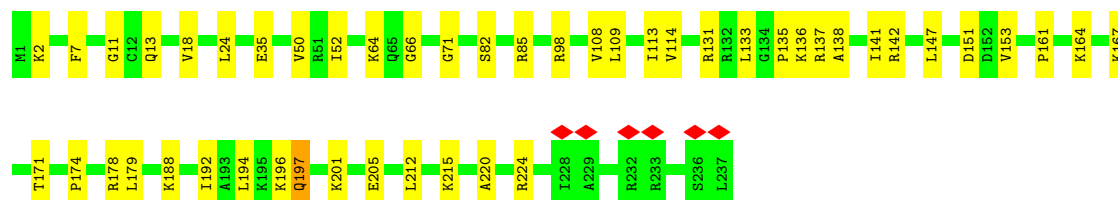
- Molecule 53: Small ribosomal subunit protein eS4, X isoform

Chain SE:  82% 18%



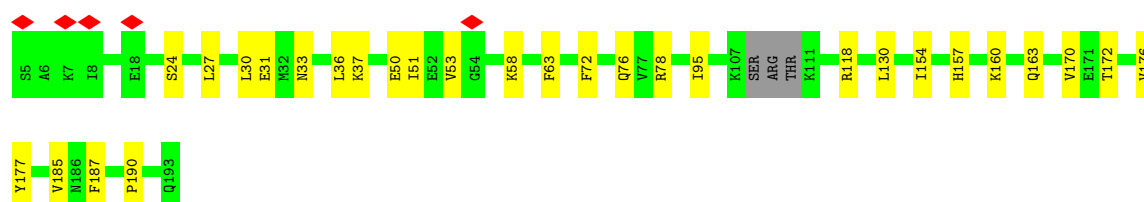
- Molecule 54: 40S ribosomal protein S6

Chain SG:  80% 20%



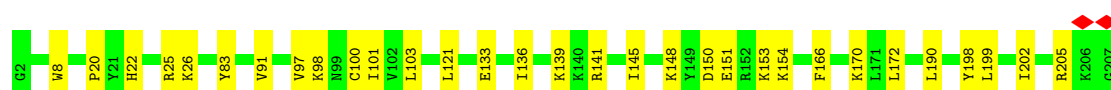
- Molecule 55: Small ribosomal subunit protein eS7

Chain SH:  83% 15%



- Molecule 56: 40S ribosomal protein S8

Chain SI:  85% 15%



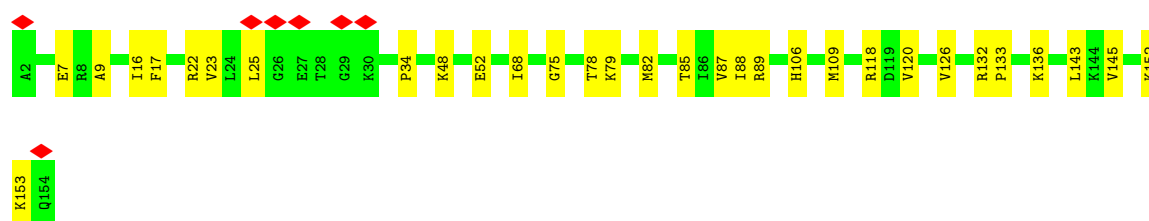
- Molecule 57: 40S ribosomal protein S9

Chain SJ:  85% 15%



- Molecule 58: 40S ribosomal protein S11

Chain SL:  5% 80% 20%



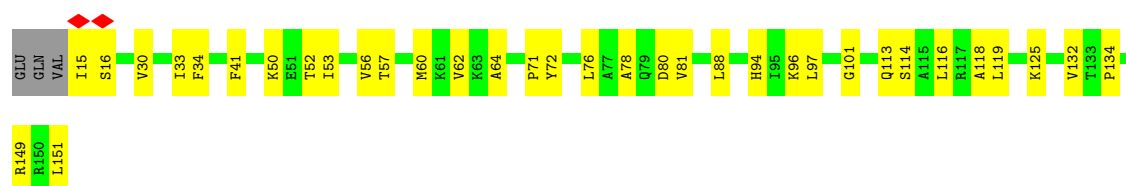
- Molecule 59: 40S ribosomal protein S13

Chain SN:  92% 8%



- Molecule 60: Small ribosomal subunit protein uS11

Chain SO:  73% 25% 2%

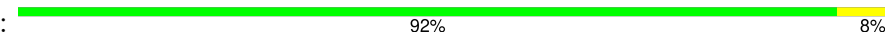


- Molecule 61: Small ribosomal subunit protein eS21

Chain SV:  82% 18%



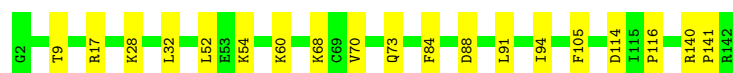
- Molecule 62: 40S ribosomal protein S15a

Chain SW:  92% 8%



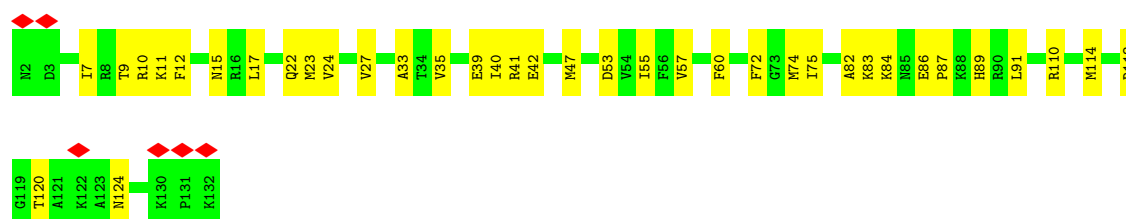
- Molecule 63: 40S ribosomal protein S23

Chain SX:  87% 13%

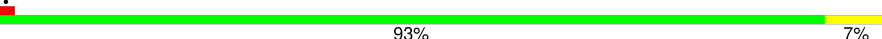


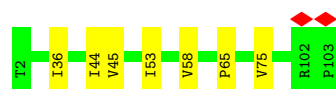
- Molecule 64: 40S ribosomal protein S24

Chain SY:  5% 72% 28%



- Molecule 65: 40S ribosomal protein S26

Chain Sa:  93% 7%



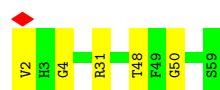
- Molecule 66: Small ribosomal subunit protein eS27

Chain Sb:  86% 14%



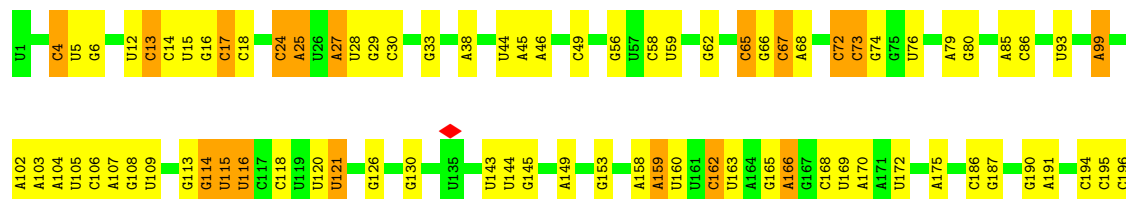
- Molecule 67: Small ribosomal subunit protein eS30

Chain Se:  91% 9%

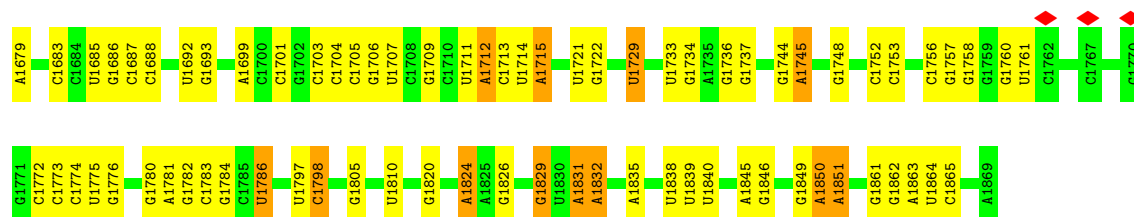


- Molecule 68: 18S rRNA

Chain S2:  58% 35% 7%

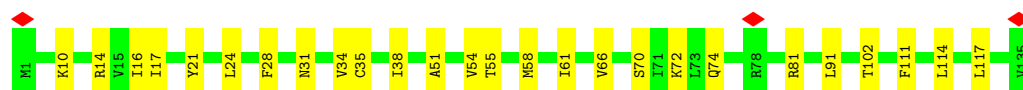


C1581	G1466	A1383	A1278	G1164	G1037	G952	G867	C739	A634	G544	U454	G351	U197
C1582	A1474	A1388	C1279	G1165	U1045	C953	A870	C746	G635	A545	A456	U352	U198
U1585	A1480	C1391	G1280	U1174	U1046	U954	A874	C748	C639	G546	C456	U354	C199
U1586	A1486	C1395	A1284	U1177	G1047	A955	A875	U749	A641	G547	C462	A360	G200
A1588	A1487	C1396	G1285	U1178	G1048	A957	A876	C751	U642	U551	A464	U361	C201
A1589	C1488	C1399	G1286	U1179	G1049	A958	A877	C752	A643	G552	A465	C362	G202
U1595	A1489	U1400	A1287	A1182	G1051	G959	C877	C753	G644	U553	A466	A363	G203
U1596	G1490	A1401	U1288	A1183	A1052	G960	C878	G785	U649	A554	A468	A364	G204
U1597	G1491	A1402	U1289	A1195	U1056	A963	C879	G786	A650	U556	G470	G207	G208
U1601	U1492	A1405	G1294	A1196	U1057	A964	C880	G787	U651	U557	G471	U367	G209
U1602	C1493	U1406	A1295	U1201	A1060	U965	C881	G788	A652	U558	G472	U368	U214
G1603	U1494	U1407	G1296	U1202	U1061	U966	U888	G789	A655	G559	C473	C369	U222
G1604	G1495	U1408	A1203	U1203	A1062	G971	U889	C790	G656	G560	G474	A371	C223
G1605	U1496	A1409	A1301	A1204	C1067	A972	U890	C791	G659	A561	G482	U372	A224
G1606	G1497	U1410	G1302	G1207	U1080	A980	U891	C792	G660	U562	C483	G373	G291
U1609	U1498	C1410	A1303	A1208	U1081	A981	U892	C793	U661	U563	A484	G377	A292
G1610	U1499	G1411	U1304	A1215	A1082	G982	U893	A794	A662	G565	U487	C382	C293
U1616	G1500	G1412	C1308	C1216	U1083	G985	U894	A795	A663	C568	C492	U384	U300
G1617	U1501	A1413	U1309	A1217	A1084	G986	U895	C796	A664	A569	A493	G385	A301
G1618	U1502	G1414	U1310	A1218	C1085	A987	U896	C797	A665	C570	C494	G386	A302
A1619	G1507	C1415	U1311	C1219	C1086	A988	U897	C798	A666	U573	C495	U387	C303
A1620	C1513	G1416	U1312	A1220	C1087	A989	U898	U799	A667	A576	C496	A389	C306
U1621	G1514	C1417	G1316	G1221	U1088	A990	U899	U800	A668	U582	C501	A398	G307
U1622	G1515	C1418	C1317	G1222	C1089	A991	U900	U801	A669	A583	C502	U406	G308
A1623	C1521	C1419	G1318	A1223	U1090	G992	U901	A809	A670	G588	G509	G407	G309
U1627	G1522	A1420	U1319	G1224	A1100	A992	A903	U814	A671	A590	A516	A414	C310
U1633	A1533	G1421	G1320	U1227	U1101	A996	U906	G821	A672	G589	A522	U428	C311
C1627	C1534	C1422	U1321	A1228	G1102	A997	U907	U822	C676	A590	A525	G432	G312
A1630	U1535	G1423	G1322	G1229	C1106	A998	A908	U823	C677	C592	A526	A433	G316
U1637	G1536	C1433	U1323	U1232	G1107	A999	U909	C824	G677	C593	A527	A434	C317
A1638	A1537	C1434	G1324	U1238	C1108	A1000	A913	A827	U681	G594	A528	A435	A318
G1639	G1540	C1435	C1331	U1242	U1109	U1001	A913	A827	G684	U591	G600	A436	C319
U1643	G1541	C1436	G1332	U1243	C1110	U1002	A913	A827	A685	C592	G601	U429	C323
C1644	C1542	A1438	U1337	U1244	C1111	G1003	A913	A827	A686	C593	A529	G432	C324
C1645	A1545	A1439	G1338	U1244	C1112	G1004	A913	A827	A687	C594	A530	A433	C325
C1646	G1546	U1442	U1339	B8N1248	A1119	A1005	G925	A837	A688	U595	A531	A434	C326
U1647	G1550	G1447	G1354	A1251	A1133	A1006	G926	A838	U689	U596	A532	C441	G327
G1648	U1551	A1448	C1355	A1252	G1134	A1007	G927	A839	G690	U597	A533	C442	G328
U1651	G1552	G1449	G1356	A1253	U1013	A1008	G928	C834	G691	A534	A534	U443	G329
G1652	U1553	C1450	A1357	G1256	C1138	A1009	G929	C835	G692	A535	A535	G444	G330
U1653	G1554	G1451	U1358	G1257	U1139	A1010	G930	C836	G693	A536	A536	U445	G331
G1654	U1555	A1454	U1359	G1258	G1140	A1011	G931	A847	G694	A537	A537	A448	G332
U1655	G1556	G1455	G1365	G1259	A1144	A1012	U940	C851	G695	A538	A538	A449	G333
A1663	U1557	A1456	U1366	A1259	A1145	A1013	C941	G852	G696	A539	A539	A450	C334
G1664	C1574	G1457	U1367	C1272	A1146	U1014	C942	G853	G697	A540	A540	C346	G335
G1665	U1575	U1458	U1371	C1273	A1147	A1015	G943	G854	G698	A541	A541	G347	C336
U1672	U1576	G1461	A1378	G1274	A1148	A1016	U944	G855	U732	A542	A542	A348	A349
	A1579	U1462	A1379	G1275	A1149	A1017	U945	G856	C733	U628	U543	G452	C350
	A1580	U1463	A1382	G1276	C1153	A1018	G946	U863	C734	A627	U544	A453	C351
				C1277	U1154	A1019	G947	A865	C735	U631	C543	C454	C352



- Molecule 69: Small ribosomal subunit protein eS17

Chain SR: 81% 19%



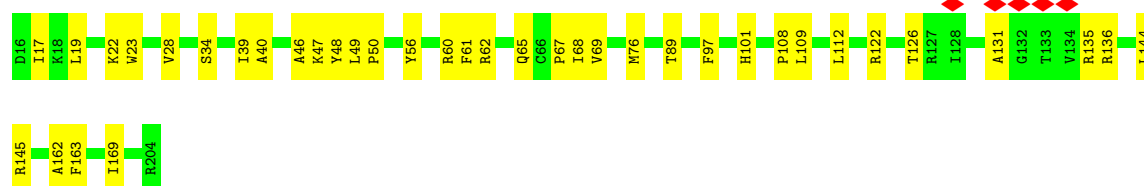
- Molecule 70: Small ribosomal subunit protein uS3

Chain SD: 82% 18%



- Molecule 71: 40S ribosomal protein S5

Chain SF: 80% 20%



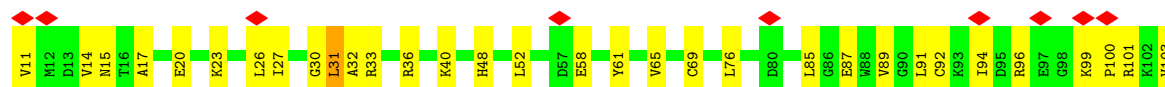
- Molecule 72: 40S ribosomal protein S10

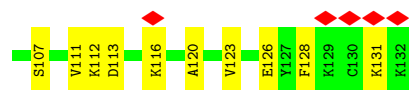
Chain SK: 74% 26%



- Molecule 73: Small ribosomal subunit protein eS12

Chain SM: 11% 66% 34%





- Molecule 74: Small ribosomal subunit protein uS19

Chain SP: 90% 10%



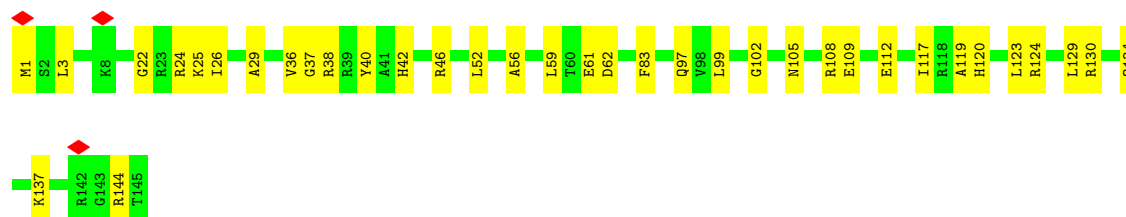
- Molecule 75: Small ribosomal subunit protein uS9

Chain SQ: 83% 17%



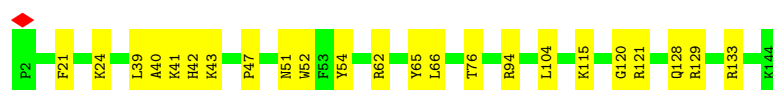
- Molecule 76: 40S ribosomal protein S18

Chain SS: 75% 25%



- Molecule 77: 40S ribosomal protein S19

Chain ST: 84% 16%



- Molecule 78: 40S ribosomal protein S20

Chain SU: 77% 23%

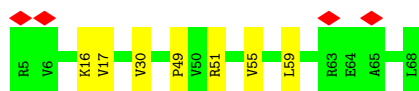
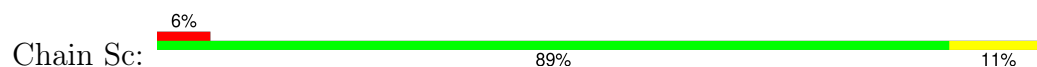


- Molecule 79: Small ribosomal subunit protein eS25

Chain SZ: 77% 23%



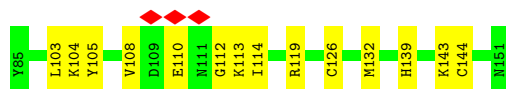
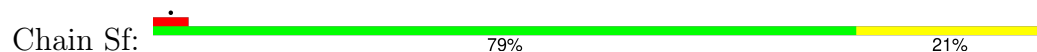
- Molecule 80: 40S ribosomal protein S28



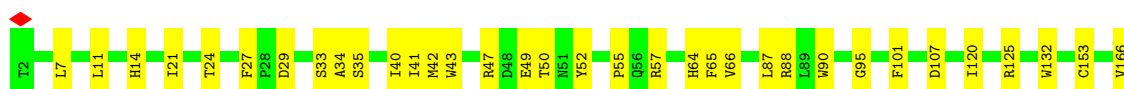
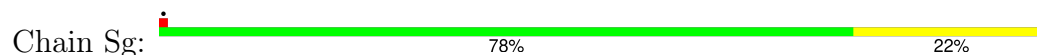
- Molecule 81: 40S ribosomal protein S29



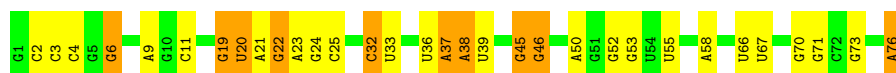
- Molecule 82: Ubiquitin-40S ribosomal protein S27a



- Molecule 83: Receptor of activated protein C kinase 1

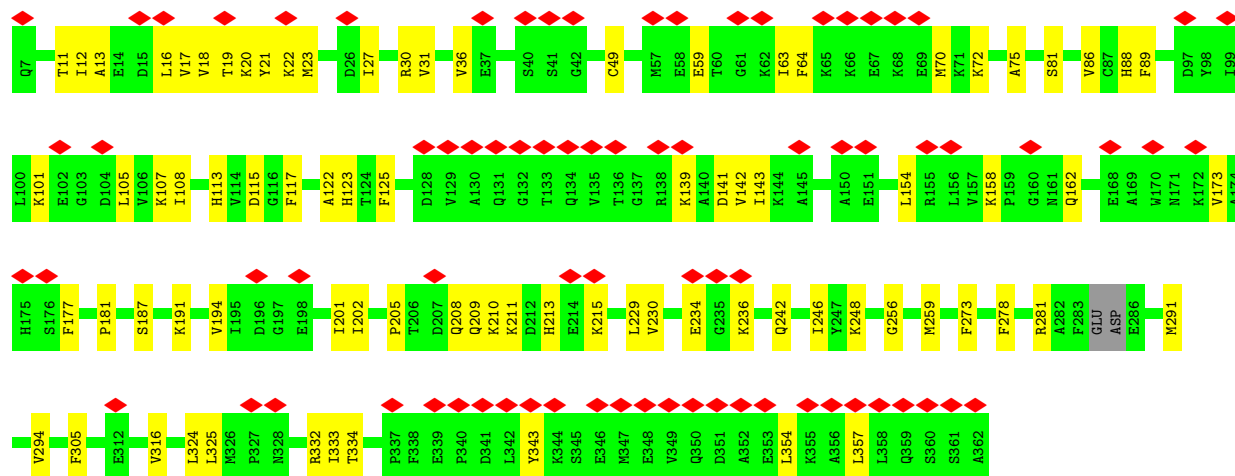
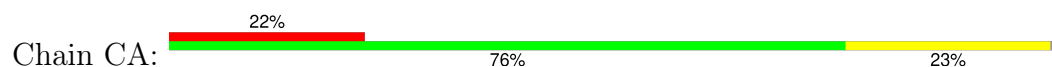


- Molecule 84: E site tRNA



- Molecule 85: Elongation factor 2

Response	Percentage
Yes	80%
No	19%
Don't know	1%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123628	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	0.391	Depositor
Minimum map value	-0.115	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.21	0/447	0.34	0/592
2	CI	0.14	0/247	0.27	0/323
3	L5	0.40	0/85098	0.35	0/132762
4	L7	0.39	0/2861	0.29	0/4459
5	L8	0.40	0/3631	0.31	0/5657
6	LA	0.40	0/1936	0.47	0/2596
7	LB	0.37	0/3306	0.43	0/4424
8	LC	0.38	0/2981	0.42	0/4002
9	LD	0.31	0/2428	0.37	0/3252
10	LE	0.30	0/1973	0.47	0/2645
11	LF	0.37	0/1905	0.38	0/2539
12	LG	0.32	0/1960	0.44	0/2637
13	LH	0.33	0/1537	0.42	0/2066
14	LI	0.33	0/1689	0.34	0/2255
15	LJ	0.27	0/1385	0.41	0/1852
16	LL	0.33	0/1732	0.37	0/2315
17	LM	0.34	0/1161	0.42	0/1554
18	LN	0.42	0/1746	0.42	0/2338
19	LO	0.38	0/1682	0.43	0/2250
20	LP	0.37	0/1268	0.43	0/1701
21	LQ	0.38	0/1537	0.41	0/2052
22	LR	0.31	0/1582	0.35	0/2091
23	LS	0.37	0/1493	0.39	0/2003
24	LT	0.35	0/1326	0.37	0/1770
25	LU	0.28	0/839	0.53	0/1126
26	LV	0.36	0/993	0.40	0/1332
27	LW	0.29	0/959	0.42	0/1270
28	LX	0.34	0/1002	0.36	0/1345
29	LY	0.34	0/1132	0.41	0/1504
30	LZ	0.32	0/1130	0.38	0/1507
31	La	0.38	0/1191	0.36	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.30	0/889	0.45	0/1175
33	Lc	0.33	0/774	0.43	0/1038
34	Ld	0.36	0/903	0.42	0/1216
35	Le	0.40	0/1071	0.39	0/1429
36	Lf	0.39	0/895	0.42	0/1198
37	Lg	0.34	0/916	0.35	0/1220
38	Lh	0.33	0/1023	0.41	0/1351
39	Li	0.27	0/843	0.37	0/1115
40	Lj	0.41	0/720	0.44	0/952
41	Lk	0.29	0/575	0.39	0/761
42	Ll	0.37	0/454	0.34	0/599
43	Lm	0.34	0/435	0.40	0/575
44	Ln	0.31	0/231	0.33	0/294
45	Lo	0.34	0/876	0.37	0/1156
46	Lp	0.36	0/718	0.39	0/953
47	Lr	0.37	0/1017	0.42	0/1364
48	Ls	0.20	0/1519	0.37	0/2052
49	Lt	0.20	0/1009	0.52	0/1363
50	SA	0.26	0/1778	0.39	0/2416
51	SB	0.22	0/1765	0.41	0/2362
52	SC	0.28	0/1744	0.41	0/2357
53	SE	0.24	0/2118	0.38	0/2849
54	SG	0.20	0/1946	0.39	0/2590
55	SH	0.21	0/1519	0.43	0/2033
56	SI	0.23	0/1715	0.41	0/2287
57	SJ	0.24	0/1550	0.39	0/2069
58	SL	0.26	0/1268	0.34	0/1696
59	SN	0.25	0/1232	0.37	0/1656
60	SO	0.26	0/1037	0.41	0/1391
61	SV	0.24	0/643	0.38	0/860
62	SW	0.28	0/1051	0.40	0/1406
63	SX	0.31	0/1116	0.41	0/1490
64	SY	0.22	0/1083	0.42	0/1438
65	Sa	0.28	0/836	0.39	0/1121
66	Sb	0.24	0/665	0.46	0/891
67	Se	0.22	0/465	0.42	0/612
68	S2	0.29	0/39756	0.30	0/61939
69	SR	0.22	0/1105	0.44	0/1484
70	SD	0.24	0/1793	0.38	0/2414
71	SF	0.20	0/1516	0.41	0/2037
72	SK	0.22	0/851	0.44	0/1147
73	SM	0.18	0/950	0.39	0/1275
74	SP	0.23	0/1003	0.41	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SQ	0.21	0/1160	0.42	0/1553
76	SS	0.19	0/1216	0.38	0/1628
77	ST	0.19	0/1131	0.37	0/1515
78	SU	0.23	0/831	0.43	0/1115
79	SZ	0.20	0/604	0.42	0/810
80	Sc	0.21	0/508	0.44	0/680
81	Sd	0.24	0/470	0.33	0/623
82	Sf	0.18	0/560	0.46	0/745
83	Sg	0.20	0/2493	0.43	0/3394
84	Et	0.24	0/1778	0.41	0/2767
85	CB	0.24	0/6734	0.42	2/9094 (0.0%)
86	CA	0.18	0/2810	0.40	0/3780
All	All	0.34	0/239825	0.37	2/350487 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	CB	665	ILE	N-CA-C	-6.82	105.84	111.91
85	CB	475	VAL	N-CA-C	-6.21	106.45	112.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CD	440	0	402	11	0
2	CI	247	0	283	3	0
3	L5	78444	0	39720	499	0
4	L7	2561	0	1295	6	0
5	L8	3315	0	1685	16	0
6	LA	1898	0	1993	23	0
7	LB	3238	0	3376	41	0
8	LC	2927	0	3104	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	LD	2382	0	2410	18	0
10	LE	1935	0	2096	16	0
11	LF	1870	0	1996	16	0
12	LG	1927	0	2074	16	0
13	LH	1518	0	1601	14	0
14	LI	1650	0	1686	14	0
15	LJ	1362	0	1399	13	0
16	LL	1701	0	1818	23	0
17	LM	1138	0	1204	11	0
18	LN	1701	0	1749	24	0
19	LO	1650	0	1794	14	0
20	LP	1242	0	1269	16	0
21	LQ	1513	0	1628	6	0
22	LR	1566	0	1729	18	0
23	LS	1453	0	1490	6	0
24	LT	1298	0	1366	10	0
25	LU	825	0	850	9	0
26	LV	979	0	1039	10	0
27	LW	945	0	1003	14	0
28	LX	985	0	1066	8	0
29	LY	1115	0	1205	7	0
30	LZ	1107	0	1182	6	0
31	La	1162	0	1213	6	0
32	Lb	876	0	948	5	0
33	Lc	764	0	804	6	0
34	Ld	888	0	930	8	0
35	Le	1053	0	1147	11	0
36	Lf	876	0	912	4	0
37	Lg	906	0	998	2	0
38	Lh	1015	0	1148	9	0
39	Li	832	0	917	5	0
40	Lj	705	0	737	3	0
41	Lk	569	0	637	11	0
42	Ll	444	0	483	7	0
43	Lm	429	0	465	1	0
44	Ln	230	0	276	2	0
45	Lo	862	0	929	8	0
46	Lp	708	0	756	3	0
47	Lr	1002	0	1068	5	0
48	Ls	1496	0	1540	21	0
49	Lt	998	0	1032	18	0
50	SA	1741	0	1746	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	SB	1738	0	1809	24	0
52	SC	1707	0	1791	22	0
53	SE	2076	0	2177	32	0
54	SG	1923	0	2089	35	0
55	SH	1497	0	1590	17	0
56	SI	1686	0	1772	23	0
57	SJ	1525	0	1640	20	0
58	SL	1247	0	1323	23	0
59	SN	1208	0	1294	7	0
60	SO	1024	0	1050	25	0
61	SV	636	0	637	12	0
62	SW	1034	0	1080	8	0
63	SX	1098	0	1167	16	0
64	SY	1065	0	1142	24	0
65	Sa	821	0	870	6	0
66	Sb	651	0	669	8	0
67	Se	459	0	503	3	0
68	S2	36952	0	18678	352	0
69	SR	1090	0	1149	20	0
70	SD	1765	0	1865	33	0
71	SF	1495	0	1549	28	0
72	SK	827	0	854	15	0
73	SM	940	0	965	28	0
74	SP	985	0	1031	9	0
75	SQ	1142	0	1213	16	0
76	SS	1198	0	1261	27	0
77	ST	1112	0	1146	16	0
78	SU	821	0	883	18	0
79	SZ	598	0	656	11	0
80	Sc	506	0	536	7	0
81	Sd	459	0	450	4	0
82	Sf	548	0	553	9	0
83	Sg	2436	0	2391	47	0
84	Et	1593	0	810	15	0
85	CB	6605	0	6679	97	0
86	CA	2764	0	2779	54	0
87	L5	178	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	LI	1	0	0	0	0
87	LP	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	LV	1	0	0	0	0
87	Le	1	0	0	0	0
87	S2	26	0	0	0	0
87	SG	1	0	0	0	0
88	L5	98	0	182	3	0
89	L5	90	0	171	3	0
89	LN	10	0	19	0	0
90	Lg	1	0	0	0	0
90	Lj	1	0	0	0	0
90	Lm	1	0	0	0	0
90	Lo	1	0	0	0	0
90	Lp	1	0	0	0	0
90	Sa	1	0	0	0	0
All	All	228141	0	172621	1955	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 (1955) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2017:A:HO2'	3:L5:2018:C:H6	1.05	0.93
68:S2:1417:C:H42	68:S2:1422:G:H22	1.14	0.91
3:L5:3754:G:H1	3:L5:3770:U:H3	1.21	0.88
16:LL:64:VAL:HA	16:LL:67:HIS:HD2	1.40	0.87
3:L5:1175:A:H2	3:L5:1185:G:H1	1.20	0.87
68:S2:1729:U:H3	68:S2:1805:G:H1	1.20	0.85
3:L5:3701:OMC:H5	3:L5:3748:A:H62	1.27	0.81
3:L5:4139:G:H21	3:L5:4140:C:H41	1.28	0.81
8:LC:5:ARG:HH22	8:LC:266:THR:HG23	1.45	0.80
68:S2:1603:G:H4'	76:SS:38:ARG:HH22	1.47	0.79
1:CD:201:ARG:HH11	70:SD:145:GLN:HG2	1.46	0.79
73:SM:99:LYS:HD2	73:SM:101:ARG:H	1.49	0.77
68:S2:925:G:H1	68:S2:1017:U:H3	1.33	0.77
3:L5:1095:A:H2	3:L5:1200:G:H1	1.32	0.76
3:L5:3937:C:H1'	18:LN:125:SER:HB3	1.68	0.75
3:L5:3951:G:H21	3:L5:4062:A:H61	1.34	0.75
75:SQ:51:LEU:HD11	75:SQ:81:ILE:HD12	1.68	0.75
49:Lt:114:ARG:HH21	49:Lt:117:ARG:HD2	1.51	0.74
68:S2:1729:U:O2	68:S2:1805:G:N2	2.20	0.74
75:SQ:58:LEU:HD22	75:SQ:108:ILE:HD11	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3946:G:H1	3:L5:4067:U:H3	1.33	0.74
54:SG:64:LYS:HE2	54:SG:82:SER:HB3	1.70	0.74
75:SQ:34:VAL:HG12	75:SQ:70:VAL:HB	1.70	0.73
64:SY:55:ILE:HG23	64:SY:75:ILE:HG22	1.69	0.73
85:CB:260:LEU:HD23	85:CB:293:ILE:HD11	1.71	0.73
3:L5:184:U:O2	3:L5:253:G:N2	2.21	0.72
7:LB:307:TYR:HE2	7:LB:366:LYS:HZ2	1.37	0.71
68:S2:1461:G:H3'	68:S2:1463:U:H3	1.55	0.71
71:SF:122:ARG:HE	80:Sc:59:LEU:HD21	1.55	0.71
86:CA:75:ALA:HB2	86:CA:113:HIS:HB3	1.72	0.71
3:L5:184:U:H3	3:L5:253:G:H1	1.37	0.71
13:LH:106:GLN:HB2	13:LH:111:LEU:HB3	1.73	0.71
54:SG:142:ARG:HG3	54:SG:147:LEU:HB2	1.72	0.71
50:SA:18:PHE:HE1	50:SA:174:MET:HE2	1.54	0.70
68:S2:1417:C:O2	68:S2:1422:G:O6	2.08	0.70
68:S2:1748:G:H1	68:S2:1786:U:H3	1.39	0.70
86:CA:154:LEU:HD11	86:CA:332:ARG:HD2	1.72	0.70
3:L5:137:G:H2'	3:L5:138:G:H8	1.56	0.70
68:S2:1354:G:H2'	68:S2:1356:G:H22	1.56	0.70
86:CA:27:ILE:HD11	86:CA:59:GLU:HG3	1.74	0.70
16:LL:64:VAL:HA	16:LL:67:HIS:CD2	2.26	0.69
3:L5:5024:C:H41	3:L5:5028:G:H21	1.39	0.69
7:LB:57:VAL:HG22	7:LB:73:VAL:HG12	1.75	0.69
3:L5:4242:U:H3	3:L5:4281:A:H2	1.38	0.69
53:SE:144:ALA:HB3	68:S2:121:OMU:HM23	1.73	0.69
71:SF:34:SER:HA	80:Sc:55:VAL:HG23	1.75	0.69
6:LA:107:MET:HB3	6:LA:111:THR:HG21	1.73	0.69
10:LE:264:ILE:HD11	10:LE:267:LEU:HD22	1.73	0.69
3:L5:2709:C:H42	86:CA:256:GLY:HA2	1.58	0.68
85:CB:745:TYR:HB2	85:CB:814:PHE:HA	1.74	0.68
3:L5:1404:G:N7	3:L5:1408:G:N2	2.40	0.68
3:L5:2458:C:H5''	18:LN:67:ARG:HD2	1.74	0.68
48:Ls:76:GLU:HA	48:Ls:79:LEU:HD13	1.74	0.68
68:S2:1354:G:H2'	68:S2:1356:G:N2	2.07	0.68
68:S2:1228:A:H2'	68:S2:1229:G:H8	1.58	0.68
20:LP:126:ARG:HH21	20:LP:140:MET:HE1	1.57	0.68
68:S2:1417:C:N4	68:S2:1422:G:H22	1.89	0.68
3:L5:4910:G:H4'	7:LB:95:THR:HG22	1.75	0.67
3:L5:758:G:H4'	13:LH:51:LYS:HE3	1.77	0.67
56:SI:91:VAL:HG21	56:SI:205:ARG:HH12	1.59	0.67
60:SO:149:ARG:HE	60:SO:151:LEU:HD11	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:CB:9:ILE:HD11	85:CB:99:LEU:HD13	1.76	0.67
76:SS:124:ARG:HE	76:SS:129:LEU:HB2	1.60	0.67
3:L5:2351:OMC:HM22	8:LC:95:MET:HG3	1.76	0.67
1:CD:195:ARG:HH21	1:CD:204:LEU:HD13	1.60	0.67
55:SH:53:VAL:HG21	55:SH:172:THR:HG22	1.77	0.67
68:S2:1581:C:H5'	68:S2:1582:C:H5	1.59	0.67
78:SU:35:VAL:HG11	78:SU:110:VAL:HG11	1.78	0.66
3:L5:1095:A:C2	3:L5:1200:G:N1	2.60	0.66
3:L5:3774:A:H2'	3:L5:3775:A:C8	2.30	0.66
25:LU:63:ILE:HG12	25:LU:72:VAL:HG22	1.78	0.66
9:LD:223:PHE:HB3	9:LD:226:TYR:HB2	1.78	0.66
68:S2:1228:A:H2'	68:S2:1229:G:C8	2.30	0.66
68:S2:1417:C:H42	68:S2:1422:G:N2	1.92	0.66
1:CD:223:ASP:HB3	70:SD:117:ARG:HG3	1.77	0.66
3:L5:2483:G:H1	3:L5:2495:U:H3	1.43	0.66
3:L5:2611:A:H5'	3:L5:2688:G:H4'	1.78	0.66
3:L5:4694:G:H4'	13:LH:71:ARG:HH12	1.61	0.66
73:SM:30:GLY:HA2	73:SM:112:LYS:HE3	1.77	0.66
85:CB:305:MET:HE1	85:CB:333:LYS:HG2	1.77	0.66
54:SG:2:LYS:HB2	54:SG:108:VAL:HG22	1.78	0.66
3:L5:3697:U:H5''	3:L5:3698:G:H5'	1.78	0.65
27:LW:4:GLU:HG2	27:LW:12:LYS:HE3	1.78	0.65
53:SE:38:LEU:HD22	68:S2:346:C:H5''	1.78	0.65
8:LC:110:ARG:HB2	18:LN:204:ARG:HH21	1.59	0.65
3:L5:3611:A:H2	3:L5:5016:A:H8	1.44	0.65
12:LG:120:LYS:HG2	12:LG:125:LYS:HB2	1.79	0.65
64:SY:10:ARG:HA	68:S2:839:C:H41	1.60	0.65
68:S2:1030:A:H2'	68:S2:1031:A2M:H8	1.78	0.65
13:LH:104:VAL:HG12	13:LH:113:GLU:HB2	1.78	0.65
54:SG:137:ARG:HD3	54:SG:178:ARG:HE	1.60	0.65
3:L5:2557:G:H1	3:L5:2570:U:H3	1.42	0.65
6:LA:137:ILE:HD11	6:LA:149:LYS:HB2	1.79	0.65
68:S2:834:C:H42	68:S2:839:C:H42	1.45	0.65
76:SS:1:MET:HG3	76:SS:3:LEU:HD23	1.78	0.64
85:CB:190:SER:HB2	85:CB:204:MET:HE1	1.80	0.64
83:Sg:257:LYS:HE2	83:Sg:259:TRP:HZ3	1.61	0.64
68:S2:12:U:HO2'	68:S2:1356:G:H8	1.45	0.64
68:S2:928:G:H2'	68:S2:929:G:C8	2.33	0.64
26:LV:13:LYS:HD2	26:LV:128:LEU:HD11	1.78	0.64
53:SE:64:ILE:HG22	53:SE:70:ILE:HD11	1.79	0.64
3:L5:1095:A:N1	3:L5:1200:G:O6	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LA:104:VAL:HA	6:LA:107:MET:HE3	1.80	0.64
9:LD:64:ILE:HD13	9:LD:109:LEU:HD22	1.80	0.64
50:SA:24:HIS:HA	50:SA:49:ILE:HG12	1.80	0.64
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.33	0.64
73:SM:128:PHE:HD1	73:SM:131:LYS:HZ3	1.45	0.64
79:SZ:58:LEU:HD12	79:SZ:62:VAL:HG21	1.78	0.64
31:La:72:THR:HG22	31:La:110:LYS:HB3	1.80	0.64
60:SO:52:THR:HG21	68:S2:952:G:H21	1.62	0.64
49:Lt:117:ARG:HG2	49:Lt:119:ARG:H	1.63	0.64
70:SD:39:VAL:HG13	70:SD:48:ILE:HG22	1.79	0.64
48:Ls:141:LEU:HD22	48:Ls:174:LEU:HD13	1.79	0.63
25:LU:47:ILE:HD12	25:LU:63:ILE:HD11	1.80	0.63
74:SP:108:LYS:HD3	76:SS:117:ILE:HG22	1.81	0.63
68:S2:981:A:H2'	68:S2:982:G:C8	2.34	0.63
79:SZ:99:LEU:HD21	79:SZ:102:LYS:HB2	1.81	0.63
49:Lt:104:ILE:HG12	49:Lt:106:PHE:HD1	1.63	0.63
3:L5:513:U:H3'	3:L5:514:U:H4'	1.81	0.63
3:L5:1995:G:H4'	49:Lt:128:THR:HB	1.80	0.63
50:SA:77:ILE:HG22	50:SA:99:ILE:HB	1.80	0.63
68:S2:1550:G:H3'	68:S2:1579:A:H61	1.64	0.63
3:L5:2495:U:H2'	3:L5:2496:G:H8	1.63	0.63
24:LT:119:ALA:HA	24:LT:122:LYS:HG2	1.80	0.63
49:Lt:65:GLN:HG3	49:Lt:67:ARG:H	1.64	0.63
83:Sg:206:LEU:HD21	83:Sg:227:LEU:HD12	1.79	0.63
86:CA:18:VAL:HG12	86:CA:22:LYS:HE2	1.81	0.63
71:SF:61:PHE:HB3	80:Sc:51:ARG:HH21	1.64	0.62
83:Sg:166:VAL:HG12	83:Sg:176:VAL:HG12	1.80	0.62
3:L5:4618:OMG:H5'	26:LV:15:ARG:HB2	1.82	0.62
3:L5:2362:U:H2'	3:L5:2363:A2M:H8	1.80	0.62
68:S2:795:A:H2'	68:S2:796:G:C8	2.34	0.62
63:SX:60:LYS:H	63:SX:114:ASP:HB2	1.64	0.62
83:Sg:259:TRP:HB3	83:Sg:266:ILE:HA	1.81	0.62
66:Sb:72:ARG:HH22	68:S2:1119:A:H2'	1.64	0.62
3:L5:4281:A:H2'	3:L5:4282:A:H2'	1.81	0.62
18:LN:62:TYR:HE2	18:LN:110:CYS:HG	1.48	0.62
68:S2:207:G:H3'	68:S2:208:G:H8	1.64	0.62
85:CB:354:ILE:HA	85:CB:358:LEU:HD23	1.80	0.62
3:L5:1270:A:H8	3:L5:2106:G:H21	1.48	0.62
86:CA:27:ILE:HG13	86:CA:30:ARG:HE	1.63	0.62
3:L5:4775:C:H41	3:L5:4859:C:H42	1.48	0.62
55:SH:31:GLU:HA	55:SH:37:LYS:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:CB:27:HIS:HB2	85:CB:139:THR:HG23	1.81	0.62
64:SY:10:ARG:HG3	64:SY:24:VAL:HG23	1.82	0.62
76:SS:129:LEU:HD23	76:SS:144:ARG:HH21	1.65	0.61
83:Sg:11:LEU:HD21	83:Sg:52:TYR:HB3	1.82	0.61
3:L5:4615:C:H5''	7:LB:357:ARG:HD2	1.83	0.61
68:S2:508:A:H3'	68:S2:509:OMG:H8	1.64	0.61
29:LY:2:LYS:HD2	29:LY:7:VAL:HG13	1.81	0.61
56:SI:190:LEU:HD21	56:SI:198:TYR:HD2	1.64	0.61
3:L5:2710:C:H41	22:LR:46:LYS:NZ	1.98	0.61
53:SE:151:ASP:HA	54:SG:212:LEU:HD21	1.81	0.61
86:CA:12:ILE:HG12	86:CA:324:LEU:HD11	1.82	0.61
55:SH:154:ILE:HB	55:SH:185:VAL:HG22	1.83	0.61
74:SP:86:LEU:HB2	74:SP:89:MET:HE3	1.81	0.61
76:SS:26:ILE:HA	76:SS:56:ALA:HB2	1.82	0.61
14:LI:54:SER:HB3	14:LI:135:ILE:HD11	1.83	0.61
3:L5:4715:C:H5''	7:LB:278:THR:HG21	1.82	0.61
7:LB:92:TYR:HB2	7:LB:159:VAL:HG13	1.82	0.61
41:Lk:26:LYS:HB2	41:Lk:69:LEU:HD12	1.81	0.61
61:SV:71:ARG:HH11	66:Sb:4:ALA:HB2	1.65	0.61
3:L5:3951:G:H21	3:L5:4062:A:N6	1.99	0.61
3:L5:4302:U:H4'	24:LT:5:LYS:HD2	1.82	0.61
54:SG:133:LEU:HD12	68:S2:65:C:C4	2.34	0.61
55:SH:51:ILE:HD11	55:SH:176:VAL:HG12	1.83	0.61
68:S2:116:OMU:HN3	68:S2:347:G:H1	1.47	0.61
50:SA:49:ILE:HD13	50:SA:163:CYS:HA	1.81	0.60
54:SG:135:PRO:HG2	54:SG:141:ILE:HD13	1.82	0.60
68:S2:588:G:H4'	68:S2:589:G:H5'	1.83	0.60
56:SI:98:LYS:HB3	68:S2:377:G:H5'	1.82	0.60
68:S2:1588:A:H2'	68:S2:1589:A:C8	2.36	0.60
71:SF:28:VAL:HG21	71:SF:109:LEU:HB2	1.83	0.60
58:SL:85:THR:HG21	68:S2:373:G:H4'	1.83	0.60
3:L5:1188:C:H2'	3:L5:1189:G:C8	2.37	0.60
88:L5:5293:SPM:H112	19:LO:91:LYS:HD3	1.84	0.60
28:LX:73:HIS:HB3	28:LX:116:LEU:HD23	1.84	0.60
72:SK:64:TRP:HB3	81:Sd:23:VAL:HA	1.83	0.60
19:LO:61:ARG:HA	19:LO:70:PRO:HD2	1.83	0.60
49:Lt:19:GLY:HA2	49:Lt:48:LYS:HZ3	1.67	0.60
73:SM:92:CYS:HB3	73:SM:103:VAL:HG12	1.84	0.60
68:S2:690:G:H3'	68:S2:691:G:H21	1.67	0.60
3:L5:4106:G:H3'	3:L5:4107:G:H8	1.66	0.60
3:L5:1254:A:H5''	3:L5:1255:A:H5''	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4279:A:H5'	3:L5:4281:A:H1'	1.84	0.60
34:Ld:64:ILE:HG23	34:Ld:68:LEU:HD23	1.83	0.60
45:Lo:33:LEU:HA	45:Lo:38:LYS:HG2	1.84	0.60
68:S2:1337:4AC:H2'	68:S2:1338:G:H8	1.66	0.60
82:Sf:110:GLU:HG2	82:Sf:113:LYS:HD3	1.84	0.60
12:LG:205:THR:HG22	12:LG:206:GLN:H	1.65	0.59
17:LM:24:LEU:H	17:LM:43:THR:HG21	1.66	0.59
68:S2:1421:A:H3'	68:S2:1422:G:C8	2.37	0.59
3:L5:261:G:H2'	3:L5:262:G:C8	2.37	0.59
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.33	0.59
6:LA:114:CYS:HB3	6:LA:165:VAL:HB	1.84	0.59
16:LL:140:SER:HA	16:LL:143:GLU:HG2	1.84	0.59
55:SH:170:VAL:HG13	55:SH:187:PHE:HB2	1.84	0.59
56:SI:22:HIS:HB3	68:S2:433:A:H5''	1.84	0.59
3:L5:4927:G:H5''	3:L5:4928:C:H5	1.68	0.59
26:LV:92:ASP:HB2	27:LW:2:LYS:HZ3	1.66	0.59
73:SM:33:ARG:HD2	73:SM:91:LEU:HD21	1.83	0.59
84:Et:6:G:H1	84:Et:67:U:H3	1.50	0.59
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.83	0.59
23:LS:15:ARG:HB3	23:LS:27:LEU:HD23	1.82	0.59
50:SA:77:ILE:HD11	50:SA:124:VAL:HG22	1.84	0.59
85:CB:196:GLU:CD	85:CB:197:SER:H	2.10	0.59
86:CA:11:THR:HG23	86:CA:13:ALA:H	1.68	0.59
3:L5:4363:A:H5''	45:Lo:36:GLN:HG2	1.83	0.59
10:LE:243:THR:HG22	10:LE:245:GLN:H	1.68	0.59
3:L5:702:U:H2'	3:L5:703:G:O4'	2.02	0.59
11:LF:105:VAL:HG13	11:LF:136:VAL:HG12	1.85	0.59
13:LH:44:GLU:HG2	13:LH:58:ASP:HB2	1.84	0.59
63:SX:70:VAL:HG11	63:SX:94:ILE:HG21	1.84	0.59
49:Lt:16:ARG:HH12	49:Lt:28:LEU:HB3	1.68	0.59
3:L5:3951:G:N2	3:L5:4062:A:H61	2.00	0.59
68:S2:1513:C:H2'	68:S2:1514:G:H8	1.68	0.59
73:SM:89:VAL:HG13	73:SM:91:LEU:HD23	1.85	0.59
3:L5:3760:A:H4'	3:L5:3761:C:H5''	1.85	0.58
53:SE:80:ILE:HG23	53:SE:81:THR:HG23	1.85	0.58
68:S2:943:U:H2'	68:S2:944:A:H8	1.68	0.58
74:SP:53:GLN:HB3	74:SP:83:MET:HE1	1.85	0.58
85:CB:607:ARG:HD3	85:CB:701:ARG:HD3	1.83	0.58
1:CD:218:TRP:HA	70:SD:115:VAL:HG22	1.85	0.58
3:L5:1503:A:H62	21:LQ:87:THR:HG21	1.68	0.58
63:SX:17:ARG:HH22	68:S2:659:G:H21	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:573:U:O2	68:S2:576:A2M:H8	2.02	0.58
3:L5:1186:U:H3'	3:L5:1187:G:H21	1.68	0.58
85:CB:693:CYS:HB3	85:CB:835:VAL:HG23	1.86	0.58
68:S2:1651:A:H2'	68:S2:1652:G:H8	1.67	0.58
69:SR:35:CYS:HA	69:SR:38:ILE:HG12	1.84	0.58
68:S2:557:U:H2'	68:S2:558:G:C8	2.39	0.58
85:CB:448:GLN:HB2	85:CB:473:VAL:HG23	1.85	0.58
3:L5:3641:U:H5	3:L5:3646:A:N7	2.01	0.58
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.38	0.58
19:LO:9:LEU:HD23	19:LO:118:MET:HB2	1.86	0.58
56:SI:25:ARG:HA	68:S2:448:A:H5''	1.85	0.58
71:SF:126:THR:HA	71:SF:135:ARG:HG2	1.86	0.58
86:CA:21:TYR:HE1	86:CA:117:PHE:HB3	1.68	0.58
51:SB:136:ARG:HB3	51:SB:216:LYS:HG3	1.86	0.58
53:SE:141:THR:HG23	53:SE:143:ASP:H	1.69	0.58
60:SO:53:ILE:HG23	60:SO:88:LEU:HD22	1.85	0.58
68:S2:562:U:H2'	68:S2:563:G:C8	2.39	0.57
68:S2:1388:A:H61	70:SD:161:GLY:HA3	1.69	0.57
27:LW:73:ARG:HD3	68:S2:1748:G:H5''	1.84	0.57
3:L5:3868:G:H22	3:L5:3900:G:H1'	1.69	0.57
9:LD:182:GLY:HA2	9:LD:194:VAL:HG13	1.86	0.57
51:SB:171:ILE:HD11	51:SB:197:ILE:HA	1.86	0.57
64:SY:11:LYS:HB2	64:SY:24:VAL:HG22	1.85	0.57
68:S2:201:C:H3'	68:S2:202:G:H21	1.68	0.57
72:SK:63:ALA:HB2	72:SK:68:TYR:HE2	1.69	0.57
76:SS:46:ARG:HE	76:SS:52:LEU:HD11	1.69	0.57
85:CB:110:ASP:HB3	85:CB:553:HIS:HB2	1.86	0.57
48:Ls:119:CYS:HB3	48:Ls:183:PHE:HB3	1.86	0.57
49:Lt:127:GLY:O	49:Lt:131:GLU:HG2	2.04	0.57
55:SH:157:HIS:HB3	55:SH:190:PRO:HG3	1.85	0.57
56:SI:141:ARG:HD3	56:SI:145:ILE:HG21	1.86	0.57
60:SO:78:ALA:HB1	60:SO:119:LEU:HG	1.84	0.57
84:Et:22:G:H2'	84:Et:23:A:H8	1.70	0.57
3:L5:1824:G:H5''	24:LT:35:LYS:HE2	1.86	0.57
3:L5:4098:A:H2'	3:L5:4099:G:H4'	1.86	0.57
9:LD:84:PRO:HB3	9:LD:89:LYS:HD2	1.87	0.57
50:SA:209:GLU:HA	50:SA:212:LYS:HG2	1.87	0.57
3:L5:1732:C:H5''	24:LT:43:LYS:HE2	1.86	0.57
54:SG:66:GLY:HA2	68:S2:1745:A:H1'	1.85	0.57
64:SY:9:THR:HB	68:S2:837:A:H61	1.69	0.57
85:CB:396:MET:HE1	85:CB:472:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.39	0.57
3:L5:1997:U:H4'	48:Ls:44:ARG:HH12	1.70	0.57
3:L5:4992:G:H2'	3:L5:4993:G:C8	2.39	0.57
51:SB:186:ASN:HA	51:SB:189:ILE:HD12	1.86	0.57
10:LE:190:HIS:HB3	10:LE:193:PHE:HD2	1.69	0.57
22:LR:105:LEU:HD23	22:LR:138:LEU:HD23	1.87	0.57
56:SI:133:GLU:HA	56:SI:136:ILE:HG12	1.87	0.57
83:Sg:64:HIS:CD2	83:Sg:65:PHE:H	2.23	0.57
3:L5:4598:C:H4'	13:LH:121:LYS:HE2	1.87	0.57
17:LM:100:ARG:HA	17:LM:103:LYS:HG2	1.87	0.57
68:S2:1627:C:H5''	77:ST:41:LYS:HD2	1.87	0.57
85:CB:56:PHE:HD1	85:CB:456:ARG:HB2	1.70	0.57
15:LJ:16:ARG:HH21	15:LJ:137:PRO:HG3	1.70	0.56
68:S2:851:C:H5''	68:S2:852:G:H5'	1.86	0.56
72:SK:91:PRO:HD2	72:SK:94:LEU:HD12	1.87	0.56
3:L5:3952:A:H2'	3:L5:3953:G:C4	2.39	0.56
16:LL:91:ALA:HB1	16:LL:96:ILE:HB	1.86	0.56
68:S2:1417:C:N3	68:S2:1422:G:N1	2.42	0.56
3:L5:1095:A:H2	3:L5:1200:G:N1	2.01	0.56
3:L5:3910:C:H2'	3:L5:3911:C:C6	2.39	0.56
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.40	0.56
57:SJ:176:LYS:HA	57:SJ:179:LYS:HE3	1.88	0.56
68:S2:1648:G:H5''	75:SQ:125:ARG:HB2	1.86	0.56
68:S2:1780:G:H3'	68:S2:1781:A:H8	1.70	0.56
70:SD:55:THR:HA	70:SD:58:VAL:HG22	1.86	0.56
85:CB:475:VAL:HG11	85:CB:485:ILE:HD11	1.87	0.56
86:CA:333:ILE:HG13	86:CA:334:THR:HG23	1.86	0.56
28:LX:73:HIS:CE1	28:LX:115:LYS:HD3	2.39	0.56
38:Lh:87:LYS:HB3	38:Lh:91:MET:HE3	1.88	0.56
85:CB:429:ILE:HG12	85:CB:485:ILE:HG12	1.86	0.56
85:CB:451:ILE:HD12	85:CB:458:VAL:HG21	1.88	0.56
3:L5:2483:G:O6	3:L5:2495:U:O4	2.23	0.56
68:S2:527:C:H2'	68:S2:528:A:H8	1.71	0.56
33:Lc:51:ASN:HB2	33:Lc:77:ASN:HB2	1.86	0.56
41:Lk:14:THR:HA	41:Lk:17:ARG:HD3	1.88	0.56
50:SA:10:MET:HB3	69:SR:111:PHE:HE2	1.70	0.56
53:SE:64:ILE:HG23	64:SY:17:LEU:HD12	1.88	0.56
85:CB:56:PHE:HB3	85:CB:456:ARG:H	1.71	0.56
57:SJ:86:VAL:HG21	57:SJ:105:PHE:HE1	1.70	0.56
68:S2:677:G:H21	68:S2:1028:A:H62	1.54	0.56
68:S2:1560:U:O2	68:S2:1575:G:O6	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SR:17:ILE:HG12	69:SR:58:MET:HE3	1.88	0.56
3:L5:497:G:N2	3:L5:498:C:H41	2.04	0.56
72:SK:15:LEU:HD21	72:SK:71:LEU:HD13	1.88	0.56
86:CA:205:PRO:HB2	86:CA:210:LYS:HG3	1.87	0.56
3:L5:267:G:H2'	3:L5:268:G:H8	1.71	0.55
57:SJ:111:GLN:HE21	57:SJ:123:ILE:HG13	1.70	0.55
70:SD:170:THR:HG22	70:SD:187:LYS:HG2	1.88	0.55
30:LZ:103:ASP:HB3	30:LZ:106:LEU:HB2	1.88	0.55
58:SL:7:GLU:HG2	58:SL:9:ALA:H	1.71	0.55
85:CB:595:SER:HA	85:CB:724:THR:HG21	1.86	0.55
3:L5:1220:G:H2'	3:L5:1221:G:C8	2.41	0.55
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.71	0.55
29:LY:4:ASN:HB3	29:LY:7:VAL:HG12	1.88	0.55
59:SN:76:LYS:HD3	59:SN:81:ALA:HB3	1.89	0.55
60:SO:56:VAL:HG12	60:SO:81:VAL:HG23	1.88	0.55
68:S2:1407:U:H2'	68:S2:1408:U:C6	2.41	0.55
78:SU:21:ARG:HD2	78:SU:88:LEU:HD22	1.88	0.55
3:L5:4966:A:H5''	7:LB:128:LYS:HG3	1.89	0.55
54:SG:18:VAL:HG11	54:SG:24:LEU:HD21	1.87	0.55
86:CA:181:PRO:HA	86:CA:230:VAL:HA	1.88	0.55
12:LG:187:LYS:HB2	12:LG:198:THR:HG23	1.88	0.55
35:Le:10:PRO:HD2	35:Le:69:MET:HE1	1.87	0.55
53:SE:60:GLU:O	53:SE:64:ILE:HD12	2.05	0.55
68:S2:640:A:H2'	68:S2:641:A:C8	2.41	0.55
68:S2:1310:U:H4'	82:Sf:143:LYS:HG3	1.89	0.55
68:S2:1705:C:H2'	68:S2:1706:G:C8	2.40	0.55
20:LP:52:THR:HG23	20:LP:85:LYS:HG3	1.87	0.55
55:SH:63:PHE:HA	55:SH:95:ILE:O	2.06	0.55
85:CB:266:PHE:HD2	85:CB:291:GLN:HG2	1.71	0.55
6:LA:115:CYS:SG	6:LA:124:GLY:HA3	2.47	0.55
7:LB:107:ALA:HB2	7:LB:201:LEU:HD22	1.88	0.55
8:LC:154:VAL:HG11	8:LC:174:LEU:HD11	1.89	0.55
68:S2:1679:A:H2'	71:Sf:60:ARG:HD2	1.87	0.55
83:Sg:233:GLY:H	83:Sg:257:LYS:HZ1	1.54	0.55
86:CA:142[A]:VAL:HG13	86:CA:143:ILE:HD12	1.87	0.55
3:L5:460:C:H2'	3:L5:461:G:H8	1.71	0.55
50:SA:205:ARG:HG3	50:SA:210:ILE:HD11	1.89	0.55
60:SO:96:LYS:HE3	60:SO:132:VAL:HG11	1.88	0.55
67:Se:2:VAL:HG13	67:Se:4:GLY:H	1.72	0.55
68:S2:323:C:H2'	68:S2:327:G:H22	1.71	0.55
83:Sg:206:LEU:HD23	83:Sg:218:LEU:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:73:A:H62	16:LL:103:ARG:HH22	1.54	0.55
3:L5:4251:A:H5''	15:LJ:108:GLY:HA3	1.89	0.55
51:SB:85:LYS:HB2	51:SB:101:HIS:HB3	1.89	0.55
57:SJ:93:LYS:HB2	57:SJ:96:TYR:HD1	1.72	0.55
62:SW:6:VAL:HG22	62:SW:34:ILE:HD11	1.89	0.55
3:L5:495:C:H2'	3:L5:496:G:C8	2.42	0.54
7:LB:56:ILE:O	7:LB:73:VAL:HA	2.07	0.54
52:SC:187:ARG:HH11	52:SC:192:LEU:HB2	1.72	0.54
82:Sf:108:VAL:HB	82:Sf:112:GLY:HA2	1.89	0.54
3:L5:4260:U:H2'	3:L5:4261:C:C6	2.43	0.54
50:SA:205:ARG:HH21	69:SR:81:ARG:HH22	1.55	0.54
68:S2:1217:A:H2'	68:S2:1218:C:C6	2.42	0.54
68:S2:1536:G:H2'	68:S2:1537:A:H8	1.72	0.54
3:L5:691:C:H2'	3:L5:692:A:C8	2.42	0.54
66:Sb:33:MET:HE2	66:Sb:48:SER:HA	1.90	0.54
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.43	0.54
83:Sg:34:ALA:HB1	83:Sg:66:VAL:HG13	1.90	0.54
3:L5:1437:C:H1'	3:L5:2098:G:H3'	1.88	0.54
3:L5:3951:G:H2'	3:L5:3952:A:C8	2.42	0.54
8:LC:116:ASN:HB2	8:LC:119:GLN:HG3	1.89	0.54
42:Ll:12:PHE:CE1	42:Ll:51:LEU:HD22	2.43	0.54
3:L5:171:U:H4'	16:LL:135:LYS:HG2	1.88	0.54
3:L5:519:C:H1'	3:L5:643:C:C2	2.43	0.54
3:L5:2495:U:H2'	3:L5:2496:G:C8	2.41	0.54
72:SK:14:LEU:HD13	72:SK:35:LEU:HD23	1.88	0.54
3:L5:3754:G:O6	3:L5:3770:U:O4	2.26	0.54
41:Lk:8:ILE:HD11	41:Lk:56:LEU:HD13	1.90	0.54
68:S2:367:U:H4'	68:S2:371:A:C8	2.42	0.54
83:Sg:120:ILE:HG23	83:Sg:132:TRP:HB2	1.89	0.54
83:Sg:212:LYS:HD2	83:Sg:235:ILE:HG21	1.89	0.54
42:Ll:28:ARG:HA	42:Ll:33:ASN:ND2	2.21	0.54
63:SX:54:LYS:HE3	63:SX:91:LEU:HG	1.90	0.54
68:S2:118:C:H1'	68:S2:445:A:C5	2.43	0.54
68:S2:554:A:HO2'	68:S2:555:A:H8	1.56	0.54
76:SS:105:ASN:HA	76:SS:108:ARG:HG3	1.90	0.54
85:CB:56:PHE:HB3	85:CB:455:GLY:HA3	1.89	0.54
3:L5:662:C:H2'	3:L5:663:G:C8	2.43	0.54
3:L5:2487:G:C4	3:L5:2489:C:H5''	2.43	0.54
3:L5:4967:A:H2'	3:L5:4968:A:H8	1.73	0.54
79:SZ:68:ILE:HG23	79:SZ:109:TYR:HB2	1.88	0.54
19:LO:34:VAL:HG22	19:LO:103:LYS:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Lc:38:ILE:HG21	33:Lc:63:TYR:HB3	1.90	0.53
60:SO:113:GLN:HE22	65:Sa:45:VAL:HA	1.73	0.53
83:Sg:233:GLY:H	83:Sg:257:LYS:NZ	2.06	0.53
3:L5:1509:C:H5''	31:La:2:PRO:HD3	1.90	0.53
8:LC:298:ILE:HD13	21:LQ:131:PRO:HB3	1.90	0.53
11:LF:59:LYS:HA	11:LF:62:ARG:HE	1.72	0.53
62:SW:107:SER:HB3	68:S2:860:G:H21	1.73	0.53
85:CB:592:LEU:HD21	85:CB:601:ARG:HD2	1.89	0.53
3:L5:159:C:H5''	39:Li:25:ARG:HG2	1.91	0.53
47:Lr:47:LYS:HB2	47:Lr:102:TYR:CZ	2.43	0.53
54:SG:147:LEU:HD12	54:SG:151:ASP:HB2	1.90	0.53
63:SX:60:LYS:HE3	63:SX:116:PRO:HB3	1.89	0.53
86:CA:141:ASP:HB2	86:CA:177:PHE:HD2	1.73	0.53
86:CA:202:ILE:HD11	86:CA:209:GLN:HB3	1.89	0.53
3:L5:2696:A:H62	41:Lk:35:LYS:NZ	2.07	0.53
20:LP:116:HIS:HB3	20:LP:149:ILE:HB	1.90	0.53
33:Lc:22:MET:O	33:Lc:23:LYS:HG3	2.08	0.53
53:SE:11:ARG:HD2	53:SE:20:LEU:HB3	1.90	0.53
55:SH:72:PHE:O	55:SH:76:GLN:HB2	2.09	0.53
68:S2:1536:G:H2'	68:S2:1537:A:C8	2.43	0.53
76:SS:25:LYS:O	76:SS:29:ALA:HB2	2.08	0.53
76:SS:36:VAL:HB	76:SS:99:LEU:HD23	1.90	0.53
1:CD:218:TRP:HE3	70:SD:115:VAL:HG21	1.73	0.53
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.43	0.53
11:LF:216:PRO:HD3	11:LF:247:MET:HE2	1.89	0.53
53:SE:44:LEU:HD22	53:SE:72:ILE:HD11	1.90	0.53
56:SI:150:ASP:HA	56:SI:153:LYS:HB3	1.91	0.53
58:SL:68:ILE:HG13	58:SL:143:LEU:HD11	1.90	0.53
68:S2:940:U:H3	68:S2:1002:U:H3	1.55	0.53
68:S2:1713:C:H2'	68:S2:1714:U:C6	2.44	0.53
85:CB:132:VAL:HG13	85:CB:167:LEU:HD11	1.91	0.53
3:L5:717:U:H2'	3:L5:718:C:C6	2.43	0.53
33:Lc:48:LEU:HD23	33:Lc:57:LYS:HG2	1.90	0.53
36:Lf:41:PHE:HE1	36:Lf:110:ILE:HD13	1.74	0.53
49:Lt:61:LYS:HA	49:Lt:75:PRO:HD2	1.91	0.53
63:SX:84:PHE:HB3	63:SX:105:PHE:HE1	1.74	0.53
84:Et:37:A:H3'	84:Et:38:A:C8	2.44	0.53
85:CB:654:PRO:HD2	85:CB:658:GLY:HA3	1.90	0.53
45:Lo:70:LEU:HD11	45:Lo:83:LEU:HD12	1.90	0.53
68:S2:349:A:H2'	68:S2:350:C:C6	2.43	0.53
68:S2:1845:A:H2'	68:S2:1846:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SD:29:LEU:HD21	70:SD:69:LEU:HD11	1.89	0.53
78:SU:80:PHE:HB3	81:Sd:52:PHE:HB3	1.89	0.53
83:Sg:247:TRP:HB3	83:Sg:258:ILE:HD11	1.91	0.53
85:CB:27:HIS:HB3	85:CB:30:HIS:CD2	2.44	0.53
3:L5:162:A:H2'	3:L5:163:A:C8	2.44	0.53
3:L5:433:A:C2	3:L5:3867:A2M:H4'	2.44	0.53
22:LR:172:ARG:HH22	68:S2:908:A:H5''	1.74	0.53
68:S2:874:G:H2'	68:S2:875:A:H8	1.73	0.53
68:S2:928:G:H1	68:S2:1013:U:H3	1.57	0.53
68:S2:1098:C:H2'	68:S2:1099:G:C8	2.44	0.53
68:S2:1709:G:H1	68:S2:1824:A:H61	1.57	0.53
85:CB:81:LEU:HD11	85:CB:89:ILE:HD11	1.89	0.53
86:CA:107:LYS:HZ2	86:CA:316:VAL:HG22	1.74	0.53
3:L5:4611:A:H2'	3:L5:4612:C:H6	1.74	0.53
51:SB:124:HIS:HA	51:SB:137:LEU:O	2.08	0.53
68:S2:543:C:H3'	68:S2:544:G:H8	1.72	0.53
10:LE:236:GLU:O	10:LE:237:LYS:HG3	2.08	0.53
60:SO:15:ILE:HG12	60:SO:16:SER:H	1.73	0.53
3:L5:3911:C:H2'	3:L5:3912:U:H6	1.74	0.52
3:L5:4441:A:H5''	14:LI:114:GLY:HA2	1.91	0.52
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.90	0.52
68:S2:186:C:H2'	68:S2:187:G:H8	1.74	0.52
86:CA:105:LEU:HD23	86:CA:139:LYS:HD2	1.91	0.52
3:L5:325:U:H2'	3:L5:326:C:C6	2.44	0.52
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.44	0.52
85:CB:228:PHE:HD2	85:CB:293:ILE:HG12	1.74	0.52
3:L5:1298:C:H2'	3:L5:1299:G:C8	2.43	0.52
3:L5:4146:G:H2'	3:L5:4147:G:C8	2.44	0.52
17:LM:122:ILE:HB	19:LO:189:ILE:HD11	1.90	0.52
27:LW:89:ASP:O	27:LW:93:LYS:HG2	2.10	0.52
63:SX:68:LYS:HB3	63:SX:91:LEU:HD22	1.90	0.52
83:Sg:87:LEU:HB2	83:Sg:101:PHE:HB2	1.91	0.52
85:CB:531:ASP:HB3	85:CB:534:VAL:HG12	1.90	0.52
86:CA:187:SER:HB2	86:CA:201:ILE:HB	1.91	0.52
3:L5:1857:C:H2'	3:L5:1858:A:H8	1.74	0.52
3:L5:3611:A:C2	3:L5:5016:A:H8	2.27	0.52
7:LB:92:TYR:HB3	7:LB:99:LEU:HD22	1.92	0.52
52:SC:64:THR:HG22	52:SC:66:LEU:H	1.74	0.52
63:SX:17:ARG:HH12	68:S2:659:G:N2	2.07	0.52
48:Ls:160:LEU:HD13	48:Ls:175:LEU:HD21	1.90	0.52
76:SS:24:ARG:HG3	76:SS:29:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:425:U:H4'	20:LP:6:LEU:HD21	1.90	0.52
3:L5:1762:C:H41	3:L5:1770:A:H2	1.57	0.52
3:L5:752:G:H1	3:L5:911:U:H3	1.56	0.52
22:LR:107:ARG:O	22:LR:111:GLU:HG2	2.10	0.52
52:SC:207:ALA:HB2	68:S2:4:C:H4'	1.92	0.52
56:SI:97:VAL:HG22	56:SI:100:CYS:HB3	1.92	0.52
3:L5:1188:C:H2'	3:L5:1189:G:H8	1.73	0.52
3:L5:1962:A:H2	3:L5:2024:G:H21	1.56	0.52
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.45	0.52
6:LA:20:VAL:HA	6:LA:23:ARG:HG3	1.91	0.52
52:SC:118:ALA:HB2	68:S2:1486:A:H4'	1.92	0.52
53:SE:100:ARG:HB2	53:SE:114:ILE:HD13	1.92	0.52
72:SK:59:LYS:HG3	72:SK:70:TYR:HD2	1.75	0.52
85:CB:120:ARG:HE	85:CB:497:MET:HG2	1.74	0.52
85:CB:279:SER:HB3	85:CB:285:LEU:HD21	1.92	0.52
3:L5:1095:A:N1	3:L5:1200:G:C6	2.77	0.52
12:LG:52:THR:HG22	28:LX:41:ARG:HG3	1.91	0.52
16:LL:80:GLU:HG3	16:LL:110:LEU:HD12	1.92	0.52
68:S2:118:C:H1'	68:S2:445:A:C4	2.45	0.52
68:S2:1653:U:H2'	68:S2:1654:G:C8	2.45	0.52
3:L5:256:G:H2'	3:L5:257:C:C6	2.45	0.52
3:L5:4457:PSU:H1'	7:LB:252:ALA:HB3	1.92	0.52
24:LT:45:MET:HE2	24:LT:47:THR:HB	1.90	0.52
82:Sf:119:ARG:HB3	82:Sf:132:MET:HB3	1.90	0.52
3:L5:662:C:H2'	3:L5:663:G:H8	1.74	0.51
3:L5:5062:G:H2'	3:L5:5063:G:H8	1.75	0.51
42:Ll:12:PHE:HE1	42:Ll:51:LEU:HD22	1.75	0.51
68:S2:107:A:H2'	68:S2:108:G:C8	2.45	0.51
79:SZ:47:LEU:HD11	79:SZ:79:ILE:HG22	1.92	0.51
86:CA:354:LEU:HD12	86:CA:357:LEU:HD21	1.92	0.51
7:LB:163:ILE:HG22	7:LB:180:LEU:HD22	1.93	0.51
22:LR:176:ARG:HH22	68:S2:909:G:H5'	1.75	0.51
25:LU:28:PRO:HB2	25:LU:34:MET:HG2	1.90	0.51
65:Sa:44:ILE:HG23	65:Sa:45:VAL:HG23	1.92	0.51
83:Sg:153:CYS:SG	83:Sg:198:VAL:HG12	2.50	0.51
3:L5:1278:C:H2'	3:L5:1279:A:O4'	2.10	0.51
59:SN:31:ASP:O	59:SN:35:GLU:HG2	2.10	0.51
3:L5:268:G:H2'	3:L5:269:G:H8	1.74	0.51
3:L5:1414:C:H2'	3:L5:1415:G:H8	1.75	0.51
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.25	0.51
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Lo:33:LEU:HD12	45:Lo:38:LYS:HE3	1.93	0.51
60:SO:56:VAL:HG11	60:SO:80:ASP:HB3	1.92	0.51
70:SD:18:LYS:HE2	70:SD:39:VAL:HB	1.92	0.51
85:CB:653:GLY:HA2	85:CB:660:ASN:HB2	1.91	0.51
18:LN:146:PRO:HB2	38:Lh:104:THR:HG23	1.92	0.51
36:Lf:71:TRP:HZ3	36:Lf:104:MET:HE3	1.75	0.51
52:SC:267:GLN:HA	52:SC:270:THR:HG23	1.92	0.51
85:CB:24:VAL:HG22	85:CB:104:ASP:HA	1.92	0.51
85:CB:225:LEU:HD21	85:CB:261:TRP:HB2	1.91	0.51
3:L5:73:A:N6	16:LL:103:ARG:HH22	2.09	0.51
3:L5:2745:A:H2'	3:L5:2746:A:C8	2.46	0.51
3:L5:4069:U:H2'	3:L5:4070:U:H6	1.75	0.51
3:L5:4489:G:H4'	89:L5:5290:SPD:H91	1.93	0.51
68:S2:1004:PSU:H2'	68:S2:1005:G:H8	1.75	0.51
71:SF:62:ARG:HD3	71:SF:65:GLN:HE21	1.75	0.51
85:CB:16:LYS:NZ	85:CB:388:CYS:HB3	2.25	0.51
3:L5:2709:C:N4	86:CA:256:GLY:HA2	2.24	0.51
53:SE:126:VAL:HG12	53:SE:139:LEU:HD21	1.93	0.51
63:SX:28:LYS:HD2	63:SX:32:LEU:HD22	1.93	0.51
68:S2:1457:U:H2'	68:S2:1458:G:H8	1.75	0.51
3:L5:1281:G:N1	10:LE:128:HIS:HB2	2.25	0.51
53:SE:159:THR:HB	53:SE:173:ILE:HB	1.92	0.51
58:SL:120:VAL:HG22	58:SL:145:VAL:HG11	1.92	0.51
68:S2:942:G:H2'	68:S2:943:U:C6	2.46	0.51
68:S2:1288:OMU:HM21	68:S2:1315:U:H1'	1.93	0.51
1:CD:218:TRP:CE3	70:SD:115:VAL:HG21	2.45	0.51
3:L5:3720:G:H22	3:L5:3733:A:H2	1.58	0.51
20:LP:54:GLN:HA	20:LP:83:TRP:CD1	2.46	0.51
68:S2:1410:C:H2'	68:S2:1411:G:H8	1.76	0.51
3:L5:5024:C:N4	3:L5:5028:G:H21	2.07	0.51
68:S2:1652:G:H1	68:S2:1672:U:H3	1.58	0.51
78:SU:20:ILE:HB	78:SU:97:ILE:HD12	1.92	0.51
3:L5:460:C:H2'	3:L5:461:G:C8	2.46	0.50
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.94	0.50
3:L5:4996:C:H4'	34:Ld:26:THR:HG23	1.93	0.50
61:SV:30:ALA:O	61:SV:60:ARG:HD3	2.11	0.50
68:S2:931:C:H2'	68:S2:932:G:C8	2.45	0.50
71:SF:131:ALA:HA	71:SF:136:ARG:HD3	1.92	0.50
6:LA:229:ALA:HB3	6:LA:234:LYS:HB3	1.93	0.50
20:LP:131:ARG:HG3	20:LP:137:ASN:OD1	2.10	0.50
50:SA:41:ARG:HD2	50:SA:47:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:5:U:H2'	68:S2:6:G:H8	1.77	0.50
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.46	0.50
3:L5:2745:A:H2'	3:L5:2746:A:H8	1.77	0.50
7:LB:294:LYS:HE3	7:LB:298:LEU:HD11	1.93	0.50
27:LW:9:SER:HA	27:LW:52:THR:HG23	1.92	0.50
68:S2:1203:G:H2'	68:S2:1204:A:C8	2.46	0.50
68:S2:1540:G:H5'	77:ST:47:PRO:HB3	1.92	0.50
86:CA:246:ILE:HB	86:CA:305:PHE:HB2	1.93	0.50
3:L5:2102:G:H1'	3:L5:2103:G:C8	2.46	0.50
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.47	0.50
3:L5:3748:A:H5''	6:LA:243:THR:HB	1.93	0.50
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.75	0.50
66:Sb:64:CYS:HB2	66:Sb:71:ALA:HB1	1.93	0.50
68:S2:28:U:H2'	68:S2:29:G:H8	1.75	0.50
68:S2:49:C:H2'	68:S2:472:C:H41	1.77	0.50
68:S2:1829:G:H1'	68:S2:1850:MA6:H2	1.94	0.50
70:SD:40:ARG:HG2	78:SU:108:PRO:HG3	1.91	0.50
73:SM:52:LEU:HD13	73:SM:65:VAL:HG21	1.94	0.50
3:L5:1333:A:H2'	3:L5:1334:A:C8	2.46	0.50
58:SL:48:LYS:O	58:SL:52:GLU:HG3	2.11	0.50
73:SM:23:LYS:O	73:SM:27:ILE:HG12	2.12	0.50
3:L5:1867:A:H2'	3:L5:1868:A:C8	2.47	0.50
3:L5:4260:U:H2'	3:L5:4261:C:H6	1.77	0.50
3:L5:4371:G:H5'	84:Et:76:A:H62	1.77	0.50
8:LC:14:LYS:HA	8:LC:173:LYS:HD3	1.94	0.50
16:LL:142:GLU:O	16:LL:146:LEU:HB2	2.12	0.50
35:Le:108:ARG:HD2	35:Le:128:ARG:HB2	1.93	0.50
53:SE:45:ILE:HG13	53:SE:61:VAL:HG11	1.94	0.50
57:SJ:63:LEU:HD23	57:SJ:70:ARG:HB2	1.93	0.50
83:Sg:185:LYS:HG3	83:Sg:186:THR:HG22	1.92	0.50
20:LP:10:ASN:HD21	20:LP:13:LYS:NZ	2.09	0.50
34:Ld:22:THR:HG23	34:Ld:122:VAL:HG23	1.94	0.50
68:S2:1221:G:H2'	68:S2:1222:G:C8	2.46	0.50
70:SD:172:VAL:HG22	70:SD:185:LYS:HG2	1.94	0.50
73:SM:120:ALA:HA	73:SM:123:VAL:HG22	1.94	0.50
3:L5:497:G:H1	3:L5:657:C:H42	1.60	0.50
3:L5:729:G:H5''	11:LF:76:ARG:HD2	1.93	0.50
3:L5:1995:G:H2'	3:L5:1996:C:C6	2.47	0.50
63:SX:9:THR:HG22	68:S2:681:PSU:H4'	1.93	0.50
68:S2:16:G:H2'	68:S2:17:C:C6	2.47	0.50
68:S2:674:C:H2'	68:S2:675:U:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:SS:36:VAL:HG23	76:SS:40:TYR:HB3	1.94	0.50
3:L5:260:C:H2'	3:L5:261:G:C8	2.47	0.50
3:L5:4508:C:N3	3:L5:4512:U:H5	2.10	0.50
3:L5:5023:C:H3'	3:L5:5024:C:H4'	1.92	0.50
25:LU:48:LYS:HG2	25:LU:53:ALA:HB2	1.92	0.50
49:Lt:151:ILE:O	49:Lt:155:ILE:HB	2.12	0.50
57:SJ:46:VAL:HG13	57:SJ:102:ILE:HD11	1.94	0.50
66:Sb:45:THR:HG23	66:Sb:82:LYS:HE3	1.94	0.50
74:SP:83:MET:HB3	74:SP:116:LEU:HD12	1.94	0.50
75:SQ:113:ILE:HD11	75:SQ:117:ARG:HG3	1.94	0.50
3:L5:5057:C:H2'	3:L5:5058:A:C8	2.47	0.49
7:LB:56:ILE:HD13	7:LB:365:LEU:HD22	1.94	0.49
35:Le:78:LEU:HB3	47:Lr:20:ARG:HD2	1.93	0.49
56:SI:172:LEU:HB3	56:SI:190:LEU:HD22	1.94	0.49
68:S2:144:U:H2'	68:S2:145:G:H8	1.76	0.49
68:S2:1595:U:H2'	68:S2:1596:U:C6	2.46	0.49
71:SF:40:ALA:HB3	71:SF:67:PRO:HA	1.93	0.49
3:L5:497:G:H21	3:L5:498:C:H41	1.60	0.49
3:L5:1802:A:H5''	3:L5:1803:G:H5'	1.93	0.49
3:L5:4239:A:H2'	3:L5:4240:G:C8	2.48	0.49
4:L7:117:G:H5'	9:LD:256:LYS:HD2	1.94	0.49
28:LX:82:THR:HG21	38:Lh:37:THR:HG22	1.94	0.49
50:SA:222:VAL:HG13	50:SA:223:THR:HG23	1.94	0.49
54:SG:85:ARG:NH2	64:SY:118:ARG:HG3	2.27	0.49
68:S2:186:C:H2'	68:S2:187:G:C8	2.47	0.49
3:L5:71:C:H1'	16:LL:62:PRO:O	2.12	0.49
3:L5:1366:G:H4'	3:L5:1367:C:OP1	2.11	0.49
14:LI:48:LEU:O	14:LI:139:ARG:HA	2.12	0.49
53:SE:57:THR:HG21	68:S2:494:C:H5''	1.95	0.49
68:S2:106:C:H2'	68:S2:107:A:H8	1.77	0.49
82:Sf:132:MET:HG2	82:Sf:139:HIS:HB3	1.94	0.49
3:L5:711:A:H2'	3:L5:712:C:C6	2.47	0.49
22:LR:70:ARG:HG2	22:LR:76:MET:HE2	1.93	0.49
42:Ll:23:ILE:HD11	42:Ll:28:ARG:HH11	1.76	0.49
53:SE:36:HIS:CG	53:SE:85:GLY:HA3	2.48	0.49
60:SO:101:GLY:HA3	60:SO:134:PRO:HD2	1.95	0.49
68:S2:1617:G:O6	74:SP:43:ARG:HD3	2.13	0.49
77:ST:115:LYS:HD3	77:ST:121:ARG:HD2	1.94	0.49
3:L5:4919:G:H2'	3:L5:4920:C:C6	2.47	0.49
16:LL:83:VAL:HG23	16:LL:114:VAL:HG11	1.95	0.49
55:SH:30:LEU:HD23	55:SH:33:ASN:HD22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:12:U:O2'	68:S2:1356:G:H8	1.95	0.49
3:L5:2448:G:H2'	3:L5:2449:A:C8	2.48	0.49
12:LG:162:ASP:HB3	12:LG:163:PRO:HD3	1.95	0.49
44:Ln:7:LYS:O	44:Ln:11:ARG:HG2	2.13	0.49
76:SS:42:HIS:O	76:SS:46:ARG:HG2	2.13	0.49
85:CB:143:LEU:O	85:CB:147:ILE:HG12	2.12	0.49
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.48	0.49
3:L5:2676:A:OP2	3:L5:2676:A:H8	1.96	0.49
34:Ld:23:ARG:HG2	34:Ld:121:ASN:HA	1.94	0.49
35:Le:76:LYS:HE2	35:Le:98:GLU:OE2	2.13	0.49
52:SC:94:ILE:HD11	52:SC:159:LYS:HG2	1.94	0.49
62:SW:2:VAL:N	68:S2:1091:C:HO2'	2.10	0.49
64:SY:12:PHE:HD1	64:SY:23:MET:HE3	1.77	0.49
68:S2:996:A:H2'	68:S2:997:A:C8	2.47	0.49
69:SR:51:ALA:O	69:SR:55:THR:HG23	2.13	0.49
3:L5:137:G:H2'	3:L5:138:G:C8	2.42	0.49
3:L5:966:A:H5''	3:L5:2092:G:H22	1.78	0.49
53:SE:87:MET:SD	53:SE:123:LEU:HB2	2.53	0.49
68:S2:694:G:H2'	68:S2:695:C:O4'	2.12	0.49
85:CB:124:GLY:HA3	85:CB:358:LEU:HD12	1.94	0.49
86:CA:162:GLN:HB3	86:CA:215[A]:LYS:HE2	1.95	0.49
3:L5:1179:U:H3'	3:L5:1180:C:H5''	1.95	0.49
3:L5:1703:C:H2'	3:L5:1704:C:O4'	2.13	0.49
3:L5:3898:G:H5'	7:LB:254:ILE:HG13	1.94	0.49
9:LD:215:ASP:HB3	9:LD:218:ALA:HB3	1.94	0.49
19:LO:168:TYR:CE2	19:LO:172:LYS:HD2	2.47	0.49
23:LS:15:ARG:HD2	23:LS:25:PRO:HG2	1.94	0.49
68:S2:907:G:H2'	68:S2:908:A:C8	2.48	0.49
68:S2:1845:A:H2'	68:S2:1846:G:H8	1.78	0.49
78:SU:20:ILE:HD11	78:SU:114:VAL:HG23	1.93	0.49
7:LB:219:VAL:HG11	7:LB:337:VAL:HG13	1.94	0.49
19:LO:108:ILE:HD13	19:LO:117:ARG:NH1	2.28	0.49
27:LW:97:LYS:HB2	27:LW:100:VAL:HG23	1.95	0.49
42:Ll:9:ILE:HD12	42:Ll:51:LEU:HD12	1.95	0.49
62:SW:28:ARG:HD3	68:S2:921:G:C5	2.47	0.49
70:SD:26:THR:O	70:SD:30:ALA:HB2	2.13	0.49
3:L5:4401:G:H2'	3:L5:4402:C:H6	1.78	0.48
3:L5:4524:G:C2	7:LB:252:ALA:HB1	2.48	0.48
9:LD:196:ARG:O	9:LD:200:MET:HG2	2.13	0.48
11:LF:52:GLU:HG3	32:Lb:96:LEU:HD13	1.95	0.48
49:Lt:127:GLY:HA2	49:Lt:130:LYS:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SB:140:VAL:HG13	51:SB:213:ARG:HB2	1.94	0.48
3:L5:2303:C:H5''	35:Le:104:SER:HB3	1.96	0.48
3:L5:4069:U:H2'	3:L5:4070:U:C6	2.48	0.48
14:LI:162:ARG:HH21	14:LI:164:LYS:HE3	1.77	0.48
18:LN:159:ARG:HB3	18:LN:164:LEU:HB2	1.94	0.48
45:Lo:24:THR:HA	45:Lo:93:LEU:HD21	1.95	0.48
53:SE:45:ILE:HB	53:SE:80:ILE:HG12	1.95	0.48
58:SL:118:ARG:HD3	58:SL:118:ARG:H	1.78	0.48
68:S2:12:U:H2'	68:S2:13:C:C6	2.47	0.48
83:Sg:24:THR:HG23	83:Sg:27:PHE:H	1.78	0.48
9:LD:62:CYS:HB3	9:LD:105:LEU:HD22	1.94	0.48
51:SB:29:ASP:HB3	51:SB:51:ARG:HE	1.77	0.48
68:S2:24:C:HO2'	68:S2:25:A:H8	1.62	0.48
68:S2:1286:G:O6	73:SM:36:ARG:HB3	2.13	0.48
68:S2:1714:U:H2'	68:S2:1715:A:C8	2.47	0.48
85:CB:286:PRO:HB2	85:CB:291:GLN:HB2	1.95	0.48
3:L5:2763:U:H4'	3:L5:2764:A:H5''	1.96	0.48
3:L5:3726:A:H2'	3:L5:3727:A:C8	2.48	0.48
3:L5:5025:C:H5''	3:L5:5026:U:H5	1.79	0.48
11:LF:157:ARG:HE	11:LF:248:ASN:HB2	1.77	0.48
22:LR:168:GLU:HA	22:LR:171:LYS:HE3	1.95	0.48
71:SF:60:ARG:HH21	80:Sc:49:PRO:HA	1.78	0.48
84:Et:22:G:H2'	84:Et:23:A:C8	2.48	0.48
85:CB:331:GLU:HA	85:CB:335:LEU:HD12	1.96	0.48
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.96	0.48
3:L5:2710:C:H41	22:LR:46:LYS:HZ3	1.62	0.48
68:S2:1201:U:H2'	68:S2:1202:U:C6	2.48	0.48
77:ST:40:ALA:HB3	77:ST:43:LYS:HG2	1.95	0.48
83:Sg:257:LYS:HD2	83:Sg:266:ILE:HD13	1.96	0.48
85:CB:16:LYS:HZ2	85:CB:388:CYS:HB3	1.79	0.48
3:L5:37:U:H2'	3:L5:38:A:O4'	2.13	0.48
3:L5:173:C:H2'	3:L5:174:C:C6	2.48	0.48
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.49	0.48
3:L5:3954:A:H1'	3:L5:4058:U:H5'	1.96	0.48
3:L5:4745:G:H1	3:L5:4955:A:H61	1.61	0.48
11:LF:182:TYR:HB3	11:LF:200:ARG:HG3	1.95	0.48
19:LO:126:VAL:HG13	19:LO:127:VAL:HG13	1.96	0.48
48:Ls:141:LEU:HD21	48:Ls:171:GLU:HG3	1.94	0.48
60:SO:57:THR:H	60:SO:60:MET:HE3	1.78	0.48
68:S2:1540:G:H2'	68:S2:1541:G:H8	1.79	0.48
69:SR:114:LEU:HB2	69:SR:117:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.79	0.48
20:LP:17:SER:HB2	20:LP:98:ALA:HB2	1.95	0.48
41:Lk:33:LYS:HG2	41:Lk:46:VAL:HG22	1.95	0.48
54:SG:201:LYS:O	54:SG:205:GLU:HG3	2.14	0.48
54:SG:212:LEU:O	54:SG:215:LYS:HG2	2.14	0.48
57:SJ:127:ARG:HD3	67:Se:31:ARG:HD3	1.96	0.48
64:SY:41:ARG:HH21	64:SY:53:ASP:HA	1.78	0.48
15:LJ:93:GLU:HG3	15:LJ:175:LEU:HD11	1.95	0.48
28:LX:87:MET:HB2	86:CA:259:MET:HE1	1.96	0.48
52:SC:183:LYS:HA	52:SC:195:LEU:O	2.14	0.48
59:SN:60:VAL:HG23	59:SN:66:VAL:HG21	1.96	0.48
68:S2:955:A:N3	68:S2:956:G:H1'	2.29	0.48
68:S2:1405:A:H2'	68:S2:1406:G:O4'	2.13	0.48
70:SD:197:LYS:HG3	70:SD:198:ILE:HG23	1.95	0.48
71:SF:162:ALA:HB3	71:SF:169:ILE:HD13	1.94	0.48
83:Sg:175:LYS:HD2	83:Sg:184:LEU:HD21	1.96	0.48
3:L5:512:U:H3	3:L5:647:G:H1	1.61	0.48
3:L5:4405:G:H5'	14:LI:8:CYS:SG	2.54	0.48
7:LB:258:HIS:HA	7:LB:260:ALA:N	2.28	0.48
17:LM:38:VAL:O	17:LM:47:ARG:HA	2.13	0.48
30:LZ:50:PRO:HD3	30:LZ:68:ILE:HG12	1.96	0.48
52:SC:173:LYS:HD3	61:SV:3:ASN:HA	1.96	0.48
68:S2:1438:A:H2'	68:S2:1439:A:C8	2.48	0.48
77:ST:129:ARG:HE	77:ST:133:ARG:HE	1.61	0.48
84:Et:23:A:H2'	84:Et:24:G:H8	1.78	0.48
85:CB:160:MET:HE3	85:CB:174:LEU:HD21	1.95	0.48
86:CA:23:MET:HE2	86:CA:63:ILE:HG13	1.96	0.48
3:L5:4063:U:H2'	3:L5:4064:C:C2	2.48	0.48
61:SV:11:LEU:HD23	61:SV:11:LEU:H	1.78	0.48
68:S2:159:A2M:O5'	68:S2:159:A2M:H8	2.13	0.48
68:S2:943:U:H2'	68:S2:944:A:C8	2.47	0.48
68:S2:1533:A:H2	68:S2:1536:G:N3	2.12	0.48
10:LE:224:LYS:HA	10:LE:227:HIS:HB3	1.96	0.47
60:SO:56:VAL:HA	60:SO:60:MET:HE3	1.95	0.47
68:S2:746:C:H42	68:S2:797:C:H42	1.61	0.47
68:S2:1839:U:H2'	68:S2:1840:U:C6	2.49	0.47
3:L5:1317:U:H2'	3:L5:1318:C:C6	2.49	0.47
3:L5:1969:G:H4'	48:Ls:36:GLY:HA2	1.96	0.47
48:Ls:91:THR:HG21	48:Ls:98:ILE:HG13	1.96	0.47
50:SA:203:PHE:HZ	69:SR:91:LEU:HD11	1.79	0.47
51:SB:171:ILE:HA	51:SB:174:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1831:A:H2'	68:S2:1832:6MZ:H8	1.96	0.47
83:Sg:256:ILE:HB	83:Sg:270:LEU:HB2	1.95	0.47
3:L5:737:C:C5	3:L5:739:G:H5''	2.49	0.47
6:LA:13:GLY:O	6:LA:17:ARG:HG3	2.15	0.47
12:LG:74:LEU:HD13	18:LN:24:ARG:HH12	1.79	0.47
14:LI:171:TRP:HB2	14:LI:178:ALA:HA	1.96	0.47
24:LT:27:LEU:HB3	24:LT:31:MET:HE3	1.96	0.47
52:SC:137:VAL:HB	52:SC:217:ALA:HA	1.95	0.47
68:S2:1277:C:H2'	68:S2:1278:A:H8	1.78	0.47
69:SR:31:ASN:HA	69:SR:34:VAL:HG22	1.96	0.47
86:CA:49:CYS:HB3	86:CA:281:ARG:NH2	2.29	0.47
5:L8:75:OMG:HM23	5:L8:75:OMG:H1'	1.73	0.47
18:LN:140:LYS:HD3	18:LN:140:LYS:HA	1.68	0.47
30:LZ:41:ALA:HB2	30:LZ:77:TYR:HE1	1.79	0.47
52:SC:70:VAL:HG21	52:SC:93:ILE:HG23	1.96	0.47
68:S2:468:A2M:H2'	68:S2:469:A:O4'	2.14	0.47
73:SM:94:ILE:HA	73:SM:96:ARG:NH1	2.29	0.47
3:L5:106:A:H2'	3:L5:107:G:O4'	2.14	0.47
3:L5:1345:A:H2'	3:L5:1346:C:C6	2.49	0.47
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.49	0.47
50:SA:48:ILE:HG21	69:SR:102:THR:HG22	1.96	0.47
51:SB:103:MET:HB3	51:SB:215:VAL:HG12	1.96	0.47
68:S2:1139:C:H2'	68:S2:1140:G:O4'	2.15	0.47
68:S2:1238:U:O2	68:S2:1242:U:H5	1.97	0.47
77:ST:65:TYR:HE2	77:ST:128:GLN:HG3	1.78	0.47
79:SZ:57:LYS:HA	79:SZ:60:LYS:HG2	1.97	0.47
83:Sg:14:HIS:HD2	83:Sg:41:ILE:HD12	1.79	0.47
83:Sg:40:ILE:HD11	83:Sg:66:VAL:HG21	1.97	0.47
83:Sg:42:MET:HE3	83:Sg:57:ARG:HB2	1.97	0.47
85:CB:305:MET:HE3	85:CB:336:LEU:HD22	1.96	0.47
85:CB:445:LYS:HB2	85:CB:445:LYS:HE3	1.59	0.47
86:CA:191:LYS:HE3	86:CA:194:VAL:HG21	1.96	0.47
3:L5:1921:C:C4	23:LS:161:ARG:HD2	2.50	0.47
3:L5:1992:U:H4'	3:L5:1993:C:H5''	1.95	0.47
51:SB:168:MET:HB2	51:SB:197:ILE:HD13	1.96	0.47
53:SE:124:CYS:HB3	53:SE:141:THR:OG1	2.14	0.47
68:S2:1010:G:H2'	68:S2:1011:A:C8	2.50	0.47
68:S2:1298:G:C8	74:SP:79:HIS:ND1	2.82	0.47
85:CB:63:GLU:HG3	85:CB:68:ILE:O	2.15	0.47
3:L5:1758:G:H2'	3:L5:1759:G:C8	2.49	0.47
3:L5:3732:A:H2'	3:L5:3733:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4238:G:H2'	3:L5:4239:A:C8	2.50	0.47
3:L5:4913:G:H4'	3:L5:4914:C:O5'	2.14	0.47
5:L8:140:C:H2'	5:L8:141:C:C6	2.49	0.47
14:LI:152:LEU:HB3	14:LI:165:ILE:HD12	1.96	0.47
39:Li:63:VAL:HG23	39:Li:65:LYS:HG3	1.97	0.47
52:SC:263:LYS:HA	52:SC:267:GLN:HE21	1.78	0.47
56:SI:139:LYS:HE2	56:SI:141:ARG:HG3	1.95	0.47
57:SJ:93:LYS:HB2	57:SJ:96:TYR:CD1	2.50	0.47
58:SL:89:ARG:HE	58:SL:106:HIS:CD2	2.32	0.47
68:S2:668:A2M:HM'3	68:S2:668:A2M:H1'	1.57	0.47
68:S2:1101:U:H2'	68:S2:1102:G:C8	2.49	0.47
68:S2:1144:A:H2'	68:S2:1145:A:C8	2.50	0.47
68:S2:1337:4AC:H2'	68:S2:1338:G:C8	2.49	0.47
70:SD:120:TYR:HB3	70:SD:124:ARG:NH1	2.30	0.47
70:SD:195:THR:HG23	70:SD:197:LYS:HG2	1.97	0.47
73:SM:31:LEU:HD12	73:SM:32:ALA:N	2.30	0.47
74:SP:16:THR:HA	74:SP:21:ASP:HA	1.95	0.47
85:CB:226:LYS:HA	85:CB:257:MET:HE2	1.95	0.47
3:L5:99:A:H5''	18:LN:184:ILE:HD12	1.96	0.47
11:LF:127:LYS:HB2	24:LT:133:ALA:HB3	1.97	0.47
15:LJ:95:ARG:HD2	15:LJ:177:GLY:HA3	1.96	0.47
26:LV:35:LYS:HB2	26:LV:67:LYS:HG3	1.97	0.47
68:S2:300:U:H2'	68:S2:301:A:H8	1.80	0.47
68:S2:1221:G:H2'	68:S2:1222:G:H8	1.80	0.47
68:S2:1338:G:H4'	78:SU:74:SER:H	1.79	0.47
73:SM:87:GLU:HG3	73:SM:103:VAL:HG21	1.95	0.47
84:Et:23:A:H2'	84:Et:24:G:C8	2.50	0.47
85:CB:539:GLU:HG2	85:CB:545:ILE:HG13	1.97	0.47
86:CA:17:VAL:HA	86:CA:20:LYS:HZ2	1.78	0.47
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.50	0.47
3:L5:1857:C:H2'	3:L5:1858:A:C8	2.49	0.47
3:L5:2539:C:H2'	3:L5:2540:C:C6	2.49	0.47
3:L5:2741:U:H2'	6:LA:50:HIS:CD2	2.50	0.47
48:Ls:187:LEU:HD23	48:Ls:187:LEU:H	1.80	0.47
51:SB:144:LYS:HD3	51:SB:208:HIS:HB3	1.97	0.47
53:SE:141:THR:HG23	53:SE:143:ASP:N	2.29	0.47
54:SG:174:PRO:HB3	68:S2:65:C:C6	2.50	0.47
64:SY:7:ILE:HD13	64:SY:27:VAL:HG12	1.97	0.47
68:S2:352:U:H2'	68:S2:353:C:C6	2.50	0.47
68:S2:1004:PSU:H2'	68:S2:1005:G:C8	2.50	0.47
68:S2:1328:OMG:HM23	68:S2:1328:OMG:H1'	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:SF:101:HIS:HB2	71:SF:108:PRO:HG3	1.97	0.47
80:Sc:17:VAL:HA	80:Sc:30:VAL:HG12	1.96	0.47
83:Sg:57:ARG:HH21	83:Sg:95:GLY:HA3	1.80	0.47
85:CB:594:LYS:HG2	85:CB:601:ARG:HG2	1.96	0.47
3:L5:4536:OMC:HM22	3:L5:4537:C:O4'	2.15	0.47
3:L5:4637:OMG:HM23	3:L5:4637:OMG:H1'	1.73	0.47
51:SB:25:PHE:CG	60:SO:88:LEU:HD21	2.50	0.47
62:SW:26:LEU:HD11	62:SW:60:LYS:HB3	1.97	0.47
71:SF:40:ALA:H	71:SF:68:ILE:HG23	1.80	0.47
85:CB:223:PHE:HB3	85:CB:344:LEU:HD13	1.96	0.47
85:CB:649:ILE:HA	85:CB:663:THR:HG22	1.97	0.47
85:CB:745:TYR:CE2	85:CB:812:CYS:HB2	2.49	0.47
3:L5:75:G:C6	16:LL:102:ARG:HA	2.50	0.46
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.49	0.46
10:LE:203:ILE:O	10:LE:206:VAL:HG22	2.15	0.46
18:LN:200:LEU:HB3	18:LN:204:ARG:NH1	2.31	0.46
68:S2:455:A:H2'	68:S2:456:C:C6	2.51	0.46
68:S2:698:G:H2'	68:S2:733:C:C4	2.50	0.46
70:SD:48:ILE:HD11	70:SD:86:LEU:HG	1.98	0.46
70:SD:219:PRO:HB2	83:Sg:192:THR:HG22	1.97	0.46
76:SS:22:GLY:HA2	76:SS:56:ALA:HB3	1.96	0.46
3:L5:1788:A:H2'	14:LI:22:PHE:CZ	2.51	0.46
3:L5:3923:A:H2'	3:L5:3924:C:C6	2.51	0.46
3:L5:4688:C:H2'	3:L5:4689:PSU:C6	2.51	0.46
8:LC:140:LYS:HD3	8:LC:245:HIS:HB2	1.96	0.46
17:LM:24:LEU:HD11	17:LM:86:TRP:CG	2.50	0.46
18:LN:38:ARG:HA	18:LN:62:TYR:HD1	1.80	0.46
55:SH:50:GLU:OE2	55:SH:58:LYS:HB3	2.15	0.46
60:SO:30:VAL:HG22	60:SO:94:HIS:HB2	1.98	0.46
68:S2:484:A2M:H8	68:S2:484:A2M:O5'	2.16	0.46
68:S2:958:G:H2'	68:S2:959:G:C8	2.50	0.46
68:S2:1451:G:H5'	83:Sg:64:HIS:HE1	1.80	0.46
68:S2:1491:G:H2'	68:S2:1492:U:C6	2.50	0.46
68:S2:1562:C:H2'	68:S2:1563:G:C8	2.50	0.46
68:S2:1780:G:H3'	68:S2:1781:A:C8	2.48	0.46
70:SD:28:GLU:HG3	70:SD:29:LEU:HD22	1.97	0.46
77:ST:76:THR:HG23	77:ST:94:ARG:HD2	1.97	0.46
3:L5:1588:U:H2'	3:L5:1589:C:C6	2.50	0.46
3:L5:1989:G:H2'	3:L5:1990:A:C8	2.49	0.46
7:LB:155:LYS:HD3	7:LB:156:TYR:CZ	2.50	0.46
7:LB:341:LYS:O	7:LB:342:LYS:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LF:197:VAL:O	11:LF:201:PHE:HB2	2.15	0.46
13:LH:95:VAL:HG12	43:Lm:82:LEU:HD13	1.97	0.46
53:SE:208:VAL:HG21	53:SE:225:ILE:HG13	1.98	0.46
63:SX:88:ASP:HA	68:S2:617:G:H4'	1.97	0.46
68:S2:194:C:H2'	68:S2:195:C:H6	1.79	0.46
85:CB:558:LEU:HD21	85:CB:572:LYS:HG2	1.97	0.46
86:CA:64:PHE:HB2	86:CA:72:LYS:HE3	1.97	0.46
5:L8:70:G:H5''	29:LY:27:ARG:CZ	2.45	0.46
6:LA:181:LYS:HB2	6:LA:184:ARG:HG3	1.97	0.46
19:LO:81:TRP:HB2	19:LO:104:VAL:HG21	1.97	0.46
25:LU:28:PRO:HB3	25:LU:100:LEU:HD21	1.98	0.46
26:LV:92:ASP:HB2	27:LW:2:LYS:NZ	2.31	0.46
29:LY:13:LYS:O	29:LY:17:ARG:HD3	2.16	0.46
60:SO:33:ILE:HG23	60:SO:97:LEU:HA	1.96	0.46
68:S2:434:G:H2'	68:S2:435:A:C8	2.51	0.46
68:S2:895:G:H3'	68:S2:896:U:H4'	1.96	0.46
69:SR:61:ILE:HD11	69:SR:66:VAL:HG22	1.96	0.46
76:SS:40:TYR:CZ	76:SS:97:GLN:HG2	2.51	0.46
79:SZ:92:LEU:HD22	79:SZ:109:TYR:HE2	1.80	0.46
85:CB:820:LEU:HB3	85:CB:831:PRO:HG3	1.97	0.46
3:L5:93:G:H2'	3:L5:94:A:C8	2.51	0.46
3:L5:1613:A:H5''	6:LA:183:GLY:CA	2.46	0.46
3:L5:2520:C:H2'	3:L5:2521:G:H8	1.81	0.46
3:L5:4196:OMG:HM23	3:L5:4196:OMG:H1'	1.68	0.46
9:LD:264:LYS:HD3	9:LD:266:TRP:CZ2	2.51	0.46
10:LE:165:LEU:HD11	10:LE:176:THR:HG22	1.95	0.46
15:LJ:146:ARG:HG2	15:LJ:147:ARG:HG3	1.97	0.46
16:LL:208:GLU:HA	16:LL:211:LYS:HG2	1.95	0.46
26:LV:91:LYS:HD3	26:LV:91:LYS:HA	1.81	0.46
31:La:100:ILE:HG13	31:La:123:ILE:HB	1.97	0.46
35:Le:35:TRP:CZ2	35:Le:56:PRO:HD2	2.51	0.46
54:SG:188:LYS:O	54:SG:192:ILE:HG12	2.16	0.46
64:SY:15:ASN:HD21	64:SY:22:GLN:HE22	1.62	0.46
68:S2:223:C:H2'	68:S2:224:A:C8	2.50	0.46
68:S2:1736:G:H2'	68:S2:1737:G:H8	1.81	0.46
71:SF:19:LEU:HD23	71:SF:109:LEU:HD21	1.97	0.46
3:L5:121:A:H62	3:L5:152:U:H3	1.64	0.46
3:L5:1705:G:H2'	3:L5:1706:A:O4'	2.14	0.46
3:L5:4389:C:H2'	3:L5:4390:A:C8	2.50	0.46
21:LQ:67:ILE:HG22	21:LQ:71:LYS:HE2	1.98	0.46
48:Ls:18:ILE:HG13	48:Ls:19:GLN:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:LS:130:LEU:HB2	48:LS:134:LYS:HE3	1.98	0.46
56:SI:199:LEU:HA	56:SI:199:LEU:HD23	1.78	0.46
57:SJ:86:VAL:HG11	57:SJ:105:PHE:CD1	2.51	0.46
86:CA:209:GLN:O	86:CA:213:HIS:HB2	2.16	0.46
3:L5:120:A:H2'	3:L5:149:A:H61	1.80	0.46
3:L5:4619:U:H2'	3:L5:4620:OMU:H6	1.98	0.46
7:LB:86:VAL:HG12	7:LB:201:LEU:HD23	1.96	0.46
26:LV:69:LYS:HB3	26:LV:71:GLU:OE1	2.15	0.46
50:SA:41:ARG:HB3	50:SA:47:TYR:CD2	2.51	0.46
51:SB:39:PHE:HE2	51:SB:86:LEU:HD11	1.80	0.46
53:SE:72:ILE:HG12	53:SE:90:ILE:HD12	1.98	0.46
60:SO:134:PRO:HB3	68:S2:944:A:H5''	1.97	0.46
68:S2:5:U:H2'	68:S2:6:G:C8	2.51	0.46
85:CB:20:ARG:HA	85:CB:20:ARG:HD3	1.82	0.46
3:L5:1733:G:N3	3:L5:4214:A:H2'	2.30	0.46
3:L5:3856:A:H5''	20:LP:83:TRP:O	2.16	0.46
14:LI:51:HIS:CD2	14:LI:168:SER:HB2	2.51	0.46
26:LV:45:ILE:HG21	26:LV:53:PRO:HB3	1.97	0.46
50:SA:63:ARG:HH11	61:SV:38:GLU:HA	1.81	0.46
51:SB:88:THR:HA	51:SB:98:THR:HA	1.98	0.46
53:SE:72:ILE:HB	53:SE:77:ARG:HG3	1.97	0.46
68:S2:85:A:H2'	68:S2:86:C:H6	1.81	0.46
68:S2:1457:U:H2'	68:S2:1458:G:C8	2.50	0.46
68:S2:1498:A:P	70:SD:27:ARG:HH22	2.39	0.46
84:ET:37:A:H3'	84:ET:38:A:H8	1.80	0.46
86:CA:113:HIS:HA	86:CA:117:PHE:O	2.16	0.46
3:L5:10:A:H2'	3:L5:11:G:C8	2.51	0.46
3:L5:162:A:H2'	3:L5:163:A:H8	1.79	0.46
3:L5:280:G:H5''	18:LN:14:LYS:HE2	1.97	0.46
3:L5:4320:G:H2'	3:L5:4321:U:C6	2.51	0.46
4:L7:63:C:H5'	4:L7:64:G:H5''	1.98	0.46
10:LE:226:ARG:HD3	10:LE:226:ARG:H	1.80	0.46
68:S2:300:U:H2'	68:S2:301:A:C8	2.51	0.46
68:S2:388:U:H2'	68:S2:389:A:C8	2.51	0.46
68:S2:1406:G:H2'	68:S2:1407:U:C6	2.51	0.46
70:SD:123:LEU:HD13	70:SD:134:CYS:SG	2.55	0.46
85:CB:57:THR:HG21	85:CB:104:ASP:OD2	2.16	0.46
3:L5:498:C:C2	3:L5:499:G:H1'	2.51	0.46
3:L5:979:C:OP2	10:LE:66:LYS:HD3	2.16	0.46
3:L5:1461:C:H2'	3:L5:1462:A:C8	2.50	0.46
3:L5:1743:A:O4'	9:LD:15:ARG:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2411:C:H2'	3:L5:2412:A:H8	1.81	0.46
3:L5:4504:C:H2'	3:L5:4505:C:C6	2.51	0.46
3:L5:4723:A:H2'	3:L5:4724:A:C8	2.51	0.46
4:L7:23:A:H2'	4:L7:24:C:C6	2.51	0.46
9:LD:205:ALA:HB1	9:LD:233:PRO:HB3	1.98	0.46
14:LI:47:PRO:HB3	14:LI:171:TRP:CZ2	2.51	0.46
75:SQ:146:ARG:NH1	84:Et:32:C:H5''	2.31	0.46
85:CB:479:LEU:HD22	85:CB:483:GLY:HA3	1.96	0.46
86:CA:12:ILE:HD13	86:CA:21:TYR:CE2	2.50	0.46
3:L5:300:A:H2'	3:L5:301:G:H8	1.81	0.45
3:L5:4919:G:H2'	3:L5:4920:C:H6	1.81	0.45
28:LX:156:ILE:HD12	28:LX:156:ILE:HA	1.86	0.45
34:Ld:19:GLU:HA	34:Ld:90:ARG:HH11	1.81	0.45
49:Lt:11:LYS:HA	49:Lt:11:LYS:HD2	1.67	0.45
54:SG:138:ALA:HB2	54:SG:179:LEU:HD12	1.97	0.45
58:SL:82:MET:HE2	58:SL:85:THR:HG23	1.97	0.45
59:SN:75:LEU:HB3	59:SN:81:ALA:HB2	1.98	0.45
62:SW:28:ARG:NH1	68:S2:921:G:H2'	2.31	0.45
68:S2:552:G:H2'	68:S2:553:U:C6	2.51	0.45
68:S2:1139:C:H5	68:S2:1149:A:H62	1.63	0.45
68:S2:1540:G:H2'	68:S2:1541:G:C8	2.51	0.45
68:S2:1709:G:H1	68:S2:1824:A:N6	2.14	0.45
69:SR:16:ILE:HD11	69:SR:54:VAL:HG21	1.98	0.45
85:CB:428:ARG:HG3	85:CB:442:LEU:HD11	1.98	0.45
3:L5:190:G:H2'	3:L5:191:G:H8	1.82	0.45
3:L5:223:G:H4'	3:L5:225:G:C8	2.50	0.45
3:L5:1326:A2M:H2'	3:L5:1327:C:C6	2.52	0.45
3:L5:1468:C:H2'	3:L5:1469:C:C6	2.51	0.45
3:L5:2079:G:H2'	3:L5:2080:U:C6	2.51	0.45
3:L5:2276:A:H2'	3:L5:2277:C:O4'	2.16	0.45
3:L5:3928:A:H2'	3:L5:3929:G:O4'	2.15	0.45
3:L5:4111:U:H2'	3:L5:4112:C:H5	1.80	0.45
3:L5:4392:OMG:HM21	3:L5:4394:A:H2'	1.98	0.45
3:L5:4571:A2M:H2'	3:L5:4572:U:H6	1.81	0.45
3:L5:5027:C:O2'	3:L5:5028:G:H5''	2.16	0.45
5:L8:92:U:H2'	5:L8:93:C:O4'	2.16	0.45
12:LG:223:ARG:HD3	12:LG:227:ASN:HB2	1.97	0.45
23:LS:16:CYS:SG	23:LS:54:MET:HG2	2.57	0.45
32:Lb:5:LYS:HE2	32:Lb:8:THR:HB	1.99	0.45
36:Lf:83:MET:HE3	36:Lf:83:MET:HB3	1.85	0.45
50:SA:3:GLY:HA2	50:SA:63:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SL:16:ILE:HG23	58:SL:34:PRO:HG2	1.99	0.45
71:SF:22:LYS:HG3	71:SF:23:TRP:CD2	2.51	0.45
73:SM:11:VAL:O	73:SM:15:ASN:HB2	2.15	0.45
76:SS:102:GLY:HA2	76:SS:105:ASN:ND2	2.31	0.45
85:CB:88:PHE:HE1	85:CB:250:ALA:HA	1.81	0.45
3:L5:99:A:H2'	3:L5:100:C:O2	2.16	0.45
3:L5:1647:U:OP1	89:L5:5291:SPD:H51	2.16	0.45
3:L5:1994:C:H2'	3:L5:1995:G:C8	2.52	0.45
3:L5:2730:U:H2'	3:L5:2731:C:C6	2.51	0.45
3:L5:4524:G:N3	7:LB:252:ALA:HB1	2.31	0.45
5:L8:141:C:H2'	5:L8:142:U:C6	2.51	0.45
14:LI:56:GLU:HG3	14:LI:161:GLY:HA3	1.98	0.45
35:Le:84:GLU:O	35:Le:87:VAL:HG22	2.16	0.45
42:Ll:28:ARG:HA	42:Ll:33:ASN:HD22	1.80	0.45
48:Ls:114:GLY:HA2	48:Ls:166:LYS:HD2	1.98	0.45
68:S2:639:C:H2'	68:S2:640:A:C8	2.51	0.45
68:S2:1101:U:H2'	68:S2:1102:G:H8	1.80	0.45
68:S2:1414:A:H2'	68:S2:1415:C:C6	2.51	0.45
76:SS:56:ALA:HA	76:SS:59:LEU:HD23	1.98	0.45
79:SZ:74:SER:HA	79:SZ:79:ILE:HG12	1.98	0.45
79:SZ:86:ALA:O	79:SZ:89:GLN:HG2	2.16	0.45
86:CA:27:ILE:O	86:CA:31:VAL:HG23	2.16	0.45
86:CA:86:VAL:HG13	86:CA:229:LEU:HD21	1.98	0.45
3:L5:257:C:H2'	3:L5:258:G:C8	2.51	0.45
3:L5:2542:G:H2'	3:L5:2543:A:C8	2.52	0.45
3:L5:4070:U:H2'	3:L5:4071:U:C6	2.51	0.45
3:L5:4911:A:OP2	7:LB:100:ARG:HD3	2.17	0.45
20:LP:23:ARG:HG2	20:LP:125:MET:HE1	1.98	0.45
68:S2:1037:G:H4'	68:S2:1845:A:H4'	1.97	0.45
68:S2:1433:C:H42	78:SU:92:HIS:HD2	1.65	0.45
86:CA:16:LEU:O	86:CA:20:LYS:HG2	2.16	0.45
2:CI:62:VAL:HG22	2:CI:71:ARG:HB3	1.97	0.45
3:L5:398:A2M:H1'	3:L5:398:A2M:HM'3	1.64	0.45
3:L5:500:G:O2'	3:L5:504:G:H3'	2.16	0.45
3:L5:1307:A:H2'	3:L5:1308:C:C6	2.50	0.45
3:L5:5004:C:H2'	3:L5:5005:G:O4'	2.16	0.45
16:LL:200:LYS:O	16:LL:204:GLU:HG2	2.16	0.45
20:LP:107:LEU:HB2	20:LP:152:GLU:OE2	2.17	0.45
50:SA:76:VAL:HG12	50:SA:123:VAL:HB	1.97	0.45
52:SC:109:ILE:HD11	52:SC:151:ILE:HD11	1.98	0.45
52:SC:130:ILE:HD13	52:SC:159:LYS:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1609:C:H2'	68:S2:1610:G:H8	1.81	0.45
75:SQ:19:ALA:HA	75:SQ:74:GLY:HA3	1.99	0.45
78:SU:22:ILE:HD11	78:SU:112:VAL:HB	1.98	0.45
83:Sg:21:ILE:HG23	83:Sg:33:SER:HB3	1.98	0.45
83:Sg:191:HIS:ND1	83:Sg:195:LEU:HD21	2.31	0.45
85:CB:26:ALA:HB2	85:CB:128:VAL:HB	1.99	0.45
3:L5:457:G:H2'	3:L5:458:C:C6	2.52	0.45
3:L5:2714:G:H2'	3:L5:2715:G:H8	1.80	0.45
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.17	0.45
64:SY:72:PHE:HE2	64:SY:74:MET:HE3	1.82	0.45
64:SY:83:LYS:HA	64:SY:91:LEU:HD11	1.97	0.45
68:S2:27:A2M:HM'3	68:S2:27:A2M:H1'	1.51	0.45
68:S2:144:U:H2'	68:S2:145:G:C8	2.52	0.45
68:S2:1365:G:H2'	68:S2:1366:G:H8	1.81	0.45
68:S2:1541:G:H2'	68:S2:1542:C:C6	2.50	0.45
68:S2:1597:C:H4'	68:S2:1603:G:C6	2.51	0.45
74:SP:93:MET:SD	74:SP:106:GLU:HB2	2.57	0.45
77:ST:21:PHE:O	77:ST:24:LYS:HG3	2.17	0.45
85:CB:39:LEU:HD11	85:CB:351:LEU:HG	1.98	0.45
46:Lp:36:LYS:HD3	46:Lp:48:LYS:HB3	1.99	0.45
54:SG:7:PHE:CD1	54:SG:113:ILE:HB	2.51	0.45
58:SL:75:GLY:HA3	58:SL:88:ILE:HD12	1.99	0.45
70:SD:14:ASP:O	70:SD:18:LYS:HG2	2.16	0.45
77:ST:42:HIS:CD2	77:ST:43:LYS:HE3	2.52	0.45
83:Sg:7:LEU:HB2	83:Sg:310:TRP:CZ3	2.52	0.45
85:CB:4:PHE:HB2	85:CB:8:GLN:NE2	2.32	0.45
85:CB:394:LEU:HD11	85:CB:421:VAL:HG22	1.99	0.45
2:CI:54:LYS:HA	2:CI:57:LYS:HG2	1.97	0.45
3:L5:1187:G:H2'	3:L5:1188:C:H6	1.81	0.45
3:L5:1855:G:OP1	32:Lb:4:SER:HB2	2.16	0.45
3:L5:5000:G:O2'	7:LB:382:MET:HE1	2.17	0.45
25:LU:18:VAL:HG13	25:LU:73:THR:HG23	1.99	0.45
38:Lh:89:ARG:O	38:Lh:93:ARG:HG2	2.17	0.45
54:SG:161:PRO:HA	54:SG:171:THR:HA	1.98	0.45
68:S2:634:A:H2'	68:S2:635:G:C8	2.52	0.45
68:S2:1284:A:C8	73:SM:33:ARG:HG3	2.51	0.45
71:SF:56:TYR:HA	71:SF:62:ARG:HG3	1.99	0.45
78:SU:24:LEU:HD13	78:SU:112:VAL:HG12	1.99	0.45
85:CB:770:VAL:HA	85:CB:786:ALA:HA	1.99	0.45
3:L5:267:G:H2'	3:L5:268:G:C8	2.50	0.45
3:L5:1327:C:H2'	3:L5:1328:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1444:G:H22	3:L5:2104:G:H21	1.65	0.45
3:L5:3599:A:H2'	3:L5:3600:G:C8	2.51	0.45
3:L5:4062:A:H2'	3:L5:4063:U:C6	2.52	0.45
3:L5:4523:A2M:HM'3	3:L5:4523:A2M:H1'	1.77	0.45
3:L5:4590:A2M:H1'	3:L5:4590:A2M:HM'3	1.63	0.45
3:L5:4685:U:H2'	3:L5:4686:G:C8	2.52	0.45
7:LB:288:GLY:HA3	7:LB:330:PHE:CE1	2.52	0.45
31:La:71:PRO:HG2	31:La:108:TYR:HA	1.97	0.45
50:SA:38:ILE:HD11	50:SA:150:THR:HG22	1.99	0.45
53:SE:99:PHE:HA	53:SE:112:HIS:O	2.16	0.45
68:S2:929:G:H2'	68:S2:930:C:O4'	2.16	0.45
68:S2:1775:U:H2'	68:S2:1776:G:C8	2.52	0.45
85:CB:8:GLN:HE21	85:CB:45:ILE:HD12	1.82	0.45
86:CA:70:MET:HE2	86:CA:115:ASP:HA	1.99	0.45
3:L5:1693:U:H2'	3:L5:1694:C:O4'	2.15	0.45
3:L5:1914:C:H4'	19:LO:89:PRO:HD3	1.99	0.45
6:LA:180:LEU:HD22	46:Lp:18:TYR:HB3	1.98	0.45
16:LL:111:GLN:O	16:LL:115:GLN:HG2	2.17	0.45
42:Ll:41:ARG:HA	42:Ll:41:ARG:HD2	1.79	0.45
47:Lr:54:ALA:HA	47:Lr:61:VAL:HG23	1.99	0.45
50:SA:8:LEU:HD23	50:SA:8:LEU:HA	1.77	0.45
59:SN:54:LEU:HG	59:SN:60:VAL:HG11	1.98	0.45
68:S2:388:U:H2'	68:S2:389:A:H8	1.81	0.45
68:S2:432:G:H2'	68:S2:433:A:C8	2.52	0.45
68:S2:1447:G:H1'	78:SU:55:ARG:HH12	1.82	0.45
75:SQ:97:GLN:HB2	75:SQ:105:LYS:HD3	1.98	0.45
3:L5:3595:U:H5''	3:L5:3597:G:OP2	2.17	0.44
3:L5:4220:6MZ:H2'	3:L5:4222:G:H5''	1.98	0.44
3:L5:4625:C:O2'	3:L5:4626:A:H5'	2.17	0.44
34:Ld:117:LEU:HD23	34:Ld:117:LEU:HA	1.83	0.44
48:Ls:82:ILE:O	48:Ls:83:ARG:HD2	2.17	0.44
54:SG:136:LYS:HB2	68:S2:65:C:H41	1.82	0.44
61:SV:1:MET:HB3	61:SV:10:ASP:HB2	1.99	0.44
68:S2:527:C:H2'	68:S2:528:A:C8	2.49	0.44
70:SD:140:GLY:HA3	70:SD:182:LEU:HD12	1.99	0.44
85:CB:6:VAL:O	85:CB:9:ILE:HG22	2.17	0.44
86:CA:123:HIS:NE2	86:CA:125:PHE:HB3	2.32	0.44
3:L5:158:A:H5''	3:L5:159:C:H2'	2.00	0.44
3:L5:223:G:H4'	3:L5:225:G:N7	2.33	0.44
3:L5:1084:C:H2'	3:L5:1085:C:H6	1.82	0.44
3:L5:2656:U:H5''	30:LZ:38:TYR:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.52	0.44
3:L5:3911:C:H2'	3:L5:3912:U:C6	2.51	0.44
3:L5:4742:G:H2'	3:L5:4743:G:H8	1.80	0.44
54:SG:220:ALA:O	54:SG:224:ARG:HG2	2.16	0.44
58:SL:133:PRO:HG2	68:S2:383:G:H21	1.83	0.44
68:S2:1298:G:C8	74:SP:79:HIS:CE1	3.06	0.44
68:S2:1736:G:H2'	68:S2:1737:G:C8	2.52	0.44
75:SQ:86:GLN:HG2	75:SQ:90:LYS:HE2	1.99	0.44
84:Et:19:G:H5''	84:Et:20:U:H5'	2.00	0.44
86:CA:173:VAL:HB	86:CA:354:LEU:HD21	1.98	0.44
3:L5:1298:C:H2'	3:L5:1299:G:H8	1.82	0.44
3:L5:2298:U:H5''	8:LC:204:ARG:HH21	1.81	0.44
3:L5:4459:U:H2'	3:L5:4460:U:C6	2.51	0.44
3:L5:4742:G:H2'	3:L5:4743:G:C8	2.52	0.44
88:L5:5293:SPM:H31	88:L5:5293:SPM:H62	1.68	0.44
18:LN:148:THR:O	18:LN:151:ILE:HG22	2.17	0.44
27:LW:96:GLN:HB2	27:LW:101:ARG:HH21	1.82	0.44
33:Lc:52:CYS:HB3	33:Lc:57:LYS:HG3	1.99	0.44
51:SB:65:ARG:HG2	60:SO:50:LYS:HD3	1.98	0.44
68:S2:386:C:H2'	68:S2:387:C:C6	2.52	0.44
68:S2:698:G:H5'	68:S2:733:C:N3	2.32	0.44
73:SM:36:ARG:O	73:SM:40:LYS:HG2	2.17	0.44
85:CB:360:SER:HB2	85:CB:362:VAL:HG22	1.99	0.44
85:CB:602:LEU:HA	85:CB:707:VAL:HG12	2.00	0.44
1:CD:195:ARG:HG2	68:S2:1701:C:C2	2.53	0.44
3:L5:1428:U:H5''	21:LQ:42:THR:HB	1.98	0.44
3:L5:3722:G:H2'	3:L5:3723:A:H8	1.82	0.44
3:L5:3932:U:H2'	3:L5:3933:G:C8	2.53	0.44
3:L5:4095:G:H2'	3:L5:4096:C:C6	2.52	0.44
8:LC:106:LYS:HD3	8:LC:108:TRP:CZ2	2.52	0.44
20:LP:117:ILE:HD12	20:LP:148:MET:HE2	1.99	0.44
40:Lj:60:GLY:HA2	40:Lj:64:MET:SD	2.58	0.44
52:SC:169:TYR:OH	61:SV:9:VAL:HG21	2.17	0.44
57:SJ:136:ARG:HA	57:SJ:141:VAL:HA	1.99	0.44
68:S2:162:C:H2'	68:S2:163:U:O4'	2.16	0.44
68:S2:634:A:H2'	68:S2:635:G:H8	1.81	0.44
68:S2:1560:U:H2'	68:S2:1561:A:H8	1.83	0.44
68:S2:1588:A:H2'	68:S2:1589:A:H8	1.81	0.44
73:SM:94:ILE:HA	73:SM:96:ARG:HH12	1.82	0.44
73:SM:99:LYS:HG2	73:SM:100:PRO:HD2	2.00	0.44
83:Sg:254:PRO:HG3	83:Sg:283:PRO:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:CA:81:SER:HB2	86:CA:107:LYS:HB2	1.99	0.44
3:L5:962:C:H5''	3:L5:963:G:C8	2.53	0.44
3:L5:2870:A:H2'	3:L5:2871:A:C8	2.52	0.44
3:L5:4345:C:H2'	3:L5:4346:U:C6	2.52	0.44
3:L5:4507:A:H2'	3:L5:4508:C:C6	2.52	0.44
3:L5:4563:U:H2'	3:L5:4564:A:C8	2.53	0.44
12:LG:70:LEU:HD23	12:LG:70:LEU:HA	1.85	0.44
13:LH:59:LYS:HE2	13:LH:66:GLU:HG3	1.99	0.44
25:LU:100:LEU:HD23	25:LU:112:LEU:HD12	1.99	0.44
49:Lt:16:ARG:HE	49:Lt:17:CYS:N	2.15	0.44
51:SB:120:MET:HE1	68:S2:987:A:C6	2.52	0.44
64:SY:35:VAL:HG13	64:SY:40:ILE:HD11	1.99	0.44
69:SR:28:PHE:HA	69:SR:55:THR:HG21	2.00	0.44
3:L5:1199:G:H2'	3:L5:1200:G:C8	2.53	0.44
3:L5:2465:C:H2'	3:L5:2466:G:O4'	2.18	0.44
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.53	0.44
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.53	0.44
5:L8:5:U:H2'	5:L8:6:C:C6	2.52	0.44
7:LB:27:GLY:HA2	7:LB:276:HIS:CD2	2.53	0.44
8:LC:318:PRO:C	8:LC:320:LYS:H	2.25	0.44
9:LD:181:PRO:HD2	9:LD:195:HIS:CD2	2.53	0.44
14:LI:43:VAL:HG21	14:LI:197:VAL:HG13	1.99	0.44
22:LR:180:LYS:O	22:LR:183:GLU:HG3	2.18	0.44
54:SG:135:PRO:HA	68:S2:169:U:H5''	2.00	0.44
57:SJ:150:ARG:HG3	68:S2:821:G:C6	2.53	0.44
64:SY:110:ARG:HG3	64:SY:114:MET:HE1	2.00	0.44
68:S2:834:C:N4	68:S2:839:C:H42	2.11	0.44
68:S2:959:G:H2'	68:S2:960:U:C6	2.53	0.44
68:S2:1051:G:H2'	68:S2:1052:A:H8	1.83	0.44
68:S2:1713:C:H2'	68:S2:1714:U:H6	1.82	0.44
70:SD:163:PRO:HA	70:SD:166:TYR:CE1	2.53	0.44
83:Sg:120:ILE:CG2	83:Sg:132:TRP:HB2	2.48	0.44
83:Sg:249:CYS:HB3	83:Sg:258:ILE:HD13	2.00	0.44
3:L5:385:A:N3	3:L5:387:G:H5''	2.33	0.44
3:L5:423:G:H5'	20:LP:26:PHE:HZ	1.83	0.44
3:L5:683:C:H2'	3:L5:684:G:O4'	2.18	0.44
3:L5:1683:PSU:H2'	3:L5:1684:A:C8	2.52	0.44
7:LB:117:ARG:HG2	7:LB:180:LEU:HD12	1.99	0.44
24:LT:44:GLY:HA2	24:LT:95:HIS:HB3	1.99	0.44
44:Ln:1:MET:HB2	68:S2:1706:G:H5'	2.00	0.44
58:SL:79:LYS:HB2	58:SL:87:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:SM:69:CYS:SG	73:SM:76:LEU:HB2	2.57	0.44
3:L5:270:U:H2'	3:L5:271:C:C6	2.53	0.44
3:L5:400:A2M:HM'3	3:L5:400:A2M:H1'	1.79	0.44
3:L5:737:C:C4	3:L5:739:G:H5''	2.53	0.44
3:L5:3861:A:H2'	3:L5:3862:A:C8	2.53	0.44
3:L5:4860:G:H2'	3:L5:4861:G:H8	1.83	0.44
5:L8:96:C:H5''	38:Lh:66:LYS:HG2	2.00	0.44
9:LD:41:LYS:HB2	24:LT:68:THR:O	2.18	0.44
9:LD:117:LYS:N	9:LD:117:LYS:HD2	2.33	0.44
12:LG:209:SER:HA	12:LG:212:LYS:HG3	1.98	0.44
49:Lt:82:ILE:HD13	49:Lt:137:GLN:HB3	2.00	0.44
50:SA:30:LEU:HD12	50:SA:38:ILE:HG13	2.00	0.44
50:SA:158:ASP:HB2	50:SA:159:ILE:HD12	2.00	0.44
68:S2:595:U:H2'	68:S2:596:U:C6	2.53	0.44
84:Et:25:C:H42	84:Et:45:G:H22	1.65	0.44
86:CA:248:LYS:HB2	86:CA:248:LYS:HE2	1.79	0.44
3:L5:138:G:H2'	3:L5:139:G:C8	2.53	0.44
3:L5:271:C:H2'	3:L5:272:U:C6	2.53	0.44
3:L5:982:U:H2'	3:L5:983:C:C6	2.53	0.44
3:L5:1359:G:H4'	18:LN:203:TYR:HB2	2.00	0.44
3:L5:1697:G:H22	3:L5:2084:C:P	2.41	0.44
3:L5:2803:U:H2'	3:L5:2804:OMC:H6	1.83	0.44
3:L5:4238:G:H2'	3:L5:4239:A:H8	1.83	0.44
3:L5:4591:U:H2'	3:L5:4592:C:C6	2.52	0.44
9:LD:156:GLY:HA2	9:LD:181:PRO:HG3	2.00	0.44
22:LR:175:GLU:O	22:LR:178:GLN:HG3	2.17	0.44
64:SY:12:PHE:CD1	64:SY:23:MET:HE3	2.53	0.44
68:S2:329:G:H2'	68:S2:330:G:H8	1.82	0.44
68:S2:943:U:C2	68:S2:944:A:C8	3.06	0.44
68:S2:1408:U:H2'	68:S2:1409:A:C8	2.53	0.44
72:SK:21:MET:HB3	72:SK:69:TRP:HB2	1.99	0.44
76:SS:61:GLU:HG2	76:SS:62:ASP:N	2.32	0.44
85:CB:400:LYS:NZ	85:CB:532:PRO:HD3	2.33	0.44
86:CA:143:ILE:HD13	86:CA:343:TYR:OH	2.18	0.44
3:L5:1251:C:H2'	3:L5:1252:C:C6	2.53	0.43
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.53	0.43
3:L5:2543:A:H2	3:L5:2773:G:H22	1.64	0.43
3:L5:2562:G:N2	3:L5:2564:G:H3'	2.33	0.43
3:L5:3861:A:H2'	3:L5:3862:A:H8	1.83	0.43
3:L5:4342:C:O3'	45:Lo:37:GLY:HA3	2.18	0.43
35:Le:99:ILE:HD13	35:Le:108:ARG:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SB:27:LYS:O	51:SB:51:ARG:HD3	2.18	0.43
68:S2:1651:A:H2'	68:S2:1652:G:C8	2.51	0.43
69:SR:31:ASN:ND2	69:SR:55:THR:HG22	2.33	0.43
77:ST:120:GLY:C	77:ST:121:ARG:HD3	2.43	0.43
83:Sg:29:ASP:HA	83:Sg:47:ARG:HH21	1.83	0.43
85:CB:697:MET:HE1	85:CB:702:PHE:HZ	1.82	0.43
86:CA:234:GLU:HG2	86:CA:236:LYS:NZ	2.33	0.43
3:L5:2844:A:O2'	3:L5:4631:G:H4'	2.18	0.43
3:L5:3652:A:H2'	3:L5:3653:A:C5	2.53	0.43
3:L5:4274:A:H2'	3:L5:4275:G:H8	1.80	0.43
5:L8:5:U:H2'	5:L8:6:C:H6	1.83	0.43
8:LC:110:ARG:HG3	18:LN:204:ARG:HE	1.83	0.43
53:SE:186:GLY:HA3	68:S2:809:A:OP1	2.18	0.43
67:Se:48:THR:HG22	67:Se:50:GLY:H	1.82	0.43
68:S2:1227:G:C2	68:S2:1228:A:C8	3.06	0.43
68:S2:1317:C:H2'	68:S2:1318:G:C8	2.53	0.43
68:S2:1621:U:O2'	68:S2:1622:U:H2'	2.18	0.43
86:CA:19:THR:HA	86:CA:22:LYS:HE3	1.99	0.43
3:L5:667:A:H5''	3:L5:668:C:H5''	1.99	0.43
3:L5:1613:A:H5''	6:LA:183:GLY:HA2	2.00	0.43
3:L5:4456:OMC:HM21	7:LB:241:PRO:HD3	1.99	0.43
5:L8:122:G:C6	5:L8:123:U:H1'	2.54	0.43
28:LX:127:LEU:HD11	28:LX:135:LYS:HE3	1.99	0.43
50:SA:51:LEU:HA	50:SA:54:THR:HG22	1.99	0.43
55:SH:118:ARG:HA	55:SH:118:ARG:HD3	1.88	0.43
56:SI:83:TYR:HB2	56:SI:202:ILE:HD11	2.00	0.43
60:SO:116:LEU:HG	65:Sa:53:ILE:HD11	2.00	0.43
68:S2:15:U:H2'	68:S2:16:G:O4'	2.18	0.43
68:S2:495:U:H2'	68:S2:496:C:O4'	2.18	0.43
68:S2:1220:A:H2'	68:S2:1221:G:O4'	2.17	0.43
68:S2:1330:G:N7	68:S2:1492:U:H3'	2.33	0.43
68:S2:1407:U:H2'	68:S2:1408:U:H6	1.80	0.43
68:S2:1616:U:H2'	68:S2:1617:G:C8	2.53	0.43
75:SQ:72:VAL:HG11	75:SQ:84:ILE:HD11	2.00	0.43
77:ST:129:ARG:HG3	77:ST:133:ARG:HH21	1.83	0.43
85:CB:36:THR:HG23	85:CB:102:LEU:HD21	2.01	0.43
1:CD:201:ARG:HD3	70:SD:145:GLN:HG2	2.00	0.43
3:L5:966:A:H2	3:L5:2093:A:H2	1.66	0.43
3:L5:1176:C:H42	3:L5:1184:A:H61	1.66	0.43
3:L5:2415:U:H2'	3:L5:2416:G:C8	2.54	0.43
10:LE:99:ASP:O	10:LE:100:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Ld:75:LYS:HB2	34:Ld:79:ASN:O	2.18	0.43
54:SG:136:LYS:HB2	68:S2:65:C:N4	2.33	0.43
68:S2:534:G:H2'	68:S2:535:G:H8	1.82	0.43
68:S2:601:OMG:HM23	68:S2:601:OMG:H1'	1.77	0.43
68:S2:1643:U:H2'	68:S2:1644:C:C6	2.53	0.43
85:CB:33:SER:HB3	85:CB:54:THR:HG23	2.00	0.43
3:L5:7:C:H2'	3:L5:8:U:C6	2.54	0.43
3:L5:500:G:H1'	3:L5:504:G:H3'	2.01	0.43
3:L5:1577:G:H5'	3:L5:1578:U:H5''	2.00	0.43
3:L5:1726:U:H5'	11:LF:135:ILE:HD11	2.00	0.43
3:L5:1753:G:H2'	3:L5:1754:U:C2	2.54	0.43
11:LF:48:LYS:HE3	32:Lb:96:LEU:HD21	2.00	0.43
11:LF:182:TYR:CZ	11:LF:203:GLU:HG2	2.53	0.43
13:LH:107:GLU:O	13:LH:107:GLU:HG2	2.18	0.43
15:LJ:15:LEU:HD12	15:LJ:165:TRP:HB2	2.01	0.43
16:LL:145:LYS:HE2	16:LL:146:LEU:HD13	2.00	0.43
19:LO:189:ILE:HD13	19:LO:189:ILE:HA	1.91	0.43
39:Li:43:MET:HE3	39:Li:43:MET:HB3	1.82	0.43
49:Lt:134:GLY:HA2	49:Lt:137:GLN:CD	2.44	0.43
50:SA:10:MET:HE1	50:SA:18:PHE:CE2	2.53	0.43
50:SA:159:ILE:HD11	61:SV:34:MET:SD	2.57	0.43
53:SE:19:MET:SD	53:SE:108:ARG:HD2	2.58	0.43
61:SV:53:TYR:CD1	61:SV:72:LEU:HD23	2.52	0.43
63:SX:60:LYS:HA	63:SX:60:LYS:HD3	1.83	0.43
64:SY:39:GLU:O	64:SY:42:GLU:HG2	2.17	0.43
68:S2:17:C:H2'	68:S2:18:C:C6	2.53	0.43
68:S2:533:A:H61	68:S2:550:C:H42	1.65	0.43
68:S2:952:G:H2'	68:S2:953:C:C6	2.52	0.43
68:S2:1217:A:H2'	68:S2:1218:C:H6	1.83	0.43
68:S2:1495:G:H4'	81:Sd:26:ASN:ND2	2.34	0.43
75:SQ:110:ASP:HA	75:SQ:113:ILE:HG22	2.01	0.43
3:L5:2101:C:H2'	3:L5:2102:G:C8	2.54	0.43
3:L5:3656:A:H2'	3:L5:3657:U:H6	1.83	0.43
3:L5:3867:A2M:HM'3	3:L5:3867:A2M:H1'	1.54	0.43
11:LF:241:ASN:O	11:LF:245:ARG:HG2	2.18	0.43
12:LG:95:LEU:HA	12:LG:218:LEU:HD11	2.00	0.43
17:LM:25:VAL:HB	17:LM:38:VAL:HG13	2.00	0.43
22:LR:19:LYS:HB2	22:LR:19:LYS:HE2	1.83	0.43
38:Lh:73:TYR:HA	38:Lh:76:LYS:HD2	2.01	0.43
48:Ls:77:LYS:HB3	48:Ls:198:ILE:HD11	2.00	0.43
48:Ls:125:ALA:HA	48:Ls:154:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ls:166:LYS:HA	48:Ls:166:LYS:HD3	1.83	0.43
49:Lt:123:ARG:HD2	49:Lt:129:ILE:HD11	2.01	0.43
50:SA:63:ARG:NH1	61:SV:38:GLU:HA	2.34	0.43
55:SH:130:LEU:HD12	55:SH:177:TYR:CZ	2.54	0.43
68:S2:116:OMU:HM23	68:S2:116:OMU:H1'	1.85	0.43
68:S2:197:U:H2'	68:S2:203:G:N2	2.34	0.43
68:S2:940:U:H2'	68:S2:941:C:C6	2.54	0.43
72:SK:3:MET:HE2	72:SK:8:ARG:HA	2.00	0.43
72:SK:10:ALA:O	72:SK:13:GLU:HG2	2.18	0.43
72:SK:21:MET:HE2	72:SK:45:VAL:HG21	1.99	0.43
79:SZ:48:VAL:HG23	79:SZ:80:ARG:HD2	2.01	0.43
86:CA:108:ILE:O	86:CA:122:ALA:HA	2.19	0.43
3:L5:269:G:H2'	3:L5:270:U:C6	2.54	0.43
3:L5:978:G:H2'	3:L5:979:C:C6	2.54	0.43
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.18	0.43
3:L5:1907:A:H2'	3:L5:1908:A:C8	2.54	0.43
10:LE:95:PRO:HA	10:LE:104:THR:HG22	2.00	0.43
27:LW:107:GLN:O	27:LW:110:ARG:HG3	2.19	0.43
33:Lc:21:VAL:HG11	33:Lc:96:ILE:HG12	2.01	0.43
54:SG:131:ARG:HH11	68:S2:168:C:H4'	1.83	0.43
68:S2:293:C:O2'	68:S2:294:U:H3'	2.19	0.43
68:S2:414:A:H2'	68:S2:415:A:H8	1.83	0.43
68:S2:1692:U:H2'	68:S2:1693:G:C8	2.53	0.43
75:SQ:146:ARG:HH11	84:Et:32:C:H5''	1.84	0.43
78:SU:104:ILE:HB	78:SU:106:ILE:HD11	2.00	0.43
3:L5:502:C:H3'	3:L5:503:C:H3'	2.01	0.43
3:L5:2267:U:OP1	47:Lr:37:SER:HB2	2.19	0.43
3:L5:3709:U:H2'	3:L5:3710:G:O4'	2.19	0.43
3:L5:4098:A:N6	3:L5:4099:G:H21	2.17	0.43
3:L5:4113:U:H4'	3:L5:4115:G:C6	2.53	0.43
3:L5:4460:U:H2'	3:L5:4461:C:C6	2.53	0.43
6:LA:48:ILE:HG22	46:Lp:54:ILE:HG12	2.00	0.43
48:Ls:16:LYS:NZ	48:Ls:20:LEU:HD22	2.34	0.43
48:Ls:128:THR:HG23	48:Ls:130:LEU:HG	2.01	0.43
50:SA:174:MET:HE3	50:SA:174:MET:HB2	1.78	0.43
51:SB:24:PRO:O	51:SB:28:LYS:HG2	2.18	0.43
51:SB:69:VAL:HG13	51:SB:74:LEU:HD11	2.00	0.43
63:SX:52:LEU:HD11	63:SX:73:GLN:HB2	2.01	0.43
68:S2:29:G:H2'	68:S2:30:C:C6	2.54	0.43
68:S2:864:A:H2'	68:S2:865:A:C8	2.53	0.43
69:SR:31:ASN:HD22	69:SR:55:THR:HG22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:SQ:106:LYS:HA	75:SQ:109:LYS:HG2	2.01	0.43
82:Sf:103:LEU:HD12	82:Sf:105:TYR:CZ	2.54	0.43
85:CB:337:LYS:HG2	85:CB:341:ARG:HH21	1.84	0.43
86:CA:89:PHE:HE1	86:CA:242:GLN:HE22	1.66	0.43
86:CA:354:LEU:HA	86:CA:357:LEU:HG	2.01	0.43
3:L5:318:A:H2'	3:L5:319:A:C8	2.54	0.43
3:L5:2474:G:H2'	3:L5:2502:G:N2	2.34	0.43
3:L5:2538:U:H2'	3:L5:2539:C:C6	2.54	0.43
3:L5:3732:A:H2'	3:L5:3733:A:H8	1.82	0.43
3:L5:5053:U:H5'	3:L5:5054:C:C4	2.53	0.43
18:LN:126:THR:HG23	18:LN:127:TYR:CD2	2.53	0.43
25:LU:80:LYS:HG2	25:LU:110:TYR:CE2	2.52	0.43
37:Lg:33:LEU:HD23	37:Lg:33:LEU:HA	1.84	0.43
52:SC:246:LYS:HB3	52:SC:246:LYS:HE2	1.74	0.43
56:SI:145:ILE:O	56:SI:148:LYS:HG2	2.19	0.43
68:S2:496:C:H2'	68:S2:497:C:H6	1.84	0.43
68:S2:980:A:H2'	68:S2:981:A:C8	2.53	0.43
68:S2:1535:U:P	71:SF:169:ILE:HG12	2.59	0.43
76:SS:40:TYR:HA	76:SS:83:PHE:HE2	1.84	0.43
77:ST:62:ARG:HH12	77:ST:66:LEU:HD11	1.84	0.43
83:Sg:183:LYS:HA	83:Sg:183:LYS:HD2	1.85	0.43
3:L5:268:G:H2'	3:L5:269:G:C8	2.53	0.43
3:L5:1167:C:H42	3:L5:1195:G:N2	2.17	0.43
3:L5:3825:A2M:H2'	3:L5:3826:C:O4'	2.19	0.43
3:L5:3925:OMU:HM23	3:L5:3925:OMU:H1'	1.88	0.43
7:LB:80:GLU:HG2	7:LB:82:PRO:HD3	2.01	0.43
8:LC:158:VAL:HG12	8:LC:217:ILE:HD12	2.01	0.43
29:LY:53:ASP:HB3	29:LY:110:LYS:H	1.84	0.43
38:Lh:52:LYS:HA	38:Lh:52:LYS:HD3	1.71	0.43
57:SJ:32:ILE:HG12	57:SJ:37:LEU:HB2	2.00	0.43
58:SL:126:VAL:HG12	58:SL:145:VAL:HG22	2.00	0.43
68:S2:348:A:H2'	68:S2:349:A:C8	2.54	0.43
68:S2:508:A:H3'	68:S2:509:OMG:C8	2.51	0.43
68:S2:569:A:H2'	68:S2:570:C:O4'	2.19	0.43
68:S2:799:OMU:HM23	68:S2:799:OMU:H1'	1.85	0.43
68:S2:1383:A2M:HM'3	68:S2:1383:A2M:H1'	1.61	0.43
68:S2:1562:C:H2'	68:S2:1563:G:H8	1.84	0.43
85:CB:23:SER:HB3	85:CB:122:THR:HG21	2.00	0.43
86:CA:88:HIS:CG	86:CA:305:PHE:HB3	2.53	0.43
3:L5:468:U:C6	3:L5:469:C:H5	2.37	0.42
3:L5:1645:C:H2'	3:L5:1646:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3690:U:H2'	3:L5:3691:G:O4'	2.19	0.42
3:L5:4113:U:H4'	3:L5:4115:G:C5	2.53	0.42
4:L7:33:U:H2'	4:L7:34:C:C6	2.53	0.42
6:LA:27:ALA:HB1	6:LA:77:ILE:HG13	2.01	0.42
7:LB:165:HIS:HA	7:LB:179:HIS:O	2.18	0.42
16:LL:42:LYS:HB3	16:LL:42:LYS:HE2	1.74	0.42
19:LO:28:LEU:HD23	19:LO:28:LEU:HA	1.92	0.42
49:Lt:16:ARG:HE	49:Lt:17:CYS:H	1.67	0.42
50:SA:206:ASP:O	50:SA:210:ILE:HD12	2.19	0.42
52:SC:167:ARG:HB3	52:SC:177:PRO:HB2	2.00	0.42
53:SE:104:ASP:HB3	53:SE:110:ALA:HB2	1.99	0.42
53:SE:128:LYS:HG2	53:SE:140:VAL:HG22	2.01	0.42
54:SG:52:ILE:HG23	54:SG:109:LEU:HD21	2.01	0.42
64:SY:84:LYS:HD2	64:SY:84:LYS:HA	1.90	0.42
68:S2:102:A:H4'	68:S2:104:A:C8	2.54	0.42
68:S2:564:A:H2'	68:S2:565:G:O4'	2.19	0.42
68:S2:800:U:H2'	68:S2:801:PSU:O4'	2.19	0.42
85:CB:208:VAL:HG13	85:CB:261:TRP:HB3	2.01	0.42
85:CB:365:GLN:NE2	85:CB:388:CYS:HB2	2.34	0.42
3:L5:25:A:H2'	3:L5:26:C:H6	1.84	0.42
3:L5:1462:A:H4'	32:Lb:27:GLN:OE1	2.19	0.42
3:L5:1751:A:H2'	3:L5:1752:G:C8	2.53	0.42
3:L5:3722:G:H2'	3:L5:3723:A:C8	2.53	0.42
4:L7:7:G:OP1	9:LD:33:ARG:HD2	2.19	0.42
5:L8:8:U:H2'	5:L8:9:A:C8	2.54	0.42
5:L8:90:C:H1'	29:LY:24:HIS:HB3	2.01	0.42
7:LB:155:LYS:HD3	7:LB:156:TYR:CE2	2.54	0.42
16:LL:110:LEU:O	16:LL:114:VAL:HG13	2.19	0.42
52:SC:191:VAL:HG11	52:SC:236:PHE:HA	2.01	0.42
58:SL:89:ARG:HE	58:SL:106:HIS:CG	2.37	0.42
68:S2:1685:U:H2'	68:S2:1686:G:O4'	2.19	0.42
69:SR:70:SER:O	69:SR:74:GLN:HG2	2.19	0.42
72:SK:42:ASN:HA	72:SK:45:VAL:HG12	2.01	0.42
85:CB:439:LYS:HA	85:CB:439:LYS:HD3	1.91	0.42
85:CB:609:PHE:CD2	85:CB:699:GLY:HA2	2.54	0.42
3:L5:272:U:H2'	3:L5:273:U:C6	2.54	0.42
3:L5:481:G:H2'	3:L5:482:G:C8	2.55	0.42
3:L5:1081:C:O2'	3:L5:1082:C:H5'	2.19	0.42
3:L5:1269:G:H2'	3:L5:1270:A:C4	2.54	0.42
3:L5:1558:A:H2'	3:L5:1559:G:C8	2.54	0.42
3:L5:1725:U:H2'	3:L5:1726:U:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3910:C:H2'	3:L5:3911:C:H6	1.83	0.42
8:LC:29:LYS:HA	8:LC:29:LYS:HD3	1.84	0.42
8:LC:33:ARG:HG3	8:LC:122:TYR:HE2	1.84	0.42
10:LE:183:ARG:HD2	10:LE:183:ARG:HA	1.71	0.42
13:LH:103:VAL:HG11	13:LH:144:LEU:HD21	2.01	0.42
15:LJ:113:ILE:HG21	15:LJ:119:TYR:HD2	1.83	0.42
17:LM:119:ARG:HG3	19:LO:189:ILE:HD12	2.02	0.42
18:LN:154:PRO:O	18:LN:157:LYS:HG2	2.20	0.42
18:LN:178:HIS:HA	18:LN:181:HIS:NE2	2.34	0.42
53:SE:58:GLY:HA2	53:SE:61:VAL:HG12	2.00	0.42
56:SI:103:LEU:HD13	56:SI:170:LYS:HD3	2.00	0.42
58:SL:78:THR:HG22	58:SL:79:LYS:HG3	2.01	0.42
68:S2:115:U:H2'	68:S2:116:OMU:C6	2.48	0.42
68:S2:329:G:H2'	68:S2:330:G:C8	2.53	0.42
68:S2:750:C:H42	68:S2:793:G:H1'	1.85	0.42
83:Sg:217:MET:HB3	83:Sg:226:HIS:CE1	2.55	0.42
3:L5:655:C:H2'	3:L5:656:C:C6	2.55	0.42
3:L5:965:G:H1'	3:L5:2093:A:N1	2.35	0.42
3:L5:1567:U:H2'	3:L5:1568:C:C6	2.53	0.42
3:L5:1875:C:H2'	3:L5:1876:U:C6	2.54	0.42
6:LA:29:LEU:O	6:LA:123:ARG:HD2	2.18	0.42
6:LA:206:PRO:HG3	6:LA:213:GLY:HA3	2.00	0.42
21:LQ:43:PHE:CD2	21:LQ:133:GLY:HA3	2.54	0.42
27:LW:5:LEU:HD12	27:LW:30:GLN:NE2	2.34	0.42
41:Lk:51:GLU:HG2	41:Lk:52:LYS:H	1.84	0.42
48:Ls:28:PHE:HZ	48:Ls:95:LEU:HA	1.84	0.42
55:SH:24:SER:HA	55:SH:27:LEU:HG	2.02	0.42
55:SH:78:ARG:HD2	55:SH:78:ARG:HA	1.89	0.42
56:SI:141:ARG:HB3	56:SI:145:ILE:HB	2.01	0.42
57:SJ:114:VAL:HG23	57:SJ:126:ALA:HB1	2.01	0.42
60:SO:34:PHE:HB3	60:SO:41:PHE:HB2	2.01	0.42
68:S2:1047:C:H2'	68:S2:1048:G:O4'	2.19	0.42
68:S2:1433:C:H42	78:SU:92:HIS:CD2	2.36	0.42
68:S2:1456:G:H2'	68:S2:1457:U:C6	2.54	0.42
70:SD:8:LYS:HG2	78:SU:61:LEU:HD21	2.01	0.42
71:SF:61:PHE:HB3	80:Sc:51:ARG:NH2	2.31	0.42
83:Sg:43:TRP:CD1	83:Sg:55:PRO:HA	2.54	0.42
85:CB:16:LYS:HB3	85:CB:16:LYS:HE2	1.87	0.42
85:CB:79:TYR:CZ	85:CB:351:LEU:HB3	2.55	0.42
85:CB:256:MET:O	85:CB:260:LEU:HD13	2.19	0.42
3:L5:411:G:H4'	3:L5:412:G:H5''	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2558:C:H2'	3:L5:2559:G:H8	1.85	0.42
3:L5:2602:G:H2'	3:L5:2603:C:C6	2.54	0.42
3:L5:4389:C:H2'	3:L5:4390:A:H8	1.84	0.42
19:LO:193:THR:HG23	19:LO:202:LEU:HD21	2.02	0.42
22:LR:182:GLU:HA	22:LR:185:ILE:HG12	2.02	0.42
48:Ls:120:GLU:HG2	48:Ls:161:ILE:O	2.20	0.42
66:Sb:8:LEU:HA	66:Sb:8:LEU:HD23	1.79	0.42
68:S2:543:C:H3'	68:S2:544:G:C8	2.53	0.42
68:S2:656:G:H5'	68:S2:662:G:N2	2.34	0.42
68:S2:946:U:H2'	68:S2:947:G:C8	2.55	0.42
68:S2:1706:G:H2'	68:S2:1707:U:H6	1.84	0.42
69:SR:24:LEU:HB2	69:SR:58:MET:HE1	2.01	0.42
73:SM:17:ALA:O	73:SM:20:GLU:HG3	2.19	0.42
73:SM:85:LEU:HD23	73:SM:107:SER:HA	2.01	0.42
85:CB:72:SER:H	85:CB:114:GLU:CD	2.27	0.42
85:CB:397:TYR:HB2	85:CB:494:MET:SD	2.59	0.42
86:CA:36:VAL:HG12	86:CA:125:PHE:CE1	2.54	0.42
3:L5:663:G:H2'	3:L5:664:G:C8	2.55	0.42
3:L5:1084:C:H2'	3:L5:1085:C:C6	2.54	0.42
3:L5:1097:C:H2'	3:L5:1098:G:C8	2.55	0.42
3:L5:2073:C:OP1	11:LF:212:LYS:HE3	2.20	0.42
3:L5:2611:A:H2'	3:L5:2612:G:C8	2.55	0.42
3:L5:3867:A2M:H2'	3:L5:3868:G:O4'	2.19	0.42
3:L5:4680:G:H2'	3:L5:4681:A:C8	2.55	0.42
3:L5:4935:C:H2'	3:L5:4936:G:C8	2.55	0.42
12:LG:138:ALA:HB2	12:LG:194:VAL:HG11	2.00	0.42
18:LN:116:LEU:HD22	18:LN:135:ILE:HD11	2.01	0.42
22:LR:165:LYS:HE3	22:LR:165:LYS:HB3	1.81	0.42
50:SA:220:LYS:HA	50:SA:220:LYS:HD3	1.85	0.42
66:Sb:70:LYS:HD2	68:S2:1106:C:H5''	2.01	0.42
68:S2:159:A2M:H1'	68:S2:159:A2M:HM'3	1.49	0.42
71:SF:17:ILE:HG13	71:SF:46:ALA:HB3	2.01	0.42
72:SK:95:ARG:HD2	72:SK:98:ARG:C	2.44	0.42
78:SU:24:LEU:HB3	78:SU:32:LEU:HD11	2.01	0.42
83:Sg:14:HIS:CE1	83:Sg:35:SER:HB2	2.54	0.42
85:CB:231:MET:HE1	85:CB:343:TRP:HZ2	1.84	0.42
3:L5:57:G:H5''	18:LN:154:PRO:HB2	2.02	0.42
3:L5:458:C:H2'	3:L5:459:C:C6	2.55	0.42
3:L5:3947:A:H3'	3:L5:3948:C:C6	2.55	0.42
3:L5:5053:U:H5'	3:L5:5054:C:C5	2.54	0.42
37:Lg:83:CYS:SG	37:Lg:86:CYS:HB2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Lj:67:LEU:HD23	40:Lj:67:LEU:HA	1.89	0.42
52:SC:173:LYS:H	52:SC:173:LYS:HG2	1.68	0.42
53:SE:195:ILE:HD13	53:SE:210:VAL:HG22	2.01	0.42
54:SG:11:GLY:HA2	68:S2:166:A2M:HM'1	2.02	0.42
54:SG:164:LYS:H	54:SG:167:LYS:HE3	1.83	0.42
60:SO:60:MET:HG2	68:S2:956:G:O5'	2.19	0.42
65:Sa:44:ILE:HG21	65:Sa:65:PRO:HD2	2.02	0.42
68:S2:964:A:H2'	68:S2:965:U:H6	1.85	0.42
68:S2:1182:A:C5	68:S2:1183:A:H1'	2.55	0.42
83:Sg:11:LEU:HB2	83:Sg:43:TRP:HZ3	1.84	0.42
3:L5:701:G:H2'	3:L5:702:U:C6	2.55	0.42
3:L5:1380:G:H4'	3:L5:1381:U:H6	1.85	0.42
3:L5:3718:A2M:H8	3:L5:3718:A2M:O5'	2.20	0.42
3:L5:4060:U:H2'	3:L5:4061:G:C8	2.55	0.42
6:LA:132:ASN:O	6:LA:169:VAL:HG12	2.20	0.42
8:LC:168:VAL:HG12	8:LC:172:LYS:HE2	2.02	0.42
17:LM:96:GLU:O	17:LM:100:ARG:HG2	2.20	0.42
50:SA:205:ARG:HH21	69:SR:81:ARG:NH2	2.17	0.42
51:SB:97:LEU:HB3	51:SB:232:HIS:CD2	2.54	0.42
60:SO:125:LYS:HB3	65:Sa:58:VAL:HG13	2.02	0.42
62:SW:3:ARG:HH22	62:SW:28:ARG:NH2	2.18	0.42
68:S2:746:C:H2'	68:S2:747:U:C6	2.54	0.42
69:SR:21:TYR:HD1	69:SR:58:MET:HE2	1.84	0.42
70:SD:120:TYR:HB3	70:SD:124:ARG:HH12	1.85	0.42
78:SU:64:THR:HA	78:SU:78:ASP:O	2.20	0.42
83:Sg:191:HIS:CD2	83:Sg:195:LEU:HD11	2.54	0.42
3:L5:1186:U:H2'	3:L5:1187:G:N3	2.34	0.42
3:L5:1662:C:H2'	3:L5:1663:C:H6	1.85	0.42
3:L5:2478:C:H2'	3:L5:2479:G:H5'	2.02	0.42
3:L5:2906:G:H1'	3:L5:2908:U:C2	2.55	0.42
3:L5:3598:C:H2'	3:L5:3599:A:C8	2.55	0.42
3:L5:3598:C:H2'	3:L5:3599:A:H8	1.84	0.42
5:L8:79:G:H2'	5:L8:80:A:O4'	2.19	0.42
7:LB:302:ASN:HB2	7:LB:314:ILE:H	1.84	0.42
9:LD:179:ARG:HD3	9:LD:179:ARG:HA	1.70	0.42
20:LP:76:TRP:CD1	20:LP:76:TRP:H	2.37	0.42
21:LQ:29:VAL:O	21:LQ:33:ARG:HB2	2.20	0.42
26:LV:21:PRO:HA	26:LV:54:ALA:HA	2.01	0.42
28:LX:155:ILE:HG22	38:Lh:33:VAL:HG13	2.01	0.42
50:SA:8:LEU:HD21	50:SA:191:ARG:HH22	1.85	0.42
50:SA:157:VAL:HG11	50:SA:160:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SO:78:ALA:HB3	60:SO:118:ALA:HB3	2.02	0.42
68:S2:958:G:C6	68:S2:959:G:C6	3.07	0.42
73:SM:31:LEU:H	73:SM:31:LEU:HG	1.70	0.42
76:SS:25:LYS:O	76:SS:29:ALA:CB	2.68	0.42
76:SS:109:GLU:HA	76:SS:112:GLU:HG2	2.02	0.42
82:Sf:126:CYS:SG	82:Sf:144:CYS:HB2	2.60	0.42
3:L5:1669:A:H4'	3:L5:1685:G:N2	2.35	0.42
3:L5:4066:U:H2'	3:L5:4067:U:C6	2.55	0.42
3:L5:4236:G:H4'	3:L5:4328:G:O2'	2.20	0.42
6:LA:142:GLU:C	6:LA:144:LYS:H	2.27	0.42
7:LB:397:ILE:HG13	7:LB:398:ALA:N	2.35	0.42
14:LI:99:ILE:HG22	14:LI:123:GLN:HB2	2.01	0.42
22:LR:149:LYS:O	22:LR:152:LYS:HG3	2.20	0.42
27:LW:111:ALA:O	27:LW:114:GLU:HG3	2.19	0.42
51:SB:109:LYS:O	51:SB:113:MET:HG2	2.19	0.42
53:SE:126:VAL:HG22	53:SE:158:ASP:H	1.85	0.42
54:SG:13:GLN:HE21	68:S2:153:G:H21	1.68	0.42
54:SG:71:GLY:O	54:SG:98:ARG:HD2	2.20	0.42
54:SG:194:LEU:HD13	54:SG:197:GLN:NE2	2.34	0.42
58:SL:17:PHE:CD2	68:S2:222:U:H5''	2.55	0.42
66:Sb:54:VAL:HG22	66:Sb:64:CYS:SG	2.60	0.42
68:S2:106:C:H2'	68:S2:107:A:C8	2.54	0.42
68:S2:165:G:H2'	68:S2:166:A2M:H8	2.02	0.42
68:S2:525:A:H2'	68:S2:526:A:H8	1.85	0.42
68:S2:1391:OMC:HM23	68:S2:1391:OMC:H1'	1.92	0.42
73:SM:30:GLY:HA3	73:SM:113:ASP:HB3	2.02	0.42
79:SZ:49:LEU:HD23	79:SZ:49:LEU:HA	1.87	0.42
85:CB:314:LYS:HE2	85:CB:314:LYS:HB2	1.85	0.42
3:L5:660:A:H2'	3:L5:661:C:C6	2.55	0.41
3:L5:716:C:OP1	8:LC:317:ASN:HB2	2.20	0.41
3:L5:2561:C:H2'	3:L5:2562:G:O4'	2.20	0.41
3:L5:2632:PSU:H2'	3:L5:2633:U:C6	2.55	0.41
3:L5:2809:G:H5''	22:LR:63:CYS:SG	2.60	0.41
3:L5:3723:A:H2'	3:L5:3724:A:C8	2.55	0.41
3:L5:4606:G:H2'	3:L5:4607:A:C8	2.55	0.41
5:L8:36:G:C5	38:Lh:89:ARG:HD3	2.55	0.41
5:L8:66:A:H2'	5:L8:67:U:C6	2.55	0.41
13:LH:92:MET:HE2	13:LH:179:ILE:HG22	2.02	0.41
15:LJ:41:GLU:HG2	15:LJ:48:PRO:HD3	2.02	0.41
22:LR:185:ILE:HA	22:LR:188:LEU:HD12	2.01	0.41
29:LY:54:GLU:HG2	29:LY:108:ARG:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SC:194:ARG:HD3	52:SC:196:ILE:HD11	2.02	0.41
55:SH:160:LYS:HA	55:SH:163:GLN:OE1	2.20	0.41
63:SX:17:ARG:NH2	68:S2:659:G:H21	2.16	0.41
68:S2:72:C:H5'	68:S2:73:C:C5	2.54	0.41
68:S2:568:C:H2'	68:S2:569:A:O4'	2.20	0.41
68:S2:1424:G:H2'	68:S2:1425:G:H8	1.84	0.41
68:S2:1797:U:H2'	68:S2:1798:C:C6	2.55	0.41
73:SM:14:VAL:HG11	73:SM:126:GLU:HG3	2.02	0.41
73:SM:48:HIS:HB2	73:SM:111:VAL:O	2.20	0.41
76:SS:102:GLY:HA2	76:SS:105:ASN:HD21	1.84	0.41
77:ST:51:ASN:HB3	77:ST:54:TYR:HD2	1.85	0.41
83:Sg:217:MET:HG2	83:Sg:229:THR:HG23	2.02	0.41
84:Et:52:G:H2'	84:Et:53:G:H8	1.84	0.41
85:CB:601:ARG:HB2	85:CB:708:THR:HG22	2.02	0.41
85:CB:604:MET:HE2	85:CB:704:VAL:HG22	2.00	0.41
3:L5:75:G:O6	16:LL:103:ARG:HD3	2.20	0.41
3:L5:179:G:H2'	3:L5:180:C:C6	2.55	0.41
3:L5:3870:C:H2'	3:L5:3871:A:C8	2.54	0.41
3:L5:3952:A:H2'	3:L5:3953:G:N9	2.35	0.41
26:LV:42:VAL:HB	26:LV:45:ILE:HG13	2.02	0.41
34:Ld:64:ILE:HD13	34:Ld:106:VAL:HG11	2.02	0.41
49:Lt:147:HIS:ND1	49:Lt:149:HIS:HB3	2.35	0.41
50:SA:34:MET:SD	50:SA:154:LEU:HD11	2.59	0.41
51:SB:182:LYS:HE3	51:SB:182:LYS:HB2	1.85	0.41
57:SJ:2:PRO:HD2	68:S2:429:C:P	2.59	0.41
57:SJ:5:ARG:HG3	68:S2:38:A:OP1	2.20	0.41
57:SJ:131:ARG:HD2	57:SJ:131:ARG:HA	1.81	0.41
60:SO:72:TYR:CZ	60:SO:76:LEU:HD11	2.55	0.41
61:SV:68:SER:HA	61:SV:71:ARG:HH21	1.84	0.41
68:S2:1272:OMC:HM23	68:S2:1272:OMC:H1'	1.89	0.41
68:S2:1775:U:H2'	68:S2:1776:G:H8	1.85	0.41
81:Sd:33:LYS:HE2	81:Sd:34:TYR:CZ	2.55	0.41
3:L5:958:G:N2	10:LE:124:LYS:HB3	2.35	0.41
3:L5:1195:G:H2'	3:L5:1196:G:C8	2.56	0.41
3:L5:1340:OMC:HM23	3:L5:1340:OMC:H1'	1.79	0.41
3:L5:2326:G:H5''	35:Le:127:ALA:HB1	2.03	0.41
3:L5:2372:U:H2'	3:L5:2373:C:C6	2.55	0.41
3:L5:2558:C:H2'	3:L5:2559:G:C8	2.55	0.41
5:L8:82:A:N7	5:L8:84:A:H3'	2.35	0.41
15:LJ:104:ASN:HB3	15:LJ:134:LEU:H	1.85	0.41
17:LM:136:LEU:O	17:LM:137:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SJ:145:PRO:HD2	68:S2:522:A:H5''	2.01	0.41
58:SL:22:ARG:NH1	58:SL:22:ARG:HA	2.35	0.41
68:S2:644:OMG:HM23	68:S2:644:OMG:H1'	1.89	0.41
68:S2:1164:G:O2'	68:S2:1165:G:H5'	2.20	0.41
68:S2:1533:A:H5'	71:SF:163:PHE:CE1	2.55	0.41
71:SF:50:PRO:HB3	71:SF:69:VAL:HG22	2.02	0.41
75:SQ:58:LEU:HD21	75:SQ:63:PHE:HE2	1.85	0.41
85:CB:288:THR:O	85:CB:292:LEU:HG	2.20	0.41
85:CB:537:ILE:HG13	85:CB:545:ILE:HB	2.01	0.41
86:CA:208:GLN:HA	86:CA:211:LYS:HE3	2.01	0.41
1:CD:287:LYS:HE2	1:CD:287:LYS:HB3	1.91	0.41
3:L5:1806:G:H2'	3:L5:1807:C:C6	2.56	0.41
3:L5:2351:OMC:HM23	3:L5:2351:OMC:H1'	1.72	0.41
3:L5:3865:A:H61	3:L5:3881:G:H1	1.68	0.41
3:L5:4306:OMU:HM23	3:L5:4306:OMU:H1'	1.86	0.41
3:L5:4393:G:O4'	3:L5:4447:5MC:HM53	2.20	0.41
10:LE:201:ILE:HG13	10:LE:203:ILE:HG23	2.02	0.41
52:SC:172:ASN:O	52:SC:174:ILE:HG12	2.20	0.41
52:SC:208:PRO:O	52:SC:212:LYS:HG2	2.20	0.41
57:SJ:3:VAL:HB	57:SJ:5:ARG:HD3	2.03	0.41
61:SV:15:ARG:HH21	61:SV:24:ILE:HG21	1.85	0.41
64:SY:82:ALA:O	64:SY:86:GLU:HB2	2.21	0.41
64:SY:87:PRO:HB2	64:SY:89:HIS:CD2	2.56	0.41
68:S2:120:U:H2'	68:S2:121:OMU:H6	2.02	0.41
68:S2:462:OMC:H1'	68:S2:462:OMC:HM23	1.75	0.41
68:S2:1521:C:N4	76:SS:137:LYS:HG3	2.35	0.41
73:SM:58:GLU:HG3	73:SM:61:TYR:H	1.86	0.41
82:Sf:103:LEU:HG	82:Sf:104:LYS:H	1.85	0.41
86:CA:158:LYS:HA	86:CA:325:LEU:HD11	2.02	0.41
3:L5:2496:G:H2'	3:L5:2497:C:H6	1.85	0.41
3:L5:3922[A]:G:H4'	3:L5:3923:A:OP2	2.19	0.41
8:LC:334:THR:HG21	11:LF:51:TYR:OH	2.21	0.41
13:LH:113:GLU:OE1	13:LH:125:ARG:HG2	2.21	0.41
16:LL:105:LYS:HE2	16:LL:105:LYS:HB3	1.88	0.41
20:LP:85:LYS:HB2	20:LP:85:LYS:HE3	1.86	0.41
22:LR:177:LEU:HD23	22:LR:177:LEU:HA	1.84	0.41
27:LW:104:GLN:O	27:LW:107:GLN:HG3	2.20	0.41
41:Lk:12:LEU:HD23	41:Lk:12:LEU:HA	1.89	0.41
54:SG:50:VAL:HG12	54:SG:113:ILE:HA	2.02	0.41
55:SH:33:ASN:ND2	55:SH:37:LYS:HE3	2.35	0.41
56:SI:8:TRP:CZ3	56:SI:20:PRO:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SY:33:ALA:HB2	68:S2:582:U:H1'	2.02	0.41
68:S2:534:G:H2'	68:S2:535:G:C8	2.55	0.41
68:S2:1289:U:H4'	72:SK:2:LEU:HD21	2.02	0.41
68:S2:1630:A:H5'	76:SS:37:GLY:N	2.35	0.41
71:SF:39:ILE:HG23	71:SF:68:ILE:HD13	2.02	0.41
71:SF:145:ARG:HA	71:SF:145:ARG:HD2	1.86	0.41
75:SQ:12:VAL:HG11	75:SQ:90:LYS:HB3	2.01	0.41
84:Et:45:G:H5'	84:Et:46:G:OP2	2.21	0.41
85:CB:480:VAL:HG13	85:CB:481:LYS:H	1.86	0.41
2:CI:55:LEU:HD22	25:LU:99:TRP:CD2	2.55	0.41
3:L5:1801:A:H4'	24:LT:102:ARG:HH21	1.85	0.41
3:L5:4108:G:H2'	3:L5:4109:G:C8	2.56	0.41
7:LB:117:ARG:HA	7:LB:177:LYS:HD2	2.02	0.41
15:LJ:94:LEU:HD23	15:LJ:94:LEU:HA	1.92	0.41
39:Li:16:LYS:HD3	39:Li:16:LYS:HA	1.78	0.41
41:Lk:55:LYS:HA	41:Lk:55:LYS:HD2	1.75	0.41
54:SG:192:ILE:O	54:SG:196:LYS:HG3	2.21	0.41
56:SI:83:TYR:HB3	56:SI:101:ILE:HD11	2.03	0.41
57:SJ:79:ARG:HA	57:SJ:82:VAL:HG22	2.02	0.41
64:SY:120:THR:O	64:SY:124:ASN:HB2	2.21	0.41
68:S2:649:PSU:H2'	68:S2:650:A:H8	1.86	0.41
68:S2:1320:G:H2'	68:S2:1321:G:O4'	2.20	0.41
68:S2:1409:A:H2'	68:S2:1410:C:C6	2.56	0.41
68:S2:1414:A:H2'	68:S2:1415:C:H6	1.85	0.41
68:S2:1643:U:H2'	68:S2:1644:C:H6	1.86	0.41
77:ST:39:LEU:HD21	77:ST:52:TRP:CZ3	2.56	0.41
78:SU:56:MET:HB2	78:SU:86:LYS:HB3	2.03	0.41
83:Sg:107:ASP:HB2	83:Sg:125:ARG:HD2	2.01	0.41
3:L5:140:G:H2'	3:L5:141:C:C6	2.56	0.41
3:L5:266:C:HO2'	3:L5:267:G:H8	1.67	0.41
3:L5:458:C:H2'	3:L5:459:C:H6	1.85	0.41
3:L5:659:G:H2'	3:L5:660:A:C8	2.55	0.41
3:L5:1194:G:H2'	3:L5:1195:G:H8	1.86	0.41
3:L5:1695:U:H2'	3:L5:1696:C:C6	2.55	0.41
3:L5:1700:G:H5'	3:L5:1702:C:OP2	2.21	0.41
3:L5:1773:U:H2'	3:L5:1774:C:C6	2.56	0.41
3:L5:4458:C:H2'	3:L5:4459:U:C6	2.55	0.41
88:L5:5292:SPM:H62	88:L5:5292:SPM:H91	1.73	0.41
6:LA:131:GLY:H	6:LA:169:VAL:HG13	1.86	0.41
12:LG:58:PRO:HD2	12:LG:61:ILE:HD12	2.01	0.41
12:LG:100:HIS:ND1	12:LG:103:ARG:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LL:111:GLN:HA	16:LL:114:VAL:HG22	2.03	0.41
16:LL:210:LYS:HD2	16:LL:210:LYS:HA	1.85	0.41
41:Lk:25:ILE:HD13	41:Lk:57:LYS:HD3	2.03	0.41
45:Lo:22:LYS:HG2	45:Lo:73:VAL:HG12	2.03	0.41
51:SB:27:LYS:HE2	51:SB:27:LYS:HB3	1.72	0.41
58:SL:132:ARG:HD3	68:S2:114:G:H5'	2.02	0.41
59:SN:38:TYR:CZ	59:SN:78:LYS:HD2	2.55	0.41
60:SO:71:PRO:HB3	60:SO:114:SER:OG	2.20	0.41
68:S2:1330:G:H4'	68:S2:1331:C:H3'	2.02	0.41
68:S2:1365:G:H2'	68:S2:1366:G:C8	2.55	0.41
68:S2:1395:C:H1'	68:S2:1474:A:C5	2.56	0.41
68:S2:1417:C:O2	68:S2:1422:G:C6	2.73	0.41
70:SD:73:VAL:HG21	70:SD:86:LEU:HD11	2.03	0.41
70:SD:119:CYS:O	70:SD:123:LEU:HD23	2.20	0.41
86:CA:27:ILE:HA	86:CA:30:ARG:HG2	2.03	0.41
86:CA:202:ILE:HG12	86:CA:205:PRO:HG3	2.01	0.41
3:L5:347:A:H2'	3:L5:348:G:C8	2.55	0.41
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.56	0.41
3:L5:1979:A:C6	3:L5:1980:U:H5	2.39	0.41
3:L5:4088:C:H2'	3:L5:4089:G:H8	1.86	0.41
3:L5:4684:A:H2'	3:L5:4685:U:O4'	2.20	0.41
7:LB:291:TYR:CD2	7:LB:327:THR:HG23	2.55	0.41
8:LC:137:VAL:HG21	8:LC:150:LEU:HD21	2.02	0.41
8:LC:207:PRO:HB3	8:LC:249:PHE:CD2	2.56	0.41
11:LF:200:ARG:HD3	11:LF:200:ARG:HA	1.80	0.41
12:LG:151:LYS:HB3	12:LG:151:LYS:HE3	1.88	0.41
16:LL:47:ALA:HB3	16:LL:48:PRO:HD3	2.03	0.41
36:Lf:47:CYS:HA	36:Lf:102:ARG:O	2.21	0.41
53:SE:136:ILE:HD12	53:SE:149:TYR:CE1	2.55	0.41
64:SY:47:MET:HE3	64:SY:47:MET:HB2	1.93	0.41
68:S2:468:A2M:HM'3	68:S2:468:A2M:H1'	1.57	0.41
68:S2:1399:C:H2'	68:S2:1400:U:H6	1.85	0.41
71:SF:47:LYS:HE3	71:SF:49:LEU:O	2.21	0.41
83:Sg:264:LYS:HE2	83:Sg:264:LYS:HB2	1.89	0.41
85:CB:221:TRP:CG	85:CB:340:MET:HB3	2.56	0.41
85:CB:287:ARG:HG3	85:CB:290:CYS:H	1.86	0.41
3:L5:138:G:H2'	3:L5:139:G:H8	1.86	0.41
3:L5:2045:G:O2'	3:L5:2046:G:H5''	2.21	0.41
3:L5:4896:G:H2'	3:L5:4897:G:H8	1.86	0.41
3:L5:4981:G:H3'	3:L5:4982:A:H8	1.86	0.41
3:L5:5006:U:H4'	3:L5:5007:A:H5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LA:60:LYS:HE2	6:LA:60:LYS:HB2	1.90	0.41
7:LB:196:TRP:O	7:LB:199:GLU:HG2	2.21	0.41
7:LB:279:GLU:HB3	7:LB:282:LYS:HZ3	1.86	0.41
7:LB:302:ASN:HD22	7:LB:313:SER:HB2	1.86	0.41
7:LB:348:ARG:HG2	7:LB:349:LYS:O	2.20	0.41
8:LC:279:LEU:HD23	8:LC:279:LEU:HA	1.87	0.41
13:LH:4:ILE:HG12	13:LH:61:TRP:CH2	2.55	0.41
13:LH:24:THR:HA	13:LH:37:ASP:HA	2.03	0.41
14:LI:169:LYS:HD2	14:LI:169:LYS:HA	1.78	0.41
15:LJ:90:ARG:HE	15:LJ:109:ILE:HG22	1.86	0.41
23:LS:157:ARG:HA	23:LS:157:ARG:HD2	1.82	0.41
27:LW:80:ARG:HH22	54:SG:131:ARG:HB3	1.86	0.41
45:Lo:4:VAL:HG23	45:Lo:93:LEU:HD12	2.03	0.41
56:SI:26:LYS:HE3	68:S2:444:G:O6	2.20	0.41
58:SL:109:MET:HE3	58:SL:109:MET:HB2	1.80	0.41
58:SL:136:LYS:HB2	68:S2:385:G:H3'	2.03	0.41
59:SN:88:LEU:O	59:SN:92:ILE:HD12	2.21	0.41
60:SO:62:VAL:HG22	60:SO:64:ALA:H	1.86	0.41
63:SX:140:ARG:HA	63:SX:141:PRO:HD3	1.95	0.41
64:SY:57:VAL:HB	64:SY:60:PHE:CE2	2.55	0.41
68:S2:382:C:H2'	68:S2:383:G:C8	2.56	0.41
68:S2:441:C:H2'	68:S2:442:C:C6	2.56	0.41
68:S2:600:G:H2'	68:S2:601:OMG:H8	1.86	0.41
68:S2:881:G:N2	68:S2:906:U:H1'	2.36	0.41
68:S2:1279:C:H2'	68:S2:1280:G:C8	2.56	0.41
68:S2:1317:C:H2'	68:S2:1318:G:H8	1.85	0.41
68:S2:1448:A:H2'	68:S2:1449:G:O4'	2.20	0.41
68:S2:1500:G:H2'	68:S2:1501:C:C6	2.56	0.41
68:S2:1622:U:C2	76:SS:120:HIS:HE1	2.39	0.41
68:S2:1711:U:H2'	68:S2:1712:A:H8	1.86	0.41
69:SR:10:LYS:O	69:SR:14:ARG:HD3	2.21	0.41
70:SD:46:THR:O	70:SD:84:VAL:HA	2.21	0.41
71:SF:97:PHE:HZ	71:SF:112:LEU:HD22	1.86	0.41
73:SM:26:LEU:HA	73:SM:31:LEU:HD23	2.03	0.41
77:ST:104:LEU:HD23	77:ST:104:LEU:HA	1.91	0.41
78:SU:90:ASP:HB3	78:SU:92:HIS:CE1	2.56	0.41
82:Sf:114:ILE:HD12	82:Sf:114:ILE:HA	1.91	0.41
85:CB:83:GLU:HG2	85:CB:84:ASN:N	2.35	0.41
85:CB:505:VAL:HG21	85:CB:550:GLY:HA2	2.03	0.41
85:CB:692:LEU:HD22	85:CB:848:ILE:HD13	2.03	0.41
3:L5:31:U:H2'	3:L5:32:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:457:G:H2'	3:L5:458:C:H6	1.86	0.41
3:L5:485:C:O2	3:L5:485:C:H2'	2.21	0.41
3:L5:644:G:H2'	3:L5:645:G:O4'	2.21	0.41
3:L5:1270:A:N7	3:L5:2107:C:H1'	2.36	0.41
3:L5:1994:C:H2'	3:L5:1995:G:H8	1.85	0.41
3:L5:2405:G:H5'	40:Lj:12:ARG:O	2.20	0.41
3:L5:2696:A:H62	41:Lk:35:LYS:HZ2	1.69	0.41
3:L5:4543:G:H2'	3:L5:4544:A:C8	2.56	0.41
7:LB:258:HIS:HA	7:LB:260:ALA:H	1.85	0.41
17:LM:135:LEU:HD12	17:LM:135:LEU:HA	1.82	0.41
30:LZ:46:ILE:HD13	30:LZ:46:ILE:HG21	1.88	0.41
35:Le:78:LEU:HD12	35:Le:98:GLU:HG3	2.03	0.41
57:SJ:86:VAL:HG11	57:SJ:105:PHE:HD1	1.85	0.41
62:SW:115:GLU:O	62:SW:119:LYS:HG2	2.21	0.41
68:S2:587:A:H1'	68:S2:590:A:H1'	2.03	0.41
68:S2:1703:OMC:H2'	68:S2:1704:C:O4'	2.21	0.41
69:SR:72:LYS:HE3	69:SR:72:LYS:HB3	1.93	0.41
76:SS:119:ALA:O	76:SS:123:LEU:HG	2.21	0.41
77:ST:39:LEU:HD23	77:ST:39:LEU:HA	1.74	0.41
86:CA:291:MET:O	86:CA:294:VAL:HG22	2.20	0.41
1:CD:195:ARG:HA	1:CD:204:LEU:HD21	2.03	0.40
3:L5:409:G:C4	20:LP:3:ARG:HD2	2.56	0.40
3:L5:462:G:H2'	3:L5:463:A:C8	2.56	0.40
3:L5:1076:C:H2'	3:L5:1077:C:C6	2.56	0.40
3:L5:2891:U:H2'	3:L5:2892:C:O4'	2.21	0.40
3:L5:4426:C:C2'	3:L5:4427:G:H5'	2.50	0.40
3:L5:4520:G:H2'	3:L5:4521:PSU:O4'	2.20	0.40
4:L7:16:A:H2'	4:L7:17:C:C6	2.56	0.40
27:LW:80:ARG:NH2	54:SG:131:ARG:HB3	2.35	0.40
35:Le:81:ASN:OD1	35:Le:84:GLU:HG3	2.22	0.40
56:SI:83:TYR:HD1	56:SI:205:ARG:HH11	1.68	0.40
56:SI:141:ARG:CZ	68:S2:191:A:H5''	2.51	0.40
68:S2:79:A:H2'	68:S2:80:G:O4'	2.22	0.40
68:S2:325:C:H3'	68:S2:326:C:H4'	2.03	0.40
68:S2:876:C:H2'	68:S2:877:C:C6	2.56	0.40
68:S2:1545:A:H2'	68:S2:1546:G:C8	2.56	0.40
68:S2:1733:U:H2'	68:S2:1734:G:O4'	2.21	0.40
70:SD:68:GLU:OE2	72:SK:20:VAL:HG12	2.20	0.40
71:SF:144:LEU:HD12	71:SF:144:LEU:HA	1.88	0.40
85:CB:266:PHE:CD2	85:CB:291:GLN:HG2	2.55	0.40
3:L5:424:U:H2'	3:L5:425:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:660:A:H2'	3:L5:661:C:H6	1.86	0.40
3:L5:964:A:H2'	3:L5:965:G:H4'	2.03	0.40
3:L5:1633:G:H5'	3:L5:1634:A:OP1	2.22	0.40
3:L5:1647:U:H5''	89:L5:5291:SPD:H71	2.02	0.40
3:L5:2497:C:H2'	3:L5:2498:C:H6	1.86	0.40
3:L5:2861:OMC:HM23	3:L5:2861:OMC:H1'	1.76	0.40
3:L5:3848:U:H2'	3:L5:3849:A:C8	2.56	0.40
3:L5:4895:C:O2'	17:LM:132:LYS:HE3	2.21	0.40
3:L5:4921:C:O2'	3:L5:4922:C:H5'	2.21	0.40
9:LD:211:LEU:HB3	9:LD:219:TYR:HB2	2.04	0.40
15:LJ:51:SER:HB2	15:LJ:69:ALA:HB3	2.02	0.40
15:LJ:104:ASN:HB2	15:LJ:133:VAL:HA	2.03	0.40
18:LN:200:LEU:HD13	18:LN:204:ARG:HH12	1.86	0.40
31:La:75:LEU:HD23	31:La:75:LEU:HA	1.92	0.40
56:SI:121:LEU:HD21	56:SI:166:PHE:CG	2.56	0.40
63:SX:17:ARG:HH22	68:S2:659:G:N2	2.16	0.40
65:Sa:36:ILE:HD11	65:Sa:75:VAL:HG12	2.03	0.40
68:S2:946:U:H2'	68:S2:947:G:H8	1.87	0.40
73:SM:116:LYS:HD3	73:SM:116:LYS:HA	1.89	0.40
79:SZ:102:LYS:HA	79:SZ:102:LYS:HD3	1.83	0.40
83:Sg:49:GLU:HG2	83:Sg:50:THR:N	2.36	0.40
85:CB:30:HIS:ND1	85:CB:130:ASP:HB2	2.36	0.40
3:L5:123:C:H2'	3:L5:124:C:H6	1.87	0.40
3:L5:965:G:N2	3:L5:2092:G:H1'	2.36	0.40
3:L5:1397:A:H8	31:La:114:LYS:HG3	1.86	0.40
3:L5:1824:G:H2'	3:L5:1825:A:C8	2.57	0.40
3:L5:2566:G:H2'	3:L5:2567:G:H8	1.86	0.40
3:L5:3610:A:H2'	3:L5:3611:A:C8	2.57	0.40
3:L5:3870:C:H2'	3:L5:3871:A:H8	1.87	0.40
3:L5:4965:U:H4'	3:L5:4966:A:H5'	2.03	0.40
10:LE:285:LYS:HE3	10:LE:285:LYS:HB3	1.84	0.40
12:LG:51:LEU:O	12:LG:55:VAL:HG23	2.22	0.40
12:LG:261:LEU:HD23	12:LG:261:LEU:HA	1.83	0.40
22:LR:46:LYS:HE3	22:LR:46:LYS:HB2	1.85	0.40
47:Lr:16:PHE:HB3	47:Lr:27:THR:H	1.86	0.40
50:SA:55:TRP:HZ3	50:SA:177:MET:HE2	1.85	0.40
51:SB:39:PHE:CD2	51:SB:74:LEU:HD22	2.56	0.40
54:SG:147:LEU:HG	54:SG:153:VAL:HG22	2.03	0.40
55:SH:33:ASN:ND2	55:SH:36:LEU:HB2	2.36	0.40
56:SI:151:GLU:HA	56:SI:154:LYS:NZ	2.36	0.40
58:SL:23:VAL:HG23	58:SL:25:LEU:HG	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SL:152:LYS:C	58:SL:153:LYS:HE2	2.46	0.40
68:S2:13:C:H4'	68:S2:1355:C:H5	1.87	0.40
68:S2:528:A:H2'	68:S2:529:A:C8	2.57	0.40
68:S2:893:U:C2	68:S2:894:G:C8	3.08	0.40
71:SF:48:TYR:CZ	75:SQ:56:LEU:HD13	2.55	0.40
76:SS:130:ARG:HD2	76:SS:134:GLN:HE21	1.86	0.40
83:Sg:88:ARG:HD3	83:Sg:90:TRP:CZ2	2.56	0.40
83:Sg:172:LYS:HG2	83:Sg:193:GLY:C	2.46	0.40
85:CB:839:ARG:HH21	85:CB:844:LEU:HD13	1.86	0.40
86:CA:273:PHE:CG	86:CA:278:PHE:HB3	2.56	0.40
1:CD:224:GLU:HB2	70:SD:116:ARG:HD3	2.04	0.40
3:L5:2459:G:H2'	3:L5:2461:G:OP2	2.22	0.40
3:L5:3934:G:H2'	3:L5:3935:C:C6	2.56	0.40
3:L5:4460:U:H2'	3:L5:4461:C:H6	1.87	0.40
39:Li:3:LEU:HD23	39:Li:3:LEU:HA	1.93	0.40
41:Lk:61:PRO:HA	41:Lk:62:PRO:HD3	1.90	0.40
48:Ls:98:ILE:HD13	48:Ls:98:ILE:HA	1.88	0.40
54:SG:35:GLU:HG2	54:SG:114:VAL:HG21	2.04	0.40
58:SL:16:ILE:HD13	58:SL:16:ILE:HA	1.92	0.40
68:S2:696:G:H4'	68:S2:735:C:C2	2.56	0.40
68:S2:991:G:N1	68:S2:1134:G:H4'	2.37	0.40
68:S2:1618:C:H2'	68:S2:1619:A:C8	2.56	0.40
68:S2:1687:C:H2'	68:S2:1688:C:H6	1.86	0.40
71:SF:76:MET:HB3	71:SF:89:THR:CG2	2.52	0.40
83:Sg:291:TRP:CE2	83:Sg:298:LEU:HD13	2.56	0.40
84:Et:2:C:H2'	84:Et:3:C:C6	2.56	0.40
85:CB:351:LEU:HA	85:CB:354:ILE:HG12	2.03	0.40
86:CA:101:LYS:HE2	86:CA:101:LYS:HB2	1.97	0.40
3:L5:279:A:C4	18:LN:12:ARG:HG2	2.57	0.40
3:L5:742:G:H2'	3:L5:743:G:H8	1.86	0.40
3:L5:1538:U:H2'	3:L5:1539:G:H8	1.87	0.40
3:L5:1558:A:H2'	3:L5:1559:G:H8	1.87	0.40
3:L5:1625:OMG:HM23	18:LN:81:TYR:HE2	1.86	0.40
3:L5:2060:G:N2	23:LS:115:ALA:HB2	2.37	0.40
3:L5:4088:C:H2'	3:L5:4089:G:C8	2.57	0.40
5:L8:40:A:H2'	5:L8:41:A:C8	2.56	0.40
6:LA:54:ARG:HG2	6:LA:56:ALA:H	1.87	0.40
7:LB:103:LYS:HE2	7:LB:149:ASP:CG	2.46	0.40
18:LN:75:VAL:HG21	18:LN:80:THR:HG23	2.04	0.40
30:LZ:28:ASN:HB2	30:LZ:77:TYR:OH	2.22	0.40
50:SA:38:ILE:HD13	50:SA:38:ILE:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SC:130:ILE:HG23	52:SC:162:ILE:HD11	2.03	0.40
68:S2:66:G:H2'	68:S2:67:C:H4'	2.02	0.40
68:S2:453:C:H2'	68:S2:454:U:H6	1.86	0.40
68:S2:497:C:H2'	68:S2:498:C:H6	1.86	0.40
72:SK:41:PRO:HG2	72:SK:44:HIS:CG	2.56	0.40
80:Sc:16:LYS:HE2	80:Sc:16:LYS:HB3	1.78	0.40
83:Sg:11:LEU:HB2	83:Sg:307:VAL:HG12	2.03	0.40
85:CB:659:PRO:HG2	85:CB:698:ARG:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CD	51/408 (12%)	49 (96%)	2 (4%)	0	100	100
2	CI	29/206 (14%)	29 (100%)	0	0	100	100
6	LA	246/248 (99%)	232 (94%)	14 (6%)	0	100	100
7	LB	400/402 (100%)	381 (95%)	19 (5%)	0	100	100
8	LC	366/368 (100%)	349 (95%)	17 (5%)	0	100	100
9	LD	291/293 (99%)	277 (95%)	14 (5%)	0	100	100
10	LE	236/250 (94%)	217 (92%)	19 (8%)	0	100	100
11	LF	223/225 (99%)	218 (98%)	5 (2%)	0	100	100
12	LG	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
13	LH	188/190 (99%)	181 (96%)	7 (4%)	0	100	100
14	LI	200/213 (94%)	198 (99%)	2 (1%)	0	100	100
15	LJ	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
16	LL	208/210 (99%)	201 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	LM	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
18	LN	201/203 (99%)	196 (98%)	5 (2%)	0	100	100
19	LO	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
20	LP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
21	LQ	185/187 (99%)	182 (98%)	3 (2%)	0	100	100
22	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
23	LS	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
24	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
25	LU	99/101 (98%)	94 (95%)	5 (5%)	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
29	LY	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
30	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
31	La	145/147 (99%)	141 (97%)	4 (3%)	0	100	100
32	Lb	105/121 (87%)	101 (96%)	4 (4%)	0	100	100
33	Lc	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
34	Ld	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
35	Le	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
36	Lf	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
37	Lg	112/114 (98%)	112 (100%)	0	0	100	100
38	Lh	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
39	Li	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
40	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
41	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
42	Ll	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
43	Lm	50/52 (96%)	50 (100%)	0	0	100	100
44	Ln	22/24 (92%)	22 (100%)	0	0	100	100
45	Lo	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
46	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
47	Lr	123/125 (98%)	117 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	Ls	194/196 (99%)	178 (92%)	16 (8%)	0	100	100
49	Lt	128/157 (82%)	100 (78%)	28 (22%)	0	100	100
50	SA	219/221 (99%)	205 (94%)	14 (6%)	0	100	100
51	SB	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
52	SC	218/222 (98%)	206 (94%)	12 (6%)	0	100	100
53	SE	260/262 (99%)	252 (97%)	8 (3%)	0	100	100
54	SG	235/237 (99%)	227 (97%)	8 (3%)	0	100	100
55	SH	182/189 (96%)	166 (91%)	16 (9%)	0	100	100
56	SI	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
57	SJ	183/185 (99%)	173 (94%)	10 (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
60	SO	135/140 (96%)	127 (94%)	8 (6%)	0	100	100
61	SV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
62	SW	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
63	SX	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
64	SY	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
65	Sa	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
66	Sb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
67	Se	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
69	SR	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
70	SD	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
71	SF	187/189 (99%)	174 (93%)	13 (7%)	0	100	100
72	SK	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
73	SM	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
74	SP	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
75	SQ	142/144 (99%)	133 (94%)	9 (6%)	0	100	100
76	SS	143/145 (99%)	132 (92%)	11 (8%)	0	100	100
77	ST	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
78	SU	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
79	SZ	73/75 (97%)	69 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
81	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
82	Sf	65/67 (97%)	59 (91%)	6 (9%)	0	100	100
83	Sg	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
85	CB	842/856 (98%)	806 (96%)	36 (4%)	0	100	100
86	CA	350/356 (98%)	334 (95%)	16 (5%)	0	100	100
All	All	12904/13702 (94%)	12329 (96%)	575 (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	25/165 (15%)	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	174/180 (97%)	174 (100%)	0	100	100
15	LJ	143/148 (97%)	143 (100%)	0	100	100
16	LL	176/176 (100%)	175 (99%)	1 (1%)	78	91
17	LM	118/118 (100%)	118 (100%)	0	100	100
18	LN	171/171 (100%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	LO	173/173 (100%)	173 (100%)	0	100	100
20	LP	134/134 (100%)	133 (99%)	1 (1%)	76	89
21	LQ	164/164 (100%)	163 (99%)	1 (1%)	78	91
22	LR	166/166 (100%)	166 (100%)	0	100	100
23	LS	156/156 (100%)	156 (100%)	0	100	100
24	LT	139/139 (100%)	139 (100%)	0	100	100
25	LU	91/91 (100%)	91 (100%)	0	100	100
26	LV	101/101 (100%)	101 (100%)	0	100	100
27	LW	95/103 (92%)	95 (100%)	0	100	100
28	LX	108/108 (100%)	108 (100%)	0	100	100
29	LY	124/124 (100%)	124 (100%)	0	100	100
30	LZ	117/117 (100%)	117 (100%)	0	100	100
31	La	120/120 (100%)	120 (100%)	0	100	100
32	Lb	88/101 (87%)	88 (100%)	0	100	100
33	Lc	83/83 (100%)	83 (100%)	0	100	100
34	Ld	98/98 (100%)	98 (100%)	0	100	100
35	Le	114/114 (100%)	114 (100%)	0	100	100
36	Lf	88/88 (100%)	88 (100%)	0	100	100
37	Lg	98/98 (100%)	98 (100%)	0	100	100
38	Lh	109/109 (100%)	109 (100%)	0	100	100
39	Li	86/86 (100%)	86 (100%)	0	100	100
40	Lj	73/73 (100%)	73 (100%)	0	100	100
41	Lk	64/64 (100%)	64 (100%)	0	100	100
42	Ll	47/47 (100%)	47 (100%)	0	100	100
43	Lm	48/48 (100%)	48 (100%)	0	100	100
44	Ln	23/23 (100%)	23 (100%)	0	100	100
45	Lo	93/93 (100%)	93 (100%)	0	100	100
46	Lp	74/74 (100%)	74 (100%)	0	100	100
47	Lr	109/109 (100%)	109 (100%)	0	100	100
48	Ls	162/164 (99%)	162 (100%)	0	100	100
49	Lt	107/130 (82%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	SA	183/183 (100%)	182 (100%)	1 (0%)	81	92
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%)	206 (100%)	1 (0%)	81	92
55	SH	166/169 (98%)	166 (100%)	0	100	100
56	SI	178/178 (100%)	178 (100%)	0	100	100
57	SJ	161/161 (100%)	161 (100%)	0	100	100
58	SL	137/137 (100%)	137 (100%)	0	100	100
59	SN	130/130 (100%)	130 (100%)	0	100	100
60	SO	107/110 (97%)	107 (100%)	0	100	100
61	SV	67/67 (100%)	67 (100%)	0	100	100
62	SW	112/112 (100%)	112 (100%)	0	100	100
63	SX	113/113 (100%)	113 (100%)	0	100	100
64	SY	113/113 (100%)	113 (100%)	0	100	100
65	Sa	89/89 (100%)	89 (100%)	0	100	100
66	Sb	75/75 (100%)	74 (99%)	1 (1%)	61	82
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%)	101 (99%)	1 (1%)	68	86
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	11212/11722 (96%)	11205 (100%)	7 (0%)	87	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	LL	59	VAL
20	LP	58	VAL
21	LQ	100	VAL
50	SA	210	ILE
54	SG	197	GLN
66	Sb	56	CYS
73	SM	31	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
6	LA	215	ASN
7	LB	68	ASN
7	LB	145	GLN
8	LC	38	ASN
8	LC	329	ASN
9	LD	122	GLN
9	LD	131	ASN
9	LD	195	HIS
9	LD	229	ASN
10	LE	182	ASN
10	LE	266	GLN
12	LG	208	ASN
13	LH	78	GLN
13	LH	188	GLN
14	LI	59	GLN
14	LI	73	ASN
16	LL	111	GLN
17	LM	34	ASN
19	LO	199	HIS
20	LP	10	ASN

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Mol	Chain	Res	Type
20	LP	34	GLN
21	LQ	162	HIS
24	LT	131	GLN
24	LT	144	ASN
26	LV	135	ASN
28	LX	111	GLN
29	LY	14	ASN
29	LY	18	HIS
29	LY	56	GLN
29	LY	61	HIS
31	La	34	ASN
31	La	62	HIS
32	Lb	11	ASN
32	Lb	60	ASN
33	Lc	72	HIS
35	Le	52	GLN
36	Lf	20	ASN
39	Li	15	HIS
43	Lm	87	GLN
48	Ls	68	HIS
48	Ls	127	ASN
48	Ls	190	GLN
48	Ls	195	ASN
49	Lt	66	ASN
49	Lt	115	GLN
51	SB	43	ASN
51	SB	202	GLN
54	SG	187	HIS
55	SH	25	GLN
55	SH	33	ASN
55	SH	126	HIS
56	SI	52	ASN
62	SW	90	GLN
63	SX	31	HIS
63	SX	61	GLN
63	SX	97	ASN
64	SY	22	GLN
66	Sb	9	HIS
69	SR	31	ASN
69	SR	74	GLN
69	SR	116	ASN
70	SD	4	GLN

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Mol	Chain	Res	Type
70	SD	179	GLN
70	SD	226	GLN
71	SF	65	GLN
71	SF	79	HIS
72	SK	61	GLN
72	SK	84	HIS
73	SM	19	GLN
73	SM	119	GLN
74	SP	53	GLN
75	SQ	86	GLN
76	SS	135	HIS
79	SZ	112	ASN
82	Sf	139	HIS
83	Sg	4	GLN
83	Sg	64	HIS
83	Sg	244	ASN
83	Sg	296	GLN
85	CB	8	GLN
85	CB	87	ASN
85	CB	101	ASN
85	CB	138	GLN
85	CB	179	GLN
85	CB	365	GLN
85	CB	468	ASN
85	CB	670	GLN
85	CB	715	HIS
85	CB	769	HIS
85	CB	803	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3643/5070 (71%)	748 (20%)	16 (0%)
4	L7	119/120 (99%)	11 (9%)	0
5	L8	155/156 (99%)	28 (18%)	0
68	S2	1715/1740 (98%)	372 (21%)	4 (0%)
84	Et	73/75 (97%)	24 (32%)	0
All	All	5705/7161 (79%)	1183 (20%)	20 (0%)

All (1183) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L5	2	G
3	L5	25	A
3	L5	30	C
3	L5	39	A
3	L5	42	A
3	L5	48	G
3	L5	56	A
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	66	A
3	L5	70	A
3	L5	73	A
3	L5	91	G
3	L5	98	A
3	L5	104	G
3	L5	108	A
3	L5	109	G
3	L5	110	C
3	L5	119	G
3	L5	120	A
3	L5	132	G
3	L5	133	C
3	L5	134	G
3	L5	135	G
3	L5	139	G
3	L5	144	G
3	L5	159	C
3	L5	165	A
3	L5	172	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	220	C

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Mol	Chain	Res	Type
3	L5	233	U
3	L5	234	G
3	L5	237	G
3	L5	255	C
3	L5	256	G
3	L5	261	G
3	L5	263	G
3	L5	264	C
3	L5	265	C
3	L5	266	C
3	L5	267	G
3	L5	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
3	L5	431	G
3	L5	432	U
3	L5	449	C
3	L5	452	A
3	L5	453	G
3	L5	454	U
3	L5	456	C
3	L5	457	G
3	L5	467	U
3	L5	485	C
3	L5	486	C
3	L5	489	C
3	L5	494	U
3	L5	497	G

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Mol	Chain	Res	Type
3	L5	498	C
3	L5	499	G
3	L5	500	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	517	C
3	L5	518	G
3	L5	643	C
3	L5	644	G
3	L5	646	G
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
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	759	G
3	L5	904	C
3	L5	905	C
3	L5	913	U
3	L5	914	U
3	L5	915	A
3	L5	916	C

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Mol	Chain	Res	Type
3	L5	917	A
3	L5	923	C
3	L5	924	C
3	L5	926	G
3	L5	932	A
3	L5	933	G
3	L5	935	A
3	L5	936	C
3	L5	942	G
3	L5	944	A
3	L5	945	U
3	L5	946	C
3	L5	958	G
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	965	G
3	L5	966	A
3	L5	967	C
3	L5	969	C
3	L5	970	G
3	L5	977	C
3	L5	982	U
3	L5	985	C
3	L5	989	U
3	L5	1070	G
3	L5	1072	C
3	L5	1075	G
3	L5	1076	C
3	L5	1082	C
3	L5	1083	U
3	L5	1095	A
3	L5	1168	G
3	L5	1171	G
3	L5	1172	C
3	L5	1173	G
3	L5	1179	U
3	L5	1180	C
3	L5	1181	C
3	L5	1182	C
3	L5	1183	C

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Mol	Chain	Res	Type
3	L5	1184	A
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	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
3	L5	1272	C
3	L5	1273	G
3	L5	1275	G
3	L5	1279	A
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	1302	U
3	L5	1326	A2M
3	L5	1337	A
3	L5	1354	A
3	L5	1359	G
3	L5	1365	C
3	L5	1366	G
3	L5	1367	C

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Mol	Chain	Res	Type
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	1411	C
3	L5	1415	G
3	L5	1417	C
3	L5	1420	A
3	L5	1437	C
3	L5	1439	C
3	L5	1443	A
3	L5	1444	G
3	L5	1446	C
3	L5	1447	C
3	L5	1481	C
3	L5	1482	G
3	L5	1483	C
3	L5	1497	A
3	L5	1498	G
3	L5	1502	G
3	L5	1517	G
3	L5	1524	A2M
3	L5	1534	A2M
3	L5	1537	A
3	L5	1547	A
3	L5	1563	A
3	L5	1566	C
3	L5	1574	G
3	L5	1578	U
3	L5	1591	U
3	L5	1596	U
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

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Mol	Chain	Res	Type
3	L5	1638	A
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	1702	C
3	L5	1704	C
3	L5	1705	G
3	L5	1717	C
3	L5	1718	C
3	L5	1719	A
3	L5	1721	G
3	L5	1731	C
3	L5	1734	G
3	L5	1740	C
3	L5	1741	G
3	L5	1742	A
3	L5	1750	G
3	L5	1757	U
3	L5	1758	G
3	L5	1760	G
3	L5	1761	G
3	L5	1762	C
3	L5	1763	C
3	L5	1764	G
3	L5	1765	A
3	L5	1766	A
3	L5	1767	A
3	L5	1768	C
3	L5	1770	A
3	L5	1787	A
3	L5	1797	G
3	L5	1803	G
3	L5	1804	A
3	L5	1806	G

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Mol	Chain	Res	Type
3	L5	1810	G
3	L5	1820	C
3	L5	1821	G
3	L5	1822	U
3	L5	1834	U
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1855	G
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
3	L5	1919	G
3	L5	1920	C
3	L5	1921	C
3	L5	1922	G
3	L5	1925	G
3	L5	1931	C
3	L5	1932	A
3	L5	1936	C
3	L5	1948	G
3	L5	1951	G
3	L5	1960	A
3	L5	1962	A
3	L5	1974	U
3	L5	1975	G
3	L5	1978	C
3	L5	1980	U
3	L5	1981	G
3	L5	1982	G
3	L5	1984	A
3	L5	1985	G
3	L5	1986	U
3	L5	1989	G
3	L5	1991	A
3	L5	1992	U
3	L5	1993	C

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Mol	Chain	Res	Type
3	L5	1997	U
3	L5	2001	G
3	L5	2002	A
3	L5	2003	G
3	L5	2004	U
3	L5	2005	G
3	L5	2016	C
3	L5	2017	A
3	L5	2018	C
3	L5	2024	G
3	L5	2025	A
3	L5	2026	A
3	L5	2046	G
3	L5	2048	U
3	L5	2055	G
3	L5	2056	G
3	L5	2069	A
3	L5	2084	C
3	L5	2092	G
3	L5	2093	A
3	L5	2095	A
3	L5	2097	U
3	L5	2098	G
3	L5	2100	A
3	L5	2101	C
3	L5	2102	G
3	L5	2107	C
3	L5	2110	C
3	L5	2112	G
3	L5	2250	C
3	L5	2252	G
3	L5	2253	A
3	L5	2256	C
3	L5	2258	C
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	2333	G
3	L5	2345	G

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Mol	Chain	Res	Type
3	L5	2348	G
3	L5	2351	OMC
3	L5	2360	A
3	L5	2364	OMG
3	L5	2383	C
3	L5	2395	A
3	L5	2397	G
3	L5	2417	A
3	L5	2425	U
3	L5	2450	G
3	L5	2453	A
3	L5	2464	C
3	L5	2465	C
3	L5	2469	C
3	L5	2471	G
3	L5	2474	G
3	L5	2475	G
3	L5	2478	C
3	L5	2479	G
3	L5	2483	G
3	L5	2484	A
3	L5	2485	U
3	L5	2487	G
3	L5	2488	C
3	L5	2489	C
3	L5	2490	U
3	L5	2491	C
3	L5	2494	U
3	L5	2504	C
3	L5	2505	C
3	L5	2506	G
3	L5	2513	A
3	L5	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	2559	G
3	L5	2560	C
3	L5	2565	A

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Mol	Chain	Res	Type
3	L5	2570	U
3	L5	2571	C
3	L5	2573	A
3	L5	2583	C
3	L5	2586	G
3	L5	2587	A
3	L5	2589	C
3	L5	2601	A
3	L5	2618	G
3	L5	2627	C
3	L5	2638	G
3	L5	2653	C
3	L5	2662	G
3	L5	2669	C
3	L5	2675	G
3	L5	2676	A
3	L5	2687	U
3	L5	2694	G
3	L5	2695	A
3	L5	2696	A
3	L5	2702	C
3	L5	2706	G
3	L5	2707	U
3	L5	2708	U
3	L5	2709	C
3	L5	2710	C
3	L5	2711	G
3	L5	2721	G
3	L5	2724	G
3	L5	2726	G
3	L5	2738	C
3	L5	2739	C
3	L5	2742	G
3	L5	2743	A
3	L5	2746	A
3	L5	2754	G
3	L5	2761	U
3	L5	2763	U
3	L5	2769	U
3	L5	2770	C
3	L5	2788	U
3	L5	2790	U

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Mol	Chain	Res	Type
3	L5	2806	A
3	L5	2812	A
3	L5	2814	C
3	L5	2815	A2M
3	L5	2826	U
3	L5	2827	G
3	L5	2835	A
3	L5	2838	G
3	L5	2842	G
3	L5	2855	G
3	L5	2867	C
3	L5	2877	G
3	L5	2892	C
3	L5	2894	A
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
3	L5	2908	U
3	L5	3585	G
3	L5	3591	C
3	L5	3592	G
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	3617	G
3	L5	3619	G
3	L5	3626	G
3	L5	3630	A
3	L5	3635	A
3	L5	3644	U
3	L5	3646	A
3	L5	3648	A
3	L5	3662	A

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Mol	Chain	Res	Type
3	L5	3670	C
3	L5	3673	C
3	L5	3674	G
3	L5	3683	C
3	L5	3685	C
3	L5	3701	OMC
3	L5	3710	G
3	L5	3711	A
3	L5	3713	U
3	L5	3726	A
3	L5	3727	A
3	L5	3748	A
3	L5	3754	G
3	L5	3756	A
3	L5	3762	U
3	L5	3764	U
3	L5	3770	U
3	L5	3772	U
3	L5	3775	A
3	L5	3776	G
3	L5	3777	G
3	L5	3785	A2M
3	L5	3786	U
3	L5	3792	OMG
3	L5	3811	G
3	L5	3814	U
3	L5	3817	A
3	L5	3819	G
3	L5	3824	A
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3867	A2M
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3880	G
3	L5	3885	G
3	L5	3897	G
3	L5	3901	A
3	L5	3906	A
3	L5	3907	G

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Mol	Chain	Res	Type
3	L5	3908	A
3	L5	3915	U
3	L5	3916	G
3	L5	3923	A
3	L5	3930	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	3953	G
3	L5	4057	C
3	L5	4058	U
3	L5	4059	C
3	L5	4060	U
3	L5	4061	G
3	L5	4062	A
3	L5	4064	C
3	L5	4068	U
3	L5	4069	U
3	L5	4076	G
3	L5	4095	G
3	L5	4097	G
3	L5	4099	G
3	L5	4101	C
3	L5	4104	G
3	L5	4106	G
3	L5	4107	G
3	L5	4108	G
3	L5	4111	U
3	L5	4112	C
3	L5	4114	C
3	L5	4115	G
3	L5	4116	C
3	L5	4117	U
3	L5	4121	G
3	L5	4122	G
3	L5	4127	A

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Mol	Chain	Res	Type
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	4149	C
3	L5	4150	G
3	L5	4162	C
3	L5	4163	U
3	L5	4168	G
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	4251	A
3	L5	4254	G
3	L5	4258	C
3	L5	4259	C
3	L5	4265	U
3	L5	4268	A
3	L5	4273	A
3	L5	4280	A
3	L5	4281	A
3	L5	4291	G
3	L5	4295	U
3	L5	4305	G
3	L5	4306	OMU
3	L5	4314	C
3	L5	4319	C
3	L5	4329	G
3	L5	4330	G
3	L5	4332	C
3	L5	4338	G
3	L5	4349	C

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Mol	Chain	Res	Type
3	L5	4350	C
3	L5	4364	G
3	L5	4373	G
3	L5	4376	A
3	L5	4377	G
3	L5	4378	A
3	L5	4379	A
3	L5	4387	C
3	L5	4391	G
3	L5	4394	A
3	L5	4405	G
3	L5	4422	A
3	L5	4427	G
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	4560	C
3	L5	4567	G
3	L5	4575	G
3	L5	4589	A
3	L5	4590	A2M
3	L5	4600	G
3	L5	4601	U
3	L5	4623	OMG
3	L5	4633	G
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4652	G
3	L5	4656	A
3	L5	4657	U

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Mol	Chain	Res	Type
3	L5	4670	C
3	L5	4672	A
3	L5	4679	G
3	L5	4687	A
3	L5	4695	C
3	L5	4700	A
3	L5	4708	A
3	L5	4709	U
3	L5	4719	G
3	L5	4734	A
3	L5	4740	G
3	L5	4741	C
3	L5	4742	G
3	L5	4745	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4765	G
3	L5	4771	C
3	L5	4772	C
3	L5	4775	C
3	L5	4859	C
3	L5	4863	G
3	L5	4864	U
3	L5	4870	G
3	L5	4871	C
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	4897	G
3	L5	4898	G
3	L5	4899	G
3	L5	4900	C
3	L5	4901	G
3	L5	4910	G
3	L5	4912	G

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Mol	Chain	Res	Type
3	L5	4914	C
3	L5	4922	C
3	L5	4925	U
3	L5	4926	C
3	L5	4927	G
3	L5	4928	C
3	L5	4934	A
3	L5	4937	C
3	L5	4940	C
3	L5	4941	G
3	L5	4943	A
3	L5	4947	U
3	L5	4951	G
3	L5	4955	A
3	L5	4960	G
3	L5	4963	G
3	L5	4976	U
3	L5	4979	A
3	L5	4988	U
3	L5	4989	U
3	L5	4991	U
3	L5	5013	C
3	L5	5017	G
3	L5	5023	C
3	L5	5024	C
3	L5	5028	G
3	L5	5030	U
3	L5	5034	A
3	L5	5041	G
3	L5	5050	C
3	L5	5054	C
3	L5	5061	A
3	L5	5069	U
4	L7	33	U
4	L7	38	U
4	L7	49	A
4	L7	53	U
4	L7	54	A
4	L7	64	G
4	L7	97	G
4	L7	100	A
4	L7	102	U

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Mol	Chain	Res	Type
4	L7	110	G
4	L7	111	C
5	L8	16	G
5	L8	23	C
5	L8	25	G
5	L8	34	U
5	L8	35	C
5	L8	38	U
5	L8	59	A
5	L8	60	G
5	L8	62	A
5	L8	63	U
5	L8	80	A
5	L8	82	A
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	104	A
5	L8	105	C
5	L8	111	U
5	L8	114	G
5	L8	123	U
5	L8	124	U
5	L8	125	C
5	L8	126	C
5	L8	127	U
5	L8	147	G
68	S2	4	C
68	S2	13	C
68	S2	14	C
68	S2	17	C
68	S2	24	C
68	S2	25	A
68	S2	33	G
68	S2	44	U
68	S2	45	A
68	S2	46	A
68	S2	56	G
68	S2	58	C

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Mol	Chain	Res	Type
68	S2	59	U
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	99	A2M
68	S2	103	A
68	S2	113	G
68	S2	114	G
68	S2	115	U
68	S2	126	G
68	S2	130	G
68	S2	143	U
68	S2	149	A
68	S2	158	A
68	S2	160	U
68	S2	162	C
68	S2	170	A
68	S2	175	A
68	S2	190	G
68	S2	196	C
68	S2	197	U
68	S2	198	U
68	S2	200	G
68	S2	203	G
68	S2	204	G
68	S2	207	G
68	S2	208	G
68	S2	214	U
68	S2	291	G
68	S2	292	A
68	S2	295	C
68	S2	302	A
68	S2	303	C
68	S2	306	C
68	S2	307	G
68	S2	308	G
68	S2	309	G

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Mol	Chain	Res	Type
68	S2	311	C
68	S2	312	G
68	S2	316	G
68	S2	318	A
68	S2	319	C
68	S2	323	C
68	S2	324	C
68	S2	325	C
68	S2	326	C
68	S2	327	G
68	S2	328	U
68	S2	329	G
68	S2	332	G
68	S2	335	G
68	S2	347	G
68	S2	360	A
68	S2	362	C
68	S2	363	A
68	S2	364	A
68	S2	368	U
68	S2	370	G
68	S2	383	G
68	S2	385	G
68	S2	386	C
68	S2	398	A
68	S2	407	G
68	S2	408	A
68	S2	409	C
68	S2	448	A
68	S2	449	A
68	S2	450	C
68	S2	452	G
68	S2	464	A
68	S2	465	A
68	S2	471	G
68	S2	472	C
68	S2	473	A
68	S2	474	G
68	S2	482	G
68	S2	487	U
68	S2	488	U
68	S2	492	C

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Mol	Chain	Res	Type
68	S2	493	A
68	S2	501	C
68	S2	502	C
68	S2	516	A
68	S2	525	A
68	S2	531	A
68	S2	532	C
68	S2	536	A
68	S2	537	C
68	S2	540	U
68	S2	542	U
68	S2	544	G
68	S2	546	G
68	S2	547	G
68	S2	557	U
68	S2	558	G
68	S2	559	G
68	S2	560	A
68	S2	563	G
68	S2	564	A
68	S2	576	A2M
68	S2	583	A
68	S2	587	A
68	S2	589	G
68	S2	590	A
68	S2	591	U
68	S2	592	C
68	S2	593	C
68	S2	604	A
68	S2	611	G
68	S2	617	G
68	S2	623	G
68	S2	627	OMU
68	S2	628	A
68	S2	631	U
68	S2	643	A
68	S2	644	OMG
68	S2	655	A
68	S2	660	C
68	S2	664	A
68	S2	668	A2M
68	S2	669	A

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Mol	Chain	Res	Type
68	S2	670	A
68	S2	671	A
68	S2	672	A
68	S2	673	G
68	S2	684	G
68	S2	688	U
68	S2	689	U
68	S2	690	G
68	S2	692	G
68	S2	693	A
68	S2	694	G
68	S2	695	C
68	S2	696	G
68	S2	697	G
68	S2	698	G
68	S2	732	U
68	S2	733	C
68	S2	736	C
68	S2	737	G
68	S2	738	C
68	S2	749	U
68	S2	751	G
68	S2	752	G
68	S2	753	C
68	S2	788	G
68	S2	789	G
68	S2	791	C
68	S2	792	C
68	S2	798	G
68	S2	799	OMU
68	S2	801	PSU
68	S2	821	G
68	S2	822	U
68	S2	823	U
68	S2	824	C
68	S2	827	A
68	S2	830	A
68	S2	834	C
68	S2	835	C
68	S2	836	G
68	S2	837	A
68	S2	838	G

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Mol	Chain	Res	Type
68	S2	839	C
68	S2	844	U
68	S2	847	A
68	S2	863	PSU
68	S2	867	OMG
68	S2	870	A
68	S2	874	G
68	S2	877	C
68	S2	878	G
68	S2	880	G
68	S2	888	U
68	S2	889	U
68	S2	891	G
68	S2	896	U
68	S2	897	U
68	S2	898	U
68	S2	899	U
68	S2	900	C
68	S2	901	G
68	S2	903	A
68	S2	913	A
68	S2	920	A
68	S2	922	A
68	S2	930	C
68	S2	933	G
68	S2	934	G
68	S2	963	A
68	S2	971	G
68	S2	972	A
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	1033	G
68	S2	1056	PSU
68	S2	1060	A
68	S2	1061	U

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Mol	Chain	Res	Type
68	S2	1062	A
68	S2	1067	C
68	S2	1080	A
68	S2	1083	A
68	S2	1085	C
68	S2	1107	G
68	S2	1109	C
68	S2	1113	A
68	S2	1116	C
68	S2	1119	A
68	S2	1133	A
68	S2	1138	C
68	S2	1139	C
68	S2	1148	A
68	S2	1153	C
68	S2	1154	U
68	S2	1195	A
68	S2	1203	G
68	S2	1207	G
68	S2	1208	A
68	S2	1215	C
68	S2	1217	A
68	S2	1220	A
68	S2	1224	G
68	S2	1227	G
68	S2	1242	U
68	S2	1243	U
68	S2	1251	A
68	S2	1253	A
68	S2	1256	G
68	S2	1257	G
68	S2	1259	A
68	S2	1274	G
68	S2	1275	G
68	S2	1284	A
68	S2	1286	G
68	S2	1294	G
68	S2	1295	A
68	S2	1301	A
68	S2	1302	G
68	S2	1303	C
68	S2	1304	U

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Mol	Chain	Res	Type
68	S2	1308	U
68	S2	1342	U
68	S2	1354	G
68	S2	1356	G
68	S2	1357	A
68	S2	1358	U
68	S2	1371	U
68	S2	1378	A
68	S2	1382	A
68	S2	1401	A
68	S2	1402	A
68	S2	1408	U
68	S2	1412	C
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	1422	G
68	S2	1423	C
68	S2	1433	C
68	S2	1434	C
68	S2	1435	C
68	S2	1438	A
68	S2	1442	OMU
68	S2	1454	A
68	S2	1462	U
68	S2	1463	U
68	S2	1466	G
68	S2	1480	A
68	S2	1486	A
68	S2	1488	C
68	S2	1489	A
68	S2	1490	OMG
68	S2	1492	U
68	S2	1494	U
68	S2	1495	G
68	S2	1497	G
68	S2	1498	A
68	S2	1507	G
68	S2	1521	C

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Mol	Chain	Res	Type
68	S2	1522	A
68	S2	1533	A
68	S2	1536	G
68	S2	1544	C
68	S2	1546	G
68	S2	1552	G
68	S2	1574	C
68	S2	1578	U
68	S2	1579	A
68	S2	1580	A
68	S2	1581	C
68	S2	1585	U
68	S2	1587	G
68	S2	1588	A
68	S2	1601	A
68	S2	1604	G
68	S2	1606	G
68	S2	1621	U
68	S2	1623	A
68	S2	1633	A
68	S2	1637	A
68	S2	1646	C
68	S2	1648	G
68	S2	1654	G
68	S2	1663	A
68	S2	1664	A
68	S2	1665	G
68	S2	1683	C
68	S2	1699	A
68	S2	1712	A
68	S2	1715	A
68	S2	1721	U
68	S2	1722	G
68	S2	1729	U
68	S2	1744	G
68	S2	1745	A
68	S2	1752	C
68	S2	1753	C
68	S2	1756	C
68	S2	1757	G
68	S2	1758	G
68	S2	1760	G

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Mol	Chain	Res	Type
68	S2	1761	U
68	S2	1772	C
68	S2	1773	C
68	S2	1774	C
68	S2	1782	G
68	S2	1783	C
68	S2	1784	G
68	S2	1786	U
68	S2	1798	C
68	S2	1810	U
68	S2	1820	G
68	S2	1824	A
68	S2	1826	G
68	S2	1829	G
68	S2	1831	A
68	S2	1835	A
68	S2	1838	U
68	S2	1849	G
68	S2	1851	MA6
68	S2	1861	G
68	S2	1862	G
68	S2	1863	A
68	S2	1864	U
68	S2	1865	C
84	Et	4	C
84	Et	6	G
84	Et	9	A
84	Et	11	C
84	Et	19	G
84	Et	20	U
84	Et	21	A
84	Et	22	G
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	45	G
84	Et	46	G
84	Et	50	A
84	Et	55	U

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Mol	Chain	Res	Type
84	Et	58	A
84	Et	66	U
84	Et	70	G
84	Et	71	G
84	Et	73	G
84	Et	76	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	406	C
3	L5	914	U
3	L5	1082	C
3	L5	1366	G
3	L5	1590	C
3	L5	1633	G
3	L5	1703	C
3	L5	1977	C
3	L5	2416	G
3	L5	2675	G
3	L5	2709	C
3	L5	2760	G
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

178 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	3825	3	22,25,26	1.26	2 (9%)	30,36,39	1.57	7 (23%)
3	PSU	L5	1792	3	18,21,22	1.02	1 (5%)	21,30,33	1.91	4 (19%)
3	OMG	L5	3792	3	23,26,27	0.63	0	32,38,41	0.54	0
3	OMC	L5	3841	3	19,22,23	0.77	1 (5%)	25,31,34	0.57	0
68	OMU	S2	1288	68	19,22,23	3.37	7 (36%)	25,31,34	1.69	4 (16%)
3	PSU	L5	1781	3	18,21,22	1.04	1 (5%)	21,30,33	1.94	4 (19%)
68	A2M	S2	668	87,68	22,25,26	1.40	2 (9%)	30,36,39	1.62	9 (30%)
3	A2M	L5	400	3	22,25,26	1.29	3 (13%)	30,36,39	1.57	10 (33%)
3	PSU	L5	4457	3	18,21,22	1.08	2 (11%)	21,30,33	2.07	5 (23%)
3	OMC	L5	2351	3	19,22,23	0.79	1 (5%)	25,31,34	0.91	1 (4%)
68	PSU	S2	109	68	18,21,22	1.12	2 (11%)	21,30,33	1.93	4 (19%)
3	PSU	L5	4500	3	18,21,22	1.13	3 (16%)	21,30,33	2.13	5 (23%)
68	PSU	S2	1177	68	18,21,22	1.07	2 (11%)	21,30,33	2.01	4 (19%)
3	OMG	L5	3744	3	23,26,27	0.61	0	32,38,41	0.49	0
3	PSU	L5	3695	3	18,21,22	1.05	2 (11%)	21,30,33	1.98	5 (23%)
68	OMU	S2	1326	68	19,22,23	3.25	7 (36%)	25,31,34	1.81	5 (20%)
3	UR3	L5	4530	3	19,22,23	2.58	6 (31%)	26,32,35	1.54	3 (11%)
3	A2M	L5	3785	87,3	22,25,26	1.18	1 (4%)	30,36,39	1.54	9 (30%)
3	OMG	L5	4392	3	23,26,27	0.69	0	32,38,41	0.49	0
3	PSU	L5	4636	3	18,21,22	1.12	3 (16%)	21,30,33	2.21	7 (33%)
3	OMC	L5	3808	3	19,22,23	0.78	1 (5%)	25,31,34	0.76	1 (4%)
68	PSU	S2	686	68	18,21,22	1.06	1 (5%)	21,30,33	1.95	5 (23%)
3	PSU	L5	3637	3	18,21,22	1.08	2 (11%)	21,30,33	2.08	5 (23%)
68	OMU	S2	428	68	19,22,23	3.30	7 (36%)	25,31,34	1.85	5 (20%)
3	A2M	L5	4571	3	22,25,26	1.37	3 (13%)	30,36,39	1.55	9 (30%)
68	OMU	S2	354	68	19,22,23	3.18	7 (36%)	25,31,34	1.85	5 (20%)
3	A2M	L5	2401	3	22,25,26	1.29	2 (9%)	30,36,39	1.60	8 (26%)
3	A2M	L5	3830	3	22,25,26	1.28	3 (13%)	30,36,39	1.57	7 (23%)
3	A2M	L5	4590	3	22,25,26	1.27	2 (9%)	30,36,39	1.57	7 (23%)
3	PSU	L5	4293	3	18,21,22	1.09	2 (11%)	21,30,33	2.00	4 (19%)
68	PSU	S2	1046	68	18,21,22	1.06	3 (16%)	21,30,33	1.96	5 (23%)
68	MA6	S2	1850	68	23,26,27	1.31	3 (13%)	33,38,41	3.34	12 (36%)
68	OMC	S2	1272	68	19,22,23	0.56	0	25,31,34	0.73	1 (4%)
68	G7M	S2	1639	68,84	23,26,27	2.64	9 (39%)	34,39,42	2.61	11 (32%)
68	PSU	S2	801	68	18,21,22	1.15	1 (5%)	21,30,33	1.83	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L5	3887	3	19,22,23	0.70	0	25,31,34	0.69	0
3	OMG	L5	3899	3	23,26,27	0.73	0	32,38,41	0.55	0
3	A2M	L5	1323	3	22,25,26	1.30	3 (13%)	30,36,39	1.61	8 (26%)
3	PSU	L5	1860	3	18,21,22	1.06	2 (11%)	21,30,33	1.89	4 (19%)
68	OMU	S2	627	68	19,22,23	3.32	7 (36%)	25,31,34	1.91	5 (20%)
3	OMC	L5	2804	3	19,22,23	0.74	0	25,31,34	0.82	1 (4%)
3	PSU	L5	4493	3	18,21,22	1.06	2 (11%)	21,30,33	1.85	4 (19%)
3	OMC	L5	2365	87,3	19,22,23	0.70	0	25,31,34	0.56	0
68	PSU	S2	681	68	18,21,22	1.05	1 (5%)	21,30,33	1.83	4 (19%)
3	PSU	L5	4689	3	18,21,22	1.11	2 (11%)	21,30,33	1.87	4 (19%)
3	PSU	L5	4576	3	18,21,22	1.11	2 (11%)	21,30,33	1.95	5 (23%)
3	OMG	L5	4228	3	23,26,27	0.65	0	32,38,41	0.68	0
68	OMC	S2	1703	68	19,22,23	0.60	0	25,31,34	0.64	0
68	OMU	S2	799	68	19,22,23	3.33	7 (36%)	25,31,34	1.79	5 (20%)
5	PSU	L8	55	5	18,21,22	1.07	2 (11%)	21,30,33	1.86	4 (19%)
3	OMU	L5	3925	3	19,22,23	3.09	7 (36%)	25,31,34	1.82	5 (20%)
3	PSU	L5	1677	3	18,21,22	1.07	3 (16%)	21,30,33	2.04	5 (23%)
3	PSU	L5	4973	3	18,21,22	1.03	2 (11%)	21,30,33	1.98	5 (23%)
3	A2M	L5	1326	3	22,25,26	1.30	2 (9%)	30,36,39	1.51	9 (30%)
3	A2M	L5	1534	87,3	22,25,26	1.30	3 (13%)	30,36,39	1.52	9 (30%)
68	A2M	S2	159	68	22,25,26	1.14	1 (4%)	30,36,39	1.48	7 (23%)
3	OMG	L5	1522	3	23,26,27	0.69	0	32,38,41	0.65	1 (3%)
3	PSU	L5	3851	3	18,21,22	1.04	1 (5%)	21,30,33	1.93	5 (23%)
3	PSU	L5	4296	3	18,21,22	1.06	2 (11%)	21,30,33	2.05	5 (23%)
68	PSU	S2	105	68	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
68	PSU	S2	866	68	18,21,22	1.11	2 (11%)	21,30,33	1.95	5 (23%)
68	PSU	S2	1004	68	18,21,22	1.11	2 (11%)	21,30,33	1.83	4 (19%)
3	OMG	L5	4196	3	23,26,27	0.64	0	32,38,41	0.44	0
68	OMG	S2	1328	68	23,26,27	0.54	0	32,38,41	0.44	0
3	OMG	L5	4618	3	23,26,27	0.67	0	32,38,41	0.49	0
3	A2M	L5	2363	87,3	22,25,26	1.35	2 (9%)	30,36,39	1.60	9 (30%)
3	PSU	L5	4361	3	18,21,22	1.06	2 (11%)	21,30,33	1.88	4 (19%)
68	OMC	S2	174	68	19,22,23	0.55	0	25,31,34	0.63	0
3	OMC	L5	2422	87,3	19,22,23	0.72	0	25,31,34	0.69	0
68	OMC	S2	517	68	19,22,23	0.64	0	25,31,34	0.65	0
3	OMG	L5	4637	3	23,26,27	0.64	0	32,38,41	0.51	0
68	6MZ	S2	1832	87,68	22,25,26	3.05	5 (22%)	29,36,39	2.28	10 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	3822	3	18,21,22	1.06	2 (11%)	21,30,33	2.04	6 (28%)
3	PSU	L5	3844	3	18,21,22	1.15	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	5001	3	18,21,22	1.11	2 (11%)	21,30,33	1.99	4 (19%)
3	PSU	L5	4442	3	18,21,22	1.11	2 (11%)	21,30,33	2.10	6 (28%)
68	OMC	S2	1391	68	19,22,23	0.58	0	25,31,34	0.67	0
3	PSU	L5	4403	3	18,21,22	1.08	3 (16%)	21,30,33	2.02	6 (28%)
68	PSU	S2	863	68	18,21,22	1.06	1 (5%)	21,30,33	1.97	4 (19%)
3	5MC	L5	4447	3	19,22,23	1.04	2 (10%)	26,32,35	0.83	0
3	OMG	L5	4499	3	23,26,27	0.60	0	32,38,41	0.44	0
68	A2M	S2	166	68	22,25,26	1.24	1 (4%)	30,36,39	1.59	8 (26%)
68	A2M	S2	468	68	22,25,26	1.24	2 (9%)	30,36,39	1.59	7 (23%)
3	PSU	L5	1683	3	18,21,22	1.08	2 (11%)	21,30,33	1.98	4 (19%)
3	OMC	L5	4536	3	19,22,23	0.73	0	25,31,34	0.70	0
68	OMU	S2	116	68	19,22,23	3.22	7 (36%)	25,31,34	1.68	5 (20%)
3	PSU	L5	4628	3	18,21,22	1.02	3 (16%)	21,30,33	1.91	4 (19%)
68	OMU	S2	172	68	19,22,23	3.27	7 (36%)	25,31,34	1.85	5 (20%)
68	OMC	S2	462	68	19,22,23	0.59	0	25,31,34	0.73	0
3	OMG	L5	1625	3	23,26,27	0.65	0	32,38,41	0.52	0
68	PSU	S2	1081	68	18,21,22	1.04	1 (5%)	21,30,33	1.87	4 (19%)
3	A2M	L5	2787	3	22,25,26	1.15	2 (9%)	30,36,39	1.50	7 (23%)
3	A2M	L5	3718	3	22,25,26	1.15	1 (4%)	30,36,39	1.52	7 (23%)
68	OMG	S2	644	68	23,26,27	0.58	0	32,38,41	0.56	0
3	A2M	L5	1524	3	22,25,26	1.40	3 (13%)	30,36,39	1.52	8 (26%)
3	OMC	L5	1340	3	19,22,23	0.75	0	25,31,34	0.79	0
3	5MC	L5	3782	87,3	19,22,23	0.82	0	26,32,35	0.77	0
3	PSU	L5	4673	87,3	18,21,22	1.07	2 (11%)	21,30,33	1.95	4 (19%)
68	OMG	S2	509	68	23,26,27	0.57	0	32,38,41	0.51	0
3	PSU	L5	4579	3	18,21,22	1.09	2 (11%)	21,30,33	1.99	4 (19%)
3	PSU	L5	1862	3	18,21,22	1.02	1 (5%)	21,30,33	2.05	4 (19%)
68	PSU	S2	651	68	18,21,22	1.07	1 (5%)	21,30,33	1.99	5 (23%)
3	OMC	L5	3869	3	19,22,23	0.70	0	25,31,34	0.64	0
3	PSU	L5	3639	3	18,21,22	1.12	2 (11%)	21,30,33	1.97	4 (19%)
3	A2M	L5	3867	3	22,25,26	1.37	2 (9%)	30,36,39	1.54	9 (30%)
3	PSU	L5	3884	3	18,21,22	1.12	2 (11%)	21,30,33	1.90	4 (19%)
68	A2M	S2	484	68	22,25,26	1.17	1 (4%)	30,36,39	1.47	7 (23%)
3	OMU	L5	4498	3	19,22,23	3.13	7 (36%)	25,31,34	1.93	5 (20%)
3	PSU	L5	4532	3	18,21,22	1.07	2 (11%)	21,30,33	1.99	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4972	3	18,21,22	1.04	2 (11%)	21,30,33	1.90	4 (19%)
3	OMU	L5	2837	3	19,22,23	3.21	7 (36%)	25,31,34	1.94	5 (20%)
3	PSU	L5	1536	3	18,21,22	1.06	2 (11%)	21,30,33	1.95	4 (19%)
68	PSU	S2	1174	68	18,21,22	1.07	2 (11%)	21,30,33	1.99	4 (19%)
3	PSU	L5	5010	3	18,21,22	1.10	2 (11%)	21,30,33	1.88	4 (19%)
5	OMG	L8	75	5	23,26,27	0.62	0	32,38,41	0.50	0
68	A2M	S2	27	68	22,25,26	1.22	2 (9%)	30,36,39	1.54	8 (26%)
68	PSU	S2	93	68	18,21,22	1.07	1 (5%)	21,30,33	1.87	4 (19%)
3	OMG	L5	4370	3	23,26,27	0.64	0	32,38,41	0.50	0
68	4AC	S2	1842	68	21,24,25	0.42	0	28,34,37	0.49	0
68	PSU	S2	406	68	18,21,22	1.07	2 (11%)	21,30,33	1.93	4 (19%)
3	PSU	L5	4471	3	18,21,22	1.12	2 (11%)	21,30,33	1.88	4 (19%)
3	PSU	L5	3853	87,3	18,21,22	1.02	1 (5%)	21,30,33	1.87	4 (19%)
68	B8N	S2	1248	68	25,29,30	3.23	7 (28%)	28,42,45	2.03	6 (21%)
68	PSU	S2	1244	68	18,21,22	1.05	2 (11%)	21,30,33	1.99	4 (19%)
68	A2M	S2	1383	68	22,25,26	1.20	1 (4%)	30,36,39	1.59	6 (20%)
3	PSU	L5	1782	3	18,21,22	1.08	2 (11%)	21,30,33	1.92	4 (19%)
68	OMG	S2	1490	68	23,26,27	0.58	0	32,38,41	0.46	0
3	OMG	L5	2364	87,3	23,26,27	0.67	0	32,38,41	0.43	0
3	OMC	L5	2861	3	19,22,23	0.70	0	25,31,34	0.75	1 (4%)
3	1MA	L5	1322	87,3	21,25,26	0.71	0	30,37,40	0.77	1 (3%)
3	A2M	L5	398	3	22,25,26	1.20	2 (9%)	30,36,39	1.67	7 (23%)
3	OMC	L5	4456	3	19,22,23	0.81	1 (5%)	25,31,34	0.66	0
68	OMU	S2	121	68	19,22,23	3.22	7 (36%)	25,31,34	1.85	5 (20%)
68	4AC	S2	1337	68	21,24,25	0.40	0	28,34,37	0.56	0
3	PSU	L5	2839	3	18,21,22	1.10	2 (11%)	21,30,33	1.95	4 (19%)
68	OMG	S2	436	68	23,26,27	0.58	0	32,38,41	0.52	0
68	A2M	S2	99	87,68	22,25,26	1.23	2 (9%)	30,36,39	1.61	8 (26%)
68	MA6	S2	1851	68	23,26,27	1.31	3 (13%)	33,38,41	3.43	12 (36%)
68	OMG	S2	867	68	23,26,27	0.51	0	32,38,41	0.51	0
68	A2M	S2	576	68	22,25,26	1.24	1 (4%)	30,36,39	1.47	5 (16%)
5	PSU	L8	69	5	18,21,22	1.08	3 (16%)	21,30,33	2.08	6 (28%)
3	OMG	L5	1316	3	23,26,27	0.77	0	32,38,41	0.60	0
3	PSU	L5	4552	3	18,21,22	1.15	2 (11%)	21,30,33	2.00	4 (19%)
3	OMG	L5	2424	3	23,26,27	0.61	0	32,38,41	0.44	0
3	A2M	L5	2815	3	22,25,26	1.22	2 (9%)	30,36,39	1.50	9 (30%)
68	OMG	S2	601	68	23,26,27	0.60	0	32,38,41	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L5	2824	3	19,22,23	0.70	0	25,31,34	0.66	0
3	OMU	L5	4306	3	19,22,23	3.13	7 (36%)	25,31,34	1.80	5 (20%)
68	PSU	S2	966	68	18,21,22	1.03	1 (5%)	21,30,33	1.94	4 (19%)
3	A2M	L5	1871	87,3	22,25,26	1.39	3 (13%)	30,36,39	1.62	8 (26%)
3	PSU	L5	3920	87,3	18,21,22	1.10	2 (11%)	21,30,33	1.99	4 (19%)
3	PSU	L5	4353	3	18,21,22	1.08	2 (11%)	21,30,33	2.02	5 (23%)
3	PSU	L5	4312	3	18,21,22	1.10	2 (11%)	21,30,33	1.93	4 (19%)
68	A2M	S2	1031	68	22,25,26	1.15	1 (4%)	30,36,39	1.55	7 (23%)
3	PSU	L5	1582	3	18,21,22	1.10	2 (11%)	21,30,33	1.78	3 (14%)
68	PSU	S2	1232	68	18,21,22	1.10	2 (11%)	21,30,33	2.06	5 (23%)
3	OMG	L5	2876	3	23,26,27	0.64	0	32,38,41	0.53	0
3	6MZ	L5	4220	3	22,25,26	2.94	6 (27%)	29,36,39	2.42	10 (34%)
3	PSU	L5	1744	87,3	18,21,22	1.07	2 (11%)	21,30,33	2.01	5 (23%)
3	PSU	L5	2632	3	18,21,22	1.02	1 (5%)	21,30,33	1.83	4 (19%)
3	OMU	L5	4227	3	19,22,23	3.17	7 (36%)	25,31,34	1.78	4 (16%)
3	OMG	L5	4494	3	23,26,27	0.64	0	32,38,41	0.51	0
3	OMG	L5	3627	3	23,26,27	0.64	0	32,38,41	0.60	0
3	UY1	L5	3818	3	19,22,23	4.67	9 (47%)	21,31,34	1.97	5 (23%)
68	PSU	S2	814	68	18,21,22	1.00	1 (5%)	21,30,33	1.77	4 (19%)
68	PSU	S2	1367	68	18,21,22	1.08	1 (5%)	21,30,33	1.83	4 (19%)
68	OMU	S2	1442	68	19,22,23	3.33	7 (36%)	25,31,34	1.86	4 (16%)
3	PSU	L5	4521	87,3	18,21,22	1.14	3 (16%)	21,30,33	2.03	5 (23%)
3	OMU	L5	4620	3	19,22,23	3.07	7 (36%)	25,31,34	1.73	5 (20%)
68	PSU	S2	649	68	18,21,22	1.09	2 (11%)	21,30,33	1.96	4 (19%)
3	PSU	L5	4431	3	18,21,22	1.04	1 (5%)	21,30,33	1.92	4 (19%)
3	A2M	L5	4523	87,3	22,25,26	1.30	3 (13%)	30,36,39	1.55	7 (23%)
3	OMG	L5	4623	3	23,26,27	0.63	0	32,38,41	0.59	0
68	OMG	S2	683	68	23,26,27	0.56	0	32,38,41	0.50	0
68	PSU	S2	1045	68	18,21,22	1.03	1 (5%)	21,30,33	1.95	4 (19%)
3	OMC	L5	3701	3	19,22,23	0.78	1 (5%)	25,31,34	1.84	4 (16%)
68	PSU	S2	1056	68	18,21,22	1.07	1 (5%)	21,30,33	1.93	5 (23%)
3	PSU	L5	4299	3	18,21,22	1.07	2 (11%)	21,30,33	1.89	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	1/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
68	OMU	S2	1288	68	-	1/9/27/28	0/2/2/2
3	PSU	L5	1781	3	-	1/7/25/26	0/2/2/2
68	A2M	S2	668	87,68	-	5/9/27/28	0/3/3/3
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2351	3	-	2/9/27/28	0/2/2/2
68	PSU	S2	109	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
68	PSU	S2	1177	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	1326	68	-	0/9/27/28	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3785	87,3	-	4/9/27/28	0/3/3/3
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4636	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	686	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	428	68	-	5/9/27/28	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
68	OMU	S2	354	68	-	0/9/27/28	0/2/2/2
3	A2M	L5	2401	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	4590	3	-	4/9/27/28	0/3/3/3
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1046	68	-	0/7/25/26	0/2/2/2
68	MA6	S2	1850	68	-	0/11/29/30	0/3/3/3
68	OMC	S2	1272	68	-	0/9/27/28	0/2/2/2
68	G7M	S2	1639	68,84	-	0/7/25/26	0/3/3/3
68	PSU	S2	801	68	-	2/7/25/26	0/2/2/2
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	3899	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	1323	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	627	68	-	2/9/27/28	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2365	87,3	-	0/9/27/28	0/2/2/2
68	PSU	S2	681	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
68	OMC	S2	1703	68	-	1/9/27/28	0/2/2/2
68	OMU	S2	799	68	-	2/9/27/28	0/2/2/2
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1677	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	3/9/27/28	0/3/3/3
3	A2M	L5	1534	87,3	-	1/9/27/28	0/3/3/3
68	A2M	S2	159	68	-	1/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3851	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	105	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	866	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	1004	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	4196	3	-	1/9/27/28	0/3/3/3
68	OMG	S2	1328	68	-	1/9/27/28	0/3/3/3
3	OMG	L5	4618	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	2363	87,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
68	OMC	S2	174	68	-	1/9/27/28	0/2/2/2
3	OMC	L5	2422	87,3	-	1/9/27/28	0/2/2/2
68	OMC	S2	517	68	-	0/9/27/28	0/2/2/2
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
68	6MZ	S2	1832	87,68	-	2/9/27/28	0/3/3/3
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
68	OMC	S2	1391	68	-	0/9/27/28	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	863	68	-	2/7/25/26	0/2/2/2
3	5MC	L5	4447	3	-	3/7/25/26	0/2/2/2
3	OMG	L5	4499	3	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	A2M	S2	166	68	-	0/9/27/28	0/3/3/3
68	A2M	S2	468	68	-	1/9/27/28	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
68	OMU	S2	116	68	-	0/9/27/28	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	172	68	-	1/9/27/28	0/2/2/2
68	OMC	S2	462	68	-	1/9/27/28	0/2/2/2
3	OMG	L5	1625	3	-	2/9/27/28	0/3/3/3
68	PSU	S2	1081	68	-	1/7/25/26	0/2/2/2
3	A2M	L5	2787	3	-	5/9/27/28	0/3/3/3
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
68	OMG	S2	644	68	-	3/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	3/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	5MC	L5	3782	87,3	-	1/7/25/26	0/2/2/2
3	PSU	L5	4673	87,3	-	0/7/25/26	0/2/2/2
68	OMG	S2	509	68	-	0/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	651	68	-	0/7/25/26	0/2/2/2
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	484	68	-	0/9/27/28	0/3/3/3
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
68	PSU	S2	1174	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
5	OMG	L8	75	5	-	2/9/27/28	0/3/3/3
68	A2M	S2	27	68	-	1/9/27/28	0/3/3/3
68	PSU	S2	93	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	4370	3	-	1/9/27/28	0/3/3/3
68	4AC	S2	1842	68	-	0/11/29/30	0/2/2/2
68	PSU	S2	406	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3853	87,3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	B8N	S2	1248	68	-	2/16/34/35	0/2/2/2
68	PSU	S2	1244	68	-	1/7/25/26	0/2/2/2
68	A2M	S2	1383	68	-	1/9/27/28	0/3/3/3
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
68	OMG	S2	1490	68	-	1/9/27/28	0/3/3/3
3	OMG	L5	2364	87,3	-	3/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	1/9/27/28	0/2/2/2
3	1MA	L5	1322	87,3	-	2/7/25/26	0/3/3/3
3	A2M	L5	398	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
68	OMU	S2	121	68	-	0/9/27/28	0/2/2/2
68	4AC	S2	1337	68	-	0/11/29/30	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
68	OMG	S2	436	68	-	2/9/27/28	0/3/3/3
68	A2M	S2	99	87,68	-	2/9/27/28	0/3/3/3
68	MA6	S2	1851	68	-	1/11/29/30	0/3/3/3
68	OMG	S2	867	68	-	1/9/27/28	0/3/3/3
68	A2M	S2	576	68	-	3/9/27/28	0/3/3/3
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
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	-	1/9/27/28	0/3/3/3
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	966	68	-	0/7/25/26	0/2/2/2
3	A2M	L5	1871	87,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3920	87,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	1031	68	-	0/9/27/28	0/3/3/3
3	PSU	L5	1582	3	-	2/7/25/26	0/2/2/2
68	PSU	S2	1232	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	6MZ	L5	4220	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	1744	87,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	UY1	L5	3818	3	-	2/9/27/28	0/2/2/2
68	PSU	S2	814	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	1367	68	-	0/7/25/26	0/2/2/2
68	OMU	S2	1442	68	-	2/9/27/28	0/2/2/2
3	PSU	L5	4521	87,3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	649	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	87,3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4623	3	-	1/9/27/28	0/3/3/3
68	OMG	S2	683	68	-	0/9/27/28	0/3/3/3
68	PSU	S2	1045	68	-	2/7/25/26	0/2/2/2
3	OMC	L5	3701	3	-	5/9/27/28	0/2/2/2
68	PSU	S2	1056	68	-	2/7/25/26	0/2/2/2
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2

All (356) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	1832	6MZ	C6-N6	12.59	1.48	1.34
3	L5	3818	UY1	C6-C5	12.12	1.48	1.35
3	L5	4220	6MZ	C6-N6	11.64	1.47	1.34
3	L5	3818	UY1	C2-N1	11.10	1.51	1.36
68	S2	1288	OMU	C2-N1	8.35	1.51	1.38
68	S2	799	OMU	C2-N1	8.25	1.51	1.38
68	S2	1442	OMU	C2-N1	8.16	1.51	1.38
68	S2	627	OMU	C2-N1	8.03	1.51	1.38
68	S2	428	OMU	C2-N1	7.99	1.51	1.38
68	S2	1248	B8N	C4-N3	-7.97	1.26	1.40
68	S2	172	OMU	C2-N1	7.87	1.50	1.38
68	S2	1326	OMU	C2-N1	7.79	1.50	1.38
68	S2	121	OMU	C2-N1	7.77	1.50	1.38
3	L5	2837	OMU	C2-N1	7.75	1.50	1.38
68	S2	116	OMU	C2-N1	7.70	1.50	1.38
68	S2	1248	B8N	C6-N1	7.67	1.55	1.36
3	L5	4227	OMU	C2-N1	7.65	1.50	1.38
68	S2	354	OMU	C2-N1	7.53	1.50	1.38
3	L5	4306	OMU	C2-N1	7.43	1.50	1.38
3	L5	3925	OMU	C2-N1	7.43	1.50	1.38
3	L5	4498	OMU	C2-N1	7.40	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	C2-N3	7.37	1.49	1.37
3	L5	4620	OMU	C2-N1	7.17	1.49	1.38
68	S2	1248	B8N	C4-C5	6.98	1.63	1.47
68	S2	1288	OMU	C2-N3	6.82	1.49	1.38
68	S2	428	OMU	C2-N3	6.80	1.49	1.38
68	S2	172	OMU	C2-N3	6.79	1.49	1.38
68	S2	627	OMU	C2-N3	6.76	1.49	1.38
68	S2	1442	OMU	C2-N3	6.75	1.49	1.38
68	S2	799	OMU	C2-N3	6.70	1.49	1.38
68	S2	116	OMU	C2-N3	6.66	1.49	1.38
68	S2	1326	OMU	C2-N3	6.64	1.49	1.38
68	S2	1639	G7M	C4-N3	6.49	1.49	1.34
68	S2	121	OMU	C2-N3	6.46	1.49	1.38
68	S2	354	OMU	C2-N3	6.45	1.49	1.38
3	L5	2837	OMU	C2-N3	6.42	1.49	1.38
3	L5	4227	OMU	C2-N3	6.35	1.49	1.38
3	L5	4306	OMU	C2-N3	6.34	1.49	1.38
3	L5	4620	OMU	C2-N3	6.29	1.48	1.38
3	L5	4498	OMU	C2-N3	6.24	1.48	1.38
3	L5	4530	UR3	C6-C5	6.13	1.49	1.35
3	L5	3925	OMU	C2-N3	6.03	1.48	1.38
68	S2	627	OMU	C6-C5	5.90	1.48	1.35
68	S2	1248	B8N	C2-N1	5.80	1.56	1.39
3	L5	4530	UR3	C2-N1	5.79	1.46	1.38
68	S2	1288	OMU	C6-C5	5.79	1.48	1.35
3	L5	4620	OMU	O4-C4	-5.79	1.13	1.24
3	L5	3925	OMU	O4-C4	-5.78	1.13	1.24
68	S2	428	OMU	C6-C5	5.76	1.48	1.35
3	L5	4306	OMU	O4-C4	-5.75	1.13	1.24
68	S2	799	OMU	C6-C5	5.74	1.48	1.35
68	S2	1326	OMU	C6-C5	5.73	1.48	1.35
68	S2	1442	OMU	C6-C5	5.71	1.48	1.35
68	S2	121	OMU	C6-C5	5.70	1.48	1.35
68	S2	172	OMU	C6-C5	5.70	1.48	1.35
3	L5	2837	OMU	C6-C5	5.69	1.48	1.35
3	L5	4227	OMU	O4-C4	-5.68	1.13	1.24
68	S2	1442	OMU	O4-C4	-5.67	1.13	1.24
68	S2	116	OMU	C6-C5	5.67	1.48	1.35
68	S2	354	OMU	O4-C4	-5.67	1.13	1.24
3	L5	2837	OMU	O4-C4	-5.67	1.13	1.24
3	L5	4498	OMU	O4-C4	-5.66	1.13	1.24
68	S2	799	OMU	O4-C4	-5.61	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	354	OMU	C6-C5	5.60	1.48	1.35
3	L5	4227	OMU	C6-C5	5.57	1.48	1.35
68	S2	116	OMU	O4-C4	-5.56	1.13	1.24
3	L5	4498	OMU	C6-C5	5.56	1.48	1.35
68	S2	428	OMU	O4-C4	-5.52	1.13	1.24
68	S2	172	OMU	O4-C4	-5.51	1.13	1.24
68	S2	1326	OMU	O4-C4	-5.49	1.13	1.24
68	S2	121	OMU	O4-C4	-5.49	1.13	1.24
3	L5	4306	OMU	C6-C5	5.49	1.47	1.35
3	L5	4530	UR3	C2-N3	5.47	1.49	1.39
68	S2	1288	OMU	O4-C4	-5.47	1.13	1.24
3	L5	4620	OMU	C6-C5	5.47	1.47	1.35
68	S2	627	OMU	O4-C4	-5.45	1.13	1.24
3	L5	3925	OMU	C6-C5	5.42	1.47	1.35
68	S2	1639	G7M	C2-N3	5.39	1.46	1.33
68	S2	1248	B8N	C6-C5	5.13	1.42	1.35
3	L5	3818	UY1	C6-N1	5.04	1.44	1.36
68	S2	1639	G7M	C5-N7	-5.04	1.33	1.39
68	S2	1639	G7M	C2-N2	4.86	1.45	1.34
68	S2	627	OMU	C4-N3	4.35	1.46	1.38
68	S2	1288	OMU	C4-N3	4.33	1.46	1.38
68	S2	172	OMU	C4-N3	4.27	1.45	1.38
68	S2	1442	OMU	C4-N3	4.26	1.45	1.38
3	L5	3818	UY1	C4-N3	4.26	1.46	1.38
68	S2	428	OMU	C4-N3	4.23	1.45	1.38
68	S2	1326	OMU	C4-N3	4.17	1.45	1.38
68	S2	799	OMU	C4-N3	4.12	1.45	1.38
68	S2	116	OMU	C4-N3	4.07	1.45	1.38
68	S2	121	OMU	C4-N3	3.97	1.45	1.38
3	L5	4498	OMU	C4-N3	3.92	1.45	1.38
68	S2	354	OMU	C4-N3	3.90	1.45	1.38
3	L5	2837	OMU	C4-N3	3.87	1.45	1.38
3	L5	3818	UY1	O4-C4	-3.75	1.16	1.23
3	L5	4227	OMU	C4-N3	3.74	1.45	1.38
3	L5	3825	A2M	O5'-C5'	-3.74	1.33	1.44
3	L5	1871	A2M	O5'-C5'	-3.70	1.33	1.44
68	S2	1639	G7M	C5-C6	3.68	1.53	1.43
3	L5	3830	A2M	O5'-C5'	-3.68	1.33	1.44
68	S2	668	A2M	O5'-C5'	-3.65	1.33	1.44
3	L5	2401	A2M	O5'-C5'	-3.63	1.33	1.44
68	S2	801	PSU	C6-C5	3.63	1.39	1.35
3	L5	400	A2M	O5'-C5'	-3.63	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4306	OMU	C4-N3	3.61	1.44	1.38
3	L5	1524	A2M	O5'-C5'	-3.60	1.33	1.44
3	L5	2363	A2M	O5'-C5'	-3.59	1.33	1.44
68	S2	468	A2M	O5'-C5'	-3.59	1.33	1.44
3	L5	3785	A2M	O5'-C5'	-3.58	1.33	1.44
3	L5	4220	6MZ	C5-C4	-3.57	1.32	1.39
3	L5	4220	6MZ	C5-N7	-3.56	1.32	1.39
3	L5	3867	A2M	O5'-C5'	-3.56	1.33	1.44
3	L5	2815	A2M	O5'-C5'	-3.56	1.33	1.44
68	S2	99	A2M	O5'-C5'	-3.55	1.33	1.44
3	L5	1323	A2M	O5'-C5'	-3.54	1.33	1.44
68	S2	484	A2M	O5'-C5'	-3.54	1.33	1.44
68	S2	1031	A2M	O5'-C5'	-3.53	1.33	1.44
68	S2	27	A2M	O5'-C5'	-3.52	1.33	1.44
3	L5	3925	OMU	C4-N3	3.51	1.44	1.38
3	L5	4620	OMU	C4-N3	3.49	1.44	1.38
3	L5	4590	A2M	O5'-C5'	-3.47	1.34	1.44
68	S2	166	A2M	O5'-C5'	-3.47	1.34	1.44
68	S2	1248	B8N	C1'-C5	3.46	1.58	1.50
68	S2	1383	A2M	O5'-C5'	-3.46	1.34	1.44
3	L5	4571	A2M	O5'-C5'	-3.46	1.34	1.44
68	S2	1004	PSU	C6-C5	3.45	1.39	1.35
68	S2	866	PSU	C6-C5	3.45	1.39	1.35
3	L5	2787	A2M	O5'-C5'	-3.45	1.34	1.44
3	L5	398	A2M	O5'-C5'	-3.44	1.34	1.44
3	L5	3718	A2M	O5'-C5'	-3.43	1.34	1.44
68	S2	668	A2M	O4'-C4'	-3.42	1.37	1.45
3	L5	2363	A2M	O4'-C4'	-3.40	1.37	1.45
3	L5	1534	A2M	O5'-C5'	-3.38	1.34	1.44
3	L5	1326	A2M	O5'-C5'	-3.38	1.34	1.44
3	L5	4523	A2M	O5'-C5'	-3.38	1.34	1.44
68	S2	1367	PSU	C6-C5	3.37	1.39	1.35
68	S2	109	PSU	C6-C5	3.36	1.39	1.35
3	L5	3844	PSU	C6-C5	3.34	1.39	1.35
3	L5	3818	UY1	O2-C2	-3.32	1.16	1.23
3	L5	5010	PSU	C6-C5	3.31	1.39	1.35
68	S2	93	PSU	C6-C5	3.30	1.38	1.35
3	L5	4552	PSU	C6-C5	3.27	1.38	1.35
68	S2	1232	PSU	C6-C5	3.26	1.38	1.35
68	S2	1832	6MZ	C5-N7	-3.25	1.33	1.39
68	S2	576	A2M	O5'-C5'	-3.23	1.34	1.44
68	S2	105	PSU	C6-C5	3.23	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	159	A2M	O5'-C5'	-3.22	1.34	1.44
68	S2	649	PSU	C6-C5	3.21	1.38	1.35
3	L5	4220	6MZ	C8-N9	-3.20	1.32	1.37
68	S2	863	PSU	C6-C5	3.19	1.38	1.35
68	S2	686	PSU	C6-C5	3.19	1.38	1.35
68	S2	1832	6MZ	C5-C4	-3.19	1.33	1.39
3	L5	4571	A2M	O4'-C4'	-3.18	1.37	1.45
68	S2	651	PSU	C6-C5	3.17	1.38	1.35
3	L5	1524	A2M	O4'-C4'	-3.17	1.37	1.45
68	S2	1832	6MZ	C8-N9	-3.17	1.32	1.37
68	S2	1056	PSU	C6-C5	3.17	1.38	1.35
3	L5	4312	PSU	C6-C5	3.16	1.38	1.35
68	S2	966	PSU	C6-C5	3.16	1.38	1.35
68	S2	1244	PSU	C6-C5	3.16	1.38	1.35
68	S2	406	PSU	C6-C5	3.16	1.38	1.35
68	S2	814	PSU	C6-C5	3.16	1.38	1.35
68	S2	1174	PSU	C6-C5	3.15	1.38	1.35
3	L5	4576	PSU	C6-C5	3.14	1.38	1.35
3	L5	4500	PSU	C6-C5	3.14	1.38	1.35
3	L5	4442	PSU	C6-C5	3.14	1.38	1.35
5	L8	55	PSU	C6-C5	3.14	1.38	1.35
68	S2	1081	PSU	C6-C5	3.12	1.38	1.35
68	S2	1850	MA6	C6-N6	3.11	1.45	1.36
3	L5	3818	UY1	C1'-C5	3.10	1.57	1.50
3	L5	1782	PSU	C6-C5	3.09	1.38	1.35
3	L5	4471	PSU	C6-C5	3.09	1.38	1.35
68	S2	1177	PSU	C6-C5	3.08	1.38	1.35
68	S2	1045	PSU	C6-C5	3.07	1.38	1.35
3	L5	4689	PSU	C6-C5	3.06	1.38	1.35
3	L5	4521	PSU	C6-C5	3.06	1.38	1.35
3	L5	2632	PSU	C6-C5	3.05	1.38	1.35
3	L5	1860	PSU	C6-C5	3.03	1.38	1.35
3	L5	1781	PSU	C6-C5	3.02	1.38	1.35
3	L5	4579	PSU	C6-C5	3.01	1.38	1.35
68	S2	1046	PSU	C6-C5	3.01	1.38	1.35
3	L5	4293	PSU	C6-C5	2.99	1.38	1.35
3	L5	4296	PSU	C6-C5	2.99	1.38	1.35
3	L5	4532	PSU	C6-C5	2.98	1.38	1.35
68	S2	1851	MA6	C6-N6	2.98	1.45	1.36
3	L5	1534	A2M	O4'-C4'	-2.98	1.38	1.45
3	L5	4353	PSU	C6-C5	2.97	1.38	1.35
3	L5	4493	PSU	C6-C5	2.97	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1744	PSU	C6-C5	2.96	1.38	1.35
3	L5	4636	PSU	C6-C5	2.96	1.38	1.35
68	S2	681	PSU	C6-C5	2.95	1.38	1.35
3	L5	2839	PSU	C6-C5	2.95	1.38	1.35
3	L5	4299	PSU	C6-C5	2.95	1.38	1.35
3	L5	4673	PSU	C6-C5	2.94	1.38	1.35
3	L5	5001	PSU	C6-C5	2.93	1.38	1.35
3	L5	4431	PSU	C6-C5	2.92	1.38	1.35
3	L5	1792	PSU	C6-C5	2.92	1.38	1.35
3	L5	3822	PSU	C6-C5	2.92	1.38	1.35
3	L5	3884	PSU	C6-C5	2.92	1.38	1.35
3	L5	3639	PSU	C6-C5	2.89	1.38	1.35
3	L5	1326	A2M	O4'-C4'	-2.89	1.38	1.45
3	L5	4972	PSU	C6-C5	2.88	1.38	1.35
68	S2	627	OMU	C5-C4	2.88	1.50	1.43
5	L8	69	PSU	C6-C5	2.88	1.38	1.35
3	L5	1862	PSU	C6-C5	2.88	1.38	1.35
3	L5	1582	PSU	C6-C5	2.86	1.38	1.35
3	L5	1323	A2M	O4'-C4'	-2.83	1.38	1.45
3	L5	4530	UR3	O2-C2	-2.81	1.17	1.22
3	L5	1683	PSU	C6-C5	2.78	1.38	1.35
68	S2	1851	MA6	C5-C4	-2.78	1.34	1.39
3	L5	3695	PSU	C6-C5	2.77	1.38	1.35
3	L5	3851	PSU	C6-C5	2.77	1.38	1.35
68	S2	1288	OMU	C5-C4	2.77	1.49	1.43
3	L5	3920	PSU	C6-C5	2.76	1.38	1.35
3	L5	4361	PSU	C6-C5	2.76	1.38	1.35
3	L5	3853	PSU	C6-C5	2.75	1.38	1.35
68	S2	1326	OMU	C5-C4	2.74	1.49	1.43
68	S2	428	OMU	C5-C4	2.73	1.49	1.43
68	S2	1288	OMU	C6-N1	2.73	1.44	1.38
3	L5	4973	PSU	C6-C5	2.73	1.38	1.35
68	S2	1442	OMU	C5-C4	2.73	1.49	1.43
68	S2	121	OMU	C5-C4	2.72	1.49	1.43
3	L5	3867	A2M	O4'-C4'	-2.72	1.39	1.45
3	L5	3637	PSU	C6-C5	2.70	1.38	1.35
3	L5	1871	A2M	O4'-C4'	-2.70	1.39	1.45
3	L5	4457	PSU	C6-C5	2.69	1.38	1.35
68	S2	799	OMU	C5-C4	2.69	1.49	1.43
3	L5	4523	A2M	O4'-C4'	-2.68	1.39	1.45
68	S2	172	OMU	C5-C4	2.67	1.49	1.43
68	S2	799	OMU	C6-N1	2.66	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4227	OMU	C5-C4	2.65	1.49	1.43
3	L5	1536	PSU	C6-C5	2.65	1.38	1.35
3	L5	4403	PSU	C6-C5	2.64	1.38	1.35
68	S2	1850	MA6	C5-C4	-2.64	1.34	1.39
68	S2	1639	G7M	C2-N1	2.64	1.44	1.37
3	L5	4220	6MZ	C6-N1	-2.63	1.30	1.35
3	L5	4628	PSU	C6-C5	2.62	1.38	1.35
68	S2	1639	G7M	O6-C6	-2.60	1.18	1.23
3	L5	2837	OMU	C5-C4	2.57	1.49	1.43
68	S2	1442	OMU	C6-N1	2.56	1.44	1.38
3	L5	400	A2M	O4'-C4'	-2.55	1.39	1.45
68	S2	354	OMU	C5-C4	2.52	1.49	1.43
68	S2	121	OMU	C6-N1	2.51	1.44	1.38
68	S2	627	OMU	C6-N1	2.50	1.44	1.38
68	S2	428	OMU	C6-N1	2.50	1.44	1.38
3	L5	4498	OMU	C5-C4	2.50	1.49	1.43
68	S2	354	OMU	C6-N1	2.50	1.44	1.38
3	L5	1677	PSU	O4'-C1'	-2.49	1.40	1.43
68	S2	116	OMU	C5-C4	2.48	1.49	1.43
3	L5	1323	A2M	O3'-C3'	-2.48	1.36	1.43
68	S2	1326	OMU	C6-N1	2.47	1.44	1.38
68	S2	1832	6MZ	C6-N1	-2.45	1.31	1.35
3	L5	3925	OMU	C5-C4	2.45	1.49	1.43
3	L5	4590	A2M	O4'-C4'	-2.45	1.39	1.45
3	L5	2815	A2M	O4'-C4'	-2.42	1.39	1.45
3	L5	4447	5MC	C4-N3	-2.42	1.30	1.34
3	L5	4498	OMU	C6-N1	2.39	1.43	1.38
3	L5	4447	5MC	C5-C4	-2.39	1.42	1.44
3	L5	4306	OMU	C5-C4	2.38	1.48	1.43
68	S2	116	OMU	C6-N1	2.37	1.43	1.38
3	L5	2837	OMU	C6-N1	2.36	1.43	1.38
3	L5	3884	PSU	C4-C5	-2.36	1.37	1.44
3	L5	4306	OMU	C6-N1	2.35	1.43	1.38
3	L5	4523	A2M	O3'-C3'	-2.35	1.37	1.43
3	L5	4530	UR3	C6-N1	2.34	1.43	1.38
3	L5	4227	OMU	C6-N1	2.33	1.43	1.38
3	L5	2401	A2M	O4'-C4'	-2.33	1.39	1.45
3	L5	1677	PSU	C6-C5	2.32	1.37	1.35
68	S2	172	OMU	C6-N1	2.32	1.43	1.38
3	L5	4620	OMU	C5-C4	2.31	1.48	1.43
3	L5	3925	OMU	C6-N1	2.31	1.43	1.38
3	L5	2839	PSU	C4-C5	-2.29	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	1639	G7M	C6-N1	2.28	1.43	1.38
3	L5	4552	PSU	C4-C5	-2.26	1.38	1.44
3	L5	3818	UY1	O4'-C1'	-2.24	1.40	1.43
3	L5	4312	PSU	C4-C5	-2.23	1.38	1.44
3	L5	4521	PSU	C4-C5	-2.23	1.38	1.44
3	L5	4456	OMC	C4-N3	-2.22	1.30	1.34
3	L5	3701	OMC	C4-N3	-2.21	1.30	1.34
3	L5	2351	OMC	C4-N3	-2.21	1.30	1.34
3	L5	1871	A2M	O3'-C3'	-2.20	1.37	1.43
3	L5	4353	PSU	C4-C5	-2.20	1.38	1.44
68	S2	99	A2M	O4'-C4'	-2.19	1.40	1.45
3	L5	1683	PSU	C4-C5	-2.19	1.38	1.44
3	L5	5001	PSU	C4-C5	-2.19	1.38	1.44
3	L5	4403	PSU	C4-C5	-2.18	1.38	1.44
3	L5	4457	PSU	C4-C5	-2.18	1.38	1.44
3	L5	1524	A2M	O3'-C3'	-2.18	1.37	1.43
68	S2	649	PSU	C4-C5	-2.18	1.38	1.44
3	L5	3920	PSU	C4-C5	-2.17	1.38	1.44
3	L5	4293	PSU	C4-C5	-2.17	1.38	1.44
3	L5	3695	PSU	C4-C5	-2.17	1.38	1.44
3	L5	4620	OMU	C6-N1	2.17	1.43	1.38
3	L5	3639	PSU	C4-C5	-2.16	1.38	1.44
3	L5	1534	A2M	O3'-C3'	-2.15	1.37	1.43
3	L5	4500	PSU	C4-C5	-2.15	1.38	1.44
3	L5	4689	PSU	C4-C5	-2.15	1.38	1.44
3	L5	3808	OMC	C4-N3	-2.15	1.30	1.34
3	L5	4636	PSU	O4'-C1'	-2.15	1.40	1.43
3	L5	4973	PSU	C4-C5	-2.14	1.38	1.44
3	L5	4576	PSU	C4-C5	-2.14	1.38	1.44
3	L5	1782	PSU	C4-C5	-2.14	1.38	1.44
68	S2	1639	G7M	C4-N9	-2.14	1.32	1.38
3	L5	4673	PSU	C4-C5	-2.14	1.38	1.44
3	L5	4571	A2M	O3'-C3'	-2.14	1.37	1.43
3	L5	1677	PSU	C4-C5	-2.14	1.38	1.44
3	L5	4636	PSU	C4-C5	-2.14	1.38	1.44
3	L5	3825	A2M	O4'-C4'	-2.13	1.40	1.45
3	L5	400	A2M	O3'-C3'	-2.11	1.37	1.43
3	L5	398	A2M	O4'-C4'	-2.11	1.40	1.45
3	L5	4471	PSU	C4-C5	-2.11	1.38	1.44
68	S2	1177	PSU	C4-C5	-2.11	1.38	1.44
68	S2	406	PSU	C4-C5	-2.10	1.38	1.44
3	L5	1860	PSU	C4-C5	-2.09	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4579	PSU	C4-C5	-2.09	1.38	1.44
3	L5	1744	PSU	C4-C5	-2.08	1.38	1.44
68	S2	27	A2M	O4'-C4'	-2.07	1.40	1.45
3	L5	5010	PSU	C4-C5	-2.07	1.38	1.44
3	L5	4530	UR3	C5-C4	2.07	1.49	1.43
5	L8	69	PSU	C4-C5	-2.07	1.38	1.44
5	L8	55	PSU	C4-C5	-2.06	1.38	1.44
3	L5	1582	PSU	C4-C5	-2.06	1.38	1.44
68	S2	1244	PSU	C4-C5	-2.06	1.38	1.44
3	L5	4972	PSU	C4-C5	-2.06	1.38	1.44
3	L5	4521	PSU	O4'-C1'	-2.06	1.41	1.43
3	L5	4493	PSU	C4-C5	-2.06	1.38	1.44
68	S2	1232	PSU	C4-C5	-2.06	1.38	1.44
3	L5	4220	6MZ	C4-N9	-2.06	1.33	1.37
68	S2	109	PSU	C4-C5	-2.05	1.38	1.44
3	L5	4628	PSU	C4-C5	-2.05	1.38	1.44
68	S2	1248	B8N	O4'-C1'	-2.05	1.41	1.43
3	L5	3841	OMC	C4-N3	-2.05	1.30	1.34
3	L5	3637	PSU	C4-C5	-2.04	1.38	1.44
3	L5	4296	PSU	C4-C5	-2.04	1.38	1.44
3	L5	3830	A2M	O4'-C4'	-2.04	1.40	1.45
3	L5	4361	PSU	C4-C5	-2.04	1.38	1.44
3	L5	4532	PSU	C4-C5	-2.03	1.38	1.44
68	S2	1046	PSU	C4-C5	-2.03	1.38	1.44
3	L5	4299	PSU	C4-C5	-2.03	1.38	1.44
68	S2	1850	MA6	C4-N9	-2.03	1.33	1.37
68	S2	468	A2M	O4'-C4'	-2.03	1.40	1.45
3	L5	3822	PSU	C4-C5	-2.03	1.38	1.44
68	S2	1851	MA6	C4-N9	-2.02	1.33	1.37
3	L5	1536	PSU	C4-C5	-2.02	1.38	1.44
68	S2	1174	PSU	C4-C5	-2.02	1.38	1.44
3	L5	4442	PSU	O4'-C1'	-2.02	1.41	1.43
68	S2	866	PSU	C4-C5	-2.02	1.38	1.44
3	L5	4403	PSU	O4'-C1'	-2.02	1.41	1.43
3	L5	4628	PSU	O4'-C1'	-2.01	1.41	1.43
68	S2	1046	PSU	O4'-C1'	-2.01	1.41	1.43
5	L8	69	PSU	O4'-C1'	-2.01	1.41	1.43
3	L5	4500	PSU	O4'-C1'	-2.01	1.41	1.43
3	L5	3830	A2M	O3'-C3'	-2.00	1.38	1.43
68	S2	1004	PSU	C4-C5	-2.00	1.38	1.44
3	L5	2787	A2M	O3'-C3'	-2.00	1.38	1.43

All (699) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1851	MA6	N1-C6-N6	-12.24	101.94	116.86
68	S2	1850	MA6	N1-C6-N6	-11.63	102.68	116.86
68	S2	1851	MA6	C5-C6-N6	8.02	138.03	125.33
68	S2	1850	MA6	C5-C6-N6	7.88	137.80	125.33
68	S2	1639	G7M	C1'-N9-C4	7.53	148.74	126.49
68	S2	1639	G7M	C1'-N9-C8	-7.42	101.70	126.74
3	L5	4498	OMU	C4-N3-C2	-6.10	119.04	126.61
68	S2	627	OMU	C4-N3-C2	-5.96	119.21	126.61
3	L5	2837	OMU	C4-N3-C2	-5.89	119.30	126.61
68	S2	1851	MA6	N1-C2-N3	-5.88	119.68	128.58
3	L5	4220	6MZ	N1-C2-N3	-5.88	119.68	128.58
68	S2	1442	OMU	C4-N3-C2	-5.85	119.35	126.61
68	S2	428	OMU	C4-N3-C2	-5.76	119.46	126.61
68	S2	172	OMU	C4-N3-C2	-5.72	119.51	126.61
3	L5	3701	OMC	C1'-N1-C2	5.71	131.05	118.44
3	L5	3925	OMU	C4-N3-C2	-5.68	119.56	126.61
3	L5	4220	6MZ	C9-N6-C6	-5.66	117.60	122.85
68	S2	1326	OMU	C4-N3-C2	-5.66	119.58	126.61
3	L5	4227	OMU	C4-N3-C2	-5.65	119.60	126.61
68	S2	121	OMU	C4-N3-C2	-5.63	119.62	126.61
3	L5	4636	PSU	C4-N3-C2	-5.62	118.64	126.37
68	S2	1850	MA6	N1-C2-N3	-5.61	120.09	128.58
68	S2	354	OMU	C4-N3-C2	-5.60	119.66	126.61
68	S2	1832	6MZ	N1-C2-N3	-5.57	120.15	128.58
68	S2	1851	MA6	N9-C8-N7	-5.56	106.05	113.94
68	S2	1850	MA6	N9-C8-N7	-5.54	106.08	113.94
3	L5	4306	OMU	C4-N3-C2	-5.48	119.81	126.61
68	S2	799	OMU	C4-N3-C2	-5.46	119.83	126.61
3	L5	4636	PSU	N1-C2-N3	5.42	120.89	115.17
3	L5	3637	PSU	N1-C2-N3	5.38	120.84	115.17
3	L5	4500	PSU	N1-C2-N3	5.36	120.83	115.17
3	L5	3637	PSU	C4-N3-C2	-5.35	119.00	126.37
3	L5	1862	PSU	C4-N3-C2	-5.33	119.03	126.37
3	L5	4530	UR3	C4-N3-C2	-5.33	120.29	124.58
3	L5	1677	PSU	C4-N3-C2	-5.33	119.03	126.37
3	L5	4457	PSU	C4-N3-C2	-5.33	119.03	126.37
3	L5	4442	PSU	N1-C2-N3	5.31	120.77	115.17
5	L8	69	PSU	N1-C2-N3	5.30	120.76	115.17
3	L5	4293	PSU	C4-N3-C2	-5.23	119.17	126.37
3	L5	3822	PSU	N1-C2-N3	5.23	120.68	115.17
3	L5	4457	PSU	N1-C2-N3	5.21	120.67	115.17
3	L5	4353	PSU	N1-C2-N3	5.19	120.64	115.17
3	L5	4296	PSU	N1-C2-N3	5.19	120.64	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1862	PSU	N1-C2-N3	5.16	120.61	115.17
68	S2	1177	PSU	C4-N3-C2	-5.16	119.27	126.37
3	L5	4442	PSU	C4-N3-C2	-5.15	119.28	126.37
68	S2	1232	PSU	C4-N3-C2	-5.14	119.29	126.37
3	L5	4296	PSU	C4-N3-C2	-5.12	119.32	126.37
68	S2	1248	B8N	C5-C4-N3	5.11	125.44	116.15
68	S2	1045	PSU	C4-N3-C2	-5.11	119.33	126.37
3	L5	4521	PSU	N1-C2-N3	5.11	120.56	115.17
68	S2	1232	PSU	N1-C2-N3	5.11	120.56	115.17
3	L5	1683	PSU	N1-C2-N3	5.11	120.55	115.17
3	L5	3920	PSU	N1-C2-N3	5.10	120.55	115.17
3	L5	4620	OMU	C4-N3-C2	-5.10	120.28	126.61
68	S2	1288	OMU	C4-N3-C2	-5.10	120.28	126.61
3	L5	4579	PSU	N1-C2-N3	5.09	120.53	115.17
68	S2	686	PSU	C4-N3-C2	-5.08	119.38	126.37
3	L5	4973	PSU	C4-N3-C2	-5.07	119.39	126.37
3	L5	4673	PSU	N1-C2-N3	5.06	120.50	115.17
3	L5	1744	PSU	N1-C2-N3	5.05	120.50	115.17
3	L5	4521	PSU	C4-N3-C2	-5.05	119.41	126.37
3	L5	4403	PSU	N1-C2-N3	5.05	120.50	115.17
3	L5	4552	PSU	N1-C2-N3	5.05	120.49	115.17
3	L5	5001	PSU	C4-N3-C2	-5.04	119.43	126.37
68	S2	1174	PSU	C4-N3-C2	-5.04	119.43	126.37
68	S2	1174	PSU	N1-C2-N3	5.04	120.48	115.17
3	L5	5001	PSU	N1-C2-N3	5.03	120.47	115.17
3	L5	4532	PSU	N1-C2-N3	5.02	120.47	115.17
68	S2	1244	PSU	C4-N3-C2	-5.02	119.45	126.37
68	S2	651	PSU	C4-N3-C2	-5.02	119.46	126.37
3	L5	4532	PSU	C4-N3-C2	-4.99	119.50	126.37
3	L5	1536	PSU	N1-C2-N3	4.99	120.43	115.17
68	S2	1177	PSU	N1-C2-N3	4.99	120.43	115.17
3	L5	3818	UY1	C4-N3-C2	-4.98	119.51	126.37
68	S2	863	PSU	N1-C2-N3	4.98	120.42	115.17
3	L5	3639	PSU	N1-C2-N3	4.98	120.42	115.17
68	S2	651	PSU	N1-C2-N3	4.98	120.42	115.17
3	L5	1781	PSU	N1-C2-N3	4.98	120.42	115.17
3	L5	3695	PSU	N1-C2-N3	4.97	120.42	115.17
3	L5	3844	PSU	N1-C2-N3	4.97	120.41	115.17
3	L5	4403	PSU	C4-N3-C2	-4.96	119.53	126.37
3	L5	4500	PSU	C4-N3-C2	-4.96	119.54	126.37
68	S2	1832	6MZ	N9-C8-N7	-4.96	106.90	113.94
3	L5	3822	PSU	C4-N3-C2	-4.96	119.54	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	863	PSU	C4-N3-C2	-4.96	119.54	126.37
68	S2	866	PSU	C4-N3-C2	-4.96	119.54	126.37
3	L5	1792	PSU	C4-N3-C2	-4.95	119.55	126.37
5	L8	69	PSU	C4-N3-C2	-4.95	119.55	126.37
3	L5	4552	PSU	C4-N3-C2	-4.95	119.55	126.37
3	L5	1582	PSU	C4-N3-C2	-4.95	119.55	126.37
3	L5	4579	PSU	C4-N3-C2	-4.94	119.56	126.37
3	L5	4293	PSU	N1-C2-N3	4.94	120.38	115.17
68	S2	1244	PSU	N1-C2-N3	4.93	120.37	115.17
68	S2	1046	PSU	N1-C2-N3	4.93	120.37	115.17
68	S2	1046	PSU	C4-N3-C2	-4.93	119.58	126.37
68	S2	116	OMU	C4-N3-C2	-4.93	120.49	126.61
3	L5	4312	PSU	N1-C2-N3	4.93	120.37	115.17
68	S2	109	PSU	C4-N3-C2	-4.92	119.59	126.37
68	S2	1056	PSU	N1-C2-N3	4.92	120.35	115.17
3	L5	3920	PSU	C4-N3-C2	-4.92	119.60	126.37
3	L5	1683	PSU	C4-N3-C2	-4.92	119.60	126.37
3	L5	1744	PSU	C4-N3-C2	-4.90	119.62	126.37
68	S2	649	PSU	N1-C2-N3	4.90	120.34	115.17
68	S2	966	PSU	N1-C2-N3	4.90	120.33	115.17
68	S2	966	PSU	C4-N3-C2	-4.90	119.62	126.37
3	L5	3851	PSU	C4-N3-C2	-4.89	119.63	126.37
3	L5	4353	PSU	C4-N3-C2	-4.89	119.64	126.37
3	L5	3851	PSU	N1-C2-N3	4.88	120.32	115.17
3	L5	1782	PSU	N1-C2-N3	4.88	120.31	115.17
3	L5	4972	PSU	C4-N3-C2	-4.88	119.66	126.37
3	L5	3639	PSU	C4-N3-C2	-4.87	119.66	126.37
3	L5	1536	PSU	C4-N3-C2	-4.87	119.67	126.37
68	S2	93	PSU	C4-N3-C2	-4.87	119.67	126.37
3	L5	1781	PSU	C4-N3-C2	-4.86	119.67	126.37
68	S2	866	PSU	N1-C2-N3	4.86	120.29	115.17
3	L5	3695	PSU	C4-N3-C2	-4.86	119.68	126.37
3	L5	4689	PSU	N1-C2-N3	4.86	120.29	115.17
3	L5	4973	PSU	N1-C2-N3	4.86	120.29	115.17
3	L5	4576	PSU	N1-C2-N3	4.85	120.28	115.17
3	L5	1860	PSU	N1-C2-N3	4.84	120.28	115.17
3	L5	4299	PSU	N1-C2-N3	4.83	120.26	115.17
3	L5	4361	PSU	N1-C2-N3	4.83	120.26	115.17
68	S2	109	PSU	N1-C2-N3	4.82	120.25	115.17
68	S2	686	PSU	N1-C2-N3	4.82	120.25	115.17
3	L5	4493	PSU	C4-N3-C2	-4.82	119.73	126.37
3	L5	2839	PSU	N1-C2-N3	4.82	120.25	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4431	PSU	N1-C2-N3	4.82	120.25	115.17
68	S2	1081	PSU	N1-C2-N3	4.81	120.25	115.17
3	L5	4361	PSU	C4-N3-C2	-4.81	119.74	126.37
3	L5	4972	PSU	N1-C2-N3	4.81	120.24	115.17
3	L5	1677	PSU	N1-C2-N3	4.81	120.24	115.17
3	L5	4471	PSU	N1-C2-N3	4.81	120.24	115.17
68	S2	1045	PSU	N1-C2-N3	4.81	120.24	115.17
68	S2	406	PSU	C4-N3-C2	-4.81	119.75	126.37
3	L5	1792	PSU	N1-C2-N3	4.80	120.23	115.17
68	S2	649	PSU	C4-N3-C2	-4.80	119.76	126.37
68	S2	105	PSU	N1-C2-N3	4.80	120.23	115.17
3	L5	3884	PSU	N1-C2-N3	4.79	120.22	115.17
3	L5	3884	PSU	C4-N3-C2	-4.79	119.78	126.37
68	S2	406	PSU	N1-C2-N3	4.78	120.21	115.17
3	L5	5010	PSU	N1-C2-N3	4.78	120.21	115.17
5	L8	55	PSU	N1-C2-N3	4.77	120.20	115.17
3	L5	2839	PSU	C4-N3-C2	-4.77	119.80	126.37
3	L5	3853	PSU	C4-N3-C2	-4.76	119.81	126.37
3	L5	4431	PSU	C4-N3-C2	-4.76	119.81	126.37
68	S2	93	PSU	N1-C2-N3	4.75	120.18	115.17
3	L5	4628	PSU	N1-C2-N3	4.74	120.17	115.17
3	L5	1782	PSU	C4-N3-C2	-4.74	119.85	126.37
3	L5	4628	PSU	C4-N3-C2	-4.72	119.87	126.37
3	L5	3853	PSU	N1-C2-N3	4.71	120.14	115.17
3	L5	4673	PSU	C4-N3-C2	-4.70	119.90	126.37
68	S2	105	PSU	C4-N3-C2	-4.69	119.91	126.37
3	L5	4576	PSU	C4-N3-C2	-4.69	119.91	126.37
68	S2	1081	PSU	C4-N3-C2	-4.68	119.92	126.37
68	S2	1248	B8N	C4-N3-C2	-4.68	119.86	125.62
3	L5	2632	PSU	C4-N3-C2	-4.67	119.94	126.37
68	S2	681	PSU	N1-C2-N3	4.67	120.09	115.17
5	L8	55	PSU	C4-N3-C2	-4.66	119.95	126.37
3	L5	2632	PSU	N1-C2-N3	4.66	120.09	115.17
68	S2	1056	PSU	C4-N3-C2	-4.66	119.95	126.37
68	S2	1832	6MZ	C5-C4-N3	-4.66	120.30	126.72
3	L5	4299	PSU	C4-N3-C2	-4.65	119.97	126.37
3	L5	4312	PSU	C4-N3-C2	-4.64	119.97	126.37
3	L5	4220	6MZ	N9-C8-N7	-4.64	107.36	113.94
68	S2	801	PSU	N1-C2-N3	4.64	120.06	115.17
68	S2	1367	PSU	N1-C2-N3	4.62	120.05	115.17
68	S2	1850	MA6	C4-N9-C8	4.62	110.58	105.74
3	L5	4471	PSU	C4-N3-C2	-4.61	120.02	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	5010	PSU	C4-N3-C2	-4.61	120.02	126.37
3	L5	1860	PSU	C4-N3-C2	-4.57	120.07	126.37
3	L5	4493	PSU	N1-C2-N3	4.56	119.98	115.17
68	S2	1004	PSU	N1-C2-N3	4.55	119.97	115.17
68	S2	1367	PSU	C4-N3-C2	-4.55	120.10	126.37
68	S2	1639	G7M	C2-N3-C4	4.54	120.12	112.30
68	S2	814	PSU	N1-C2-N3	4.54	119.95	115.17
68	S2	1004	PSU	C4-N3-C2	-4.53	120.13	126.37
3	L5	3701	OMC	C1'-N1-C6	-4.53	111.10	120.78
68	S2	681	PSU	C4-N3-C2	-4.51	120.16	126.37
3	L5	4220	6MZ	C5-C4-N3	-4.51	120.51	126.72
3	L5	4689	PSU	C4-N3-C2	-4.49	120.19	126.37
68	S2	814	PSU	C4-N3-C2	-4.47	120.22	126.37
68	S2	1851	MA6	C5-C4-N3	-4.42	120.64	126.72
68	S2	1851	MA6	C4-N9-C8	4.40	110.36	105.74
3	L5	1582	PSU	N1-C2-N3	4.38	119.78	115.17
68	S2	801	PSU	C4-N3-C2	-4.36	120.36	126.37
3	L5	3844	PSU	C4-N3-C2	-4.35	120.38	126.37
3	L5	2837	OMU	N3-C2-N1	4.35	120.55	114.89
68	S2	1248	B8N	C1'-C5-C4	4.34	124.20	117.61
68	S2	1850	MA6	C5-C4-N3	-4.24	120.87	126.72
3	L5	3818	UY1	N1-C2-N3	4.24	119.64	115.17
68	S2	121	OMU	N3-C2-N1	4.20	120.36	114.89
68	S2	627	OMU	N3-C2-N1	4.14	120.29	114.89
68	S2	1639	G7M	C5-C6-N1	4.12	120.36	111.84
3	L5	1871	A2M	C3'-C2'-C1'	-4.11	94.93	102.81
68	S2	1639	G7M	C5-C4-N3	-4.11	120.39	128.15
3	L5	4523	A2M	C3'-C2'-C1'	-4.10	94.96	102.81
3	L5	4498	OMU	N3-C2-N1	4.10	120.23	114.89
3	L5	398	A2M	C3'-C2'-C1'	-4.10	94.96	102.81
3	L5	3830	A2M	C3'-C2'-C1'	-4.05	95.05	102.81
68	S2	1442	OMU	C5-C4-N3	4.03	120.44	114.80
3	L5	4498	OMU	C5-C4-N3	3.99	120.38	114.80
3	L5	4306	OMU	N3-C2-N1	3.94	120.02	114.89
3	L5	3925	OMU	N3-C2-N1	3.89	119.96	114.89
68	S2	428	OMU	N3-C2-N1	3.80	119.84	114.89
3	L5	3925	OMU	C5-C4-N3	3.80	120.12	114.80
3	L5	1323	A2M	C2'-C1'-N9	3.79	120.00	113.75
68	S2	99	A2M	C3'-C2'-C1'	-3.79	95.55	102.81
68	S2	354	OMU	C5-C4-N3	3.78	120.09	114.80
68	S2	354	OMU	N3-C2-N1	3.77	119.80	114.89
3	L5	4227	OMU	N3-C2-N1	3.76	119.79	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3718	A2M	C3'-C2'-C1'	-3.76	95.62	102.81
68	S2	1326	OMU	C5-C4-N3	3.75	120.06	114.80
3	L5	4620	OMU	N3-C2-N1	3.75	119.77	114.89
68	S2	799	OMU	C5-C4-N3	3.74	120.03	114.80
68	S2	799	OMU	N3-C2-N1	3.74	119.76	114.89
3	L5	4227	OMU	C5-C4-N3	3.74	120.03	114.80
3	L5	398	A2M	O3'-C3'-C2'	3.74	121.64	111.19
68	S2	172	OMU	C5-C4-N3	3.71	120.00	114.80
68	S2	428	OMU	C5-C4-N3	3.70	119.98	114.80
3	L5	4530	UR3	C5-C4-N3	3.67	119.88	115.04
68	S2	1326	OMU	N3-C2-N1	3.66	119.66	114.89
68	S2	172	OMU	N3-C2-N1	3.65	119.65	114.89
3	L5	3825	A2M	C3'-C2'-C1'	-3.64	95.84	102.81
68	S2	1442	OMU	N3-C2-N1	3.63	119.62	114.89
3	L5	2837	OMU	C5-C4-N3	3.63	119.88	114.80
68	S2	1850	MA6	C2-N1-C6	3.62	120.67	111.83
3	L5	4306	OMU	C5-C4-N3	3.61	119.86	114.80
68	S2	627	OMU	C5-C4-N3	3.60	119.84	114.80
68	S2	1850	MA6	C4-C5-C6	3.60	119.63	115.91
68	S2	121	OMU	C5-C4-N3	3.60	119.84	114.80
68	S2	1248	B8N	N3-C2-N1	3.58	121.10	116.72
68	S2	1383	A2M	C3'-C2'-C1'	-3.58	95.96	102.81
68	S2	116	OMU	N3-C2-N1	3.56	119.52	114.89
68	S2	1851	MA6	C2-N1-C6	3.55	120.50	111.83
68	S2	1288	OMU	C5-C4-N3	3.55	119.77	114.80
68	S2	1832	6MZ	C5-N7-C8	3.49	108.94	103.45
3	L5	2787	A2M	O3'-C3'-C2'	3.48	120.92	111.19
68	S2	576	A2M	O3'-C3'-C2'	3.47	120.89	111.19
68	S2	1288	OMU	N3-C2-N1	3.44	119.37	114.89
68	S2	468	A2M	C3'-C2'-C1'	-3.43	96.23	102.81
68	S2	1639	G7M	O6-C6-C5	-3.43	120.35	128.01
3	L5	4620	OMU	C5-C4-N3	3.42	119.59	114.80
3	L5	2363	A2M	C2'-C1'-N9	3.42	119.37	113.75
68	S2	1031	A2M	C3'-C2'-C1'	-3.40	96.30	102.81
68	S2	1383	A2M	O3'-C3'-C2'	3.39	120.68	111.19
3	L5	4220	6MZ	C2-N3-C4	3.39	120.11	111.83
68	S2	1832	6MZ	C2-N3-C4	3.38	120.08	111.83
68	S2	166	A2M	C3'-C2'-C1'	-3.35	96.40	102.81
68	S2	1850	MA6	N3-C4-N9	3.33	132.83	127.17
68	S2	1639	G7M	N9-C4-N3	3.33	132.61	125.95
68	S2	116	OMU	C5-C4-N3	3.32	119.45	114.80
68	S2	1851	MA6	N3-C4-N9	3.30	132.78	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	99	A2M	O3'-C3'-C2'	3.30	120.41	111.19
3	L5	4590	A2M	C3'-C2'-C1'	-3.29	96.50	102.81
3	L5	2401	A2M	O3'-C3'-C2'	3.29	120.39	111.19
68	S2	1851	MA6	C2-N3-C4	3.29	119.86	111.83
3	L5	4532	PSU	O2-C2-N1	-3.27	119.41	122.79
68	S2	1851	MA6	C4-C5-C6	3.27	119.30	115.91
68	S2	1639	G7M	CN7-N7-C5	3.26	130.87	126.80
3	L5	3867	A2M	C2'-C1'-N9	3.26	119.11	113.75
3	L5	1536	PSU	O2-C2-N1	-3.25	119.44	122.79
68	S2	166	A2M	O3'-C3'-C2'	3.25	120.28	111.19
3	L5	4628	PSU	O2-C2-N1	-3.24	119.44	122.79
3	L5	1534	A2M	C3'-C2'-C1'	-3.22	96.64	102.81
68	S2	1244	PSU	O2-C2-N1	-3.21	119.48	122.79
68	S2	1832	6MZ	C4-N9-C8	3.20	109.09	105.74
68	S2	27	A2M	C3'-C2'-C1'	-3.19	96.69	102.81
68	S2	468	A2M	O3'-C3'-C2'	3.19	120.13	111.19
3	L5	2401	A2M	C3'-C2'-C1'	-3.17	96.73	102.81
68	S2	1851	MA6	C5-N7-C8	3.17	108.43	103.45
68	S2	668	A2M	C4-N9-C1'	-3.17	119.23	126.63
68	S2	863	PSU	O2-C2-N1	-3.16	119.53	122.79
3	L5	4590	A2M	C4-N9-C1'	-3.14	119.28	126.63
68	S2	428	OMU	O4-C4-C5	-3.14	119.74	125.16
68	S2	1850	MA6	C5-N7-C8	3.14	108.39	103.45
68	S2	1031	A2M	O3'-C3'-C2'	3.14	119.97	111.19
68	S2	1442	OMU	O4-C4-C5	-3.13	119.77	125.16
68	S2	1639	G7M	C2-N1-C6	-3.13	119.44	125.11
3	L5	3701	OMC	O2-C2-N3	-3.12	117.42	122.33
3	L5	4579	PSU	O2-C2-N1	-3.10	119.59	122.79
3	L5	3718	A2M	O3'-C3'-C2'	3.10	119.86	111.19
3	L5	3844	PSU	C6-N1-C2	-3.09	119.82	122.69
3	L5	1744	PSU	O2-C2-N1	-3.09	119.60	122.79
3	L5	4220	6MZ	C4-N9-C8	3.09	108.98	105.74
3	L5	2815	A2M	C2'-C1'-N9	3.09	118.83	113.75
3	L5	4689	PSU	C6-N1-C2	-3.08	119.83	122.69
3	L5	1323	A2M	C3'-C2'-C1'	-3.08	96.90	102.81
3	L5	4500	PSU	O2-C2-N1	-3.08	119.61	122.79
3	L5	4500	PSU	C6-N1-C2	-3.08	119.83	122.69
3	L5	1781	PSU	O2-C2-N1	-3.07	119.62	122.79
3	L5	1323	A2M	O3'-C3'-C2'	3.06	119.76	111.19
3	L5	3785	A2M	O3'-C3'-C2'	3.06	119.76	111.19
3	L5	4220	6MZ	N3-C4-N9	3.06	132.37	127.17
3	L5	400	A2M	C3'-C2'-C1'	-3.05	96.96	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	172	OMU	O4-C4-C5	-3.05	119.90	125.16
3	L5	4296	PSU	O2-C2-N1	-3.05	119.64	122.79
68	S2	1174	PSU	O2-C2-N1	-3.05	119.64	122.79
68	S2	649	PSU	O2-C2-N1	-3.05	119.65	122.79
3	L5	4431	PSU	O2-C2-N1	-3.05	119.65	122.79
3	L5	4498	OMU	O4-C4-C5	-3.03	119.93	125.16
3	L5	2363	A2M	C3'-C2'-C1'	-3.03	97.01	102.81
68	S2	1850	MA6	C2-N3-C4	3.03	119.22	111.83
3	L5	4500	PSU	C6-C5-C4	3.02	120.22	118.17
3	L5	2839	PSU	O2-C2-N1	-3.01	119.69	122.79
3	L5	2401	A2M	C4-N9-C1'	-3.00	119.61	126.63
3	L5	1860	PSU	C6-N1-C2	-3.00	119.91	122.69
3	L5	1871	A2M	O3'-C3'-C2'	3.00	119.59	111.19
3	L5	3822	PSU	O2-C2-N1	-3.00	119.70	122.79
68	S2	1177	PSU	O2-C2-N1	-2.98	119.71	122.79
3	L5	4312	PSU	C6-N1-C2	-2.97	119.93	122.69
3	L5	4636	PSU	C6-C5-C4	2.97	120.18	118.17
3	L5	4442	PSU	O2-C2-N1	-2.96	119.73	122.79
68	S2	668	A2M	C1'-N9-C8	2.96	133.67	127.09
3	L5	3830	A2M	O3'-C3'-C2'	2.96	119.48	111.19
68	S2	966	PSU	O2-C2-N1	-2.96	119.73	122.79
3	L5	1871	A2M	C4-N9-C1'	-2.96	119.71	126.63
68	S2	27	A2M	C4-N9-C1'	-2.96	119.71	126.63
68	S2	354	OMU	O4-C4-C5	-2.96	120.06	125.16
68	S2	159	A2M	O3'-C3'-C2'	2.96	119.46	111.19
3	L5	4552	PSU	O2-C2-N1	-2.95	119.74	122.79
68	S2	1046	PSU	O2-C2-N1	-2.95	119.74	122.79
3	L5	3818	UY1	C6-C5-C4	2.95	120.17	118.17
68	S2	576	A2M	C3'-C2'-C1'	-2.94	97.18	102.81
3	L5	1524	A2M	O3'-C3'-C2'	2.94	119.41	111.19
68	S2	801	PSU	C6-N1-C2	-2.94	119.96	122.69
3	L5	3639	PSU	O2-C2-N1	-2.94	119.76	122.79
3	L5	1524	A2M	C4'-O4'-C1'	-2.93	102.99	109.47
68	S2	406	PSU	O2-C2-N1	-2.93	119.77	122.79
3	L5	3853	PSU	O2-C2-N1	-2.93	119.77	122.79
68	S2	166	A2M	C4-N9-C1'	-2.92	119.79	126.63
5	L8	69	PSU	O2-C2-N1	-2.92	119.77	122.79
3	L5	1862	PSU	O2-C2-N1	-2.92	119.77	122.79
68	S2	484	A2M	O3'-C3'-C2'	2.92	119.36	111.19
3	L5	4673	PSU	O2-C2-N1	-2.92	119.78	122.79
68	S2	468	A2M	C4-N9-C1'	-2.91	119.82	126.63
3	L5	400	A2M	O3'-C3'-C2'	2.91	119.34	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	651	PSU	O2-C2-N1	-2.91	119.78	122.79
68	S2	668	A2M	O3'-C3'-C2'	2.91	119.34	111.19
68	S2	1288	OMU	O4-C4-C5	-2.91	120.14	125.16
3	L5	3695	PSU	O2-C2-N1	-2.91	119.79	122.79
68	S2	1832	6MZ	N3-C4-N9	2.91	132.11	127.17
68	S2	116	OMU	O4-C4-C5	-2.90	120.16	125.16
68	S2	799	OMU	O4-C4-C5	-2.89	120.17	125.16
5	L8	69	PSU	C6-N1-C2	-2.89	120.01	122.69
3	L5	4312	PSU	O2-C2-N1	-2.88	119.81	122.79
68	S2	1832	6MZ	C4-C5-C6	2.88	119.17	116.78
68	S2	1326	OMU	O4-C4-C5	-2.87	120.21	125.16
68	S2	1383	A2M	C4-N9-C1'	-2.87	119.92	126.63
3	L5	4220	6MZ	C5-N7-C8	2.87	107.95	103.45
3	L5	4590	A2M	C1'-N9-C8	2.87	133.46	127.09
3	L5	1792	PSU	O2-C2-N1	-2.86	119.84	122.79
3	L5	4293	PSU	O2-C2-N1	-2.85	119.85	122.79
3	L5	4673	PSU	C6-N1-C2	-2.84	120.05	122.69
68	S2	99	A2M	C4-N9-C1'	-2.84	119.99	126.63
3	L5	3701	OMC	O2-C2-N1	2.83	124.45	118.90
68	S2	1248	B8N	O4-C4-N3	-2.83	115.39	119.99
3	L5	4457	PSU	O2-C2-N1	-2.83	119.87	122.79
68	S2	1056	PSU	C6-N1-C2	-2.83	120.07	122.69
3	L5	2837	OMU	O4-C4-C5	-2.83	120.29	125.16
3	L5	4353	PSU	C6-N1-C2	-2.82	120.07	122.69
3	L5	2839	PSU	C6-N1-C2	-2.81	120.09	122.69
3	L5	4353	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L5	3825	A2M	O3'-C3'-C2'	2.80	119.03	111.19
3	L5	4523	A2M	O3'-C3'-C2'	2.80	119.02	111.19
68	S2	627	OMU	O4-C4-C5	-2.80	120.34	125.16
3	L5	3851	PSU	O2-C2-N1	-2.80	119.90	122.79
68	S2	801	PSU	O2-C2-N1	-2.79	119.91	122.79
68	S2	681	PSU	C6-N1-C2	-2.79	120.10	122.69
68	S2	121	OMU	O4-C4-C5	-2.78	120.37	125.16
3	L5	4571	A2M	C4-N9-C1'	-2.78	120.13	126.63
3	L5	3825	A2M	C4-N9-C1'	-2.77	120.16	126.63
68	S2	27	A2M	O3'-C3'-C2'	2.77	118.93	111.19
3	L5	2401	A2M	C1'-N9-C8	2.76	133.23	127.09
3	L5	1860	PSU	O2-C2-N1	-2.76	119.95	122.79
3	L5	3830	A2M	C4-N9-C1'	-2.76	120.19	126.63
3	L5	1683	PSU	C6-N1-C2	-2.76	120.13	122.69
3	L5	3639	PSU	C6-N1-C2	-2.76	120.13	122.69
3	L5	4306	OMU	O4-C4-C5	-2.75	120.41	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1871	A2M	C1'-N9-C8	2.75	133.20	127.09
3	L5	5010	PSU	C6-N1-C2	-2.75	120.14	122.69
3	L5	3920	PSU	O2-C2-N1	-2.75	119.96	122.79
68	S2	27	A2M	C1'-N9-C8	2.73	133.16	127.09
3	L5	1534	A2M	C2'-C1'-N9	2.73	118.25	113.75
3	L5	4552	PSU	C6-N1-C2	-2.73	120.16	122.69
68	S2	1232	PSU	C6-C5-C4	2.73	120.01	118.17
3	L5	3925	OMU	O4-C4-C5	-2.73	120.46	125.16
3	L5	4403	PSU	O2-C2-N1	-2.72	119.98	122.79
3	L5	3867	A2M	C4-N9-C1'	-2.72	120.27	126.63
3	L5	1782	PSU	C6-N1-C2	-2.72	120.17	122.69
68	S2	1004	PSU	C6-N1-C2	-2.72	120.17	122.69
68	S2	1832	6MZ	C4-C5-N7	-2.72	107.47	110.58
3	L5	2632	PSU	O2-C2-N1	-2.71	119.99	122.79
3	L5	2351	OMC	C1'-N1-C2	2.71	124.43	118.44
3	L5	3822	PSU	C6-N1-C2	-2.71	120.18	122.69
3	L5	3884	PSU	C6-N1-C2	-2.70	120.19	122.69
3	L5	1677	PSU	O2-C2-N1	-2.70	120.01	122.79
68	S2	668	A2M	O4'-C1'-C2'	2.69	111.22	106.59
3	L5	5010	PSU	O2-C2-N1	-2.69	120.02	122.79
3	L5	4571	A2M	O3'-C3'-C2'	2.69	118.70	111.19
3	L5	3818	UY1	O2-C2-N1	-2.68	120.02	122.79
3	L5	1683	PSU	O2-C2-N1	-2.68	120.02	122.79
3	L5	4636	PSU	O2-C2-N1	-2.68	120.03	122.79
68	S2	166	A2M	C1'-N9-C8	2.68	133.03	127.09
68	S2	649	PSU	C6-N1-C2	-2.67	120.21	122.69
3	L5	3695	PSU	C6-N1-C2	-2.67	120.21	122.69
3	L5	5001	PSU	O2-C2-N1	-2.67	120.04	122.79
68	S2	1639	G7M	CN7-N7-C8	-2.66	120.76	124.79
68	S2	1046	PSU	C6-N1-C2	-2.66	120.22	122.69
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	3830	A2M	C1'-N9-C8	2.65	132.98	127.09
3	L5	4431	PSU	C6-N1-C2	-2.65	120.23	122.69
68	S2	105	PSU	O2-C2-N1	-2.65	120.06	122.79
3	L5	4576	PSU	C6-C5-C4	2.65	119.96	118.17
3	L5	3920	PSU	C6-N1-C2	-2.65	120.23	122.69
3	L5	2363	A2M	O3'-C3'-C2'	2.65	118.60	111.19
3	L5	1326	A2M	C3'-C2'-C1'	-2.64	97.75	102.81
3	L5	1536	PSU	C6-N1-C2	-2.64	120.24	122.69
68	S2	1004	PSU	O2-C2-N1	-2.64	120.07	122.79
3	L5	1326	A2M	C4-N9-C1'	-2.64	120.47	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4973	PSU	O2-C2-N1	-2.63	120.07	122.79
68	S2	1081	PSU	C6-N1-C2	-2.63	120.25	122.69
68	S2	105	PSU	C6-N1-C2	-2.63	120.25	122.69
68	S2	99	A2M	C1'-N9-C8	2.63	132.92	127.09
3	L5	4620	OMU	O4-C4-C5	-2.62	120.64	125.16
3	L5	2363	A2M	C4-N9-C1'	-2.62	120.51	126.63
3	L5	4471	PSU	C6-N1-C2	-2.62	120.26	122.69
3	L5	398	A2M	C4-N9-C1'	-2.62	120.52	126.63
3	L5	4972	PSU	C6-N1-C2	-2.62	120.26	122.69
3	L5	1326	A2M	O3'-C3'-C2'	2.62	118.51	111.19
3	L5	4579	PSU	C6-N1-C2	-2.61	120.27	122.69
3	L5	4220	6MZ	C4-C5-C6	2.61	118.95	116.78
3	L5	4299	PSU	C6-N1-C2	-2.61	120.27	122.69
3	L5	2815	A2M	O3'-C3'-C2'	2.61	118.48	111.19
68	S2	468	A2M	C1'-N9-C8	2.60	132.87	127.09
68	S2	159	A2M	C4-N9-C1'	-2.60	120.55	126.63
3	L5	3867	A2M	C1'-N9-C8	2.59	132.85	127.09
3	L5	4227	OMU	O4-C4-C5	-2.59	120.69	125.16
68	S2	1045	PSU	O2-C2-N1	-2.59	120.12	122.79
5	L8	55	PSU	C6-N1-C2	-2.59	120.29	122.69
3	L5	4628	PSU	C6-N1-C2	-2.59	120.29	122.69
3	L5	3785	A2M	C4'-O4'-C1'	-2.59	103.75	109.47
68	S2	1367	PSU	C6-N1-C2	-2.58	120.29	122.69
68	S2	484	A2M	C4-N9-C1'	-2.58	120.60	126.63
3	L5	3818	UY1	C6-N1-C2	-2.57	120.30	122.69
68	S2	1383	A2M	C1'-N9-C8	2.57	132.80	127.09
3	L5	4521	PSU	O2-C2-N1	-2.57	120.14	122.79
68	S2	1031	A2M	C4-N9-C1'	-2.57	120.62	126.63
3	L5	4571	A2M	C1'-N9-C8	2.57	132.79	127.09
68	S2	406	PSU	C6-N1-C2	-2.57	120.31	122.69
68	S2	863	PSU	C6-N1-C2	-2.56	120.31	122.69
68	S2	814	PSU	C6-N1-C2	-2.56	120.31	122.69
3	L5	1782	PSU	O2-C2-N1	-2.56	120.15	122.79
68	S2	93	PSU	O2-C2-N1	-2.56	120.15	122.79
3	L5	2787	A2M	O4'-C1'-C2'	2.56	111.00	106.59
68	S2	109	PSU	C6-N1-C2	-2.56	120.31	122.69
3	L5	4590	A2M	C6-C5-C4	-2.56	113.69	117.18
3	L5	4590	A2M	O3'-C3'-C2'	2.56	118.34	111.19
3	L5	3884	PSU	O2-C2-N1	-2.55	120.15	122.79
3	L5	4493	PSU	O2-C2-N1	-2.55	120.15	122.79
3	L5	4576	PSU	C6-N1-C2	-2.55	120.33	122.69
68	S2	866	PSU	O2-C2-N1	-2.54	120.17	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2363	A2M	C1'-N9-C8	2.54	132.74	127.09
3	L5	4471	PSU	O2-C2-N1	-2.54	120.17	122.79
3	L5	4576	PSU	O2-C2-N1	-2.54	120.17	122.79
3	L5	4361	PSU	O2-C2-N1	-2.54	120.17	122.79
68	S2	159	A2M	C1'-N9-C8	2.54	132.73	127.09
68	S2	681	PSU	O2-C2-N1	-2.53	120.17	122.79
3	L5	1524	A2M	O4'-C1'-C2'	2.53	110.95	106.59
3	L5	4523	A2M	C4-N9-C1'	-2.53	120.71	126.63
3	L5	4299	PSU	O2-C2-N1	-2.53	120.18	122.79
68	S2	1056	PSU	O2-C2-N1	-2.53	120.18	122.79
3	L5	3825	A2M	C1'-N9-C8	2.53	132.70	127.09
3	L5	1781	PSU	C6-N1-C2	-2.52	120.35	122.69
68	S2	484	A2M	C1'-N9-C8	2.52	132.69	127.09
3	L5	400	A2M	C4-N9-C1'	-2.52	120.75	126.63
3	L5	1744	PSU	C6-N1-C2	-2.51	120.36	122.69
68	S2	966	PSU	C6-N1-C2	-2.51	120.36	122.69
3	L5	4442	PSU	C6-N1-C2	-2.51	120.36	122.69
68	S2	1174	PSU	C6-N1-C2	-2.51	120.36	122.69
3	L5	400	A2M	C2'-C1'-N9	2.51	117.88	113.75
5	L8	69	PSU	C6-C5-C4	2.51	119.86	118.17
68	S2	1244	PSU	C6-N1-C2	-2.50	120.37	122.69
68	S2	1367	PSU	O2-C2-N1	-2.50	120.21	122.79
3	L5	2804	OMC	C1'-N1-C2	2.50	123.97	118.44
3	L5	4220	6MZ	C5-C6-N1	2.50	120.83	118.15
3	L5	4442	PSU	C6-C5-C4	2.50	119.86	118.17
3	L5	1326	A2M	C1'-N9-C8	2.50	132.64	127.09
3	L5	4403	PSU	C6-N1-C2	-2.49	120.38	122.69
3	L5	4571	A2M	C3'-C2'-C1'	-2.49	98.04	102.81
3	L5	2632	PSU	C6-N1-C2	-2.49	120.38	122.69
3	L5	1534	A2M	O3'-C3'-C4'	-2.48	103.96	111.08
3	L5	5001	PSU	C6-N1-C2	-2.48	120.39	122.69
3	L5	4521	PSU	C6-N1-C2	-2.47	120.39	122.69
3	L5	4571	A2M	O4'-C1'-C2'	2.46	110.83	106.59
5	L8	55	PSU	O2-C2-N1	-2.46	120.25	122.79
3	L5	398	A2M	C1'-N9-C8	2.46	132.56	127.09
68	S2	1031	A2M	C1'-N9-C8	2.46	132.55	127.09
68	S2	686	PSU	O2-C2-N1	-2.46	120.25	122.79
3	L5	2363	A2M	O4'-C1'-C2'	2.45	110.80	106.59
3	L5	4403	PSU	C6-C5-C4	2.45	119.83	118.17
3	L5	2815	A2M	C3'-C2'-C1'	-2.44	98.14	102.81
68	S2	1081	PSU	O2-C2-N1	-2.44	120.27	122.79
3	L5	1871	A2M	C6-C5-C4	-2.43	113.86	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4296	PSU	C6-N1-C2	-2.43	120.44	122.69
68	S2	651	PSU	C6-N1-C2	-2.43	120.44	122.69
68	S2	1177	PSU	C6-N1-C2	-2.42	120.45	122.69
68	S2	484	A2M	O4'-C1'-C2'	2.42	110.75	106.59
68	S2	354	OMU	O2-C2-N1	-2.41	119.66	122.80
3	L5	4523	A2M	C1'-N9-C8	2.41	132.44	127.09
68	S2	627	OMU	O2-C2-N1	-2.40	119.67	122.80
68	S2	93	PSU	C6-N1-C2	-2.39	120.47	122.69
3	L5	400	A2M	C1'-N9-C8	2.39	132.41	127.09
3	L5	4361	PSU	C6-N1-C2	-2.39	120.47	122.69
3	L5	3637	PSU	C6-C5-C4	2.39	119.79	118.17
3	L5	3718	A2M	C2'-C1'-N9	2.39	117.68	113.75
3	L5	1534	A2M	C4-N9-C1'	-2.38	121.08	126.63
3	L5	1744	PSU	C6-C5-C4	2.37	119.77	118.17
3	L5	1534	A2M	C1'-N9-C8	2.37	132.35	127.09
68	S2	668	A2M	C2'-C1'-N9	2.36	117.64	113.75
3	L5	2837	OMU	O2-C2-N1	-2.36	119.72	122.80
3	L5	3844	PSU	O2-C2-N1	-2.36	120.36	122.79
3	L5	3867	A2M	C6-C5-C4	-2.35	113.97	117.18
3	L5	1326	A2M	O4'-C1'-C2'	2.35	110.63	106.59
3	L5	3718	A2M	C1'-N9-C8	2.35	132.31	127.09
3	L5	4532	PSU	C6-N1-C2	-2.35	120.51	122.69
68	S2	814	PSU	O2-C2-N1	-2.34	120.37	122.79
3	L5	1677	PSU	C6-C5-C4	2.34	119.76	118.17
3	L5	4972	PSU	O2-C2-N1	-2.34	120.37	122.79
68	S2	866	PSU	C6-N1-C2	-2.34	120.52	122.69
68	S2	1850	MA6	C1'-N9-C8	-2.33	121.91	127.09
3	L5	1524	A2M	C4-N9-C1'	-2.33	121.17	126.63
3	L5	2861	OMC	C1'-N1-C2	2.33	123.59	118.44
68	S2	576	A2M	C4-N9-C1'	-2.33	121.18	126.63
68	S2	159	A2M	O4'-C1'-C2'	2.33	110.59	106.59
3	L5	4521	PSU	C6-C5-C4	2.32	119.74	118.17
3	L5	3808	OMC	C1'-N1-C2	2.32	123.56	118.44
68	S2	668	A2M	C6-C5-C4	-2.32	114.02	117.18
68	S2	1232	PSU	C6-N1-C2	-2.31	120.54	122.69
3	L5	4498	OMU	O2-C2-N1	-2.31	119.79	122.80
68	S2	1248	B8N	O4'-C1'-C2'	2.31	108.35	105.15
68	S2	27	A2M	C6-C5-C4	-2.30	114.03	117.18
3	L5	3785	A2M	C2-N1-C6	-2.30	114.95	118.73
3	L5	4636	PSU	O4'-C1'-C2'	2.30	108.33	105.15
68	S2	172	OMU	O2-C2-N1	-2.29	119.81	122.80
3	L5	2401	A2M	C6-C5-C4	-2.29	114.05	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4973	PSU	C6-C5-C4	2.29	119.72	118.17
68	S2	1851	MA6	C1'-N9-C8	-2.28	122.03	127.09
3	L5	3785	A2M	C4-N9-C1'	-2.28	121.30	126.63
68	S2	576	A2M	C1'-N9-C8	2.28	132.15	127.09
3	L5	4530	UR3	C6-N1-C2	-2.28	119.94	121.80
3	L5	3637	PSU	O2-C2-N1	-2.28	120.44	122.79
3	L5	1322	1MA	N1-C6-N6	2.27	125.42	119.71
3	L5	3830	A2M	C6-C5-C4	-2.27	114.08	117.18
68	S2	1639	G7M	N9-C8-N7	-2.27	106.97	112.48
3	L5	3637	PSU	C6-N1-C2	-2.27	120.58	122.69
3	L5	1323	A2M	O4'-C1'-C2'	2.27	110.49	106.59
68	S2	166	A2M	C6-C5-C4	-2.26	114.09	117.18
3	L5	4306	OMU	O2-C2-N1	-2.26	119.86	122.80
3	L5	3785	A2M	C3'-C2'-C1'	-2.26	98.48	102.81
3	L5	4296	PSU	C6-C5-C4	2.25	119.69	118.17
3	L5	2815	A2M	C4-N9-C1'	-2.25	121.38	126.63
3	L5	398	A2M	C2-N1-C6	-2.25	115.04	118.73
68	S2	1326	OMU	O2-C2-N1	-2.24	119.88	122.80
68	S2	468	A2M	C6-C5-C4	-2.24	114.12	117.18
3	L5	2787	A2M	C4-N9-C1'	-2.23	121.41	126.63
3	L5	1522	OMG	C2'-C1'-N9	-2.23	110.00	114.24
3	L5	4571	A2M	C6-C5-C4	-2.23	114.13	117.18
68	S2	1383	A2M	C6-C5-C4	-2.23	114.13	117.18
3	L5	3853	PSU	C6-N1-C2	-2.23	120.62	122.69
3	L5	4620	OMU	O2-C2-N1	-2.23	119.90	122.80
3	L5	4973	PSU	C6-N1-C2	-2.22	120.63	122.69
3	L5	3867	A2M	O3'-C3'-C2'	2.21	117.39	111.19
68	S2	668	A2M	O3'-C3'-C4'	-2.21	104.74	111.08
3	L5	4457	PSU	C6-C5-C4	2.21	119.66	118.17
3	L5	4523	A2M	C6-C5-C4	-2.20	114.17	117.18
3	L5	4442	PSU	O4'-C1'-C2'	2.20	108.20	105.15
3	L5	2815	A2M	C1'-N9-C8	2.20	131.98	127.09
3	L5	4457	PSU	C6-N1-C2	-2.20	120.65	122.69
3	L5	3825	A2M	C6-C5-C4	-2.20	114.18	117.18
3	L5	1862	PSU	C6-N1-C2	-2.19	120.66	122.69
5	L8	69	PSU	O4'-C1'-C2'	2.19	108.19	105.15
3	L5	398	A2M	C5-C6-N1	2.18	123.06	117.51
3	L5	2815	A2M	C6-C5-C4	-2.18	114.20	117.18
3	L5	1326	A2M	C6-C5-C4	-2.18	114.20	117.18
3	L5	4571	A2M	C2'-C1'-N9	2.18	117.33	113.75
3	L5	400	A2M	C6-C5-C4	-2.18	114.21	117.18
3	L5	3785	A2M	C5-C6-N1	2.17	123.03	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4403	PSU	O4'-C1'-C2'	2.17	108.16	105.15
3	L5	2815	A2M	O4'-C1'-C2'	2.17	110.32	106.59
68	S2	799	OMU	C1'-N1-C2	2.17	121.49	117.59
3	L5	4493	PSU	C6-N1-C2	-2.17	120.68	122.69
3	L5	4590	A2M	O4'-C1'-C2'	2.17	110.32	106.59
3	L5	1323	A2M	C2-N1-C6	-2.17	115.17	118.73
3	L5	1524	A2M	C1'-N9-C8	2.16	131.90	127.09
3	L5	4636	PSU	C5-C6-N1	-2.16	119.14	122.14
3	L5	1534	A2M	C6-C5-C4	-2.16	114.23	117.18
3	L5	3822	PSU	O4'-C1'-C2'	2.15	108.13	105.15
3	L5	1871	A2M	C4'-O4'-C1'	-2.15	104.72	109.47
68	S2	27	A2M	O4'-C1'-C2'	2.15	110.28	106.59
68	S2	651	PSU	C6-C5-C4	2.15	119.62	118.17
68	S2	686	PSU	C6-N1-C2	-2.14	120.70	122.69
3	L5	3785	A2M	C1'-N9-C8	2.14	131.85	127.09
3	L5	3785	A2M	O4'-C1'-N9	2.14	112.20	108.09
3	L5	1534	A2M	C2-N1-C6	-2.14	115.21	118.73
3	L5	2401	A2M	O4'-C1'-C2'	2.14	110.28	106.59
68	S2	1045	PSU	C6-C5-C4	2.14	119.62	118.17
3	L5	398	A2M	C6-C5-C4	-2.13	114.26	117.18
3	L5	4523	A2M	C5-C6-N1	2.13	122.92	117.51
68	S2	159	A2M	C2-N1-C6	-2.13	115.23	118.73
3	L5	400	A2M	C2-N1-C6	-2.13	115.23	118.73
3	L5	3718	A2M	C4-N9-C1'	-2.13	121.66	126.63
68	S2	866	PSU	C6-C5-C4	2.12	119.61	118.17
3	L5	3925	OMU	O2-C2-N1	-2.12	120.03	122.80
68	S2	99	A2M	C6-C5-C4	-2.12	114.28	117.18
68	S2	99	A2M	C5-C6-N1	2.12	122.89	117.51
3	L5	1792	PSU	C6-N1-C2	-2.12	120.72	122.69
68	S2	1031	A2M	C2-N1-C6	-2.12	115.25	118.73
3	L5	2787	A2M	C2-N1-C6	-2.11	115.26	118.73
3	L5	3825	A2M	C5-C6-N1	2.11	122.87	117.51
68	S2	121	OMU	O2-C2-N1	-2.11	120.05	122.80
3	L5	3822	PSU	C6-C5-C4	2.11	119.60	118.17
3	L5	3825	A2M	C2-N1-C6	-2.11	115.27	118.73
3	L5	1326	A2M	C5-C6-N1	2.10	122.85	117.51
3	L5	3867	A2M	O4'-C1'-C2'	2.10	110.21	106.59
3	L5	4523	A2M	C2-N1-C6	-2.10	115.28	118.73
3	L5	1677	PSU	O4'-C1'-C2'	2.10	108.06	105.15
3	L5	3867	A2M	C2-N1-C6	-2.10	115.28	118.73
68	S2	428	OMU	O2-C2-N1	-2.10	120.06	122.80
68	S2	1056	PSU	C6-C5-C4	2.10	119.59	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1031	A2M	C6-C5-C4	-2.10	114.31	117.18
68	S2	468	A2M	O4'-C1'-C2'	2.09	110.19	106.59
3	L5	4689	PSU	O2-C2-N1	-2.09	120.63	122.79
3	L5	1326	A2M	C2-N1-C6	-2.09	115.29	118.73
3	L5	400	A2M	C5-C6-N1	2.09	122.83	117.51
3	L5	2787	A2M	C1'-N9-C8	2.09	131.74	127.09
68	S2	484	A2M	C5-C6-N1	2.09	122.82	117.51
68	S2	1031	A2M	C5-C6-N1	2.09	122.82	117.51
3	L5	2363	A2M	C2-N1-C6	-2.09	115.30	118.73
3	L5	1323	A2M	C5-C6-N1	2.09	122.81	117.51
3	L5	4353	PSU	C6-C5-C4	2.09	119.58	118.17
3	L5	400	A2M	O4'-C1'-C2'	2.09	110.18	106.59
3	L5	1524	A2M	C2-N1-C6	-2.09	115.30	118.73
3	L5	2815	A2M	C2-N1-C6	-2.09	115.30	118.73
3	L5	3830	A2M	C5-C6-N1	2.09	122.81	117.51
68	S2	99	A2M	C2-N1-C6	-2.08	115.31	118.73
3	L5	1323	A2M	C4-N9-C1'	-2.08	121.76	126.63
3	L5	3867	A2M	C3'-C2'-C1'	-2.08	98.82	102.81
68	S2	484	A2M	C6-C5-C4	-2.08	114.34	117.18
3	L5	2787	A2M	C5-C6-N1	2.08	122.79	117.51
3	L5	1326	A2M	C2'-C1'-N9	2.08	117.17	113.75
3	L5	3718	A2M	C5-C6-N1	2.08	122.78	117.51
3	L5	2815	A2M	C5-C6-N1	2.07	122.78	117.51
68	S2	27	A2M	C5-C6-N1	2.07	122.77	117.51
68	S2	159	A2M	C5-C6-N1	2.07	122.77	117.51
68	S2	668	A2M	C5-C6-N1	2.07	122.76	117.51
68	S2	166	A2M	C2-N1-C6	-2.07	115.34	118.73
3	L5	3867	A2M	C5-C6-N1	2.06	122.75	117.51
68	S2	1832	6MZ	C5-C6-N1	2.06	120.37	118.15
68	S2	116	OMU	O2-C2-N1	-2.06	120.11	122.80
3	L5	1534	A2M	C5-C6-N1	2.06	122.74	117.51
3	L5	3851	PSU	C6-C5-C4	2.06	119.56	118.17
3	L5	2363	A2M	C6-C5-C4	-2.06	114.37	117.18
3	L5	3718	A2M	C2-N1-C6	-2.06	115.35	118.73
3	L5	4293	PSU	C6-N1-C2	-2.05	120.79	122.69
3	L5	1871	A2M	O4'-C1'-C2'	2.05	110.12	106.59
3	L5	3851	PSU	C6-N1-C2	-2.05	120.79	122.69
68	S2	159	A2M	O4'-C4'-C3'	2.05	109.22	105.15
3	L5	4571	A2M	C5-C6-N1	2.05	122.72	117.51
68	S2	668	A2M	C2-N1-C6	-2.05	115.36	118.73
68	S2	166	A2M	C5-C6-N1	2.04	122.70	117.51
3	L5	2401	A2M	C2-N1-C6	-2.04	115.38	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3830	A2M	C4'-O4'-C1'	-2.03	104.97	109.47
3	L5	2363	A2M	C5-C6-N1	2.03	122.67	117.51
68	S2	1383	A2M	C5-C6-N1	2.03	122.67	117.51
3	L5	1323	A2M	C1'-N9-C8	2.03	131.60	127.09
68	S2	484	A2M	C2-N1-C6	-2.03	115.39	118.73
68	S2	166	A2M	O4'-C1'-C2'	2.03	110.08	106.59
3	L5	3695	PSU	C6-C5-C4	2.03	119.54	118.17
68	S2	468	A2M	C5-C6-N1	2.03	122.66	117.51
3	L5	1582	PSU	C5-C4-N3	2.02	121.00	116.55
68	S2	27	A2M	C2-N1-C6	-2.02	115.41	118.73
3	L5	1524	A2M	C6-C5-C4	-2.02	114.42	117.18
3	L5	1534	A2M	O4'-C1'-C2'	2.02	110.07	106.59
68	S2	99	A2M	O4'-C1'-C2'	2.02	110.06	106.59
68	S2	576	A2M	C6-C5-C4	-2.02	114.42	117.18
3	L5	1871	A2M	C5-C6-N1	2.01	122.63	117.51
68	S2	1272	OMC	C1'-N1-C2	2.01	122.89	118.44
3	L5	1524	A2M	C5-C6-N1	2.01	122.62	117.51
3	L5	3785	A2M	O4'-C4'-C3'	2.01	109.14	105.15
3	L5	400	A2M	O3'-C3'-C4'	-2.01	105.31	111.08
3	L5	4636	PSU	C6-N1-C2	-2.01	120.83	122.69
3	L5	2787	A2M	C3'-C2'-C1'	-2.01	98.96	102.81
3	L5	4590	A2M	C5-C6-N1	2.01	122.61	117.51
68	S2	686	PSU	C6-C5-C4	2.00	119.53	118.17
68	S2	1046	PSU	O4'-C1'-C2'	2.00	107.92	105.15
3	L5	4571	A2M	O3'-C3'-C4'	-2.00	105.33	111.08
3	L5	2401	A2M	C5-C6-N1	2.00	122.59	117.51

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L8	75	OMG	C1'-C2'-O2'-CM2
3	L5	1326	A2M	O4'-C4'-C5'-O5'
3	L5	1625	OMG	O4'-C4'-C5'-O5'
3	L5	2351	OMC	C1'-C2'-O2'-CM2
3	L5	2364	OMG	O4'-C4'-C5'-O5'
3	L5	2787	A2M	C1'-C2'-O2'-CM'
3	L5	2815	A2M	O4'-C4'-C5'-O5'
3	L5	2861	OMC	C1'-C2'-O2'-CM2
3	L5	3701	OMC	C2'-C1'-N1-C2
3	L5	3792	OMG	O4'-C4'-C5'-O5'
3	L5	3867	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
3	L5	4196	OMG	C1'-C2'-O2'-CM2
3	L5	4590	A2M	C1'-C2'-O2'-CM'
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	159	A2M	C1'-C2'-O2'-CM'
68	S2	462	OMC	C1'-C2'-O2'-CM2
68	S2	468	A2M	C1'-C2'-O2'-CM'
68	S2	576	A2M	O4'-C4'-C5'-O5'
68	S2	627	OMU	O4'-C4'-C5'-O5'
68	S2	644	OMG	O4'-C4'-C5'-O5'
68	S2	668	A2M	C1'-C2'-O2'-CM'
68	S2	799	OMU	C3'-C4'-C5'-O5'
68	S2	799	OMU	O4'-C4'-C5'-O5'
68	S2	801	PSU	C3'-C4'-C5'-O5'
68	S2	863	PSU	O4'-C4'-C5'-O5'
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-C6
3	L5	1326	A2M	C3'-C4'-C5'-O5'
3	L5	1536	PSU	C3'-C4'-C5'-O5'
3	L5	3701	OMC	C3'-C4'-C5'-O5'
3	L5	3701	OMC	O4'-C4'-C5'-O5'
3	L5	3867	A2M	C3'-C4'-C5'-O5'
3	L5	4500	PSU	C3'-C4'-C5'-O5'
3	L5	4500	PSU	O4'-C4'-C5'-O5'
3	L5	4590	A2M	O4'-C4'-C5'-O5'
3	L5	4590	A2M	C3'-C4'-C5'-O5'
68	S2	99	A2M	O4'-C4'-C5'-O5'
68	S2	576	A2M	C3'-C4'-C5'-O5'
68	S2	627	OMU	C3'-C4'-C5'-O5'
68	S2	863	PSU	C3'-C4'-C5'-O5'
68	S2	1442	OMU	O4'-C4'-C5'-O5'
3	L5	1536	PSU	O4'-C4'-C5'-O5'
3	L5	1625	OMG	C3'-C4'-C5'-O5'
3	L5	3785	A2M	O4'-C4'-C5'-O5'
3	L5	3867	A2M	O4'-C4'-C5'-O5'
3	L5	3899	OMG	C3'-C4'-C5'-O5'
3	L5	4637	OMG	C3'-C4'-C5'-O5'
68	S2	801	PSU	O4'-C4'-C5'-O5'
68	S2	1442	OMU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
68	S2	1248	B8N	N34-C33-C34-O36
3	L5	2815	A2M	C3'-C4'-C5'-O5'
3	L5	3785	A2M	C3'-C4'-C5'-O5'
3	L5	3792	OMG	C3'-C4'-C5'-O5'
68	S2	644	OMG	C3'-C4'-C5'-O5'
3	L5	2364	OMG	C3'-C4'-C5'-O5'
68	S2	99	A2M	C3'-C4'-C5'-O5'
68	S2	668	A2M	O4'-C4'-C5'-O5'
3	L5	3899	OMG	O4'-C4'-C5'-O5'
3	L5	4618	OMG	C3'-C4'-C5'-O5'
68	S2	668	A2M	C3'-C4'-C5'-O5'
68	S2	428	OMU	C2'-C1'-N1-C6
3	L5	4220	6MZ	O4'-C4'-C5'-O5'
68	S2	1045	PSU	O4'-C4'-C5'-O5'
3	L5	3818	UY1	C4'-C5'-O5'-P
3	L5	1524	A2M	O4'-C4'-C5'-O5'
3	L5	1524	A2M	C3'-C4'-C5'-O5'
3	L5	4220	6MZ	C3'-C4'-C5'-O5'
3	L5	2787	A2M	C2'-C1'-N9-C8
3	L5	2364	OMG	C1'-C2'-O2'-CM2
68	S2	1045	PSU	C3'-C4'-C5'-O5'
68	S2	436	OMG	C3'-C4'-C5'-O5'
3	L5	1582	PSU	C3'-C4'-C5'-O5'
3	L5	2787	A2M	C3'-C4'-C5'-O5'
3	L5	4618	OMG	O4'-C4'-C5'-O5'
68	S2	1056	PSU	C3'-C4'-C5'-O5'
68	S2	1288	OMU	C3'-C4'-C5'-O5'
68	S2	428	OMU	O4'-C1'-N1-C6
3	L5	1323	A2M	O4'-C4'-C5'-O5'
3	L5	4590	A2M	C4'-C5'-O5'-P
68	S2	867	OMG	C4'-C5'-O5'-P
68	S2	436	OMG	O4'-C4'-C5'-O5'
68	S2	1056	PSU	O4'-C4'-C5'-O5'
3	L5	1322	1MA	C2'-C1'-N9-C8
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	4500	PSU	C4'-C5'-O5'-P
68	S2	1490	OMG	C4'-C5'-O5'-P
68	S2	1851	MA6	C4'-C5'-O5'-P
3	L5	1677	PSU	O4'-C1'-C5-C4
3	L5	3818	UY1	O4'-C1'-C5-C4
3	L5	2787	A2M	C2'-C1'-N9-C4
3	L5	4447	5MC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
68	S2	644	OMG	C4'-C5'-O5'-P
68	S2	1081	PSU	C4'-C5'-O5'-P
68	S2	428	OMU	C2'-C1'-N1-C2
3	L5	1524	A2M	C3'-C2'-O2'-CM'
3	L5	4370	OMG	C3'-C2'-O2'-CM2
3	L5	1322	1MA	C2'-C1'-N9-C4
5	L8	75	OMG	C4'-C5'-O5'-P
3	L5	1326	A2M	C4'-C5'-O5'-P
3	L5	3844	PSU	C4'-C5'-O5'-P
68	S2	576	A2M	C4'-C5'-O5'-P
3	L5	398	A2M	O4'-C4'-C5'-O5'
3	L5	1781	PSU	C3'-C4'-C5'-O5'
3	L5	3782	5MC	O4'-C4'-C5'-O5'
68	S2	172	OMU	O4'-C4'-C5'-O5'
68	S2	1244	PSU	O4'-C4'-C5'-O5'
68	S2	428	OMU	O4'-C1'-N1-C2
3	L5	3887	OMC	C4'-C5'-O5'-P
3	L5	4623	OMG	C3'-C4'-C5'-O5'
3	L5	398	A2M	C1'-C2'-O2'-CM'
68	S2	174	OMC	C1'-C2'-O2'-CM2
68	S2	601	OMG	C1'-C2'-O2'-CM2
68	S2	1328	OMG	C1'-C2'-O2'-CM2
3	L5	1792	PSU	O4'-C4'-C5'-O5'
3	L5	2422	OMC	C3'-C4'-C5'-O5'
3	L5	1677	PSU	O4'-C1'-C5-C6
3	L5	3785	A2M	C3'-C2'-O2'-CM'
68	S2	1703	OMC	O4'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C6
68	S2	428	OMU	O4'-C4'-C5'-O5'
3	L5	2401	A2M	C3'-C2'-O2'-CM'
3	L5	4499	OMG	C3'-C2'-O2'-CM2
3	L5	3701	OMC	O4'-C1'-N1-C6
3	L5	1582	PSU	O4'-C4'-C5'-O5'
3	L5	4447	5MC	O4'-C1'-N1-C2
3	L5	2787	A2M	O4'-C1'-N9-C8
68	S2	668	A2M	O4'-C1'-N9-C8
3	L5	2351	OMC	C2'-C1'-N1-C2
3	L5	3785	A2M	C2'-C1'-N9-C8
68	S2	668	A2M	C2'-C1'-N9-C8
68	S2	1248	B8N	N34-C33-C34-O35
3	L5	2824	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

62 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3825	A2M	1	0
68	S2	1288	OMU	1	0
68	S2	668	A2M	1	0
3	L5	400	A2M	1	0
3	L5	4457	PSU	1	0
3	L5	2351	OMC	2	0
3	L5	4392	OMG	1	0
3	L5	4571	A2M	1	0
3	L5	4590	A2M	1	0
68	S2	1850	MA6	1	0
68	S2	1272	OMC	1	0
68	S2	801	PSU	1	0
3	L5	2804	OMC	1	0
68	S2	681	PSU	1	0
3	L5	4689	PSU	1	0
68	S2	1703	OMC	1	0
68	S2	799	OMU	1	0
3	L5	3925	OMU	1	0
3	L5	1326	A2M	1	0
68	S2	159	A2M	2	0
68	S2	1004	PSU	2	0
3	L5	4196	OMG	1	0
68	S2	1328	OMG	1	0
3	L5	4618	OMG	1	0
3	L5	2363	A2M	1	0
3	L5	4637	OMG	1	0
68	S2	1832	6MZ	1	0
68	S2	1391	OMC	1	0
3	L5	4447	5MC	1	0
68	S2	166	A2M	2	0
68	S2	468	A2M	2	0
3	L5	1683	PSU	1	0
3	L5	4536	OMC	1	0
68	S2	116	OMU	3	0
68	S2	462	OMC	1	0
3	L5	1625	OMG	1	0
3	L5	3718	A2M	3	0
68	S2	644	OMG	1	0
3	L5	1340	OMC	2	0
68	S2	509	OMG	2	0
3	L5	3867	A2M	3	0
68	S2	484	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L8	75	OMG	1	0
68	S2	27	A2M	1	0
68	S2	1383	A2M	1	0
3	L5	2861	OMC	1	0
3	L5	398	A2M	1	0
3	L5	4456	OMC	1	0
68	S2	121	OMU	2	0
68	S2	1337	4AC	2	0
68	S2	576	A2M	1	0
68	S2	601	OMG	2	0
3	L5	4306	OMU	1	0
3	L5	1871	A2M	1	0
68	S2	1031	A2M	1	0
3	L5	4220	6MZ	1	0
3	L5	2632	PSU	1	0
3	L5	4521	PSU	1	0
3	L5	4620	OMU	1	0
68	S2	649	PSU	1	0
3	L5	4523	A2M	1	0
3	L5	3701	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
89	SPD	L5	5261	-	9,9,9	0.34	0	8,8,8	1.09	0
89	SPD	L5	5283	-	9,9,9	0.32	0	8,8,8	0.90	0
89	SPD	L5	5286	-	9,9,9	0.33	0	8,8,8	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	SPM	L5	5259	-	13,13,13	0.39	0	12,12,12	1.04	0
89	SPD	LN	301	-	9,9,9	0.34	0	8,8,8	0.85	0
88	SPM	L5	5292	-	13,13,13	0.37	0	12,12,12	0.91	0
88	SPM	L5	5289	-	13,13,13	0.37	0	12,12,12	1.01	0
88	SPM	L5	5293	-	13,13,13	0.36	0	12,12,12	0.83	0
89	SPD	L5	5285	-	9,9,9	0.33	0	8,8,8	0.85	0
89	SPD	L5	5284	-	9,9,9	0.31	0	8,8,8	0.92	0
88	SPM	L5	5264	-	13,13,13	0.38	0	12,12,12	1.02	0
88	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	0.98	0
89	SPD	L5	5287	-	9,9,9	0.33	0	8,8,8	0.95	0
88	SPM	L5	5267	-	13,13,13	0.40	0	12,12,12	1.24	1 (8%)
89	SPD	L5	5291	-	9,9,9	0.34	0	8,8,8	0.91	0
89	SPD	L5	5288	-	9,9,9	0.32	0	8,8,8	0.86	0
89	SPD	L5	5290	-	9,9,9	0.32	0	8,8,8	0.80	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	5261	-	-	1/7/7/7	-
89	SPD	L5	5283	-	-	1/7/7/7	-
89	SPD	L5	5286	-	-	2/7/7/7	-
88	SPM	L5	5259	-	-	6/11/11/11	-
89	SPD	LN	301	-	-	0/7/7/7	-
88	SPM	L5	5292	-	-	6/11/11/11	-
88	SPM	L5	5289	-	-	5/11/11/11	-
88	SPM	L5	5293	-	-	4/11/11/11	-
89	SPD	L5	5285	-	-	5/7/7/7	-
89	SPD	L5	5284	-	-	2/7/7/7	-
88	SPM	L5	5264	-	-	5/11/11/11	-
88	SPM	L5	5263	-	-	6/11/11/11	-
89	SPD	L5	5287	-	-	3/7/7/7	-
88	SPM	L5	5267	-	-	5/11/11/11	-
89	SPD	L5	5291	-	-	3/7/7/7	-
89	SPD	L5	5288	-	-	3/7/7/7	-
89	SPD	L5	5290	-	-	3/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	L5	5267	SPM	C3-C4-N5	-2.01	106.68	112.07

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	L5	5267	SPM	C7-C8-C9-N10
88	L5	5263	SPM	C7-C8-C9-N10
89	L5	5284	SPD	C8-C7-N6-C5
88	L5	5292	SPM	C7-C8-C9-N10
89	L5	5285	SPD	C3-C4-C5-N6
88	L5	5263	SPM	N10-C11-C12-C13
88	L5	5264	SPM	C2-C3-C4-N5
89	L5	5285	SPD	N6-C7-C8-C9
89	L5	5288	SPD	N6-C7-C8-C9
89	L5	5287	SPD	C3-C4-C5-N6
88	L5	5264	SPM	C3-C4-N5-C6
88	L5	5264	SPM	N5-C6-C7-C8
88	L5	5289	SPM	C8-C9-N10-C11
88	L5	5259	SPM	C2-C3-C4-N5
88	L5	5292	SPM	N10-C11-C12-C13
88	L5	5267	SPM	C12-C11-N10-C9
88	L5	5289	SPM	C12-C11-N10-C9
88	L5	5293	SPM	C8-C9-N10-C11
89	L5	5288	SPD	C8-C7-N6-C5
88	L5	5267	SPM	N10-C11-C12-C13
89	L5	5288	SPD	N1-C2-C3-C4
88	L5	5289	SPM	C7-C6-N5-C4
89	L5	5285	SPD	C2-C3-C4-C5
88	L5	5267	SPM	C6-C7-C8-C9
88	L5	5264	SPM	C6-C7-C8-C9
88	L5	5259	SPM	C6-C7-C8-C9
89	L5	5290	SPD	C2-C3-C4-C5
88	L5	5263	SPM	C6-C7-C8-C9
88	L5	5293	SPM	C6-C7-C8-C9
88	L5	5259	SPM	C7-C6-N5-C4
88	L5	5264	SPM	N1-C2-C3-C4
88	L5	5293	SPM	C7-C6-N5-C4
89	L5	5291	SPD	C8-C7-N6-C5
88	L5	5289	SPM	C2-C3-C4-N5

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Mol	Chain	Res	Type	Atoms
89	L5	5290	SPD	N1-C2-C3-C4
89	L5	5287	SPD	N6-C7-C8-C9
88	L5	5259	SPM	C3-C4-N5-C6
89	L5	5291	SPD	C4-C5-N6-C7
88	L5	5292	SPM	N5-C6-C7-C8
89	L5	5287	SPD	C2-C3-C4-C5
88	L5	5263	SPM	C7-C6-N5-C4
88	L5	5289	SPM	N1-C2-C3-C4
89	L5	5284	SPD	C7-C8-C9-N10
89	L5	5290	SPD	C7-C8-C9-N10
89	L5	5291	SPD	C7-C8-C9-N10
89	L5	5286	SPD	C2-C3-C4-C5
89	L5	5261	SPD	C8-C7-N6-C5
88	L5	5259	SPM	N5-C6-C7-C8
89	L5	5286	SPD	C3-C4-C5-N6
88	L5	5292	SPM	C6-C7-C8-C9
88	L5	5263	SPM	C8-C9-N10-C11
88	L5	5292	SPM	C7-C6-N5-C4
88	L5	5293	SPM	C3-C4-N5-C6
88	L5	5263	SPM	C3-C4-N5-C6
88	L5	5259	SPM	C11-C12-C13-N14
88	L5	5267	SPM	N1-C2-C3-C4
88	L5	5292	SPM	C11-C12-C13-N14
89	L5	5285	SPD	C7-C8-C9-N10
89	L5	5285	SPD	C4-C5-N6-C7
89	L5	5283	SPD	C2-C3-C4-C5

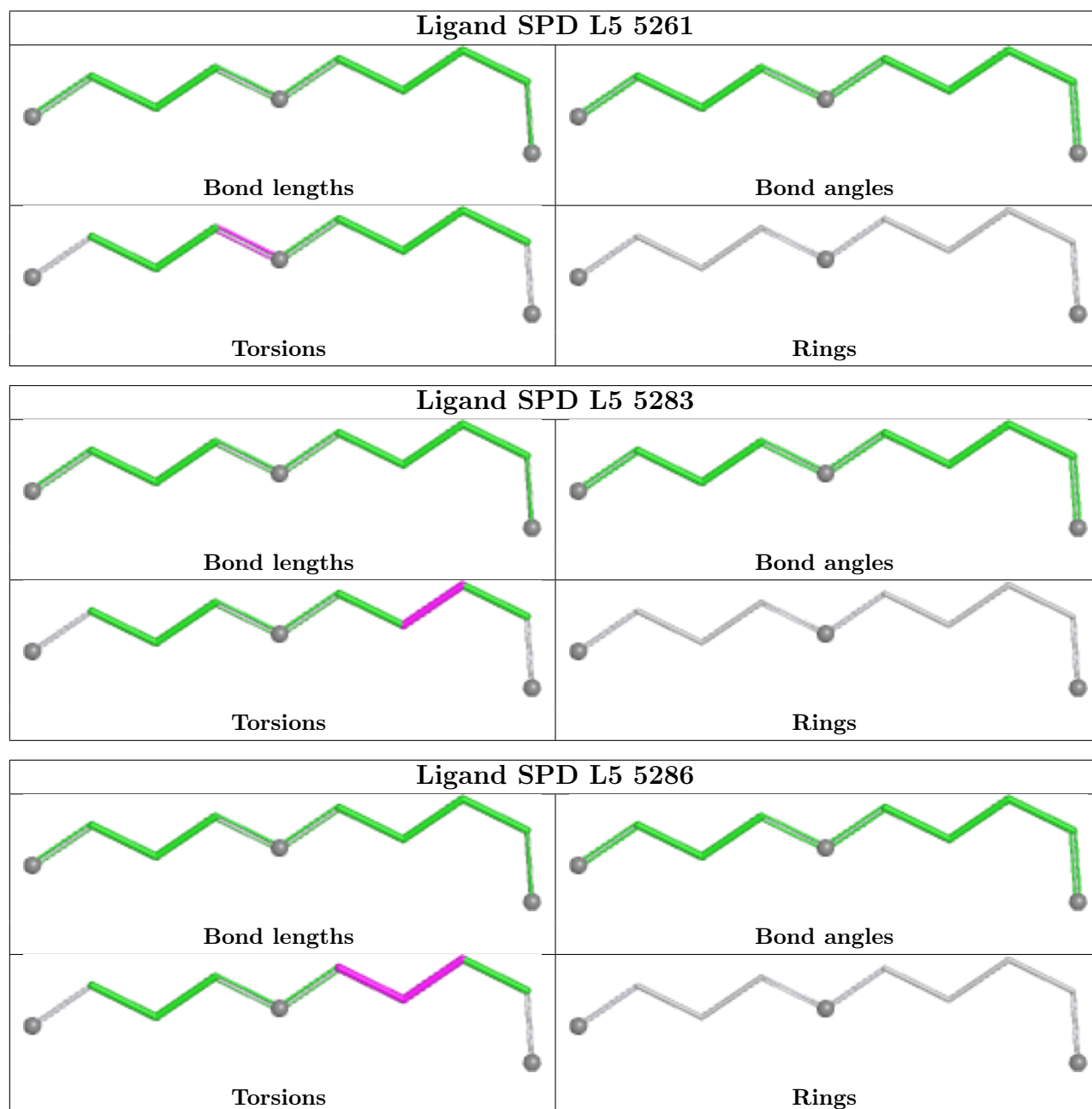
There are no ring outliers.

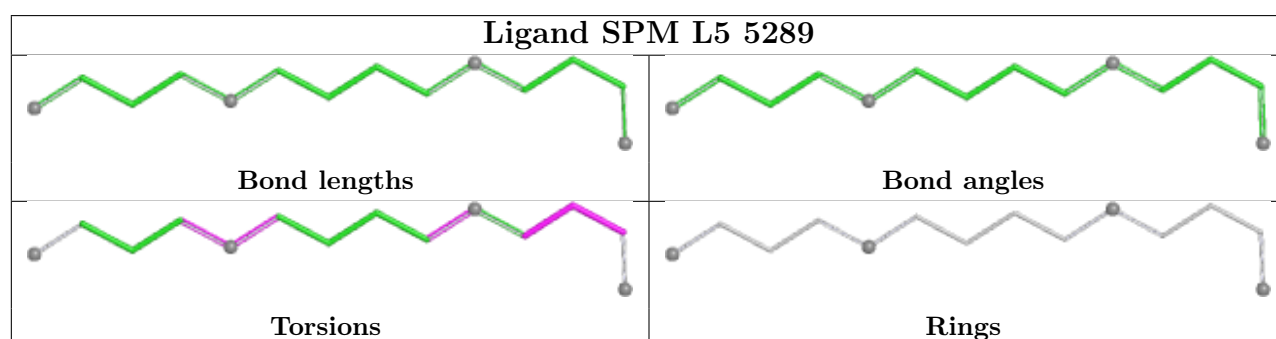
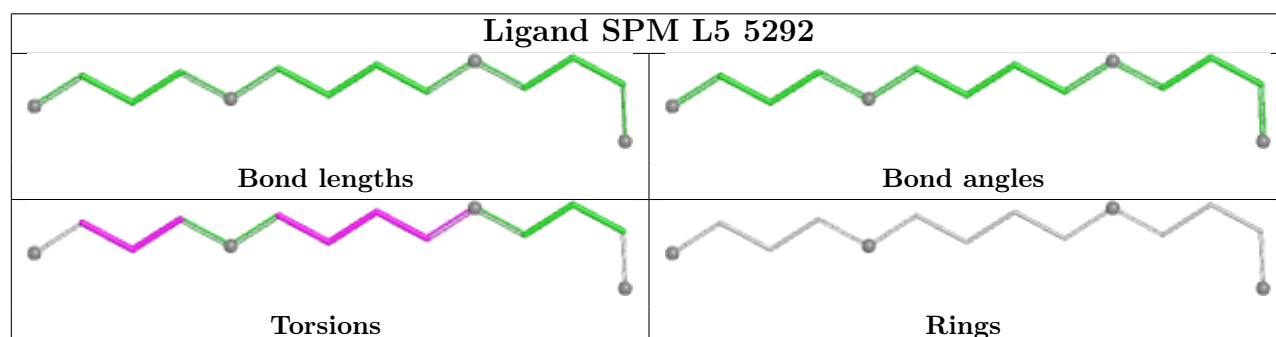
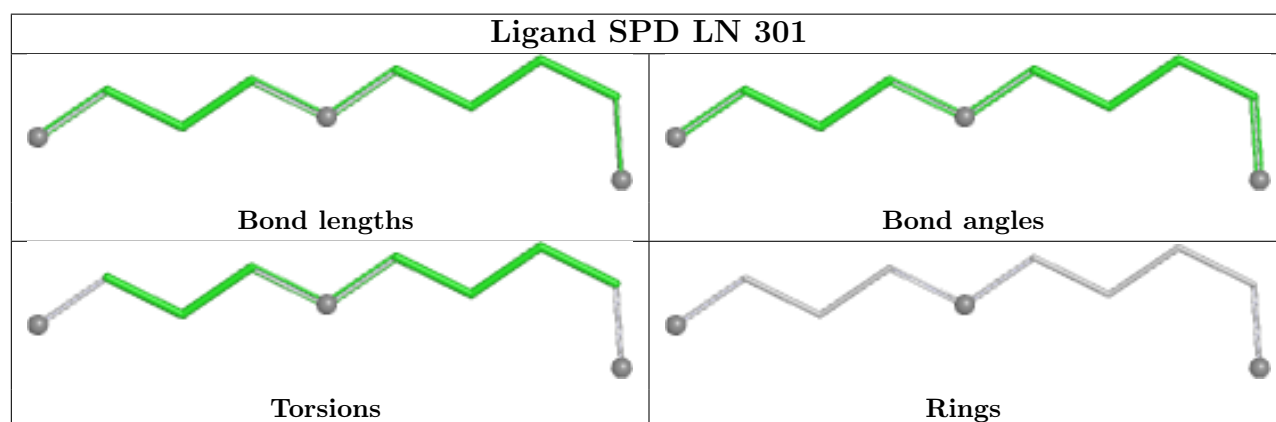
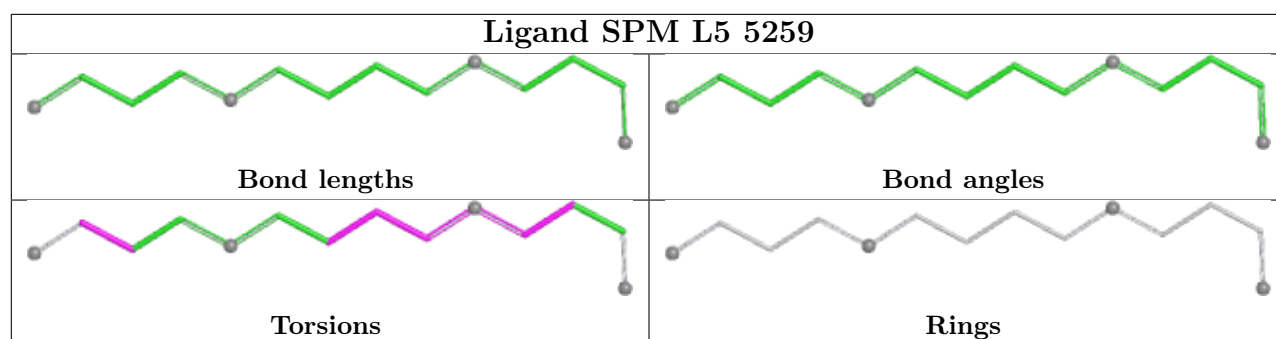
4 monomers are involved in 6 short contacts:

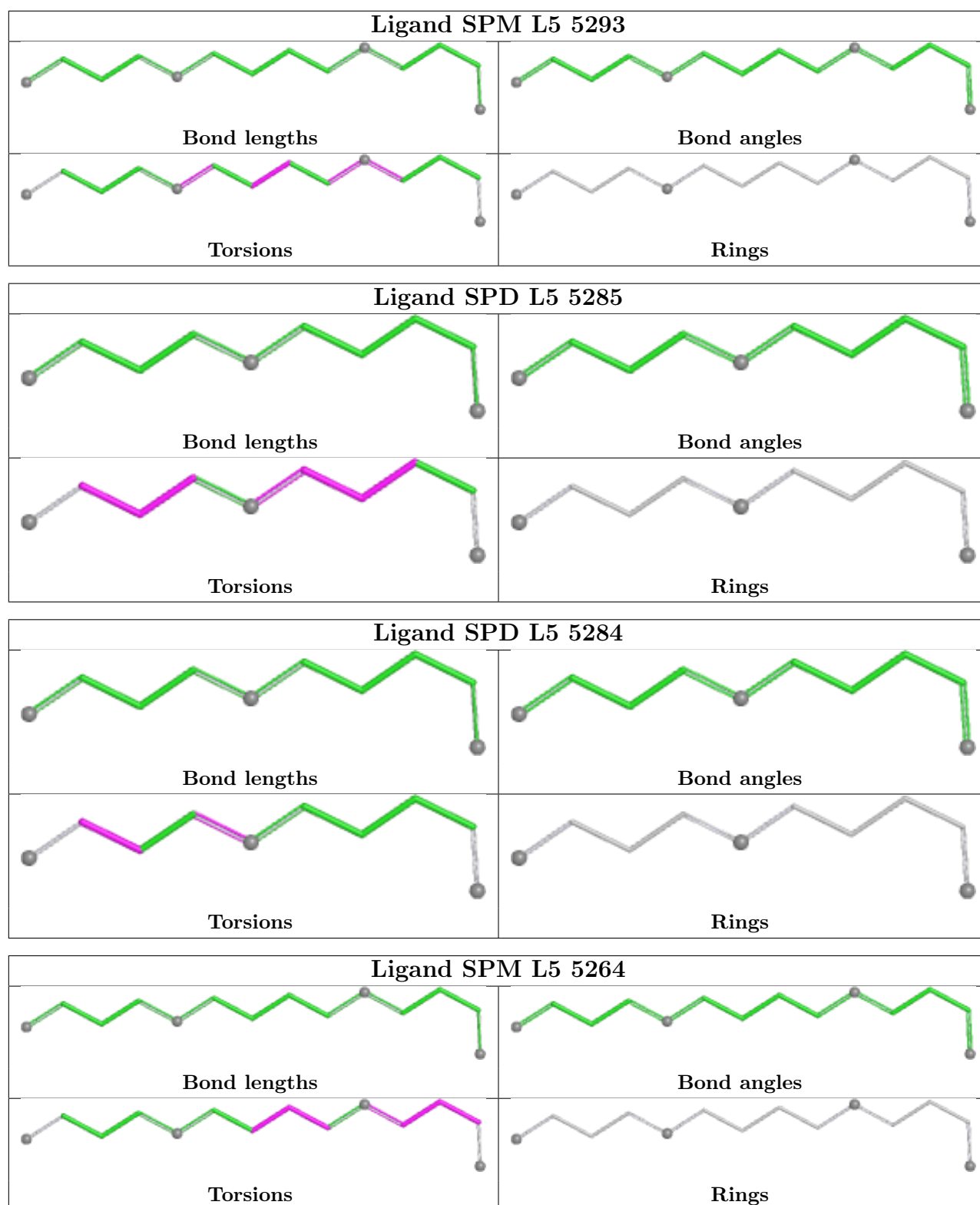
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5292	SPM	1	0
88	L5	5293	SPM	2	0
89	L5	5291	SPD	2	0
89	L5	5290	SPD	1	0

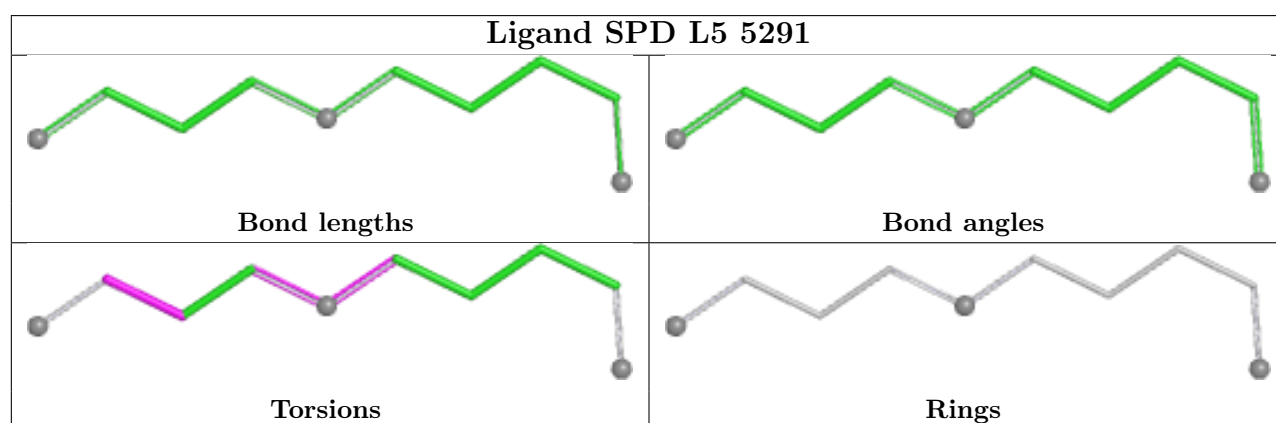
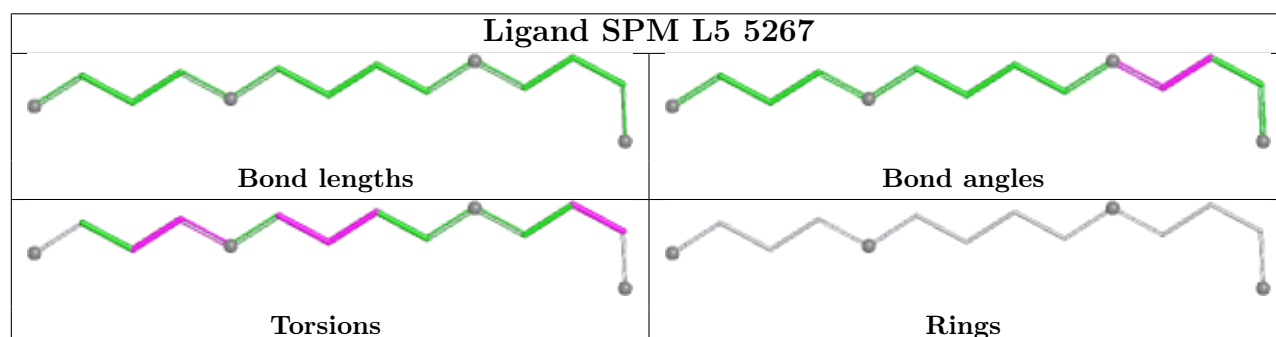
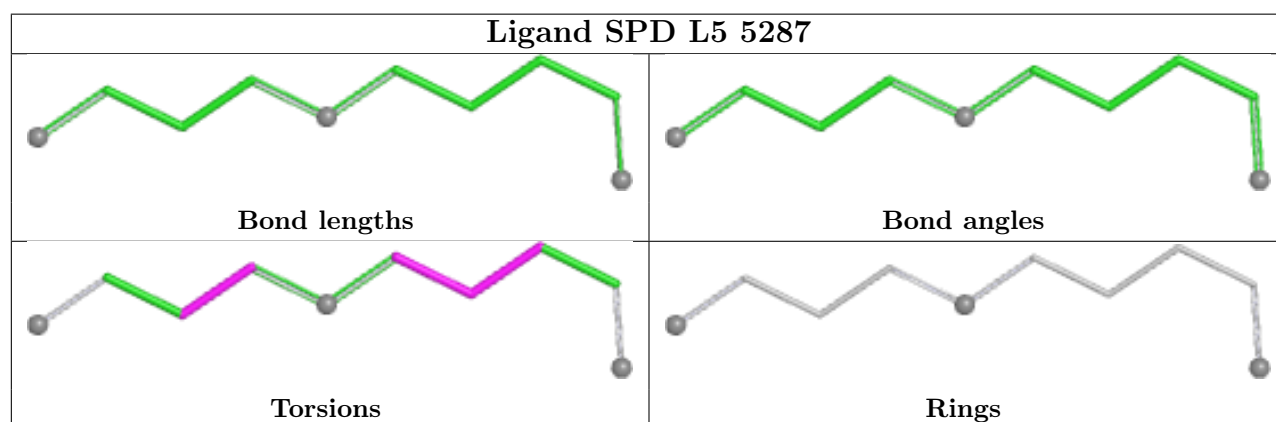
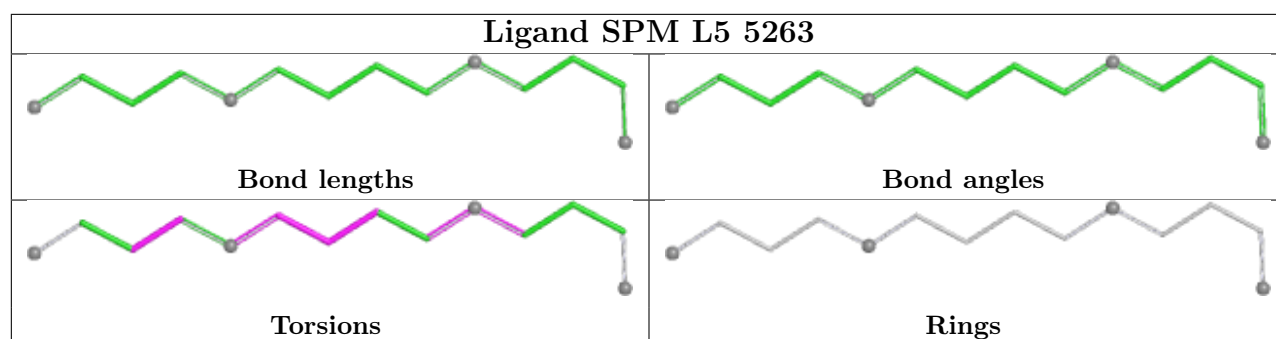
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

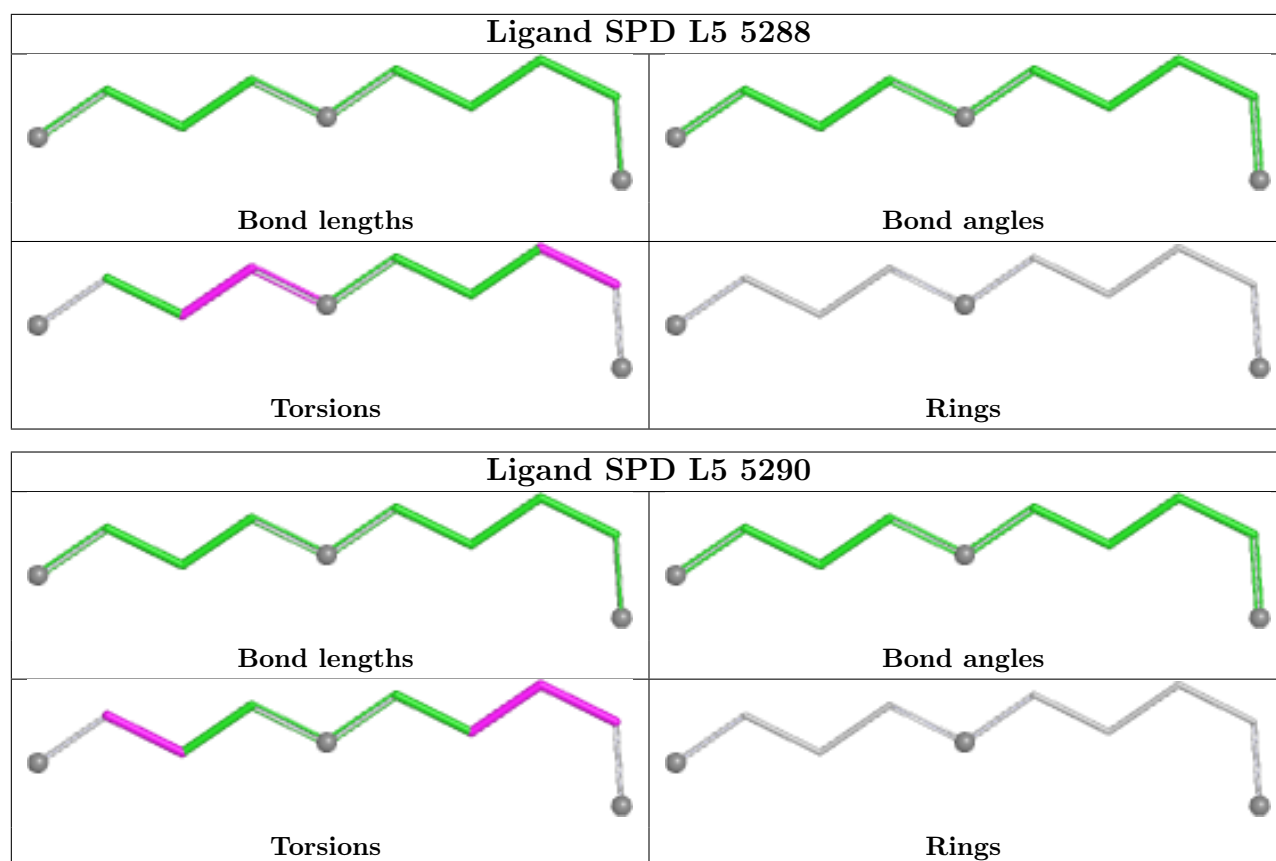
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	28.56
1	S2	698:G	O3'	730:C	P	13.86
1	S2	739:C	O3'	746:C	P	13.02
1	Et	16:C	O3'	18:U	P	7.35
1	S2	225:G	O3'	287:U	P	6.63

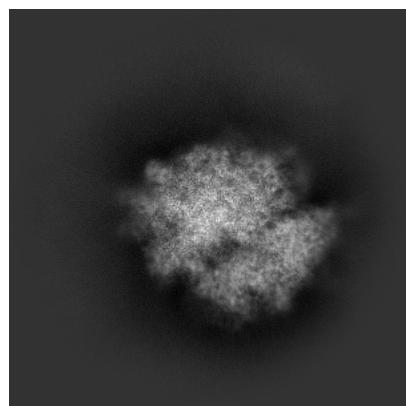
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71339. These allow visual inspection of the internal detail of the map and identification of artifacts.

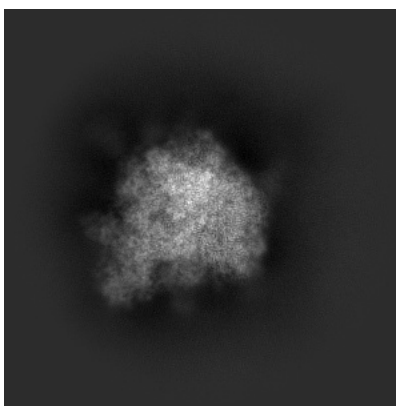
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

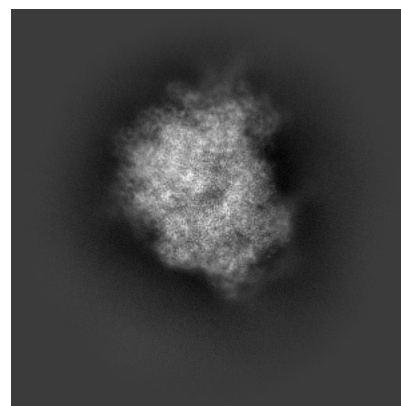
6.1.1 Primary map



X

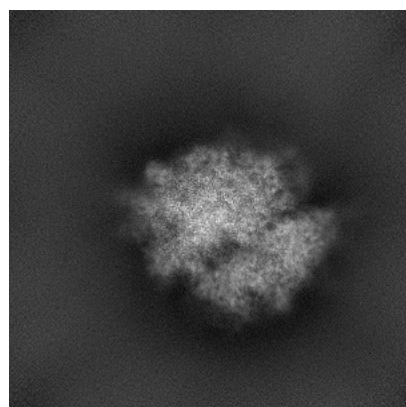


Y

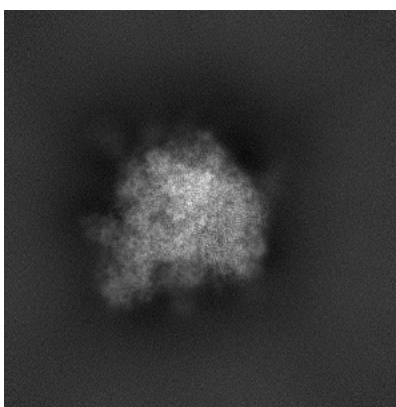


Z

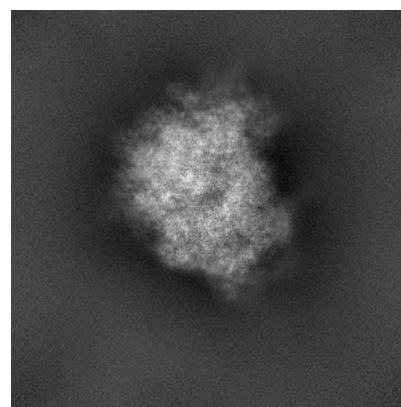
6.1.2 Raw map



X



Y

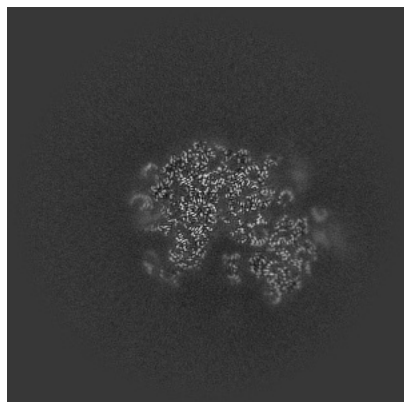


Z

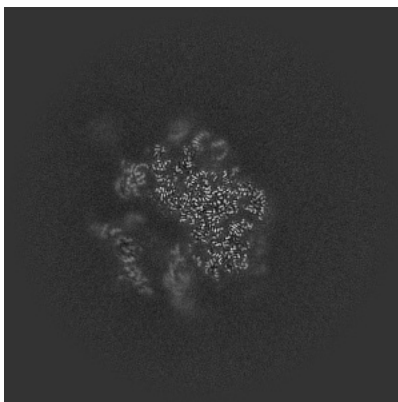
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

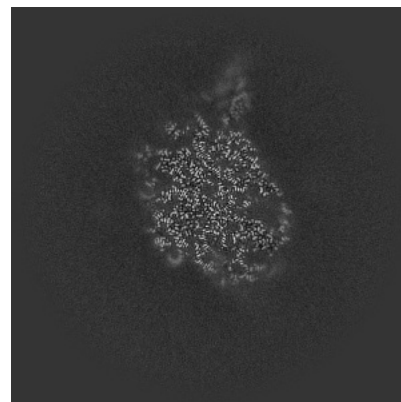
6.2.1 Primary map



X Index: 256



Y Index: 256

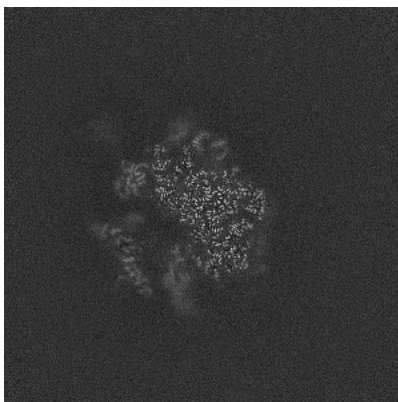


Z Index: 256

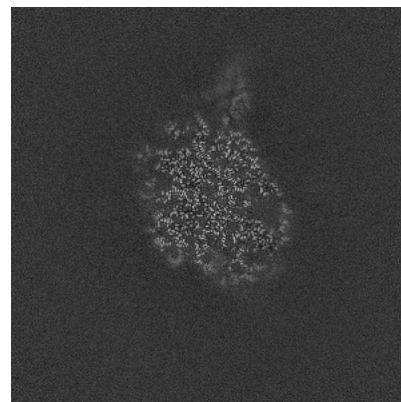
6.2.2 Raw map



X Index: 256



Y Index: 256

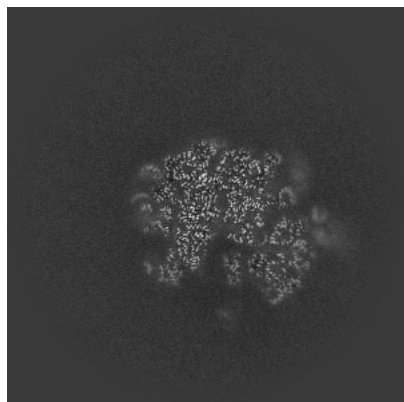


Z Index: 256

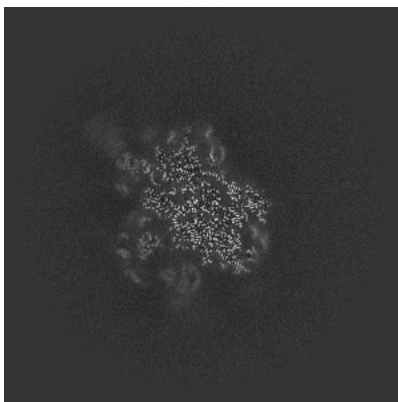
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

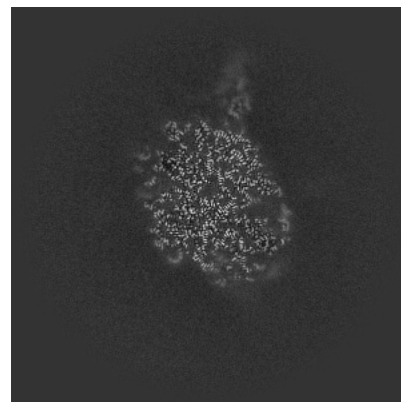
6.3.1 Primary map



X Index: 253

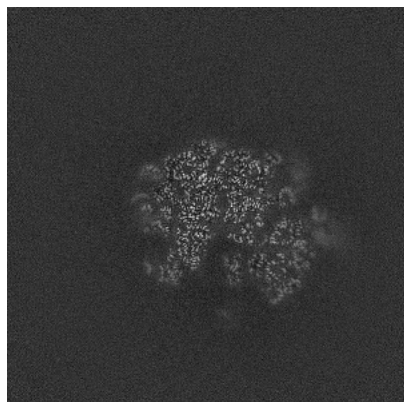


Y Index: 243

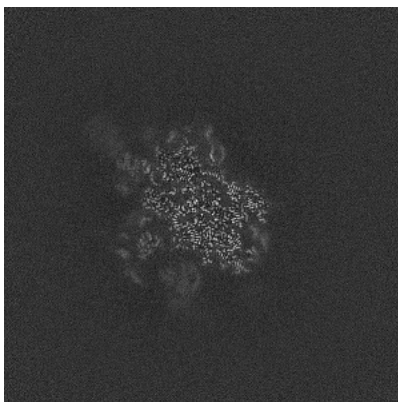


Z Index: 258

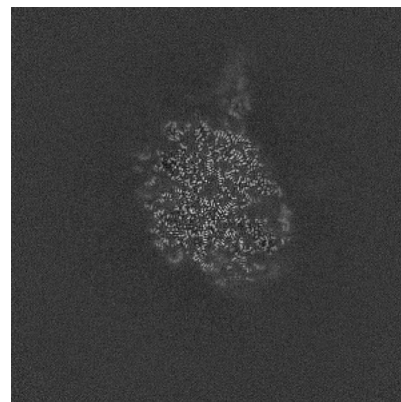
6.3.2 Raw map



X Index: 253



Y Index: 243

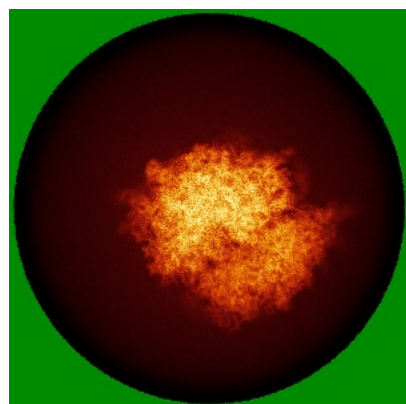


Z Index: 258

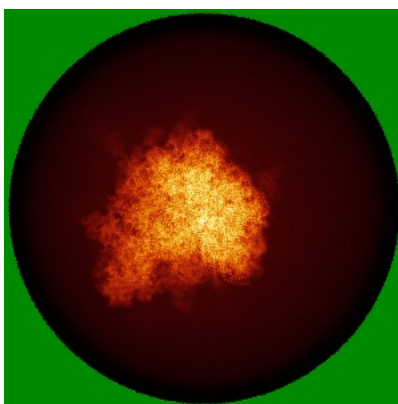
The images above show the largest variance slices of the map in three orthogonal directions.

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

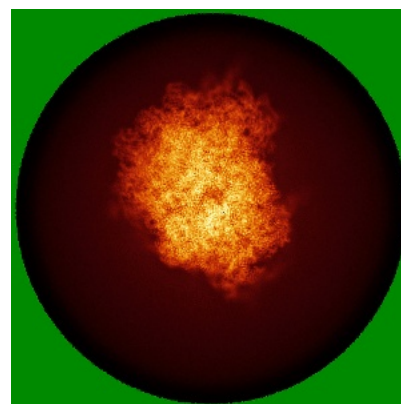
6.4.1 Primary map



X

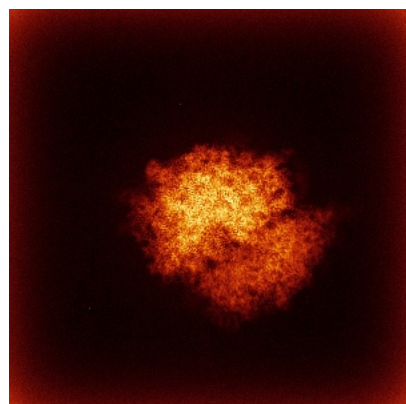


Y

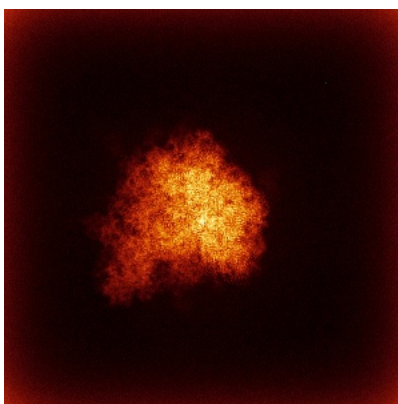


Z

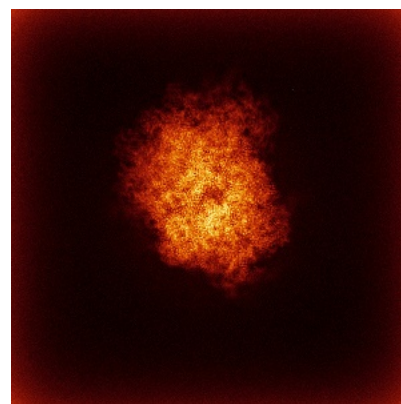
6.4.2 Raw map



X



Y

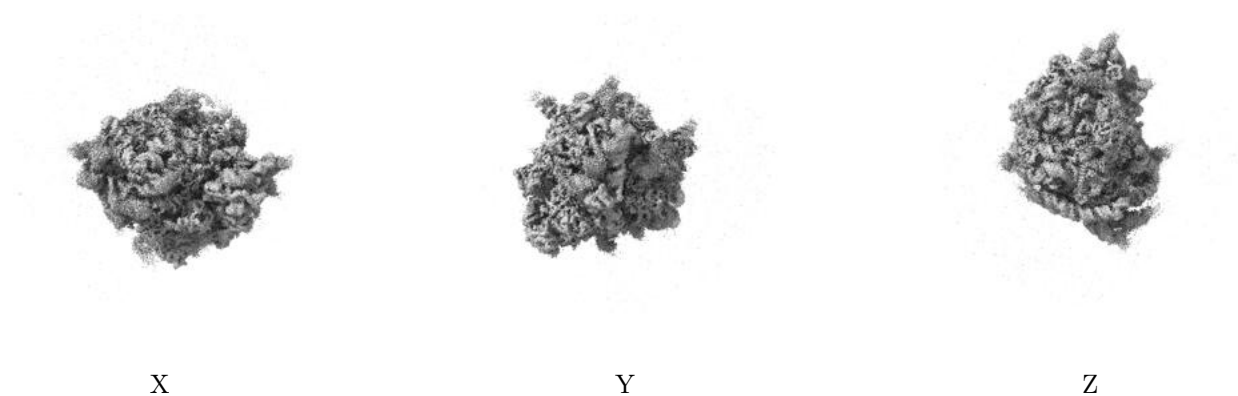


Z

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

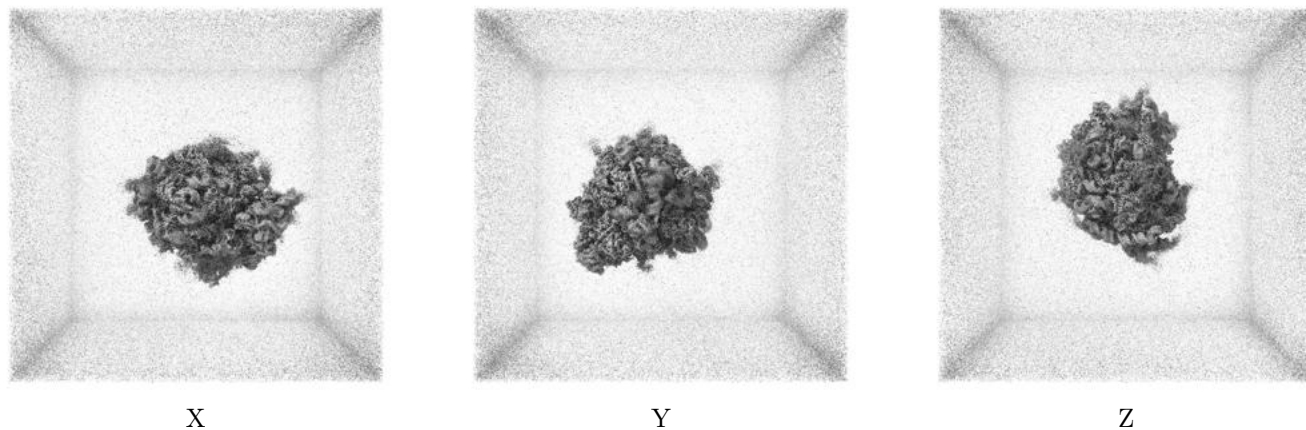
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

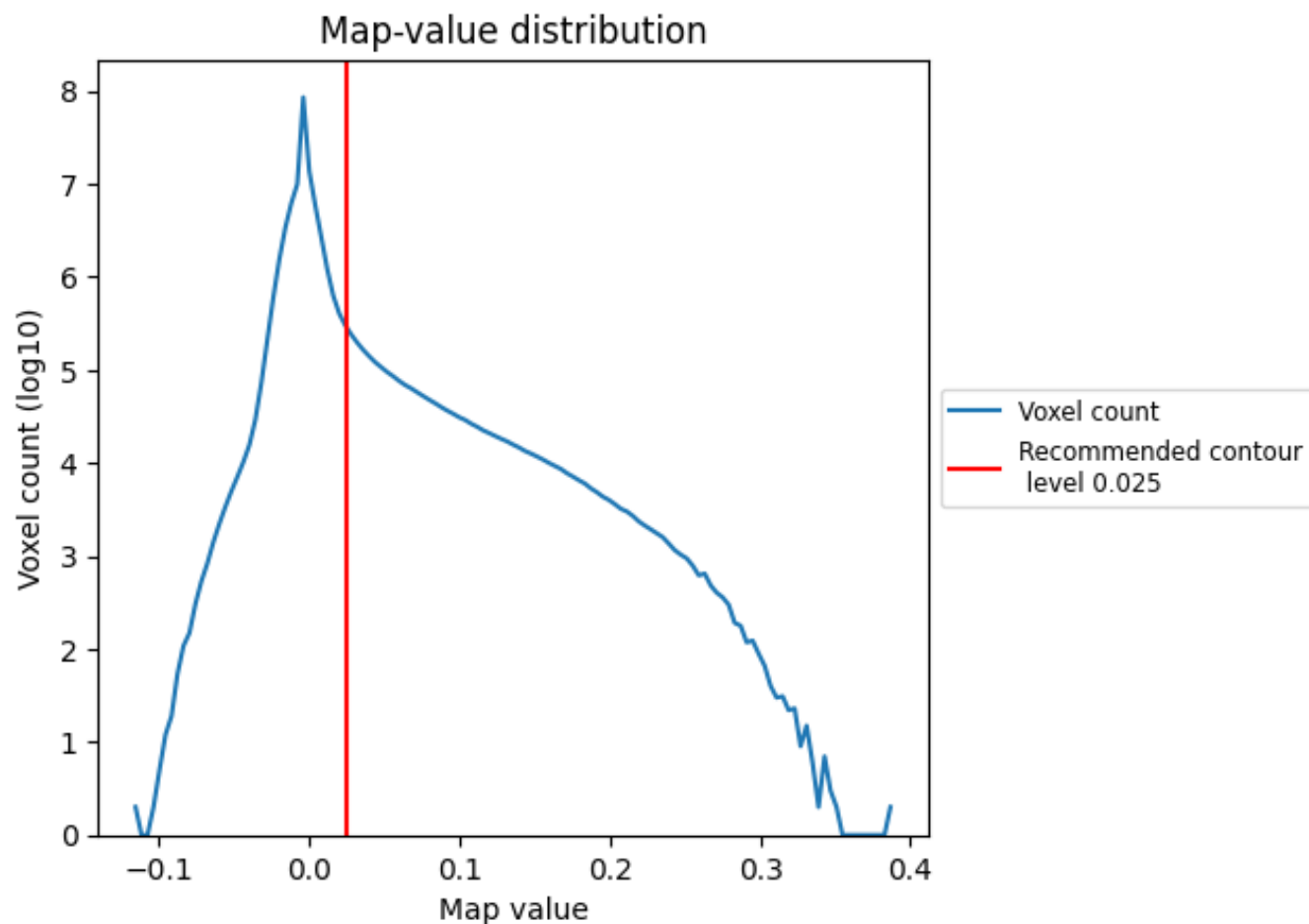
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

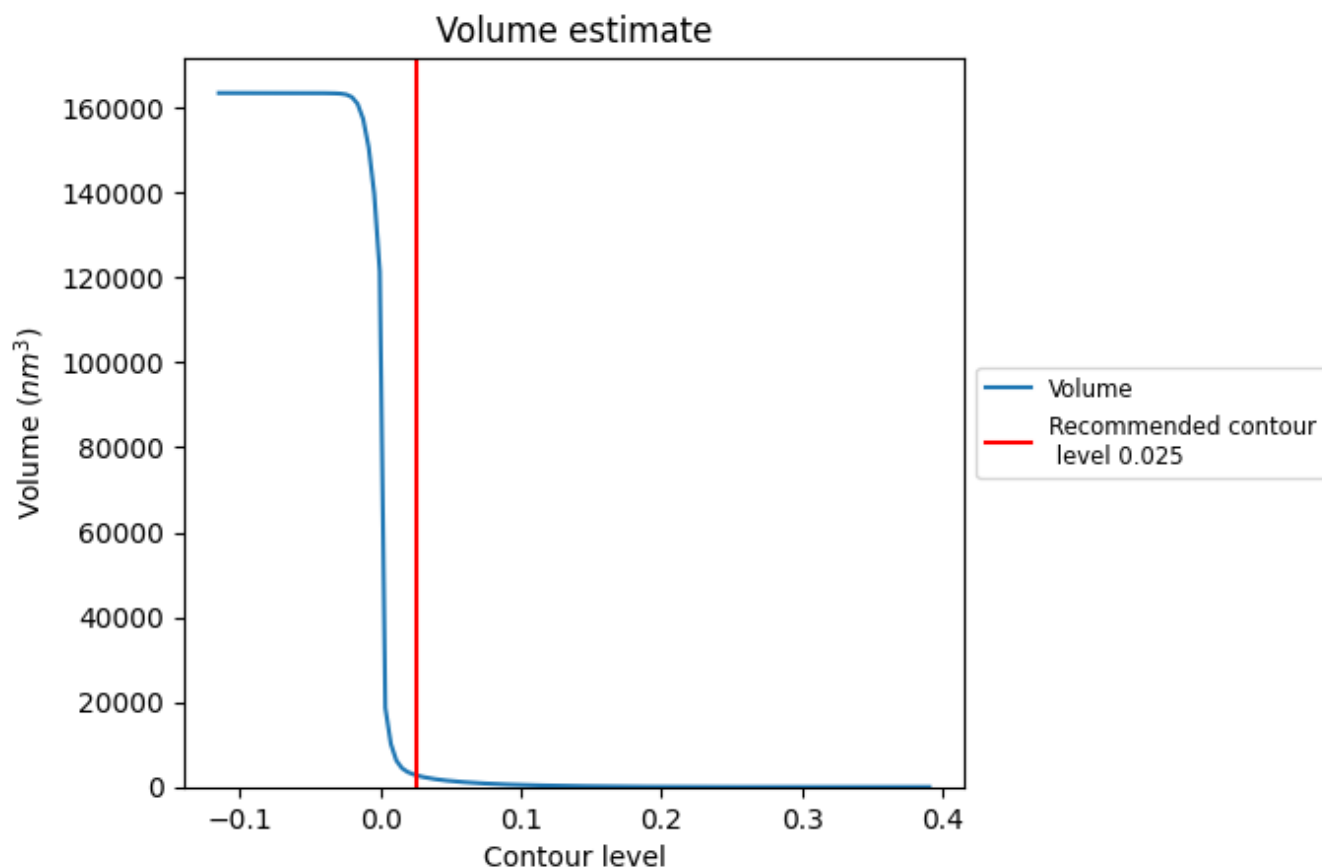
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

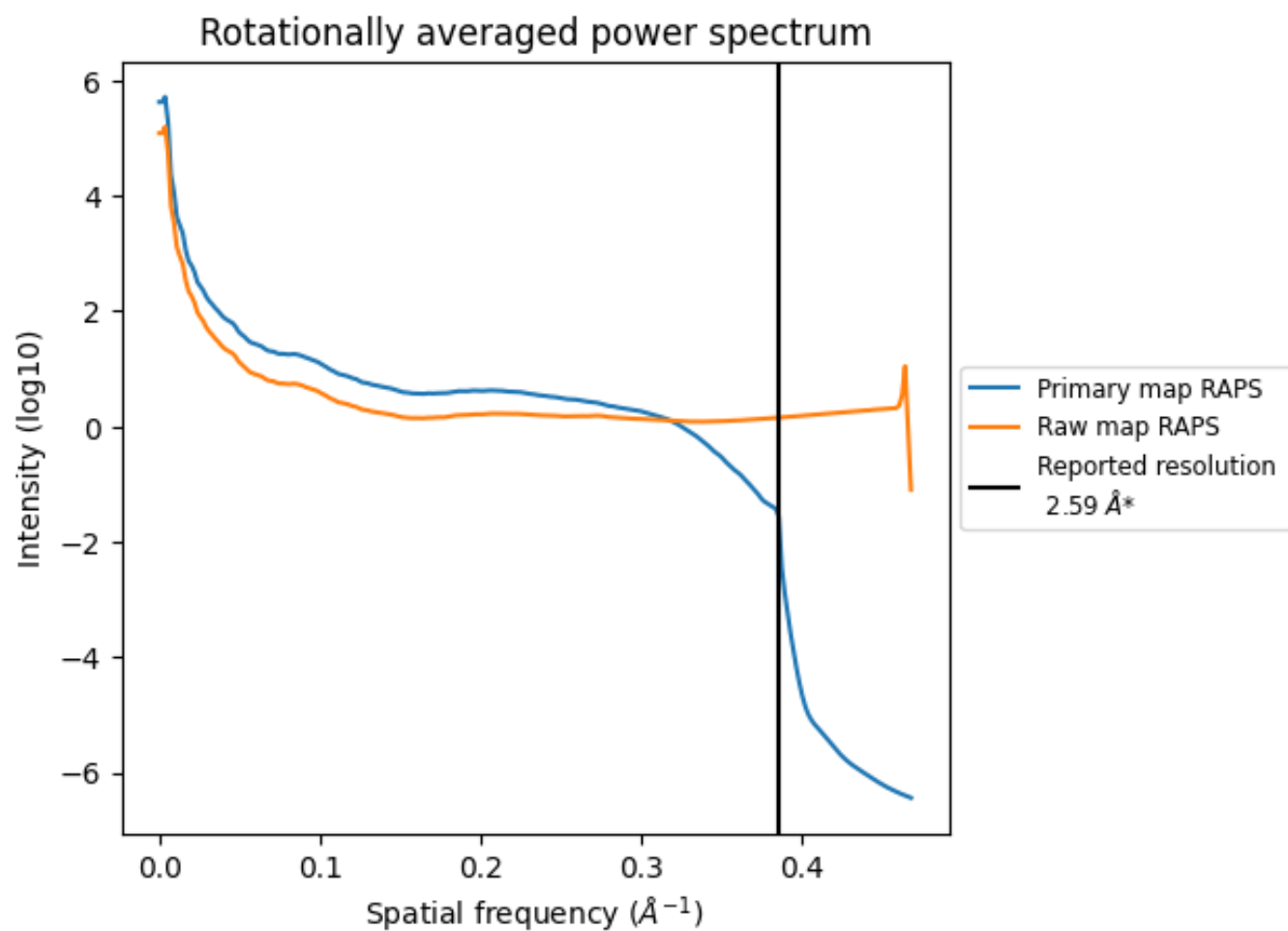
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2818 nm³; this corresponds to an approximate mass of 2545 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 ⓘ

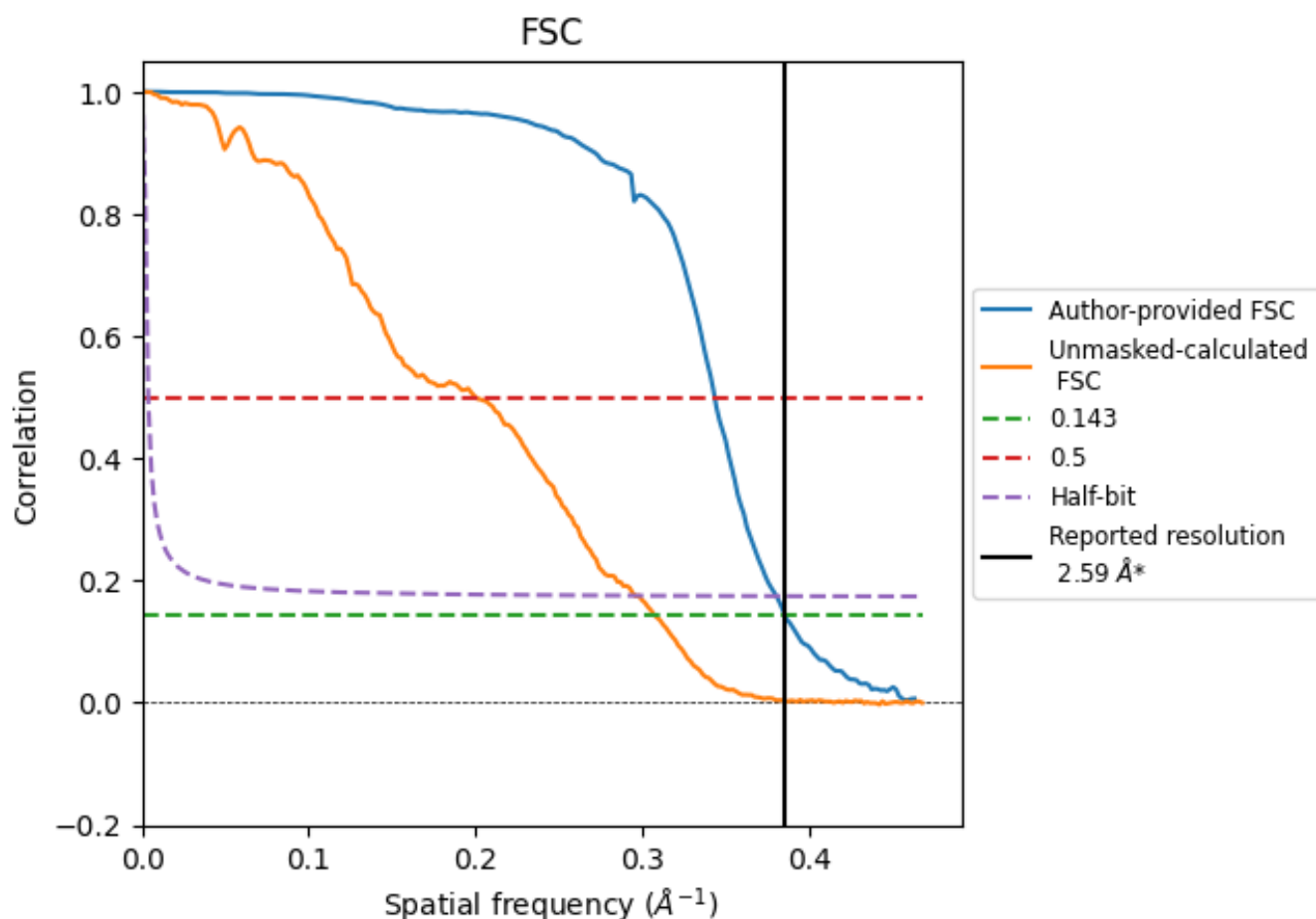


*Reported resolution corresponds to spatial frequency of 0.386 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.386 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

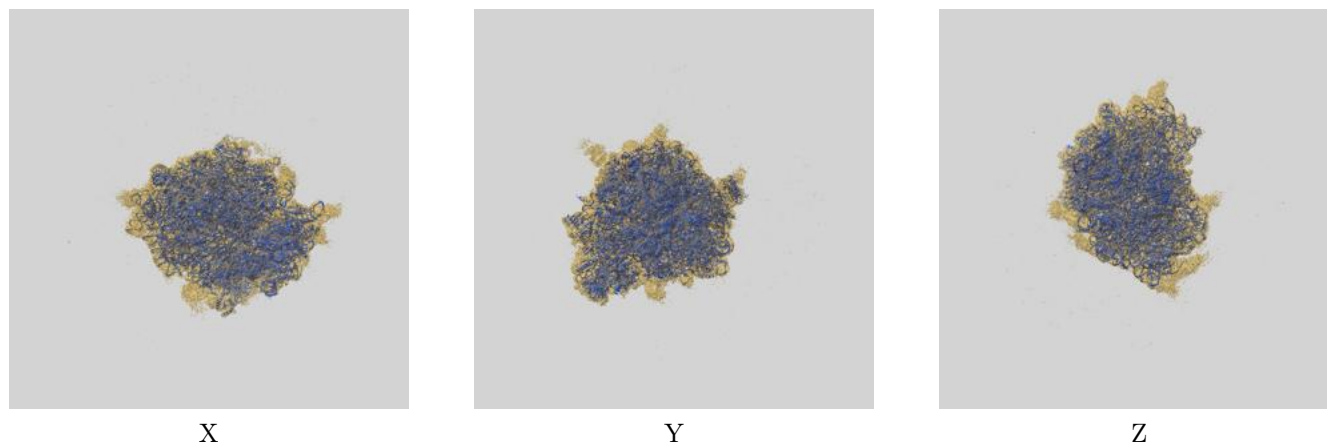
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.59	-	-
Author-provided FSC curve	2.59	2.91	2.63
Unmasked-calculated*	3.25	5.00	3.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.59 by more than 10 %

9 Map-model fit [i](#)

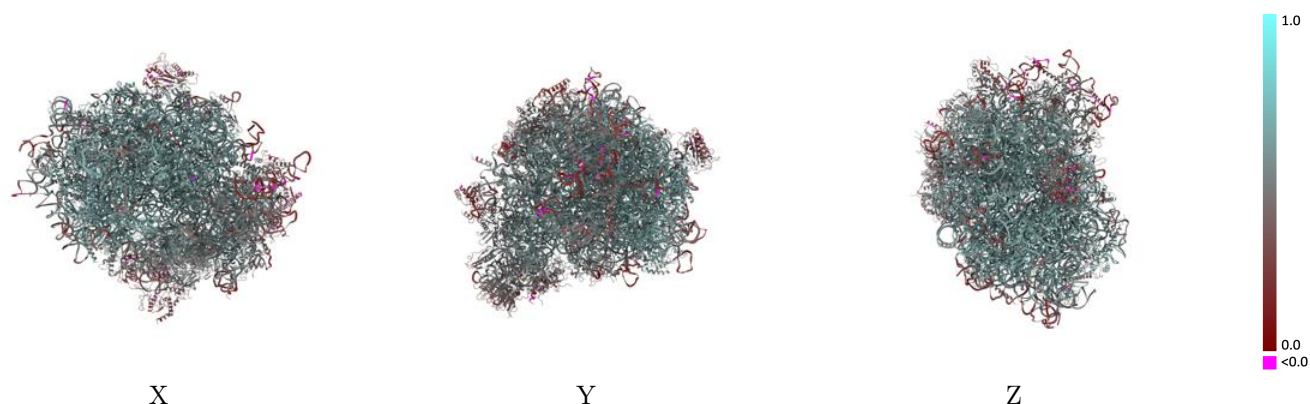
This section contains information regarding the fit between EMDB map EMD-71339 and PDB model 9P7E. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



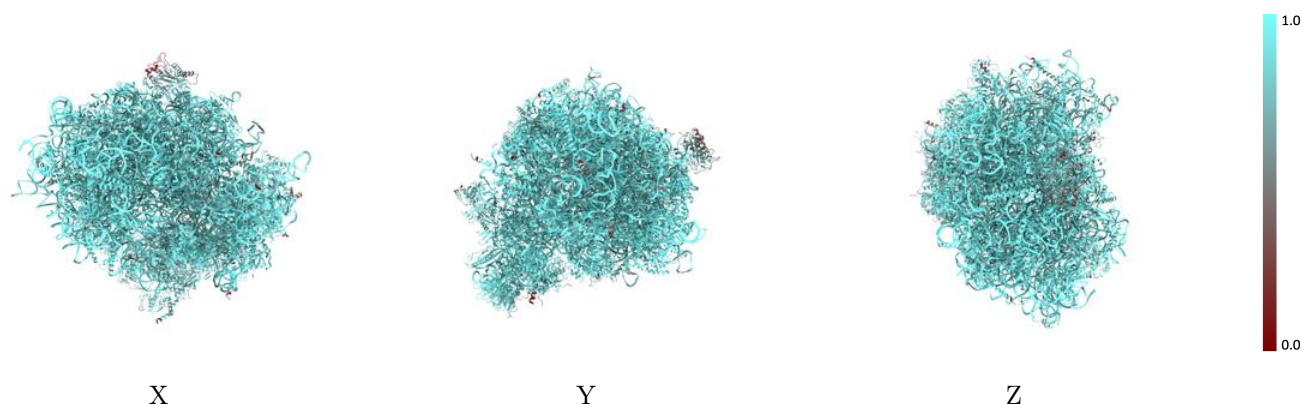
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



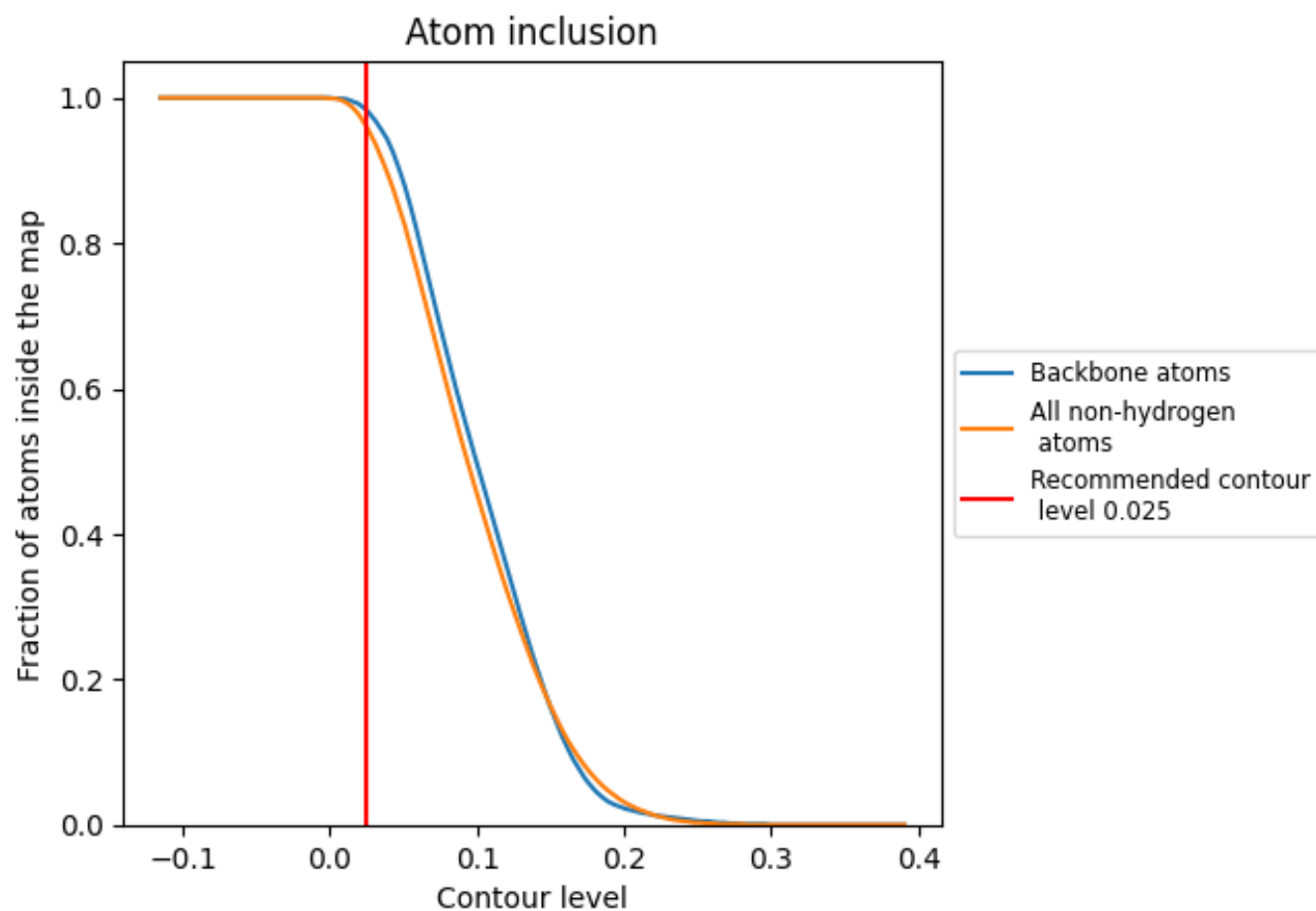
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.9600	 0.5430
CA	 0.6100	 0.3490
CB	 0.9060	 0.5110
CD	 0.9230	 0.4910
CI	 0.7570	 0.4680
Et	 0.9750	 0.4720
L5	 0.9850	 0.5700
L7	 0.9980	 0.6100
L8	 0.9900	 0.5890
LA	 0.9890	 0.6210
LB	 0.9690	 0.6090
LC	 0.9790	 0.6100
LD	 0.9660	 0.5810
LE	 0.9410	 0.5450
LF	 0.9880	 0.6120
LG	 0.9380	 0.5590
LH	 0.9790	 0.6010
LI	 0.9710	 0.6110
LJ	 0.9370	 0.5470
LL	 0.9440	 0.5850
LM	 0.9820	 0.5960
LN	 0.9980	 0.6360
LO	 0.9840	 0.6140
LP	 0.9840	 0.6190
LQ	 0.9920	 0.6310
LR	 0.9310	 0.5520
LS	 0.9890	 0.6240
LT	 0.9690	 0.5980
LU	 0.9480	 0.5270
LV	 0.9770	 0.6130
LW	 0.8840	 0.4600
LX	 0.9680	 0.5980
LY	 0.9800	 0.5970
LZ	 0.9870	 0.5850
La	 0.9890	 0.6310



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Chain	Atom inclusion	Q-score
Lb	 0.9360	 0.5490
Lc	 0.9510	 0.5630
Ld	 0.9640	 0.5960
Le	 0.9890	 0.6260
Lf	 0.9920	 0.6300
Lg	 0.9790	 0.6040
Lh	 0.9690	 0.5930
Li	 0.9640	 0.5860
Lj	 0.9910	 0.6220
Lk	 0.9120	 0.5440
Ll	 0.9860	 0.6180
Lm	 0.9740	 0.6140
Ln	 0.9860	 0.5940
Lo	 0.9630	 0.6100
Lp	 0.9770	 0.6080
Lr	 0.9830	 0.6150
Ls	 0.8940	 0.4490
Lt	 0.7040	 0.2570
S2	 0.9870	 0.5070
SA	 0.9110	 0.5020
SB	 0.9170	 0.5070
SC	 0.9680	 0.5530
SD	 0.9230	 0.4950
SE	 0.9550	 0.5160
SF	 0.8750	 0.4230
SG	 0.8830	 0.4350
SH	 0.8730	 0.4390
SI	 0.9170	 0.4940
SJ	 0.9320	 0.5220
SK	 0.9130	 0.4480
SL	 0.9150	 0.5300
SM	 0.7450	 0.2710
SN	 0.9610	 0.5370
SO	 0.9230	 0.5030
SP	 0.9090	 0.4450
SQ	 0.9020	 0.4600
SR	 0.8780	 0.4510
SS	 0.8670	 0.4040
ST	 0.9170	 0.4210
SU	 0.8990	 0.4490
SV	 0.9370	 0.5180
SW	 0.9750	 0.5610

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Chain	Atom inclusion	Q-score
SX	 0.9710	 0.5750
SY	 0.8980	 0.4590
SZ	 0.8200	 0.3790
Sa	 0.9480	 0.5440
Sb	 0.9080	 0.4900
Sc	 0.8330	 0.3930
Sd	 0.9640	 0.5240
Se	 0.9010	 0.5110
Sf	 0.8350	 0.3280
Sg	 0.9030	 0.4160