



Full wwPDB EM Validation Report ⓘ

Jul 6, 2026 – 08:32 PM EDT

PDB ID : 9PKB / pdb_00009pkb
EMDB ID : EMD-71690
Title : In situ HHT and CHX treated human hibernating state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-07-14
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

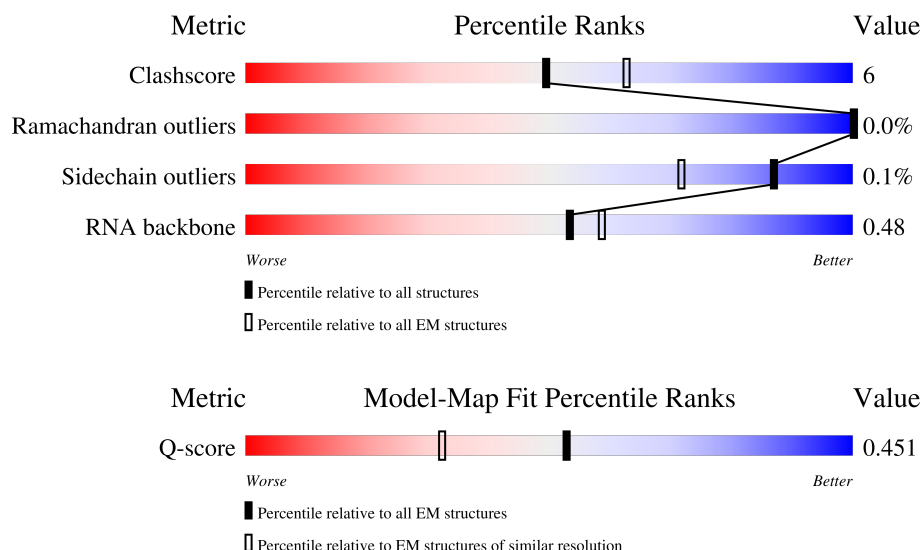
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.05 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.



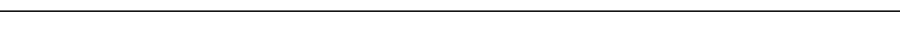
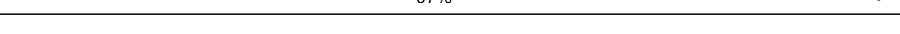
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13971 (2.55 - 3.55)

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	55	
2	CI	31	
3	L5	3655	

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

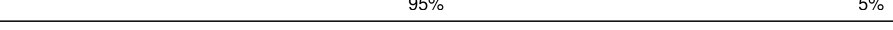
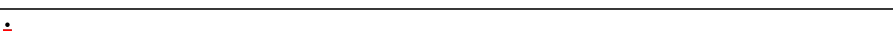
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Mol	Chain	Length	Quality of chain
29	LY	134	
30	LZ	135	
31	La	147	
32	Lb	121	
33	Lc	98	
34	Ld	107	
35	Le	128	
36	Lf	109	
37	Lg	114	
38	Lh	122	
39	Li	102	
40	Lj	86	
41	Lk	69	
42	Ll	50	
43	Lm	52	
44	Ln	24	
45	Lo	105	
46	Lp	91	
47	Lr	125	
48	Ls	196	
49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

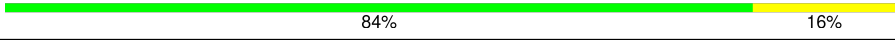
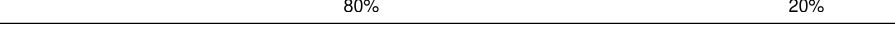
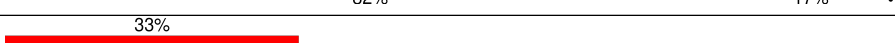
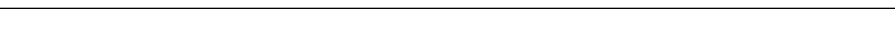
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Mol	Chain	Length	Quality of chain
54	SG	237	
55	SH	189	
56	SI	206	
57	SJ	185	
58	SL	153	
59	SN	150	
60	SO	140	
61	SV	83	
62	SW	129	
63	SX	141	
64	SY	131	
65	Sa	102	
66	Sb	83	
67	Se	58	
68	S2	1740	
69	SR	135	
70	SD	227	
71	SF	189	
72	SK	98	
73	SM	122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

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Mol	Chain	Length	Quality of chain
79	SZ	75	 80%20%
80	Sc	64	 78%22%
81	Sd	55	 84%16%
82	Sf	67	 82%18%
83	Sg	313	 80%20%
84	CB	856	 82%17%.
85	CA	356	 33%79%21%.

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 226615 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 Isoform 2 of SERPINE1 mRNA-binding protein 1.

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

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CD	183	ASP	-	expression tag	UNP Q8NC51
CD	184	GLY	-	expression tag	UNP Q8NC51
CD	283	LEU	-	insertion	UNP Q8NC51
CD	284	ASP	GLU	conflict	UNP Q8NC51
CD	285	GLU	SER	conflict	UNP Q8NC51
CD	286	TRP	PRO	conflict	UNP Q8NC51
CD	288	ALA	TYR	conflict	UNP Q8NC51
CD	291	ASN	LYS	conflict	UNP Q8NC51
CD	292	LYS	GLN	conflict	UNP Q8NC51
CD	293	ASP	-	expression tag	UNP Q8NC51

- Molecule 2 is a protein called Transcription factor BTF3.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LE	240	Total	C	N	O	S	0	0
			1935	1242	368	321	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LI	205	Total	C	N	O	S	0	0
			1658	1052	318	274	14		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

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

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

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

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

- Molecule 25 is a protein called Heparin-binding protein HBp15.

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

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

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

- Molecule 27 is a protein called Ribosomal protein L24.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

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

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

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

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

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

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

- Molecule 32 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 68 is a RNA chain called 18S rRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 84 is a protein called Elongation factor 2.

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

- Molecule 85 is a protein called Proliferation-associated protein 2G4.

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

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

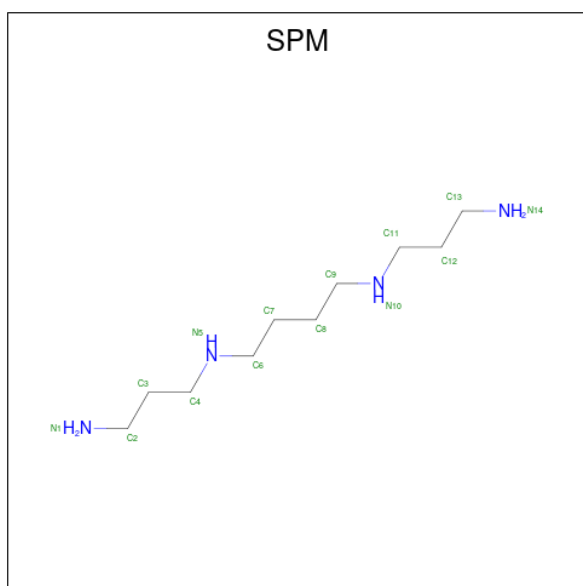
Mol	Chain	Residues	Atoms		AltConf
86	L5	179	Total	Mg	0
			179	179	
86	L7	3	Total	Mg	0
			3	3	
86	L8	4	Total	Mg	0
			4	4	
86	LA	1	Total	Mg	0
			1	1	
86	LP	1	Total	Mg	0
			1	1	
86	LV	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
86	Le	1	Total	Mg	0
			1	1	
86	Lj	1	Total	Mg	0
			1	1	
86	S2	27	Total	Mg	0
			27	27	

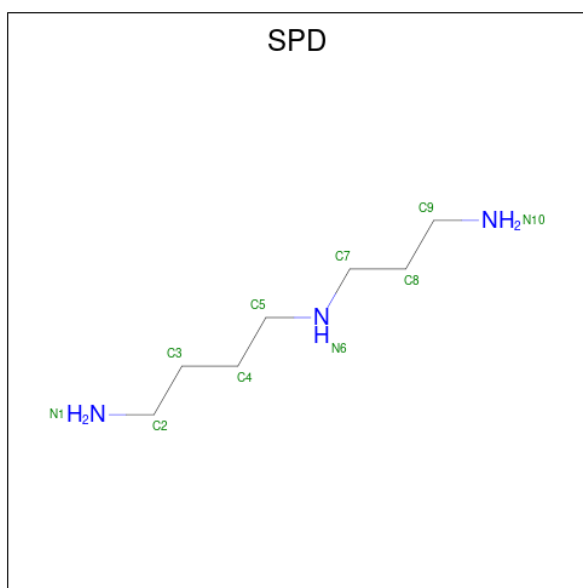
- Molecule 87 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



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

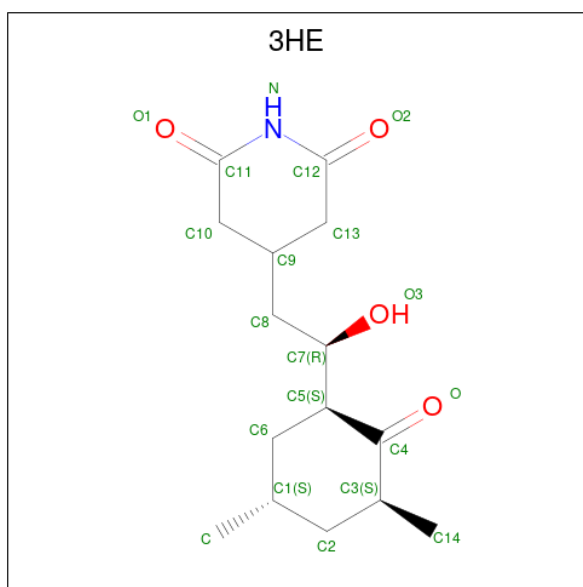
- Molecule 88 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of

Interest" by depositor).



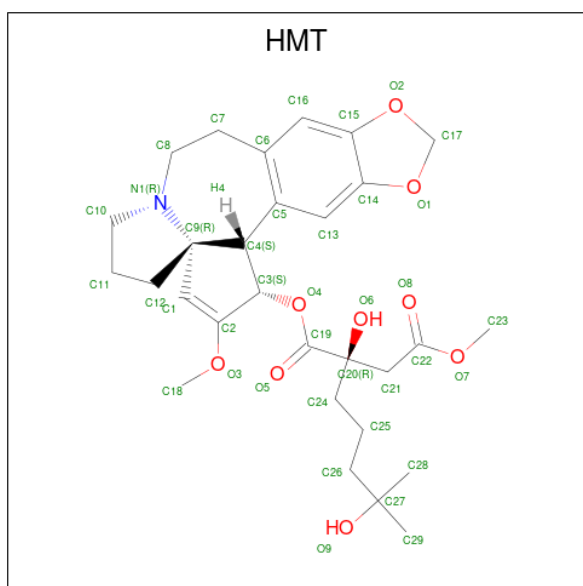
Mol	Chain	Residues	Atoms			AltConf
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	
88	L5	1	Total	C	N	0
			10	7	3	

- Molecule 89 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: C₁₅H₂₃NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
89	L5	1	Total	C	N	O	0
			20	15	1	4	

- Molecule 90 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptanoyl]cephalotaxine (CCD ID: HMT) (formula: $C_{29}H_{39}NO_9$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
90	L5	1	Total	C	N	O	0
			39	29	1	9	

- Molecule 91 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by

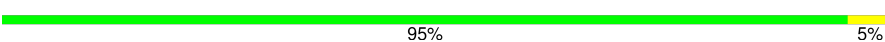
depositor).

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

3 Residue-property plots

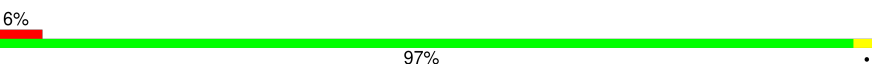
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

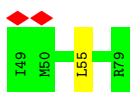
- Molecule 1: Isoform 2 of SERPINE1 mRNA-binding protein 1

Chain CD: 



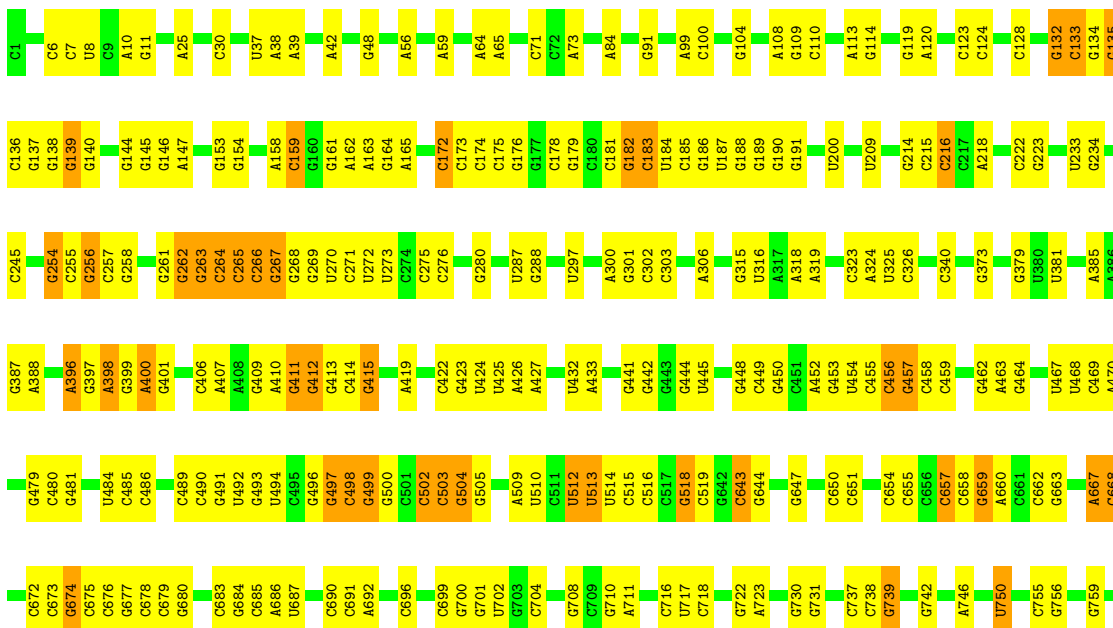
- Molecule 2: Transcription factor BTF3

Chain CI: 



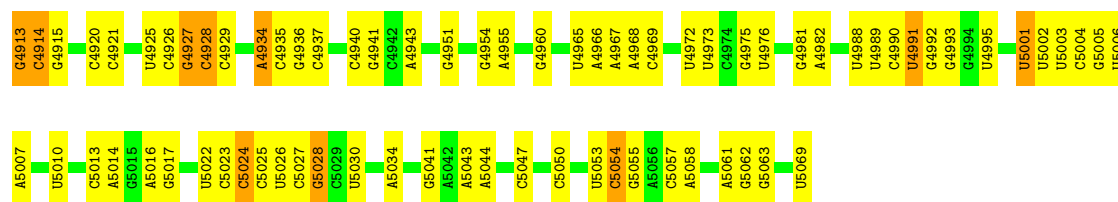
- Molecule 3: 28S rRNA

Chain L5: 



C2558	C2469	C2335	G1948	G1836	G1741	C1628	C1501	A1397	A1294	C904
C2559	C2470	G2336	G1951	A1837	A1742	A1631	G1502	A1398	C1295	C905
C2560	C2471	C2340	G1952	G1842	A1743	A1632	G1503	G1404	G1296	C906
C2563	G2474	G2348	A1962	G1846	G1750	A1633	G1504	G1405	C1297	C907
C2564	G2475	C2351	G1974	C1847	A1751	A1634	C1505	G1406	C1298	G908
C2565	C2476	C2358	G1975	C1848	G1752	C1640	A1508	G1407	G1299	A909
C2568	C2478	G2359	G1976	G1855	U1757	G1641	C1509	G1408	G1301	G910
C2569	G2479	G2360	G1977	G1858	G1758	C1645	U1510	U1410	C1304	U913
C2570	G2480	A2361	C1978	U1859	G1759	A1646	U1511	C1411	C1305	U914
C2571	G2481	G2362	A1979	U1860	U1760	G1654	U1512	C1414	C1306	A915
C2572	G2482	U2363	G1980	U1861	G1761	G1655	U1513	G1415	A1307	C916
C2573	A2483	A2364	G1981	U1862	C1762	C1661	A1515	G1416	C1308	C917
C2583	U2484	G2365	A1982	U1866	G1763	C1662	G1516	C1417	C1309	C918
C2586	G2485	A2374	A1983	U1867	G1764	C1663	A1524	A1420	G1316	C919
C2587	G2486	C2381	G1984	G1869	A1765	A1669	A1534	C1431	U1317	C1082
C2588	G2487	A2382	G1985	C1870	A1766	A1676	U1535	G1432	U1318	C920
C2589	C2488	C2383	A1986	A1871	A1767	U1677	U1536	C1437	C1322	U1083
C2606	G2489	U2384	G1987	U1876	G1769	U1683	U1537	U1438	A1323	C1084
C2607	G2490	G2385	C1988	G1877	A1770	U1684	U1538	C1439	C1324	C922
C2608	G2491	U2386	C1989	G1878	U1773	A1684	G1539	C1442	A1326	C923
C2609	G2492	G2387	C1990	C1879	U1774	G1685	G1540	C1443	C1327	C924
C2610	G2493	A2388	G1991	C1880	C1774	G1686	C1541	A1444	G1328	C925
C2611	G2494	C2389	A1992	C1881	U1775	U1687	A1547	G1445	C1329	G926
C2612	U2495	A2390	G1993	C1882	U1776	U1688	A1548	C1446	C1332	A932
C2627	G2496	C2391	C1994	U1879	U1777	G1689	A1563	U1447	A1333	G933
C2632	U2500	A2392	G1995	C1883	U1778	U1690	A1564	C1458	A1334	C934
C2633	C2501	G2393	A1996	G1884	U1779	C1694	U1565	C1459	A1337	A935
C2634	C2502	C2394	G1997	C1885	A1780	U1695	C1566	C1460	A1338	C936
C2635	C2503	G2395	A1998	G1886	U1781	U1696	G1574	C1461	C1339	U937
C2638	C2504	A2396	G1999	C1887	U1782	U1697	G1575	A1462	C1340	A944
U2639	C2505	U2397	G2000	U1906	U1783	U1698	U1577	C1463	A1384	A956
G2640	G2400	C2398	U2001	A1907	U1784	U1699	U1578	C1464	G1355	G957
A2641	C2401	A2401	C2011	A1908	A1787	U1700	U1579	C1468	U1356	G958
C2644	C2411	C2411	C2016	A1909	U1792	C1702	U1582	C1469	C1357	G959
A2647	A2412	A2412	A2017	G1912	U1802	C1703	U1586	C1470	G1358	G961
G2648	G2416	G2416	U2020	G1916	G1803	C1704	G1586	U1471	G1359	G962
G2649	G2417	G2417	G2021	A1917	A1804	C1705	U1591	C1472	C1365	G963
C2653	G2421	G2421	G2024	U1918	A1805	C1706	U1596	C1478	G1370	A964
C2654	C2422	A2423	A2025	U1919	G1806	C1707	U1597	C1479	G1377	G965
C2655	G2423	G2423	A2026	U1920	C1807	U1708	U1598	C1480	C1378	A966
U2656	U2424	U2424	G2046	C1921	C1808	C1709	U1599	U1483	C1379	C967
C2663	U2425	U2425	A2047	G1922	U1810	C1710	U1599	U1484	U1381	C968
C2664	G2448	G2448	U2048	G1925	G1811	C1711	U1599	C1495	G1387	G970
C2665	A2449	A2449	G2052	G1931	C1812	C1712	U1599	G1496	C1287	C974
U2666	G2450	G2450	G2055	U1932	U1813	C1713	U1599	G1497	C1288	G978
U2667	A2453	A2453	G2056	U1933	U1814	C1714	U1599	C1498	C1289	C979
C2668	C2458	C2458	G2057	U1934	U1815	C1715	U1599	C1499	C1290	U982
C2669	C2464	C2464	G2058	U1935	U1816	C1716	U1599	C1500	C1291	
C2672	U2465	U2465	G2059	U1936	G1824	C1717	U1599	C1501	C1292	
C2673	U2466	U2466	G2060	G1940	A1825	C1718	U1599	C1502	C1293	
C2674	C2467	C2467	C2068	A1941	G1826	C1719	U1599	C1503		
C2675	U2554	U2554	A2069	A1942	G1827	C1720	U1599	C1504		
C2676	C2555	C2555	G2076	A1943	U1834	C1721	U1599	C1505		

A4723	A4611	C4519	G4391	G4291	G4196	G4104	C3919	U3844	G3754	A3648	C2898	U2761	C2670
A4724	A4616	C4520	G4392	A4292	A4203	A4105	U3920	U3848	G3755	G3661	C2899	G2762	C2671
A4727	A4617	U4521	G4393	U4293	A4203	G4106	U3921	A3849	A3756	A3662	U2900	A2763	C2672
U4728	A4618	A4522	A4394	U4294	U4208	G4108	A3923	C3850	G3757	A3663	G2901	A2764	
C4733	G4619	A4523	G4401	U4296	G4209	U4111	C3924	C3851	A3760	A3664	G2902	A2765	A2675
A4734	U4620	A4524	C4402	G4297	A4212	C4112	U3925	A3852		G3665	U2904	A2766	
G4735	C4621	U4525	U4403	A4298		G4113	U3930	U3853	U3764	C3666	G2905		G2677
G4736	A4622	U4526	C4421	U4299	A4220	U4113	C3931	C3854	G3765	C3667	C2906	U2769	U2687
G4737	G4623	U4530	A4422	U4301	A4221	C4114	U3932	C3855	A3766		G2907	G2770	G2688
C4738	U4531	U4532	C4422	U4301	G4222	C4115	A3933	A3856		C3670	U2908	G2773	
G4739	G4430	A4304	G4430	A4304	G4225	C4119	C3937	A3860	U3770	C3673	G3585	U2780	U2691
G4740	U4431	G4305	U4431	G4305	G4225		C3938	A3861	U3772	G3674		G2781	U2692
G4741	C4432	U4306	G4432	U4306	U4227	G4122		A3862	U3773			G2693	G2693
G4742	G4433	A4311	G4433	A4311	U4227				A3774			A2787	G2694
G4743	U4438	A4312	U4438	A4312	C4228	C4126	A3942	A3867	A3775	G3684	G3588	U2788	A2695
A4744	U4439	A4313	A4439	A4313	U4229	A4127	G3944	C3868	A3776	C3885	C3591	A2789	A2696
G4745	U4442	C4314	A4442	C4314	U4232		A3945	C3870	G3777	A3692		U2790	
					A4233	G4139	G3946	C3871	U3778				G2703
G4754	A4651	U4548	C4447	G4319	A4234	C4140	A3947	A3872	C3782	U3695	C3594	A2806	G2704
G4757	G4652	G4549	A4448	G4320	U4235	G4141	A3952	G3879	U3805	C3696	U3595	G2705	G2706
U4758	A4653	U4552	A4449	G4321		C4142	A3953	C3881	G3806	U3697	A3596	A2815	U2707
G4760	U4654			G4322		G4143	A3954	C3882	U3807	C3698	C3597	G2816	U2708
G4761	U4655			A4333		G4144	A3955	C3883	A3808	C3699	C3598	A2709	U2708
				G4334		C4145	A4056	U3884	G3710	C3700	C3600	G2710	G2710
G4765	A4656	U4558	C4453	G4330	A4239	C4146	A4057	A3885	U3811	C3701		G2826	G2711
		A4559	G4454	G4331	G4240	G4147	U4058		G3814			G2827	G2712
G4766	C4670	U4560	G4455	A4332		G4148	A4059	A3890	U3814			U2828	
A4672	A4671	C4561	A4456	C4336	C4243	G4149	A4060	A3891	A3817	A3717	G3615	A2835	G2724
U4673	U4672	U4562	U4457	A4337	A4244	C4150	A4061	C3892	U13818	A3718	G3616	A2836	A2725
C4674	C4673	U4563	C4337	G4338	G4245		U4062	C3893	G3819	A3719	G3617	U2837	G2726
		A4564	G4338			G4151	U4063	A3894	G3820	G3720	A3624	U2839	G2727
G4775	G4678	U4567	U4460	G4344	G4249	C4153	A4064	C3896	A3821	U3721	G3627	G2855	U2718
				A4345	A4251	G4154	U4065	G3897	U3822	G3722	A3628	G2731	G2731
G4689	A4688	U4571	A4464	C4346		G4155		C3898	G3823	A3723	A3629	G2732	G2732
		A4572	U4465	A4348	G4254	C4156	U4068	G3899	A3824			G2859	C2733
G4863	A4681	G4573	C4466	C4349	A4257	C4160	U4069	G3900	A3825	A3726	C3633	C2860	
		U4574	A4467	C4350	U4258	G4161	U4070	A3901	C3826	A3727	G3634	C2861	G2739
G4870	U4685	U4575	U4471	U4353	C4259	C4162	A4068	A3906	A3830	A3732	A3635	A2870	U2740
C4871	A4687	U4576	U4475	U4354	U4260	U4163	C4069	A3907	U3831	A3733	C3636	A2743	G2742
	U4688	U4577	G4475	U4355	G4261	C4164	U4090	A3908	C3833	A3736	U3637	A2744	A2745
G4875	U4689	U4578	C4475	U4356	C4262	A4170	G4095	A3912	C3837	A3737	U3639	A2746	
		U4579	U4481	U4361	G4262		C4096	U3915	U3838	G3744	U3641	G2749	G2749
U4881	G4694	U4584	U4482	A4363	C4263	U4174	C4097	G3916	U3839	A3745	U3644	A2885	G2750
U4882	C4695	U4585	U4488	G4364	U4264	G4175	A4097	A3917	U3840	A3746	U3645	G2754	
C4883		G4586		C4365	U4265	G4180	A4098	A3918	C3841	A3748	A3646	C2892	G2754
									C3842			G2897	G2760
G4889	U4699	U4589	U4493	G4370	A4268	G4183	U4071		C3843				
		A4589				G4184	G4076						
C4895	A4707	A4590	U4498	G4373	A4273		C4088	A3908	U3832				
G4896	U4708	U4591	A4499	G4377	A4275	G4187	C4089	C3910	C3833				
		C4592	U4500	G4378	G4276	U4188	U4090	U3912					
G4899	C4710	C4593	U4501	A4379	G4277	U4189			C3837				
C4900	C4711	U4594	U4507	C4387	C4278	U4190			U3839				
G4901	G4712	G4595	C4508	A4388	A4279	C4191			U3840				
				C4389	A4281	A4192			C3841				
G4910	G4713	U4600	U4512	A4602		A4193			C3842				
A4911		U4601	A4513						C3843				
G4912	G4719												



- Molecule 4: 5S rRNA

Chain L7: 77% 22%



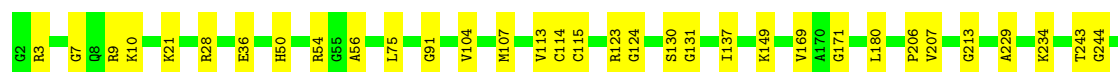
- Molecule 5: 5.8S rRNA

Chain L8: 62% 37%



- Molecule 6: 60S ribosomal protein L8

Chain LA: 87% 13%



- Molecule 7: Large ribosomal subunit protein uL3

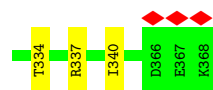
Chain LB: 89% 11%



- Molecule 8: 60S ribosomal protein L4

Chain LC: 91% 9%





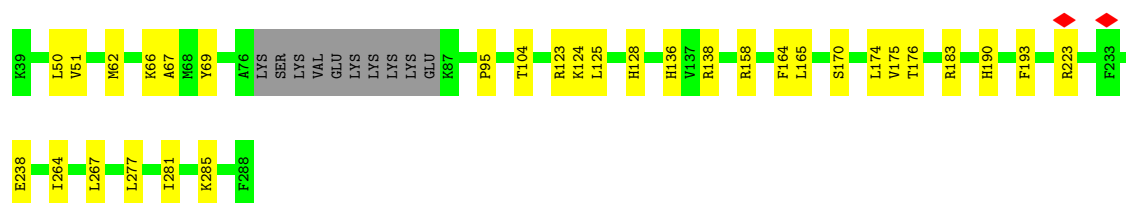
- Molecule 9: Large ribosomal subunit protein uL18

Chain LD: 90% 10%



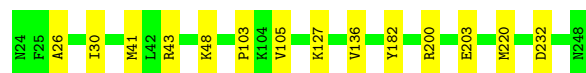
- Molecule 10: Large ribosomal subunit protein eL6

Chain LE: 84% 12%



- Molecule 11: 60S ribosomal protein L7

Chain LF: 94% 6%



- Molecule 12: 60S ribosomal protein L7a

Chain LG: 91% 9%



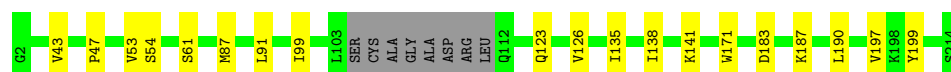
- Molecule 13: 60S ribosomal protein L9

Chain LH: 89% 11%



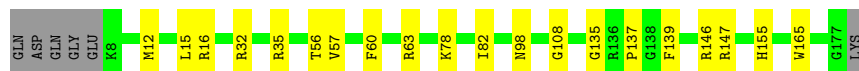
- Molecule 14: Ribosomal protein uL16-like

Chain LI: 87% 9%

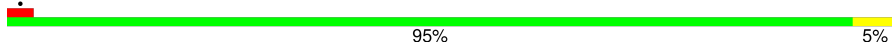


- Molecule 15: 60S ribosomal protein L11

Chain LJ:  85% 11%



- Molecule 16: Large ribosomal subunit protein eL13

Chain LL:  95% 5%

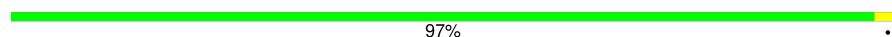


- Molecule 17: 60S ribosomal protein L14

Chain LM:  92% 8%



- Molecule 18: 60S ribosomal protein L15

Chain LN:  97%

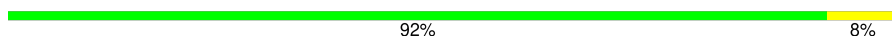


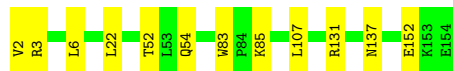
- Molecule 19: 60S ribosomal protein L13a

Chain LO:  88% 12%

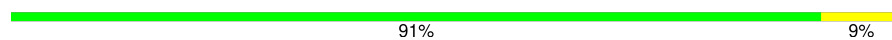


- Molecule 20: 60S ribosomal protein L17

Chain LP:  92% 8%

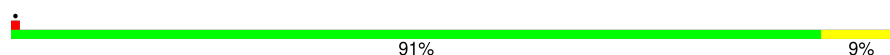


- Molecule 21: 60S ribosomal protein L18

Chain LQ:  91% 9%



- Molecule 22: 60S ribosomal protein L19

Chain LR:  91% 9%

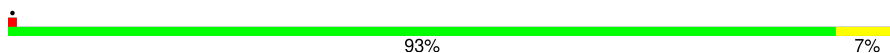


- Molecule 23: 60S ribosomal protein L18a

Chain LS:  92% 8%



- Molecule 24: 60S ribosomal protein L21

Chain LT:  93% 7%

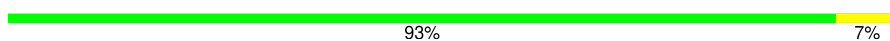


- Molecule 25: Heparin-binding protein HBp15

Chain LU:  88% 12%



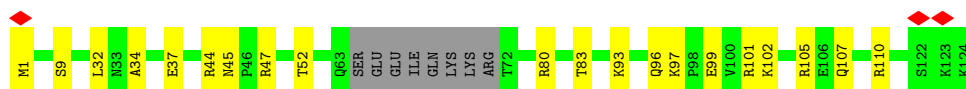
- Molecule 26: 60S ribosomal protein L23

Chain LV:  93% 7%

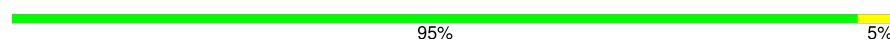


- Molecule 27: Ribosomal protein L24

Chain LW:  77% 16% 6%

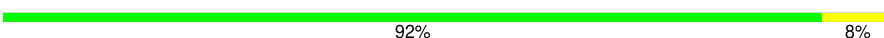


- Molecule 28: 60S ribosomal protein L23a

Chain LX:  95% 5%



• Molecule 29: 60S ribosomal protein L26

Chain LY:  92% 8%

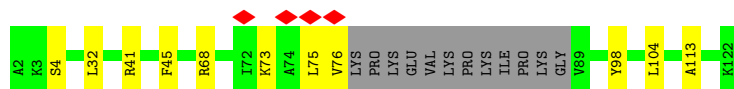
• Molecule 30: 60S ribosomal protein L27

Chain LZ:  86% 14%

• Molecule 31: 60S ribosomal protein L27a

Chain La:  91% 9%

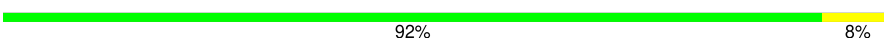
• Molecule 32: Large ribosomal subunit protein eL29

Chain Lb:  81% 9% 10%

• Molecule 33: 60S ribosomal protein L30

Chain Lc:  89% 11%

• Molecule 34: 60S ribosomal protein L31

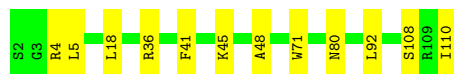
Chain Ld:  92% 8%

• Molecule 35: 60S ribosomal protein L32

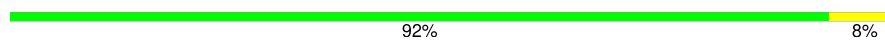
Chain Le:  92% 8%

- Molecule 36: 60S ribosomal protein L35a

Chain Lf:  89% 11%



- Molecule 37: 60S ribosomal protein L34

Chain Lg:  92% 8%

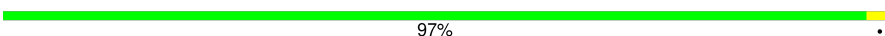


- Molecule 38: 60S ribosomal protein L35

Chain Lh:  84% 16%



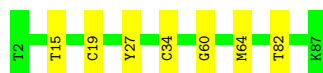
- Molecule 39: 60S ribosomal protein L36

Chain Li:  97% 3%



- Molecule 40: 60S ribosomal protein L37

Chain Lj:  92% 8%

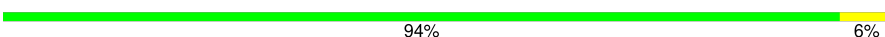


- Molecule 41: 60S ribosomal protein L38

Chain Lk:  84% 16%



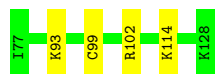
- Molecule 42: 60S ribosomal protein L39

Chain Ll:  94% 6%



- Molecule 43: Large ribosomal subunit protein eL40

Chain Lm:  92% 8%

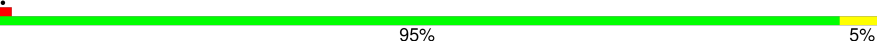


- Molecule 44: 60S ribosomal protein L41

Chain Ln:  88% 12%

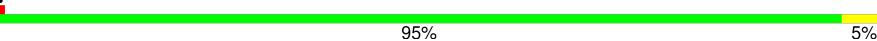


- Molecule 45: 60S ribosomal protein L36a

Chain Lo:  95% 5%

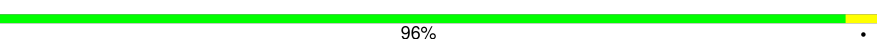


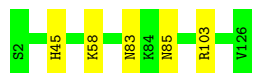
- Molecule 46: 60S ribosomal protein L37a

Chain Lp:  95% 5%



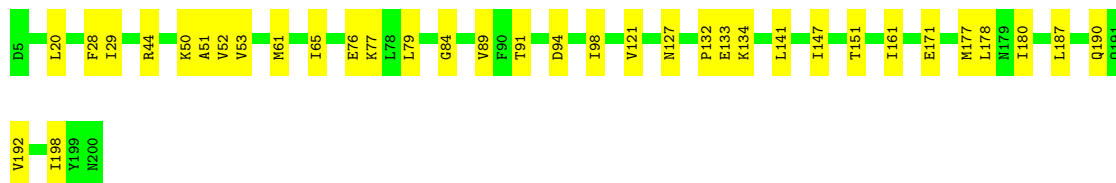
- Molecule 47: 60S ribosomal protein L28

Chain Lr:  96% 4%



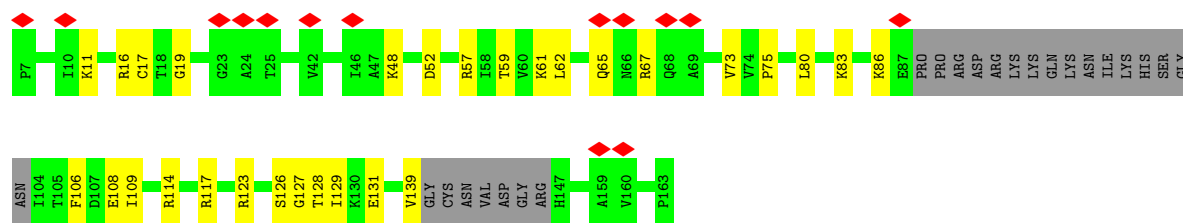
- Molecule 48: 60S acidic ribosomal protein P0

Chain Ls:  82% 18%



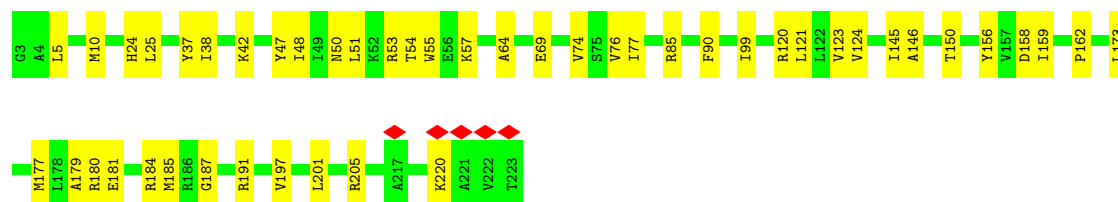
- Molecule 49: Large ribosomal subunit protein uL11

Chain Lt:  9% 67% 18% 15%



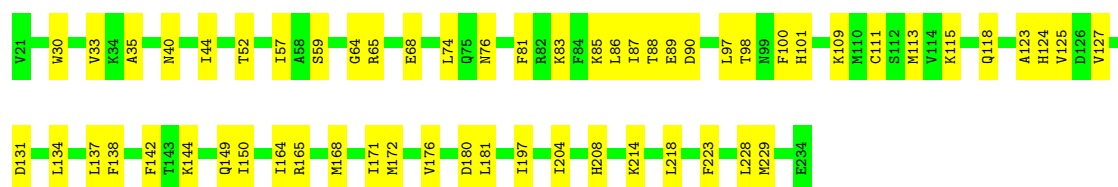
- Molecule 50: 40S ribosomal protein SA

Chain SA: 79% 21%



- Molecule 51: 40S ribosomal protein S3a

Chain SB: 73% 27%



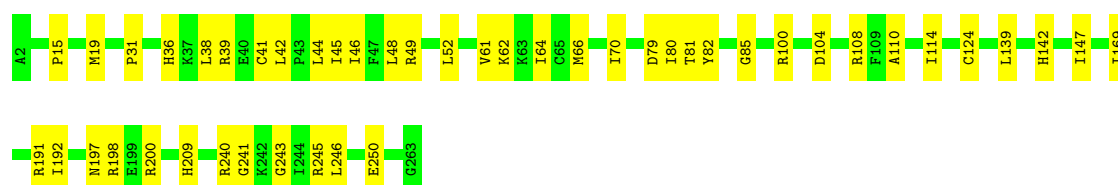
- Molecule 52: 40S ribosomal protein S2

Chain SC: 87% 12%



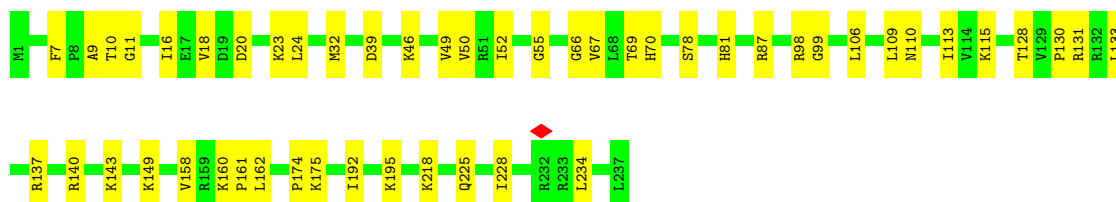
- Molecule 53: Small ribosomal subunit protein eS4, X isoform

Chain SE: 82% 18%



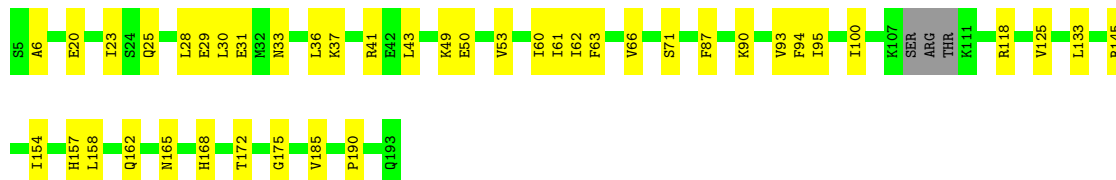
- Molecule 54: 40S ribosomal protein S6

Chain SG: 79% 21%



- Molecule 55: Small ribosomal subunit protein eS7

Chain SH: 76% 22%



- Molecule 56: 40S ribosomal protein S8

Chain SI: 81% 19%



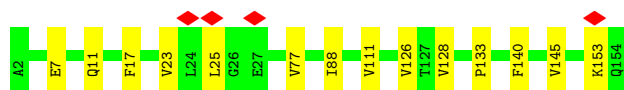
- Molecule 57: 40S ribosomal protein S9

Chain SJ: 86% 14%



- Molecule 58: 40S ribosomal protein S11

Chain SL: 91% 9%

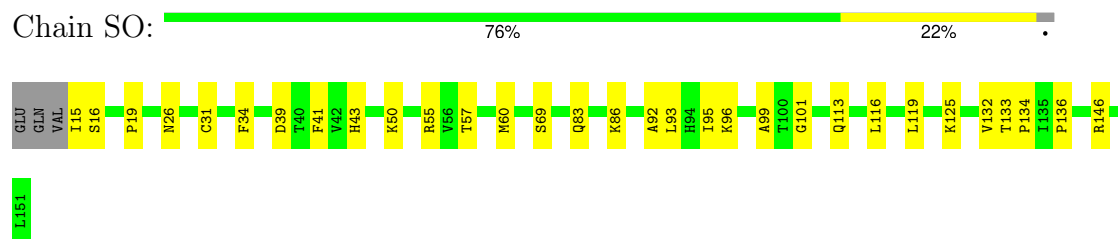


- Molecule 59: 40S ribosomal protein S13

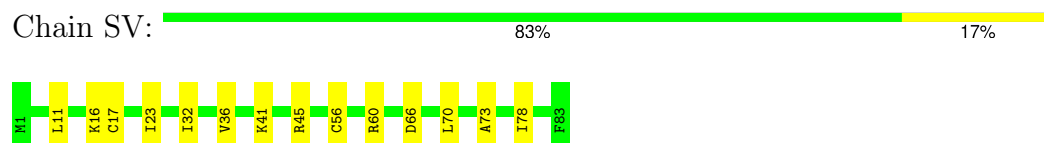
Chain SN: 91% 9%



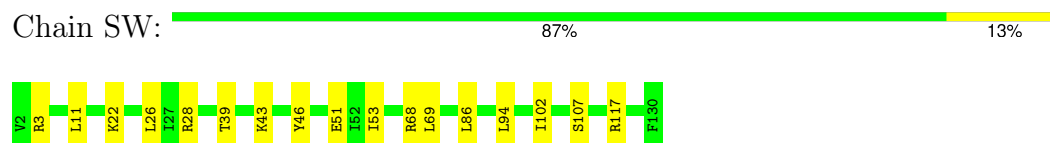
- Molecule 60: Small ribosomal subunit protein uS11



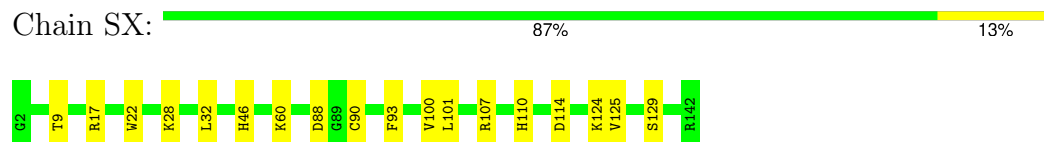
- Molecule 61: Small ribosomal subunit protein eS21



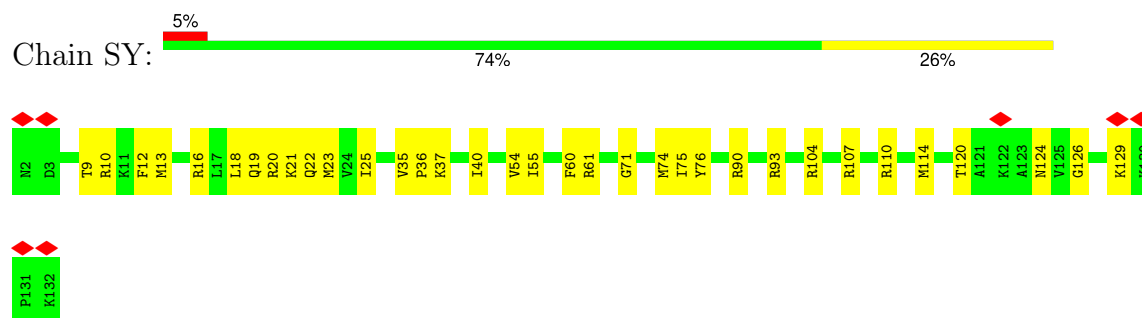
- Molecule 62: 40S ribosomal protein S15a



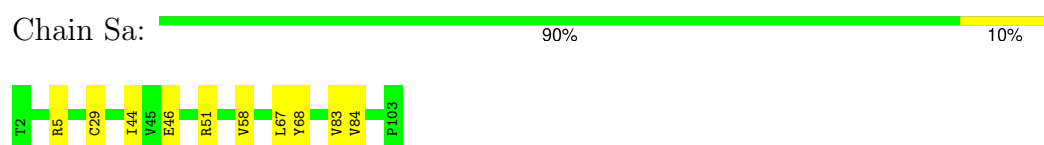
- Molecule 63: 40S ribosomal protein S23



- Molecule 64: 40S ribosomal protein S24



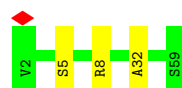
- Molecule 65: 40S ribosomal protein S26



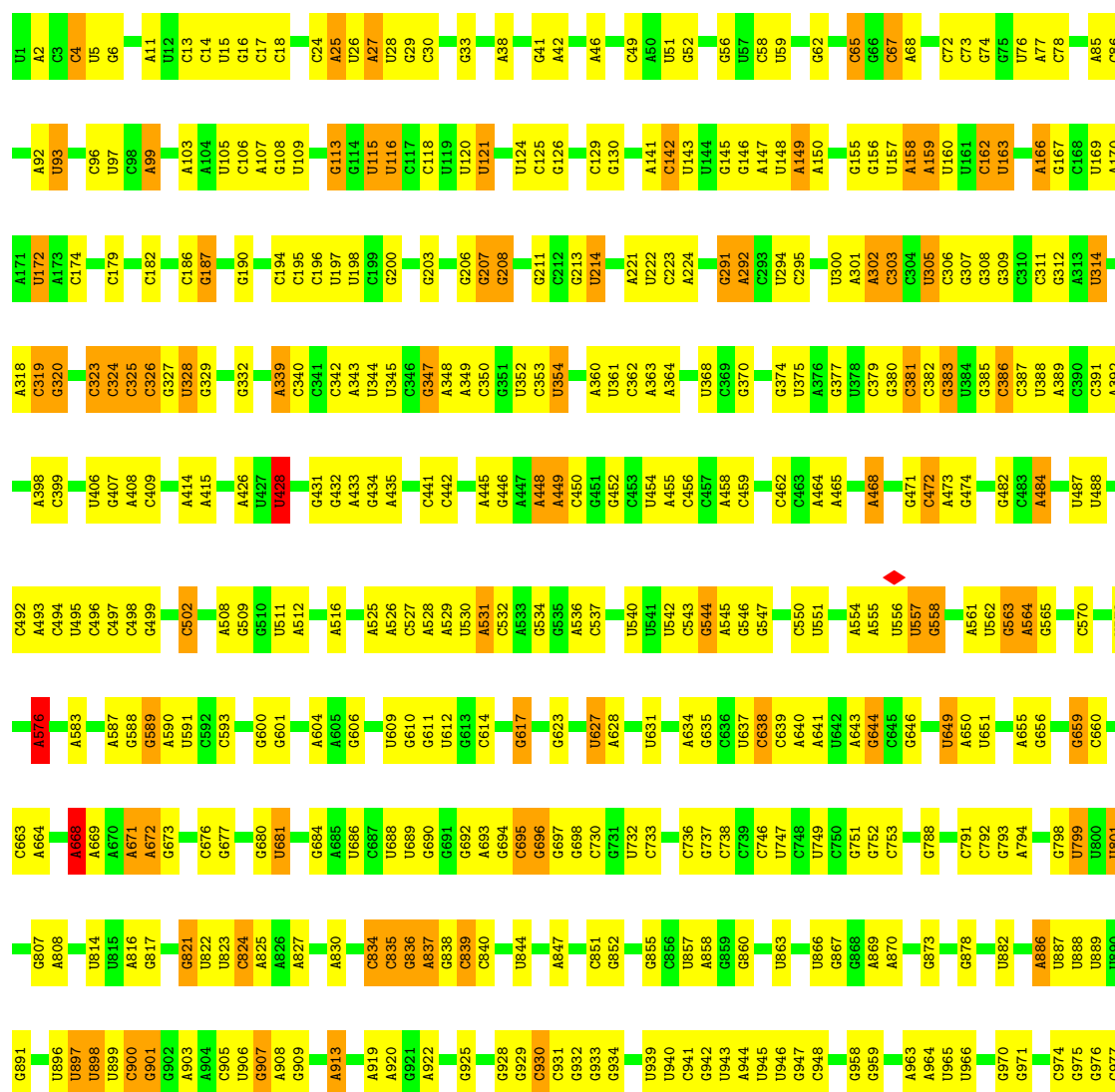
- Molecule 66: Small ribosomal subunit protein eS27

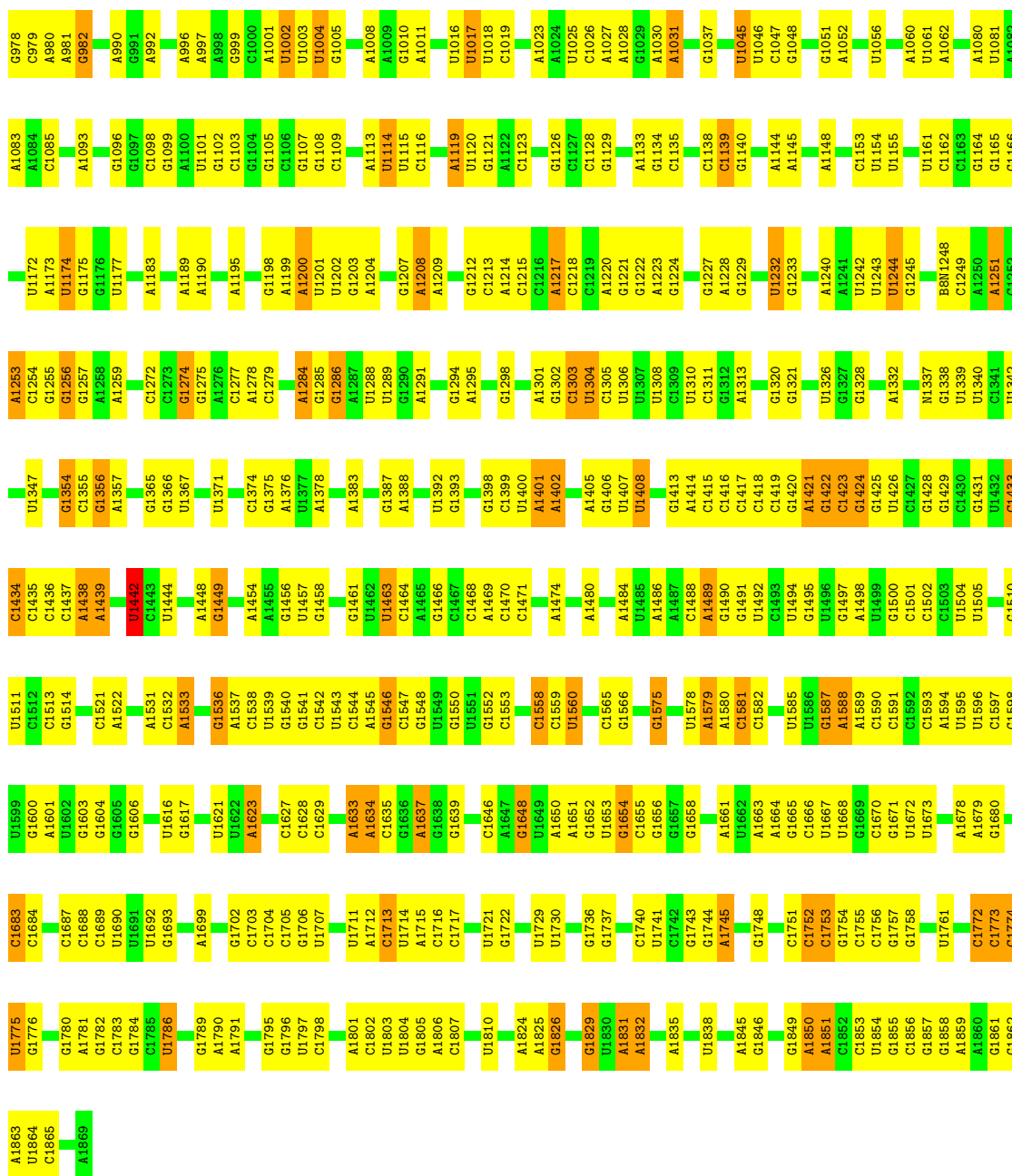


- Molecule 67: Small ribosomal subunit protein eS30



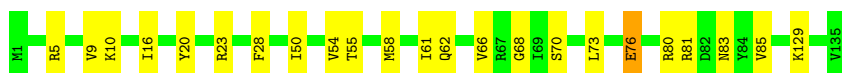
- Molecule 68: 18S rRNA





- Molecule 69: Small ribosomal subunit protein eS17

Chain SR: 83% 16%

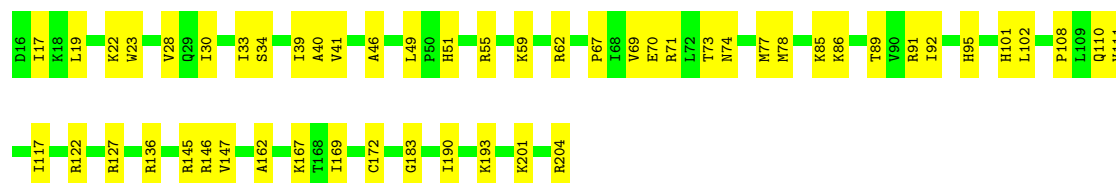


- Molecule 70: Small ribosomal subunit protein uS3

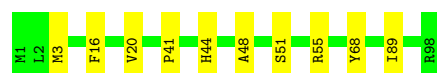
Chain SD: 86% 14%



- Molecule 71: 40S ribosomal protein S5



- Molecule 72: 40S ribosomal protein S10



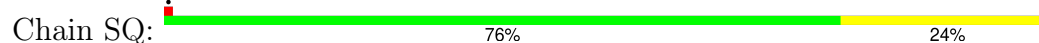
- Molecule 73: Small ribosomal subunit protein eS12



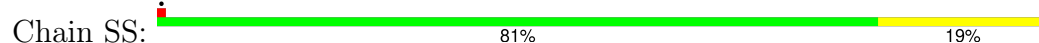
- Molecule 74: Small ribosomal subunit protein uS19



- Molecule 75: Small ribosomal subunit protein uS9



- Molecule 76: 40S ribosomal protein S18



- Molecule 77: 40S ribosomal protein S19

Chain ST:  83% 17%



- Molecule 78: 40S ribosomal protein S20

Chain SU:  81% 19%



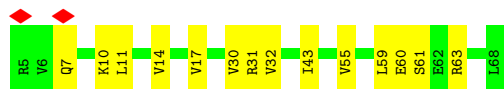
- Molecule 79: Small ribosomal subunit protein eS25

Chain SZ:  80% 20%



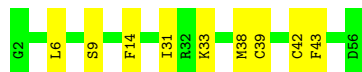
- Molecule 80: 40S ribosomal protein S28

Chain Sc:  78% 22%



- Molecule 81: 40S ribosomal protein S29

Chain Sd:  84% 16%



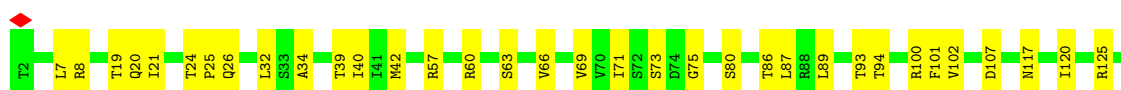
- Molecule 82: Ubiquitin-40S ribosomal protein S27a

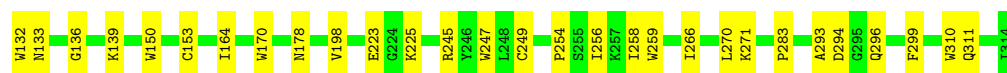
Chain Sf:  82% 18%



- Molecule 83: Receptor of activated protein C kinase 1

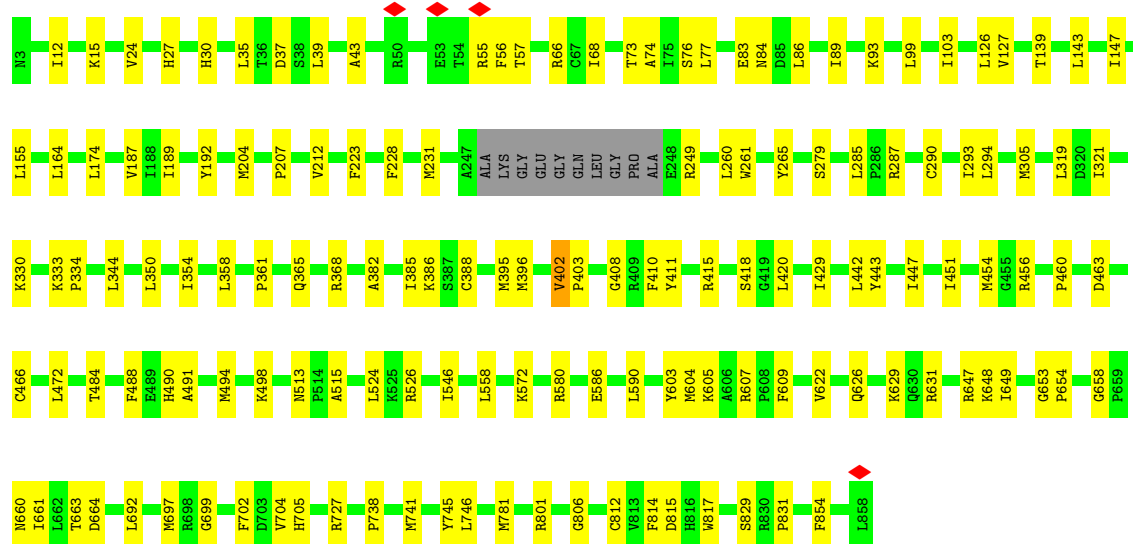
Chain Sg:  80% 20%





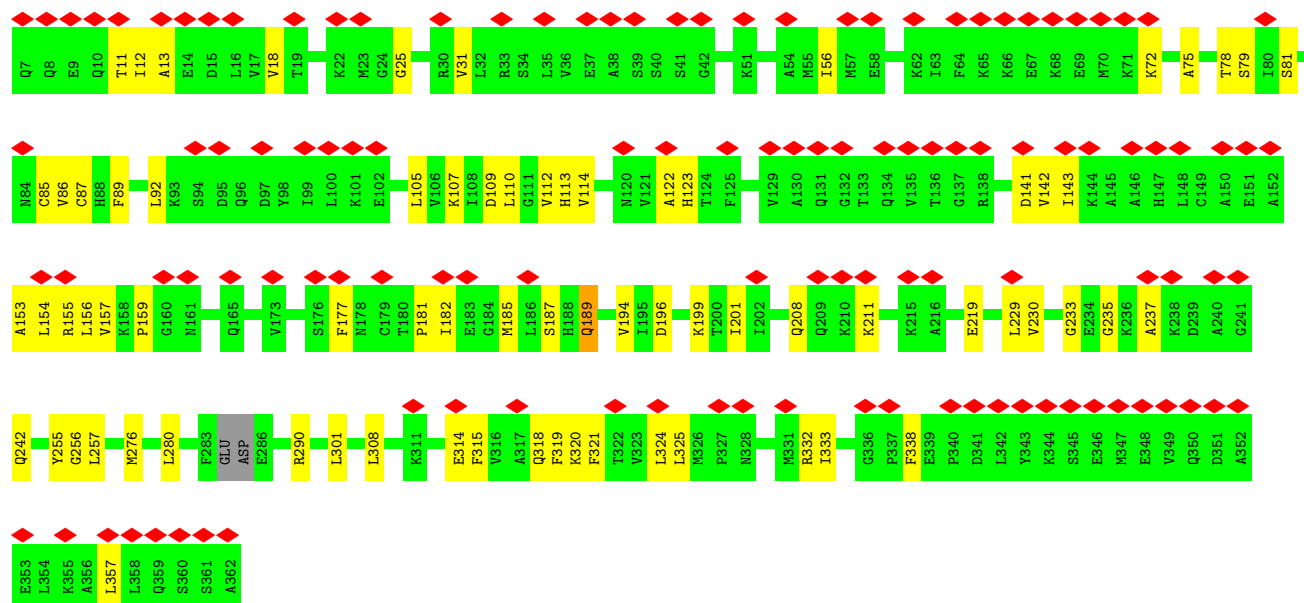
• Molecule 84: Elongation factor 2

Chain CB: 82% 17%



• Molecule 85: Proliferation-associated protein 2G4

Chain CA: 33% 79% 21%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52735	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	0.781	Depositor
Minimum map value	-0.311	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.0746	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: 6MZ, SPM, OMU, SPD, UR3, MA6, PSU, MG, 4AC, ZN, G7M, B8N, HMT, OMG, A2M, OMC, 1MA, 3HE, 5MC, UY1

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	0.22	0/447	0.34	0/592
2	CI	0.15	0/247	0.31	0/323
3	L5	0.34	0/85098	0.34	1/132762 (0.0%)
4	L7	0.32	0/2861	0.28	0/4459
5	L8	0.33	0/3631	0.30	0/5657
6	LA	0.34	0/1936	0.41	0/2596
7	LB	0.33	0/3306	0.38	0/4424
8	LC	0.34	0/2981	0.41	0/4002
9	LD	0.27	0/2428	0.37	0/3252
10	LE	0.27	0/1973	0.43	0/2645
11	LF	0.34	0/1905	0.35	0/2539
12	LG	0.27	0/1960	0.39	0/2637
13	LH	0.31	0/1537	0.37	0/2066
14	LI	0.30	0/1697	0.35	0/2266
15	LJ	0.25	0/1385	0.37	0/1852
16	LL	0.30	0/1732	0.37	0/2315
17	LM	0.30	0/1161	0.38	0/1554
18	LN	0.35	0/1746	0.37	0/2338
19	LO	0.34	0/1682	0.37	0/2250
20	LP	0.32	0/1268	0.39	0/1701
21	LQ	0.34	0/1537	0.39	0/2052
22	LR	0.27	0/1582	0.32	0/2091
23	LS	0.34	0/1493	0.34	0/2003
24	LT	0.32	0/1326	0.35	0/1770
25	LU	0.23	0/839	0.38	0/1126
26	LV	0.32	0/993	0.39	0/1332
27	LW	0.24	0/959	0.35	0/1270
28	LX	0.29	0/1002	0.33	0/1345
29	LY	0.31	0/1132	0.39	0/1504
30	LZ	0.28	0/1130	0.38	0/1507
31	La	0.34	0/1191	0.36	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.26	0/889	0.38	0/1175
33	Lc	0.28	0/774	0.37	0/1038
34	Ld	0.30	0/903	0.38	0/1216
35	Le	0.34	0/1071	0.35	0/1429
36	Lf	0.35	0/895	0.41	0/1198
37	Lg	0.29	0/916	0.35	0/1220
38	Lh	0.28	0/1023	0.32	0/1351
39	Li	0.25	0/843	0.34	0/1115
40	Lj	0.36	0/720	0.44	0/952
41	Lk	0.25	0/575	0.33	0/761
42	Ll	0.31	0/454	0.35	0/599
43	Lm	0.30	0/435	0.37	0/575
44	Ln	0.22	0/231	0.25	0/294
45	Lo	0.29	0/876	0.39	0/1156
46	Lp	0.31	0/718	0.35	0/953
47	Lr	0.32	0/1017	0.40	0/1364
48	Ls	0.20	0/1519	0.38	0/2052
49	Lt	0.21	0/1009	0.52	0/1363
50	SA	0.27	0/1778	0.44	0/2416
51	SB	0.18	0/1765	0.35	0/2362
52	SC	0.26	0/1744	0.40	0/2357
53	SE	0.21	0/2118	0.39	0/2849
54	SG	0.17	0/1946	0.34	0/2590
55	SH	0.20	0/1519	0.44	0/2033
56	SI	0.20	0/1715	0.40	0/2287
57	SJ	0.20	0/1550	0.32	0/2069
58	SL	0.23	0/1268	0.34	0/1696
59	SN	0.23	0/1232	0.33	0/1656
60	SO	0.20	0/1037	0.40	0/1391
61	SV	0.27	0/643	0.41	0/860
62	SW	0.27	0/1051	0.41	0/1406
63	SX	0.26	0/1116	0.42	0/1490
64	SY	0.18	0/1083	0.35	0/1438
65	Sa	0.24	0/836	0.37	0/1121
66	Sb	0.23	0/665	0.45	0/891
67	Se	0.19	0/465	0.36	0/612
68	S2	0.27	0/39756	0.32	0/61939
69	SR	0.20	0/1105	0.41	0/1484
70	SD	0.22	0/1793	0.34	0/2414
71	SF	0.19	0/1516	0.37	0/2037
72	SK	0.19	0/851	0.41	0/1147
73	SM	0.16	0/950	0.36	0/1275
74	SP	0.21	0/1003	0.37	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SQ	0.31	0/1160	0.52	0/1553
76	SS	0.19	0/1216	0.37	0/1628
77	ST	0.19	0/1131	0.36	0/1515
78	SU	0.28	0/831	0.49	0/1115
79	SZ	0.22	0/604	0.40	0/810
80	Sc	0.17	0/508	0.35	0/680
81	Sd	0.28	0/470	0.52	0/623
82	Sf	0.21	0/560	0.58	0/745
83	Sg	0.17	0/2493	0.37	0/3394
84	CB	0.22	0/6734	0.38	0/9094
85	CA	0.16	0/2810	0.40	0/3780
All	All	0.30	0/238055	0.35	1/347731 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1703	C	C2'-C3'-O3'	5.29	117.44	109.50

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	2	0
2	CI	247	0	283	1	0
3	L5	78444	0	39717	741	0
4	L7	2561	0	1295	15	0
5	L8	3315	0	1685	27	0
6	LA	1898	0	1993	24	0
7	LB	3238	0	3376	32	0
8	LC	2927	0	3104	23	0
9	LD	2382	0	2410	18	0
10	LE	1935	0	2096	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	LF	1870	0	1996	10	0
12	LG	1927	0	2074	13	0
13	LH	1518	0	1601	13	0
14	LI	1658	0	1697	11	0
15	LJ	1362	0	1399	12	0
16	LL	1701	0	1818	8	0
17	LM	1138	0	1204	7	0
18	LN	1701	0	1749	6	0
19	LO	1650	0	1794	15	0
20	LP	1242	0	1269	9	0
21	LQ	1513	0	1628	12	0
22	LR	1566	0	1729	11	0
23	LS	1453	0	1490	11	0
24	LT	1298	0	1366	9	0
25	LU	825	0	850	7	0
26	LV	979	0	1039	5	0
27	LW	945	0	1003	13	0
28	LX	985	0	1066	4	0
29	LY	1115	0	1205	7	0
30	LZ	1107	0	1182	13	0
31	La	1162	0	1213	8	0
32	Lb	876	0	948	8	0
33	Lc	764	0	804	7	0
34	Ld	888	0	930	7	0
35	Le	1053	0	1147	5	0
36	Lf	876	0	912	8	0
37	Lg	906	0	998	6	0
38	Lh	1015	0	1148	16	0
39	Li	832	0	917	3	0
40	Lj	705	0	737	5	0
41	Lk	569	0	637	7	0
42	Ll	444	0	483	3	0
43	Lm	429	0	465	2	0
44	Ln	230	0	276	2	0
45	Lo	862	0	929	4	0
46	Lp	708	0	756	4	0
47	Lr	1002	0	1068	4	0
48	Ls	1496	0	1540	23	0
49	Lt	998	0	1032	19	0
50	SA	1741	0	1744	38	0
51	SB	1738	0	1809	35	0
52	SC	1707	0	1791	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	SE	2076	0	2177	29	0
54	SG	1923	0	2089	41	0
55	SH	1497	0	1590	25	0
56	SI	1686	0	1772	30	0
57	SJ	1525	0	1640	17	0
58	SL	1247	0	1323	9	0
59	SN	1208	0	1294	9	0
60	SO	1024	0	1050	24	0
61	SV	636	0	637	13	0
62	SW	1034	0	1080	15	0
63	SX	1098	0	1167	14	0
64	SY	1065	0	1142	24	0
65	Sa	821	0	870	8	0
66	Sb	651	0	669	21	0
67	Se	459	0	503	2	0
68	S2	36952	0	18678	482	0
69	SR	1090	0	1149	18	0
70	SD	1765	0	1865	20	0
71	SF	1495	0	1549	40	0
72	SK	827	0	854	7	0
73	SM	940	0	965	7	0
74	SP	985	0	1031	19	0
75	SQ	1142	0	1213	30	0
76	SS	1198	0	1261	21	0
77	ST	1112	0	1146	18	0
78	SU	821	0	883	14	0
79	SZ	598	0	656	12	0
80	Sc	506	0	536	11	0
81	Sd	459	0	449	8	0
82	Sf	548	0	551	9	0
83	Sg	2436	0	2391	40	0
84	CB	6605	0	6679	87	0
85	CA	2764	0	2779	47	0
86	L5	179	0	0	0	0
86	L7	3	0	0	0	0
86	L8	4	0	0	0	0
86	LA	1	0	0	0	0
86	LP	1	0	0	0	0
86	LV	1	0	0	0	0
86	Le	1	0	0	0	0
86	Lj	1	0	0	0	0
86	S2	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
87	L5	98	0	182	4	0
88	L5	100	0	190	1	0
89	L5	20	0	23	0	0
90	L5	39	0	39	0	0
91	Lg	1	0	0	0	0
91	Lj	1	0	0	0	0
91	Lm	1	0	0	0	0
91	Lo	1	0	0	0	0
91	Lp	1	0	0	0	0
91	Sa	1	0	0	0	0
All	All	226615	0	171876	2251	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 6.

All (2251) 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)
60:SO:99:ALA:H	60:SO:133:THR:HG22	1.40	0.85
49:Lt:19:GLY:HA2	49:Lt:48:LYS:HZ3	1.44	0.81
3:L5:1095:A:H2	3:L5:1200:G:H1	1.30	0.79
83:Sg:26:GLN:HE22	83:Sg:75:GLY:HA3	1.48	0.79
68:S2:1337:4AC:H2'	68:S2:1338:G:H8	1.48	0.78
80:Sc:10:LYS:HZ1	80:Sc:61:SER:HB2	1.47	0.78
3:L5:512:U:H3	3:L5:647:G:H1	1.30	0.78
7:LB:90:VAL:HG23	7:LB:163:ILE:HD11	1.65	0.78
75:SQ:134:GLY:HA3	75:SQ:140:ARG:HA	1.65	0.77
15:LJ:16:ARG:HH21	15:LJ:137:PRO:HG3	1.50	0.77
3:L5:3944:G:H1	3:L5:4069:U:H3	1.31	0.76
13:LH:106:GLN:HB2	13:LH:111:LEU:HB3	1.68	0.76
83:Sg:120:ILE:HB	83:Sg:132:TRP:HB2	1.68	0.76
74:SP:34:MET:HB3	74:SP:42:ARG:HG3	1.68	0.75
8:LC:212:ASN:HD22	8:LC:255:SER:HB3	1.52	0.75
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.69	0.75
68:S2:1536:G:H2'	68:S2:1537:A:H8	1.51	0.74
68:S2:1748:G:H1	68:S2:1786:U:H3	0.81	0.74
45:Lo:69:ARG:HH21	45:Lo:80:LYS:HE2	1.52	0.74
56:SI:98:LYS:HB3	68:S2:377:G:H5'	1.68	0.74
50:SA:145:ILE:HG12	50:SA:159:ILE:HD13	1.70	0.73
71:SF:17:ILE:HG21	71:SF:46:ALA:HB1	1.71	0.73
68:S2:1286:G:H21	68:S2:1313:A:H62	1.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1997:U:H4'	48:Ls:44:ARG:HH12	1.52	0.73
22:LR:169:ALA:HA	22:LR:172:ARG:HE	1.53	0.72
49:Lt:83:LYS:HD2	49:Lt:86:LYS:HZ1	1.54	0.72
71:SF:49:LEU:HD12	75:SQ:50:LYS:HG2	1.69	0.72
54:SG:137:ARG:HB3	54:SG:140:ARG:HG3	1.70	0.72
48:Ls:76:GLU:HA	48:Ls:79:LEU:HD13	1.72	0.72
71:SF:34:SER:HA	80:Sc:55:VAL:HG13	1.72	0.71
84:CB:155:LEU:HB3	84:CB:212:VAL:HG23	1.71	0.71
53:SE:45:ILE:HG13	53:SE:61:VAL:HG11	1.72	0.71
85:CA:189:GLN:HG2	85:CA:199:LYS:HB3	1.71	0.71
10:LE:223:ARG:HH22	10:LE:238:GLU:HG2	1.56	0.71
3:L5:690:C:H4'	47:Lr:85:ASN:HD22	1.56	0.71
81:Sd:39:CYS:HB2	81:Sd:42:CYS:H	1.56	0.71
84:CB:745:TYR:HB2	84:CB:814:PHE:HA	1.73	0.71
58:SL:133:PRO:HG2	68:S2:383:G:H21	1.54	0.70
68:S2:1030:A:H2'	68:S2:1031:A2M:H8	1.72	0.70
26:LV:13:LYS:HD2	26:LV:128:LEU:HD11	1.74	0.70
50:SA:123:VAL:HA	50:SA:145:ILE:O	1.91	0.70
3:L5:4775:C:H41	3:L5:4859:C:H42	1.39	0.70
76:SS:36:VAL:HG23	76:SS:40:TYR:HB3	1.73	0.70
83:Sg:256:ILE:HB	83:Sg:270:LEU:HB2	1.74	0.70
77:ST:143:LYS:HG2	77:ST:144:LYS:HG2	1.72	0.70
68:S2:943:U:H2'	68:S2:944:A:H8	1.57	0.70
85:CA:187:SER:HB2	85:CA:201:ILE:HB	1.72	0.70
9:LD:103:LEU:HD11	9:LD:248:ARG:HE	1.57	0.69
3:L5:4139:G:H21	3:L5:4140:C:H41	1.41	0.69
30:LZ:77:TYR:HD2	33:Lc:39:ARG:HD3	1.57	0.69
3:L5:679:C:H2'	3:L5:680:G:H8	1.58	0.69
50:SA:85:ARG:HH22	69:SR:83:ASN:HA	1.58	0.69
3:L5:3754:G:H1	3:L5:3770:U:H3	1.41	0.69
3:L5:2458:C:H5''	18:LN:67:ARG:HD2	1.74	0.68
68:S2:1228:A:H2'	68:S2:1229:G:C8	2.28	0.68
7:LB:57:VAL:HG22	7:LB:73:VAL:HG12	1.76	0.68
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.59	0.68
68:S2:1652:G:H1	68:S2:1672:U:H3	1.40	0.67
85:CA:79:SER:HB3	85:CA:109:ASP:HB2	1.76	0.67
68:S2:1228:A:H2'	68:S2:1229:G:H8	1.59	0.67
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.58	0.67
3:L5:4910:G:H4'	7:LB:95:THR:HG22	1.77	0.67
3:L5:966:A:H5''	3:L5:2092:G:H22	1.59	0.67
64:SY:9:THR:H	68:S2:837:A:H61	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SY:36:PRO:HG3	68:S2:570:C:H4'	1.76	0.67
68:S2:1854:U:H2'	68:S2:1855:G:H8	1.58	0.67
53:SE:191:ARG:HD2	53:SE:245:ARG:HH11	1.59	0.67
64:SY:37:LYS:HA	64:SY:40:ILE:HD12	1.76	0.67
3:L5:2611:A:H5'	3:L5:2688:G:H4'	1.77	0.67
50:SA:205:ARG:HE	69:SR:81:ARG:HH12	1.40	0.67
68:S2:1532:C:H3'	68:S2:1637:A:H62	1.60	0.67
85:CA:75:ALA:HB2	85:CA:113:HIS:HB3	1.77	0.67
3:L5:3772:U:H3	3:L5:3776:G:H1	1.43	0.66
60:SO:92:ALA:HA	60:SO:125:LYS:HB2	1.77	0.66
68:S2:1780:G:H3'	68:S2:1781:A:H8	1.61	0.66
82:Sf:132:MET:HA	82:Sf:141:CYS:HA	1.76	0.66
15:LJ:146:ARG:HG2	15:LJ:147:ARG:HG3	1.77	0.66
74:SP:108:LYS:H	74:SP:111:MET:HE2	1.60	0.66
56:SI:129:LEU:HB3	56:SI:133:GLU:HB3	1.78	0.66
41:Lk:8:ILE:HD11	41:Lk:56:LEU:HD21	1.78	0.66
3:L5:1326:A2M:H2'	3:L5:1327:C:C6	2.31	0.66
3:L5:5024:C:H41	3:L5:5028:G:H21	1.41	0.66
3:L5:502:C:H3'	3:L5:503:C:H3'	1.78	0.65
50:SA:50:ASN:HD22	50:SA:53:ARG:HH11	1.44	0.65
75:SQ:32:ILE:HG23	75:SQ:68:ILE:HB	1.78	0.65
3:L5:3930:U:H3	3:L5:4180:G:H1	1.43	0.65
27:LW:96:GLN:HB2	27:LW:101:ARG:HH21	1.60	0.65
68:S2:1743:G:H21	68:S2:1791:A:H62	1.43	0.65
3:L5:300:A:H2'	3:L5:301:G:H8	1.62	0.65
68:S2:1513:C:H2'	68:S2:1514:G:H8	1.61	0.65
84:CB:12:ILE:HD12	84:CB:15:LYS:HD2	1.77	0.65
6:LA:104:VAL:HA	6:LA:107:MET:HE2	1.77	0.65
54:SG:20:ASP:HB3	54:SG:23:LYS:HG2	1.78	0.65
68:S2:388:U:H2'	68:S2:389:A:H8	1.61	0.65
68:S2:928:G:H2'	68:S2:929:G:C8	2.31	0.65
68:S2:1536:G:H2'	68:S2:1537:A:C8	2.30	0.65
71:SF:162:ALA:HB3	71:SF:169:ILE:HD13	1.79	0.65
85:CA:142[A]:VAL:HG23	85:CA:143:ILE:HD12	1.78	0.65
3:L5:1179:U:H3'	3:L5:1180:C:H5''	1.77	0.65
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.77	0.65
68:S2:1433:C:H42	78:SU:92:HIS:HD2	1.43	0.64
84:CB:84:ASN:HB2	84:CB:249:ARG:HH21	1.62	0.64
51:SB:131:ASP:HB2	51:SB:180:ASP:HB2	1.78	0.64
22:LR:188:LEU:HD22	55:SH:41:ARG:HH11	1.62	0.64
23:LS:127:MET:HE1	24:LT:155:PRO:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SE:19:MET:HE1	53:SE:108:ARG:HD2	1.78	0.64
85:CA:72:LYS:HG2	85:CA:114:VAL:HG12	1.79	0.64
31:La:72:THR:HG22	31:La:110:LYS:HB3	1.79	0.64
76:SS:80:PRO:HG2	77:ST:36:THR:HG21	1.80	0.64
51:SB:149:GLN:HE21	68:S2:1123:C:H4'	1.63	0.64
84:CB:164:LEU:HD21	84:CB:174:LEU:HD22	1.78	0.64
84:CB:354:ILE:HG23	84:CB:358:LEU:HD12	1.80	0.64
85:CA:81:SER:HB2	85:CA:85:CYS:HB3	1.79	0.64
62:SW:51:GLU:HG3	66:Sb:8:LEU:HD11	1.79	0.64
52:SC:191:VAL:HG11	52:SC:236:PHE:HA	1.80	0.64
60:SO:146:ARG:HG3	65:Sa:29:CYS:HB2	1.80	0.64
74:SP:34:MET:HE2	74:SP:45:LEU:HB3	1.78	0.64
68:S2:508:A:H3'	68:S2:509:OMG:H8	1.63	0.63
3:L5:2745:A:H2'	3:L5:2746:A:H8	1.63	0.63
3:L5:1178:G:H2'	3:L5:1178:G:N3	2.13	0.63
3:L5:3697:U:H5''	3:L5:3698:G:H5'	1.79	0.63
68:S2:834:C:H42	68:S2:839:C:H42	1.46	0.63
77:ST:104:LEU:HD23	77:ST:121:ARG:HD2	1.81	0.63
84:CB:484:THR:HG21	84:CB:494:MET:H	1.63	0.63
68:S2:1365:G:H2'	68:S2:1366:G:H8	1.64	0.63
68:S2:1748:G:O6	68:S2:1786:U:O4	2.16	0.63
3:L5:1180:C:H5''	3:L5:1180:C:H6	1.64	0.63
3:L5:1994:C:H2'	3:L5:1995:G:C8	2.34	0.63
3:L5:4250:G:H5''	15:LJ:98:ASN:HD22	1.64	0.63
68:S2:1277:C:H2'	68:S2:1278:A:H8	1.64	0.63
3:L5:2709:C:H42	85:CA:257:LEU:H	1.47	0.63
60:SO:34:PHE:HB3	60:SO:41:PHE:HB2	1.81	0.62
68:S2:1829:G:H1'	68:S2:1850:MA6:H2	1.81	0.62
19:LO:126:VAL:HG13	19:LO:127:VAL:HG13	1.82	0.62
85:CA:185:MET:HG3	85:CA:229:LEU:HD23	1.80	0.62
3:L5:1254:A:H5''	3:L5:1255:A:H5''	1.80	0.62
3:L5:4163:U:H5'	3:L5:4164:C:H5''	1.81	0.62
27:LW:45:ASN:HD21	27:LW:47:ARG:HH21	1.47	0.62
68:S2:116:OMU:HN3	68:S2:347:G:H1	1.47	0.62
3:L5:268:G:H2'	3:L5:269:G:H8	1.65	0.62
43:Lm:99:CYS:HB2	43:Lm:114:LYS:HE2	1.82	0.62
48:Ls:29:ILE:HG23	48:Ls:190:GLN:HB2	1.82	0.62
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.35	0.62
3:L5:2020:U:H2'	3:L5:2021:G:H8	1.64	0.62
51:SB:35:ALA:HB2	51:SB:44:ILE:HD11	1.82	0.62
55:SH:154:ILE:HB	55:SH:185:VAL:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LF:105:VAL:HG13	11:LF:136:VAL:HG12	1.82	0.62
68:S2:166:A2M:H2'	68:S2:167:G:H8	1.65	0.62
3:L5:2016:C:H2'	3:L5:2017:A:H8	1.63	0.61
49:Lt:114:ARG:HD3	49:Lt:129:ILE:HG22	1.82	0.61
66:Sb:19:HIS:HB3	66:Sb:22:LYS:HG3	1.82	0.61
3:L5:2845:A:H61	3:L5:3843:C:H42	1.47	0.61
50:SA:120:ARG:HD2	52:SC:266:TYR:HB3	1.83	0.61
64:SY:110:ARG:HG3	64:SY:114:MET:HE1	1.80	0.61
66:Sb:14:GLU:HB2	66:Sb:17:ARG:HH21	1.65	0.61
85:CA:11:THR:HG23	85:CA:13:ALA:H	1.66	0.61
49:Lt:65:GLN:HG3	49:Lt:67:ARG:H	1.65	0.61
50:SA:145:ILE:CG1	50:SA:159:ILE:HD13	2.29	0.61
68:S2:207:G:H3'	68:S2:208:G:H8	1.63	0.61
85:CA:208:GLN:HA	85:CA:211:LYS:HE3	1.82	0.61
3:L5:1802:A:H5''	3:L5:1803:G:H5'	1.81	0.61
3:L5:3774:A:H2'	3:L5:3775:A:C8	2.36	0.61
51:SB:138:PHE:HD2	51:SB:214:LYS:HB3	1.65	0.61
68:S2:24:C:HO2'	68:S2:25:A:H8	1.46	0.61
3:L5:4174:U:H2'	3:L5:4175:G:H8	1.65	0.61
8:LC:298:ILE:HD13	21:LQ:131:PRO:HB3	1.83	0.61
54:SG:32:MET:HA	54:SG:52:ILE:HB	1.82	0.61
60:SO:95:ILE:HD13	60:SO:116:LEU:HD11	1.82	0.61
84:CB:586:GLU:HG2	84:CB:607:ARG:HB2	1.82	0.61
3:L5:1181:C:H1'	3:L5:1182:C:H3'	1.82	0.61
3:L5:497:G:H21	3:L5:498:C:H41	1.48	0.61
3:L5:1414:C:H2'	3:L5:1415:G:H8	1.65	0.61
3:L5:2554:U:O2	3:L5:2764:A:N7	2.33	0.61
84:CB:408:GLY:HA2	84:CB:526:ARG:HD3	1.81	0.61
71:SF:59:LYS:HG2	71:SF:62:ARG:HE	1.65	0.60
3:L5:662:C:H2'	3:L5:663:G:H8	1.66	0.60
3:L5:2362:U:H2'	3:L5:2363:A2M:H8	1.82	0.60
16:LL:64:VAL:HA	16:LL:67:HIS:CD2	2.36	0.60
71:SF:127:ARG:HA	71:SF:136:ARG:HD3	1.84	0.60
54:SG:162:LEU:HD21	68:S2:67:C:H6	1.65	0.60
60:SO:101:GLY:HA3	60:SO:134:PRO:HD2	1.84	0.60
68:S2:835:C:H4'	68:S2:836:G:H8	1.66	0.60
51:SB:168:MET:HG2	51:SB:172:MET:HE2	1.82	0.60
56:SI:49:ARG:HE	68:S2:446:G:H5''	1.66	0.60
56:SI:91:VAL:HG21	56:SI:205:ARG:HH12	1.66	0.60
3:L5:1500:A:H5''	3:L5:1501:C:H5''	1.83	0.60
9:LD:65:ALA:HB2	9:LD:74:ILE:HG13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Lh:95:LEU:HB3	38:Lh:99:GLU:HG3	1.84	0.60
68:S2:1461:G:H3'	68:S2:1463:U:H3	1.66	0.60
83:Sg:87:LEU:HB2	83:Sg:101:PHE:HB2	1.82	0.60
84:CB:56:PHE:HB3	84:CB:456:ARG:H	1.65	0.60
3:L5:5006:U:H4'	3:L5:5007:A:H5'	1.84	0.60
10:LE:165:LEU:HD11	10:LE:176:THR:HG22	1.84	0.60
84:CB:279:SER:HB3	84:CB:285:LEU:HD21	1.83	0.60
64:SY:90:ARG:HA	64:SY:93:ARG:HD2	1.82	0.60
68:S2:106:C:H2'	68:S2:107:A:H8	1.67	0.60
68:S2:600:G:H2'	68:S2:601:OMG:H8	1.67	0.60
3:L5:4153:C:H2'	3:L5:4154:G:H8	1.67	0.60
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.66	0.60
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.83	0.60
83:Sg:247:TRP:HB3	83:Sg:258:ILE:HD11	1.81	0.60
3:L5:659:G:H2'	3:L5:660:A:H8	1.66	0.60
3:L5:1175:A:H2	3:L5:1185:G:H22	1.49	0.60
51:SB:33:VAL:HG12	51:SB:44:ILE:HD13	1.82	0.60
52:SC:90:GLU:HB2	52:SC:93:ILE:HG13	1.83	0.60
55:SH:49:LYS:HB2	55:SH:61:ILE:HD11	1.83	0.60
60:SO:96:LYS:HE3	60:SO:132:VAL:HG11	1.84	0.59
64:SY:9:THR:HG22	64:SY:25:ILE:HG22	1.84	0.59
68:S2:1004:PSU:H2'	68:S2:1005:G:H8	1.66	0.59
68:S2:1221:G:H2'	68:S2:1222:G:H8	1.67	0.59
3:L5:1095:A:N1	3:L5:1200:G:O6	2.35	0.59
3:L5:1188:C:H2'	3:L5:1189:G:C8	2.38	0.59
42:Ll:28:ARG:HA	42:Ll:33:ASN:ND2	2.18	0.59
51:SB:68:GLU:HB3	51:SB:83:LYS:HD3	1.84	0.59
3:L5:1697:G:H22	3:L5:2084:C:P	2.26	0.59
11:LF:127:LYS:HB2	24:LT:133:ALA:HB3	1.84	0.59
50:SA:64:ALA:HB3	50:SA:145:ILE:HD11	1.84	0.59
53:SE:42:LEU:HG	53:SE:46:ILE:HD11	1.85	0.59
56:SI:75:LYS:HE3	68:S2:303:C:H5'	1.84	0.59
62:SW:28:ARG:HH22	68:S2:1093:A:H5''	1.67	0.59
3:L5:1503:A:H62	21:LQ:87:THR:HG21	1.65	0.59
50:SA:37:TYR:HA	50:SA:53:ARG:HD3	1.85	0.59
50:SA:77:ILE:HG12	50:SA:99:ILE:HB	1.84	0.59
54:SG:49:VAL:HB	54:SG:115:LYS:HB3	1.83	0.59
68:S2:1286:G:N2	68:S2:1313:A:H62	2.00	0.59
70:SD:172:VAL:HG22	70:SD:185:LYS:HG2	1.83	0.59
71:SF:71:ARG:HH22	71:SF:147:VAL:HG23	1.66	0.59
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SJ:164:PRO:HB3	57:SJ:170:PRO:HA	1.83	0.59
64:SY:55:ILE:HG23	64:SY:75:ILE:HG22	1.84	0.59
71:SF:102:LEU:HD11	79:SZ:110:THR:HB	1.84	0.59
15:LJ:56:THR:HG23	15:LJ:63:ARG:HA	1.85	0.59
3:L5:3870:C:H2'	3:L5:3871:A:H8	1.68	0.59
23:LS:161:ARG:HE	23:LS:164:LYS:HB2	1.67	0.59
68:S2:172:OMU:H6	68:S2:314:U:H1'	1.84	0.59
70:SD:127:MET:HE1	70:SD:133:GLY:HA2	1.84	0.59
68:S2:1831:A:H2'	68:S2:1832:6MZ:H8	1.83	0.59
85:CA:107:LYS:HD2	85:CA:318:GLN:HG3	1.85	0.59
85:CA:255:TYR:HB3	85:CA:301:LEU:HD11	1.83	0.59
58:SL:126:VAL:HG22	58:SL:145:VAL:HG22	1.85	0.58
68:S2:588:G:H4'	68:S2:589:G:H5'	1.85	0.58
68:S2:1421:A:H3'	68:S2:1422:G:C8	2.38	0.58
78:SU:66:ARG:HH22	78:SU:75:LYS:HD3	1.68	0.58
5:L8:90:C:H1'	29:LY:24:HIS:HB3	1.85	0.58
10:LE:164:PHE:HA	10:LE:175:VAL:HG12	1.85	0.58
52:SC:207:ALA:HB2	68:S2:4:C:H4'	1.84	0.58
68:S2:158:A:H2'	68:S2:159:A2M:H8	1.85	0.58
68:S2:925:G:H1	68:S2:1017:U:H3	1.51	0.58
25:LU:19:LEU:HD12	25:LU:78:PHE:HB3	1.85	0.58
85:CA:123:HIS:HE1	85:CA:338:PHE:HB2	1.68	0.58
3:L5:1095:A:C2	3:L5:1200:G:N1	2.59	0.58
3:L5:3932:U:H2'	3:L5:3933:G:H8	1.67	0.58
3:L5:462:G:H2'	3:L5:463:A:C8	2.39	0.58
3:L5:1086:C:H2'	3:L5:1087:A:H8	1.69	0.58
7:LB:29:VAL:HG12	7:LB:31:SER:H	1.69	0.58
68:S2:851:C:H5''	68:S2:852:G:H5'	1.86	0.58
74:SP:86:LEU:H	74:SP:89:MET:HE2	1.69	0.58
85:CA:182:ILE:HD13	85:CA:235:GLY:HA2	1.85	0.58
33:Lc:38:ILE:HD11	33:Lc:46:VAL:HG21	1.85	0.58
45:Lo:69:ARG:HE	45:Lo:80:LYS:HG2	1.67	0.58
51:SB:150:ILE:HD13	69:SR:129:LYS:HB2	1.86	0.58
76:SS:40:TYR:HA	76:SS:83:PHE:HE2	1.68	0.58
84:CB:74:ALA:HA	84:CB:103:ILE:HG22	1.84	0.58
3:L5:3898:G:H5'	7:LB:254:ILE:HG13	1.85	0.58
54:SG:7:PHE:HD1	54:SG:113:ILE:HB	1.68	0.58
68:S2:1804:U:H2'	68:S2:1805:G:C8	2.38	0.58
69:SR:58:MET:HA	69:SR:61:ILE:HG12	1.86	0.58
7:LB:92:TYR:HB2	7:LB:159:VAL:HG13	1.86	0.57
21:LQ:119:LYS:HE3	21:LQ:121:LEU:HD21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SE:31:PRO:HG2	53:SE:38:LEU:HB2	1.85	0.57
64:SY:10:ARG:HA	68:S2:839:C:H41	1.69	0.57
68:S2:1845:A:H2'	68:S2:1846:G:H8	1.69	0.57
3:L5:2489:C:H4'	3:L5:2491:C:H42	1.68	0.57
65:Sa:5:ARG:HH21	68:S2:1864:U:H3'	1.68	0.57
83:Sg:20:GLN:HG2	83:Sg:69:VAL:H	1.69	0.57
84:CB:629:LYS:HD3	84:CB:647:ARG:HH22	1.69	0.57
3:L5:1097:C:H2'	3:L5:1098:G:H8	1.69	0.57
3:L5:1444:G:H22	3:L5:2104:G:H21	1.52	0.57
3:L5:4239:A:H2'	3:L5:4240:G:C8	2.40	0.57
15:LJ:78:LYS:HE3	15:LJ:82:ILE:HD11	1.87	0.57
50:SA:124:VAL:HB	50:SA:146:ALA:HB1	1.85	0.57
84:CB:260:LEU:HD23	84:CB:293:ILE:HD11	1.86	0.57
48:Ls:134:LYS:HG2	48:Ls:177:MET:HE2	1.86	0.57
68:S2:1218:C:H1'	68:S2:1683:C:H42	1.69	0.57
3:L5:257:C:H2'	3:L5:258:G:C8	2.40	0.57
7:LB:165:HIS:HB3	7:LB:180:LEU:HD23	1.86	0.57
50:SA:5:LEU:HD13	61:SV:41:LYS:HA	1.85	0.57
84:CB:745:TYR:CE2	84:CB:812:CYS:HB3	2.39	0.57
85:CA:25:GLY:HA3	85:CA:333:ILE:HG22	1.87	0.57
3:L5:497:G:N2	3:L5:498:C:H41	2.03	0.57
68:S2:554:A:HO2'	68:S2:555:A:H8	1.51	0.57
83:Sg:164:ILE:HG22	83:Sg:178:ASN:HA	1.87	0.57
3:L5:10:A:H2'	3:L5:11:G:H8	1.69	0.57
3:L5:1820:C:H2'	3:L5:1822:U:H5'	1.86	0.57
49:Lt:108:GLU:HG2	49:Lt:109:ILE:HD12	1.87	0.57
53:SE:64:ILE:HD11	64:SY:18:LEU:HD11	1.86	0.57
68:S2:694:G:H5''	68:S2:730:C:H5	1.68	0.57
3:L5:2568:C:H2'	3:L5:2569:G:C8	2.40	0.57
3:L5:4069:U:H2'	3:L5:4070:U:H6	1.70	0.57
3:L5:4742:G:H2'	3:L5:4743:G:H8	1.70	0.57
50:SA:57:LYS:HD3	61:SV:70:LEU:HD12	1.86	0.57
68:S2:1291:A:H62	82:Sf:95:ARG:HH12	1.51	0.57
68:S2:1737:G:H1	68:S2:1797:U:H3	1.52	0.57
68:S2:1856:C:H2'	68:S2:1857:G:H8	1.70	0.57
3:L5:1702:C:H4'	8:LC:308:LYS:HD2	1.87	0.57
84:CB:361:PRO:HB3	84:CB:415:ARG:HH12	1.69	0.57
84:CB:396:MET:HE1	84:CB:472:LEU:HD11	1.87	0.57
8:LC:340:ILE:HG21	10:LE:50:LEU:HD13	1.87	0.57
70:SD:69:LEU:HA	70:SD:72:VAL:HG12	1.86	0.57
85:CA:181:PRO:HA	85:CA:230:VAL:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:907:C:H2'	3:L5:908:G:H8	1.70	0.56
3:L5:3932:U:H2'	3:L5:3933:G:C8	2.39	0.56
68:S2:1438:A:H2'	68:S2:1439:A:C8	2.40	0.56
68:S2:1714:U:H2'	68:S2:1715:A:C8	2.40	0.56
71:SF:89:THR:HA	71:SF:92:ILE:HD12	1.85	0.56
3:L5:691:C:H2'	3:L5:692:A:C8	2.40	0.56
57:SJ:115:PHE:HA	57:SJ:120:ALA:HB3	1.86	0.56
68:S2:28:U:H2'	68:S2:29:G:H8	1.70	0.56
68:S2:1588:A:H2'	68:S2:1589:A:C8	2.40	0.56
84:CB:590:LEU:HD21	84:CB:603:TYR:HB3	1.87	0.56
3:L5:448:G:H2'	3:L5:450:G:H5'	1.87	0.56
3:L5:1974:U:H3	3:L5:2002:A:H8	1.52	0.56
3:L5:2859:G:H21	3:L5:3837:C:H1'	1.70	0.56
3:L5:3950:U:H3'	3:L5:3951:G:C8	2.40	0.56
3:L5:4966:A:H5''	7:LB:128:LYS:HG3	1.87	0.56
12:LG:214:ALA:HA	12:LG:217:LYS:HD2	1.85	0.56
13:LH:44:GLU:HG3	17:LM:2:VAL:HG12	1.86	0.56
13:LH:102:ASN:HB2	13:LH:115:ARG:HB2	1.86	0.56
25:LU:18:VAL:HG23	25:LU:73:THR:HG23	1.88	0.56
75:SQ:134:GLY:CA	75:SQ:140:ARG:HA	2.35	0.56
85:CA:122:ALA:HB3	85:CA:320:LYS:HG2	1.85	0.56
85:CA:159:PRO:HD3	85:CA:325:LEU:HD11	1.87	0.56
3:L5:325:U:H2'	3:L5:326:C:C6	2.41	0.56
3:L5:1172:C:HO2'	3:L5:1173:G:H8	1.54	0.56
9:LD:223:PHE:HB3	9:LD:226:TYR:HB2	1.87	0.56
55:SH:53:VAL:HG21	55:SH:172:THR:HG22	1.88	0.56
66:Sb:24:LEU:HD23	66:Sb:25:VAL:HG23	1.85	0.56
68:S2:1420:G:H21	68:S2:1421:A:H1'	1.71	0.56
68:S2:1581:C:H5'	68:S2:1582:C:H5	1.69	0.56
84:CB:147:ILE:HD11	84:CB:192:TYR:HB2	1.87	0.56
68:S2:527:C:H2'	68:S2:528:A:H8	1.70	0.56
84:CB:365:GLN:HA	84:CB:368:ARG:HB2	1.88	0.56
3:L5:2517:A:H5'	37:Lg:62:LYS:HD3	1.88	0.56
68:S2:981:A:H2'	68:S2:982:G:C8	2.41	0.56
69:SR:28:PHE:HA	69:SR:55:THR:HG21	1.87	0.56
84:CB:27:HIS:HB2	84:CB:139:THR:HG23	1.87	0.56
3:L5:1306:C:H2'	3:L5:1307:A:H8	1.70	0.56
3:L5:2411:C:H2'	3:L5:2412:A:H8	1.71	0.56
87:L5:5294:SPM:H112	19:LO:91:LYS:HD3	1.87	0.56
6:LA:137:ILE:HD11	6:LA:149:LYS:HB2	1.88	0.56
68:S2:1221:G:H2'	68:S2:1222:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:SM:36:ARG:HH21	73:SM:40:LYS:HB3	1.69	0.56
79:SZ:84:ALA:O	79:SZ:88:LEU:HB2	2.04	0.56
84:CB:83:GLU:HA	84:CB:86:LEU:HD12	1.88	0.56
53:SE:36:HIS:ND1	53:SE:85:GLY:HA3	2.21	0.56
5:L8:67:U:H2'	5:L8:68:G:H8	1.71	0.56
3:L5:1761:G:H1'	3:L5:1764:G:H22	1.69	0.56
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.38	0.56
3:L5:4965:U:H5''	7:LB:128:LYS:HZ1	1.70	0.56
12:LG:58:PRO:HD2	12:LG:61:ILE:HD12	1.88	0.56
59:SN:91:LEU:HB3	59:SN:122:ILE:HG12	1.88	0.56
3:L5:4088:C:H2'	3:L5:4089:G:H8	1.71	0.55
65:Sa:44:ILE:HD13	65:Sa:67:LEU:HG	1.88	0.55
78:SU:56:MET:HB2	78:SU:86:LYS:HB3	1.87	0.55
83:Sg:223:GLU:HB3	83:Sg:225:LYS:HG2	1.87	0.55
85:CA:78:THR:HG22	85:CA:110:LEU:HD12	1.87	0.55
83:Sg:24:THR:HB	83:Sg:71:ILE:HG21	1.87	0.55
3:L5:4126:C:H5''	3:L5:4127:A:H5''	1.88	0.55
14:LI:54:SER:HB3	14:LI:135:ILE:HD11	1.87	0.55
44:Ln:1:MET:HB2	68:S2:1706:G:H5'	1.87	0.55
62:SW:107:SER:HB2	68:S2:860:G:H21	1.70	0.55
71:SF:201:LYS:HD2	71:SF:204:ARG:HD2	1.88	0.55
3:L5:3722:G:H2'	3:L5:3723:A:H8	1.71	0.55
3:L5:4153:C:H2'	3:L5:4154:G:C8	2.42	0.55
3:L5:4238:G:H2'	3:L5:4239:A:H8	1.70	0.55
9:LD:64:ILE:HD13	9:LD:109:LEU:HD22	1.88	0.55
68:S2:1743:G:N2	68:S2:1791:A:H62	2.04	0.55
83:Sg:26:GLN:NE2	83:Sg:75:GLY:HA3	2.20	0.55
68:S2:166:A2M:H2'	68:S2:167:G:C8	2.40	0.55
68:S2:391:C:H2'	68:S2:392:A:H8	1.71	0.55
68:S2:1560:U:O2	68:S2:1575:G:O6	2.24	0.55
70:SD:109:LEU:HD12	70:SD:184:ILE:HD11	1.88	0.55
81:Sd:6:LEU:HA	81:Sd:9:SER:HB3	1.88	0.55
84:CB:265:TYR:HA	84:CB:287:ARG:HA	1.88	0.55
68:S2:1285:G:H5'	73:SM:35:ILE:HG12	1.89	0.55
75:SQ:131:LYS:C	75:SQ:133:GLY:H	2.15	0.55
84:CB:801:ARG:HG2	84:CB:806:GLY:HA2	1.89	0.55
3:L5:3599:A:H2'	3:L5:3600:G:C8	2.41	0.55
3:L5:4238:G:H2'	3:L5:4239:A:C8	2.42	0.55
54:SG:11:GLY:HA2	68:S2:166:A2M:HM'1	1.89	0.55
68:S2:1670:C:H2'	68:S2:1671:G:C8	2.42	0.55
83:Sg:32:LEU:HA	83:Sg:42:MET:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:276:C:H2'	39:Li:29:ARG:HH22	1.72	0.55
3:L5:2400:G:H21	37:Lg:6:THR:HG22	1.72	0.55
59:SN:14:SER:HB2	68:S2:1016:U:H5''	1.89	0.55
60:SO:93:LEU:HD23	60:SO:119:LEU:HD21	1.88	0.55
3:L5:964:A:H2'	3:L5:965:G:H4'	1.89	0.55
3:L5:4364:G:H2'	3:L5:4365:C:H6	1.72	0.55
87:L5:5289:SPM:H32	88:L5:5290:SPD:H102	1.72	0.55
56:SI:22:HIS:HB3	68:S2:433:A:H5''	1.89	0.55
56:SI:87:ASN:HB3	56:SI:90:LEU:HD23	1.89	0.55
63:SX:9:THR:HG22	68:S2:681:PSU:H4'	1.89	0.55
68:S2:677:G:H21	68:S2:1028:A:H62	1.53	0.55
84:CB:692:LEU:HD11	84:CB:738:PRO:HB2	1.89	0.55
3:L5:257:C:H2'	3:L5:258:G:H8	1.71	0.54
10:LE:277:LEU:HB2	36:Lf:4:ARG:HB3	1.89	0.54
38:Lh:80:PRO:HD2	38:Lh:83:LEU:HD12	1.89	0.54
68:S2:186:C:H2'	68:S2:187:G:C8	2.41	0.54
68:S2:1748:G:N2	68:S2:1786:U:O2	2.27	0.54
85:CA:92:LEU:HD22	85:CA:290:ARG:HD3	1.88	0.54
3:L5:3917:A:H2'	3:L5:3918:G:H8	1.72	0.54
3:L5:4279:A:H5'	3:L5:4281:A:H1'	1.89	0.54
6:LA:3:ARG:HB3	6:LA:207:VAL:HG22	1.89	0.54
69:SR:70:SER:HB3	69:SR:73:LEU:HB2	1.89	0.54
3:L5:173:C:H5''	16:LL:129:ARG:HH12	1.72	0.54
3:L5:1175:A:H2	3:L5:1185:G:H1	1.52	0.54
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.40	0.54
50:SA:10:MET:HE3	50:SA:55:TRP:HB2	1.90	0.54
55:SH:157:HIS:HB3	55:SH:190:PRO:HG3	1.89	0.54
68:S2:996:A:H2'	68:S2:997:A:C8	2.42	0.54
84:CB:43:ALA:HB3	84:CB:77:LEU:HD23	1.88	0.54
3:L5:662:C:H2'	3:L5:663:G:C8	2.42	0.54
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.42	0.54
7:LB:258:HIS:HA	7:LB:260:ALA:H	1.72	0.54
12:LG:209:SER:HA	12:LG:212:LYS:HG3	1.88	0.54
63:SX:46:HIS:HB3	63:SX:101:LEU:HD11	1.90	0.54
68:S2:1468:C:H2'	68:S2:1469:A:C8	2.42	0.54
68:S2:1856:C:H2'	68:S2:1857:G:C8	2.43	0.54
69:SR:83:ASN:HB3	69:SR:85:VAL:HG13	1.89	0.54
84:CB:429:ILE:HB	84:CB:443:TYR:HB2	1.89	0.54
3:L5:158:A:H5''	3:L5:159:C:H2'	1.88	0.54
5:L8:8:U:H2'	5:L8:9:A:H8	1.73	0.54
6:LA:131:GLY:H	6:LA:169:VAL:HG13	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Lk:26:LYS:HB2	41:Lk:69:LEU:HD12	1.89	0.54
50:SA:205:ARG:HE	69:SR:81:ARG:NH1	2.03	0.54
85:CA:12:ILE:HG12	85:CA:324:LEU:HD21	1.89	0.54
68:S2:223:C:H2'	68:S2:224:A:C8	2.42	0.54
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.43	0.54
7:LB:107:ALA:HB2	7:LB:201:LEU:HD22	1.90	0.54
48:Ls:127:ASN:HD21	48:Ls:151:THR:HG23	1.72	0.54
68:S2:49:C:H2'	68:S2:472:C:H41	1.72	0.54
68:S2:1405:A:H2'	68:S2:1406:G:O4'	2.08	0.54
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.43	0.54
3:L5:4088:C:H2'	3:L5:4089:G:C8	2.43	0.54
26:LV:106:VAL:HG12	26:LV:112:MET:HA	1.90	0.54
3:L5:1994:C:H2'	3:L5:1995:G:H8	1.69	0.54
3:L5:4578:G:H2'	3:L5:4579:PSU:H6	1.72	0.54
52:SC:167:ARG:HB3	52:SC:177:PRO:HB2	1.90	0.54
54:SG:10:THR:HA	54:SG:128:THR:HG23	1.89	0.54
68:S2:1144:A:H2'	68:S2:1145:A:C8	2.42	0.54
83:Sg:249:CYS:HB3	83:Sg:258:ILE:HD13	1.90	0.54
85:CA:154:LEU:HD11	85:CA:332:ARG:HD2	1.89	0.54
3:L5:4319:C:H2'	3:L5:4320:G:H8	1.72	0.54
3:L5:4775:C:H41	3:L5:4859:C:N4	2.05	0.54
48:Ls:77:LYS:HB3	48:Ls:198:ILE:HD11	1.89	0.54
68:S2:1407:U:H2'	68:S2:1408:U:C6	2.43	0.54
3:L5:2079:G:H2'	3:L5:2080:U:C6	2.44	0.53
3:L5:3661:G:H4'	3:L5:3662:A:H5'	1.89	0.53
68:S2:388:U:H2'	68:S2:389:A:C8	2.41	0.53
3:L5:1327:C:H2'	3:L5:1328:G:C8	2.43	0.53
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.90	0.53
3:L5:2633:U:H2'	3:L5:2634:C:H6	1.73	0.53
3:L5:381:U:H4'	3:L5:415:G:H5'	1.89	0.53
3:L5:956:A:H1'	3:L5:2076:G:H5''	1.90	0.53
3:L5:1404:G:N7	3:L5:1408:G:N2	2.56	0.53
53:SE:104:ASP:HB3	53:SE:110:ALA:HB2	1.90	0.53
69:SR:66:VAL:HG23	69:SR:68:GLY:H	1.73	0.53
75:SQ:34:VAL:HG12	75:SQ:70:VAL:HB	1.89	0.53
79:SZ:92:LEU:HD12	79:SZ:109:TYR:HE2	1.73	0.53
3:L5:10:A:H2'	3:L5:11:G:C8	2.43	0.53
3:L5:175:C:H2'	3:L5:176:G:H8	1.73	0.53
3:L5:3911:C:H2'	3:L5:3912:U:H6	1.74	0.53
5:L8:8:U:H2'	5:L8:9:A:C8	2.44	0.53
7:LB:258:HIS:HA	7:LB:260:ALA:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SC:121:ARG:HH12	68:S2:1347:U:H5''	1.73	0.53
68:S2:1845:A:H2'	68:S2:1846:G:C8	2.43	0.53
84:CB:649:ILE:HA	84:CB:663:THR:HG22	1.91	0.53
3:L5:178:C:H2'	3:L5:179:G:C8	2.44	0.53
3:L5:1366:G:C2	16:LL:33:ILE:HG21	2.44	0.53
3:L5:2745:A:H2'	3:L5:2746:A:C8	2.42	0.53
3:L5:3910:C:H2'	3:L5:3911:C:C6	2.44	0.53
3:L5:3910:C:H2'	3:L5:3911:C:H6	1.73	0.53
18:LN:146:PRO:HB2	38:Lh:104:THR:HG23	1.90	0.53
27:LW:93:LYS:HA	27:LW:96:GLN:HG3	1.89	0.53
68:S2:1468:C:H2'	68:S2:1469:A:H8	1.73	0.53
73:SM:92:CYS:HB3	73:SM:103:VAL:HG12	1.91	0.53
3:L5:137:G:H2'	3:L5:138:G:C8	2.44	0.53
3:L5:3848:U:H2'	3:L5:3849:A:H8	1.74	0.53
3:L5:4274:A:H2'	3:L5:4275:G:H8	1.73	0.53
5:L8:19:C:H2'	5:L8:20:A:C8	2.44	0.53
50:SA:76:VAL:HG12	50:SA:123:VAL:HB	1.89	0.53
68:S2:1201:U:H2'	68:S2:1202:U:C6	2.43	0.53
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.44	0.53
51:SB:88:THR:HG22	51:SB:98:THR:HG22	1.90	0.53
51:SB:111:CYS:HB3	65:Sa:68:TYR:HB2	1.91	0.53
53:SE:197:ASN:HB3	53:SE:209:HIS:HD2	1.74	0.53
64:SY:12:PHE:HZ	64:SY:21:LYS:HE2	1.73	0.53
68:S2:85:A:H2'	68:S2:86:C:H6	1.74	0.53
68:S2:1199:A:H2'	68:S2:1200:A:C8	2.44	0.53
68:S2:1595:U:H2'	68:S2:1596:U:C6	2.43	0.53
68:S2:1656:G:H1	68:S2:1668:U:H3	1.57	0.53
3:L5:1509:C:H5''	31:La:2:PRO:HD3	1.91	0.53
9:LD:51:MET:HE1	9:LD:163:LEU:HA	1.91	0.53
9:LD:123:VAL:HG22	9:LD:248:ARG:HH12	1.73	0.53
59:SN:35:GLU:HA	59:SN:38:TYR:HD1	1.73	0.53
66:Sb:72:ARG:NH1	68:S2:1120:U:H5'	2.24	0.53
68:S2:1310:U:H5''	82:Sf:130:VAL:HB	1.90	0.53
70:SD:195:THR:HG23	70:SD:197:LYS:H	1.73	0.53
83:Sg:259:TRP:HB3	83:Sg:266:ILE:HA	1.91	0.53
3:L5:2520:C:H2'	3:L5:2521:G:H8	1.74	0.53
6:LA:36:GLU:HG3	6:LA:91:GLY:HA2	1.90	0.53
33:Lc:13:SER:HB3	33:Lc:17:ARG:HH21	1.73	0.53
56:SI:172:LEU:HB3	56:SI:190:LEU:HD12	1.89	0.53
68:S2:897:U:H2'	68:S2:898:U:H4'	1.91	0.53
74:SP:20:VAL:HG11	74:SP:28:MET:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L7:112:U:H2'	4:L7:113:G:H8	1.74	0.53
48:LS:20:LEU:HD11	48:LS:52:VAL:HG11	1.91	0.53
51:SB:127:VAL:HG11	51:SB:176:VAL:HB	1.90	0.53
71:SF:122:ARG:HE	80:Sc:59:LEU:HD21	1.74	0.53
3:L5:432:U:H1'	87:L5:5294:SPM:H82	1.90	0.52
71:SF:30:ILE:HG23	71:SF:117:ILE:HD11	1.92	0.52
76:SS:124:ARG:HE	76:SS:129:LEU:HB2	1.74	0.52
4:L7:92:C:H2'	4:L7:93:G:H8	1.73	0.52
17:LM:122:ILE:HB	19:LO:189:ILE:HD11	1.91	0.52
27:LW:9:SER:HA	27:LW:52:THR:HG23	1.91	0.52
27:LW:80:ARG:H	54:SG:131:ARG:HH12	1.55	0.52
28:LX:80:PRO:HG2	28:LX:155:ILE:HG21	1.91	0.52
45:Lo:10:THR:HG21	45:Lo:70:LEU:HD13	1.91	0.52
68:S2:1244:PSU:H2'	68:S2:1245:G:H8	1.73	0.52
68:S2:1277:C:H2'	68:S2:1278:A:C8	2.44	0.52
68:S2:1667:U:H2'	68:S2:1668:U:C6	2.43	0.52
85:CA:233:GLY:HA3	85:CA:314:GLU:HG2	1.91	0.52
3:L5:691:C:H2'	3:L5:692:A:H8	1.73	0.52
3:L5:1095:A:N1	3:L5:1200:G:C6	2.78	0.52
3:L5:1468:C:H2'	3:L5:1469:C:H6	1.73	0.52
3:L5:2401:A2M:H5''	3:L5:2401:A2M:H8	1.90	0.52
50:SA:74:VAL:HG12	50:SA:121:LEU:HB3	1.90	0.52
68:S2:1365:G:H2'	68:S2:1366:G:C8	2.44	0.52
62:SW:39:THR:HG22	62:SW:43:LYS:HE2	1.92	0.52
68:S2:1751:C:H42	68:S2:1782:G:N2	2.06	0.52
78:SU:21:ARG:HD3	78:SU:88:LEU:HD22	1.92	0.52
78:SU:55:ARG:HG2	78:SU:87:ARG:HD3	1.91	0.52
3:L5:1751:A:H2'	3:L5:1752:G:C8	2.45	0.52
3:L5:4251:A:H5''	15:LJ:108:GLY:HA3	1.91	0.52
55:SH:62:ILE:HD12	55:SH:94:PHE:HE1	1.75	0.52
85:CA:157:VAL:HG22	85:CA:325:LEU:HD13	1.91	0.52
3:L5:138:G:H2'	3:L5:139:G:H8	1.74	0.52
3:L5:267:G:H2'	3:L5:268:G:H8	1.75	0.52
3:L5:2521:G:H5'	3:L5:2640:G:H1'	1.91	0.52
3:L5:2539:C:H2'	3:L5:2540:C:C6	2.45	0.52
3:L5:2696:A:H62	41:Lk:35:LYS:NZ	2.08	0.52
3:L5:4459:U:H2'	3:L5:4460:U:C6	2.44	0.52
66:Sb:72:ARG:HH22	68:S2:1119:A:H2'	1.73	0.52
84:CB:89:ILE:HB	84:CB:93:LYS:HD3	1.91	0.52
3:L5:4113:U:H4'	3:L5:4115:G:C4	2.45	0.52
3:L5:4619:U:H2'	3:L5:4620:OMU:H6	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LW:34:ALA:HA	27:LW:37:GLU:HG2	1.91	0.52
76:SS:88:LYS:H	76:SS:95:TYR:HD1	1.58	0.52
77:ST:22:LEU:HD13	77:ST:28:LEU:HD13	1.91	0.52
84:CB:558:LEU:HD13	84:CB:572:LYS:HG2	1.92	0.52
3:L5:1188:C:H2'	3:L5:1189:G:H8	1.75	0.52
3:L5:3860:A:H2	20:LP:131:ARG:HH22	1.58	0.52
5:L8:141:C:H2'	5:L8:142:U:C6	2.45	0.52
53:SE:48:LEU:HD23	53:SE:52:LEU:HD12	1.92	0.52
3:L5:3641:U:H5	3:L5:3646:A:N7	2.06	0.52
3:L5:3805:U:H2'	3:L5:3806:G:H8	1.74	0.52
3:L5:4992:G:H2'	3:L5:4993:G:C8	2.44	0.52
28:LX:73:HIS:HB3	28:LX:116:LEU:HD23	1.92	0.52
30:LZ:103:ASP:HB3	30:LZ:106:LEU:HB2	1.91	0.52
48:Ls:50:LYS:NZ	48:Ls:98:ILE:HD12	2.25	0.52
49:Lt:127:GLY:O	49:Lt:131:GLU:HG2	2.09	0.52
3:L5:4991:U:H2'	3:L5:4992:G:H8	1.75	0.52
6:LA:206:PRO:HG3	6:LA:213:GLY:HA3	1.91	0.52
22:LR:115:ILE:HG22	22:LR:119:MET:HE3	1.92	0.52
33:Lc:99:PRO:HG3	33:Lc:104:ILE:HD12	1.91	0.52
68:S2:557:U:H2'	68:S2:558:G:C8	2.45	0.52
3:L5:2558:C:H2'	3:L5:2559:G:C8	2.44	0.51
3:L5:4954:G:H2'	3:L5:4955:A:C8	2.46	0.51
7:LB:367:PHE:HB2	27:LW:1:MET:HB2	1.91	0.51
68:S2:494:C:N4	68:S2:509:OMG:HN22	2.07	0.51
3:L5:323:C:H2'	3:L5:324:A:H8	1.75	0.51
3:L5:3607:U:H2'	3:L5:3608:A:H8	1.74	0.51
3:L5:3861:A:H2'	3:L5:3862:A:H8	1.75	0.51
71:SF:22:LYS:HG3	71:SF:23:TRP:CD2	2.45	0.51
75:SQ:19:ALA:HB2	75:SQ:75:GLY:HA3	1.92	0.51
82:Sf:103:LEU:HG	82:Sf:104:LYS:H	1.74	0.51
3:L5:518:G:H1	3:L5:643:C:H2'	1.75	0.51
26:LV:37:LEU:HD23	26:LV:65:VAL:HG12	1.93	0.51
32:Lb:75:LEU:HD23	32:Lb:76:VAL:HG22	1.91	0.51
56:SI:57:ALA:HB2	56:SI:183:GLY:HA2	1.91	0.51
3:L5:2568:C:H2'	3:L5:2569:G:H8	1.76	0.51
3:L5:2780:C:H2'	3:L5:2781:G:H8	1.75	0.51
3:L5:3771:C:H2'	3:L5:3772:U:C6	2.45	0.51
8:LC:334:THR:HG22	8:LC:337:ARG:HH21	1.75	0.51
56:SI:106:SER:HB3	56:SI:171:LEU:HG	1.93	0.51
63:SX:28:LYS:HE2	63:SX:32:LEU:HD22	1.92	0.51
68:S2:1420:G:N2	68:S2:1421:A:H1'	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:SP:85:ILE:HG23	74:SP:107:ILE:HD11	1.92	0.51
77:ST:51:ASN:HB3	77:ST:54:TYR:HD2	1.74	0.51
3:L5:2090:U:H4'	3:L5:2091:C:H3'	1.90	0.51
3:L5:3870:C:H2'	3:L5:3871:A:C8	2.46	0.51
19:LO:12:ARG:HB2	19:LO:37:ARG:HH11	1.75	0.51
50:SA:158:ASP:HB2	50:SA:159:ILE:HD12	1.92	0.51
68:S2:1037:G:H4'	68:S2:1845:A:H4'	1.92	0.51
70:SD:135:GLU:HB2	70:SD:153:VAL:HG23	1.93	0.51
71:SF:28:VAL:HG12	71:SF:110:GLN:HB2	1.92	0.51
3:L5:717:U:H2'	3:L5:718:C:C6	2.46	0.51
3:L5:2558:C:H2'	3:L5:2559:G:H8	1.76	0.51
3:L5:5027:C:O2'	3:L5:5028:G:H5''	2.11	0.51
5:L8:96:C:H5''	38:Lh:66:LYS:HG2	1.92	0.51
56:SI:9:HIS:HE1	68:S2:386:C:H4'	1.76	0.51
64:SY:18:LEU:HD22	64:SY:20:ARG:NH1	2.25	0.51
81:Sd:38:MET:HE3	81:Sd:43:PHE:HA	1.92	0.51
3:L5:175:C:H2'	3:L5:176:G:C8	2.45	0.51
3:L5:266:C:HO2'	3:L5:267:G:H8	1.57	0.51
3:L5:490:C:H2'	3:L5:491:G:C8	2.46	0.51
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.46	0.51
50:SA:69:GLU:HB2	52:SC:270:THR:HG21	1.93	0.51
66:Sb:54:VAL:HG23	66:Sb:63:LEU:HB2	1.92	0.51
3:L5:1494:U:H2'	3:L5:1495:G:H8	1.76	0.51
3:L5:2491:C:H2'	3:L5:2492:C:C6	2.46	0.51
3:L5:2543:A:H2	3:L5:2773:G:H22	1.58	0.51
3:L5:3950:U:H3	3:L5:4063:U:H3	1.59	0.51
4:L7:55:A:H4'	15:LJ:155:HIS:HB2	1.92	0.51
13:LH:118:LEU:HD11	13:LH:167:VAL:HG22	1.93	0.51
68:S2:1550:G:H3'	68:S2:1579:A:H61	1.75	0.51
69:SR:5:ARG:HB2	69:SR:10:LYS:HE2	1.93	0.51
3:L5:1333:A:H2'	3:L5:1334:A:C8	2.46	0.51
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.46	0.51
48:Ls:133:GLU:HG2	48:Ls:134:LYS:HD2	1.93	0.51
51:SB:74:LEU:HD21	51:SB:86:LEU:HD11	1.92	0.51
60:SO:15:ILE:HG23	60:SO:16:SER:H	1.75	0.51
68:S2:1398:G:H1'	83:Sg:63:SER:HB2	1.91	0.51
68:S2:1597:C:H4'	68:S2:1603:G:O6	2.11	0.51
76:SS:47:LYS:HE3	76:SS:79:ILE:HA	1.92	0.51
84:CB:654:PRO:HD2	84:CB:658:GLY:HA3	1.92	0.51
3:L5:182:G:H2'	3:L5:183:C:H4'	1.92	0.51
3:L5:5002:U:H2'	3:L5:5003:U:H6	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LB:117:ARG:HA	7:LB:177:LYS:HD2	1.92	0.51
23:LS:82:LEU:HA	23:LS:127:MET:HG2	1.93	0.51
68:S2:1850:MA6:H8	68:S2:1850:MA6:O5'	2.11	0.51
79:SZ:99:LEU:HD11	79:SZ:102:LYS:HE2	1.93	0.51
83:Sg:133:ASN:HB3	83:Sg:139:LYS:HD2	1.93	0.51
3:L5:153:G:H2'	3:L5:154:G:H8	1.76	0.50
3:L5:1180:C:H5''	3:L5:1180:C:C6	2.45	0.50
3:L5:1248:C:H2'	3:L5:1249:C:C6	2.46	0.50
3:L5:3607:U:H2'	3:L5:3608:A:C8	2.46	0.50
3:L5:3954:A:H1'	3:L5:4058:U:H5'	1.93	0.50
3:L5:4260:U:H2'	3:L5:4261:C:C6	2.47	0.50
3:L5:4680:G:H2'	3:L5:4681:A:C8	2.46	0.50
7:LB:59:GLU:HB2	7:LB:366:LYS:HE2	1.92	0.50
23:LS:15:ARG:HB3	23:LS:27:LEU:HD23	1.93	0.50
51:SB:97:LEU:HG	51:SB:229:MET:HE1	1.93	0.50
68:S2:808:A:H2	68:S2:855:G:H22	1.59	0.50
68:S2:835:C:H4'	68:S2:836:G:C8	2.46	0.50
68:S2:980:A:H2'	68:S2:981:A:C8	2.45	0.50
68:S2:1203:G:H2'	68:S2:1204:A:C8	2.46	0.50
68:S2:1491:G:H2'	68:S2:1492:U:C6	2.46	0.50
68:S2:1628:C:H2'	68:S2:1629:C:C6	2.46	0.50
68:S2:1666:C:H2'	68:S2:1667:U:O4'	2.10	0.50
69:SR:58:MET:O	69:SR:62:GLN:HG2	2.11	0.50
3:L5:1514:U:H2'	3:L5:1515:A:C8	2.46	0.50
3:L5:4070:U:H2'	3:L5:4071:U:H6	1.76	0.50
27:LW:97:LYS:HG3	27:LW:99:GLU:H	1.76	0.50
30:LZ:115:LYS:O	30:LZ:119:GLU:HG2	2.11	0.50
38:Lh:99:GLU:HA	38:Lh:102:LEU:HD22	1.93	0.50
48:Ls:187:LEU:HD23	48:Ls:187:LEU:H	1.76	0.50
51:SB:171:ILE:HD11	51:SB:197:ILE:HD13	1.92	0.50
68:S2:496:C:H2'	68:S2:497:C:H6	1.75	0.50
68:S2:976:G:H2'	68:S2:977:C:C6	2.46	0.50
68:S2:1623:A:C6	76:SS:132:ARG:HD3	2.46	0.50
68:S2:1670:C:H2'	68:S2:1671:G:H8	1.76	0.50
3:L5:1695:U:H2'	3:L5:1696:C:C6	2.46	0.50
3:L5:5024:C:H41	3:L5:5028:G:N2	2.07	0.50
7:LB:224:LYS:HG2	7:LB:340:THR:HG22	1.92	0.50
8:LC:218:ILE:HA	8:LC:229:LEU:HD22	1.93	0.50
53:SE:80:ILE:HG23	53:SE:81:THR:HG23	1.93	0.50
55:SH:30:LEU:HG	55:SH:33:ASN:HD22	1.77	0.50
60:SO:146:ARG:NH1	68:S2:1857:G:H3'	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SY:35:VAL:HG23	64:SY:40:ILE:HD11	1.94	0.50
68:S2:323:C:H2'	68:S2:327:G:H1	1.76	0.50
68:S2:1399:C:H2'	68:S2:1400:U:H6	1.77	0.50
71:SF:70:GLU:HA	71:SF:73:THR:HG22	1.94	0.50
77:ST:77:LYS:HG3	77:ST:94:ARG:HH21	1.76	0.50
3:L5:2897:G:H2'	3:L5:2898:G:H8	1.77	0.50
68:S2:1298:G:H4'	74:SP:78:THR:HA	1.93	0.50
69:SR:16:ILE:HD11	69:SR:54:VAL:HG21	1.93	0.50
84:CB:305:MET:HE1	84:CB:333:LYS:HA	1.94	0.50
3:L5:163:A:H2'	3:L5:164:G:H8	1.76	0.50
3:L5:1478:C:H2'	3:L5:1479:G:H8	1.77	0.50
3:L5:4363:A:H5''	45:Lo:36:GLN:HG2	1.93	0.50
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.47	0.50
51:SB:123:ALA:HB2	51:SB:165:ARG:HG3	1.93	0.50
53:SE:198:ARG:NH1	53:SE:200:ARG:HH21	2.10	0.50
66:Sb:72:ARG:HH12	68:S2:1120:U:H5'	1.77	0.50
68:S2:1424:G:H2'	68:S2:1425:G:H8	1.76	0.50
75:SQ:43:GLU:HB2	75:SQ:44:PRO:HD3	1.94	0.50
76:SS:43:VAL:HG21	77:ST:36:THR:HG23	1.92	0.50
83:Sg:40:ILE:HD11	83:Sg:66:VAL:HG21	1.93	0.50
85:CA:154:LEU:HD21	85:CA:332:ARG:HB2	1.92	0.50
3:L5:1669:A:H4'	3:L5:1685:G:N2	2.26	0.50
3:L5:3868:G:H22	3:L5:3900:G:H1'	1.76	0.50
3:L5:4688:C:H2'	3:L5:4689:PSU:C6	2.46	0.50
12:LG:103:ARG:HD3	12:LG:195:HIS:CE1	2.46	0.50
68:S2:525:A:H2'	68:S2:526:A:C8	2.46	0.50
85:CA:89:PHE:HE1	85:CA:242:GLN:HE22	1.58	0.50
3:L5:2495:U:H2'	3:L5:2496:G:C8	2.47	0.50
3:L5:4967:A:H2'	3:L5:4968:A:H8	1.76	0.50
3:L5:5024:C:N4	3:L5:5028:G:H21	2.09	0.50
23:LS:127:MET:HB3	24:LT:153:PRO:HG2	1.94	0.50
30:LZ:50:PRO:HD3	30:LZ:68:ILE:HG12	1.93	0.50
56:SI:141:ARG:HD3	56:SI:145:ILE:HG21	1.94	0.50
68:S2:1354:G:H2'	68:S2:1356:G:H21	1.77	0.50
82:Sf:103:LEU:HB2	82:Sf:105:TYR:CE2	2.46	0.50
85:CA:123:HIS:HA	85:CA:319:PHE:HD1	1.76	0.50
3:L5:690:C:H2'	3:L5:691:C:C6	2.47	0.50
3:L5:1824:G:H2'	3:L5:1825:A:C8	2.47	0.50
3:L5:4685:U:H2'	3:L5:4686:G:C8	2.47	0.50
3:L5:4935:C:H2'	3:L5:4936:G:C8	2.47	0.50
6:LA:115:CYS:SG	6:LA:124:GLY:HA3	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LO:7:LEU:HB2	19:LO:31:ARG:HH11	1.75	0.50
23:LS:121:ALA:HA	23:LS:124:ILE:HD12	1.94	0.50
50:SA:180:ARG:HD3	50:SA:184:ARG:CZ	2.41	0.50
50:SA:181:GLU:HG3	50:SA:185:MET:HE3	1.94	0.50
54:SG:87:ARG:HH22	68:S2:162:C:H5'	1.77	0.50
56:SI:83:TYR:HB2	56:SI:202:ILE:HD11	1.94	0.50
60:SO:43:HIS:CD2	60:SO:55:ARG:HB2	2.46	0.50
68:S2:1010:G:H2'	68:S2:1011:A:H8	1.76	0.50
3:L5:1906:U:H2'	3:L5:1907:A:H8	1.77	0.50
3:L5:2661:U:C4	22:LR:118:HIS:CE1	3.00	0.50
3:L5:3911:C:H2'	3:L5:3912:U:C6	2.47	0.50
56:SI:174:CYS:HB2	56:SI:190:LEU:HD21	1.93	0.50
68:S2:525:A:H2'	68:S2:526:A:H8	1.77	0.50
68:S2:640:A:H2'	68:S2:641:A:C8	2.47	0.50
68:S2:746:C:H2'	68:S2:747:U:C6	2.47	0.50
68:S2:1650:A:H5'	75:SQ:139:ALA:HB2	1.92	0.50
3:L5:908:G:H2'	3:L5:909:A:H8	1.77	0.49
3:L5:1097:C:H2'	3:L5:1098:G:C8	2.46	0.49
3:L5:2676:A:OP2	3:L5:2676:A:H8	1.95	0.49
3:L5:2706:G:H22	3:L5:2709:C:H5'	1.77	0.49
3:L5:3867:A2M:H2'	3:L5:3868:G:C8	2.47	0.49
3:L5:4991:U:H2'	3:L5:4992:G:C8	2.47	0.49
22:LR:105:LEU:HD23	22:LR:138:LEU:HD23	1.93	0.49
50:SA:38:ILE:HD12	50:SA:47:TYR:HB3	1.93	0.49
68:S2:1591:C:H5'	71:SF:85:LYS:HE3	1.93	0.49
84:CB:76:SER:HB2	84:CB:454:MET:HE1	1.93	0.49
85:CA:105:LEU:HD21	85:CA:315:PHE:HB3	1.94	0.49
19:LO:61:ARG:HA	19:LO:70:PRO:HD2	1.93	0.49
34:Ld:64:ILE:HG23	34:Ld:68:LEU:HD23	1.93	0.49
68:S2:5:U:H2'	68:S2:6:G:H8	1.76	0.49
68:S2:145:G:H2'	68:S2:146:G:C8	2.48	0.49
68:S2:349:A:H2'	68:S2:350:C:C6	2.48	0.49
70:SD:72:VAL:HG22	72:SK:68:TYR:HD1	1.76	0.49
3:L5:2295:C:H2'	3:L5:2296:G:H8	1.77	0.49
3:L5:3732:A:H2'	3:L5:3733:A:H8	1.77	0.49
3:L5:5053:U:H5'	3:L5:5054:C:C4	2.47	0.49
48:Ls:178:LEU:HB3	48:Ls:180:ILE:HG23	1.94	0.49
50:SA:197:VAL:HG13	50:SA:201:LEU:HD23	1.93	0.49
68:S2:550:C:H2'	68:S2:551:U:C6	2.46	0.49
3:L5:268:G:H2'	3:L5:269:G:C8	2.46	0.49
3:L5:710:G:H2'	3:L5:711:A:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4389:C:H2'	3:L5:4390:A:H8	1.76	0.49
10:LE:95:PRO:HA	10:LE:104:THR:HG22	1.94	0.49
40:Lj:27:TYR:HA	40:Lj:34:CYS:HA	1.94	0.49
55:SH:33:ASN:HD21	55:SH:37:LYS:HG2	1.77	0.49
75:SQ:58:LEU:HB2	75:SQ:63:PHE:HE1	1.77	0.49
77:ST:12:GLN:HG2	77:ST:16:ARG:HH21	1.78	0.49
10:LE:277:LEU:HA	10:LE:281:ILE:HD11	1.93	0.49
50:SA:42:LYS:HB3	50:SA:48:ILE:HD11	1.93	0.49
61:SV:17:CYS:HB2	61:SV:56:CYS:HB3	1.93	0.49
65:Sa:51:ARG:NH1	80:Sc:63:ARG:HG2	2.27	0.49
3:L5:71:C:H1'	16:LL:62:PRO:O	2.13	0.49
3:L5:1504:G:H2'	3:L5:1505:C:H6	1.77	0.49
5:L8:81:C:H5'	38:Lh:3:LYS:HE3	1.93	0.49
51:SB:87:ILE:H	51:SB:101:HIS:HB2	1.78	0.49
68:S2:1423:C:H41	75:SQ:4:LYS:HA	1.78	0.49
84:CB:488:PHE:CZ	84:CB:490:HIS:HB2	2.48	0.49
3:L5:491:G:H2'	3:L5:492:U:C6	2.48	0.49
3:L5:1323:A2M:H2'	3:L5:1324:A:O4'	2.12	0.49
3:L5:2540:C:H2'	3:L5:2541:G:H8	1.77	0.49
3:L5:2732:G:H2'	3:L5:2733:C:C6	2.48	0.49
3:L5:4273:A:H2'	3:L5:4274:A:C8	2.48	0.49
26:LV:45:ILE:HG21	26:LV:53:PRO:HB3	1.94	0.49
52:SC:210:PRO:HD3	52:SC:236:PHE:CE2	2.47	0.49
56:SI:37:LYS:HB2	56:SI:59:ARG:HG2	1.94	0.49
79:SZ:99:LEU:HD11	79:SZ:102:LYS:HB2	1.93	0.49
84:CB:653:GLY:HA2	84:CB:660:ASN:HB2	1.93	0.49
3:L5:398:A2M:O5'	3:L5:398:A2M:H8	2.12	0.49
3:L5:1248:C:H2'	3:L5:1249:C:H6	1.78	0.49
3:L5:4389:C:H2'	3:L5:4390:A:C8	2.47	0.49
5:L8:94:G:H21	40:Lj:82:THR:HB	1.76	0.49
64:SY:12:PHE:HD1	64:SY:23:MET:HB3	1.78	0.49
68:S2:609:U:H2'	68:S2:610:G:H8	1.78	0.49
68:S2:907:G:H2'	68:S2:908:A:C8	2.48	0.49
68:S2:1174:PSU:H2'	68:S2:1175:G:H8	1.77	0.49
68:S2:1858:G:H2'	68:S2:1859:A:H8	1.78	0.49
84:CB:745:TYR:HE2	84:CB:812:CYS:HB3	1.76	0.49
3:L5:1508:A:H5''	8:LC:113:ARG:HD2	1.95	0.49
3:L5:2743:A:H2'	3:L5:2744:A:C8	2.48	0.49
3:L5:4723:A:H2'	3:L5:4724:A:C8	2.48	0.49
29:LY:85:VAL:HG11	29:LY:99:ILE:HD11	1.94	0.49
68:S2:528:A:H2'	68:S2:529:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1661:A:H8	81:Sd:14:PHE:HB2	1.78	0.49
70:SD:136:VAL:HG12	70:SD:186:VAL:HG22	1.94	0.49
76:SS:5:ILE:HD11	76:SS:9:PHE:CD1	2.48	0.49
3:L5:512:U:O4	3:L5:647:G:O6	2.31	0.49
3:L5:1194:G:H2'	3:L5:1195:G:H8	1.78	0.49
3:L5:2640:G:H2'	3:L5:2641:A:H8	1.78	0.49
3:L5:3709:U:H2'	3:L5:3710:G:O4'	2.12	0.49
3:L5:3726:A:H2'	3:L5:3727:A:C8	2.48	0.49
6:LA:28:ARG:HE	6:LA:123:ARG:HG3	1.77	0.49
10:LE:136:HIS:HB2	10:LE:138:ARG:HH12	1.78	0.49
53:SE:44:LEU:HD11	53:SE:70:ILE:HG21	1.94	0.49
68:S2:352:U:H2'	68:S2:353:C:C6	2.48	0.49
68:S2:468:A2M:HM'3	68:S2:468:A2M:H1'	1.57	0.49
68:S2:940:U:H3	68:S2:1002:U:H3	1.58	0.49
68:S2:1538:C:H2'	68:S2:1539:U:C6	2.47	0.49
68:S2:1658:G:H5'	81:Sd:33:LYS:HD2	1.94	0.49
71:SF:91:ARG:HD2	79:SZ:103:HIS:CE1	2.48	0.49
74:SP:87:PRO:HB3	74:SP:112:ILE:HD13	1.94	0.49
78:SU:93:SER:H	78:SU:97:ILE:HD11	1.77	0.49
3:L5:1962:A:H2	3:L5:2024:G:H21	1.60	0.48
3:L5:2831:G:H2'	3:L5:2832:A:H8	1.77	0.48
3:L5:4457:PSU:H1'	7:LB:252:ALA:HB3	1.95	0.48
3:L5:4571:A2M:H2'	3:L5:4572:U:H6	1.78	0.48
3:L5:4611:A:H2	13:LH:120:GLU:HB3	1.78	0.48
3:L5:4742:G:H2'	3:L5:4743:G:C8	2.48	0.48
35:Le:7:LEU:HB2	35:Le:93:LYS:HB3	1.95	0.48
50:SA:51:LEU:HA	50:SA:54:THR:HG22	1.95	0.48
51:SB:40:ASN:HD21	51:SB:76:ASN:HB2	1.78	0.48
51:SB:85:LYS:HB2	51:SB:101:HIS:HB3	1.93	0.48
51:SB:125:VAL:HG22	51:SB:137:LEU:HB2	1.95	0.48
54:SG:50:VAL:HG12	54:SG:113:ILE:HA	1.94	0.48
55:SH:66:VAL:HG11	68:S2:913:A:N3	2.27	0.48
57:SJ:136:ARG:HA	57:SJ:141:VAL:HA	1.95	0.48
62:SW:22:LYS:HA	66:Sb:3:LEU:HB3	1.95	0.48
68:S2:432:G:H2'	68:S2:433:A:C8	2.48	0.48
68:S2:508:A:H3'	68:S2:509:OMG:C8	2.46	0.48
84:CB:420:LEU:HD11	84:CB:463:ASP:HB2	1.94	0.48
85:CA:153:ALA:HA	85:CA:156:LEU:HG	1.94	0.48
3:L5:138:G:H2'	3:L5:139:G:C8	2.47	0.48
3:L5:398:A2M:HM'3	3:L5:398:A2M:H1'	1.61	0.48
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1751:A:H2'	3:L5:1752:G:H8	1.78	0.48
3:L5:2765:A:H2'	3:L5:2766:A:C8	2.47	0.48
3:L5:4069:U:H2'	3:L5:4070:U:C6	2.49	0.48
3:L5:5002:U:H2'	3:L5:5003:U:C6	2.48	0.48
41:Lk:35:LYS:HB3	41:Lk:42:LEU:HD11	1.94	0.48
47:Lr:58:LYS:HG3	47:Lr:83:ASN:HD21	1.79	0.48
56:SI:83:TYR:HB3	56:SI:101:ILE:HB	1.94	0.48
74:SP:81:ARG:HB2	74:SP:117:GLY:HA3	1.94	0.48
84:CB:626:GLN:NE2	84:CB:631:ARG:HB2	2.29	0.48
84:CB:697:MET:HE1	84:CB:702:PHE:HZ	1.78	0.48
3:L5:498:C:C2	3:L5:499:G:H1'	2.49	0.48
3:L5:2634:C:H2'	3:L5:2635:U:H6	1.78	0.48
13:LH:93:ARG:HD2	13:LH:143:GLU:HG3	1.94	0.48
63:SX:17:ARG:HH22	68:S2:659:G:H21	1.58	0.48
68:S2:382:C:H2'	68:S2:383:G:C8	2.48	0.48
68:S2:458:A:H2'	68:S2:459:C:H6	1.77	0.48
3:L5:178:C:H2'	3:L5:179:G:H8	1.78	0.48
3:L5:1504:G:H2'	3:L5:1505:C:C6	2.47	0.48
3:L5:4401:G:H2'	3:L5:4402:C:H6	1.78	0.48
4:L7:58:A:H2'	4:L7:59:G:H8	1.76	0.48
9:LD:55:VAL:HG11	9:LD:158:LYS:HE3	1.95	0.48
9:LD:181:PRO:HD2	9:LD:195:HIS:CD2	2.48	0.48
19:LO:81:TRP:HB2	19:LO:104:VAL:HG21	1.95	0.48
36:Lf:45:LYS:NZ	36:Lf:108:SER:HA	2.29	0.48
54:SG:81:HIS:CE1	68:S2:1790:A:H5''	2.48	0.48
68:S2:561:A:H2'	68:S2:562:U:C6	2.48	0.48
68:S2:639:C:H2'	68:S2:640:A:C8	2.48	0.48
68:S2:1240:A:C2	74:SP:100:LYS:HB3	2.49	0.48
3:L5:137:G:H2'	3:L5:138:G:H8	1.77	0.48
3:L5:3595:U:H5''	3:L5:3597:G:OP2	2.14	0.48
3:L5:4319:C:H2'	3:L5:4320:G:C8	2.49	0.48
6:LA:107:MET:HE1	6:LA:113:VAL:HG11	1.95	0.48
7:LB:206:PRO:HG2	7:LB:209:GLN:HG2	1.94	0.48
13:LH:61:TRP:CZ3	17:LM:33:GLN:HG3	2.49	0.48
14:LI:87:MET:HG2	14:LI:138:ILE:HG12	1.95	0.48
50:SA:173:LEU:HD11	50:SA:177:MET:HE3	1.94	0.48
52:SC:68:ARG:HG2	52:SC:277:HIS:HB2	1.94	0.48
67:Se:5:SER:HB3	67:Se:8:ARG:HH21	1.78	0.48
68:S2:1172:U:H2'	68:S2:1173:A:H8	1.79	0.48
71:SF:55:ARG:HH21	75:SQ:125:ARG:HD3	1.77	0.48
3:L5:1333:A:H2'	3:L5:1334:A:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1951:G:H1'	23:LS:117:HIS:HE1	1.78	0.48
3:L5:4523:A2M:H5''	3:L5:4524:G:H5'	1.95	0.48
4:L7:110:G:H2'	4:L7:111:C:C6	2.48	0.48
14:LI:47:PRO:HD2	14:LI:141:LYS:HA	1.96	0.48
37:Lg:83:CYS:SG	37:Lg:86:CYS:HB2	2.54	0.48
68:S2:495:U:H2'	68:S2:496:C:O4'	2.14	0.48
68:S2:1134:G:H2'	68:S2:1135:C:C6	2.49	0.48
75:SQ:97:GLN:HB2	75:SQ:105:LYS:HD2	1.96	0.48
84:CB:513:ASN:HD21	84:CB:515:ALA:HB3	1.78	0.48
3:L5:318:A:H2'	3:L5:319:A:H8	1.79	0.48
3:L5:2845:A:H61	3:L5:3843:C:N4	2.12	0.48
3:L5:3597:G:H2'	3:L5:3598:C:H6	1.78	0.48
54:SG:175:LYS:HG3	68:S2:77:A:H2	1.79	0.48
56:SI:36:THR:O	56:SI:95:THR:HA	2.14	0.48
68:S2:149:A:N7	68:S2:169:U:O2	2.47	0.48
68:S2:300:U:H2'	68:S2:301:A:H8	1.79	0.48
68:S2:1801:A:H2'	68:S2:1802:C:H6	1.78	0.48
3:L5:958:G:H21	10:LE:125:LEU:H	1.61	0.48
3:L5:1323:A2M:HM'3	3:L5:1323:A2M:H1'	1.51	0.48
3:L5:1992:U:H4'	3:L5:1993:C:H5''	1.95	0.48
3:L5:3825:A2M:H1'	3:L5:3825:A2M:HM'3	1.54	0.48
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.49	0.48
4:L7:4:U:H2'	4:L7:5:A:H8	1.79	0.48
52:SC:113:GLN:HG2	68:S2:11:A:H4'	1.95	0.48
55:SH:93:VAL:HG21	55:SH:133:LEU:HD12	1.96	0.48
66:Sb:22:LYS:HE3	68:S2:1129:G:H5''	1.96	0.48
68:S2:348:A:H2'	68:S2:349:A:C8	2.48	0.48
68:S2:544:G:H2'	68:S2:545:A:C8	2.48	0.48
68:S2:1398:G:H22	68:S2:1448:A:H2	1.62	0.48
70:SD:70:THR:HG22	70:SD:86:LEU:HD13	1.96	0.48
84:CB:395:MET:HE2	84:CB:494:MET:HE2	1.95	0.48
3:L5:187:U:H2'	3:L5:245:C:H1'	1.95	0.48
3:L5:1683:PSU:H2'	3:L5:1684:A:C8	2.49	0.48
3:L5:3736:A:H2'	3:L5:3737:A:H8	1.79	0.48
22:LR:160:GLU:HA	22:LR:163:ARG:HG2	1.95	0.48
52:SC:70:VAL:HG21	52:SC:93:ILE:HG23	1.95	0.48
53:SE:62:LYS:HB2	53:SE:80:ILE:HD12	1.95	0.48
68:S2:496:C:H2'	68:S2:497:C:C6	2.49	0.48
84:CB:727:ARG:HG2	84:CB:854:PHE:HD1	1.78	0.48
3:L5:135:G:H5''	38:Lh:96:ASN:HB2	1.96	0.48
3:L5:2079:G:H2'	3:L5:2080:U:H6	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3720:G:H22	3:L5:3733:A:H2	1.61	0.48
3:L5:3744:OMG:HM23	3:L5:3744:OMG:H1'	1.71	0.48
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.48	0.48
51:SB:113:MET:HB3	51:SB:142:PHE:CE2	2.49	0.48
56:SI:110:ARG:HH21	56:SI:123:ARG:HH11	1.61	0.48
57:SJ:63:LEU:HD23	57:SJ:70:ARG:HB2	1.95	0.48
68:S2:1144:A:H5'	68:S2:1355:C:H42	1.78	0.48
68:S2:1406:G:H2'	68:S2:1407:U:C6	2.49	0.48
68:S2:1687:C:H2'	68:S2:1688:C:C6	2.49	0.48
71:SF:95:HIS:CD2	79:SZ:106:GLN:HB3	2.48	0.48
82:Sf:108:VAL:HB	82:Sf:112:GLY:HA2	1.96	0.48
3:L5:907:C:H2'	3:L5:908:G:C8	2.47	0.47
3:L5:4591:U:H2'	3:L5:4592:C:C6	2.49	0.47
17:LM:36:ALA:HB3	17:LM:55:MET:HE1	1.96	0.47
68:S2:562:U:H2'	68:S2:563:G:C8	2.49	0.47
68:S2:1217:A:H2'	68:S2:1218:C:C6	2.49	0.47
76:SS:124:ARG:HH21	76:SS:129:LEU:HB3	1.79	0.47
3:L5:1494:U:H2'	3:L5:1495:G:C8	2.49	0.47
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.13	0.47
3:L5:2654:C:H2'	3:L5:2655:C:H6	1.79	0.47
3:L5:3848:U:H2'	3:L5:3849:A:C8	2.49	0.47
3:L5:4336:A:H5''	3:L5:4337:C:H5'	1.96	0.47
3:L5:4448:G:H5''	3:L5:4449:A:H5'	1.96	0.47
13:LH:24:THR:HA	13:LH:37:ASP:HA	1.96	0.47
68:S2:929:G:H2'	68:S2:930:C:O4'	2.14	0.47
71:SF:108:PRO:HA	71:SF:111:VAL:HG12	1.96	0.47
80:Sc:17:VAL:HA	80:Sc:30:VAL:HG23	1.95	0.47
84:CB:27:HIS:HB3	84:CB:30:HIS:CD2	2.49	0.47
84:CB:524:LEU:HD22	84:CB:546:ILE:HD11	1.96	0.47
3:L5:2293:U:H2'	3:L5:2294:G:C8	2.49	0.47
3:L5:2815:A2M:H2'	3:L5:2816:G:C8	2.49	0.47
10:LE:190:HIS:HB3	10:LE:193:PHE:HD2	1.79	0.47
53:SE:61:VAL:HG13	53:SE:80:ILE:HD11	1.96	0.47
58:SL:23:VAL:HG23	58:SL:25:LEU:HG	1.96	0.47
68:S2:1392:U:H2'	68:S2:1393:G:H8	1.79	0.47
3:L5:318:A:H2'	3:L5:319:A:C8	2.50	0.47
3:L5:1563:A:H2'	3:L5:1564:A:C8	2.49	0.47
3:L5:2656:U:H5''	30:LZ:38:TYR:HB3	1.94	0.47
51:SB:64:GLY:HA2	51:SB:87:ILE:HD11	1.96	0.47
54:SG:67:VAL:HG12	54:SG:69:THR:HG22	1.95	0.47
56:SI:56:ARG:HA	56:SI:180:GLY:HA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:469:C:H2'	3:L5:470:A:H8	1.80	0.47
3:L5:1327:C:H2'	3:L5:1328:G:H8	1.79	0.47
3:L5:4736:C:H2'	3:L5:4737:G:H8	1.79	0.47
53:SE:191:ARG:HD2	53:SE:245:ARG:NH1	2.29	0.47
68:S2:28:U:H2'	68:S2:29:G:C8	2.49	0.47
68:S2:671:A:H4'	68:S2:672:A:H5''	1.96	0.47
68:S2:1775:U:H2'	68:S2:1776:G:C8	2.49	0.47
3:L5:162:A:H2'	3:L5:163:A:C8	2.50	0.47
3:L5:441:G:H2'	3:L5:442:G:H8	1.80	0.47
3:L5:490:C:H2'	3:L5:491:G:H8	1.80	0.47
3:L5:1306:C:H2'	3:L5:1307:A:C8	2.48	0.47
3:L5:1822:U:H2'	3:L5:1823:G:H8	1.79	0.47
3:L5:3923:A:H2'	3:L5:3924:C:C6	2.50	0.47
4:L7:7:G:H5''	9:LD:22:ARG:HD3	1.95	0.47
29:LY:47:MET:HE3	29:LY:48:PRO:HD2	1.95	0.47
57:SJ:5:ARG:HG3	68:S2:38:A:OP1	2.14	0.47
68:S2:166:A2M:HM'3	68:S2:166:A2M:H1'	1.49	0.47
68:S2:1222:G:H2'	68:S2:1223:A:C8	2.49	0.47
68:S2:1711:U:H2'	68:S2:1712:A:H8	1.80	0.47
68:S2:1797:U:H2'	68:S2:1798:C:C6	2.49	0.47
75:SQ:133:GLY:HA3	75:SQ:140:ARG:NH1	2.30	0.47
81:Sd:39:CYS:HB2	81:Sd:42:CYS:N	2.26	0.47
83:Sg:8:ARG:HH11	83:Sg:311:GLN:HG3	1.78	0.47
3:L5:99:A:H2'	3:L5:100:C:O2	2.15	0.47
3:L5:737:C:C5	3:L5:739:G:H5''	2.50	0.47
3:L5:1538:U:H2'	3:L5:1539:G:H8	1.80	0.47
3:L5:1806:G:H2'	3:L5:1807:C:C6	2.50	0.47
3:L5:4239:A:H2'	3:L5:4240:G:H8	1.78	0.47
3:L5:4392:OMG:N3	3:L5:4447:5MC:HM52	2.29	0.47
3:L5:4759:C:H2'	3:L5:4760:G:C8	2.50	0.47
3:L5:4920:C:H2'	3:L5:4921:C:C6	2.49	0.47
5:L8:119:C:H2'	5:L8:120:G:H8	1.78	0.47
21:LQ:176:ARG:HA	21:LQ:180:ARG:HG3	1.95	0.47
36:Lf:36:ARG:HB2	36:Lf:80:ASN:HA	1.96	0.47
53:SE:15:PRO:HG3	53:SE:39:ARG:HD3	1.97	0.47
58:SL:7:GLU:OE2	58:SL:11:GLN:HG2	2.15	0.47
68:S2:319:C:H2'	68:S2:320:G:H8	1.80	0.47
68:S2:649:PSU:H2'	68:S2:650:A:H8	1.80	0.47
68:S2:1388:A:H61	70:SD:161:GLY:HA3	1.80	0.47
69:SR:9:VAL:HG23	69:SR:50:ILE:HA	1.97	0.47
70:SD:29:LEU:HB2	70:SD:34:TYR:HB2	1.96	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	1.96	0.47
84:CB:189:ILE:HD11	84:CB:204:MET:HA	1.95	0.47
3:L5:1822:U:H2'	3:L5:1823:G:C8	2.49	0.47
48:Ls:91:THR:HG21	48:Ls:98:ILE:HG13	1.97	0.47
61:SV:11:LEU:HD23	61:SV:11:LEU:H	1.80	0.47
66:Sb:47:PHE:CE2	66:Sb:49:HIS:HB2	2.50	0.47
68:S2:5:U:H2'	68:S2:6:G:C8	2.50	0.47
68:S2:882:U:H1'	68:S2:905:C:C2	2.49	0.47
68:S2:941:C:H2'	68:S2:942:G:C8	2.50	0.47
68:S2:1470:C:H2'	68:S2:1471:C:H6	1.80	0.47
68:S2:1531:A:H2'	68:S2:1532:C:C6	2.50	0.47
82:Sf:121:CYS:HB2	82:Sf:145:CYS:HB3	1.56	0.47
3:L5:2448:G:H2'	3:L5:2449:A:C8	2.50	0.47
3:L5:3945:A:H2'	3:L5:3946:G:C8	2.50	0.47
3:L5:4098:A:N7	3:L5:4099:G:H1'	2.30	0.47
53:SE:100:ARG:HB2	53:SE:114:ILE:HD13	1.96	0.47
60:SO:134:PRO:HB3	68:S2:944:A:H5''	1.97	0.47
68:S2:945:U:H2'	68:S2:946:U:C6	2.49	0.47
68:S2:1545:A:H2'	68:S2:1546:G:C8	2.49	0.47
68:S2:1692:U:H2'	68:S2:1693:G:C8	2.49	0.47
68:S2:1716:C:H2'	68:S2:1717:C:H6	1.80	0.47
3:L5:1461:C:H2'	3:L5:1462:A:H8	1.79	0.47
3:L5:2021:G:H4'	48:Ls:84:GLY:C	2.40	0.47
3:L5:4524:G:C2	7:LB:252:ALA:HB1	2.50	0.47
40:Lj:19:CYS:SG	40:Lj:34:CYS:HB2	2.54	0.47
53:SE:41:CYS:HA	53:SE:85:GLY:HA2	1.96	0.47
54:SG:7:PHE:CE2	54:SG:9:ALA:HB3	2.50	0.47
60:SO:26:ASN:HD21	65:Sa:58:VAL:HG21	1.80	0.47
66:Sb:45:THR:HG23	66:Sb:82:LYS:HE3	1.96	0.47
68:S2:15:U:H2'	68:S2:16:G:O4'	2.15	0.47
68:S2:1590:C:H42	75:SQ:77:HIS:CE1	2.33	0.47
68:S2:1651:A:H2'	68:S2:1652:G:H8	1.79	0.47
3:L5:272:U:H2'	3:L5:273:U:C6	2.50	0.46
3:L5:444:G:H2'	3:L5:445:U:C6	2.50	0.46
3:L5:755:C:H2'	3:L5:756:G:H8	1.80	0.46
3:L5:2633:U:H2'	3:L5:2634:C:C6	2.51	0.46
3:L5:3615:G:H1'	27:LW:44:ARG:HD2	1.98	0.46
3:L5:4299:PSU:H2'	3:L5:4300:U:H6	1.80	0.46
3:L5:4578:G:H2'	3:L5:4579:PSU:C6	2.50	0.46
3:L5:5025:C:H42	3:L5:5027:C:H42	1.62	0.46
6:LA:54:ARG:HG2	6:LA:56:ALA:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LM:100:ARG:HA	17:LM:103:LYS:HG2	1.97	0.46
48:Ls:61:MET:O	48:Ls:65:ILE:HG12	2.14	0.46
51:SB:65:ARG:HG2	60:SO:50:LYS:HD3	1.97	0.46
52:SC:206:SER:HB2	52:SC:210:PRO:HG2	1.97	0.46
54:SG:174:PRO:HB3	68:S2:65:C:C6	2.49	0.46
63:SX:88:ASP:HA	68:S2:617:G:H4'	1.97	0.46
68:S2:454:U:H2'	68:S2:455:A:C8	2.51	0.46
68:S2:1392:U:H2'	68:S2:1393:G:C8	2.50	0.46
68:S2:1423:C:C5	75:SQ:4:LYS:HG2	2.50	0.46
68:S2:1780:G:H3'	68:S2:1781:A:C8	2.45	0.46
84:CB:66:ARG:HB2	84:CB:68:ILE:HG22	1.96	0.46
3:L5:270:U:H2'	3:L5:271:C:H6	1.80	0.46
3:L5:1281:G:C6	10:LE:128:HIS:HB2	2.50	0.46
3:L5:2385:U:H2'	3:L5:2386:U:C6	2.50	0.46
7:LB:219:VAL:HG11	7:LB:337:VAL:HG13	1.97	0.46
36:Lf:41:PHE:HE1	36:Lf:110:ILE:HD13	1.79	0.46
55:SH:87:PHE:HB3	55:SH:90:LYS:HG3	1.96	0.46
61:SV:16:LYS:HG2	61:SV:23:ILE:HD13	1.96	0.46
61:SV:32:ILE:HD13	61:SV:60:ARG:HE	1.80	0.46
63:SX:124:LYS:HG2	63:SX:129:SER:HA	1.97	0.46
68:S2:344:U:H2'	68:S2:345:U:C6	2.51	0.46
68:S2:931:C:H2'	68:S2:932:G:C8	2.50	0.46
84:CB:609:PHE:CZ	84:CB:661:ILE:HG12	2.50	0.46
3:L5:979:C:OP2	10:LE:66:LYS:HD3	2.16	0.46
3:L5:1316:OMG:HM23	3:L5:1316:OMG:H1'	1.70	0.46
3:L5:1995:G:H4'	49:Lt:128:THR:HB	1.98	0.46
3:L5:2098:G:H2'	3:L5:2099:G:C8	2.49	0.46
3:L5:3855:C:H2'	3:L5:3856:A:H8	1.80	0.46
5:L8:67:U:H2'	5:L8:68:G:C8	2.48	0.46
9:LD:56:THR:HG22	9:LD:57:ASN:H	1.81	0.46
10:LE:67:ALA:HA	10:LE:69:TYR:CE2	2.51	0.46
19:LO:14:HIS:CE1	19:LO:119:VAL:HG23	2.49	0.46
21:LQ:50:ARG:HH12	21:LQ:140:SER:HB2	1.79	0.46
40:Lj:60:GLY:HA2	40:Lj:64:MET:SD	2.55	0.46
51:SB:57:ILE:HG13	51:SB:59:SER:H	1.80	0.46
57:SJ:46:VAL:HG13	57:SJ:102:ILE:HD11	1.98	0.46
58:SL:111:VAL:HG11	58:SL:128:VAL:HG11	1.98	0.46
64:SY:104:ARG:HG3	64:SY:107:ARG:HH21	1.80	0.46
68:S2:141:A:H4'	68:S2:142:C:H3'	1.96	0.46
71:SF:39:ILE:HG22	71:SF:41:VAL:HG23	1.97	0.46
83:Sg:7:LEU:HB2	83:Sg:310:TRP:CZ3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:215:C:H5''	3:L5:216:C:H5''	1.97	0.46
3:L5:269:G:H2'	3:L5:270:U:C6	2.50	0.46
3:L5:419:A:H61	5:L8:15:G:H1'	1.80	0.46
3:L5:701:G:H2'	3:L5:702:U:C6	2.51	0.46
3:L5:1194:G:H2'	3:L5:1195:G:C8	2.50	0.46
3:L5:3830:A2M:H1'	3:L5:3830:A2M:HM'3	1.51	0.46
33:Lc:48:LEU:HD21	33:Lc:60:ILE:HG21	1.96	0.46
49:Lt:62:LEU:HB3	49:Lt:73:VAL:HG23	1.96	0.46
49:Lt:123:ARG:HD2	49:Lt:129:ILE:HD11	1.96	0.46
68:S2:1212:G:H2'	68:S2:1213:C:C6	2.51	0.46
68:S2:1688:C:H2'	68:S2:1689:C:H6	1.81	0.46
84:CB:37:ASP:CG	84:CB:55:ARG:HG2	2.40	0.46
84:CB:55:ARG:HD2	84:CB:55:ARG:HA	1.72	0.46
3:L5:161:G:H2'	3:L5:162:A:H8	1.79	0.46
3:L5:1086:C:H2'	3:L5:1087:A:C8	2.49	0.46
3:L5:1190:C:H2'	3:L5:1191:C:C6	2.51	0.46
3:L5:2256:C:H2'	3:L5:2257:C:O4'	2.15	0.46
3:L5:4508:C:N3	3:L5:4512:U:H5	2.13	0.46
8:LC:207:PRO:HB3	8:LC:249:PHE:CD2	2.51	0.46
37:Lg:33:LEU:HD23	37:Lg:33:LEU:HA	1.78	0.46
54:SG:195:LYS:NZ	68:S2:126:G:H5'	2.30	0.46
68:S2:835:C:H5'	68:S2:836:G:H5'	1.98	0.46
68:S2:1031:A2M:HM'3	68:S2:1031:A2M:H1'	1.56	0.46
68:S2:1588:A:H2'	68:S2:1589:A:H8	1.81	0.46
68:S2:1593:C:H2'	68:S2:1594:A:H8	1.81	0.46
68:S2:1633:A:H2'	68:S2:1634:A:C8	2.50	0.46
3:L5:499:G:H2'	3:L5:499:G:N3	2.30	0.46
3:L5:667:A:H5''	3:L5:668:C:H5''	1.97	0.46
3:L5:1725:U:H2'	3:L5:1726:U:H6	1.80	0.46
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.50	0.46
3:L5:2385:U:H2'	3:L5:2386:U:H6	1.81	0.46
3:L5:4364:G:H2'	3:L5:4365:C:C6	2.51	0.46
4:L7:23:A:H2'	4:L7:24:C:C6	2.51	0.46
9:LD:182:GLY:HA2	9:LD:194:VAL:HG23	1.98	0.46
14:LI:43:VAL:HG21	14:LI:197:VAL:HG13	1.97	0.46
30:LZ:41:ALA:HB2	30:LZ:77:TYR:HE1	1.80	0.46
51:SB:144:LYS:HB2	51:SB:208:HIS:HB3	1.98	0.46
68:S2:601:OMG:HM23	68:S2:601:OMG:H1'	1.65	0.46
68:S2:1687:C:H2'	68:S2:1688:C:H6	1.80	0.46
78:SU:20:ILE:HD12	78:SU:116:ILE:HA	1.97	0.46
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1806:G:H2'	3:L5:1807:C:H6	1.80	0.46
23:LS:15:ARG:HD2	23:LS:25:PRO:HG2	1.96	0.46
27:LW:102:LYS:HA	27:LW:105:ARG:HE	1.80	0.46
50:SA:38:ILE:HD11	50:SA:150:THR:HG22	1.98	0.46
62:SW:53:ILE:HG12	66:Sb:24:LEU:HD21	1.97	0.46
68:S2:573:U:O2	68:S2:576:A2M:H8	2.14	0.46
68:S2:1338:G:H2'	68:S2:1339:U:H6	1.81	0.46
68:S2:1546:G:H22	68:S2:1655:C:H1'	1.81	0.46
85:CA:31:VAL:HG21	85:CA:56:ILE:HD11	1.97	0.46
3:L5:256:G:H2'	3:L5:257:C:C6	2.50	0.46
3:L5:302:C:H2'	3:L5:303:C:C6	2.50	0.46
3:L5:513:U:H1'	3:L5:516:C:H41	1.79	0.46
3:L5:2570:U:H2'	3:L5:2571:C:C6	2.51	0.46
3:L5:3611:A:H4'	56:SI:92:ARG:CZ	2.46	0.46
3:L5:3841:OMC:HM23	3:L5:3841:OMC:H1'	1.76	0.46
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.49	0.46
6:LA:180:LEU:HD21	46:Lp:22:LEU:HB3	1.98	0.46
9:LD:179:ARG:HD3	9:LD:179:ARG:HA	1.70	0.46
64:SY:13:MET:HE3	64:SY:22:GLN:HE21	1.80	0.46
68:S2:77:A:H2'	68:S2:78:C:C6	2.51	0.46
68:S2:434:G:H2'	68:S2:435:A:C8	2.51	0.46
68:S2:907:G:H2'	68:S2:908:A:H8	1.81	0.46
68:S2:1616:U:H2'	68:S2:1617:G:C8	2.50	0.46
3:L5:267:G:H2'	3:L5:268:G:C8	2.50	0.46
3:L5:411:G:H5''	3:L5:414:C:H1'	1.97	0.46
3:L5:1366:G:N2	16:LL:33:ILE:HD13	2.30	0.46
3:L5:1858:A:H2'	3:L5:1859:C:H6	1.81	0.46
3:L5:3722:G:H2'	3:L5:3723:A:C8	2.50	0.46
3:L5:3746:A:H5''	6:LA:244:GLY:HA3	1.98	0.46
3:L5:4392:OMG:HM23	3:L5:4392:OMG:H1'	1.73	0.46
3:L5:4530:UR3:H2'	3:L5:4531:U:H2'	1.97	0.46
68:S2:639:C:H2'	68:S2:640:A:H8	1.81	0.46
77:ST:28:LEU:HG	77:ST:106:ALA:HB1	1.96	0.46
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.51	0.46
3:L5:1461:C:H2'	3:L5:1462:A:C8	2.51	0.46
3:L5:2732:G:H2'	3:L5:2733:C:H6	1.81	0.46
3:L5:3664:G:H2'	3:L5:3665:G:H8	1.81	0.46
9:LD:216:GLU:O	9:LD:220:LYS:HG2	2.16	0.46
15:LJ:32:ARG:HA	15:LJ:35:ARG:HH21	1.80	0.46
31:La:102:ASP:HA	31:La:125:LYS:HB2	1.98	0.46
51:SB:90:ASP:HB2	51:SB:228:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SG:140:ARG:HA	54:SG:143:LYS:HG2	1.97	0.46
57:SJ:138:ARG:HH21	57:SJ:153:SER:HA	1.81	0.46
68:S2:494:C:H42	68:S2:509:OMG:HN22	1.62	0.46
3:L5:2521:G:H2'	3:L5:2522:G:H8	1.81	0.45
3:L5:3883:U:H2'	3:L5:3884:PSU:C6	2.50	0.45
3:L5:4299:PSU:H2'	3:L5:4300:U:C6	2.52	0.45
11:LF:26:ALA:O	11:LF:30:ILE:HG12	2.16	0.45
58:SL:17:PHE:CD2	68:S2:222:U:H5''	2.51	0.45
68:S2:458:A:H2'	68:S2:459:C:C6	2.51	0.45
68:S2:462:OMC:HM23	68:S2:462:OMC:H1'	1.79	0.45
68:S2:644:OMG:HM23	68:S2:644:OMG:H1'	1.72	0.45
3:L5:1084:C:H2'	3:L5:1085:C:H6	1.80	0.45
3:L5:2080:U:H2'	3:L5:2081:C:C6	2.50	0.45
3:L5:2741:U:OP2	6:LA:50:HIS:HE1	2.00	0.45
3:L5:3856:A:H5''	20:LP:83:TRP:O	2.16	0.45
3:L5:3952:A:H2'	3:L5:3953:G:C4	2.51	0.45
12:LG:182:CYS:HB3	12:LG:222:ILE:HD12	1.98	0.45
16:LL:58:ILE:HG12	16:LL:157:VAL:HG13	1.99	0.45
20:LP:107:LEU:HB2	20:LP:152:GLU:OE2	2.16	0.45
21:LQ:178:ARG:N	31:La:51:GLY:HA2	2.32	0.45
54:SG:70:HIS:HA	54:SG:98:ARG:HH12	1.81	0.45
68:S2:120:U:H2'	68:S2:121:OMU:H6	1.97	0.45
72:SK:3:MET:HG2	72:SK:44:HIS:HD2	1.81	0.45
72:SK:41:PRO:HG2	72:SK:44:HIS:ND1	2.31	0.45
76:SS:40:TYR:CZ	76:SS:97:GLN:HG2	2.51	0.45
77:ST:114:GLU:HG2	77:ST:115:LYS:O	2.16	0.45
83:Sg:89:LEU:HB2	83:Sg:101:PHE:HE1	1.81	0.45
83:Sg:93:THR:HG22	83:Sg:94:THR:HG23	1.98	0.45
3:L5:397:G:N2	20:LP:22:LEU:HD22	2.30	0.45
3:L5:921:C:H2'	3:L5:922:C:C6	2.52	0.45
3:L5:1354:A:OP2	21:LQ:87:THR:HG23	2.16	0.45
3:L5:3732:A:H2'	3:L5:3733:A:C8	2.51	0.45
3:L5:4743:G:H2'	3:L5:4744:A:C8	2.51	0.45
5:L8:5:U:H2'	5:L8:6:C:H6	1.81	0.45
8:LC:134:PRO:HG3	8:LC:150:LEU:HD13	1.98	0.45
15:LJ:57:VAL:HG12	15:LJ:60:PHE:H	1.81	0.45
46:Lp:26:VAL:HG22	46:Lp:30:GLU:HG3	1.98	0.45
54:SG:106:LEU:HD13	54:SG:109:LEU:HD21	1.97	0.45
56:SI:133:GLU:HA	56:SI:136:ILE:HG12	1.98	0.45
68:S2:1213:C:H2'	68:S2:1214:A:C8	2.52	0.45
68:S2:1338:G:H2'	68:S2:1339:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1500:G:H2'	68:S2:1501:C:C6	2.52	0.45
68:S2:1671:G:H2'	68:S2:1672:U:H6	1.82	0.45
70:SD:66:ILE:HD13	70:SD:66:ILE:HA	1.84	0.45
83:Sg:39:THR:HG23	83:Sg:60:ARG:HG2	1.98	0.45
3:L5:1878:G:H2'	3:L5:1879:C:C6	2.51	0.45
3:L5:2608:G:H2'	3:L5:2609:G:H8	1.81	0.45
3:L5:4563:U:H2'	3:L5:4564:A:H8	1.81	0.45
5:L8:106:G:H4'	5:L8:137:A:H5'	1.97	0.45
22:LR:170:ARG:NH1	22:LR:174:GLU:HG2	2.31	0.45
41:Lk:61:PRO:HA	41:Lk:62:PRO:HD3	1.89	0.45
53:SE:38:LEU:HA	53:SE:41:CYS:SG	2.57	0.45
62:SW:3:ARG:HH12	62:SW:28:ARG:HH21	1.65	0.45
64:SY:126:GLY:HA2	64:SY:129:LYS:HG2	1.98	0.45
68:S2:155:G:H2'	68:S2:156:G:C8	2.52	0.45
68:S2:159:A2M:HM'3	68:S2:159:A2M:H1'	1.51	0.45
68:S2:174:OMC:HM23	68:S2:174:OMC:H1'	1.70	0.45
68:S2:386:C:H2'	68:S2:387:C:C6	2.51	0.45
68:S2:527:C:H2'	68:S2:528:A:C8	2.50	0.45
68:S2:543:C:H3'	68:S2:544:G:H8	1.81	0.45
68:S2:1533:A:H2	68:S2:1536:G:N3	2.15	0.45
68:S2:1600:G:OP1	79:SZ:44:LEU:HD22	2.16	0.45
77:ST:28:LEU:HD12	77:ST:110:LEU:HD22	1.98	0.45
83:Sg:101:PHE:CD2	83:Sg:136:GLY:HA2	2.52	0.45
3:L5:3700:C:H2'	3:L5:3746:A:H61	1.81	0.45
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.51	0.45
25:LU:29:VAL:HG11	25:LU:36:ALA:HB2	1.98	0.45
55:SH:43:LEU:HD11	55:SH:71:SER:HB3	1.98	0.45
61:SV:73:ALA:HB1	61:SV:78:ILE:HB	1.99	0.45
68:S2:29:G:H2'	68:S2:30:C:C6	2.51	0.45
68:S2:51:U:H2'	68:S2:52:G:H8	1.82	0.45
68:S2:1457:U:H2'	68:S2:1458:G:C8	2.52	0.45
83:Sg:150:TRP:HB2	83:Sg:170:TRP:CD1	2.51	0.45
3:L5:1511:U:H2'	3:L5:1512:G:H8	1.81	0.45
3:L5:2465:C:H2'	3:L5:2466:G:O4'	2.16	0.45
3:L5:4063:U:H2'	3:L5:4064:C:C2	2.51	0.45
3:L5:4196:OMG:HM23	3:L5:4196:OMG:H1'	1.69	0.45
28:LX:148:ASP:HA	28:LX:151:ASN:HD22	1.81	0.45
52:SC:275:LYS:HG3	52:SC:276:THR:HG23	1.98	0.45
55:SH:31:GLU:HA	55:SH:37:LYS:HG3	1.99	0.45
68:S2:149:A:H3'	68:S2:150:A:H8	1.81	0.45
68:S2:886:A:H2'	68:S2:887:U:O4'	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1558:C:H2'	68:S2:1559:C:C6	2.52	0.45
74:SP:20:VAL:HG13	74:SP:24:GLN:HE21	1.81	0.45
74:SP:133:ILE:HG22	74:SP:134:GLY:H	1.81	0.45
84:CB:402:VAL:HG13	84:CB:411:TYR:HB2	1.97	0.45
84:CB:447:ILE:HG12	84:CB:472:LEU:HD13	1.99	0.45
3:L5:426:A:H2'	3:L5:427:A:H8	1.81	0.45
3:L5:659:G:H2'	3:L5:660:A:C8	2.50	0.45
3:L5:676:C:H2'	3:L5:677:G:H8	1.81	0.45
3:L5:1091:C:H2'	3:L5:1092:G:C8	2.51	0.45
3:L5:1377:G:H4'	3:L5:1378:C:H3'	1.98	0.45
3:L5:2730:U:H2'	3:L5:2731:C:C6	2.52	0.45
3:L5:4727:A:H2'	3:L5:4728:U:O4'	2.17	0.45
4:L7:57:C:H2'	4:L7:58:A:H8	1.82	0.45
7:LB:46:PHE:CZ	7:LB:84:MET:HG3	2.51	0.45
8:LC:284:MET:HE3	21:LQ:28:LEU:HB3	1.99	0.45
51:SB:52:THR:HG23	51:SB:57:ILE:HA	1.99	0.45
60:SO:146:ARG:HH12	68:S2:1857:G:H3'	1.82	0.45
68:S2:1134:G:H2'	68:S2:1135:C:H6	1.81	0.45
68:S2:1510:G:H2'	68:S2:1511:U:O4'	2.17	0.45
68:S2:1713:C:H2'	68:S2:1714:U:C6	2.52	0.45
75:SQ:134:GLY:HA3	75:SQ:140:ARG:CA	2.41	0.45
85:CA:194:VAL:HG22	85:CA:196:ASP:H	1.82	0.45
3:L5:422:C:H2'	3:L5:423:G:H8	1.82	0.45
3:L5:1081:C:O2'	3:L5:1082:C:H5'	2.16	0.45
3:L5:3628:G:H2'	3:L5:3629:A:H8	1.81	0.45
3:L5:4935:C:H2'	3:L5:4936:G:H8	1.81	0.45
8:LC:163:LYS:HE3	8:LC:163:LYS:HB3	1.80	0.45
18:LN:140:LYS:HD3	18:LN:140:LYS:HA	1.66	0.45
52:SC:256:TRP:CE2	62:SW:68:ARG:HD3	2.52	0.45
59:SN:40:LEU:HD23	59:SN:43:LYS:HE3	1.98	0.45
68:S2:668:A2M:H1'	68:S2:668:A2M:HM'3	1.48	0.45
68:S2:1442:OMU:HM23	68:S2:1442:OMU:H1'	1.78	0.45
76:SS:22:GLY:HA2	76:SS:56:ALA:HB3	1.99	0.45
83:Sg:25:PRO:HA	83:Sg:293:ALA:HB2	1.99	0.45
84:CB:57:THR:HA	84:CB:73:THR:HG21	1.99	0.45
3:L5:173:C:H2'	3:L5:174:C:C6	2.51	0.45
3:L5:1405:C:H2'	3:L5:1406:G:H8	1.82	0.45
3:L5:3867:A2M:HM'3	3:L5:3867:A2M:H1'	1.41	0.45
3:L5:4454:G:H2'	3:L5:4455:G:C8	2.52	0.45
3:L5:4507:A:H2'	3:L5:4508:C:C6	2.51	0.45
30:LZ:109:LYS:HB3	30:LZ:109:LYS:HE2	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:694:G:H2'	68:S2:695:C:O4'	2.17	0.45
68:S2:1018:U:H2'	68:S2:1019:C:C6	2.52	0.45
68:S2:1457:U:H2'	68:S2:1458:G:H8	1.81	0.45
71:SF:122:ARG:NH1	71:SF:193:LYS:HZ1	2.15	0.45
79:SZ:49:LEU:HD23	79:SZ:49:LEU:HA	1.89	0.45
80:Sc:31:ARG:HD3	80:Sc:43:ILE:HG13	1.98	0.45
83:Sg:19:THR:HG21	83:Sg:66:VAL:O	2.17	0.45
83:Sg:153:CYS:SG	83:Sg:198:VAL:HG12	2.56	0.45
84:CB:451:ILE:HG22	84:CB:460:PRO:HA	1.99	0.45
3:L5:1176:C:H2'	3:L5:1177:U:C6	2.52	0.45
3:L5:2374:A:H5'	34:Ld:64:ILE:O	2.17	0.45
3:L5:2648:G:H2'	3:L5:2649:G:H8	1.80	0.45
3:L5:3920:PSU:H2'	3:L5:3921:U:C6	2.51	0.45
3:L5:4454:G:H1	3:L5:4526:U:H3	1.64	0.45
7:LB:288:GLY:HA3	7:LB:330:PHE:CE1	2.52	0.45
22:LR:170:ARG:HH12	22:LR:174:GLU:HG2	1.81	0.45
57:SJ:65:GLU:O	57:SJ:66:LYS:HG2	2.17	0.45
64:SY:20:ARG:HD2	64:SY:74:MET:HE3	1.97	0.45
64:SY:120:THR:O	64:SY:124:ASN:HB2	2.16	0.45
68:S2:379:C:H2'	68:S2:380:G:C8	2.52	0.45
68:S2:1547:C:H1'	68:S2:1670:C:H4'	1.99	0.45
68:S2:1634:A:H2'	68:S2:1635:C:O4'	2.17	0.45
84:CB:609:PHE:CD2	84:CB:699:GLY:HA2	2.52	0.45
3:L5:133:C:C4	38:Lh:74:LYS:HG3	2.52	0.44
3:L5:139:G:H2'	3:L5:140:G:H8	1.82	0.44
3:L5:423:G:H2'	3:L5:424:U:C6	2.52	0.44
3:L5:1764:G:H4'	3:L5:1769:G:C6	2.52	0.44
3:L5:1976:G:H21	49:Lt:139:VAL:HG12	1.81	0.44
3:L5:2664:G:H4'	3:L5:2677:G:H4'	1.99	0.44
3:L5:4927:G:H5''	3:L5:4928:C:C5	2.52	0.44
24:LT:27:LEU:HB3	24:LT:31:MET:HE3	1.99	0.44
54:SG:78:SER:H	54:SG:81:HIS:HD2	1.65	0.44
62:SW:94:LEU:HD21	62:SW:102:ILE:HG13	1.98	0.44
68:S2:162:C:H2'	68:S2:163:U:O4'	2.17	0.44
68:S2:433:A:H2'	68:S2:434:G:C8	2.51	0.44
68:S2:1139:C:H2'	68:S2:1140:G:O4'	2.17	0.44
68:S2:1198:G:H2'	68:S2:1199:A:C8	2.53	0.44
83:Sg:245:ARG:HD2	83:Sg:247:TRP:CD2	2.52	0.44
84:CB:386:LYS:HD3	84:CB:386:LYS:HA	1.84	0.44
3:L5:2358:G:H2'	3:L5:2359:U:O4'	2.17	0.44
3:L5:3951:G:H2'	3:L5:3952:A:C4	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LL:48:PRO:HB2	38:Lh:120:ALA:HB2	1.99	0.44
68:S2:155:G:H2'	68:S2:156:G:H8	1.80	0.44
68:S2:323:C:H4'	68:S2:324:C:C5	2.52	0.44
68:S2:958:G:H2'	68:S2:959:G:C8	2.52	0.44
68:S2:1415:C:H2'	68:S2:1416:C:C6	2.52	0.44
83:Sg:107:ASP:HB2	83:Sg:125:ARG:HD2	1.99	0.44
84:CB:746:LEU:HB2	84:CB:815:ASP:OD2	2.17	0.44
3:L5:750:U:H1'	3:L5:917:A:C8	2.52	0.44
3:L5:1645:C:H2'	3:L5:1646:A:C8	2.52	0.44
3:L5:1846:G:H2'	3:L5:1847:C:H6	1.82	0.44
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.53	0.44
3:L5:2648:G:H2'	3:L5:2649:G:C8	2.52	0.44
3:L5:2726:G:H2'	3:L5:2727:C:C6	2.52	0.44
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.16	0.44
6:LA:229:ALA:HB3	6:LA:234:LYS:HB3	1.99	0.44
19:LO:47:PHE:HA	19:LO:136:ALA:HB2	1.99	0.44
36:Lf:48:ALA:HB2	36:Lf:71:TRP:CZ3	2.53	0.44
42:Ll:28:ARG:HA	42:Ll:33:ASN:HD22	1.82	0.44
52:SC:166:ARG:HG2	52:SC:181:PRO:HG3	2.00	0.44
55:SH:145:ARG:HG2	62:SW:51:GLU:OE1	2.17	0.44
68:S2:696:G:H21	68:S2:737:G:N2	2.15	0.44
68:S2:1705:C:H2'	68:S2:1706:G:C8	2.53	0.44
84:CB:403:PRO:HA	84:CB:410:PHE:HD1	1.81	0.44
84:CB:622:VAL:HG13	84:CB:631:ARG:HD3	1.99	0.44
85:CA:75:ALA:H	85:CA:112:VAL:HA	1.82	0.44
3:L5:1683:PSU:H2'	3:L5:1684:A:H8	1.82	0.44
3:L5:2634:C:H2'	3:L5:2635:U:C6	2.52	0.44
3:L5:3606:U:H2'	3:L5:3607:U:H6	1.82	0.44
3:L5:4965:U:H4'	3:L5:4966:A:H5'	2.00	0.44
20:LP:131:ARG:HG3	20:LP:137:ASN:OD1	2.16	0.44
24:LT:44:GLY:HA2	24:LT:95:HIS:HB3	1.98	0.44
37:Lg:41:ALA:O	37:Lg:52:ARG:HD3	2.17	0.44
41:Lk:14:THR:HA	41:Lk:17:ARG:HD3	1.99	0.44
68:S2:484:A2M:H8	68:S2:484:A2M:O5'	2.17	0.44
68:S2:1256:G:H1	81:Sd:31:ILE:HG12	1.83	0.44
84:CB:654:PRO:HD3	84:CB:660:ASN:HD22	1.81	0.44
85:CA:12:ILE:HG13	85:CA:18:VAL:HG22	2.00	0.44
3:L5:233:U:O2'	3:L5:234:G:H2'	2.18	0.44
3:L5:270:U:H2'	3:L5:271:C:C6	2.53	0.44
3:L5:302:C:H2'	3:L5:303:C:H6	1.83	0.44
3:L5:1185:G:O2'	3:L5:1186:U:H5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1431:C:H2'	3:L5:1432:G:O4'	2.17	0.44
3:L5:1577:G:H5'	3:L5:1578:U:H5''	1.99	0.44
3:L5:2709:C:N4	85:CA:257:LEU:H	2.14	0.44
3:L5:4454:G:H2'	3:L5:4455:G:H8	1.81	0.44
3:L5:4590:A2M:HM'3	3:L5:4590:A2M:H1'	1.59	0.44
6:LA:75:LEU:HD12	6:LA:75:LEU:HA	1.84	0.44
10:LE:285:LYS:HE2	10:LE:285:LYS:HB3	1.68	0.44
33:Lc:38:ILE:HG21	33:Lc:63:TYR:HB3	1.99	0.44
59:SN:13:GLN:NE2	66:Sb:21:LYS:HE2	2.33	0.44
68:S2:554:A:O2'	68:S2:555:A:H8	1.99	0.44
68:S2:897:U:C4	68:S2:898:U:H1'	2.53	0.44
68:S2:1772:C:P	68:S2:1773:C:H5''	2.58	0.44
68:S2:1795:G:H2'	68:S2:1796:G:H8	1.83	0.44
70:SD:72:VAL:HB	72:SK:20:VAL:HG11	1.98	0.44
73:SM:128:PHE:O	73:SM:132:LYS:HG2	2.18	0.44
74:SP:68:PRO:O	74:SP:71:GLU:HG2	2.18	0.44
3:L5:139:G:H2'	3:L5:140:G:C8	2.52	0.44
3:L5:480:C:H2'	3:L5:481:G:H8	1.81	0.44
3:L5:1541:C:H5''	6:LA:21:LYS:HG2	2.00	0.44
3:L5:3861:A:H2'	3:L5:3862:A:C8	2.52	0.44
3:L5:4113:U:H4'	3:L5:4115:G:C5	2.52	0.44
7:LB:378:ARG:HE	27:LW:32:LEU:HD21	1.82	0.44
27:LW:83:THR:N	54:SG:130:PRO:HB2	2.32	0.44
52:SC:256:TRP:CD2	62:SW:68:ARG:HD3	2.51	0.44
54:SG:81:HIS:HE1	68:S2:1790:A:H5''	1.82	0.44
55:SH:53:VAL:HG12	55:SH:175:GLY:HA3	2.00	0.44
56:SI:41:ARG:CZ	68:S2:305:U:H4'	2.48	0.44
58:SL:77:VAL:HA	58:SL:88:ILE:HG22	1.99	0.44
62:SW:86:LEU:HB3	62:SW:117:ARG:NH2	2.33	0.44
68:S2:1806:A:H2'	68:S2:1807:C:C6	2.53	0.44
77:ST:104:LEU:HD23	77:ST:121:ARG:HH11	1.83	0.44
83:Sg:69:VAL:HG12	83:Sg:80:SER:HB3	1.99	0.44
3:L5:457:G:H2'	3:L5:458:C:C6	2.53	0.44
3:L5:2538:U:H2'	3:L5:2539:C:C6	2.53	0.44
3:L5:3611:A:C2	3:L5:5016:A:H8	2.36	0.44
3:L5:3748:A:H5''	6:LA:243:THR:HB	2.00	0.44
3:L5:4311:A:H2'	3:L5:4312:PSU:H6	1.83	0.44
3:L5:4927:G:H5''	3:L5:4928:C:H5	1.82	0.44
3:L5:4934:A:H2'	3:L5:4935:C:C6	2.52	0.44
5:L8:144:U:H2'	5:L8:145:C:C6	2.53	0.44
8:LC:7:LEU:HG	8:LC:21:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Lt:123:ARG:HH21	49:Lt:126:SER:N	2.15	0.44
51:SB:81:PHE:CG	51:SB:109:LYS:HE3	2.53	0.44
68:S2:291:G:H2'	68:S2:292:A:C8	2.53	0.44
68:S2:1320:G:H2'	68:S2:1321:G:O4'	2.17	0.44
68:S2:1541:G:H2'	68:S2:1542:C:C6	2.53	0.44
68:S2:1653:U:H2'	68:S2:1654:G:C8	2.53	0.44
84:CB:228:PHE:HA	84:CB:231:MET:HE3	1.99	0.44
84:CB:781:MET:HE3	84:CB:781:MET:HB3	1.83	0.44
3:L5:755:C:H2'	3:L5:756:G:C8	2.53	0.44
3:L5:1247:U:H2'	3:L5:1248:C:C6	2.53	0.44
3:L5:1278:C:H2'	3:L5:1279:A:O4'	2.18	0.44
3:L5:1514:U:H2'	3:L5:1515:A:H8	1.83	0.44
3:L5:2293:U:H2'	3:L5:2294:G:H8	1.82	0.44
3:L5:4678:G:N2	3:L5:4713:G:H1'	2.33	0.44
8:LC:242:PRO:HG3	8:LC:248:ARG:HD2	1.99	0.44
10:LE:264:ILE:HG23	10:LE:267:LEU:HB2	2.00	0.44
12:LG:125:LYS:HD3	12:LG:125:LYS:HA	1.82	0.44
49:Lt:16:ARG:HE	49:Lt:17:CYS:H	1.64	0.44
50:SA:124:VAL:HB	50:SA:146:ALA:CB	2.48	0.44
50:SA:220:LYS:HA	50:SA:220:LYS:HD3	1.83	0.44
56:SI:147:LYS:HD2	56:SI:147:LYS:HA	1.84	0.44
67:Se:32:ALA:HB2	68:S2:525:A:H5''	1.99	0.44
68:S2:29:G:H2'	68:S2:30:C:H6	1.83	0.44
68:S2:339:A:H2'	68:S2:340:C:H5	1.83	0.44
68:S2:1018:U:H2'	68:S2:1019:C:H6	1.83	0.44
68:S2:1208:A:H2'	68:S2:1209:A:H8	1.82	0.44
68:S2:1339:U:H2'	68:S2:1340:U:C6	2.53	0.44
68:S2:1678:A:H2'	68:S2:1679:A:N3	2.33	0.44
71:SF:204:ARG:NH2	80:Sc:60:GLU:HB2	2.32	0.44
74:SP:28:MET:HG3	74:SP:32:GLN:HE21	1.82	0.44
83:Sg:73:SER:HB3	83:Sg:117:ASN:HD21	1.81	0.44
84:CB:24:VAL:HG12	84:CB:126:LEU:HB3	2.00	0.44
3:L5:426:A:H2'	3:L5:427:A:C8	2.53	0.44
3:L5:497:G:H1	3:L5:657:C:H42	1.66	0.44
3:L5:700:G:C2	3:L5:701:G:C5	3.05	0.44
3:L5:1468:C:H2'	3:L5:1469:C:C6	2.53	0.44
3:L5:2045:G:O2'	3:L5:2046:G:H5''	2.17	0.44
3:L5:3832:U:H2'	3:L5:3833:C:C6	2.53	0.44
3:L5:4064:C:H2'	3:L5:4065:G:H8	1.83	0.44
3:L5:4920:C:H2'	3:L5:4921:C:H6	1.82	0.44
10:LE:183:ARG:HA	10:LE:183:ARG:HD2	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:LG:98:LEU:HA	12:LG:101:LYS:HZ3	1.83	0.44
13:LH:114:ILE:HB	13:LH:124:ARG:HB2	2.00	0.44
19:LO:168:TYR:CE2	19:LO:172:LYS:HD2	2.53	0.44
48:Ls:141:LEU:HD11	48:Ls:171:GLU:HG3	2.00	0.44
49:Lt:61:LYS:HA	49:Lt:75:PRO:HD2	1.99	0.44
55:SH:6:ALA:HB3	55:SH:28:LEU:HD13	1.99	0.44
68:S2:16:G:H2'	68:S2:17:C:C6	2.53	0.44
68:S2:1278:A:H2'	68:S2:1279:C:C6	2.52	0.44
69:SR:73:LEU:HA	69:SR:76:GLU:OE2	2.17	0.44
74:SP:75:VAL:HG22	74:SP:93:MET:HB3	2.00	0.44
74:SP:96:VAL:HG11	74:SP:117:GLY:HA2	1.99	0.44
3:L5:677:G:H2'	3:L5:678:C:C6	2.53	0.43
11:LF:41:MET:HE2	32:Lb:113:ALA:HB2	1.99	0.43
12:LG:103:ARG:HG3	12:LG:193:LEU:O	2.18	0.43
14:LI:183:ASP:O	14:LI:187:LYS:HG2	2.18	0.43
20:LP:52:THR:HG23	20:LP:85:LYS:HG3	1.99	0.43
35:Le:35:TRP:CZ2	35:Le:56:PRO:HD2	2.53	0.43
47:Lr:103:ARG:HD3	47:Lr:103:ARG:HA	1.79	0.43
53:SE:49:ARG:HE	53:SE:49:ARG:HB3	1.66	0.43
54:SG:133:LEU:HD12	68:S2:65:C:C2	2.52	0.43
54:SG:225:GLN:HA	54:SG:228:ILE:HG22	1.99	0.43
55:SH:25:GLN:HE21	55:SH:29:GLU:HG2	1.83	0.43
62:SW:26:LEU:HB2	66:Sb:7:LEU:HD23	1.99	0.43
63:SX:60:LYS:HD3	63:SX:60:LYS:HA	1.72	0.43
63:SX:90:CYS:HA	63:SX:93:PHE:HD2	1.83	0.43
68:S2:352:U:H2'	68:S2:353:C:H6	1.82	0.43
68:S2:498:C:H2'	68:S2:499:G:C8	2.53	0.43
68:S2:996:A:H2'	68:S2:997:A:H8	1.82	0.43
3:L5:300:A:H2'	3:L5:301:G:C8	2.48	0.43
3:L5:710:G:H2'	3:L5:711:A:C8	2.53	0.43
3:L5:1270:A:H8	3:L5:2106:G:H21	1.64	0.43
3:L5:1307:A:H2'	3:L5:1308:C:H6	1.83	0.43
3:L5:1340:OMC:HM23	3:L5:1340:OMC:H1'	1.71	0.43
3:L5:1628:C:OP2	6:LA:9:ARG:HD2	2.18	0.43
3:L5:1693:U:H2'	3:L5:1694:C:O4'	2.18	0.43
3:L5:2815:A2M:HM'3	3:L5:2815:A2M:H1'	1.47	0.43
3:L5:2897:G:H2'	3:L5:2898:G:C8	2.52	0.43
3:L5:3917:A:H2'	3:L5:3918:G:C8	2.51	0.43
3:L5:4089:G:H2'	3:L5:4090:G:C8	2.52	0.43
3:L5:5004:C:H2'	3:L5:5005:G:O4'	2.17	0.43
4:L7:4:U:H2'	4:L7:5:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LB:66:LYS:HB2	26:LV:14:PHE:HE2	1.83	0.43
13:LH:41:ILE:HG22	13:LH:43:VAL:HG13	1.99	0.43
30:LZ:9:LYS:HD2	30:LZ:83:THR:O	2.18	0.43
48:Ls:50:LYS:HZ3	48:Ls:98:ILE:HD12	1.81	0.43
68:S2:115:U:H2'	68:S2:116:OMU:C6	2.48	0.43
68:S2:186:C:H2'	68:S2:187:G:H8	1.83	0.43
68:S2:300:U:H2'	68:S2:301:A:C8	2.54	0.43
68:S2:1047:C:H2'	68:S2:1048:G:O4'	2.18	0.43
68:S2:1289:U:C5	82:Sf:97:LYS:HE2	2.52	0.43
68:S2:1587:G:N7	77:ST:67:ARG:HD2	2.32	0.43
68:S2:1653:U:H3	68:S2:1671:G:H1	1.66	0.43
76:SS:25:LYS:HD3	76:SS:55:ARG:HD3	1.98	0.43
85:CA:237:ALA:HB1	85:CA:308:LEU:HB3	2.00	0.43
3:L5:269:G:H2'	3:L5:270:U:H6	1.82	0.43
3:L5:1095:A:H2	3:L5:1200:G:N1	2.06	0.43
3:L5:1175:A:H2	3:L5:1185:G:N2	2.16	0.43
3:L5:2095:A:H1'	3:L5:2096:G:N2	2.34	0.43
3:L5:3765:G:H21	3:L5:3766:A:N6	2.16	0.43
3:L5:4089:G:H2'	3:L5:4090:G:H8	1.83	0.43
3:L5:4523:A2M:H1'	3:L5:4558:U:C4	2.53	0.43
3:L5:5062:G:C2	3:L5:5063:G:C8	3.06	0.43
8:LC:279:LEU:HD23	8:LC:279:LEU:HA	1.82	0.43
54:SG:98:ARG:HH11	54:SG:99:GLY:H	1.65	0.43
56:SI:151:GLU:HA	56:SI:154:LYS:HZ2	1.83	0.43
60:SO:31:CYS:HB2	60:SO:93:LEU:HD11	1.99	0.43
60:SO:113:GLN:HG3	65:Sa:46:GLU:HG3	1.99	0.43
68:S2:1004:PSU:H2'	68:S2:1005:G:C8	2.49	0.43
68:S2:1051:G:H2'	68:S2:1052:A:C8	2.53	0.43
68:S2:1114:U:O2'	68:S2:1115:U:H2'	2.18	0.43
68:S2:1208:A:H2'	68:S2:1209:A:C8	2.53	0.43
68:S2:1745:A:H62	68:S2:1789:G:H21	1.66	0.43
70:SD:175:VAL:HB	70:SD:182:LEU:HB3	1.99	0.43
84:CB:330:LYS:HD3	84:CB:334:PRO:HB2	1.99	0.43
84:CB:498:LYS:HB3	84:CB:498:LYS:HE3	1.86	0.43
3:L5:480:C:H2'	3:L5:481:G:C8	2.53	0.43
3:L5:959:G:C8	10:LE:123:ARG:HG2	2.53	0.43
3:L5:2254:G:H4'	3:L5:2255:C:C5	2.54	0.43
3:L5:2335:C:H2'	3:L5:2336:G:H8	1.84	0.43
3:L5:3633:C:H2'	3:L5:3634:G:C8	2.54	0.43
15:LJ:135:GLY:HA2	15:LJ:139:PHE:CE2	2.53	0.43
20:LP:54:GLN:HA	20:LP:83:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Lr:45:HIS:CG	47:Lr:103:ARG:HH22	2.36	0.43
61:SV:32:ILE:HG12	61:SV:60:ARG:HD2	2.01	0.43
68:S2:323:C:H4'	68:S2:324:C:H5	1.82	0.43
68:S2:414:A:H2'	68:S2:415:A:H8	1.82	0.43
68:S2:656:G:N2	68:S2:663:C:H5''	2.33	0.43
71:SF:49:LEU:HD11	75:SQ:49:TYR:HB2	2.00	0.43
76:SS:5:ILE:HD11	76:SS:9:PHE:CG	2.54	0.43
78:SU:20:ILE:HG22	78:SU:91:LEU:HB2	2.00	0.43
83:Sg:270:LEU:HD23	83:Sg:310:TRP:CD2	2.54	0.43
84:CB:207:PRO:HG2	84:CB:261:TRP:CE2	2.53	0.43
84:CB:604:MET:HE2	84:CB:704:VAL:HG22	1.99	0.43
3:L5:162:A:H2'	3:L5:163:A:H8	1.83	0.43
3:L5:1076:C:H2'	3:L5:1077:C:C6	2.53	0.43
3:L5:1195:G:H2'	3:L5:1196:G:H8	1.82	0.43
3:L5:2691:U:H2'	3:L5:2692:U:H6	1.84	0.43
3:L5:3925:OMU:HM23	3:L5:3925:OMU:H1'	1.70	0.43
3:L5:4062:A:H2'	3:L5:4063:U:C6	2.54	0.43
3:L5:4344:U:H2'	3:L5:4345:C:H6	1.82	0.43
14:LI:47:PRO:HB3	14:LI:171:TRP:CZ2	2.53	0.43
29:LY:131:GLU:HA	29:LY:134:LYS:HD3	2.00	0.43
54:SG:55:GLY:HA2	54:SG:110:ASN:HD22	1.84	0.43
57:SJ:113:GLN:HG3	57:SJ:149:VAL:HG21	2.01	0.43
66:Sb:69:GLY:HA3	68:S2:1105:G:O3'	2.18	0.43
68:S2:1101:U:H2'	68:S2:1102:G:H8	1.83	0.43
68:S2:1399:C:H2'	68:S2:1400:U:C6	2.53	0.43
3:L5:455:C:O2'	3:L5:456:C:H5'	2.18	0.43
3:L5:716:C:OP1	8:LC:317:ASN:HB2	2.17	0.43
3:L5:1084:C:H2'	3:L5:1085:C:C6	2.53	0.43
3:L5:3719:A:C4	3:L5:3720:G:C8	3.07	0.43
3:L5:4481:U:H2'	3:L5:4482:U:H6	1.82	0.43
4:L7:58:A:H2'	4:L7:59:G:C8	2.54	0.43
6:LA:130:SER:HB2	6:LA:171:GLY:HA3	1.99	0.43
56:SI:51:GLY:HA3	68:S2:445:A:H5''	1.99	0.43
68:S2:325:C:H3'	68:S2:326:C:H4'	2.00	0.43
68:S2:381:C:H2'	68:S2:382:C:C6	2.54	0.43
68:S2:441:C:H2'	68:S2:442:C:C6	2.54	0.43
68:S2:1703:OMC:H2'	68:S2:1704:C:O4'	2.19	0.43
69:SR:20:TYR:HD2	69:SR:23:ARG:HG3	1.84	0.43
75:SQ:8:GLN:CD	75:SQ:27:ARG:HE	2.25	0.43
76:SS:23:ARG:O	79:SZ:48:VAL:HG21	2.19	0.43
3:L5:679:C:H2'	3:L5:680:G:C8	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4637:OMG:H2'	3:L5:4638:U:C6	2.54	0.43
57:SJ:134:HIS:CE1	57:SJ:164:PRO:HD2	2.54	0.43
58:SL:153:LYS:HD3	58:SL:153:LYS:HA	1.81	0.43
68:S2:26:U:H2'	68:S2:27:A2M:H8	1.99	0.43
68:S2:1189:A:H2'	68:S2:1190:A:H8	1.84	0.43
68:S2:1284:A:C8	73:SM:33:ARG:HG3	2.53	0.43
68:S2:1431:G:H4'	68:S2:1434:C:N4	2.34	0.43
68:S2:1752:C:N4	68:S2:1755:C:H41	2.16	0.43
70:SD:163:PRO:HA	70:SD:166:TYR:CE2	2.53	0.43
73:SM:69:CYS:SG	73:SM:76:LEU:HB2	2.58	0.43
78:SU:50:VAL:HG22	78:SU:91:LEU:HD22	2.01	0.43
84:CB:319:LEU:O	84:CB:321:ILE:HG13	2.19	0.43
1:CD:195:ARG:HD3	68:S2:1489:A:OP2	2.19	0.43
3:L5:1912:G:N2	19:LO:87:MET:HE2	2.33	0.43
3:L5:3619:G:H22	3:L5:3624:A:H1'	1.84	0.43
3:L5:4159:C:H2'	3:L5:4160:C:C6	2.54	0.43
3:L5:4622:A:H2'	3:L5:4623:OMG:C8	2.53	0.43
8:LC:292:ILE:HG23	21:LQ:128:LEU:HD21	2.00	0.43
30:LZ:95:VAL:HG12	30:LZ:110:ALA:HA	2.01	0.43
39:Li:76:ARG:HD3	39:Li:76:ARG:HA	1.76	0.43
49:Lt:48:LYS:HE3	49:Lt:52:ASP:OD1	2.19	0.43
57:SJ:129:LEU:HB3	57:SJ:135:ILE:HD11	1.99	0.43
68:S2:353:C:H2'	68:S2:354:OMU:H6	2.00	0.43
68:S2:611:G:H2'	68:S2:612:U:H6	1.84	0.43
68:S2:1119:A:H3'	68:S2:1120:U:H6	1.82	0.43
68:S2:1253:A:H4'	68:S2:1254:C:H5''	2.00	0.43
68:S2:1689:C:H2'	68:S2:1690:U:H6	1.84	0.43
2:CI:55:LEU:HD22	25:LU:99:TRP:CG	2.53	0.43
3:L5:132:G:H2'	3:L5:133:C:H4'	2.00	0.43
3:L5:400:A2M:H2'	3:L5:401:G:O4'	2.19	0.43
3:L5:441:G:H2'	3:L5:442:G:C8	2.54	0.43
3:L5:500:G:O2'	3:L5:504:G:H3'	2.19	0.43
3:L5:674:G:H2'	3:L5:675:C:C6	2.53	0.43
3:L5:2481:G:H2'	3:L5:2482:C:C6	2.54	0.43
3:L5:2671:C:H2'	3:L5:2672:C:C6	2.54	0.43
3:L5:4344:U:H2'	3:L5:4345:C:C6	2.53	0.43
3:L5:4521:PSU:H1'	7:LB:253:CYS:SG	2.59	0.43
34:Ld:90:ARG:HD3	34:Ld:102:LEU:HD13	2.00	0.43
49:Lt:57:ARG:HG3	49:Lt:83:LYS:HB3	2.01	0.43
51:SB:89:GLU:HB3	51:SB:223:PHE:HE1	1.84	0.43
53:SE:79:ASP:HB3	53:SE:82:TYR:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:SX:17:ARG:NH2	68:S2:659:G:H21	2.17	0.43
64:SY:54:VAL:HG22	64:SY:76:TYR:HB2	2.00	0.43
68:S2:116:OMU:H1'	68:S2:116:OMU:HM23	1.73	0.43
68:S2:342:C:H2'	68:S2:343:A:H8	1.84	0.43
68:S2:1328:OMG:HM23	68:S2:1328:OMG:H1'	1.64	0.43
68:S2:1399:C:H5''	83:Sg:100:ARG:CZ	2.49	0.43
71:SF:122:ARG:HG2	71:SF:146:ARG:NH1	2.34	0.43
71:SF:162:ALA:HB2	71:SF:172:CYS:SG	2.58	0.43
76:SS:66:ARG:O	76:SS:70:ILE:HG12	2.19	0.43
83:Sg:101:PHE:CE2	83:Sg:136:GLY:HA2	2.54	0.43
84:CB:580:ARG:HB2	84:CB:741:MET:HB2	2.01	0.43
85:CA:92:LEU:HD21	85:CA:280:LEU:HB3	2.00	0.43
3:L5:937:U:C6	17:LM:46:ARG:HD2	2.54	0.43
3:L5:4456:OMC:H1'	3:L5:4456:OMC:HM23	1.74	0.43
8:LC:324:ILE:HD13	8:LC:327:LYS:HE2	2.01	0.43
12:LG:120:LYS:HE3	12:LG:125:LYS:HG2	2.01	0.43
49:Lt:59:THR:HA	49:Lt:80:LEU:HD11	2.01	0.43
50:SA:177:MET:HG2	50:SA:180:ARG:HH21	1.84	0.43
53:SE:66:MET:HG3	68:S2:502:C:O4'	2.19	0.43
53:SE:139:LEU:HD22	53:SE:147:ILE:HD11	2.01	0.43
53:SE:192:ILE:HD12	53:SE:243:GLY:HA3	2.00	0.43
55:SH:165:ASN:HA	55:SH:168:HIS:CE1	2.53	0.43
56:SI:110:ARG:NH2	56:SI:123:ARG:HD3	2.34	0.43
60:SO:116:LEU:HA	60:SO:116:LEU:HD12	1.78	0.43
68:S2:448:A:H4'	68:S2:449:A:H5''	2.01	0.43
68:S2:1538:C:H2'	68:S2:1539:U:H6	1.83	0.43
68:S2:1672:U:H2'	68:S2:1673:U:H6	1.84	0.43
68:S2:1706:G:H2'	68:S2:1707:U:H6	1.82	0.43
70:SD:137:VAL:HG22	70:SD:151:LYS:HG3	1.99	0.43
76:SS:34:LYS:HE3	76:SS:34:LYS:HB2	1.85	0.43
85:CA:155:ARG:HD2	85:CA:357:LEU:HB2	2.00	0.43
3:L5:7:C:H2'	3:L5:8:U:C6	2.54	0.42
3:L5:37:U:H2'	3:L5:38:A:O4'	2.19	0.42
3:L5:1662:C:H2'	3:L5:1663:C:H6	1.84	0.42
3:L5:1705:G:H2'	3:L5:1706:A:O4'	2.18	0.42
3:L5:2297:G:H4'	8:LC:242:PRO:HB2	2.00	0.42
3:L5:2588:C:H4'	3:L5:2589:C:H5''	2.01	0.42
3:L5:2611:A:H2'	3:L5:2612:G:C8	2.54	0.42
3:L5:2870:A:H2'	3:L5:2871:A:C8	2.54	0.42
4:L7:60:G:H2'	4:L7:61:G:H8	1.83	0.42
19:LO:124:LEU:HA	19:LO:124:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LP:2:VAL:HG22	20:LP:3:ARG:H	1.84	0.42
36:Lf:92:LEU:HD23	36:Lf:92:LEU:HA	1.85	0.42
37:Lg:22:LEU:HD23	37:Lg:30:ILE:HG21	2.00	0.42
57:SJ:142:VAL:HG12	57:SJ:144:ILE:H	1.84	0.42
68:S2:398:A:H4'	68:S2:399:C:H5''	2.00	0.42
68:S2:556:U:H3'	68:S2:557:U:H4'	2.01	0.42
68:S2:1736:G:H2'	68:S2:1737:G:H8	1.84	0.42
76:SS:138:THR:HA	76:SS:141:ARG:NH2	2.33	0.42
3:L5:190:G:H2'	3:L5:191:G:H8	1.83	0.42
3:L5:433:A:C2	3:L5:3867:A2M:H4'	2.54	0.42
3:L5:701:G:H2'	3:L5:702:U:H6	1.85	0.42
3:L5:1405:C:H2'	3:L5:1406:G:C8	2.55	0.42
3:L5:2521:G:H2'	3:L5:2522:G:C8	2.54	0.42
3:L5:5026:U:C4	56:SI:124:LYS:HD2	2.54	0.42
5:L8:36:G:C5	38:Lh:89:ARG:HD3	2.54	0.42
10:LE:50:LEU:HD12	10:LE:51:VAL:N	2.34	0.42
10:LE:138:ARG:HH21	10:LE:170:SER:HA	1.84	0.42
10:LE:158:ARG:HG2	36:Lf:5:LEU:HD13	2.02	0.42
49:Lt:11:LYS:HA	49:Lt:11:LYS:HD2	1.69	0.42
50:SA:187:GLY:HA2	61:SV:45:ARG:NH1	2.33	0.42
53:SE:124:CYS:HA	53:SE:142:HIS:HE1	1.84	0.42
62:SW:11:LEU:HD23	62:SW:11:LEU:HA	1.87	0.42
62:SW:46:TYR:HB3	62:SW:69:LEU:HD13	2.00	0.42
68:S2:1010:G:H2'	68:S2:1011:A:C8	2.53	0.42
68:S2:1374:C:H2'	68:S2:1375:G:O4'	2.19	0.42
68:S2:1774:C:C5	68:S2:1775:U:H1'	2.55	0.42
71:SF:51:HIS:CD2	71:SF:86:LYS:HE3	2.54	0.42
82:Sf:141:CYS:HB3	82:Sf:145:CYS:HB2	1.51	0.42
85:CA:113:HIS:CD2	85:CA:276:MET:HE3	2.53	0.42
3:L5:1195:G:H2'	3:L5:1196:G:C8	2.55	0.42
3:L5:1876:U:O3'	11:LF:103:PRO:HD3	2.19	0.42
3:L5:3700:C:O2'	3:L5:3774:A:H1'	2.19	0.42
3:L5:4968:A:H2'	3:L5:4969:C:C6	2.54	0.42
18:LN:6:TYR:CZ	39:Li:40:VAL:HG22	2.54	0.42
32:Lb:98:TYR:CE1	32:Lb:104:LEU:HB3	2.53	0.42
48:Ls:132:PRO:HB3	48:Ls:147:ILE:HD12	2.01	0.42
50:SA:156:TYR:HB3	61:SV:60:ARG:HH12	1.84	0.42
55:SH:50:GLU:OE1	55:SH:60:ILE:HG12	2.19	0.42
56:SI:110:ARG:HH21	56:SI:123:ARG:NH1	2.16	0.42
63:SX:60:LYS:H	63:SX:114:ASP:HB2	1.85	0.42
68:S2:85:A:H2'	68:S2:86:C:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:807:G:H2'	68:S2:808:A:H8	1.84	0.42
68:S2:939:U:H2'	68:S2:940:U:C6	2.54	0.42
68:S2:1222:G:H5''	71:SF:78:MET:HE1	2.00	0.42
68:S2:1470:C:H2'	68:S2:1471:C:C6	2.54	0.42
71:SF:19:LEU:HD11	71:SF:69:VAL:HG11	2.00	0.42
78:SU:66:ARG:HH12	78:SU:75:LYS:HA	1.84	0.42
3:L5:222:C:H2'	3:L5:223:G:O4'	2.20	0.42
3:L5:424:U:H2'	3:L5:425:U:C6	2.54	0.42
3:L5:1177:U:C2	3:L5:1180:C:N4	2.88	0.42
3:L5:1187:G:H1'	9:LD:275:GLN:HE21	1.84	0.42
3:L5:1779:U:H2'	3:L5:1780:A:C8	2.55	0.42
3:L5:3754:G:O6	3:L5:3770:U:O4	2.37	0.42
5:L8:130:C:H2'	5:L8:131:G:H8	1.83	0.42
8:LC:5:ARG:HH22	8:LC:266:THR:HG23	1.85	0.42
23:LS:47:PHE:HE1	23:LS:125:GLN:HG3	1.84	0.42
38:Lh:52:LYS:HA	38:Lh:52:LYS:HD3	1.77	0.42
51:SB:134:LEU:HB3	51:SB:218:LEU:HB2	2.00	0.42
57:SJ:131:ARG:HD2	57:SJ:131:ARG:HA	1.81	0.42
60:SO:39:ASP:H	60:SO:69:SER:HB3	1.85	0.42
60:SO:83:GLN:HA	60:SO:86:LYS:HE2	2.00	0.42
68:S2:1164:G:O2'	68:S2:1165:G:H5'	2.19	0.42
68:S2:1423:C:H5	75:SQ:4:LYS:HG2	1.82	0.42
71:SF:33:ILE:HG22	80:Sc:11:LEU:HD13	2.00	0.42
72:SK:51:SER:O	72:SK:55:ARG:HD3	2.20	0.42
84:CB:39:LEU:HD21	84:CB:350:LEU:HD22	2.00	0.42
3:L5:254:G:H8	3:L5:254:G:O5'	2.03	0.42
3:L5:2421:G:OP2	3:L5:2828:U:H1'	2.20	0.42
3:L5:3684:G:H2'	3:L5:3685:C:C6	2.54	0.42
3:L5:4174:U:H2'	3:L5:4175:G:C8	2.49	0.42
3:L5:4500:PSU:H2'	3:L5:4501:U:C6	2.54	0.42
3:L5:4600:G:H4'	3:L5:4601:U:O5'	2.19	0.42
3:L5:4637:OMG:H1'	3:L5:4637:OMG:HM23	1.64	0.42
3:L5:5001:PSU:H2'	3:L5:5002:U:O4'	2.18	0.42
3:L5:5043:A:H2'	3:L5:5044:A:C8	2.54	0.42
7:LB:161:ARG:HG2	7:LB:184:GLN:HA	2.02	0.42
35:Le:91:CYS:HB3	35:Le:95:TYR:HD2	1.85	0.42
48:Ls:53:VAL:HG22	48:Ls:89:VAL:HG12	2.01	0.42
53:SE:246:LEU:HD22	53:SE:250:GLU:HG3	2.01	0.42
68:S2:497:C:H2'	68:S2:498:C:H6	1.84	0.42
68:S2:857:U:H2'	68:S2:858:A:C8	2.54	0.42
68:S2:1337:4AC:H2'	68:S2:1338:G:C8	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:S2:1683:C:H2'	68:S2:1684:C:H6	1.84	0.42
84:CB:99:LEU:HD12	84:CB:99:LEU:HA	1.89	0.42
84:CB:358:LEU:HD23	84:CB:358:LEU:HA	1.90	0.42
85:CA:219:GLU:O	85:CA:325:LEU:HD23	2.19	0.42
3:L5:419:A:N6	5:L8:15:G:H1'	2.35	0.42
3:L5:425:U:H4'	20:LP:6:LEU:HD21	2.00	0.42
3:L5:457:G:H2'	3:L5:458:C:H6	1.85	0.42
3:L5:1323:A2M:O5'	3:L5:1323:A2M:H8	2.20	0.42
3:L5:4095:G:H2'	3:L5:4096:C:C6	2.55	0.42
3:L5:4144:C:C2	3:L5:4145:C:H5	2.38	0.42
7:LB:341:LYS:O	7:LB:342:LYS:HG2	2.19	0.42
14:LI:61:SER:HA	14:LI:126:VAL:HG12	2.02	0.42
51:SB:100:PHE:HD2	51:SB:181:LEU:HD11	1.85	0.42
52:SC:248:TYR:O	61:SV:23:ILE:HG21	2.19	0.42
54:SG:195:LYS:HZ3	68:S2:126:G:H5'	1.84	0.42
68:S2:1003:U:H2'	68:S2:1004:PSU:C6	2.54	0.42
68:S2:1274:G:H5'	68:S2:1274:G:N3	2.34	0.42
68:S2:1627:C:H5''	77:ST:41:LYS:HD2	2.01	0.42
76:SS:75:ARG:NH1	76:SS:95:TYR:HB2	2.35	0.42
84:CB:385:ILE:HG22	84:CB:418:SER:HB2	2.02	0.42
85:CA:154:LEU:HD23	85:CA:154:LEU:HA	1.84	0.42
3:L5:163:A:H2'	3:L5:164:G:C8	2.54	0.42
3:L5:676:C:H2'	3:L5:677:G:C8	2.55	0.42
3:L5:1318:C:H2'	3:L5:1319:U:O4'	2.20	0.42
3:L5:2563:C:H2'	3:L5:2564:G:O4'	2.20	0.42
3:L5:4481:U:H2'	3:L5:4482:U:C6	2.55	0.42
14:LI:53:VAL:HG11	24:LT:158:PHE:HZ	1.85	0.42
22:LR:15:LEU:HD13	22:LR:52:ARG:HB2	2.00	0.42
68:S2:24:C:O2'	68:S2:25:A:H8	2.01	0.42
68:S2:291:G:H8	68:S2:291:G:OP1	2.03	0.42
68:S2:1456:G:H2'	68:S2:1457:U:C6	2.55	0.42
68:S2:1672:U:H2'	68:S2:1673:U:C6	2.54	0.42
71:SF:183:GLY:HA2	71:SF:190:ILE:HG13	2.01	0.42
74:SP:22:LEU:HA	74:SP:25:LEU:HB2	2.01	0.42
76:SS:63:GLU:HG2	76:SS:66:ARG:HH22	1.85	0.42
83:Sg:86:THR:HG22	83:Sg:102:VAL:HG23	2.01	0.42
85:CA:321:PHE:CD2	85:CA:332:ARG:HG3	2.54	0.42
3:L5:261:G:H2'	3:L5:262:G:C8	2.55	0.42
3:L5:411:G:H4'	3:L5:412:G:H5''	2.02	0.42
3:L5:1091:C:H2'	3:L5:1092:G:H8	1.85	0.42
3:L5:1294:A:H1'	3:L5:1296:G:N1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1687:U:H2'	3:L5:1688:G:C8	2.54	0.42
3:L5:2424:OMG:HM23	3:L5:2424:OMG:H1'	1.78	0.42
3:L5:4458:C:H2'	3:L5:4459:U:C6	2.54	0.42
6:LA:7:GLY:HA2	6:LA:10:LYS:HG3	2.02	0.42
15:LJ:12:MET:HE3	15:LJ:12:MET:HB3	1.88	0.42
28:LX:148:ASP:HA	28:LX:151:ASN:HB2	2.02	0.42
31:La:36:GLY:HA3	31:La:40:HIS:CE1	2.55	0.42
38:Lh:73:TYR:HA	38:Lh:76:LYS:HD2	2.02	0.42
51:SB:30:TRP:CE2	60:SO:19:PRO:HD3	2.55	0.42
52:SC:114:LYS:HB3	52:SC:121:ARG:HG2	2.02	0.42
54:SG:149:LYS:HD3	54:SG:149:LYS:HA	1.92	0.42
55:SH:158:LEU:HD23	55:SH:158:LEU:HA	1.87	0.42
59:SN:5:HIS:HD2	68:S2:676:C:H5''	1.84	0.42
60:SO:43:HIS:CG	60:SO:55:ARG:HD3	2.55	0.42
68:S2:194:C:H2'	68:S2:195:C:C6	2.55	0.42
68:S2:497:C:H2'	68:S2:498:C:C6	2.55	0.42
68:S2:1425:G:H2'	68:S2:1426:U:H6	1.83	0.42
68:S2:1858:G:H2'	68:S2:1859:A:C8	2.55	0.42
83:Sg:42:MET:HE3	83:Sg:57:ARG:HB3	2.02	0.42
3:L5:264:C:H2'	3:L5:265:C:C4	2.55	0.42
3:L5:1172:C:O2'	3:L5:1173:G:H8	2.01	0.42
3:L5:2638:G:H22	3:L5:2719:C:P	2.42	0.42
3:L5:2831:G:H2'	3:L5:2832:A:C8	2.55	0.42
3:L5:3606:U:H2'	3:L5:3607:U:C6	2.55	0.42
3:L5:3937:C:H1'	18:LN:125:SER:HB3	2.02	0.42
3:L5:4616:A:H2'	3:L5:4617:G:O4'	2.19	0.42
4:L7:49:A:H5''	9:LD:224:SER:OG	2.19	0.42
19:LO:93:LYS:HA	19:LO:93:LYS:HD3	1.81	0.42
38:Lh:89:ARG:O	38:Lh:93:ARG:HG2	2.19	0.42
54:SG:78:SER:H	54:SG:81:HIS:CD2	2.38	0.42
55:SH:20:GLU:HA	55:SH:23:ILE:HG22	2.01	0.42
68:S2:344:U:H2'	68:S2:345:U:H6	1.84	0.42
68:S2:1098:C:H2'	68:S2:1099:G:C8	2.54	0.42
68:S2:1407:U:H4'	75:SQ:71:ARG:CZ	2.50	0.42
68:S2:1543:U:H4'	75:SQ:43:GLU:CD	2.44	0.42
75:SQ:48:GLN:HA	75:SQ:51:LEU:HD23	2.02	0.42
83:Sg:34:ALA:HB1	83:Sg:66:VAL:HG13	2.02	0.42
85:CA:141:ASP:HB2	85:CA:177:PHE:HD2	1.85	0.42
3:L5:1174:G:H1	3:L5:1186:U:H3	1.67	0.42
3:L5:1356:U:H2'	3:L5:1357:C:C6	2.54	0.42
3:L5:2295:C:H2'	3:L5:2296:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2299:G:H2'	3:L5:2301:G:O4'	2.20	0.42
3:L5:2884:G:H2'	3:L5:2885:A:H8	1.85	0.42
3:L5:4981:G:H3'	3:L5:4982:A:H8	1.84	0.42
57:SJ:150:ARG:HG3	68:S2:821:G:C6	2.55	0.42
68:S2:221:A:H2'	68:S2:222:U:C6	2.55	0.42
68:S2:374:G:H2'	68:S2:375:U:C6	2.54	0.42
68:S2:1174:PSU:H2'	68:S2:1175:G:C8	2.55	0.42
68:S2:1752:C:C5	68:S2:1753:C:H1'	2.55	0.42
71:SF:127:ARG:HG2	71:SF:136:ARG:HE	1.85	0.42
1:CD:286:TRP:HA	1:CD:289:ILE:HG12	2.02	0.41
3:L5:958:G:N2	10:LE:124:LYS:HB3	2.35	0.41
3:L5:1076:C:H2'	3:L5:1077:C:H6	1.85	0.41
3:L5:1458:C:C2	3:L5:1459:A:C8	3.08	0.41
3:L5:1460:C:H2'	3:L5:1461:C:H6	1.85	0.41
3:L5:1778:C:H5''	9:LD:5:LYS:HG3	2.02	0.41
3:L5:1811:G:H2'	3:L5:1812:C:C6	2.54	0.41
3:L5:2340:C:H4'	8:LC:42:THR:HG23	2.02	0.41
3:L5:2538:U:H2'	3:L5:2539:C:H6	1.85	0.41
3:L5:4233:A:C8	3:L5:4235:G:C8	3.08	0.41
3:L5:4653:C:H2'	3:L5:4654:C:C6	2.55	0.41
12:LG:125:LYS:HG3	12:LG:126:GLY:H	1.84	0.41
21:LQ:43:PHE:CD2	21:LQ:133:GLY:HA3	2.55	0.41
25:LU:28:PRO:HB2	25:LU:34:MET:HB3	2.02	0.41
34:Ld:23:ARG:HG2	34:Ld:121:ASN:HA	2.01	0.41
38:Lh:88:THR:HG22	38:Lh:90:ALA:H	1.84	0.41
44:Ln:2:ARG:HB3	44:Ln:5:TRP:CD1	2.55	0.41
51:SB:164:ILE:HD11	51:SB:204:ILE:HB	2.02	0.41
55:SH:100:ILE:HG12	55:SH:125:VAL:HG21	2.02	0.41
66:Sb:33:MET:HE2	66:Sb:48:SER:HA	2.01	0.41
68:S2:455:A:H2'	68:S2:456:C:H6	1.84	0.41
68:S2:455:A:H2'	68:S2:456:C:C6	2.55	0.41
68:S2:974:C:C2	68:S2:975:G:C8	3.08	0.41
68:S2:1540:G:H5'	77:ST:47:PRO:HB3	2.02	0.41
68:S2:1801:A:H2'	68:S2:1802:C:C6	2.54	0.41
68:S2:1853:C:H2'	68:S2:1854:U:C6	2.55	0.41
78:SU:66:ARG:NH1	78:SU:75:LYS:HA	2.34	0.41
83:Sg:254:PRO:HG3	83:Sg:283:PRO:HG2	2.02	0.41
84:CB:223:PHE:HB3	84:CB:344:LEU:HD13	2.00	0.41
3:L5:974:C:H5''	11:LF:43:ARG:NH1	2.34	0.41
3:L5:1534:A2M:H8	40:Lj:15:THR:OG1	2.20	0.41
3:L5:1847:C:H2'	3:L5:1848:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2519:U:H1'	3:L5:2520:C:C6	2.55	0.41
3:L5:3773:U:HO2'	3:L5:3774:A:H8	1.67	0.41
3:L5:4296:PSU:H2'	3:L5:4297:G:O4'	2.20	0.41
3:L5:4585:U:H2'	3:L5:4586:G:H8	1.85	0.41
5:L8:37:A:OP2	38:Lh:89:ARG:HD2	2.20	0.41
6:LA:171:GLY:O	46:Lp:68:ALA:HB2	2.20	0.41
12:LG:95:LEU:HA	12:LG:218:LEU:HD11	2.02	0.41
15:LJ:15:LEU:HD12	15:LJ:165:TRP:HB2	2.02	0.41
52:SC:253:PRO:HA	52:SC:256:TRP:CE2	2.55	0.41
54:SG:160:LYS:HD2	54:SG:161:PRO:HD2	2.01	0.41
54:SG:175:LYS:HG3	68:S2:77:A:C2	2.55	0.41
56:SI:123:ARG:NH2	56:SI:129:LEU:HD13	2.35	0.41
57:SJ:87:LEU:HD12	57:SJ:87:LEU:HA	1.89	0.41
68:S2:17:C:H2'	68:S2:18:C:C6	2.56	0.41
68:S2:637:U:H2'	68:S2:638:C:C6	2.55	0.41
68:S2:1128:C:H2'	68:S2:1129:G:C8	2.55	0.41
68:S2:1199:A:H2'	68:S2:1200:A:H8	1.85	0.41
68:S2:1303:C:H2'	68:S2:1304:U:C6	2.55	0.41
68:S2:1597:C:H4'	68:S2:1603:G:C6	2.56	0.41
77:ST:18:LEU:HD22	77:ST:58:ALA:HA	2.01	0.41
84:CB:829:SER:HB2	84:CB:831:PRO:HD2	2.01	0.41
3:L5:951:G:H2'	3:L5:952:G:H8	1.86	0.41
3:L5:1773:U:H2'	3:L5:1774:C:C6	2.56	0.41
3:L5:1830:G:H4'	32:Lb:68:ARG:NH1	2.34	0.41
3:L5:4192:A:H2'	3:L5:4193:C:H6	1.84	0.41
3:L5:4401:G:H2'	3:L5:4402:C:C6	2.55	0.41
3:L5:4573:G:H2'	3:L5:4574:U:C6	2.56	0.41
3:L5:4710:C:H2'	3:L5:4711:C:C6	2.55	0.41
5:L8:45:C:H2'	5:L8:46:G:H8	1.86	0.41
10:LE:165:LEU:HD12	10:LE:174:LEU:HG	2.02	0.41
17:LM:6:PHE:H	17:LM:11:ARG:NH2	2.19	0.41
18:LN:75:VAL:HG11	18:LN:80:THR:HG22	2.01	0.41
25:LU:86:LEU:HD23	25:LU:86:LEU:HA	1.83	0.41
48:Ls:147:ILE:HD11	84:CB:187:VAL:HG12	2.02	0.41
58:SL:111:VAL:HG12	58:SL:140:PHE:HB2	2.02	0.41
69:SR:80:ARG:HG2	69:SR:81:ARG:H	1.85	0.41
78:SU:26:SER:HB3	78:SU:110:VAL:HG22	2.01	0.41
3:L5:161:G:H2'	3:L5:162:A:C8	2.55	0.41
3:L5:172:C:H4'	3:L5:173:C:H5'	2.02	0.41
3:L5:458:C:H2'	3:L5:459:C:H6	1.85	0.41
3:L5:515:C:H2'	3:L5:516:C:H5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:690:C:H2'	3:L5:691:C:H6	1.85	0.41
3:L5:2381:A:H1'	3:L5:2383:C:OP2	2.20	0.41
3:L5:2484:A:H3'	3:L5:2486:G:H22	1.86	0.41
3:L5:2654:C:H2'	3:L5:2655:C:C6	2.55	0.41
3:L5:2693:G:H2'	3:L5:2694:G:N2	2.35	0.41
3:L5:4651:A:H2'	3:L5:4652:G:O4'	2.20	0.41
11:LF:182:TYR:CZ	11:LF:203:GLU:HG2	2.54	0.41
11:LF:220:MET:HB3	11:LF:232:ASP:OD2	2.20	0.41
14:LI:99:ILE:HG22	14:LI:123:GLN:HB2	2.03	0.41
32:Lb:41:ARG:HH21	32:Lb:45:PHE:HE2	1.69	0.41
48:Ls:28:PHE:CD1	48:Ls:192:VAL:HG23	2.55	0.41
50:SA:158:ASP:O	61:SV:66:ASP:HA	2.21	0.41
54:SG:39:ASP:HB3	54:SG:46:LYS:HD2	2.02	0.41
55:SH:63:PHE:HA	55:SH:95:ILE:O	2.19	0.41
68:S2:1101:U:H2'	68:S2:1102:G:C8	2.56	0.41
68:S2:1213:C:H2'	68:S2:1214:A:H8	1.84	0.41
68:S2:1501:C:H2'	68:S2:1502:C:H6	1.85	0.41
68:S2:1702:G:H2'	68:S2:1703:OMC:O4'	2.20	0.41
68:S2:1729:U:H2'	68:S2:1730:U:C6	2.56	0.41
71:SF:74:ASN:HA	71:SF:77:MET:HE3	2.02	0.41
75:SQ:16:LYS:HG2	75:SQ:17:LYS:HG3	2.02	0.41
3:L5:722:G:H2'	3:L5:723:A:C8	2.55	0.41
3:L5:1281:G:N1	10:LE:128:HIS:HB2	2.36	0.41
3:L5:1916:G:O6	36:Lf:18:LEU:HB2	2.20	0.41
3:L5:1980:U:O2'	3:L5:1981:G:H5''	2.21	0.41
3:L5:2709:C:H42	85:CA:256:GLY:HA2	1.85	0.41
3:L5:4103:C:H4'	3:L5:4104:G:N7	2.35	0.41
5:L8:148:A:H2'	5:L8:149:G:C8	2.55	0.41
13:LH:4:ILE:HG12	13:LH:61:TRP:CH2	2.56	0.41
29:LY:50:ARG:HG3	29:LY:51:LYS:N	2.35	0.41
31:La:71:PRO:HG2	31:La:108:TYR:HA	2.03	0.41
35:Le:26:ASP:OD1	35:Le:27:ARG:HG3	2.20	0.41
53:SE:240:ARG:HD3	53:SE:241:GLY:H	1.86	0.41
54:SG:218:LYS:HE3	54:SG:218:LYS:HB3	1.89	0.41
66:Sb:16:LYS:HA	66:Sb:23:ARG:HH21	1.86	0.41
66:Sb:37:CYS:HB3	66:Sb:63:LEU:HD21	2.03	0.41
68:S2:327:G:H5''	68:S2:328:U:C2	2.55	0.41
68:S2:1504:U:H2'	68:S2:1505:U:C6	2.55	0.41
71:SF:145:ARG:HA	71:SF:145:ARG:HD2	1.91	0.41
71:SF:201:LYS:HA	71:SF:204:ARG:HD2	2.02	0.41
72:SK:16:PHE:HE1	72:SK:89:ILE:HG22	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Sg:21:ILE:HG21	83:Sg:299:PHE:HB2	2.01	0.41
3:L5:135:G:C4	38:Lh:97:LYS:HG3	2.55	0.41
3:L5:146:G:H2'	3:L5:147:A:H8	1.85	0.41
3:L5:262:G:H2'	3:L5:263:G:C8	2.55	0.41
3:L5:271:C:H2'	3:L5:272:U:C6	2.56	0.41
3:L5:399:G:H2'	3:L5:400:A2M:H8	2.03	0.41
3:L5:1092:G:H2'	3:L5:1093:C:C6	2.56	0.41
3:L5:1464:C:H5''	32:Lb:32:LEU:HD12	2.02	0.41
3:L5:1471:U:H2'	3:L5:1472:C:H6	1.86	0.41
3:L5:1982:G:H8	3:L5:1982:G:OP2	2.03	0.41
3:L5:2273:G:H2'	3:L5:2274:C:C6	2.56	0.41
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.52	0.41
3:L5:2484:A:H3'	3:L5:2486:G:N2	2.36	0.41
3:L5:2696:A:H5'	41:Lk:70:LYS:HE2	2.01	0.41
3:L5:3772:U:O4	3:L5:3776:G:N2	2.53	0.41
3:L5:4208:U:H2'	3:L5:4209:G:H8	1.86	0.41
3:L5:4739:C:H2'	3:L5:4740:G:H5'	2.02	0.41
5:L8:119:C:H2'	5:L8:120:G:C8	2.55	0.41
14:LI:190:LEU:HD23	14:LI:199:TYR:HA	2.02	0.41
33:Lc:35:LEU:O	33:Lc:39:ARG:HG2	2.20	0.41
54:SG:16:ILE:HD13	54:SG:16:ILE:HA	1.89	0.41
54:SG:18:VAL:HG11	54:SG:24:LEU:HD21	2.02	0.41
59:SN:7:PRO:HG3	68:S2:996:A:H5''	2.01	0.41
60:SO:57:THR:O	60:SO:60:MET:HG2	2.21	0.41
68:S2:107:A:H2'	68:S2:108:G:C8	2.55	0.41
68:S2:564:A:H2'	68:S2:565:G:O4'	2.20	0.41
68:S2:1102:G:H2'	68:S2:1103:C:C6	2.55	0.41
68:S2:1387:G:H2'	68:S2:1388:A:O4'	2.20	0.41
70:SD:132:LYS:HB2	70:SD:189:MET:HG2	2.02	0.41
74:SP:28:MET:HG3	74:SP:32:GLN:NE2	2.36	0.41
3:L5:214:G:H2'	3:L5:215:C:C6	2.56	0.41
3:L5:2728:U:H2'	3:L5:2729:C:C6	2.55	0.41
3:L5:3916:G:H2'	3:L5:3917:A:C8	2.55	0.41
3:L5:4070:U:H2'	3:L5:4071:U:C6	2.55	0.41
3:L5:4263:C:H2'	3:L5:4264:G:O4'	2.20	0.41
3:L5:4674:C:H5''	7:LB:334:LYS:NZ	2.36	0.41
7:LB:29:VAL:HA	7:LB:220:ILE:HD13	2.03	0.41
13:LH:92:MET:HE2	13:LH:179:ILE:HG22	2.03	0.41
31:La:75:LEU:HD23	31:La:75:LEU:HA	1.91	0.41
48:Ls:50:LYS:HD2	48:Ls:51:ALA:HB2	2.02	0.41
48:Ls:94:ASP:O	48:Ls:98:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Lt:106:PHE:HB2	49:Lt:109:ILE:HB	2.03	0.41
49:Lt:114:ARG:HH21	49:Lt:117:ARG:HD2	1.86	0.41
52:SC:263:LYS:HA	52:SC:267:GLN:HE21	1.85	0.41
54:SG:7:PHE:HD2	54:SG:10:THR:HG22	1.85	0.41
64:SY:61:ARG:HA	64:SY:61:ARG:HD3	1.87	0.41
66:Sb:34:ASP:O	66:Sb:79:PHE:HA	2.21	0.41
68:S2:29:G:C6	68:S2:646:G:C6	3.09	0.41
68:S2:511:U:H2'	68:S2:512:A:C8	2.55	0.41
68:S2:943:U:H2'	68:S2:944:A:C8	2.45	0.41
68:S2:1310:U:H2'	68:S2:1311:C:C6	2.56	0.41
68:S2:1401:A:H2'	68:S2:1402:A:C8	2.55	0.41
3:L5:113:A:H2'	3:L5:114:G:O4'	2.21	0.41
3:L5:919:C:H2'	3:L5:920:C:H6	1.85	0.41
3:L5:978:G:H2'	3:L5:979:C:C6	2.55	0.41
3:L5:978:G:OP1	10:LE:62:MET:HG3	2.21	0.41
3:L5:1317:U:H2'	3:L5:1318:C:C6	2.56	0.41
3:L5:2543:A:H4'	3:L5:2544:G:N7	2.36	0.41
3:L5:2610:G:H2'	3:L5:2611:A:C8	2.56	0.41
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.55	0.41
3:L5:3760:A:C5	68:S2:1826:G:H4'	2.55	0.41
3:L5:3825:A2M:H2'	3:L5:3826:C:O4'	2.21	0.41
3:L5:3893:C:H2'	3:L5:3894:A:C8	2.55	0.41
4:L7:114:U:H2'	4:L7:115:A:C8	2.55	0.41
6:LA:131:GLY:N	6:LA:169:VAL:HG13	2.35	0.41
9:LD:60:ILE:HB	9:LD:80:ALA:HB2	2.02	0.41
19:LO:58:LEU:HD23	19:LO:58:LEU:HA	1.83	0.41
22:LR:181:LYS:HA	22:LR:181:LYS:HD3	1.81	0.41
30:LZ:30:ASP:HA	30:LZ:39:SER:OG	2.21	0.41
34:Ld:29:ILE:O	34:Ld:33:ILE:HG12	2.20	0.41
55:SH:118:ARG:HD3	55:SH:118:ARG:HA	1.93	0.41
64:SY:60:PHE:CD1	64:SY:71:GLY:HA3	2.55	0.41
65:Sa:83:VAL:HG12	65:Sa:84:VAL:HG13	2.02	0.41
68:S2:96:C:H2'	68:S2:97:U:C6	2.56	0.41
68:S2:432:G:H2'	68:S2:433:A:H8	1.84	0.41
68:S2:793:G:H2'	68:S2:794:A:H8	1.86	0.41
68:S2:1249:C:OP1	68:S2:1251:A:H5''	2.20	0.41
68:S2:1332:A:C6	68:S2:1500:G:C5	3.09	0.41
70:SD:25:LEU:HD23	70:SD:25:LEU:HA	1.82	0.41
83:Sg:294:ASP:OD2	83:Sg:296:GLN:HB2	2.20	0.41
3:L5:6:C:H2'	3:L5:7:C:H6	1.86	0.41
3:L5:683:C:H2'	3:L5:684:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1247:U:H2'	3:L5:1248:C:H6	1.86	0.41
3:L5:1326:A2M:HM'3	3:L5:1326:A2M:H1'	1.54	0.41
3:L5:1812:C:H2'	3:L5:1813:U:C6	2.56	0.41
3:L5:1995:G:H2'	3:L5:1996:C:C6	2.56	0.41
3:L5:2539:C:H2'	3:L5:2540:C:H6	1.84	0.41
3:L5:2787:A2M:H1'	3:L5:2787:A2M:HM'2	1.66	0.41
3:L5:2861:OMC:HM23	3:L5:2861:OMC:H1'	1.58	0.41
3:L5:3588:C:H2'	3:L5:3589:G:O4'	2.21	0.41
3:L5:3754:G:C4	3:L5:3755:G:C8	3.09	0.41
3:L5:3851:PSU:H2'	3:L5:3852:A:O4'	2.21	0.41
3:L5:4187:G:OP2	87:L5:5268:SPM:H131	2.21	0.41
3:L5:4227:OMU:H1'	3:L5:4227:OMU:HM23	1.77	0.41
3:L5:4277:G:H2'	3:L5:4278:C:C6	2.56	0.41
3:L5:4300:U:H4'	24:LT:89:ILE:HG22	2.03	0.41
3:L5:4311:A:H2'	3:L5:4312:PSU:C6	2.55	0.41
3:L5:4370:OMG:H1'	3:L5:4370:OMG:HM23	1.85	0.41
3:L5:4913:G:H4'	3:L5:4914:C:O5'	2.21	0.41
5:L8:66:A:H2'	5:L8:67:U:C6	2.56	0.41
6:LA:114:CYS:SG	6:LA:169:VAL:HB	2.61	0.41
8:LC:138:MET:HE2	8:LC:144:ILE:O	2.21	0.41
9:LD:111:ASN:HA	9:LD:116:ASP:OD2	2.20	0.41
13:LH:34:LEU:HD23	13:LH:34:LEU:HA	1.86	0.41
19:LO:9:LEU:HD23	19:LO:118:MET:HB2	2.03	0.41
30:LZ:73:LYS:HE3	30:LZ:73:LYS:HB3	1.79	0.41
30:LZ:121:ARG:HA	30:LZ:121:ARG:HD3	1.90	0.41
31:La:87:ARG:NH1	31:La:118:PRO:HG3	2.35	0.41
50:SA:24:HIS:CE1	50:SA:25:LEU:HG	2.55	0.41
50:SA:54:THR:HA	50:SA:162:PRO:HG2	2.03	0.41
54:SG:234:LEU:HD12	54:SG:234:LEU:HA	1.95	0.41
55:SH:33:ASN:ND2	55:SH:36:LEU:HB2	2.36	0.41
68:S2:113:G:N2	68:S2:292:A:H2'	2.36	0.41
68:S2:124:U:H2'	68:S2:125:C:C6	2.56	0.41
68:S2:428:OMU:H2'	68:S2:428:OMU:H6	1.88	0.41
68:S2:964:A:H2'	68:S2:965:U:H6	1.86	0.41
68:S2:1448:A:H2'	68:S2:1449:G:O4'	2.21	0.41
68:S2:1484:A:H4'	70:SD:159:HIS:ND1	2.36	0.41
68:S2:1547:C:H3'	68:S2:1548:G:H8	1.85	0.41
68:S2:1716:C:H2'	68:S2:1717:C:C6	2.55	0.41
68:S2:1802:C:H2'	68:S2:1803:U:H6	1.86	0.41
78:SU:32:LEU:HA	78:SU:32:LEU:HD12	1.86	0.41
81:Sd:39:CYS:HB2	81:Sd:42:CYS:HB2	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:Sg:271:LYS:HD2	83:Sg:271:LYS:HA	1.90	0.41
84:CB:35:LEU:HD23	84:CB:35:LEU:HA	1.83	0.41
3:L5:323:C:H2'	3:L5:324:A:C8	2.54	0.41
3:L5:650:C:H2'	3:L5:651:C:C6	2.56	0.41
3:L5:1093:C:H2'	3:L5:1094:G:O4'	2.20	0.41
3:L5:1503:A:H1'	3:L5:1504:G:C8	2.56	0.41
3:L5:1511:U:H2'	3:L5:1512:G:C8	2.56	0.41
3:L5:2638:G:N1	3:L5:2718:U:H2'	2.36	0.41
3:L5:4301:U:H4'	24:LT:54:HIS:CD2	2.56	0.41
3:L5:4601:U:H2'	3:L5:4602:A:H8	1.85	0.41
3:L5:4934:A:H2'	3:L5:4935:C:H6	1.86	0.41
7:LB:19:ARG:HB2	7:LB:234:ARG:NH2	2.36	0.41
12:LG:37:LYS:HE2	12:LG:37:LYS:HB3	1.88	0.41
12:LG:51:LEU:O	12:LG:55:VAL:HG23	2.21	0.41
14:LI:91:LEU:HD12	14:LI:135:ILE:HG23	2.03	0.41
29:LY:24:HIS:CE1	29:LY:25:ILE:HG23	2.56	0.41
48:Ls:121:VAL:HG22	48:Ls:161:ILE:HB	2.02	0.41
51:SB:115:LYS:HB2	51:SB:118:GLN:CD	2.46	0.41
53:SE:169:ILE:HD13	53:SE:169:ILE:HA	1.85	0.41
64:SY:18:LEU:HD22	64:SY:20:ARG:CZ	2.51	0.41
66:Sb:47:PHE:HE2	66:Sb:49:HIS:HB2	1.85	0.41
68:S2:824:C:H2'	68:S2:825:A:C8	2.56	0.41
68:S2:906:U:H2'	68:S2:907:G:C8	2.56	0.41
68:S2:1539:U:H2'	68:S2:1540:G:C8	2.56	0.41
68:S2:1617:G:O6	74:SP:43:ARG:HD3	2.21	0.41
75:SQ:42:ILE:HD12	75:SQ:42:ILE:HA	1.96	0.41
78:SU:24:LEU:HD22	78:SU:112:VAL:HG12	2.02	0.41
85:CA:86:VAL:HG12	85:CA:87:CYS:SG	2.61	0.41
85:CA:123:HIS:HA	85:CA:319:PHE:CD1	2.55	0.41
3:L5:1578:U:H2'	3:L5:1579:C:C6	2.56	0.40
3:L5:4466:C:H2'	3:L5:4467:A:H8	1.86	0.40
3:L5:4593:C:H2'	3:L5:4594:U:H6	1.85	0.40
4:L7:92:C:H2'	4:L7:93:G:C8	2.54	0.40
5:L8:52:A:H4'	42:Ll:19:GLN:HA	2.03	0.40
5:L8:89:U:H2'	5:L8:90:C:C6	2.56	0.40
8:LC:76:ILE:HG12	8:LC:96:CYS:SG	2.61	0.40
16:LL:14:PHE:HD2	16:LL:18:TRP:CD1	2.39	0.40
23:LS:83:ARG:HG3	23:LS:125:GLN:HB3	2.03	0.40
27:LW:107:GLN:HB2	27:LW:110:ARG:HH21	1.85	0.40
30:LZ:135:ARG:HA	30:LZ:135:ARG:HD2	1.81	0.40
35:Le:85:LEU:HD22	35:Le:111:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:Lm:93:LYS:HD3	43:Lm:102:ARG:HG2	2.04	0.40
50:SA:90:PHE:CD1	50:SA:179:ALA:HB2	2.56	0.40
60:SO:136:PRO:HB3	68:S2:944:A:H1'	2.02	0.40
68:S2:221:A:H2'	68:S2:222:U:H6	1.86	0.40
68:S2:1803:U:O2'	68:S2:1804:U:H5'	2.21	0.40
71:SF:23:TRP:CE2	71:SF:108:PRO:HG2	2.57	0.40
75:SQ:72:VAL:HG21	75:SQ:84:ILE:HD11	2.03	0.40
77:ST:47:PRO:HG2	77:ST:52:TRP:CD1	2.56	0.40
80:Sc:7:GLN:HE22	80:Sc:10:LYS:HZ2	1.68	0.40
3:L5:123:C:H2'	3:L5:124:C:H6	1.86	0.40
3:L5:1907:A:H2'	3:L5:1908:A:C8	2.56	0.40
3:L5:2571:C:H2'	3:L5:2572:C:C6	2.56	0.40
3:L5:2647:A:H3'	3:L5:2648:G:H8	1.86	0.40
3:L5:2749:C:H2'	3:L5:2750:G:C8	2.56	0.40
3:L5:4146:G:H2'	3:L5:4147:G:C8	2.57	0.40
3:L5:4561:C:H2'	3:L5:4562:C:C6	2.57	0.40
3:L5:4563:U:H2'	3:L5:4564:A:C8	2.55	0.40
3:L5:4593:C:H2'	3:L5:4594:U:C6	2.55	0.40
3:L5:4771:C:H2'	3:L5:4772:C:C6	2.56	0.40
5:L8:88:A:H2'	5:L8:89:U:O4'	2.22	0.40
8:LC:128:LEU:HD23	8:LC:128:LEU:HA	1.88	0.40
29:LY:38:LEU:HD23	29:LY:38:LEU:HA	1.87	0.40
46:Lp:86:LEU:HD23	46:Lp:86:LEU:HA	1.94	0.40
50:SA:184:ARG:HD3	50:SA:191:ARG:HD3	2.02	0.40
51:SB:88:THR:HA	51:SB:98:THR:HA	2.03	0.40
51:SB:124:HIS:HA	51:SB:137:LEU:O	2.20	0.40
54:SG:66:GLY:HA2	68:S2:1745:A:H1'	2.02	0.40
68:S2:342:C:H2'	68:S2:343:A:C8	2.56	0.40
68:S2:919:A:OP2	68:S2:919:A:H8	2.03	0.40
68:S2:979:C:H2'	68:S2:980:A:C8	2.56	0.40
68:S2:1189:A:H2'	68:S2:1190:A:C8	2.56	0.40
68:S2:1305:C:H2'	68:S2:1306:U:C6	2.57	0.40
68:S2:1444:U:P	75:SQ:15:ARG:HH22	2.44	0.40
68:S2:1688:C:H2'	68:S2:1689:C:C6	2.56	0.40
68:S2:1740:C:H2'	68:S2:1741:U:C6	2.56	0.40
69:SR:83:ASN:HB3	69:SR:85:VAL:H	1.86	0.40
71:SF:167:LYS:HA	79:SZ:71:ALA:HB1	2.03	0.40
75:SQ:134:GLY:H	75:SQ:140:ARG:CZ	2.35	0.40
80:Sc:14:VAL:HA	80:Sc:32:VAL:HG12	2.03	0.40
84:CB:294:LEU:HA	84:CB:294:LEU:HD23	1.85	0.40
84:CB:605:LYS:HD3	84:CB:705:HIS:CE1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:CA:86:VAL:HG13	85:CA:229:LEU:HD21	2.03	0.40
3:L5:400:A2M:H1'	3:L5:400:A2M:HM'3	1.51	0.40
3:L5:1239:C:P	11:LF:48:LYS:HZ1	2.44	0.40
3:L5:1510:G:H2'	3:L5:1511:U:C6	2.56	0.40
3:L5:2422:OMC:HM23	3:L5:2422:OMC:H1'	1.78	0.40
3:L5:3628:G:H2'	3:L5:3629:A:C8	2.57	0.40
3:L5:3896:C:H1'	7:LB:268:ARG:NH2	2.36	0.40
3:L5:4244:A:H2'	3:L5:4245:G:O4'	2.21	0.40
3:L5:4348:A:C6	3:L5:4350:C:C4	3.09	0.40
3:L5:4459:U:H2'	3:L5:4460:U:H6	1.84	0.40
3:L5:4536:OMC:HM22	3:L5:4537:C:O4'	2.22	0.40
3:L5:4708:A:N3	3:L5:4709:U:H5'	2.36	0.40
5:L8:19:C:H2'	5:L8:20:A:H8	1.83	0.40
24:LT:87:LYS:HA	24:LT:87:LYS:HD2	1.92	0.40
54:SG:98:ARG:HH11	54:SG:99:GLY:N	2.18	0.40
57:SJ:138:ARG:HB3	57:SJ:139:LYS:H	1.71	0.40
63:SX:100:VAL:HG12	63:SX:125:VAL:HA	2.04	0.40
63:SX:107:ARG:HG3	63:SX:110:HIS:HB3	2.02	0.40
68:S2:156:G:H2'	68:S2:157:U:C6	2.56	0.40
68:S2:302:A:H2'	68:S2:303:C:C6	2.56	0.40
68:S2:348:A:H2'	68:S2:349:A:H8	1.83	0.40
68:S2:634:A:H2'	68:S2:635:G:H8	1.87	0.40
68:S2:680:G:H2'	68:S2:681:PSU:C6	2.56	0.40
68:S2:816:A:H2'	68:S2:817:G:O4'	2.22	0.40
68:S2:947:G:H2'	68:S2:948:C:H6	1.87	0.40
68:S2:1232:PSU:H2'	68:S2:1233:G:C8	2.57	0.40
68:S2:1284:A:C4	73:SM:91:LEU:HD21	2.57	0.40
70:SD:25:LEU:HD12	70:SD:37:VAL:HG21	2.03	0.40
71:SF:33:ILE:HG23	80:Sc:55:VAL:HG11	2.04	0.40
84:CB:127:VAL:HB	84:CB:155:LEU:HD12	2.02	0.40
84:CB:442:LEU:HA	84:CB:442:LEU:HD23	1.81	0.40
84:CB:648:LYS:HB3	84:CB:664:ASP:OD1	2.22	0.40
3:L5:469:C:H2'	3:L5:470:A:C8	2.56	0.40
3:L5:699:C:H2'	3:L5:700:G:H8	1.85	0.40
3:L5:1290:G:H2'	3:L5:1291:G:C8	2.56	0.40
3:L5:1298:C:H2'	3:L5:1299:G:C8	2.55	0.40
3:L5:1855:G:OP1	32:Lb:4:SER:HB2	2.21	0.40
3:L5:2500:U:H2'	3:L5:2501:C:C6	2.56	0.40
3:L5:3667:C:P	6:LA:234:LYS:HD2	2.61	0.40
3:L5:4561:C:H2'	3:L5:4562:C:H6	1.86	0.40
3:L5:4625:C:OP1	7:LB:224:LYS:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4928:C:H2'	3:L5:4929:C:C6	2.57	0.40
21:LQ:27:LEU:HD23	21:LQ:27:LEU:HA	1.80	0.40
22:LR:19:LYS:HB2	22:LR:19:LYS:HE2	1.96	0.40
23:LS:25:PRO:HA	23:LS:26:PRO:HD3	1.98	0.40
25:LU:21:PHE:HD1	25:LU:108:GLU:HA	1.86	0.40
32:Lb:73:LYS:HA	32:Lb:73:LYS:HD3	1.87	0.40
34:Ld:33:ILE:HD12	34:Ld:33:ILE:HG23	1.91	0.40
57:SJ:138:ARG:HD3	57:SJ:138:ARG:HA	1.86	0.40
59:SN:37:ILE:HG23	59:SN:50:ILE:HG21	2.04	0.40
59:SN:102:LEU:HD11	59:SN:112:LYS:HA	2.04	0.40
61:SV:36:VAL:HG11	61:SV:78:ILE:HG21	2.03	0.40
63:SX:129:SER:HB2	68:S2:29:G:H4'	2.04	0.40
64:SY:16:ARG:H	64:SY:16:ARG:HG2	1.71	0.40
64:SY:16:ARG:HA	64:SY:19:GLN:HA	2.03	0.40
68:S2:530:U:H5'	68:S2:531:A:OP2	2.22	0.40
68:S2:1025:U:H2'	68:S2:1026:C:O4'	2.21	0.40
68:S2:1272:OMC:H1'	68:S2:1272:OMC:HM23	1.85	0.40
68:S2:1565:C:H2'	68:S2:1566:G:C8	2.56	0.40
68:S2:1593:C:H2'	68:S2:1594:A:C8	2.57	0.40
68:S2:1648:G:H5''	75:SQ:125:ARG:HB2	2.02	0.40
71:SF:40:ALA:HB3	71:SF:67:PRO:HA	2.04	0.40
72:SK:3:MET:SD	72:SK:48:ALA:HB2	2.61	0.40
75:SQ:8:GLN:HG3	75:SQ:99:TYR:CE2	2.57	0.40
76:SS:16:LEU:HD13	76:SS:16:LEU:HA	1.92	0.40
84:CB:143:LEU:HD23	84:CB:143:LEU:HA	1.85	0.40
84:CB:290:CYS:HA	84:CB:294:LEU:HB2	2.03	0.40
84:CB:488:PHE:HB3	84:CB:491:ALA:HB2	2.03	0.40
84:CB:814:PHE:HZ	84:CB:817:TRP:NE1	2.20	0.40
3:L5:287:U:H2'	3:L5:288:G:C8	2.57	0.40
3:L5:396:A:H2'	3:L5:397:G:C8	2.56	0.40
3:L5:1304:C:H2'	3:L5:1305:C:C6	2.57	0.40
3:L5:1942:A:H2'	3:L5:1943:A:H8	1.82	0.40
3:L5:2386:U:C2	3:L5:2387:G:C8	3.10	0.40
3:L5:3819:G:H2'	3:L5:3820:G:H8	1.86	0.40
3:L5:4232:U:H1'	3:L5:4233:A:C2	2.56	0.40
3:L5:4743:G:H2'	3:L5:4744:A:H8	1.86	0.40
3:L5:4954:G:H2'	3:L5:4955:A:H8	1.85	0.40
3:L5:5057:C:H2'	3:L5:5058:A:C8	2.56	0.40
11:LF:182:TYR:HB3	11:LF:200:ARG:HG3	2.02	0.40
21:LQ:177:ALA:O	21:LQ:184:ARG:HB2	2.21	0.40
34:Ld:117:LEU:HA	34:Ld:117:LEU:HD23	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SA:85:ARG:HD2	69:SR:81:ARG:HE	1.86	0.40
54:SG:192:ILE:HD13	54:SG:195:LYS:HD2	2.03	0.40
56:SI:5:ARG:HA	56:SI:5:ARG:HD2	1.89	0.40
63:SX:22:TRP:HE3	63:SX:28:LYS:HD2	1.86	0.40
68:S2:106:C:H5''	68:S2:431:G:O2'	2.22	0.40
68:S2:118:C:H1'	68:S2:445:A:C5	2.56	0.40
68:S2:129:C:OP2	68:S2:214:U:H2'	2.22	0.40
68:S2:900:C:H5'	68:S2:901:G:N7	2.36	0.40
68:S2:1627:C:H2'	68:S2:1628:C:C6	2.55	0.40
68:S2:1714:U:H2'	68:S2:1715:A:H8	1.86	0.40
77:ST:135:ALA:HA	77:ST:138:VAL:HG12	2.03	0.40
79:SZ:86:ALA:O	79:SZ:90:GLU:HG2	2.21	0.40
84:CB:382:ALA:O	84:CB:386:LYS:HG2	2.22	0.40
84:CB:388:CYS:HB2	84:CB:466:CYS:HB2	1.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CD	51/55 (93%)	51 (100%)	0	0	100	100
2	CI	29/31 (94%)	29 (100%)	0	0	100	100
6	LA	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
7	LB	400/402 (100%)	385 (96%)	14 (4%)	1 (0%)	36	63
8	LC	366/368 (100%)	351 (96%)	15 (4%)	0	100	100
9	LD	291/293 (99%)	281 (97%)	10 (3%)	0	100	100
10	LE	236/250 (94%)	217 (92%)	19 (8%)	0	100	100
11	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
12	LG	239/241 (99%)	226 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	LH	188/190 (99%)	182 (97%)	6 (3%)	0	100	100
14	LI	201/213 (94%)	199 (99%)	2 (1%)	0	100	100
15	LJ	168/176 (96%)	164 (98%)	4 (2%)	0	100	100
16	LL	208/210 (99%)	201 (97%)	7 (3%)	0	100	100
17	LM	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
18	LN	201/203 (99%)	196 (98%)	5 (2%)	0	100	100
19	LO	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
20	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
21	LQ	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
22	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
23	LS	173/175 (99%)	167 (96%)	6 (4%)	0	100	100
24	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
25	LU	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
26	LV	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
27	LW	112/124 (90%)	110 (98%)	2 (2%)	0	100	100
28	LX	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
29	LY	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
30	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
31	La	145/147 (99%)	139 (96%)	6 (4%)	0	100	100
32	Lb	105/121 (87%)	98 (93%)	7 (7%)	0	100	100
33	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
34	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
35	Le	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
36	Lf	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
37	Lg	112/114 (98%)	112 (100%)	0	0	100	100
38	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
39	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
40	Lj	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
41	Lk	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
42	Ll	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
43	Lm	50/52 (96%)	50 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	Ln	22/24 (92%)	22 (100%)	0	0	100	100
45	Lo	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
46	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
47	Lr	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
48	Ls	194/196 (99%)	181 (93%)	13 (7%)	0	100	100
49	Lt	128/157 (82%)	104 (81%)	24 (19%)	0	100	100
50	SA	219/221 (99%)	208 (95%)	11 (5%)	0	100	100
51	SB	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
52	SC	218/222 (98%)	207 (95%)	11 (5%)	0	100	100
53	SE	260/262 (99%)	249 (96%)	11 (4%)	0	100	100
54	SG	235/237 (99%)	227 (97%)	8 (3%)	0	100	100
55	SH	182/189 (96%)	171 (94%)	11 (6%)	0	100	100
56	SI	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
57	SJ	183/185 (99%)	172 (94%)	11 (6%)	0	100	100
58	SL	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
59	SN	148/150 (99%)	144 (97%)	4 (3%)	0	100	100
60	SO	135/140 (96%)	122 (90%)	13 (10%)	0	100	100
61	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
62	SW	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
63	SX	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
64	SY	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
65	Sa	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
66	Sb	81/83 (98%)	71 (88%)	10 (12%)	0	100	100
67	Se	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
69	SR	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
70	SD	225/227 (99%)	223 (99%)	2 (1%)	0	100	100
71	SF	187/189 (99%)	176 (94%)	11 (6%)	0	100	100
72	SK	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
73	SM	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
74	SP	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
75	SQ	142/144 (99%)	134 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
76	SS	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
77	ST	141/143 (99%)	139 (99%)	2 (1%)	0	100	100
78	SU	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
79	SZ	73/75 (97%)	65 (89%)	8 (11%)	0	100	100
80	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
81	Sd	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
82	Sf	65/67 (97%)	54 (83%)	11 (17%)	0	100	100
83	Sg	311/313 (99%)	289 (93%)	22 (7%)	0	100	100
84	CB	842/856 (98%)	814 (97%)	28 (3%)	0	100	100
85	CA	350/356 (98%)	333 (95%)	17 (5%)	0	100	100
All	All	12905/13174 (98%)	12355 (96%)	549 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	LB	295	ASP

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	46/46 (100%)	46 (100%)	0	100	100
2	CI	25/25 (100%)	25 (100%)	0	100	100
6	LA	190/190 (100%)	190 (100%)	0	100	100
7	LB	348/348 (100%)	348 (100%)	0	100	100
8	LC	306/306 (100%)	306 (100%)	0	100	100
9	LD	246/247 (100%)	246 (100%)	0	100	100
10	LE	212/222 (96%)	212 (100%)	0	100	100
11	LF	194/194 (100%)	194 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	LG	203/205 (99%)	203 (100%)	0	100	100
13	LH	169/169 (100%)	169 (100%)	0	100	100
14	LI	175/180 (97%)	175 (100%)	0	100	100
15	LJ	143/148 (97%)	143 (100%)	0	100	100
16	LL	176/176 (100%)	175 (99%)	1 (1%)	78	81
17	LM	118/118 (100%)	117 (99%)	1 (1%)	73	79
18	LN	171/171 (100%)	171 (100%)	0	100	100
19	LO	173/173 (100%)	173 (100%)	0	100	100
20	LP	134/134 (100%)	134 (100%)	0	100	100
21	LQ	164/164 (100%)	164 (100%)	0	100	100
22	LR	166/166 (100%)	166 (100%)	0	100	100
23	LS	156/156 (100%)	156 (100%)	0	100	100
24	LT	139/139 (100%)	139 (100%)	0	100	100
25	LU	91/91 (100%)	91 (100%)	0	100	100
26	LV	101/101 (100%)	101 (100%)	0	100	100
27	LW	95/103 (92%)	95 (100%)	0	100	100
28	LX	108/108 (100%)	108 (100%)	0	100	100
29	LY	124/124 (100%)	124 (100%)	0	100	100
30	LZ	117/117 (100%)	117 (100%)	0	100	100
31	La	120/120 (100%)	120 (100%)	0	100	100
32	Lb	88/101 (87%)	88 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	Lm	48/48 (100%)	48 (100%)	0	100	100
44	Ln	23/23 (100%)	23 (100%)	0	100	100
45	Lo	93/93 (100%)	93 (100%)	0	100	100
46	Lp	74/74 (100%)	74 (100%)	0	100	100
47	Lr	109/109 (100%)	109 (100%)	0	100	100
48	Ls	162/164 (99%)	162 (100%)	0	100	100
49	Lt	107/130 (82%)	107 (100%)	0	100	100
50	SA	183/183 (100%)	183 (100%)	0	100	100
51	SB	195/195 (100%)	195 (100%)	0	100	100
52	SC	186/188 (99%)	186 (100%)	0	100	100
53	SE	224/224 (100%)	224 (100%)	0	100	100
54	SG	207/207 (100%)	206 (100%)	1 (0%)	81	82
55	SH	166/169 (98%)	165 (99%)	1 (1%)	78	81
56	SI	178/178 (100%)	178 (100%)	0	100	100
57	SJ	161/161 (100%)	161 (100%)	0	100	100
58	SL	137/137 (100%)	137 (100%)	0	100	100
59	SN	130/130 (100%)	130 (100%)	0	100	100
60	SO	107/110 (97%)	107 (100%)	0	100	100
61	SV	67/67 (100%)	67 (100%)	0	100	100
62	SW	112/112 (100%)	112 (100%)	0	100	100
63	SX	113/113 (100%)	113 (100%)	0	100	100
64	SY	113/113 (100%)	113 (100%)	0	100	100
65	Sa	89/89 (100%)	89 (100%)	0	100	100
66	Sb	75/75 (100%)	75 (100%)	0	100	100
67	Se	47/47 (100%)	47 (100%)	0	100	100
69	SR	122/122 (100%)	121 (99%)	1 (1%)	73	79
70	SD	190/190 (100%)	190 (100%)	0	100	100
71	SF	159/159 (100%)	159 (100%)	0	100	100
72	SK	89/89 (100%)	89 (100%)	0	100	100
73	SM	102/104 (98%)	102 (100%)	0	100	100
74	SP	107/107 (100%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
75	SQ	119/119 (100%)	119 (100%)	0	100	100
76	SS	126/126 (100%)	126 (100%)	0	100	100
77	ST	113/113 (100%)	113 (100%)	0	100	100
78	SU	94/94 (100%)	94 (100%)	0	100	100
79	SZ	66/66 (100%)	66 (100%)	0	100	100
80	Sc	57/57 (100%)	57 (100%)	0	100	100
81	Sd	48/48 (100%)	48 (100%)	0	100	100
82	Sf	60/60 (100%)	60 (100%)	0	100	100
83	Sg	272/272 (100%)	272 (100%)	0	100	100
84	CB	722/728 (99%)	721 (100%)	1 (0%)	88	89
85	CA	303/305 (99%)	302 (100%)	1 (0%)	86	85
All	All	11213/11300 (99%)	11206 (100%)	7 (0%)	87	89

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

Mol	Chain	Res	Type
16	LL	59	VAL
17	LM	31	ILE
54	SG	158	VAL
55	SH	162	GLN
69	SR	76	GLU
84	CB	402	VAL
85	CA	189	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	CD	206	HIS
6	LA	22	HIS
7	LB	68	ASN
7	LB	184	GLN
7	LB	289	GLN
7	LB	354	GLN
7	LB	376	HIS
8	LC	38	ASN
8	LC	212	ASN
8	LC	347	HIS

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Mol	Chain	Res	Type
8	LC	362	GLN
9	LD	131	ASN
10	LE	266	GLN
11	LF	58	HIS
11	LF	80	ASN
12	LG	85	GLN
13	LH	102	ASN
13	LH	138	GLN
13	LH	188	GLN
14	LI	59	GLN
14	LI	73	ASN
14	LI	92	HIS
15	LJ	71	HIS
15	LJ	98	ASN
15	LJ	110	GLN
15	LJ	155	HIS
16	LL	15	HIS
17	LM	20	HIS
17	LM	48	GLN
18	LN	15	GLN
19	LO	180	GLN
20	LP	21	ASN
20	LP	137	ASN
21	LQ	125	GLN
22	LR	143	HIS
23	LS	108	GLN
23	LS	125	GLN
24	LT	98	HIS
24	LT	144	ASN
25	LU	50	ASN
27	LW	45	ASN
28	LX	125	ASN
29	LY	14	ASN
29	LY	61	HIS
31	La	28	HIS
31	La	34	ASN
31	La	62	HIS
31	La	67	GLN
32	Lb	49	HIS
32	Lb	60	ASN
35	Le	107	ASN
36	Lf	21	GLN

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Mol	Chain	Res	Type
38	Lh	107	GLN
39	Li	15	HIS
39	Li	26	HIS
40	Lj	13	ASN
41	Lk	28	ASN
41	Lk	31	ASN
47	Lr	4	HIS
47	Lr	30	ASN
47	Lr	83	ASN
48	Ls	68	HIS
48	Ls	71	ASN
48	Ls	127	ASN
48	Ls	179	ASN
49	Lt	115	GLN
50	SA	50	ASN
51	SB	75	GLN
51	SB	92	GLN
51	SB	101	HIS
52	SC	136	HIS
54	SG	4	ASN
54	SG	81	HIS
54	SG	110	ASN
55	SH	126	HIS
55	SH	157	HIS
55	SH	162	GLN
55	SH	168	HIS
56	SI	7	ASN
56	SI	9	HIS
56	SI	52	ASN
57	SJ	75	ASN
57	SJ	140	GLN
61	SV	82	ASN
63	SX	97	ASN
65	Sa	72	HIS
66	Sb	29	ASN
71	SF	83	ASN
71	SF	95	HIS
71	SF	110	GLN
71	SF	118	ASN
72	SK	66	HIS
73	SM	15	ASN
73	SM	46	GLN

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Mol	Chain	Res	Type
73	SM	119	GLN
74	SP	53	GLN
74	SP	103	ASN
75	SQ	86	GLN
75	SQ	142	GLN
76	SS	11	HIS
76	SS	19	ASN
79	SZ	106	GLN
80	Sc	7	GLN
81	Sd	3	HIS
84	CB	168	GLN
84	CB	202	ASN
84	CB	513	ASN
84	CB	626	GLN
84	CB	660	ASN
84	CB	803	ASN
85	CA	113	HIS
85	CA	161	ASN
85	CA	165	GLN
85	CA	203	GLN
85	CA	303	GLN
85	CA	306	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3643/3655 (99%)	743 (20%)	20 (0%)
4	L7	119/120 (99%)	10 (8%)	0
5	L8	155/156 (99%)	25 (16%)	0
68	S2	1715/1740 (98%)	397 (23%)	5 (0%)
All	All	5632/5671 (99%)	1175 (20%)	25 (0%)

All (1175) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L5	25	A
3	L5	30	C
3	L5	39	A
3	L5	42	A
3	L5	48	G
3	L5	56	A

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Mol	Chain	Res	Type
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	73	A
3	L5	84	A
3	L5	91	G
3	L5	104	G
3	L5	108	A
3	L5	109	G
3	L5	110	C
3	L5	119	G
3	L5	120	A
3	L5	128	C
3	L5	132	G
3	L5	133	C
3	L5	134	G
3	L5	135	G
3	L5	136	C
3	L5	139	G
3	L5	144	G
3	L5	145	G
3	L5	159	C
3	L5	165	A
3	L5	172	C
3	L5	181	C
3	L5	182	G
3	L5	183	C
3	L5	184	U
3	L5	185	C
3	L5	186	G
3	L5	188	G
3	L5	189	G
3	L5	200	U
3	L5	209	U
3	L5	216	C
3	L5	218	A
3	L5	255	C
3	L5	256	G
3	L5	262	G
3	L5	263	G
3	L5	264	C
3	L5	265	C

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Mol	Chain	Res	Type
3	L5	266	C
3	L5	267	G
3	L5	275	C
3	L5	280	G
3	L5	297	U
3	L5	306	A
3	L5	315	G
3	L5	316	U
3	L5	340	C
3	L5	373	G
3	L5	379	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	415	G
3	L5	449	C
3	L5	452	A
3	L5	453	G
3	L5	454	U
3	L5	456	C
3	L5	457	G
3	L5	464	G
3	L5	467	U
3	L5	468	U
3	L5	479	G
3	L5	484	U
3	L5	485	C
3	L5	486	C
3	L5	489	C
3	L5	493	G
3	L5	494	U
3	L5	496	G
3	L5	497	G
3	L5	498	C
3	L5	499	G

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Mol	Chain	Res	Type
3	L5	502	C
3	L5	503	C
3	L5	504	G
3	L5	505	G
3	L5	509	A
3	L5	510	U
3	L5	512	U
3	L5	513	U
3	L5	514	U
3	L5	518	G
3	L5	519	C
3	L5	643	C
3	L5	644	G
3	L5	654	C
3	L5	655	C
3	L5	657	C
3	L5	658	C
3	L5	659	G
3	L5	667	A
3	L5	668	C
3	L5	672	C
3	L5	673	C
3	L5	674	G
3	L5	685	C
3	L5	686	A
3	L5	687	U
3	L5	696	C
3	L5	704	C
3	L5	708	G
3	L5	730	G
3	L5	731	G
3	L5	738	C
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	910	G
3	L5	913	U
3	L5	914	U

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Mol	Chain	Res	Type
3	L5	915	A
3	L5	917	A
3	L5	923	C
3	L5	924	C
3	L5	926	G
3	L5	932	A
3	L5	933	G
3	L5	935	A
3	L5	936	C
3	L5	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	968	C
3	L5	969	C
3	L5	970	G
3	L5	982	U
3	L5	985	C
3	L5	989	U
3	L5	1066	G
3	L5	1070	G
3	L5	1072	C
3	L5	1075	G
3	L5	1082	C
3	L5	1083	U
3	L5	1168	G
3	L5	1171	G
3	L5	1172	C
3	L5	1173	G
3	L5	1178	G
3	L5	1179	U
3	L5	1180	C
3	L5	1181	C
3	L5	1182	C
3	L5	1183	C

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Mol	Chain	Res	Type
3	L5	1187	G
3	L5	1202	C
3	L5	1203	G
3	L5	1205	G
3	L5	1210	C
3	L5	1211	G
3	L5	1214	C
3	L5	1215	C
3	L5	1218	G
3	L5	1219	G
3	L5	1221	G
3	L5	1222	A
3	L5	1242	G
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	1277	G
3	L5	1280	C
3	L5	1284	G
3	L5	1285	U
3	L5	1287	G
3	L5	1293	G
3	L5	1294	A
3	L5	1295	C
3	L5	1296	G
3	L5	1301	C
3	L5	1326	A2M
3	L5	1337	A
3	L5	1354	A
3	L5	1359	G
3	L5	1365	C
3	L5	1366	G

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Mol	Chain	Res	Type
3	L5	1370	G
3	L5	1379	C
3	L5	1381	U
3	L5	1387	A
3	L5	1394	G
3	L5	1397	A
3	L5	1398	A
3	L5	1404	G
3	L5	1407	C
3	L5	1408	G
3	L5	1409	C
3	L5	1410	U
3	L5	1411	C
3	L5	1415	G
3	L5	1416	G
3	L5	1417	C
3	L5	1420	A
3	L5	1437	C
3	L5	1439	C
3	L5	1442	C
3	L5	1443	A
3	L5	1444	G
3	L5	1446	C
3	L5	1447	C
3	L5	1480	C
3	L5	1483	C
3	L5	1497	A
3	L5	1498	G
3	L5	1502	G
3	L5	1504	G
3	L5	1517	G
3	L5	1524	A2M
3	L5	1534	A2M
3	L5	1537	A
3	L5	1547	A
3	L5	1564	A
3	L5	1566	C
3	L5	1574	G
3	L5	1578	U
3	L5	1586	G
3	L5	1591	U
3	L5	1596	U

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Mol	Chain	Res	Type
3	L5	1612	G
3	L5	1613	A
3	L5	1621	A
3	L5	1624	G
3	L5	1625	OMG
3	L5	1626	G
3	L5	1631	A
3	L5	1633	G
3	L5	1634	A
3	L5	1640	C
3	L5	1641	G
3	L5	1654	G
3	L5	1661	C
3	L5	1676	C
3	L5	1677	PSU
3	L5	1694	C
3	L5	1697	G
3	L5	1699	A
3	L5	1700	G
3	L5	1701	A
3	L5	1704	C
3	L5	1705	G
3	L5	1717	C
3	L5	1718	C
3	L5	1719	A
3	L5	1721	G
3	L5	1731	C
3	L5	1733	G
3	L5	1734	G
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

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Mol	Chain	Res	Type
3	L5	1768	C
3	L5	1770	A
3	L5	1787	A
3	L5	1804	A
3	L5	1806	G
3	L5	1810	G
3	L5	1821	G
3	L5	1822	U
3	L5	1834	U
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1855	G
3	L5	1866	U
3	L5	1869	G
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	1940	G
3	L5	1948	G
3	L5	1962	A
3	L5	1974	U
3	L5	1975	G
3	L5	1978	C
3	L5	1980	U
3	L5	1981	G
3	L5	1982	G
3	L5	1984	A
3	L5	1985	G
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	2002	A
3	L5	2003	G
3	L5	2005	G
3	L5	2011	C
3	L5	2024	G
3	L5	2025	A
3	L5	2026	A
3	L5	2046	G
3	L5	2048	U
3	L5	2052	G
3	L5	2055	G
3	L5	2056	G
3	L5	2068	C
3	L5	2069	A
3	L5	2084	C
3	L5	2085	G
3	L5	2092	G
3	L5	2093	A
3	L5	2094	G
3	L5	2095	A
3	L5	2097	U
3	L5	2098	G
3	L5	2101	C
3	L5	2102	G
3	L5	2103	G
3	L5	2107	C
3	L5	2112	G
3	L5	2252	G
3	L5	2253	A
3	L5	2254	G
3	L5	2256	C
3	L5	2258	C
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2306	G
3	L5	2313	A
3	L5	2331	G
3	L5	2333	G
3	L5	2348	G
3	L5	2351	OMC

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Mol	Chain	Res	Type
3	L5	2360	A
3	L5	2364	OMG
3	L5	2389	A
3	L5	2395	A
3	L5	2397	G
3	L5	2398	U
3	L5	2401	A2M
3	L5	2411	C
3	L5	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	2511	A
3	L5	2513	A
3	L5	2518	G
3	L5	2519	U
3	L5	2520	C
3	L5	2529	A
3	L5	2537	A
3	L5	2544	G
3	L5	2546	G
3	L5	2547	G
3	L5	2554	U
3	L5	2555	G

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Mol	Chain	Res	Type
3	L5	2559	G
3	L5	2560	C
3	L5	2565	A
3	L5	2573	A
3	L5	2583	C
3	L5	2586	G
3	L5	2587	A
3	L5	2589	C
3	L5	2606	G
3	L5	2627	C
3	L5	2644	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	2703	G
3	L5	2705	G
3	L5	2707	U
3	L5	2708	U
3	L5	2709	C
3	L5	2710	C
3	L5	2711	G
3	L5	2712	G
3	L5	2721	G
3	L5	2724	G
3	L5	2726	G
3	L5	2739	C
3	L5	2742	G
3	L5	2743	A
3	L5	2754	G
3	L5	2761	U
3	L5	2762	G
3	L5	2763	U
3	L5	2764	A
3	L5	2769	U
3	L5	2770	C
3	L5	2788	U

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Mol	Chain	Res	Type
3	L5	2790	U
3	L5	2806	A
3	L5	2826	U
3	L5	2827	G
3	L5	2829	U
3	L5	2835	A
3	L5	2855	G
3	L5	2867	C
3	L5	2877	G
3	L5	2892	C
3	L5	2900	U
3	L5	2901	G
3	L5	2902	G
3	L5	2903	G
3	L5	2904	U
3	L5	2905	C
3	L5	2907	G
3	L5	2908	U
3	L5	3585	G
3	L5	3590	G
3	L5	3591	C
3	L5	3594	C
3	L5	3595	U
3	L5	3596	A
3	L5	3597	G
3	L5	3599	A
3	L5	3605	C
3	L5	3615	G
3	L5	3626	G
3	L5	3630	A
3	L5	3635	A
3	L5	3644	U
3	L5	3646	A
3	L5	3648	A
3	L5	3662	A
3	L5	3664	G
3	L5	3670	C
3	L5	3673	C
3	L5	3674	G
3	L5	3692	A
3	L5	3701	OMC
3	L5	3710	G

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Mol	Chain	Res	Type
3	L5	3711	A
3	L5	3713	U
3	L5	3714	G
3	L5	3727	A
3	L5	3736	A
3	L5	3748	A
3	L5	3756	A
3	L5	3757	G
3	L5	3764	U
3	L5	3771	C
3	L5	3775	A
3	L5	3776	G
3	L5	3777	G
3	L5	3778	U
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	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3885	G
3	L5	3890	A
3	L5	3892	U
3	L5	3897	G
3	L5	3898	G
3	L5	3901	A
3	L5	3906	A
3	L5	3907	G
3	L5	3908	A
3	L5	3915	U
3	L5	3923	A
3	L5	3938	G
3	L5	3942	A
3	L5	3943	A

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Mol	Chain	Res	Type
3	L5	3946	G
3	L5	3947	A
3	L5	3948	C
3	L5	3949	A
3	L5	3950	U
3	L5	3951	G
3	L5	3952	A
3	L5	3953	G
3	L5	4057	C
3	L5	4058	U
3	L5	4059	C
3	L5	4060	U
3	L5	4061	G
3	L5	4062	A
3	L5	4064	C
3	L5	4068	U
3	L5	4069	U
3	L5	4076	G
3	L5	4088	C
3	L5	4095	G
3	L5	4097	G
3	L5	4099	G
3	L5	4101	C
3	L5	4104	G
3	L5	4105	A
3	L5	4106	G
3	L5	4108	G
3	L5	4111	U
3	L5	4114	C
3	L5	4115	G
3	L5	4116	C
3	L5	4119	C
3	L5	4122	G
3	L5	4127	A
3	L5	4141	G
3	L5	4142	C
3	L5	4143	G
3	L5	4144	C
3	L5	4146	G
3	L5	4150	G
3	L5	4162	C
3	L5	4163	U

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Mol	Chain	Res	Type
3	L5	4170	A
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4203	A
3	L5	4212	A
3	L5	4220	6MZ
3	L5	4222	G
3	L5	4225	G
3	L5	4229	U
3	L5	4232	U
3	L5	4233	A
3	L5	4234	A
3	L5	4243	C
3	L5	4249	G
3	L5	4251	A
3	L5	4254	G
3	L5	4257	A
3	L5	4258	C
3	L5	4265	U
3	L5	4268	A
3	L5	4273	A
3	L5	4291	G
3	L5	4295	U
3	L5	4304	A
3	L5	4305	G
3	L5	4314	C
3	L5	4319	C
3	L5	4329	G
3	L5	4330	G
3	L5	4332	C
3	L5	4338	G
3	L5	4349	C
3	L5	4373	G
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	4421	C
3	L5	4422	A

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Mol	Chain	Res	Type
3	L5	4430	G
3	L5	4433	G
3	L5	4438	U
3	L5	4448	G
3	L5	4449	A
3	L5	4453	C
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	4532	PSU
3	L5	4545	G
3	L5	4548	A
3	L5	4549	G
3	L5	4560	C
3	L5	4567	G
3	L5	4573	G
3	L5	4575	G
3	L5	4589	A
3	L5	4590	A2M
3	L5	4601	U
3	L5	4618	OMG
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4652	G
3	L5	4656	A
3	L5	4670	C
3	L5	4672	A
3	L5	4694	G
3	L5	4695	C
3	L5	4700	A
3	L5	4707	A
3	L5	4708	A
3	L5	4709	U
3	L5	4719	G
3	L5	4733	C

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Mol	Chain	Res	Type
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	4870	G
3	L5	4871	C
3	L5	4875	G
3	L5	4881	U
3	L5	4882	U
3	L5	4883	C
3	L5	4889	G
3	L5	4895	C
3	L5	4896	G
3	L5	4899	G
3	L5	4900	C
3	L5	4901	G
3	L5	4910	G
3	L5	4912	G
3	L5	4914	C
3	L5	4915	G
3	L5	4925	U
3	L5	4926	C
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	4951	G
3	L5	4960	G

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Mol	Chain	Res	Type
3	L5	4975	G
3	L5	4976	U
3	L5	4988	U
3	L5	4989	U
3	L5	4990	C
3	L5	4991	U
3	L5	4995	U
3	L5	5013	C
3	L5	5014	A
3	L5	5017	G
3	L5	5022	U
3	L5	5023	C
3	L5	5024	C
3	L5	5028	G
3	L5	5030	U
3	L5	5034	A
3	L5	5041	G
3	L5	5047	C
3	L5	5050	C
3	L5	5054	C
3	L5	5055	G
3	L5	5061	A
3	L5	5069	U
4	L7	22	A
4	L7	33	U
4	L7	38	U
4	L7	53	U
4	L7	54	A
4	L7	64	G
4	L7	97	G
4	L7	100	A
4	L7	110	G
4	L7	111	C
5	L8	25	G
5	L8	34	U
5	L8	35	C
5	L8	59	A
5	L8	62	A
5	L8	63	U
5	L8	75	OMG
5	L8	80	A
5	L8	82	A

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Mol	Chain	Res	Type
5	L8	83	C
5	L8	84	A
5	L8	85	U
5	L8	87	G
5	L8	94	G
5	L8	103	A
5	L8	105	C
5	L8	111	U
5	L8	114	G
5	L8	123	U
5	L8	124	U
5	L8	125	C
5	L8	126	C
5	L8	127	U
5	L8	150	C
5	L8	153	C
68	S2	2	A
68	S2	4	C
68	S2	13	C
68	S2	14	C
68	S2	25	A
68	S2	33	G
68	S2	41	G
68	S2	42	A
68	S2	46	A
68	S2	56	G
68	S2	58	C
68	S2	59	U
68	S2	62	G
68	S2	65	C
68	S2	67	C
68	S2	68	A
68	S2	72	C
68	S2	73	C
68	S2	74	G
68	S2	76	U
68	S2	92	A
68	S2	93	PSU
68	S2	99	A2M
68	S2	103	A
68	S2	113	G
68	S2	115	U

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Mol	Chain	Res	Type
68	S2	130	G
68	S2	142	C
68	S2	143	U
68	S2	147	A
68	S2	148	U
68	S2	149	A
68	S2	158	A
68	S2	160	U
68	S2	162	C
68	S2	163	U
68	S2	170	A
68	S2	179	C
68	S2	182	C
68	S2	187	G
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	206	G
68	S2	207	G
68	S2	208	G
68	S2	211	G
68	S2	213	G
68	S2	214	U
68	S2	291	G
68	S2	292	A
68	S2	294	U
68	S2	295	C
68	S2	302	A
68	S2	303	C
68	S2	305	U
68	S2	306	C
68	S2	307	G
68	S2	308	G
68	S2	309	G
68	S2	311	C
68	S2	312	G
68	S2	314	U
68	S2	318	A
68	S2	319	C

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Mol	Chain	Res	Type
68	S2	320	G
68	S2	323	C
68	S2	324	C
68	S2	325	C
68	S2	326	C
68	S2	328	U
68	S2	329	G
68	S2	332	G
68	S2	339	A
68	S2	347	G
68	S2	360	A
68	S2	361	U
68	S2	362	C
68	S2	363	A
68	S2	364	A
68	S2	368	U
68	S2	370	G
68	S2	381	C
68	S2	383	G
68	S2	385	G
68	S2	386	C
68	S2	407	G
68	S2	408	A
68	S2	409	C
68	S2	426	A
68	S2	428	OMU
68	S2	448	A
68	S2	449	A
68	S2	450	C
68	S2	452	G
68	S2	464	A
68	S2	465	A
68	S2	471	G
68	S2	472	C
68	S2	473	A
68	S2	474	G
68	S2	482	G
68	S2	487	U
68	S2	488	U
68	S2	492	C
68	S2	493	A
68	S2	502	C

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Mol	Chain	Res	Type
68	S2	516	A
68	S2	531	A
68	S2	532	C
68	S2	534	G
68	S2	536	A
68	S2	537	C
68	S2	540	U
68	S2	542	U
68	S2	544	G
68	S2	546	G
68	S2	547	G
68	S2	557	U
68	S2	558	G
68	S2	563	G
68	S2	564	A
68	S2	576	A2M
68	S2	583	A
68	S2	587	A
68	S2	589	G
68	S2	590	A
68	S2	591	U
68	S2	593	C
68	S2	604	A
68	S2	606	G
68	S2	614	C
68	S2	617	G
68	S2	623	G
68	S2	627	OMU
68	S2	628	A
68	S2	631	U
68	S2	638	C
68	S2	643	A
68	S2	644	OMG
68	S2	655	A
68	S2	659	G
68	S2	660	C
68	S2	664	A
68	S2	668	A2M
68	S2	669	A
68	S2	671	A
68	S2	672	A
68	S2	673	G

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Mol	Chain	Res	Type
68	S2	684	G
68	S2	688	U
68	S2	689	U
68	S2	690	G
68	S2	692	G
68	S2	693	A
68	S2	695	C
68	S2	696	G
68	S2	697	G
68	S2	698	G
68	S2	732	U
68	S2	733	C
68	S2	736	C
68	S2	738	C
68	S2	749	U
68	S2	751	G
68	S2	752	G
68	S2	753	C
68	S2	788	G
68	S2	791	C
68	S2	792	C
68	S2	798	G
68	S2	799	OMU
68	S2	801	PSU
68	S2	821	G
68	S2	822	U
68	S2	823	U
68	S2	824	C
68	S2	827	A
68	S2	830	A
68	S2	834	C
68	S2	835	C
68	S2	836	G
68	S2	837	A
68	S2	838	G
68	S2	839	C
68	S2	840	C
68	S2	844	U
68	S2	847	A
68	S2	867	OMG
68	S2	869	A
68	S2	870	A

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Mol	Chain	Res	Type
68	S2	873	G
68	S2	878	G
68	S2	886	A
68	S2	888	U
68	S2	889	U
68	S2	891	G
68	S2	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	907	G
68	S2	909	G
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	970	G
68	S2	971	G
68	S2	978	G
68	S2	982	G
68	S2	990	A
68	S2	992	A
68	S2	999	G
68	S2	1001	A
68	S2	1002	U
68	S2	1008	A
68	S2	1017	U
68	S2	1023	A
68	S2	1027	A
68	S2	1045	PSU
68	S2	1060	A
68	S2	1061	U
68	S2	1062	A
68	S2	1080	A
68	S2	1083	A
68	S2	1085	C

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Mol	Chain	Res	Type
68	S2	1096	G
68	S2	1107	G
68	S2	1108	G
68	S2	1109	C
68	S2	1113	A
68	S2	1114	U
68	S2	1116	C
68	S2	1119	A
68	S2	1121	G
68	S2	1126	G
68	S2	1133	A
68	S2	1138	C
68	S2	1139	C
68	S2	1148	A
68	S2	1153	C
68	S2	1154	U
68	S2	1155	U
68	S2	1161	U
68	S2	1162	C
68	S2	1166	G
68	S2	1183	A
68	S2	1195	A
68	S2	1200	A
68	S2	1207	G
68	S2	1208	A
68	S2	1215	C
68	S2	1217	A
68	S2	1220	A
68	S2	1224	G
68	S2	1227	G
68	S2	1242	U
68	S2	1243	U
68	S2	1251	A
68	S2	1253	A
68	S2	1255	G
68	S2	1256	G
68	S2	1257	G
68	S2	1259	A
68	S2	1274	G
68	S2	1275	G
68	S2	1284	A
68	S2	1286	G

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Mol	Chain	Res	Type
68	S2	1294	G
68	S2	1295	A
68	S2	1301	A
68	S2	1302	G
68	S2	1303	C
68	S2	1304	U
68	S2	1308	U
68	S2	1342	U
68	S2	1354	G
68	S2	1356	G
68	S2	1357	A
68	S2	1371	U
68	S2	1376	A
68	S2	1378	A
68	S2	1401	A
68	S2	1402	A
68	S2	1408	U
68	S2	1413	G
68	S2	1414	A
68	S2	1417	C
68	S2	1418	C
68	S2	1419	C
68	S2	1421	A
68	S2	1423	C
68	S2	1424	G
68	S2	1428	G
68	S2	1429	G
68	S2	1433	C
68	S2	1434	C
68	S2	1435	C
68	S2	1436	C
68	S2	1437	C
68	S2	1438	A
68	S2	1439	A
68	S2	1442	OMU
68	S2	1449	G
68	S2	1454	A
68	S2	1463	U
68	S2	1464	C
68	S2	1466	G
68	S2	1474	A
68	S2	1480	A

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Mol	Chain	Res	Type
68	S2	1486	A
68	S2	1488	C
68	S2	1489	A
68	S2	1490	OMG
68	S2	1494	U
68	S2	1495	G
68	S2	1497	G
68	S2	1498	A
68	S2	1521	C
68	S2	1522	A
68	S2	1533	A
68	S2	1536	G
68	S2	1544	C
68	S2	1546	G
68	S2	1552	G
68	S2	1553	C
68	S2	1558	C
68	S2	1560	U
68	S2	1575	G
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	1598	G
68	S2	1601	A
68	S2	1604	G
68	S2	1606	G
68	S2	1621	U
68	S2	1623	A
68	S2	1633	A
68	S2	1634	A
68	S2	1637	A
68	S2	1646	C
68	S2	1648	G
68	S2	1654	G
68	S2	1663	A
68	S2	1664	A
68	S2	1665	G
68	S2	1680	G

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Mol	Chain	Res	Type
68	S2	1683	C
68	S2	1699	A
68	S2	1713	C
68	S2	1721	U
68	S2	1722	G
68	S2	1744	G
68	S2	1745	A
68	S2	1752	C
68	S2	1753	C
68	S2	1754	G
68	S2	1756	C
68	S2	1757	G
68	S2	1758	G
68	S2	1761	U
68	S2	1772	C
68	S2	1773	C
68	S2	1774	C
68	S2	1775	U
68	S2	1783	C
68	S2	1784	G
68	S2	1786	U
68	S2	1810	U
68	S2	1824	A
68	S2	1825	A
68	S2	1826	G
68	S2	1829	G
68	S2	1831	A
68	S2	1835	A
68	S2	1838	U
68	S2	1849	G
68	S2	1851	MA6
68	S2	1861	G
68	S2	1862	G
68	S2	1863	A
68	S2	1865	C

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	254	G
3	L5	406	C
3	L5	914	U

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Mol	Chain	Res	Type
3	L5	1082	C
3	L5	1178	G
3	L5	1633	G
3	L5	1698	C
3	L5	1703	C
3	L5	1977	C
3	L5	2252	G
3	L5	2416	G
3	L5	2559	G
3	L5	2675	G
3	L5	2760	G
3	L5	2763	U
3	L5	3673	C
3	L5	4061	G
3	L5	4600	G
3	L5	4699	U
3	L5	4913	G
68	S2	291	G
68	S2	531	A
68	S2	563	G
68	S2	688	U
68	S2	1422	G

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	OMG	L5	3627	3	23,26,27	0.57	0	32,38,41	0.58	0
68	OMU	S2	116	68	19,22,23	3.33	7 (36%)	25,31,34	1.74	5 (20%)
68	PSU	S2	1177	68	18,21,22	1.11	2 (11%)	21,30,33	1.94	4 (19%)
3	PSU	L5	4403	3	18,21,22	1.10	3 (16%)	21,30,33	2.08	6 (28%)
68	OMC	S2	1703	68	19,22,23	0.59	0	25,31,34	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L5	3841	3	19,22,23	0.68	0	25,31,34	0.55	0
3	PSU	L5	1860	3	18,21,22	1.07	2 (11%)	21,30,33	1.88	4 (19%)
3	PSU	L5	4293	3	18,21,22	1.06	2 (11%)	21,30,33	2.01	5 (23%)
68	PSU	S2	109	68	18,21,22	1.06	2 (11%)	21,30,33	1.90	5 (23%)
68	PSU	S2	93	68	18,21,22	1.00	1 (5%)	21,30,33	1.90	4 (19%)
3	PSU	L5	1862	3	18,21,22	1.03	2 (11%)	21,30,33	1.98	4 (19%)
3	OMG	L5	4637	3	23,26,27	0.57	0	32,38,41	0.48	0
3	PSU	L5	4312	3	18,21,22	1.05	2 (11%)	21,30,33	1.92	4 (19%)
3	PSU	L5	3637	3	18,21,22	1.06	1 (5%)	21,30,33	1.98	4 (19%)
3	OMG	L5	4618	3	23,26,27	0.61	0	32,38,41	0.49	0
3	A2M	L5	2401	3	22,25,26	1.20	2 (9%)	30,36,39	1.55	7 (23%)
3	OMU	L5	3925	3	19,22,23	3.15	7 (36%)	25,31,34	1.92	5 (20%)
3	A2M	L5	3785	3,86	22,25,26	1.24	1 (4%)	30,36,39	1.69	9 (30%)
3	OMG	L5	4494	3	23,26,27	0.59	0	32,38,41	0.52	0
3	A2M	L5	2787	3	22,25,26	1.17	2 (9%)	30,36,39	1.48	8 (26%)
3	PSU	L5	4299	3	18,21,22	1.05	2 (11%)	21,30,33	1.90	4 (19%)
3	A2M	L5	1326	3	22,25,26	1.28	2 (9%)	30,36,39	1.48	9 (30%)
3	OMU	L5	4306	3	19,22,23	3.14	7 (36%)	25,31,34	1.78	5 (20%)
3	OMC	L5	2804	3	19,22,23	0.67	0	25,31,34	0.61	0
3	PSU	L5	4471	3	18,21,22	1.09	2 (11%)	21,30,33	2.00	4 (19%)
3	PSU	L5	1792	3	18,21,22	1.03	1 (5%)	21,30,33	1.90	4 (19%)
68	MA6	S2	1850	68	23,26,27	1.31	3 (13%)	33,38,41	3.32	12 (36%)
3	PSU	L5	1683	3	18,21,22	1.09	2 (11%)	21,30,33	1.91	4 (19%)
3	OMG	L5	4196	3	23,26,27	0.57	0	32,38,41	0.46	0
3	5MC	L5	4447	3	19,22,23	0.90	1 (5%)	26,32,35	0.87	0
68	OMC	S2	1391	68	19,22,23	0.60	0	25,31,34	0.70	0
68	OMG	S2	867	68	23,26,27	0.52	0	32,38,41	0.48	0
3	PSU	L5	2632	3	18,21,22	1.05	2 (11%)	21,30,33	2.05	5 (23%)
3	PSU	L5	1582	3	18,21,22	1.10	2 (11%)	21,30,33	2.01	5 (23%)
3	PSU	L5	4296	3	18,21,22	1.10	2 (11%)	21,30,33	2.05	5 (23%)
3	OMG	L5	3899	3	23,26,27	0.62	0	32,38,41	0.51	0
3	PSU	L5	4628	3	18,21,22	1.02	1 (5%)	21,30,33	1.85	4 (19%)
3	PSU	L5	4552	3	18,21,22	1.16	2 (11%)	21,30,33	1.94	4 (19%)
68	PSU	S2	866	68	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
68	OMU	S2	172	68	19,22,23	3.31	7 (36%)	25,31,34	1.90	4 (16%)
3	6MZ	L5	4220	3	22,25,26	2.96	5 (22%)	29,36,39	2.43	10 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	3718	3	22,25,26	1.22	2 (9%)	30,36,39	1.53	6 (20%)
68	OMG	S2	436	68	23,26,27	0.55	0	32,38,41	0.54	0
68	PSU	S2	1244	68	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
3	OMG	L5	4228	3	23,26,27	0.59	0	32,38,41	0.66	0
68	OMU	S2	354	68	19,22,23	3.25	7 (36%)	25,31,34	1.85	5 (20%)
3	OMG	L5	4499	3	23,26,27	0.57	0	32,38,41	0.46	0
3	OMC	L5	3887	3	19,22,23	0.64	0	25,31,34	0.70	0
3	OMC	L5	4536	3	19,22,23	0.68	0	25,31,34	0.61	0
3	OMG	L5	4370	3	23,26,27	0.57	0	32,38,41	0.49	0
68	MA6	S2	1851	68	23,26,27	1.30	2 (8%)	33,38,41	3.38	12 (36%)
68	OMC	S2	462	68	19,22,23	0.57	0	25,31,34	0.54	0
5	PSU	L8	55	5	18,21,22	1.07	2 (11%)	21,30,33	1.86	4 (19%)
68	PSU	S2	651	68	18,21,22	1.06	1 (5%)	21,30,33	1.98	4 (19%)
3	A2M	L5	400	3	22,25,26	1.32	2 (9%)	30,36,39	1.57	9 (30%)
68	PSU	S2	406	68	18,21,22	1.10	2 (11%)	21,30,33	1.89	4 (19%)
3	PSU	L5	1782	3	18,21,22	1.09	2 (11%)	21,30,33	1.91	4 (19%)
3	PSU	L5	4442	3	18,21,22	1.08	3 (16%)	21,30,33	2.04	6 (28%)
3	PSU	L5	4353	3	18,21,22	1.07	2 (11%)	21,30,33	2.02	6 (28%)
68	PSU	S2	1367	68	18,21,22	1.07	1 (5%)	21,30,33	1.93	4 (19%)
3	A2M	L5	4590	3	22,25,26	1.26	2 (9%)	30,36,39	1.56	7 (23%)
3	OMG	L5	1316	3	23,26,27	0.67	0	32,38,41	0.53	0
68	4AC	S2	1842	68	21,24,25	0.40	0	28,34,37	0.45	0
3	PSU	L5	4457	3	18,21,22	1.08	3 (16%)	21,30,33	1.99	5 (23%)
3	A2M	L5	1323	3	22,25,26	1.33	3 (13%)	30,36,39	1.53	9 (30%)
3	OMG	L5	4623	3	23,26,27	0.59	0	32,38,41	0.48	0
3	OMG	L5	1522	3	23,26,27	0.59	0	32,38,41	0.54	0
3	A2M	L5	4523	3,86	22,25,26	1.39	3 (13%)	30,36,39	1.54	9 (30%)
68	PSU	S2	1045	68	18,21,22	1.10	1 (5%)	21,30,33	1.99	4 (19%)
3	OMG	L5	2424	3	23,26,27	0.55	0	32,38,41	0.49	0
68	A2M	S2	159	68	22,25,26	1.10	1 (4%)	30,36,39	1.51	9 (30%)
68	PSU	S2	686	68	18,21,22	1.11	2 (11%)	21,30,33	1.91	4 (19%)
3	OMG	L5	2876	3	23,26,27	0.60	0	32,38,41	0.49	0
68	PSU	S2	814	68	18,21,22	1.11	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L5	1781	3	18,21,22	1.05	1 (5%)	21,30,33	1.91	4 (19%)
3	PSU	L5	3695	3	18,21,22	1.05	2 (11%)	21,30,33	1.94	4 (19%)
68	G7M	S2	1639	68	23,26,27	2.66	9 (39%)	34,39,42	2.49	11 (32%)
68	PSU	S2	1004	68	18,21,22	1.08	1 (5%)	21,30,33	1.95	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	3744	3	23,26,27	0.58	0	32,38,41	0.45	0
3	PSU	L5	4579	3	18,21,22	1.01	1 (5%)	21,30,33	1.90	4 (19%)
3	PSU	L5	3822	3	18,21,22	1.08	2 (11%)	21,30,33	2.04	6 (28%)
68	OMU	S2	1326	68	19,22,23	3.28	7 (36%)	25,31,34	1.83	5 (20%)
3	PSU	L5	3853	3,86	18,21,22	1.05	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L5	1536	3	18,21,22	1.11	2 (11%)	21,30,33	2.05	4 (19%)
3	PSU	L5	4972	3	18,21,22	1.06	1 (5%)	21,30,33	1.97	4 (19%)
3	OMC	L5	3701	3	19,22,23	0.68	0	25,31,34	1.31	3 (12%)
3	1MA	L5	1322	3,86	21,25,26	0.67	0	30,37,40	0.76	1 (3%)
68	OMG	S2	644	68	23,26,27	0.54	0	32,38,41	0.45	0
3	A2M	L5	398	3	22,25,26	1.24	2 (9%)	30,36,39	1.59	7 (23%)
3	PSU	L5	3920	3,86	18,21,22	1.09	3 (16%)	21,30,33	2.12	6 (28%)
68	OMC	S2	517	68	19,22,23	0.62	0	25,31,34	0.74	0
3	OMG	L5	1625	3	23,26,27	0.61	0	32,38,41	0.52	0
5	PSU	L8	69	5	18,21,22	1.09	2 (11%)	21,30,33	1.92	5 (23%)
3	OMU	L5	4227	3	19,22,23	3.22	7 (36%)	25,31,34	1.88	5 (20%)
3	PSU	L5	4636	3	18,21,22	1.11	3 (16%)	21,30,33	2.18	6 (28%)
3	A2M	L5	1524	3	22,25,26	1.39	3 (13%)	30,36,39	1.52	7 (23%)
68	OMG	S2	601	68	23,26,27	0.58	0	32,38,41	0.45	0
3	A2M	L5	3830	3	22,25,26	1.29	3 (13%)	30,36,39	1.55	5 (16%)
3	A2M	L5	2815	3	22,25,26	1.21	1 (4%)	30,36,39	1.47	7 (23%)
3	PSU	L5	3639	3	18,21,22	1.12	2 (11%)	21,30,33	1.90	4 (19%)
3	A2M	L5	3825	3	22,25,26	1.22	2 (9%)	30,36,39	1.52	8 (26%)
3	OMC	L5	1340	3	19,22,23	0.66	0	25,31,34	0.65	0
68	B8N	S2	1248	68	25,29,30	3.25	6 (24%)	28,42,45	1.94	8 (28%)
68	A2M	S2	1031	68	22,25,26	1.21	1 (4%)	30,36,39	1.53	8 (26%)
3	PSU	L5	3851	3	18,21,22	1.08	1 (5%)	21,30,33	1.89	4 (19%)
68	OMC	S2	174	68	19,22,23	0.56	0	25,31,34	0.65	0
3	OMC	L5	4456	3	19,22,23	0.72	0	25,31,34	0.80	1 (4%)
3	A2M	L5	4571	3	22,25,26	1.33	2 (9%)	30,36,39	1.60	7 (23%)
3	A2M	L5	1871	3,86	22,25,26	1.35	2 (9%)	30,36,39	1.58	7 (23%)
68	OMG	S2	509	68	23,26,27	0.54	0	32,38,41	0.56	0
3	PSU	L5	4532	3	18,21,22	1.09	2 (11%)	21,30,33	1.92	4 (19%)
3	PSU	L5	2839	3	18,21,22	1.12	2 (11%)	21,30,33	1.97	5 (23%)
68	OMU	S2	428	68	19,22,23	3.33	7 (36%)	25,31,34	1.84	5 (20%)
3	OMU	L5	4498	3	19,22,23	3.16	7 (36%)	25,31,34	1.91	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	1534	3,86	22,25,26	1.29	3 (13%)	30,36,39	1.53	8 (26%)
68	A2M	S2	468	68	22,25,26	1.28	1 (4%)	30,36,39	1.62	8 (26%)
68	PSU	S2	1081	68	18,21,22	1.07	2 (11%)	21,30,33	2.02	6 (28%)
68	4AC	S2	1337	68	21,24,25	0.39	0	28,34,37	0.54	0
68	A2M	S2	668	68,86	22,25,26	1.38	2 (9%)	30,36,39	1.63	9 (30%)
3	PSU	L5	3844	3	18,21,22	1.09	2 (11%)	21,30,33	1.90	4 (19%)
3	PSU	L5	5001	3	18,21,22	1.13	2 (11%)	21,30,33	2.08	5 (23%)
3	PSU	L5	4500	3	18,21,22	1.05	2 (11%)	21,30,33	2.01	6 (28%)
68	PSU	S2	801	68	18,21,22	1.15	1 (5%)	21,30,33	1.79	4 (19%)
3	OMG	L5	3792	3	23,26,27	0.59	0	32,38,41	0.53	0
68	A2M	S2	484	68	22,25,26	1.19	1 (4%)	30,36,39	1.51	8 (26%)
68	6MZ	S2	1832	68,86	22,25,26	3.04	5 (22%)	29,36,39	2.27	10 (34%)
68	PSU	S2	1232	68	18,21,22	1.09	1 (5%)	21,30,33	2.02	6 (28%)
68	PSU	S2	1056	68	18,21,22	1.06	1 (5%)	21,30,33	1.89	4 (19%)
3	UR3	L5	4530	3	19,22,23	2.68	7 (36%)	26,32,35	1.55	3 (11%)
3	OMG	L5	4392	3	23,26,27	0.61	0	32,38,41	0.49	0
3	OMC	L5	3808	3,86	19,22,23	0.68	0	25,31,34	0.93	2 (8%)
68	PSU	S2	863	68	18,21,22	1.09	1 (5%)	21,30,33	1.94	5 (23%)
3	PSU	L5	4689	3	18,21,22	1.09	2 (11%)	21,30,33	1.92	4 (19%)
68	PSU	S2	1046	68	18,21,22	1.06	1 (5%)	21,30,33	1.88	4 (19%)
3	OMC	L5	2422	3,86	19,22,23	0.63	0	25,31,34	0.67	0
3	OMC	L5	2861	3	19,22,23	0.62	0	25,31,34	0.79	1 (4%)
3	5MC	L5	3782	3,86	19,22,23	0.74	0	26,32,35	0.86	1 (3%)
68	A2M	S2	166	68	22,25,26	1.29	1 (4%)	30,36,39	1.61	7 (23%)
68	OMU	S2	121	68	19,22,23	3.27	7 (36%)	25,31,34	1.73	4 (16%)
3	OMC	L5	2365	3,86	19,22,23	0.65	0	25,31,34	0.53	0
68	OMU	S2	1442	68	19,22,23	3.33	7 (36%)	25,31,34	1.81	4 (16%)
3	PSU	L5	4673	3	18,21,22	1.07	2 (11%)	21,30,33	1.90	4 (19%)
68	OMU	S2	799	68	19,22,23	3.40	7 (36%)	25,31,34	1.84	5 (20%)
5	OMG	L8	75	5	23,26,27	0.53	0	32,38,41	0.48	0
68	PSU	S2	681	68	18,21,22	1.02	2 (11%)	21,30,33	1.92	4 (19%)
68	A2M	S2	576	68	22,25,26	1.23	1 (4%)	30,36,39	1.53	4 (13%)
68	PSU	S2	1174	68	18,21,22	1.06	2 (11%)	21,30,33	1.87	4 (19%)
3	OMU	L5	4620	3	19,22,23	3.17	7 (36%)	25,31,34	1.84	5 (20%)
68	PSU	S2	966	68,86	18,21,22	1.12	1 (5%)	21,30,33	1.99	6 (28%)
3	A2M	L5	2363	3,86	22,25,26	1.25	3 (13%)	30,36,39	1.48	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	OMG	S2	683	68	23,26,27	0.57	0	32,38,41	0.54	0
68	A2M	S2	99	68,86	22,25,26	1.25	1 (4%)	30,36,39	1.54	7 (23%)
68	OMU	S2	627	68	19,22,23	3.28	7 (36%)	25,31,34	1.88	5 (20%)
3	PSU	L5	4576	3	18,21,22	1.06	1 (5%)	21,30,33	1.95	4 (19%)
3	OMC	L5	2824	3	19,22,23	0.64	0	25,31,34	0.65	0
3	OMC	L5	3869	3	19,22,23	0.64	0	25,31,34	0.69	0
68	A2M	S2	27	68	22,25,26	1.23	2 (9%)	30,36,39	1.55	8 (26%)
3	OMC	L5	2351	3,86	19,22,23	0.67	0	25,31,34	0.84	1 (4%)
3	PSU	L5	3884	3	18,21,22	1.12	2 (11%)	21,30,33	2.00	5 (23%)
3	PSU	L5	1744	3,86	18,21,22	1.11	2 (11%)	21,30,33	1.91	4 (19%)
3	OMG	L5	2364	3,86	23,26,27	0.61	0	32,38,41	0.43	0
3	OMU	L5	2837	3	19,22,23	3.20	7 (36%)	25,31,34	1.93	5 (20%)
68	OMC	S2	1272	68	19,22,23	0.57	0	25,31,34	0.73	0
3	A2M	L5	3867	3	22,25,26	1.31	2 (9%)	30,36,39	1.61	8 (26%)
68	PSU	S2	105	68	18,21,22	1.08	1 (5%)	21,30,33	2.00	5 (23%)
68	OMU	S2	1288	68	19,22,23	3.32	7 (36%)	25,31,34	1.65	4 (16%)
68	OMG	S2	1328	68	23,26,27	0.55	0	32,38,41	0.43	0
3	PSU	L5	5010	3	18,21,22	1.12	2 (11%)	21,30,33	1.92	4 (19%)
3	PSU	L5	4493	3	18,21,22	1.09	2 (11%)	21,30,33	1.99	5 (23%)
3	PSU	L5	1677	3	18,21,22	1.07	3 (16%)	21,30,33	1.98	6 (28%)
3	PSU	L5	4431	3	18,21,22	1.08	2 (11%)	21,30,33	1.98	4 (19%)
3	UY1	L5	3818	3	19,22,23	4.73	9 (47%)	21,31,34	1.94	5 (23%)
3	PSU	L5	4521	3,86	18,21,22	1.06	2 (11%)	21,30,33	1.99	5 (23%)
3	PSU	L5	4361	3	18,21,22	1.05	1 (5%)	21,30,33	1.87	4 (19%)
68	A2M	S2	1383	68	22,25,26	1.22	1 (4%)	30,36,39	1.70	7 (23%)
3	PSU	L5	4973	3	18,21,22	1.06	2 (11%)	21,30,33	2.00	5 (23%)
68	PSU	S2	649	68	18,21,22	1.16	2 (11%)	21,30,33	1.88	5 (23%)
68	OMG	S2	1490	68	23,26,27	0.52	0	32,38,41	0.49	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
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
68	OMU	S2	116	68	-	1/9/27/28	0/2/2/2
68	PSU	S2	1177	68	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
68	OMC	S2	1703	68	-	1/9/27/28	0/2/2/2
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	109	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	93	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4618	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	2401	3	-	3/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
3	A2M	L5	3785	3,86	-	2/9/27/28	0/3/3/3
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2787	3	-	5/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	4/9/27/28	0/3/3/3
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
68	MA6	S2	1850	68	-	0/11/29/30	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4196	3	-	1/9/27/28	0/3/3/3
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
68	OMC	S2	1391	68	-	0/9/27/28	0/2/2/2
68	OMG	S2	867	68	-	2/9/27/28	0/3/3/3
3	PSU	L5	2632	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	4/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	866	68	-	0/7/25/26	0/2/2/2
68	OMU	S2	172	68	-	0/9/27/28	0/2/2/2
3	6MZ	L5	4220	3	-	2/9/27/28	0/3/3/3
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
68	OMG	S2	436	68	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
68	PSU	S2	1244	68	-	1/7/25/26	0/2/2/2
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
68	OMU	S2	354	68	-	1/9/27/28	0/2/2/2
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
68	MA6	S2	1851	68	-	1/11/29/30	0/3/3/3
68	OMC	S2	462	68	-	1/9/27/28	0/2/2/2
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
68	PSU	S2	651	68	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3
68	PSU	S2	406	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1367	68	-	0/7/25/26	0/2/2/2
3	A2M	L5	4590	3	-	4/9/27/28	0/3/3/3
3	OMG	L5	1316	3	-	1/9/27/28	0/3/3/3
68	4AC	S2	1842	68	-	0/11/29/30	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1323	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	4623	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	4523	3,86	-	0/9/27/28	0/3/3/3
68	PSU	S2	1045	68	-	2/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
68	A2M	S2	159	68	-	1/9/27/28	0/3/3/3
68	PSU	S2	686	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
68	PSU	S2	814	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
68	G7M	S2	1639	68	-	0/7/25/26	0/3/3/3
68	PSU	S2	1004	68	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	1326	68	-	0/9/27/28	0/2/2/2
3	PSU	L5	3853	3,86	-	0/7/25/26	0/2/2/2
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3701	3	-	6/9/27/28	0/2/2/2
3	1MA	L5	1322	3,86	-	2/7/25/26	0/3/3/3
68	OMG	S2	644	68	-	4/9/27/28	0/3/3/3
3	A2M	L5	398	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	3920	3,86	-	0/7/25/26	0/2/2/2
68	OMC	S2	517	68	-	0/9/27/28	0/2/2/2
3	OMG	L5	1625	3	-	2/9/27/28	0/3/3/3
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4636	3	-	3/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	2/9/27/28	0/3/3/3
68	OMG	S2	601	68	-	1/9/27/28	0/3/3/3
3	A2M	L5	3830	3	-	3/9/27/28	0/3/3/3
3	A2M	L5	2815	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3825	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
68	B8N	S2	1248	68	-	4/16/34/35	0/2/2/2
68	A2M	S2	1031	68	-	1/9/27/28	0/3/3/3
3	PSU	L5	3851	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	4456	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1871	3,86	-	0/9/27/28	0/3/3/3
68	OMG	S2	509	68	-	0/9/27/28	0/3/3/3
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	428	68	-	6/9/27/28	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	1534	3,86	-	2/9/27/28	0/3/3/3
68	A2M	S2	468	68	-	1/9/27/28	0/3/3/3
68	PSU	S2	1081	68	-	1/7/25/26	0/2/2/2
68	4AC	S2	1337	68	-	0/11/29/30	0/2/2/2
68	A2M	S2	668	68,86	-	3/9/27/28	0/3/3/3
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	4500	3	-	3/7/25/26	0/2/2/2
68	PSU	S2	801	68	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
68	A2M	S2	484	68	-	0/9/27/28	0/3/3/3
68	6MZ	S2	1832	68,86	-	2/9/27/28	0/3/3/3
68	PSU	S2	1232	68	-	0/7/25/26	0/2/2/2
68	PSU	S2	1056	68	-	0/7/25/26	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	3808	3,86	-	0/9/27/28	0/2/2/2
68	PSU	S2	863	68	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	1046	68	-	1/7/25/26	0/2/2/2
3	OMC	L5	2422	3,86	-	3/9/27/28	0/2/2/2
3	OMC	L5	2861	3	-	1/9/27/28	0/2/2/2
3	5MC	L5	3782	3,86	-	0/7/25/26	0/2/2/2
68	A2M	S2	166	68	-	3/9/27/28	0/3/3/3
68	OMU	S2	121	68	-	0/9/27/28	0/2/2/2
3	OMC	L5	2365	3,86	-	0/9/27/28	0/2/2/2
68	OMU	S2	1442	68	-	2/9/27/28	0/2/2/2
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
68	OMU	S2	799	68	-	2/9/27/28	0/2/2/2
5	OMG	L8	75	5	-	2/9/27/28	0/3/3/3
68	PSU	S2	681	68	-	0/7/25/26	0/2/2/2
68	A2M	S2	576	68	-	3/9/27/28	0/3/3/3
68	PSU	S2	1174	68	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
68	PSU	S2	966	68,86	-	0/7/25/26	0/2/2/2
3	A2M	L5	2363	3,86	-	0/9/27/28	0/3/3/3
68	OMG	S2	683	68	-	1/9/27/28	0/3/3/3
68	A2M	S2	99	68,86	-	2/9/27/28	0/3/3/3
68	OMU	S2	627	68	-	2/9/27/28	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	3869	3	-	1/9/27/28	0/2/2/2
68	A2M	S2	27	68	-	1/9/27/28	0/3/3/3
3	OMC	L5	2351	3,86	-	1/9/27/28	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1744	3,86	-	0/7/25/26	0/2/2/2
3	OMG	L5	2364	3,86	-	2/9/27/28	0/3/3/3
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
68	OMC	S2	1272	68	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	3867	3	-	2/9/27/28	0/3/3/3
68	PSU	S2	105	68	-	0/7/25/26	0/2/2/2
68	OMU	S2	1288	68	-	0/9/27/28	0/2/2/2
68	OMG	S2	1328	68	-	1/9/27/28	0/3/3/3
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	UY1	L5	3818	3	-	3/9/27/28	0/2/2/2
3	PSU	L5	4521	3,86	-	0/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
68	A2M	S2	1383	68	-	3/9/27/28	0/3/3/3
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
68	PSU	S2	649	68	-	0/7/25/26	0/2/2/2
68	OMG	S2	1490	68	-	1/9/27/28	0/3/3/3

All (338) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	1832	6MZ	C6-N6	12.55	1.48	1.34
3	L5	3818	UY1	C6-C5	12.21	1.48	1.35
3	L5	4220	6MZ	C6-N6	11.87	1.47	1.34
3	L5	3818	UY1	C2-N1	11.33	1.51	1.36
68	S2	799	OMU	C2-N1	8.61	1.51	1.38
68	S2	172	OMU	C2-N1	8.24	1.51	1.38
68	S2	1442	OMU	C2-N1	8.14	1.51	1.38
68	S2	1288	OMU	C2-N1	8.11	1.51	1.38
68	S2	1248	B8N	C4-N3	-8.08	1.26	1.40
68	S2	428	OMU	C2-N1	8.07	1.51	1.38
68	S2	116	OMU	C2-N1	7.98	1.51	1.38
68	S2	121	OMU	C2-N1	7.92	1.50	1.38
68	S2	354	OMU	C2-N1	7.87	1.50	1.38
68	S2	1326	OMU	C2-N1	7.84	1.50	1.38
68	S2	627	OMU	C2-N1	7.78	1.50	1.38
68	S2	1248	B8N	C6-N1	7.76	1.55	1.36
3	L5	4227	OMU	C2-N1	7.64	1.50	1.38
3	L5	2837	OMU	C2-N1	7.59	1.50	1.38
3	L5	4620	OMU	C2-N1	7.52	1.50	1.38
3	L5	3818	UY1	C2-N3	7.46	1.49	1.37
3	L5	4498	OMU	C2-N1	7.43	1.50	1.38
3	L5	4306	OMU	C2-N1	7.38	1.50	1.38
3	L5	3925	OMU	C2-N1	7.35	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	116	OMU	C2-N3	6.98	1.50	1.38
68	S2	1248	B8N	C4-C5	6.93	1.63	1.47
68	S2	799	OMU	C2-N3	6.89	1.50	1.38
68	S2	428	OMU	C2-N3	6.78	1.49	1.38
68	S2	172	OMU	C2-N3	6.77	1.49	1.38
68	S2	1326	OMU	C2-N3	6.75	1.49	1.38
68	S2	627	OMU	C2-N3	6.74	1.49	1.38
68	S2	1442	OMU	C2-N3	6.70	1.49	1.38
68	S2	1288	OMU	C2-N3	6.69	1.49	1.38
3	L5	4227	OMU	C2-N3	6.64	1.49	1.38
68	S2	121	OMU	C2-N3	6.56	1.49	1.38
68	S2	1639	G7M	C4-N3	6.56	1.49	1.34
68	S2	354	OMU	C2-N3	6.53	1.49	1.38
3	L5	4620	OMU	C2-N3	6.50	1.49	1.38
3	L5	4498	OMU	C2-N3	6.45	1.49	1.38
3	L5	3925	OMU	C2-N3	6.41	1.49	1.38
3	L5	2837	OMU	C2-N3	6.40	1.49	1.38
3	L5	4306	OMU	C2-N3	6.32	1.49	1.38
3	L5	4530	UR3	C2-N1	6.29	1.47	1.38
3	L5	4530	UR3	C6-C5	6.11	1.49	1.35
3	L5	2837	OMU	C6-C5	5.89	1.48	1.35
68	S2	428	OMU	C6-C5	5.87	1.48	1.35
68	S2	1288	OMU	C6-C5	5.86	1.48	1.35
68	S2	121	OMU	C6-C5	5.83	1.48	1.35
68	S2	116	OMU	C6-C5	5.80	1.48	1.35
68	S2	1248	B8N	C2-N1	5.80	1.56	1.39
68	S2	1326	OMU	C6-C5	5.79	1.48	1.35
68	S2	1442	OMU	C6-C5	5.79	1.48	1.35
3	L5	4530	UR3	C2-N3	5.75	1.50	1.39
68	S2	627	OMU	C6-C5	5.74	1.48	1.35
68	S2	799	OMU	C6-C5	5.74	1.48	1.35
68	S2	172	OMU	C6-C5	5.73	1.48	1.35
3	L5	4227	OMU	C6-C5	5.72	1.48	1.35
3	L5	3925	OMU	O4-C4	-5.72	1.13	1.24
68	S2	354	OMU	C6-C5	5.72	1.48	1.35
3	L5	4306	OMU	C6-C5	5.67	1.48	1.35
3	L5	4620	OMU	O4-C4	-5.64	1.13	1.24
3	L5	4306	OMU	O4-C4	-5.63	1.13	1.24
3	L5	4620	OMU	C6-C5	5.63	1.48	1.35
3	L5	3925	OMU	C6-C5	5.63	1.48	1.35
68	S2	1442	OMU	O4-C4	-5.62	1.13	1.24
3	L5	4498	OMU	C6-C5	5.61	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	354	OMU	O4-C4	-5.60	1.13	1.24
3	L5	4227	OMU	O4-C4	-5.58	1.13	1.24
68	S2	799	OMU	O4-C4	-5.55	1.13	1.24
3	L5	4498	OMU	O4-C4	-5.53	1.13	1.24
68	S2	627	OMU	O4-C4	-5.51	1.13	1.24
68	S2	1326	OMU	O4-C4	-5.50	1.13	1.24
3	L5	2837	OMU	O4-C4	-5.49	1.13	1.24
68	S2	1288	OMU	O4-C4	-5.48	1.13	1.24
68	S2	121	OMU	O4-C4	-5.47	1.13	1.24
68	S2	428	OMU	O4-C4	-5.47	1.13	1.24
68	S2	116	OMU	O4-C4	-5.45	1.13	1.24
68	S2	1639	G7M	C2-N3	5.39	1.46	1.33
68	S2	172	OMU	O4-C4	-5.39	1.14	1.24
3	L5	3818	UY1	C6-N1	5.22	1.44	1.36
68	S2	1248	B8N	C6-C5	5.21	1.42	1.35
68	S2	1639	G7M	C2-N2	4.93	1.45	1.34
68	S2	1639	G7M	C5-N7	-4.76	1.33	1.39
68	S2	116	OMU	C4-N3	4.44	1.46	1.38
68	S2	627	OMU	C4-N3	4.37	1.46	1.38
68	S2	428	OMU	C4-N3	4.36	1.46	1.38
3	L5	3818	UY1	C4-N3	4.31	1.46	1.38
68	S2	1326	OMU	C4-N3	4.28	1.45	1.38
68	S2	1288	OMU	C4-N3	4.25	1.45	1.38
68	S2	799	OMU	C4-N3	4.24	1.45	1.38
68	S2	172	OMU	C4-N3	4.23	1.45	1.38
68	S2	1442	OMU	C4-N3	4.22	1.45	1.38
68	S2	121	OMU	C4-N3	4.12	1.45	1.38
3	L5	4227	OMU	C4-N3	4.04	1.45	1.38
3	L5	4498	OMU	C4-N3	4.01	1.45	1.38
68	S2	354	OMU	C4-N3	3.99	1.45	1.38
3	L5	4620	OMU	C4-N3	3.91	1.45	1.38
3	L5	2837	OMU	C4-N3	3.87	1.45	1.38
3	L5	3925	OMU	C4-N3	3.84	1.45	1.38
68	S2	1639	G7M	C5-C6	3.81	1.53	1.43
3	L5	4306	OMU	C4-N3	3.72	1.45	1.38
3	L5	3818	UY1	O4-C4	-3.68	1.16	1.23
68	S2	801	PSU	C6-C5	3.68	1.39	1.35
3	L5	2815	A2M	O5'-C5'	-3.64	1.33	1.44
3	L5	1871	A2M	O5'-C5'	-3.63	1.33	1.44
68	S2	668	A2M	O5'-C5'	-3.60	1.33	1.44
3	L5	4220	6MZ	C5-C4	-3.57	1.32	1.39
3	L5	4571	A2M	O5'-C5'	-3.57	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	966	PSU	C6-C5	3.57	1.39	1.35
3	L5	3785	A2M	O5'-C5'	-3.56	1.33	1.44
68	S2	99	A2M	O5'-C5'	-3.56	1.33	1.44
3	L5	3825	A2M	O5'-C5'	-3.55	1.33	1.44
3	L5	1524	A2M	O5'-C5'	-3.55	1.33	1.44
68	S2	814	PSU	C6-C5	3.55	1.39	1.35
68	S2	686	PSU	C6-C5	3.53	1.39	1.35
68	S2	27	A2M	O5'-C5'	-3.53	1.33	1.44
68	S2	1248	B8N	C1'-C5	3.53	1.58	1.50
3	L5	1323	A2M	O5'-C5'	-3.53	1.33	1.44
68	S2	1045	PSU	C6-C5	3.52	1.39	1.35
68	S2	866	PSU	C6-C5	3.51	1.39	1.35
68	S2	576	A2M	O5'-C5'	-3.50	1.34	1.44
3	L5	2787	A2M	O5'-C5'	-3.48	1.34	1.44
3	L5	3830	A2M	O5'-C5'	-3.48	1.34	1.44
3	L5	400	A2M	O5'-C5'	-3.48	1.34	1.44
68	S2	484	A2M	O5'-C5'	-3.48	1.34	1.44
68	S2	649	PSU	C6-C5	3.48	1.39	1.35
3	L5	398	A2M	O5'-C5'	-3.46	1.34	1.44
68	S2	1177	PSU	C6-C5	3.45	1.39	1.35
68	S2	468	A2M	O5'-C5'	-3.44	1.34	1.44
3	L5	3718	A2M	O5'-C5'	-3.43	1.34	1.44
3	L5	4590	A2M	O5'-C5'	-3.41	1.34	1.44
68	S2	1244	PSU	C6-C5	3.41	1.39	1.35
68	S2	166	A2M	O5'-C5'	-3.41	1.34	1.44
68	S2	1031	A2M	O5'-C5'	-3.40	1.34	1.44
3	L5	3867	A2M	O5'-C5'	-3.40	1.34	1.44
3	L5	2363	A2M	O5'-C5'	-3.39	1.34	1.44
68	S2	1383	A2M	O5'-C5'	-3.38	1.34	1.44
3	L5	5010	PSU	C6-C5	3.38	1.39	1.35
68	S2	406	PSU	C6-C5	3.37	1.39	1.35
3	L5	1326	A2M	O5'-C5'	-3.37	1.34	1.44
68	S2	1004	PSU	C6-C5	3.37	1.39	1.35
3	L5	4523	A2M	O5'-C5'	-3.37	1.34	1.44
3	L5	2401	A2M	O5'-C5'	-3.36	1.34	1.44
3	L5	4220	6MZ	C5-N7	-3.35	1.33	1.39
68	S2	1056	PSU	C6-C5	3.35	1.39	1.35
3	L5	4552	PSU	C6-C5	3.33	1.39	1.35
68	S2	863	PSU	C6-C5	3.33	1.39	1.35
3	L5	1534	A2M	O5'-C5'	-3.33	1.34	1.44
3	L5	1744	PSU	C6-C5	3.32	1.39	1.35
68	S2	1046	PSU	C6-C5	3.31	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	O2-C2	-3.31	1.16	1.23
68	S2	1367	PSU	C6-C5	3.30	1.38	1.35
68	S2	1232	PSU	C6-C5	3.27	1.38	1.35
3	L5	1860	PSU	C6-C5	3.25	1.38	1.35
5	L8	55	PSU	C6-C5	3.22	1.38	1.35
3	L5	4296	PSU	C6-C5	3.21	1.38	1.35
3	L5	1782	PSU	C6-C5	3.21	1.38	1.35
3	L5	3851	PSU	C6-C5	3.21	1.38	1.35
5	L8	69	PSU	C6-C5	3.20	1.38	1.35
3	L5	5001	PSU	C6-C5	3.19	1.38	1.35
68	S2	109	PSU	C6-C5	3.19	1.38	1.35
68	S2	1832	6MZ	C5-N7	-3.16	1.33	1.39
68	S2	651	PSU	C6-C5	3.16	1.38	1.35
68	S2	1832	6MZ	C5-C4	-3.16	1.33	1.39
3	L5	3818	UY1	C1'-C5	3.16	1.57	1.50
3	L5	3844	PSU	C6-C5	3.15	1.38	1.35
3	L5	4220	6MZ	C8-N9	-3.15	1.32	1.37
68	S2	159	A2M	O5'-C5'	-3.15	1.35	1.44
68	S2	1851	MA6	C6-N6	3.14	1.45	1.36
68	S2	105	PSU	C6-C5	3.14	1.38	1.35
3	L5	4972	PSU	C6-C5	3.13	1.38	1.35
3	L5	4493	PSU	C6-C5	3.12	1.38	1.35
68	S2	1174	PSU	C6-C5	3.12	1.38	1.35
3	L5	3637	PSU	C6-C5	3.11	1.38	1.35
3	L5	1781	PSU	C6-C5	3.11	1.38	1.35
3	L5	1683	PSU	C6-C5	3.10	1.38	1.35
68	S2	93	PSU	C6-C5	3.09	1.38	1.35
68	S2	1832	6MZ	C8-N9	-3.09	1.32	1.37
3	L5	2632	PSU	C6-C5	3.08	1.38	1.35
3	L5	3639	PSU	C6-C5	3.08	1.38	1.35
3	L5	2839	PSU	C6-C5	3.07	1.38	1.35
3	L5	4471	PSU	C6-C5	3.06	1.38	1.35
3	L5	3822	PSU	C6-C5	3.06	1.38	1.35
68	S2	1081	PSU	C6-C5	3.06	1.38	1.35
3	L5	4532	PSU	C6-C5	3.06	1.38	1.35
3	L5	4361	PSU	C6-C5	3.05	1.38	1.35
68	S2	1850	MA6	C6-N6	3.05	1.45	1.36
3	L5	1536	PSU	C6-C5	3.03	1.38	1.35
3	L5	4442	PSU	C6-C5	3.02	1.38	1.35
3	L5	4403	PSU	C6-C5	3.01	1.38	1.35
3	L5	4431	PSU	C6-C5	3.01	1.38	1.35
3	L5	1582	PSU	C6-C5	3.01	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3695	PSU	C6-C5	3.00	1.38	1.35
3	L5	1524	A2M	O4'-C4'	-3.00	1.38	1.45
68	S2	668	A2M	O4'-C4'	-3.00	1.38	1.45
3	L5	4576	PSU	C6-C5	2.98	1.38	1.35
3	L5	4673	PSU	C6-C5	2.97	1.38	1.35
3	L5	3853	PSU	C6-C5	2.97	1.38	1.35
3	L5	4353	PSU	C6-C5	2.96	1.38	1.35
3	L5	1862	PSU	C6-C5	2.96	1.38	1.35
3	L5	3884	PSU	C6-C5	2.96	1.38	1.35
3	L5	4312	PSU	C6-C5	2.95	1.38	1.35
3	L5	1792	PSU	C6-C5	2.95	1.38	1.35
3	L5	4636	PSU	C6-C5	2.94	1.38	1.35
3	L5	4293	PSU	C6-C5	2.93	1.38	1.35
3	L5	4299	PSU	C6-C5	2.90	1.38	1.35
3	L5	4689	PSU	C6-C5	2.89	1.38	1.35
68	S2	1442	OMU	C5-C4	2.88	1.50	1.43
3	L5	4457	PSU	C6-C5	2.87	1.38	1.35
68	S2	1639	G7M	C2-N1	2.85	1.44	1.37
3	L5	4579	PSU	C6-C5	2.85	1.38	1.35
3	L5	4973	PSU	C6-C5	2.85	1.38	1.35
68	S2	428	OMU	C5-C4	2.82	1.49	1.43
3	L5	4521	PSU	C6-C5	2.79	1.38	1.35
3	L5	4500	PSU	C6-C5	2.79	1.38	1.35
3	L5	4628	PSU	C6-C5	2.79	1.38	1.35
68	S2	1288	OMU	C5-C4	2.79	1.49	1.43
68	S2	627	OMU	C5-C4	2.77	1.49	1.43
68	S2	121	OMU	C5-C4	2.75	1.49	1.43
68	S2	1326	OMU	C5-C4	2.75	1.49	1.43
68	S2	354	OMU	C5-C4	2.75	1.49	1.43
3	L5	3920	PSU	C6-C5	2.73	1.38	1.35
68	S2	172	OMU	C5-C4	2.73	1.49	1.43
68	S2	116	OMU	C5-C4	2.71	1.49	1.43
68	S2	799	OMU	C5-C4	2.71	1.49	1.43
68	S2	1288	OMU	C6-N1	2.71	1.44	1.38
3	L5	2837	OMU	C5-C4	2.69	1.49	1.43
68	S2	681	PSU	C6-C5	2.67	1.38	1.35
68	S2	799	OMU	C6-N1	2.65	1.44	1.38
3	L5	4523	A2M	O3'-C3'	-2.64	1.36	1.43
3	L5	1677	PSU	C6-C5	2.64	1.38	1.35
68	S2	1442	OMU	C6-N1	2.62	1.44	1.38
3	L5	4523	A2M	O4'-C4'	-2.62	1.39	1.45
3	L5	3867	A2M	O4'-C4'	-2.61	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	S2	121	OMU	C6-N1	2.61	1.44	1.38
3	L5	4227	OMU	C5-C4	2.61	1.49	1.43
68	S2	1850	MA6	C5-C4	-2.60	1.34	1.39
3	L5	4530	UR3	O2-C2	-2.59	1.17	1.22
3	L5	4571	A2M	O4'-C4'	-2.59	1.39	1.45
68	S2	1851	MA6	C5-C4	-2.58	1.34	1.39
3	L5	4306	OMU	C5-C4	2.57	1.49	1.43
68	S2	428	OMU	C6-N1	2.56	1.44	1.38
68	S2	116	OMU	C6-N1	2.56	1.44	1.38
68	S2	1639	G7M	O6-C6	-2.55	1.18	1.23
3	L5	1326	A2M	O4'-C4'	-2.54	1.39	1.45
3	L5	4498	OMU	C5-C4	2.53	1.49	1.43
3	L5	1323	A2M	O4'-C4'	-2.51	1.39	1.45
3	L5	3925	OMU	C5-C4	2.50	1.49	1.43
3	L5	2363	A2M	O4'-C4'	-2.50	1.39	1.45
3	L5	4220	6MZ	C6-N1	-2.49	1.31	1.35
68	S2	1326	OMU	C6-N1	2.48	1.44	1.38
68	S2	627	OMU	C6-N1	2.46	1.44	1.38
3	L5	4620	OMU	C5-C4	2.46	1.49	1.43
68	S2	354	OMU	C6-N1	2.45	1.43	1.38
68	S2	1639	G7M	C6-N1	2.43	1.43	1.38
3	L5	1534	A2M	O4'-C4'	-2.42	1.39	1.45
68	S2	172	OMU	C6-N1	2.42	1.43	1.38
3	L5	4530	UR3	C6-N1	2.40	1.43	1.38
3	L5	4306	OMU	C6-N1	2.39	1.43	1.38
3	L5	400	A2M	O4'-C4'	-2.39	1.39	1.45
3	L5	1677	PSU	O4'-C1'	-2.38	1.40	1.43
3	L5	4227	OMU	C6-N1	2.37	1.43	1.38
3	L5	4552	PSU	C4-C5	-2.35	1.37	1.44
3	L5	3884	PSU	C4-C5	-2.35	1.37	1.44
3	L5	2837	OMU	C6-N1	2.34	1.43	1.38
3	L5	2839	PSU	C4-C5	-2.34	1.37	1.44
3	L5	3925	OMU	C6-N1	2.33	1.43	1.38
68	S2	1832	6MZ	C6-N1	-2.31	1.31	1.35
3	L5	3639	PSU	C4-C5	-2.31	1.37	1.44
3	L5	4498	OMU	C6-N1	2.30	1.43	1.38
3	L5	4620	OMU	C6-N1	2.29	1.43	1.38
3	L5	1524	A2M	O3'-C3'	-2.27	1.37	1.43
3	L5	1323	A2M	O3'-C3'	-2.27	1.37	1.43
3	L5	4431	PSU	C4-C5	-2.26	1.38	1.44
3	L5	4471	PSU	C4-C5	-2.26	1.38	1.44
3	L5	3830	A2M	O4'-C4'	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4689	PSU	C4-C5	-2.26	1.38	1.44
3	L5	4293	PSU	C4-C5	-2.26	1.38	1.44
3	L5	1582	PSU	C4-C5	-2.24	1.38	1.44
3	L5	3920	PSU	C4-C5	-2.23	1.38	1.44
3	L5	1871	A2M	O4'-C4'	-2.23	1.40	1.45
3	L5	5001	PSU	C4-C5	-2.21	1.38	1.44
68	S2	649	PSU	C4-C5	-2.20	1.38	1.44
3	L5	1536	PSU	C4-C5	-2.20	1.38	1.44
3	L5	4636	PSU	C4-C5	-2.20	1.38	1.44
68	S2	1639	G7M	C4-N9	-2.20	1.32	1.38
3	L5	1677	PSU	C4-C5	-2.19	1.38	1.44
3	L5	4521	PSU	C4-C5	-2.19	1.38	1.44
3	L5	1534	A2M	O3'-C3'	-2.19	1.37	1.43
3	L5	3818	UY1	O4'-C1'	-2.18	1.40	1.43
3	L5	3825	A2M	O4'-C4'	-2.17	1.40	1.45
3	L5	2401	A2M	O4'-C4'	-2.17	1.40	1.45
3	L5	4493	PSU	C4-C5	-2.17	1.38	1.44
3	L5	4403	PSU	C4-C5	-2.16	1.38	1.44
3	L5	4403	PSU	O4'-C1'	-2.16	1.40	1.43
3	L5	3920	PSU	O4'-C1'	-2.15	1.40	1.43
3	L5	4973	PSU	C4-C5	-2.15	1.38	1.44
3	L5	4457	PSU	C4-C5	-2.15	1.38	1.44
3	L5	1683	PSU	C4-C5	-2.15	1.38	1.44
3	L5	4312	PSU	C4-C5	-2.15	1.38	1.44
3	L5	4532	PSU	C4-C5	-2.14	1.38	1.44
3	L5	4673	PSU	C4-C5	-2.13	1.38	1.44
3	L5	4590	A2M	O4'-C4'	-2.13	1.40	1.45
3	L5	4500	PSU	O4'-C1'	-2.12	1.40	1.43
3	L5	4530	UR3	C3U-N3	2.12	1.50	1.47
3	L5	5010	PSU	C4-C5	-2.11	1.38	1.44
3	L5	1744	PSU	C4-C5	-2.11	1.38	1.44
3	L5	4447	5MC	C4-N3	-2.11	1.30	1.34
3	L5	398	A2M	O3'-C3'	-2.11	1.37	1.43
3	L5	3830	A2M	O3'-C3'	-2.11	1.37	1.43
3	L5	3822	PSU	O4'-C1'	-2.10	1.40	1.43
3	L5	3695	PSU	C4-C5	-2.10	1.38	1.44
3	L5	4353	PSU	C4-C5	-2.10	1.38	1.44
68	S2	681	PSU	C4-C5	-2.10	1.38	1.44
68	S2	1081	PSU	C4-C5	-2.10	1.38	1.44
3	L5	3844	PSU	C4-C5	-2.09	1.38	1.44
68	S2	406	PSU	C4-C5	-2.09	1.38	1.44
68	S2	1174	PSU	C4-C5	-2.08	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4530	UR3	C5-C4	2.08	1.49	1.43
3	L5	2363	A2M	O3'-C3'	-2.07	1.37	1.43
3	L5	3718	A2M	O4'-C4'	-2.07	1.40	1.45
3	L5	1782	PSU	C4-C5	-2.07	1.38	1.44
3	L5	4299	PSU	C4-C5	-2.07	1.38	1.44
3	L5	4636	PSU	O4'-C1'	-2.06	1.41	1.43
3	L5	4457	PSU	O4'-C1'	-2.06	1.41	1.43
3	L5	4296	PSU	C4-C5	-2.05	1.38	1.44
68	S2	27	A2M	O4'-C4'	-2.05	1.40	1.45
3	L5	4442	PSU	C4-C5	-2.04	1.38	1.44
5	L8	55	PSU	C4-C5	-2.03	1.38	1.44
68	S2	109	PSU	C4-C5	-2.03	1.38	1.44
3	L5	1862	PSU	C4-C5	-2.03	1.38	1.44
3	L5	2632	PSU	C4-C5	-2.02	1.38	1.44
68	S2	686	PSU	C4-C5	-2.02	1.38	1.44
3	L5	1860	PSU	C4-C5	-2.02	1.38	1.44
68	S2	1850	MA6	C5-N7	-2.02	1.35	1.39
68	S2	1177	PSU	C4-C5	-2.01	1.38	1.44
5	L8	69	PSU	C4-C5	-2.01	1.38	1.44
3	L5	2787	A2M	O4'-C4'	-2.00	1.40	1.45
3	L5	4442	PSU	O4'-C1'	-2.00	1.41	1.43

All (703) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1850	MA6	N1-C6-N6	-11.85	102.42	116.86
68	S2	1851	MA6	N1-C6-N6	-11.74	102.55	116.86
68	S2	1851	MA6	C5-C6-N6	7.81	137.70	125.33
68	S2	1850	MA6	C5-C6-N6	7.79	137.66	125.33
68	S2	1639	G7M	C1'-N9-C8	-7.16	102.57	126.74
68	S2	1639	G7M	C1'-N9-C4	7.12	147.52	126.49
68	S2	627	OMU	C4-N3-C2	-5.99	119.17	126.61
3	L5	4498	OMU	C4-N3-C2	-5.96	119.22	126.61
3	L5	3925	OMU	C4-N3-C2	-5.95	119.23	126.61
3	L5	4227	OMU	C4-N3-C2	-5.87	119.33	126.61
3	L5	2837	OMU	C4-N3-C2	-5.82	119.38	126.61
68	S2	172	OMU	C4-N3-C2	-5.80	119.41	126.61
68	S2	428	OMU	C4-N3-C2	-5.80	119.42	126.61
68	S2	354	OMU	C4-N3-C2	-5.79	119.42	126.61
68	S2	1326	OMU	C4-N3-C2	-5.76	119.46	126.61
68	S2	1442	OMU	C4-N3-C2	-5.76	119.46	126.61
3	L5	4220	6MZ	N1-C2-N3	-5.72	119.92	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1832	6MZ	N1-C2-N3	-5.69	119.96	128.58
68	S2	1850	MA6	N1-C2-N3	-5.65	120.03	128.58
68	S2	1851	MA6	N1-C2-N3	-5.63	120.06	128.58
3	L5	4620	OMU	C4-N3-C2	-5.56	119.71	126.61
68	S2	799	OMU	C4-N3-C2	-5.50	119.79	126.61
3	L5	4306	OMU	C4-N3-C2	-5.48	119.81	126.61
68	S2	1851	MA6	N9-C8-N7	-5.39	106.30	113.94
68	S2	121	OMU	C4-N3-C2	-5.34	119.99	126.61
3	L5	4636	PSU	C4-N3-C2	-5.33	119.02	126.37
68	S2	1850	MA6	N9-C8-N7	-5.31	106.40	113.94
68	S2	116	OMU	C4-N3-C2	-5.29	120.05	126.61
68	S2	1248	B8N	C5-C4-N3	5.28	125.74	116.15
3	L5	3637	PSU	N1-C2-N3	5.26	120.72	115.17
3	L5	3920	PSU	C4-N3-C2	-5.24	119.15	126.37
3	L5	4636	PSU	N1-C2-N3	5.22	120.68	115.17
3	L5	1536	PSU	N1-C2-N3	5.20	120.66	115.17
3	L5	4530	UR3	C4-N3-C2	-5.20	120.39	124.58
3	L5	1582	PSU	C4-N3-C2	-5.20	119.22	126.37
3	L5	3920	PSU	N1-C2-N3	5.19	120.65	115.17
3	L5	4442	PSU	C4-N3-C2	-5.19	119.22	126.37
3	L5	2632	PSU	N1-C2-N3	5.18	120.63	115.17
3	L5	4973	PSU	C4-N3-C2	-5.17	119.25	126.37
3	L5	4353	PSU	C4-N3-C2	-5.17	119.25	126.37
3	L5	5001	PSU	C4-N3-C2	-5.17	119.25	126.37
3	L5	4471	PSU	C4-N3-C2	-5.15	119.27	126.37
3	L5	4403	PSU	N1-C2-N3	5.13	120.58	115.17
3	L5	4293	PSU	C4-N3-C2	-5.13	119.31	126.37
3	L5	4521	PSU	C4-N3-C2	-5.11	119.33	126.37
3	L5	4296	PSU	C4-N3-C2	-5.09	119.36	126.37
68	S2	1045	PSU	N1-C2-N3	5.09	120.54	115.17
3	L5	3822	PSU	N1-C2-N3	5.09	120.53	115.17
68	S2	1232	PSU	N1-C2-N3	5.09	120.53	115.17
3	L5	4296	PSU	N1-C2-N3	5.08	120.53	115.17
3	L5	5001	PSU	N1-C2-N3	5.08	120.52	115.17
68	S2	105	PSU	N1-C2-N3	5.07	120.52	115.17
3	L5	4220	6MZ	N9-C8-N7	-5.05	106.77	113.94
68	S2	1081	PSU	C4-N3-C2	-5.03	119.44	126.37
3	L5	4972	PSU	C4-N3-C2	-5.03	119.45	126.37
68	S2	1045	PSU	C4-N3-C2	-5.03	119.45	126.37
68	S2	651	PSU	C4-N3-C2	-5.00	119.48	126.37
68	S2	1177	PSU	C4-N3-C2	-5.00	119.48	126.37
3	L5	3695	PSU	C4-N3-C2	-4.99	119.49	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1288	OMU	C4-N3-C2	-4.99	120.41	126.61
3	L5	4500	PSU	C4-N3-C2	-4.99	119.50	126.37
3	L5	4442	PSU	N1-C2-N3	4.99	120.43	115.17
3	L5	1862	PSU	N1-C2-N3	4.99	120.43	115.17
3	L5	4431	PSU	C4-N3-C2	-4.99	119.50	126.37
68	S2	1232	PSU	C4-N3-C2	-4.98	119.51	126.37
3	L5	1862	PSU	C4-N3-C2	-4.97	119.52	126.37
3	L5	4457	PSU	C4-N3-C2	-4.96	119.53	126.37
3	L5	4972	PSU	N1-C2-N3	4.96	120.40	115.17
68	S2	1004	PSU	N1-C2-N3	4.96	120.40	115.17
68	S2	1081	PSU	N1-C2-N3	4.95	120.39	115.17
3	L5	2632	PSU	C4-N3-C2	-4.95	119.55	126.37
68	S2	966	PSU	N1-C2-N3	4.95	120.39	115.17
3	L5	1677	PSU	C4-N3-C2	-4.95	119.55	126.37
3	L5	4457	PSU	N1-C2-N3	4.95	120.39	115.17
3	L5	4493	PSU	N1-C2-N3	4.95	120.39	115.17
3	L5	4353	PSU	N1-C2-N3	4.94	120.38	115.17
3	L5	4431	PSU	N1-C2-N3	4.94	120.38	115.17
68	S2	651	PSU	N1-C2-N3	4.94	120.38	115.17
3	L5	3884	PSU	N1-C2-N3	4.93	120.37	115.17
3	L5	3822	PSU	C4-N3-C2	-4.93	119.58	126.37
3	L5	3818	UY1	C4-N3-C2	-4.93	119.58	126.37
68	S2	1832	6MZ	N9-C8-N7	-4.92	106.95	113.94
3	L5	4576	PSU	C4-N3-C2	-4.92	119.59	126.37
3	L5	4689	PSU	N1-C2-N3	4.92	120.35	115.17
3	L5	1683	PSU	C4-N3-C2	-4.91	119.61	126.37
68	S2	93	PSU	C4-N3-C2	-4.91	119.61	126.37
3	L5	4471	PSU	N1-C2-N3	4.90	120.34	115.17
3	L5	1781	PSU	N1-C2-N3	4.90	120.34	115.17
3	L5	4500	PSU	N1-C2-N3	4.90	120.34	115.17
3	L5	3637	PSU	C4-N3-C2	-4.89	119.63	126.37
3	L5	4403	PSU	C4-N3-C2	-4.89	119.63	126.37
3	L5	1781	PSU	C4-N3-C2	-4.89	119.63	126.37
3	L5	1792	PSU	N1-C2-N3	4.89	120.33	115.17
3	L5	5010	PSU	C4-N3-C2	-4.89	119.64	126.37
68	S2	863	PSU	C4-N3-C2	-4.88	119.64	126.37
68	S2	105	PSU	C4-N3-C2	-4.88	119.64	126.37
3	L5	4521	PSU	N1-C2-N3	4.88	120.32	115.17
3	L5	4973	PSU	N1-C2-N3	4.88	120.31	115.17
68	S2	681	PSU	C4-N3-C2	-4.87	119.66	126.37
68	S2	1004	PSU	C4-N3-C2	-4.87	119.66	126.37
3	L5	1582	PSU	N1-C2-N3	4.87	120.31	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4576	PSU	N1-C2-N3	4.87	120.31	115.17
3	L5	4293	PSU	N1-C2-N3	4.87	120.30	115.17
68	S2	1056	PSU	N1-C2-N3	4.87	120.30	115.17
68	S2	1177	PSU	N1-C2-N3	4.87	120.30	115.17
68	S2	863	PSU	N1-C2-N3	4.86	120.29	115.17
3	L5	1536	PSU	C4-N3-C2	-4.86	119.68	126.37
3	L5	4493	PSU	C4-N3-C2	-4.86	119.68	126.37
3	L5	4579	PSU	C4-N3-C2	-4.85	119.69	126.37
3	L5	1792	PSU	C4-N3-C2	-4.84	119.70	126.37
3	L5	3851	PSU	N1-C2-N3	4.84	120.27	115.17
3	L5	4532	PSU	N1-C2-N3	4.83	120.27	115.17
68	S2	93	PSU	N1-C2-N3	4.83	120.27	115.17
3	L5	1683	PSU	N1-C2-N3	4.83	120.26	115.17
3	L5	4299	PSU	C4-N3-C2	-4.83	119.72	126.37
3	L5	4579	PSU	N1-C2-N3	4.82	120.26	115.17
68	S2	966	PSU	C4-N3-C2	-4.82	119.73	126.37
3	L5	4312	PSU	N1-C2-N3	4.82	120.25	115.17
3	L5	1782	PSU	C4-N3-C2	-4.82	119.74	126.37
3	L5	3884	PSU	C4-N3-C2	-4.81	119.74	126.37
3	L5	3844	PSU	N1-C2-N3	4.81	120.25	115.17
3	L5	2839	PSU	N1-C2-N3	4.81	120.24	115.17
3	L5	4552	PSU	N1-C2-N3	4.81	120.24	115.17
68	S2	814	PSU	C4-N3-C2	-4.81	119.75	126.37
68	S2	686	PSU	C4-N3-C2	-4.80	119.76	126.37
3	L5	3695	PSU	N1-C2-N3	4.80	120.23	115.17
68	S2	866	PSU	N1-C2-N3	4.79	120.22	115.17
3	L5	1744	PSU	C4-N3-C2	-4.79	119.77	126.37
3	L5	4220	6MZ	C9-N6-C6	-4.79	118.41	122.85
68	S2	1367	PSU	C4-N3-C2	-4.79	119.78	126.37
3	L5	3853	PSU	N1-C2-N3	4.79	120.22	115.17
68	S2	1367	PSU	N1-C2-N3	4.78	120.21	115.17
3	L5	4552	PSU	C4-N3-C2	-4.78	119.79	126.37
3	L5	1782	PSU	N1-C2-N3	4.78	120.20	115.17
3	L5	1860	PSU	C4-N3-C2	-4.78	119.79	126.37
3	L5	3851	PSU	C4-N3-C2	-4.77	119.80	126.37
68	S2	681	PSU	N1-C2-N3	4.77	120.20	115.17
3	L5	4532	PSU	C4-N3-C2	-4.77	119.80	126.37
3	L5	4673	PSU	C4-N3-C2	-4.77	119.80	126.37
3	L5	4312	PSU	C4-N3-C2	-4.76	119.81	126.37
68	S2	109	PSU	C4-N3-C2	-4.76	119.81	126.37
68	S2	1244	PSU	N1-C2-N3	4.75	120.18	115.17
5	L8	69	PSU	C4-N3-C2	-4.75	119.83	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L8	69	PSU	N1-C2-N3	4.74	120.17	115.17
68	S2	1244	PSU	C4-N3-C2	-4.74	119.84	126.37
3	L5	4673	PSU	N1-C2-N3	4.74	120.17	115.17
3	L5	4299	PSU	N1-C2-N3	4.74	120.17	115.17
68	S2	686	PSU	N1-C2-N3	4.73	120.16	115.17
68	S2	1046	PSU	N1-C2-N3	4.73	120.16	115.17
68	S2	1056	PSU	C4-N3-C2	-4.73	119.86	126.37
3	L5	4361	PSU	C4-N3-C2	-4.73	119.86	126.37
3	L5	3853	PSU	C4-N3-C2	-4.72	119.86	126.37
3	L5	5010	PSU	N1-C2-N3	4.72	120.15	115.17
68	S2	1046	PSU	C4-N3-C2	-4.72	119.87	126.37
3	L5	1744	PSU	N1-C2-N3	4.70	120.12	115.17
3	L5	3639	PSU	N1-C2-N3	4.70	120.12	115.17
68	S2	406	PSU	C4-N3-C2	-4.69	119.91	126.37
3	L5	4361	PSU	N1-C2-N3	4.69	120.12	115.17
68	S2	1174	PSU	C4-N3-C2	-4.69	119.91	126.37
68	S2	1174	PSU	N1-C2-N3	4.69	120.12	115.17
68	S2	866	PSU	C4-N3-C2	-4.68	119.92	126.37
68	S2	1851	MA6	C5-C4-N3	-4.68	120.27	126.72
68	S2	649	PSU	N1-C2-N3	4.68	120.11	115.17
3	L5	2839	PSU	C4-N3-C2	-4.67	119.93	126.37
5	L8	55	PSU	N1-C2-N3	4.67	120.10	115.17
68	S2	1832	6MZ	C5-C4-N3	-4.67	120.29	126.72
3	L5	1677	PSU	N1-C2-N3	4.66	120.08	115.17
68	S2	814	PSU	N1-C2-N3	4.66	120.08	115.17
3	L5	4628	PSU	N1-C2-N3	4.65	120.07	115.17
68	S2	801	PSU	N1-C2-N3	4.65	120.07	115.17
3	L5	1860	PSU	N1-C2-N3	4.64	120.06	115.17
3	L5	3639	PSU	C4-N3-C2	-4.64	119.98	126.37
68	S2	406	PSU	N1-C2-N3	4.63	120.05	115.17
68	S2	109	PSU	N1-C2-N3	4.60	120.02	115.17
3	L5	4220	6MZ	C5-C4-N3	-4.58	120.41	126.72
68	S2	649	PSU	C4-N3-C2	-4.56	120.09	126.37
5	L8	55	PSU	C4-N3-C2	-4.55	120.10	126.37
3	L5	4628	PSU	C4-N3-C2	-4.55	120.10	126.37
68	S2	1248	B8N	C4-N3-C2	-4.54	120.03	125.62
3	L5	3844	PSU	C4-N3-C2	-4.54	120.12	126.37
3	L5	2837	OMU	N3-C2-N1	4.52	120.77	114.89
68	S2	1850	MA6	C5-C4-N3	-4.44	120.60	126.72
3	L5	4689	PSU	C4-N3-C2	-4.27	120.48	126.37
68	S2	1639	G7M	C2-N3-C4	4.27	119.65	112.30
68	S2	1851	MA6	C4-N9-C8	4.25	110.20	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3925	OMU	N3-C2-N1	4.24	120.42	114.89
68	S2	801	PSU	C4-N3-C2	-4.24	120.53	126.37
3	L5	4498	OMU	N3-C2-N1	4.23	120.40	114.89
3	L5	4227	OMU	N3-C2-N1	4.20	120.36	114.89
3	L5	3818	UY1	N1-C2-N3	4.19	119.58	115.17
68	S2	1850	MA6	C4-N9-C8	4.06	110.00	105.74
3	L5	398	A2M	C3'-C2'-C1'	-4.02	95.10	102.81
68	S2	172	OMU	N3-C2-N1	4.02	120.13	114.89
3	L5	4306	OMU	N3-C2-N1	3.99	120.08	114.89
68	S2	354	OMU	N3-C2-N1	3.95	120.04	114.89
68	S2	1383	A2M	C3'-C2'-C1'	-3.92	95.31	102.81
68	S2	627	OMU	C5-C4-N3	3.91	120.28	114.80
3	L5	4620	OMU	N3-C2-N1	3.90	119.97	114.89
68	S2	1442	OMU	C5-C4-N3	3.87	120.23	114.80
68	S2	1639	G7M	C5-C6-N1	3.86	119.82	111.84
68	S2	428	OMU	N3-C2-N1	3.83	119.88	114.89
68	S2	1851	MA6	C4-C5-C6	3.82	119.86	115.91
3	L5	1871	A2M	C3'-C2'-C1'	-3.81	95.52	102.81
68	S2	799	OMU	C5-C4-N3	3.79	120.11	114.80
3	L5	3701	OMC	C1'-N1-C2	3.79	126.80	118.44
3	L5	3925	OMU	C5-C4-N3	3.78	120.09	114.80
68	S2	1639	G7M	C5-C4-N3	-3.77	121.03	128.15
68	S2	116	OMU	N3-C2-N1	3.76	119.79	114.89
68	S2	1442	OMU	N3-C2-N1	3.76	119.78	114.89
68	S2	354	OMU	C5-C4-N3	3.75	120.06	114.80
68	S2	1326	OMU	N3-C2-N1	3.75	119.78	114.89
68	S2	1326	OMU	C5-C4-N3	3.74	120.03	114.80
68	S2	1383	A2M	O3'-C3'-C2'	3.67	121.47	111.19
3	L5	4498	OMU	C5-C4-N3	3.67	119.94	114.80
3	L5	4220	6MZ	C4-N9-C8	3.67	109.59	105.74
3	L5	4571	A2M	O3'-C3'-C2'	3.67	121.45	111.19
68	S2	428	OMU	C5-C4-N3	3.66	119.93	114.80
68	S2	627	OMU	N3-C2-N1	3.65	119.64	114.89
3	L5	4530	UR3	C5-C4-N3	3.65	119.84	115.04
3	L5	4620	OMU	C5-C4-N3	3.64	119.91	114.80
68	S2	121	OMU	N3-C2-N1	3.64	119.63	114.89
3	L5	4689	PSU	C6-N1-C2	-3.61	119.34	122.69
68	S2	799	OMU	N3-C2-N1	3.60	119.58	114.89
3	L5	1536	PSU	O2-C2-N1	-3.59	119.09	122.79
68	S2	121	OMU	C5-C4-N3	3.59	119.82	114.80
3	L5	4523	A2M	C3'-C2'-C1'	-3.57	95.98	102.81
3	L5	4227	OMU	C5-C4-N3	3.55	119.78	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	172	OMU	C5-C4-N3	3.54	119.76	114.80
68	S2	1850	MA6	C4-C5-C6	3.53	119.56	115.91
3	L5	4636	PSU	C6-C5-C4	3.53	120.55	118.17
68	S2	1851	MA6	N3-C4-N9	3.52	133.16	127.17
68	S2	1288	OMU	C5-C4-N3	3.52	119.73	114.80
3	L5	4306	OMU	C5-C4-N3	3.51	119.71	114.80
68	S2	468	A2M	C3'-C2'-C1'	-3.49	96.13	102.81
68	S2	1850	MA6	C2-N1-C6	3.48	120.34	111.83
68	S2	99	A2M	C3'-C2'-C1'	-3.45	96.20	102.81
68	S2	1851	MA6	C2-N1-C6	3.45	120.26	111.83
68	S2	166	A2M	O3'-C3'-C2'	3.44	120.81	111.19
68	S2	1832	6MZ	C2-N3-C4	3.43	120.22	111.83
68	S2	1832	6MZ	C5-N7-C8	3.40	108.79	103.45
3	L5	3830	A2M	C3'-C2'-C1'	-3.39	96.32	102.81
68	S2	576	A2M	O3'-C3'-C2'	3.38	120.66	111.19
3	L5	4571	A2M	C3'-C2'-C1'	-3.37	96.35	102.81
3	L5	2837	OMU	C5-C4-N3	3.37	119.52	114.80
3	L5	4220	6MZ	C2-N3-C4	3.36	120.03	111.83
68	S2	116	OMU	C5-C4-N3	3.36	119.50	114.80
3	L5	1534	A2M	C3'-C2'-C1'	-3.36	96.38	102.81
3	L5	3785	A2M	C4'-O4'-C1'	-3.35	102.06	109.47
68	S2	1639	G7M	O6-C6-C5	-3.33	120.57	128.01
68	S2	1288	OMU	N3-C2-N1	3.32	119.21	114.89
3	L5	5001	PSU	O2-C2-N1	-3.27	119.41	122.79
3	L5	3867	A2M	C2'-C1'-N9	3.27	119.14	113.75
3	L5	4220	6MZ	N3-C4-N9	3.27	132.72	127.17
68	S2	1851	MA6	C2-N3-C4	3.26	119.80	111.83
68	S2	1248	B8N	C1'-C5-C4	3.26	122.55	117.61
68	S2	1383	A2M	C4-N9-C1'	-3.26	119.02	126.63
3	L5	4296	PSU	O2-C2-N1	-3.24	119.44	122.79
68	S2	1248	B8N	N3-C2-N1	3.24	120.68	116.72
3	L5	3718	A2M	C3'-C2'-C1'	-3.22	96.63	102.81
68	S2	1850	MA6	N3-C4-N9	3.21	132.62	127.17
68	S2	468	A2M	C4-N9-C1'	-3.19	119.16	126.63
3	L5	4500	PSU	O2-C2-N1	-3.18	119.51	122.79
3	L5	2632	PSU	O2-C2-N1	-3.17	119.52	122.79
68	S2	1850	MA6	C2-N3-C4	3.16	119.55	111.83
68	S2	1851	MA6	C5-N7-C8	3.16	108.41	103.45
68	S2	1832	6MZ	C4-N9-C8	3.15	109.05	105.74
3	L5	4590	A2M	C3'-C2'-C1'	-3.14	96.80	102.81
3	L5	3718	A2M	O3'-C3'-C2'	3.12	119.93	111.19
3	L5	1536	PSU	C6-N1-C2	-3.12	119.80	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	166	A2M	C3'-C2'-C1'	-3.12	96.84	102.81
68	S2	668	A2M	C4-N9-C1'	-3.11	119.36	126.63
68	S2	468	A2M	O3'-C3'-C2'	3.10	119.88	111.19
68	S2	27	A2M	C3'-C2'-C1'	-3.10	96.87	102.81
3	L5	2401	A2M	O3'-C3'-C2'	3.10	119.86	111.19
3	L5	4532	PSU	O2-C2-N1	-3.08	119.61	122.79
68	S2	1850	MA6	C5-N7-C8	3.08	108.29	103.45
68	S2	799	OMU	O4-C4-C5	-3.08	119.86	125.16
68	S2	627	OMU	O4-C4-C5	-3.07	119.86	125.16
3	L5	4590	A2M	C4-N9-C1'	-3.07	119.45	126.63
68	S2	576	A2M	C3'-C2'-C1'	-3.07	96.93	102.81
68	S2	1367	PSU	O2-C2-N1	-3.07	119.62	122.79
3	L5	3920	PSU	O2-C2-N1	-3.07	119.62	122.79
3	L5	3785	A2M	C4-N9-C1'	-3.06	119.47	126.63
68	S2	801	PSU	C6-N1-C2	-3.06	119.85	122.69
3	L5	3701	OMC	C1'-N1-C6	-3.06	114.24	120.78
3	L5	398	A2M	O3'-C3'-C2'	3.06	119.74	111.19
5	L8	69	PSU	O2-C2-N1	-3.05	119.64	122.79
3	L5	3818	UY1	C6-C5-C4	3.05	120.23	118.17
3	L5	3822	PSU	O2-C2-N1	-3.05	119.64	122.79
3	L5	3853	PSU	O2-C2-N1	-3.05	119.64	122.79
3	L5	4498	OMU	O4-C4-C5	-3.04	119.91	125.16
3	L5	3844	PSU	O2-C2-N1	-3.04	119.65	122.79
3	L5	3867	A2M	C4-N9-C1'	-3.04	119.52	126.63
3	L5	4220	6MZ	C5-N7-C8	3.02	108.19	103.45
3	L5	4628	PSU	O2-C2-N1	-3.02	119.68	122.79
3	L5	4299	PSU	O2-C2-N1	-3.01	119.68	122.79
68	S2	1046	PSU	O2-C2-N1	-3.01	119.68	122.79
3	L5	400	A2M	O3'-C3'-C2'	3.00	119.58	111.19
3	L5	2401	A2M	C3'-C2'-C1'	-2.99	97.07	102.81
68	S2	1326	OMU	O4-C4-C5	-2.99	120.00	125.16
68	S2	1639	G7M	CN7-N7-C5	2.98	130.51	126.80
68	S2	99	A2M	O3'-C3'-C2'	2.97	119.50	111.19
68	S2	1244	PSU	O2-C2-N1	-2.97	119.72	122.79
3	L5	1860	PSU	O2-C2-N1	-2.97	119.73	122.79
3	L5	4620	OMU	O4-C4-C5	-2.97	120.05	125.16
68	S2	1639	G7M	N9-C4-N3	2.97	131.88	125.95
68	S2	166	A2M	C4-N9-C1'	-2.97	119.69	126.63
68	S2	1031	A2M	C3'-C2'-C1'	-2.96	97.14	102.81
68	S2	863	PSU	O2-C2-N1	-2.96	119.74	122.79
68	S2	428	OMU	O4-C4-C5	-2.96	120.06	125.16
3	L5	3844	PSU	C6-N1-C2	-2.95	119.95	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4673	PSU	O2-C2-N1	-2.95	119.74	122.79
3	L5	1862	PSU	O2-C2-N1	-2.95	119.75	122.79
3	L5	3884	PSU	C6-N1-C2	-2.95	119.96	122.69
3	L5	4431	PSU	O2-C2-N1	-2.95	119.75	122.79
3	L5	4457	PSU	O2-C2-N1	-2.94	119.75	122.79
3	L5	1871	A2M	O3'-C3'-C2'	2.94	119.42	111.19
68	S2	116	OMU	O4-C4-C5	-2.94	120.09	125.16
3	L5	4523	A2M	C4-N9-C1'	-2.93	119.78	126.63
68	S2	966	PSU	O2-C2-N1	-2.93	119.77	122.79
3	L5	400	A2M	C3'-C2'-C1'	-2.93	97.20	102.81
3	L5	1871	A2M	C4-N9-C1'	-2.93	119.78	126.63
3	L5	3925	OMU	O4-C4-C5	-2.92	120.12	125.16
3	L5	4689	PSU	O2-C2-N1	-2.92	119.77	122.79
3	L5	3825	A2M	O3'-C3'-C2'	2.92	119.37	111.19
3	L5	3830	A2M	C4-N9-C1'	-2.92	119.80	126.63
3	L5	3808	OMC	C1'-N1-C2	2.92	124.88	118.44
68	S2	1031	A2M	C4-N9-C1'	-2.91	119.83	126.63
3	L5	4973	PSU	O2-C2-N1	-2.91	119.79	122.79
3	L5	4227	OMU	O4-C4-C5	-2.91	120.15	125.16
3	L5	3884	PSU	O2-C2-N1	-2.91	119.79	122.79
68	S2	105	PSU	O2-C2-N1	-2.90	119.80	122.79
68	S2	27	A2M	O3'-C3'-C2'	2.90	119.30	111.19
3	L5	2787	A2M	O3'-C3'-C2'	2.89	119.28	111.19
68	S2	686	PSU	O2-C2-N1	-2.89	119.81	122.79
3	L5	4312	PSU	O2-C2-N1	-2.88	119.82	122.79
3	L5	4493	PSU	O2-C2-N1	-2.87	119.82	122.79
68	S2	1288	OMU	O4-C4-C5	-2.87	120.21	125.16
68	S2	1031	A2M	O3'-C3'-C2'	2.87	119.22	111.19
68	S2	172	OMU	O4-C4-C5	-2.87	120.21	125.16
3	L5	4361	PSU	O2-C2-N1	-2.87	119.83	122.79
68	S2	1832	6MZ	N3-C4-N9	2.87	132.04	127.17
68	S2	468	A2M	C1'-N9-C8	2.87	133.46	127.09
3	L5	3830	A2M	O3'-C3'-C2'	2.86	119.20	111.19
3	L5	4521	PSU	O2-C2-N1	-2.86	119.84	122.79
3	L5	4403	PSU	C6-N1-C2	-2.86	120.03	122.69
3	L5	398	A2M	C4-N9-C1'	-2.86	119.94	126.63
68	S2	1056	PSU	O2-C2-N1	-2.86	119.84	122.79
68	S2	1639	G7M	C2-N1-C6	-2.86	119.93	125.11
3	L5	2839	PSU	O2-C2-N1	-2.85	119.85	122.79
3	L5	3695	PSU	O2-C2-N1	-2.85	119.85	122.79
68	S2	1832	6MZ	C4-C5-C6	2.85	119.14	116.78
68	S2	1383	A2M	C1'-N9-C8	2.84	133.41	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3785	A2M	O3'-C3'-C2'	2.84	119.14	111.19
68	S2	1248	B8N	O4-C4-N3	-2.84	115.38	119.99
68	S2	668	A2M	C1'-N9-C8	2.84	133.40	127.09
68	S2	484	A2M	O3'-C3'-C2'	2.83	119.12	111.19
68	S2	109	PSU	O2-C2-N1	-2.83	119.87	122.79
68	S2	651	PSU	O2-C2-N1	-2.83	119.87	122.79
3	L5	3785	A2M	C3'-C2'-C1'	-2.83	97.39	102.81
68	S2	1442	OMU	O4-C4-C5	-2.83	120.29	125.16
3	L5	4471	PSU	O2-C2-N1	-2.82	119.88	122.79
68	S2	1045	PSU	O2-C2-N1	-2.82	119.88	122.79
68	S2	354	OMU	O4-C4-C5	-2.81	120.31	125.16
3	L5	2815	A2M	O3'-C3'-C2'	2.81	119.06	111.19
5	L8	55	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L5	4403	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L5	5010	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L5	4576	PSU	O2-C2-N1	-2.81	119.89	122.79
68	S2	1004	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L5	3637	PSU	C6-N1-C2	-2.81	120.09	122.69
3	L5	2839	PSU	C6-N1-C2	-2.80	120.09	122.69
3	L5	4293	PSU	O2-C2-N1	-2.80	119.90	122.79
68	S2	27	A2M	C4-N9-C1'	-2.80	120.09	126.63
3	L5	1524	A2M	O3'-C3'-C2'	2.79	119.00	111.19
3	L5	4442	PSU	O2-C2-N1	-2.79	119.91	122.79
3	L5	4628	PSU	C6-N1-C2	-2.79	120.10	122.69
3	L5	4220	6MZ	C4-C5-C6	2.79	119.10	116.78
68	S2	1174	PSU	O2-C2-N1	-2.79	119.91	122.79
3	L5	4636	PSU	O2-C2-N1	-2.78	119.92	122.79
68	S2	1081	PSU	O2-C2-N1	-2.78	119.92	122.79
3	L5	4590	A2M	C1'-N9-C8	2.78	133.26	127.09
3	L5	3825	A2M	C4-N9-C1'	-2.77	120.14	126.63
68	S2	1174	PSU	C6-N1-C2	-2.77	120.12	122.69
3	L5	2632	PSU	C6-N1-C2	-2.77	120.12	122.69
68	S2	159	A2M	O3'-C3'-C2'	2.77	118.93	111.19
68	S2	121	OMU	O4-C4-C5	-2.77	120.39	125.16
68	S2	681	PSU	O2-C2-N1	-2.77	119.94	122.79
3	L5	4312	PSU	C6-N1-C2	-2.76	120.13	122.69
3	L5	3825	A2M	C3'-C2'-C1'	-2.76	97.53	102.81
3	L5	3867	A2M	C1'-N9-C8	2.75	133.20	127.09
68	S2	105	PSU	C6-N1-C2	-2.75	120.14	122.69
3	L5	1871	A2M	C1'-N9-C8	2.74	133.19	127.09
3	L5	1792	PSU	O2-C2-N1	-2.74	119.96	122.79
68	S2	866	PSU	O2-C2-N1	-2.74	119.96	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	398	A2M	C1'-N9-C8	2.74	133.17	127.09
68	S2	1031	A2M	C1'-N9-C8	2.74	133.17	127.09
3	L5	1534	A2M	O3'-C3'-C4'	-2.74	103.22	111.08
3	L5	1323	A2M	C4-N9-C1'	-2.74	120.23	126.63
68	S2	406	PSU	O2-C2-N1	-2.74	119.97	122.79
68	S2	966	PSU	C6-N1-C2	-2.73	120.16	122.69
68	S2	484	A2M	C4-N9-C1'	-2.73	120.24	126.63
3	L5	3639	PSU	O2-C2-N1	-2.73	119.98	122.79
3	L5	1781	PSU	O2-C2-N1	-2.72	119.98	122.79
3	L5	1323	A2M	C2'-C1'-N9	2.72	118.23	113.75
3	L5	4532	PSU	C6-N1-C2	-2.72	120.17	122.69
3	L5	1326	A2M	O3'-C3'-C2'	2.72	118.80	111.19
3	L5	1582	PSU	O2-C2-N1	-2.72	119.98	122.79
3	L5	3639	PSU	C6-N1-C2	-2.72	120.17	122.69
68	S2	166	A2M	C1'-N9-C8	2.72	133.12	127.09
3	L5	3785	A2M	C1'-N9-C8	2.72	133.12	127.09
68	S2	93	PSU	O2-C2-N1	-2.72	119.99	122.79
68	S2	1177	PSU	O2-C2-N1	-2.71	119.99	122.79
68	S2	668	A2M	O3'-C3'-C2'	2.71	118.76	111.19
3	L5	2401	A2M	C4-N9-C1'	-2.70	120.31	126.63
3	L5	4431	PSU	C6-N1-C2	-2.70	120.18	122.69
3	L5	4972	PSU	O2-C2-N1	-2.70	120.00	122.79
3	L5	4590	A2M	O3'-C3'-C2'	2.70	118.75	111.19
68	S2	799	OMU	C1'-N1-C2	2.70	122.45	117.59
3	L5	4220	6MZ	C5-C6-N1	2.70	121.05	118.15
68	S2	649	PSU	C6-N1-C2	-2.70	120.19	122.69
3	L5	4579	PSU	O2-C2-N1	-2.70	120.00	122.79
3	L5	4552	PSU	C6-N1-C2	-2.70	120.19	122.69
3	L5	3920	PSU	C6-C5-C4	2.69	119.99	118.17
68	S2	681	PSU	C6-N1-C2	-2.69	120.19	122.69
68	S2	866	PSU	C6-N1-C2	-2.69	120.19	122.69
68	S2	668	A2M	O4'-C1'-C2'	2.68	111.21	106.59
3	L5	4571	A2M	C4-N9-C1'	-2.68	120.36	126.63
3	L5	3851	PSU	O2-C2-N1	-2.68	120.03	122.79
68	S2	814	PSU	O2-C2-N1	-2.68	120.03	122.79
68	S2	99	A2M	C4-N9-C1'	-2.68	120.37	126.63
3	L5	4403	PSU	C6-C5-C4	2.68	119.98	118.17
68	S2	1851	MA6	C1'-N9-C8	-2.67	121.17	127.09
5	L8	55	PSU	C6-N1-C2	-2.67	120.21	122.69
3	L5	1683	PSU	O2-C2-N1	-2.66	120.04	122.79
68	S2	27	A2M	C1'-N9-C8	2.66	133.01	127.09
3	L5	3925	OMU	O2-C2-N1	-2.66	119.33	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1744	PSU	O2-C2-N1	-2.66	120.05	122.79
3	L5	4306	OMU	O4-C4-C5	-2.66	120.58	125.16
68	S2	159	A2M	C2'-C1'-N9	2.65	118.12	113.75
68	S2	1832	6MZ	C4-C5-N7	-2.65	107.55	110.58
3	L5	400	A2M	C4-N9-C1'	-2.65	120.43	126.63
3	L5	3830	A2M	C1'-N9-C8	2.65	132.98	127.09
3	L5	3818	UY1	C6-N1-C2	-2.65	120.23	122.69
5	L8	69	PSU	C6-N1-C2	-2.65	120.24	122.69
3	L5	1323	A2M	C1'-N9-C8	2.64	132.96	127.09
3	L5	4353	PSU	O2-C2-N1	-2.64	120.06	122.79
3	L5	4498	OMU	O2-C2-N1	-2.64	119.36	122.80
3	L5	1792	PSU	C6-N1-C2	-2.63	120.25	122.69
3	L5	1677	PSU	O2-C2-N1	-2.62	120.08	122.79
3	L5	4523	A2M	C1'-N9-C8	2.62	132.92	127.09
3	L5	1782	PSU	O2-C2-N1	-2.62	120.08	122.79
3	L5	2363	A2M	C2'-C1'-N9	2.62	118.07	113.75
68	S2	1232	PSU	C6-C5-C4	2.62	119.94	118.17
3	L5	1524	A2M	O4'-C1'-C2'	2.62	111.09	106.59
3	L5	2837	OMU	O4-C4-C5	-2.62	120.65	125.16
68	S2	1244	PSU	C6-N1-C2	-2.62	120.26	122.69
3	L5	2787	A2M	C4-N9-C1'	-2.61	120.53	126.63
68	S2	484	A2M	C1'-N9-C8	2.61	132.88	127.09
3	L5	3825	A2M	C1'-N9-C8	2.61	132.88	127.09
68	S2	1004	PSU	C6-N1-C2	-2.60	120.27	122.69
3	L5	1683	PSU	C6-N1-C2	-2.59	120.28	122.69
3	L5	3853	PSU	C6-N1-C2	-2.59	120.29	122.69
3	L5	3822	PSU	C6-N1-C2	-2.59	120.29	122.69
68	S2	1639	G7M	CN7-N7-C8	-2.59	120.88	124.79
68	S2	801	PSU	O2-C2-N1	-2.59	120.12	122.79
3	L5	4493	PSU	C6-N1-C2	-2.59	120.29	122.69
3	L5	2815	A2M	C2'-C1'-N9	2.58	117.99	113.75
3	L5	1524	A2M	C4'-O4'-C1'	-2.57	103.78	109.47
68	S2	99	A2M	C1'-N9-C8	2.57	132.80	127.09
68	S2	1232	PSU	O2-C2-N1	-2.57	120.14	122.79
3	L5	4457	PSU	C6-N1-C2	-2.57	120.31	122.69
3	L5	4227	OMU	O2-C2-N1	-2.56	119.47	122.80
3	L5	4552	PSU	O2-C2-N1	-2.55	120.15	122.79
68	S2	1056	PSU	C6-N1-C2	-2.55	120.32	122.69
3	L5	3718	A2M	C1'-N9-C8	2.55	132.76	127.09
3	L5	4493	PSU	C6-C5-C4	2.55	119.89	118.17
68	S2	668	A2M	C2'-C1'-N9	2.54	117.94	113.75
3	L5	2401	A2M	C1'-N9-C8	2.54	132.73	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	1046	PSU	C6-N1-C2	-2.54	120.33	122.69
3	L5	4500	PSU	C6-N1-C2	-2.54	120.34	122.69
3	L5	3851	PSU	C6-N1-C2	-2.53	120.34	122.69
3	L5	4530	UR3	C6-N1-C2	-2.53	119.73	121.80
3	L5	1862	PSU	C6-N1-C2	-2.53	120.34	122.69
3	L5	400	A2M	C1'-N9-C8	2.53	132.71	127.09
3	L5	4296	PSU	C6-N1-C2	-2.53	120.34	122.69
3	L5	4299	PSU	C6-N1-C2	-2.53	120.35	122.69
68	S2	406	PSU	C6-N1-C2	-2.53	120.35	122.69
3	L5	2351	OMC	C1'-N1-C2	2.52	124.01	118.44
3	L5	3818	UY1	O2-C2-N1	-2.52	120.19	122.79
68	S2	484	A2M	O4'-C1'-C2'	2.52	110.93	106.59
3	L5	4579	PSU	C6-N1-C2	-2.52	120.36	122.69
3	L5	2787	A2M	O4'-C1'-C2'	2.51	110.92	106.59
68	S2	159	A2M	C4-N9-C1'	-2.51	120.77	126.63
3	L5	3920	PSU	C6-N1-C2	-2.50	120.37	122.69
3	L5	4361	PSU	C6-N1-C2	-2.50	120.37	122.69
68	S2	686	PSU	C6-N1-C2	-2.50	120.37	122.69
3	L5	4673	PSU	C6-N1-C2	-2.49	120.38	122.69
3	L5	5001	PSU	C6-N1-C2	-2.49	120.38	122.69
68	S2	159	A2M	C1'-N9-C8	2.49	132.62	127.09
68	S2	1367	PSU	C6-N1-C2	-2.49	120.39	122.69
3	L5	4576	PSU	C6-N1-C2	-2.48	120.39	122.69
68	S2	1232	PSU	C6-N1-C2	-2.48	120.39	122.69
3	L5	1744	PSU	C6-N1-C2	-2.48	120.39	122.69
3	L5	4571	A2M	C1'-N9-C8	2.48	132.59	127.09
68	S2	863	PSU	C6-N1-C2	-2.46	120.40	122.69
68	S2	651	PSU	C6-N1-C2	-2.46	120.41	122.69
68	S2	576	A2M	C4-N9-C1'	-2.46	120.88	126.63
3	L5	2363	A2M	O4'-C1'-C2'	2.45	110.81	106.59
68	S2	1639	G7M	N9-C8-N7	-2.45	106.53	112.48
68	S2	93	PSU	C6-N1-C2	-2.45	120.42	122.69
3	L5	5010	PSU	C6-N1-C2	-2.45	120.42	122.69
3	L5	3808	OMC	C1'-N1-C6	-2.44	115.57	120.78
3	L5	4972	PSU	C6-N1-C2	-2.44	120.43	122.69
3	L5	2363	A2M	C4-N9-C1'	-2.43	120.94	126.63
3	L5	2787	A2M	C1'-N9-C8	2.43	132.50	127.09
68	S2	1177	PSU	C6-N1-C2	-2.43	120.43	122.69
3	L5	1860	PSU	C6-N1-C2	-2.43	120.44	122.69
3	L5	3718	A2M	C2'-C1'-N9	2.42	117.73	113.75
3	L5	1782	PSU	C6-N1-C2	-2.42	120.45	122.69
3	L5	1323	A2M	O4'-C1'-C2'	2.41	110.74	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2632	PSU	C6-C5-C4	2.41	119.80	118.17
3	L5	4471	PSU	C6-N1-C2	-2.41	120.45	122.69
68	S2	159	A2M	O4'-C1'-C2'	2.41	110.74	106.59
3	L5	3867	A2M	O3'-C3'-C2'	2.41	117.92	111.19
3	L5	3867	A2M	O4'-C1'-C2'	2.41	110.73	106.59
68	S2	1045	PSU	C6-N1-C2	-2.40	120.46	122.69
3	L5	1781	PSU	C6-N1-C2	-2.40	120.47	122.69
3	L5	2839	PSU	C6-C5-C4	2.40	119.79	118.17
3	L5	3867	A2M	C3'-C2'-C1'	-2.40	98.22	102.81
3	L5	4403	PSU	O4'-C1'-C2'	2.40	108.47	105.15
68	S2	166	A2M	O4'-C1'-C2'	2.39	110.70	106.59
3	L5	1677	PSU	C6-N1-C2	-2.38	120.48	122.69
3	L5	2363	A2M	C1'-N9-C8	2.38	132.39	127.09
3	L5	1524	A2M	C4-N9-C1'	-2.38	121.06	126.63
3	L5	2837	OMU	O2-C2-N1	-2.38	119.70	122.80
3	L5	1677	PSU	O4'-C1'-C2'	2.38	108.44	105.15
3	L5	4353	PSU	C6-C5-C4	2.38	119.78	118.17
3	L5	3718	A2M	C4-N9-C1'	-2.37	121.08	126.63
3	L5	4636	PSU	C6-N1-C2	-2.37	120.49	122.69
3	L5	3695	PSU	C6-N1-C2	-2.37	120.50	122.69
3	L5	2363	A2M	O3'-C3'-C2'	2.36	117.80	111.19
68	S2	116	OMU	O2-C2-N1	-2.35	119.74	122.80
3	L5	4293	PSU	C6-C5-C4	2.34	119.75	118.17
68	S2	468	A2M	C6-C5-C4	-2.34	113.98	117.18
3	L5	4442	PSU	C6-N1-C2	-2.34	120.52	122.69
3	L5	4306	OMU	O2-C2-N1	-2.33	119.76	122.80
68	S2	1248	B8N	O4'-C1'-C2'	2.33	108.38	105.15
68	S2	1081	PSU	C6-N1-C2	-2.33	120.53	122.69
3	L5	3822	PSU	O4'-C1'-C2'	2.33	108.37	105.15
3	L5	1534	A2M	C2'-C1'-N9	2.33	117.58	113.75
3	L5	1524	A2M	C1'-N9-C8	2.32	132.25	127.09
68	S2	649	PSU	O2-C2-N1	-2.32	120.40	122.79
3	L5	4590	A2M	C6-C5-C4	-2.32	114.01	117.18
3	L5	1323	A2M	C3'-C2'-C1'	-2.31	98.38	102.81
3	L5	3867	A2M	C6-C5-C4	-2.31	114.02	117.18
3	L5	5001	PSU	C6-C5-C4	2.31	119.73	118.17
68	S2	814	PSU	C6-N1-C2	-2.31	120.55	122.69
68	S2	966	PSU	C6-C5-C4	2.31	119.73	118.17
68	S2	627	OMU	O2-C2-N1	-2.31	119.80	122.80
68	S2	1081	PSU	C6-C5-C4	2.30	119.73	118.17
68	S2	576	A2M	C1'-N9-C8	2.30	132.20	127.09
3	L5	1323	A2M	O3'-C3'-C2'	2.29	117.60	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	109	PSU	C6-N1-C2	-2.28	120.57	122.69
3	L5	1582	PSU	C6-C5-C4	2.28	119.72	118.17
3	L5	1534	A2M	C4-N9-C1'	-2.28	121.29	126.63
68	S2	166	A2M	C6-C5-C4	-2.28	114.06	117.18
3	L5	2861	OMC	C1'-N1-C2	2.28	123.48	118.44
3	L5	3785	A2M	C2-N1-C6	-2.28	114.99	118.73
3	L5	4442	PSU	O4'-C1'-C2'	2.27	108.30	105.15
68	S2	1326	OMU	O2-C2-N1	-2.27	119.84	122.80
3	L5	1326	A2M	C4-N9-C1'	-2.26	121.35	126.63
3	L5	1326	A2M	O3'-C3'-C4'	-2.26	104.60	111.08
3	L5	3782	5MC	C1'-N1-C6	-2.25	117.44	121.15
3	L5	3637	PSU	O2-C2-N1	-2.25	120.46	122.79
3	L5	4590	A2M	O4'-C1'-C2'	2.24	110.45	106.59
3	L5	4523	A2M	O3'-C3'-C2'	2.23	117.42	111.19
68	S2	428	OMU	O2-C2-N1	-2.23	119.90	122.80
68	S2	1383	A2M	C6-C5-C4	-2.23	114.14	117.18
3	L5	1534	A2M	O3'-C3'-C2'	2.23	117.42	111.19
3	L5	3822	PSU	C6-C5-C4	2.23	119.68	118.17
3	L5	400	A2M	C2'-C1'-N9	2.22	117.41	113.75
68	S2	668	A2M	C6-C5-C4	-2.22	114.15	117.18
3	L5	4620	OMU	O2-C2-N1	-2.22	119.91	122.80
3	L5	1534	A2M	C1'-N9-C8	2.22	132.01	127.09
3	L5	4636	PSU	O4'-C1'-C2'	2.21	108.21	105.15
3	L5	4973	PSU	C6-N1-C2	-2.21	120.64	122.69
3	L5	2363	A2M	C2-N1-C6	-2.21	115.10	118.73
3	L5	398	A2M	C6-C5-C4	-2.21	114.16	117.18
3	L5	4500	PSU	O4'-C1'-C2'	2.21	108.21	105.15
3	L5	3785	A2M	C6-C5-C4	-2.20	114.17	117.18
3	L5	4521	PSU	C6-N1-C2	-2.20	120.65	122.69
3	L5	2815	A2M	C2-N1-C6	-2.20	115.11	118.73
68	S2	1031	A2M	C6-C5-C4	-2.20	114.18	117.18
3	L5	4456	OMC	C1'-N1-C2	2.19	123.29	118.44
3	L5	4293	PSU	C6-N1-C2	-2.19	120.66	122.69
3	L5	2815	A2M	C4-N9-C1'	-2.19	121.52	126.63
3	L5	1582	PSU	C6-N1-C2	-2.19	120.66	122.69
3	L5	2363	A2M	C3'-C2'-C1'	-2.18	98.62	102.81
3	L5	1534	A2M	C2-N1-C6	-2.18	115.14	118.73
68	S2	668	A2M	O3'-C3'-C4'	-2.18	104.81	111.08
3	L5	2815	A2M	C1'-N9-C8	2.18	131.93	127.09
3	L5	1326	A2M	C2'-C1'-N9	2.18	117.33	113.75
3	L5	4296	PSU	C6-C5-C4	2.18	119.64	118.17
68	S2	109	PSU	C6-C5-C4	2.17	119.64	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3785	A2M	C5-C6-N1	2.17	123.02	117.51
68	S2	1031	A2M	O4'-C1'-C2'	2.17	110.33	106.59
68	S2	105	PSU	C6-C5-C4	2.17	119.64	118.17
3	L5	4353	PSU	C6-N1-C2	-2.16	120.68	122.69
3	L5	4523	A2M	C6-C5-C4	-2.16	114.22	117.18
3	L5	4523	A2M	C4'-O4'-C1'	-2.16	104.69	109.47
3	L5	1326	A2M	O4'-C1'-C2'	2.16	110.31	106.59
5	L8	69	PSU	O4'-C1'-C2'	2.16	108.14	105.15
3	L5	3825	A2M	C2-N1-C6	-2.16	115.18	118.73
3	L5	1326	A2M	C1'-N9-C8	2.16	131.88	127.09
3	L5	4500	PSU	C6-C5-C4	2.16	119.63	118.17
68	S2	354	OMU	O2-C2-N1	-2.15	119.99	122.80
68	S2	159	A2M	C2-N1-C6	-2.15	115.20	118.73
3	L5	1871	A2M	C6-C5-C4	-2.14	114.25	117.18
68	S2	99	A2M	C2-N1-C6	-2.14	115.21	118.73
3	L5	2787	A2M	C3'-C2'-C1'	-2.14	98.71	102.81
68	S2	1248	B8N	O4-C4-C5	-2.14	118.88	122.58
3	L5	4523	A2M	C2-N1-C6	-2.13	115.23	118.73
3	L5	4571	A2M	C6-C5-C4	-2.13	114.27	117.18
3	L5	1323	A2M	C6-C5-C4	-2.13	114.27	117.18
3	L5	3830	A2M	C6-C5-C4	-2.13	114.27	117.18
3	L5	1326	A2M	C5-C6-N1	2.13	122.92	117.51
3	L5	1524	A2M	C2-N1-C6	-2.13	115.23	118.73
68	S2	1081	PSU	O4'-C1'-C2'	2.13	108.10	105.15
3	L5	1326	A2M	C2-N1-C6	-2.12	115.24	118.73
3	L5	400	A2M	C6-C5-C4	-2.12	114.28	117.18
68	S2	27	A2M	C6-C5-C4	-2.12	114.28	117.18
3	L5	3920	PSU	O4'-C1'-C2'	2.12	108.08	105.15
68	S2	484	A2M	C2-N1-C6	-2.11	115.26	118.73
3	L5	2401	A2M	C2-N1-C6	-2.11	115.26	118.73
3	L5	4523	A2M	C5-C6-N1	2.11	122.87	117.51
68	S2	99	A2M	C5-C6-N1	2.11	122.87	117.51
68	S2	1383	A2M	O4'-C1'-C2'	2.11	110.22	106.59
68	S2	166	A2M	C5-C6-N1	2.11	122.87	117.51
3	L5	1871	A2M	C4'-O4'-C1'	-2.11	104.81	109.47
68	S2	159	A2M	C5-C6-N1	2.11	122.86	117.51
68	S2	1832	6MZ	C5-C6-N1	2.11	120.41	118.15
3	L5	4973	PSU	C6-C5-C4	2.11	119.60	118.17
3	L5	1323	A2M	C2-N1-C6	-2.10	115.28	118.73
3	L5	3718	A2M	C2-N1-C6	-2.10	115.28	118.73
3	L5	398	A2M	C5-C6-N1	2.10	122.83	117.51
3	L5	1534	A2M	C5-C6-N1	2.10	122.83	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
68	S2	159	A2M	C6-C5-C4	-2.09	114.32	117.18
68	S2	668	A2M	C2-N1-C6	-2.09	115.29	118.73
3	L5	2401	A2M	C5-C6-N1	2.09	122.82	117.51
68	S2	159	A2M	O4'-C4'-C3'	2.08	109.29	105.15
68	S2	1031	A2M	C5-C6-N1	2.08	122.80	117.51
68	S2	27	A2M	O4'-C1'-C2'	2.08	110.17	106.59
3	L5	3867	A2M	C2-N1-C6	-2.08	115.32	118.73
3	L5	2787	A2M	C6-C5-C4	-2.07	114.35	117.18
3	L5	2815	A2M	C5-C6-N1	2.07	122.77	117.51
68	S2	668	A2M	C5-C6-N1	2.07	122.77	117.51
3	L5	2787	A2M	C2-N1-C6	-2.07	115.33	118.73
3	L5	1323	A2M	C5-C6-N1	2.07	122.76	117.51
68	S2	649	PSU	C6-C5-C4	2.06	119.57	118.17
3	L5	1524	A2M	C5-C6-N1	2.06	122.75	117.51
68	S2	966	PSU	O4'-C1'-C2'	2.06	108.00	105.15
68	S2	484	A2M	O4'-C4'-C3'	2.06	109.24	105.15
68	S2	484	A2M	C6-C5-C4	-2.06	114.37	117.18
3	L5	2363	A2M	C5-C6-N1	2.06	122.73	117.51
3	L5	3825	A2M	O4'-C1'-C2'	2.06	110.13	106.59
3	L5	2787	A2M	C5-C6-N1	2.06	122.73	117.51
3	L5	1322	1MA	CM1-N1-C6	-2.06	116.96	120.15
3	L5	400	A2M	O3'-C3'-C4'	-2.05	105.18	111.08
3	L5	3825	A2M	C5-C6-N1	2.05	122.72	117.51
3	L5	1677	PSU	C6-C5-C4	2.05	119.56	118.17
68	S2	1248	B8N	C31-N3-C2	2.05	120.67	117.64
3	L5	398	A2M	C2-N1-C6	-2.05	115.36	118.73
68	S2	484	A2M	C5-C6-N1	2.05	122.72	117.51
68	S2	27	A2M	C2-N1-C6	-2.05	115.36	118.73
3	L5	2815	A2M	O3'-C3'-C4'	-2.05	105.20	111.08
68	S2	1031	A2M	C2-N1-C6	-2.04	115.38	118.73
3	L5	1871	A2M	C5-C6-N1	2.04	122.69	117.51
3	L5	3785	A2M	O4'-C4'-C3'	2.04	109.20	105.15
3	L5	3825	A2M	C6-C5-C4	-2.03	114.40	117.18
3	L5	4571	A2M	C2-N1-C6	-2.03	115.39	118.73
68	S2	468	A2M	O4'-C1'-C2'	2.03	110.09	106.59
68	S2	468	A2M	C5-C6-N1	2.03	122.66	117.51
68	S2	1850	MA6	C1'-N9-C8	-2.03	122.60	127.09
3	L5	3884	PSU	C6-C5-C4	2.03	119.54	118.17
3	L5	1326	A2M	C6-C5-C4	-2.03	114.41	117.18
3	L5	4571	A2M	C5-C6-N1	2.02	122.65	117.51
3	L5	400	A2M	O4'-C1'-C2'	2.02	110.07	106.59
3	L5	4353	PSU	O4'-C1'-C2'	2.02	107.95	105.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3701	OMC	O2-C2-N3	-2.02	119.14	122.33
68	S2	863	PSU	O4'-C1'-C2'	2.02	107.95	105.15
3	L5	4457	PSU	O4'-C1'-C2'	2.02	107.95	105.15
3	L5	400	A2M	C5-C6-N1	2.02	122.64	117.51
68	S2	1383	A2M	C5-C6-N1	2.02	122.63	117.51
3	L5	4442	PSU	C6-C5-C4	2.02	119.53	118.17
3	L5	2401	A2M	C6-C5-C4	-2.01	114.43	117.18
3	L5	4521	PSU	C6-C5-C4	2.01	119.53	118.17
3	L5	4590	A2M	C5-C6-N1	2.01	122.61	117.51
68	S2	27	A2M	C5-C6-N1	2.01	122.61	117.51
68	S2	468	A2M	C4'-O4'-C1'	-2.01	105.04	109.47
68	S2	99	A2M	C6-C5-C4	-2.00	114.44	117.18
68	S2	1232	PSU	O4'-C1'-C2'	2.00	107.92	105.15
3	L5	4523	A2M	CM'-O2'-C2'	-2.00	109.34	114.47

There are no chirality outliers.

All (154) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L8	75	OMG	C1'-C2'-O2'-CM2
3	L5	398	A2M	C1'-C2'-O2'-CM'
3	L5	400	A2M	C1'-C2'-O2'-CM'
3	L5	1316	OMG	C1'-C2'-O2'-CM2
3	L5	1323	A2M	C1'-C2'-O2'-CM'
3	L5	1326	A2M	O4'-C4'-C5'-O5'
3	L5	1326	A2M	C3'-C4'-C5'-O5'
3	L5	1326	A2M	C1'-C2'-O2'-CM'
3	L5	1340	OMC	C1'-C2'-O2'-CM2
3	L5	1625	OMG	O4'-C4'-C5'-O5'
3	L5	2364	OMG	O4'-C4'-C5'-O5'
3	L5	2401	A2M	C1'-C2'-O2'-CM'
3	L5	2787	A2M	C1'-C2'-O2'-CM'
3	L5	2815	A2M	C1'-C2'-O2'-CM'
3	L5	2861	OMC	C1'-C2'-O2'-CM2
3	L5	3701	OMC	O4'-C4'-C5'-O5'
3	L5	3744	OMG	C1'-C2'-O2'-CM2
3	L5	3792	OMG	O4'-C4'-C5'-O5'
3	L5	3825	A2M	C1'-C2'-O2'-CM'
3	L5	3830	A2M	C1'-C2'-O2'-CM'
3	L5	3867	A2M	C1'-C2'-O2'-CM'
3	L5	3925	OMU	C1'-C2'-O2'-CM2
3	L5	4196	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
3	L5	4590	A2M	O4'-C4'-C5'-O5'
3	L5	4590	A2M	C1'-C2'-O2'-CM'
3	L5	4636	PSU	C2'-C1'-C5-C4
3	L5	4637	OMG	O4'-C4'-C5'-O5'
3	L5	4637	OMG	C1'-C2'-O2'-CM2
68	S2	27	A2M	C1'-C2'-O2'-CM'
68	S2	116	OMU	C1'-C2'-O2'-CM2
68	S2	159	A2M	C1'-C2'-O2'-CM'
68	S2	166	A2M	C1'-C2'-O2'-CM'
68	S2	174	OMC	C1'-C2'-O2'-CM2
68	S2	354	OMU	C1'-C2'-O2'-CM2
68	S2	428	OMU	C2'-C1'-N1-C2
68	S2	428	OMU	C2'-C1'-N1-C6
68	S2	468	A2M	C1'-C2'-O2'-CM'
68	S2	601	OMG	C1'-C2'-O2'-CM2
68	S2	627	OMU	O4'-C4'-C5'-O5'
68	S2	644	OMG	O4'-C4'-C5'-O5'
68	S2	644	OMG	C1'-C2'-O2'-CM2
68	S2	668	A2M	C1'-C2'-O2'-CM'
68	S2	801	PSU	C3'-C4'-C5'-O5'
68	S2	867	OMG	C3'-C4'-C5'-O5'
68	S2	1031	A2M	C1'-C2'-O2'-CM'
68	S2	1248	B8N	C31-C32-C33-C34
68	S2	1328	OMG	C1'-C2'-O2'-CM2
68	S2	1383	A2M	C1'-C2'-O2'-CM'
68	S2	1832	6MZ	C5-C6-N6-C9
68	S2	1832	6MZ	N1-C6-N6-C9
3	L5	1536	PSU	C3'-C4'-C5'-O5'
3	L5	1536	PSU	O4'-C4'-C5'-O5'
3	L5	1625	OMG	C3'-C4'-C5'-O5'
3	L5	2401	A2M	C3'-C4'-C5'-O5'
3	L5	4590	A2M	C3'-C4'-C5'-O5'
68	S2	99	A2M	O4'-C4'-C5'-O5'
68	S2	627	OMU	C3'-C4'-C5'-O5'
68	S2	867	OMG	O4'-C4'-C5'-O5'
68	S2	1045	PSU	O4'-C4'-C5'-O5'
68	S2	1442	OMU	O4'-C4'-C5'-O5'
3	L5	2364	OMG	C3'-C4'-C5'-O5'
3	L5	3701	OMC	C3'-C4'-C5'-O5'
3	L5	3899	OMG	C3'-C4'-C5'-O5'
3	L5	4500	PSU	O4'-C4'-C5'-O5'
68	S2	428	OMU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
68	S2	428	OMU	O4'-C4'-C5'-O5'
68	S2	801	PSU	O4'-C4'-C5'-O5'
68	S2	1045	PSU	C3'-C4'-C5'-O5'
68	S2	1442	OMU	C3'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C6
3	L5	3792	OMG	C3'-C4'-C5'-O5'
3	L5	4500	PSU	C3'-C4'-C5'-O5'
68	S2	644	OMG	C3'-C4'-C5'-O5'
3	L5	1524	A2M	C3'-C4'-C5'-O5'
3	L5	2401	A2M	O4'-C4'-C5'-O5'
3	L5	4618	OMG	C3'-C4'-C5'-O5'
3	L5	4637	OMG	C3'-C4'-C5'-O5'
68	S2	99	A2M	C3'-C4'-C5'-O5'
68	S2	576	A2M	C3'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C2
3	L5	1524	A2M	O4'-C4'-C5'-O5'
3	L5	3899	OMG	O4'-C4'-C5'-O5'
3	L5	4220	6MZ	O4'-C4'-C5'-O5'
68	S2	576	A2M	O4'-C4'-C5'-O5'
3	L5	3818	UY1	C4'-C5'-O5'-P
3	L5	2422	OMC	O4'-C4'-C5'-O5'
3	L5	3830	A2M	O4'-C4'-C5'-O5'
3	L5	4220	6MZ	C3'-C4'-C5'-O5'
68	S2	166	A2M	O4'-C4'-C5'-O5'
3	L5	2422	OMC	C3'-C4'-C5'-O5'
68	S2	668	A2M	O4'-C4'-C5'-O5'
3	L5	4590	A2M	C4'-C5'-O5'-P
68	S2	166	A2M	C3'-C4'-C5'-O5'
68	S2	668	A2M	C3'-C4'-C5'-O5'
68	S2	1248	B8N	N34-C33-C34-O36
3	L5	2787	A2M	C2'-C1'-N9-C8
3	L5	3841	OMC	C1'-C2'-O2'-CM2
3	L5	4392	OMG	C1'-C2'-O2'-CM2
3	L5	3830	A2M	C3'-C4'-C5'-O5'
3	L5	4618	OMG	O4'-C4'-C5'-O5'
68	S2	799	OMU	C3'-C4'-C5'-O5'
68	S2	1046	PSU	O4'-C4'-C5'-O5'
3	L5	4447	5MC	O4'-C1'-N1-C6
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	1534	A2M	C3'-C2'-O2'-CM'
3	L5	3869	OMC	C3'-C2'-O2'-CM2
68	S2	576	A2M	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
68	S2	1851	MA6	C4'-C5'-O5'-P
3	L5	3818	UY1	O4'-C1'-C5-C4
3	L5	4636	PSU	O4'-C1'-C5-C4
68	S2	1248	B8N	O4'-C1'-C5-C4
3	L5	2787	A2M	C2'-C1'-N9-C4
3	L5	4447	5MC	O4'-C1'-N1-C2
3	L5	4623	OMG	C3'-C4'-C5'-O5'
68	S2	1383	A2M	C3'-C4'-C5'-O5'
3	L5	3844	PSU	C4'-C5'-O5'-P
3	L5	3701	OMC	O4'-C1'-N1-C6
3	L5	1322	1MA	C2'-C1'-N9-C8
3	L5	3701	OMC	C2'-C1'-N1-C2
68	S2	428	OMU	O4'-C1'-N1-C6
3	L5	3701	OMC	C2'-C1'-N1-C6
3	L5	1322	1MA	C2'-C1'-N9-C4
3	L5	4500	PSU	C4'-C5'-O5'-P
68	S2	1081	PSU	C4'-C5'-O5'-P
68	S2	1490	OMG	C4'-C5'-O5'-P
3	L5	1326	A2M	C4'-C5'-O5'-P
68	S2	644	OMG	C4'-C5'-O5'-P
3	L5	2815	A2M	O4'-C4'-C5'-O5'
68	S2	1244	PSU	O4'-C4'-C5'-O5'
68	S2	1383	A2M	O4'-C4'-C5'-O5'
3	L5	3701	OMC	O4'-C1'-N1-C2
3	L5	2422	OMC	C1'-C2'-O2'-CM2
3	L5	3899	OMG	C1'-C2'-O2'-CM2
68	S2	462	OMC	C1'-C2'-O2'-CM2
3	L5	2632	PSU	C3'-C4'-C5'-O5'
3	L5	3867	A2M	C3'-C4'-C5'-O5'
3	L5	4623	OMG	O4'-C4'-C5'-O5'
68	S2	1703	OMC	O4'-C4'-C5'-O5'
3	L5	3818	UY1	O4'-C1'-C5-C6
68	S2	1248	B8N	O4'-C1'-C5-C6
3	L5	3899	OMG	C3'-C2'-O2'-CM2
68	S2	428	OMU	O4'-C1'-N1-C2
3	L5	3887	OMC	C4'-C5'-O5'-P
68	S2	683	OMG	C3'-C4'-C5'-O5'
3	L5	2787	A2M	C3'-C4'-C5'-O5'
3	L5	3785	A2M	O4'-C4'-C5'-O5'
3	L5	2787	A2M	O4'-C1'-N9-C8
3	L5	2351	OMC	O4'-C4'-C5'-O5'
3	L5	398	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
68	S2	799	OMU	O4'-C4'-C5'-O5'
3	L5	3785	A2M	O4'-C1'-N9-C8
5	L8	75	OMG	C4'-C5'-O5'-P
3	L5	2632	PSU	O4'-C4'-C5'-O5'
3	L5	4636	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

80 monomers are involved in 116 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
68	S2	116	OMU	3	0
68	S2	1703	OMC	2	0
3	L5	3841	OMC	1	0
3	L5	4637	OMG	2	0
3	L5	4312	PSU	2	0
3	L5	2401	A2M	1	0
3	L5	3925	OMU	1	0
3	L5	2787	A2M	1	0
3	L5	4299	PSU	2	0
3	L5	1326	A2M	2	0
68	S2	1850	MA6	2	0
3	L5	1683	PSU	2	0
3	L5	4196	OMG	1	0
3	L5	4447	5MC	1	0
3	L5	4296	PSU	1	0
68	S2	172	OMU	1	0
3	L5	3718	A2M	2	0
68	S2	1244	PSU	1	0
68	S2	354	OMU	1	0
3	L5	4536	OMC	1	0
3	L5	4370	OMG	1	0
68	S2	462	OMC	1	0
3	L5	400	A2M	3	0
3	L5	4590	A2M	1	0
3	L5	1316	OMG	1	0
3	L5	4457	PSU	1	0
3	L5	1323	A2M	3	0
3	L5	4623	OMG	1	0
3	L5	4523	A2M	2	0
3	L5	2424	OMG	1	0
68	S2	159	A2M	2	0
68	S2	1004	PSU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3744	OMG	1	0
3	L5	4579	PSU	2	0
68	S2	644	OMG	1	0
3	L5	398	A2M	2	0
3	L5	3920	PSU	1	0
3	L5	4227	OMU	1	0
68	S2	601	OMG	2	0
3	L5	3830	A2M	1	0
3	L5	2815	A2M	2	0
3	L5	3825	A2M	2	0
3	L5	1340	OMC	2	0
68	S2	1031	A2M	2	0
3	L5	3851	PSU	1	0
68	S2	174	OMC	1	0
3	L5	4456	OMC	1	0
3	L5	4571	A2M	1	0
3	L5	1871	A2M	1	0
68	S2	509	OMG	4	0
68	S2	428	OMU	1	0
3	L5	1534	A2M	1	0
68	S2	468	A2M	1	0
68	S2	1337	4AC	2	0
68	S2	668	A2M	1	0
3	L5	5001	PSU	1	0
3	L5	4500	PSU	1	0
68	S2	484	A2M	1	0
68	S2	1832	6MZ	1	0
68	S2	1232	PSU	1	0
3	L5	4530	UR3	1	0
3	L5	4392	OMG	2	0
3	L5	4689	PSU	1	0
3	L5	2422	OMC	1	0
3	L5	2861	OMC	1	0
68	S2	166	A2M	4	0
68	S2	121	OMU	1	0
68	S2	1442	OMU	1	0
68	S2	681	PSU	2	0
68	S2	576	A2M	1	0
68	S2	1174	PSU	2	0
3	L5	4620	OMU	1	0
3	L5	2363	A2M	1	0
68	S2	27	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	3884	PSU	1	0
68	S2	1272	OMC	1	0
3	L5	3867	A2M	3	0
68	S2	1328	OMG	1	0
3	L5	4521	PSU	1	0
68	S2	649	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 243 ligands modelled in this entry, 224 are monoatomic - leaving 19 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	$\# Z > 2$
87	SPM	L5	5268	-	13,13,13	0.36	0	12,12,12	0.97	0
87	SPM	L5	5294	-	13,13,13	0.34	0	12,12,12	0.87	0
87	SPM	L5	5289	-	13,13,13	0.37	0	12,12,12	0.99	0
87	SPM	L5	5264	-	13,13,13	0.37	0	12,12,12	1.01	0
88	SPD	L5	5293	-	9,9,9	0.32	0	8,8,8	0.81	0
89	3HE	L5	5295	-	21,21,21	0.54	0	23,30,30	0.82	1 (4%)
87	SPM	L5	5265	-	13,13,13	0.35	0	12,12,12	1.09	0
88	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.83	0
88	SPD	L5	5285	-	9,9,9	0.31	0	8,8,8	0.88	0
90	HMT	L5	5296	-	41,43,43	0.78	1 (2%)	43,66,66	0.73	1 (2%)
88	SPD	L5	5284	-	9,9,9	0.30	0	8,8,8	0.84	0
87	SPM	L5	5259	-	13,13,13	0.36	0	12,12,12	0.97	0
88	SPD	L5	5290	-	9,9,9	0.32	0	8,8,8	0.86	0
88	SPD	L5	5288	-	9,9,9	0.31	0	8,8,8	0.81	0
88	SPD	L5	5287	-	9,9,9	0.33	0	8,8,8	0.82	0
88	SPD	L5	5291	-	9,9,9	0.33	0	8,8,8	0.82	0
87	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	SPD	L5	5286	-	9,9,9	0.33	0	8,8,8	0.78	0
88	SPD	L5	5262	-	9,9,9	0.32	0	8,8,8	1.06	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
87	SPM	L5	5268	-	-	3/11/11/11	-
87	SPM	L5	5294	-	-	1/11/11/11	-
87	SPM	L5	5289	-	-	5/11/11/11	-
87	SPM	L5	5264	-	-	3/11/11/11	-
88	SPD	L5	5293	-	-	4/7/7/7	-
89	3HE	L5	5295	-	-	2/8/36/36	0/2/2/2
87	SPM	L5	5265	-	-	4/11/11/11	-
88	SPD	L5	5283	-	-	0/7/7/7	-
88	SPD	L5	5285	-	-	1/7/7/7	-
90	HMT	L5	5296	-	-	0/27/74/74	0/5/5/5
88	SPD	L5	5284	-	-	2/7/7/7	-
87	SPM	L5	5259	-	-	3/11/11/11	-
88	SPD	L5	5290	-	-	0/7/7/7	-
88	SPD	L5	5288	-	-	3/7/7/7	-
88	SPD	L5	5287	-	-	1/7/7/7	-
88	SPD	L5	5291	-	-	5/7/7/7	-
87	SPM	L5	5292	-	-	5/11/11/11	-
88	SPD	L5	5286	-	-	0/7/7/7	-
88	SPD	L5	5262	-	-	2/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	L5	5296	HMT	C20-C19	-3.58	1.49	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	L5	5296	HMT	C25-C24-C20	-2.84	108.72	115.34
89	L5	5295	3HE	C9-C13-C12	-2.41	110.41	114.46

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	L5	5295	3HE	C7-C8-C9-C13
87	L5	5264	SPM	N10-C11-C12-C13
87	L5	5259	SPM	N5-C6-C7-C8
87	L5	5268	SPM	C7-C8-C9-N10
88	L5	5293	SPD	C3-C4-C5-N6
87	L5	5292	SPM	C7-C8-C9-N10
88	L5	5262	SPD	N6-C7-C8-C9
87	L5	5264	SPM	C7-C6-N5-C4
88	L5	5293	SPD	C8-C7-N6-C5
89	L5	5295	3HE	C7-C8-C9-C10
88	L5	5287	SPD	C4-C5-N6-C7
87	L5	5264	SPM	N5-C6-C7-C8
88	L5	5293	SPD	N6-C7-C8-C9
87	L5	5289	SPM	C12-C11-N10-C9
88	L5	5291	SPD	C4-C5-N6-C7
87	L5	5292	SPM	N10-C11-C12-C13
88	L5	5288	SPD	N1-C2-C3-C4
88	L5	5293	SPD	C2-C3-C4-C5
87	L5	5265	SPM	C6-C7-C8-C9
88	L5	5288	SPD	C2-C3-C4-C5
87	L5	5265	SPM	C7-C8-C9-N10
88	L5	5285	SPD	C2-C3-C4-C5
87	L5	5259	SPM	C6-C7-C8-C9
88	L5	5291	SPD	C3-C4-C5-N6
87	L5	5294	SPM	C8-C9-N10-C11
88	L5	5284	SPD	C7-C8-C9-N10
87	L5	5289	SPM	C8-C9-N10-C11
88	L5	5284	SPD	C8-C7-N6-C5
88	L5	5291	SPD	C8-C7-N6-C5
87	L5	5268	SPM	C6-C7-C8-C9
88	L5	5291	SPD	N1-C2-C3-C4
87	L5	5265	SPM	C2-C3-C4-N5
87	L5	5289	SPM	N1-C2-C3-C4
87	L5	5292	SPM	C11-C12-C13-N14
88	L5	5262	SPD	C7-C8-C9-N10
88	L5	5288	SPD	C8-C7-N6-C5
88	L5	5291	SPD	C7-C8-C9-N10
87	L5	5289	SPM	C7-C6-N5-C4
87	L5	5292	SPM	C12-C11-N10-C9
87	L5	5292	SPM	C7-C6-N5-C4

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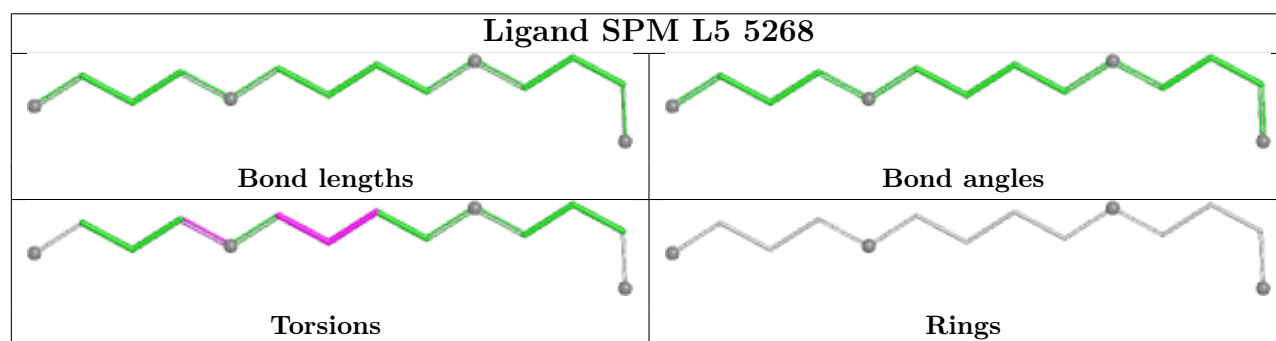
Mol	Chain	Res	Type	Atoms
87	L5	5268	SPM	C12-C11-N10-C9
87	L5	5259	SPM	N1-C2-C3-C4
87	L5	5265	SPM	N1-C2-C3-C4
87	L5	5289	SPM	C2-C3-C4-N5

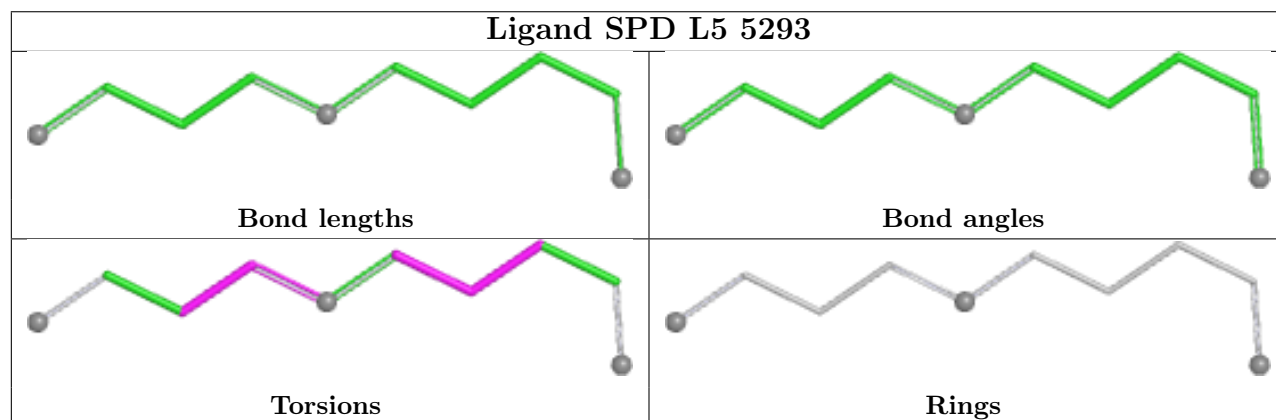
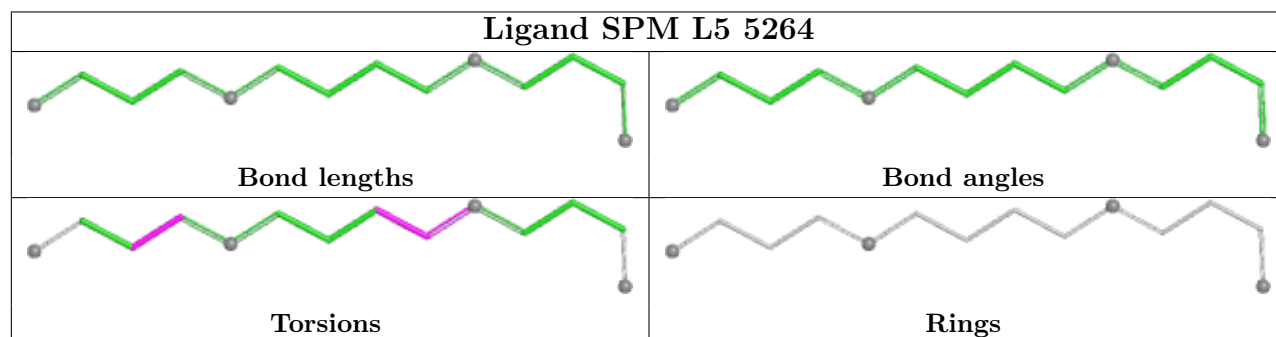
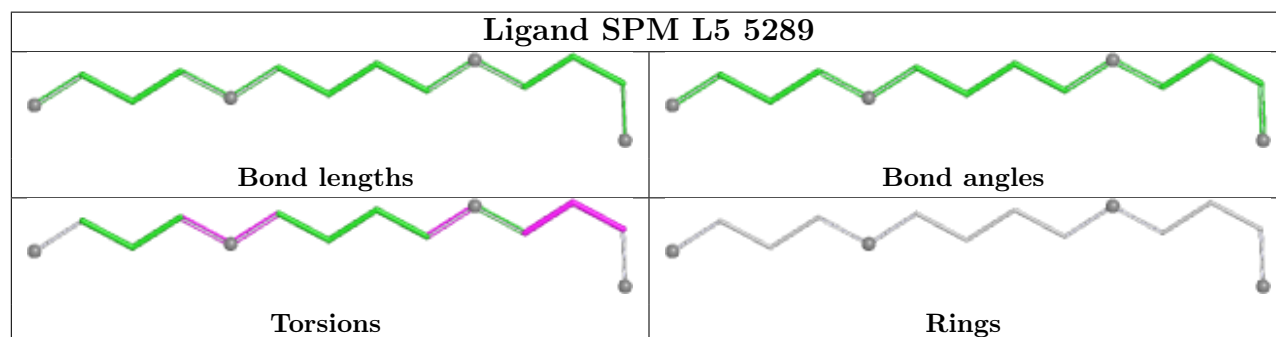
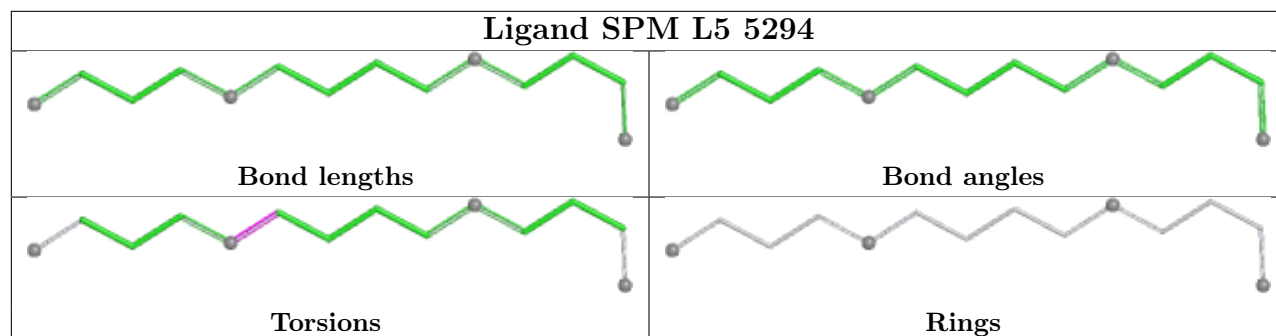
There are no ring outliers.

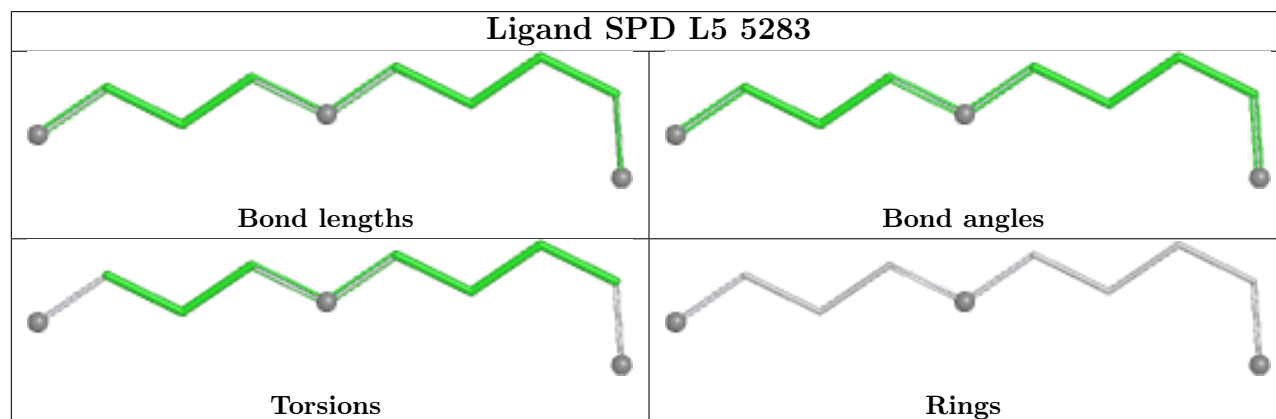
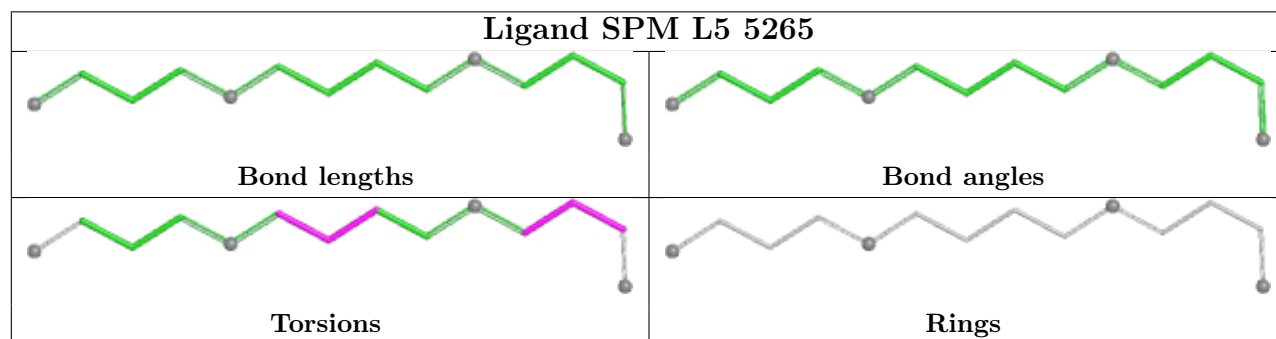
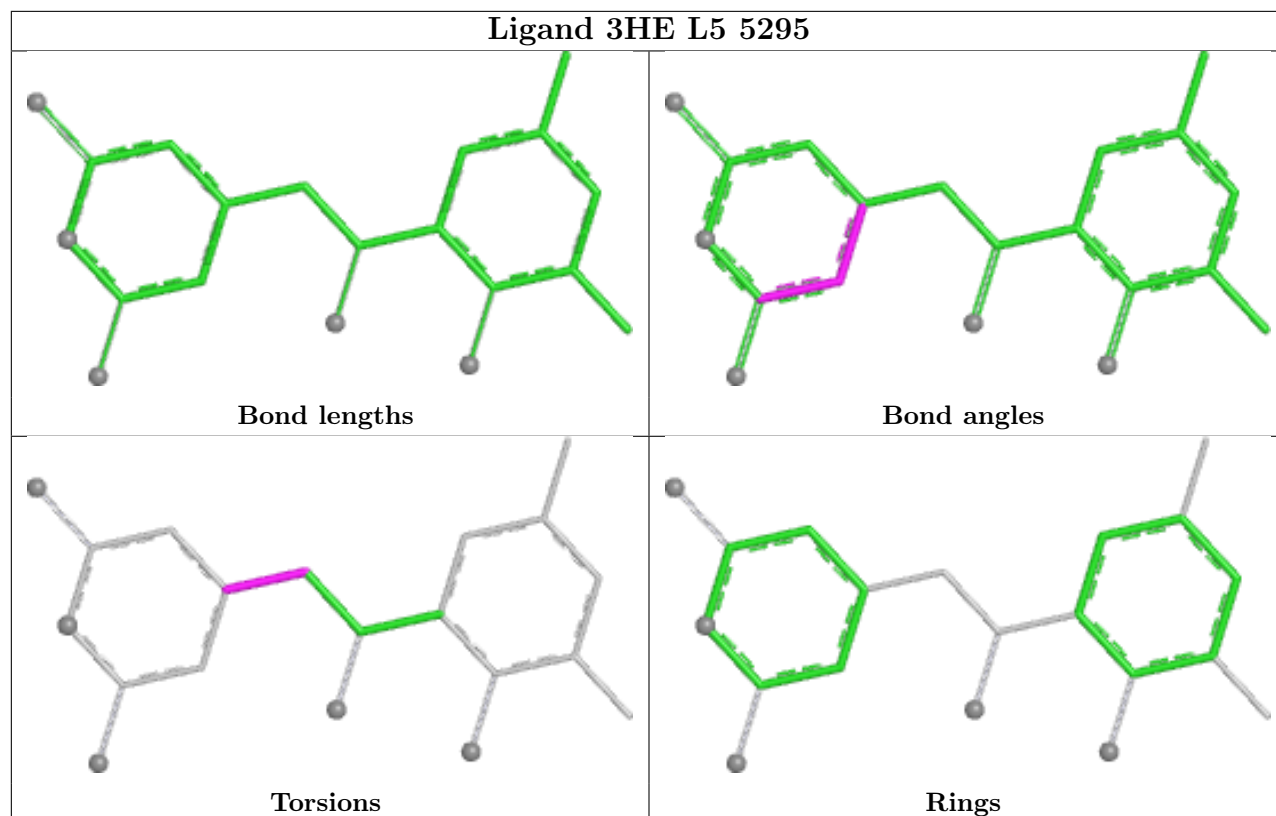
4 monomers are involved in 4 short contacts:

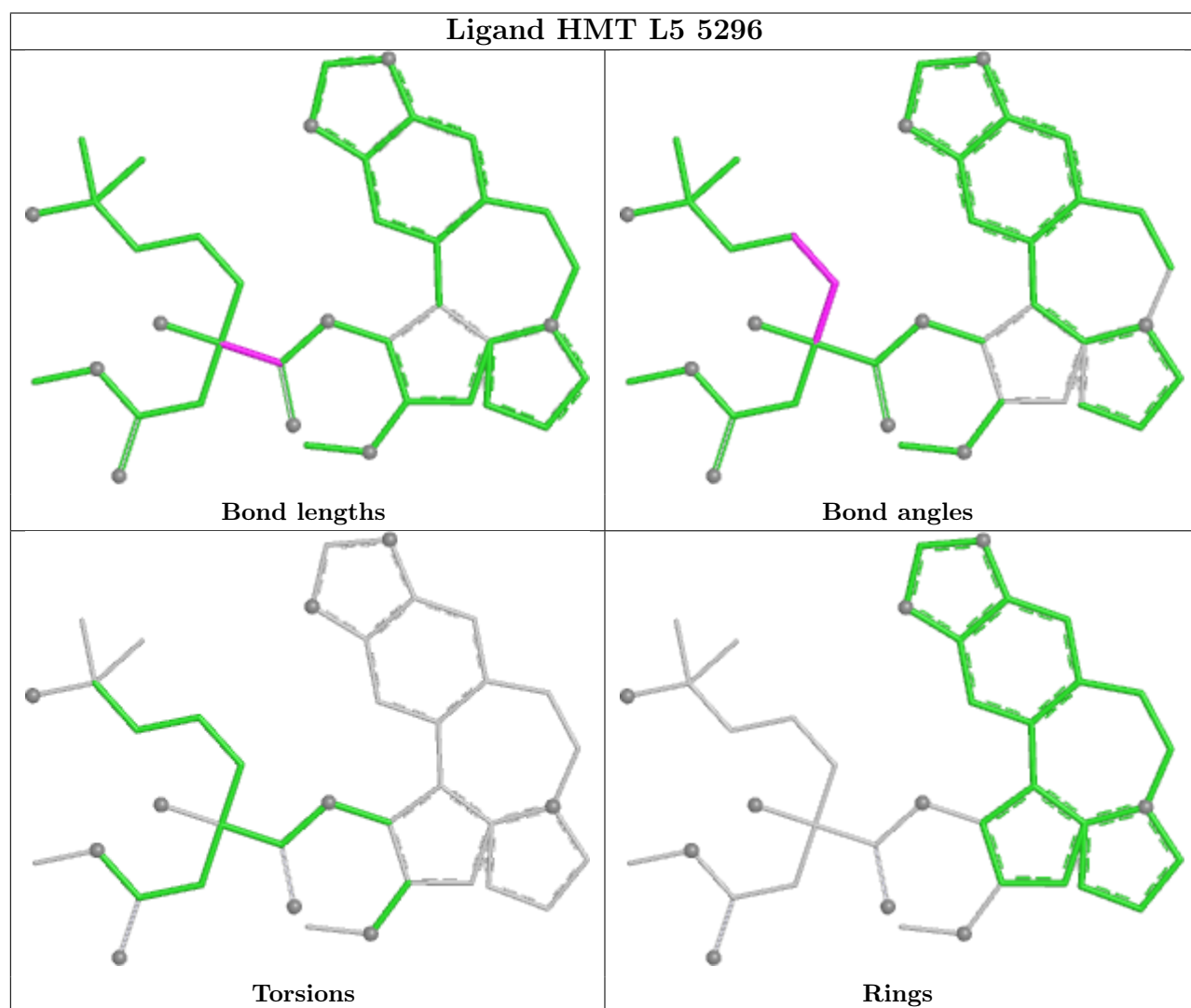
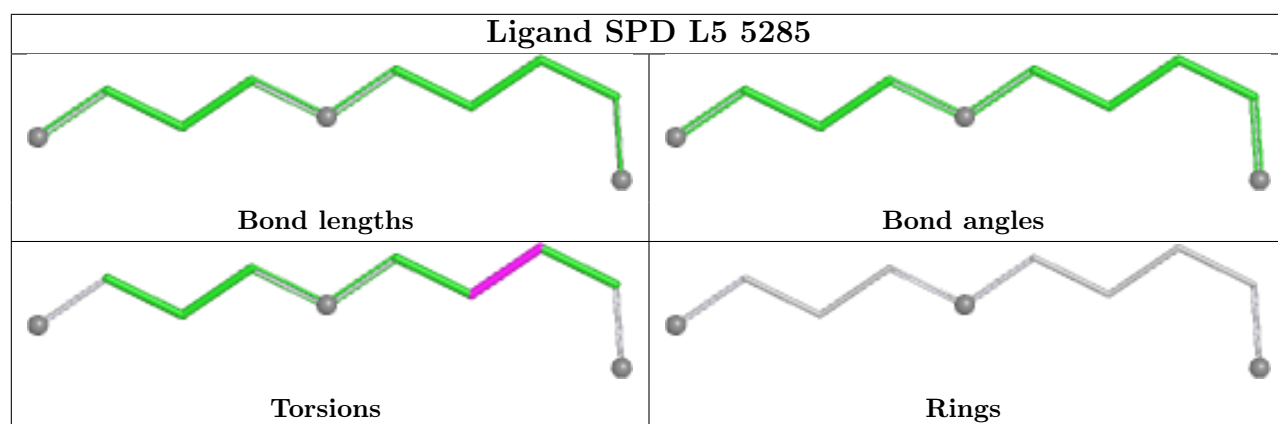
Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	L5	5268	SPM	1	0
87	L5	5294	SPM	2	0
87	L5	5289	SPM	1	0
88	L5	5290	SPD	1	0

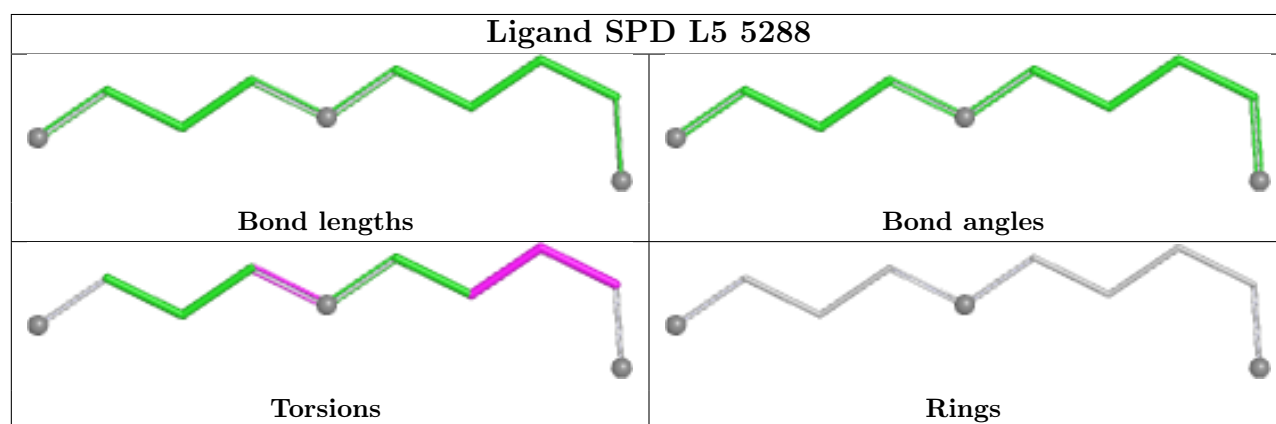
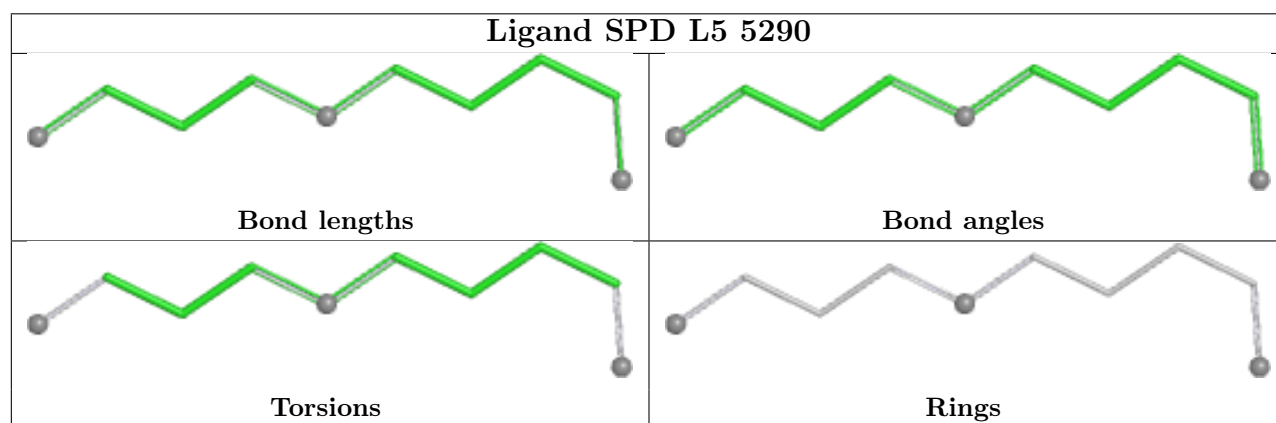
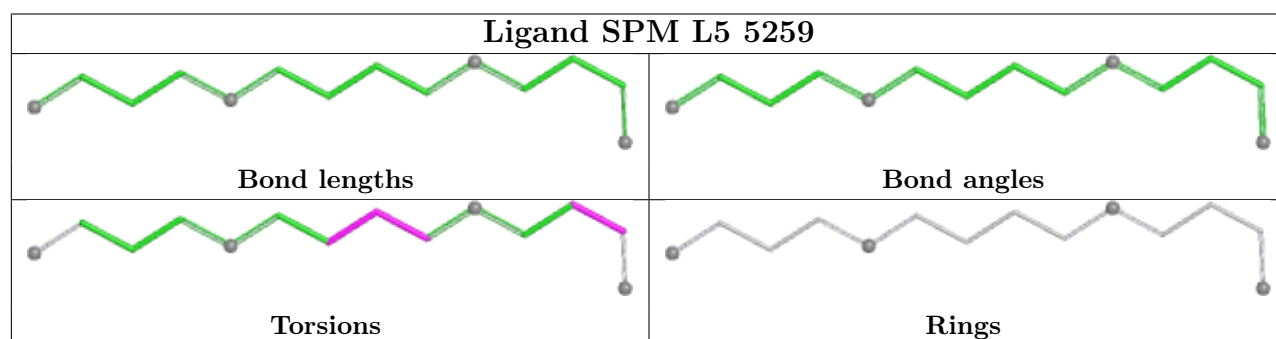
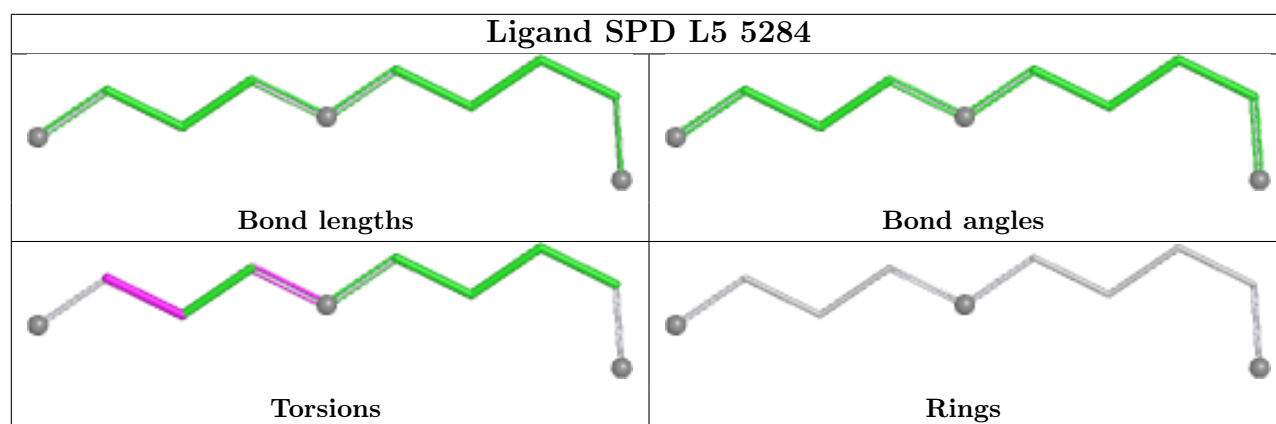
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

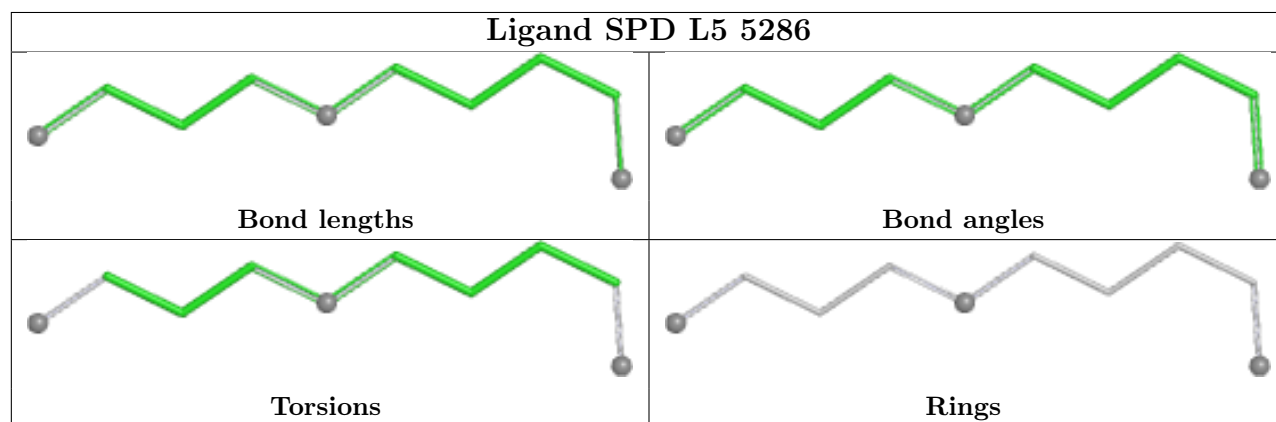
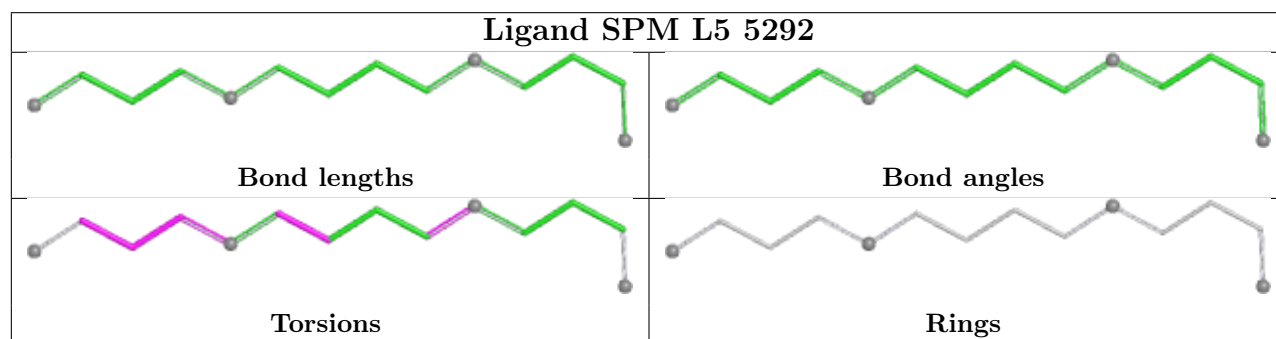
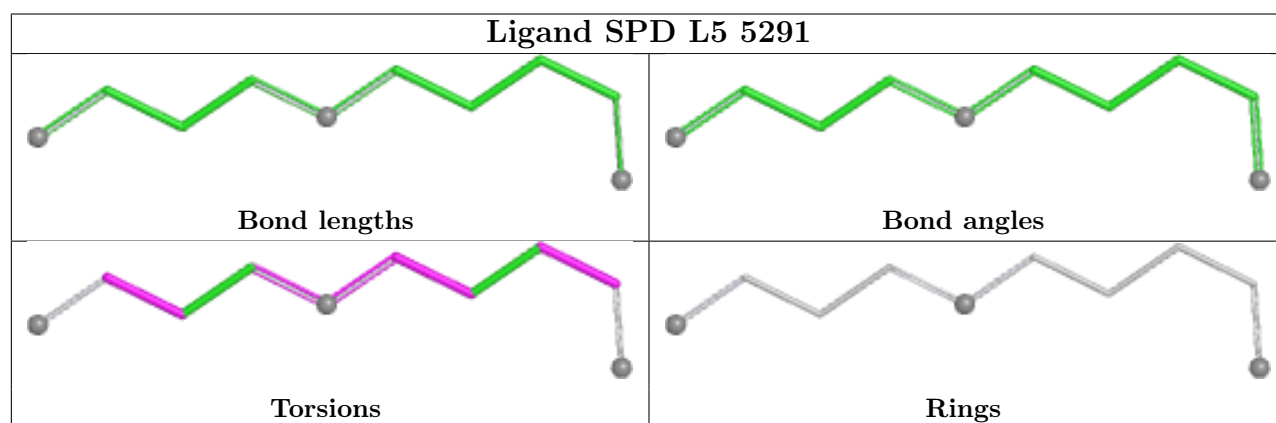
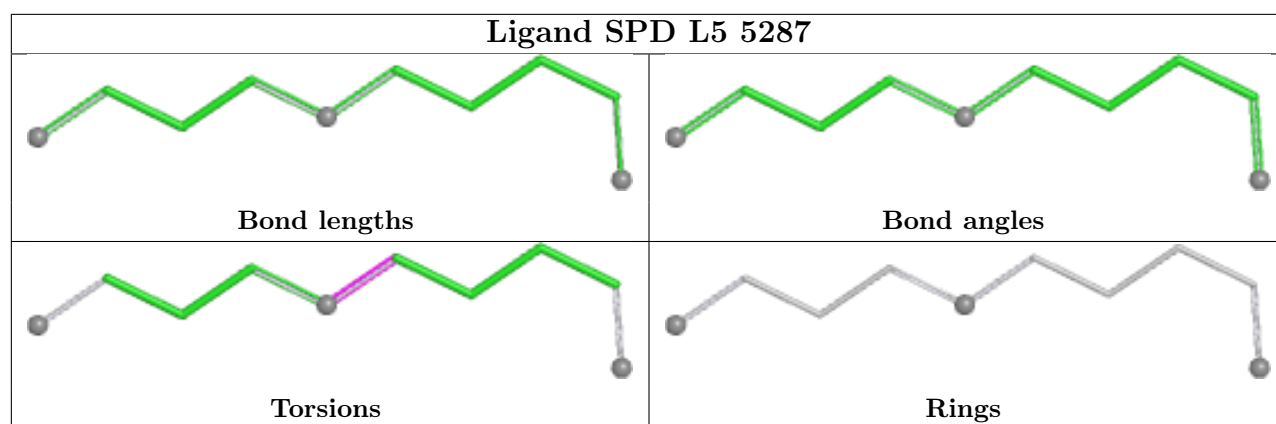


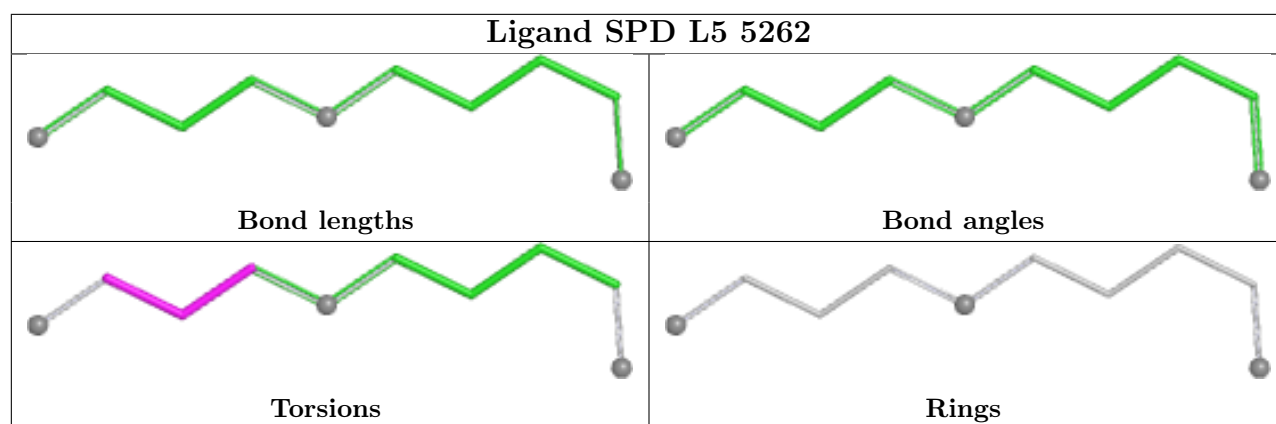












5.7 Other polymers [i](#)

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
3	L5	10
68	S2	4
1	CD	1
84	CB	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	225:LEU	C	282:THR	N	58.36
1	S2	753:C	O3'	785:C	P	28.46
1	L5	1706:A	O3'	1716:G	P	21.63
1	L5	2910:G	O3'	3584:C	P	21.13
1	L5	760:G	O3'	903:C	P	16.94
1	CB	236:PHE	C	247:ALA	N	16.69
1	L5	519:C	O3'	642:G	P	15.60
1	L5	3954:A	O3'	4056:A	P	14.59
1	S2	698:G	O3'	730:C	P	14.38
1	L5	4776:G	O3'	4858:C	P	13.75
1	L5	2112:G	O3'	2249:C	P	13.71
1	S2	739:C	O3'	746:C	P	13.08
1	L5	990:C	O3'	1064:G	P	12.18
1	L5	1222:A	O3'	1234:G	P	11.37
1	S2	225:G	O3'	287:U	P	7.10

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L5	1100:U	O3'	1167:C	P	6.86

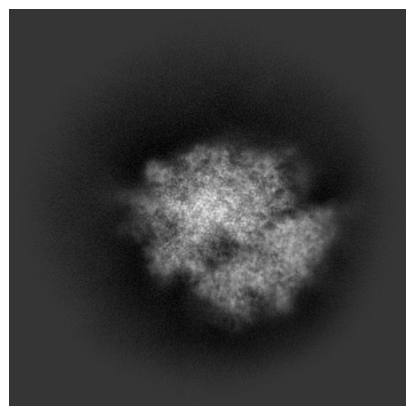
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71690. These allow visual inspection of the internal detail of the map and identification of artifacts.

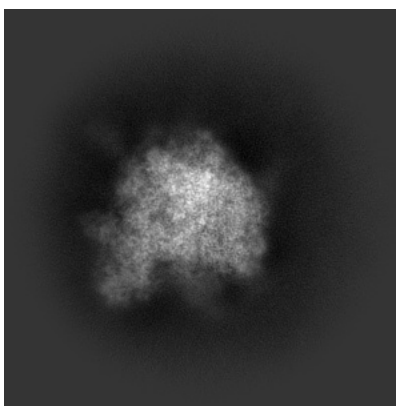
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

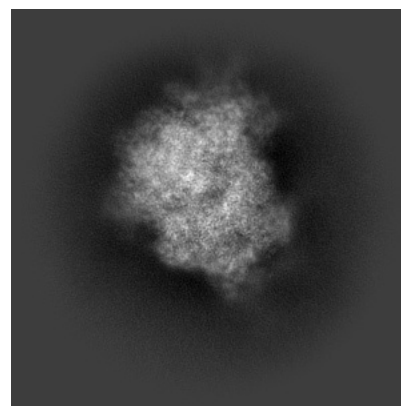
6.1.1 Primary map



X

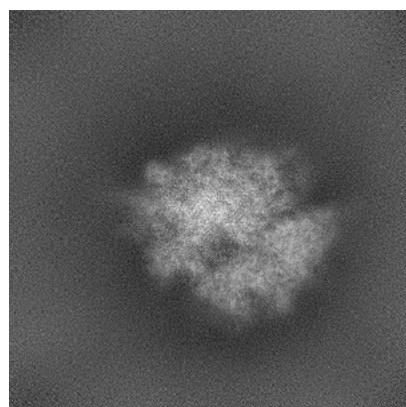


Y

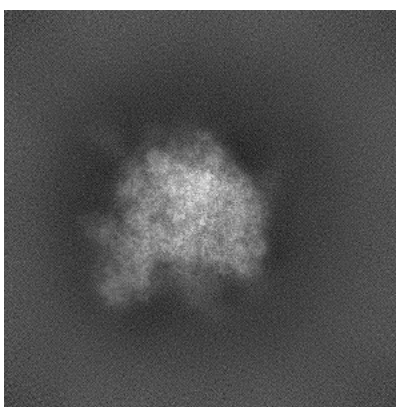


Z

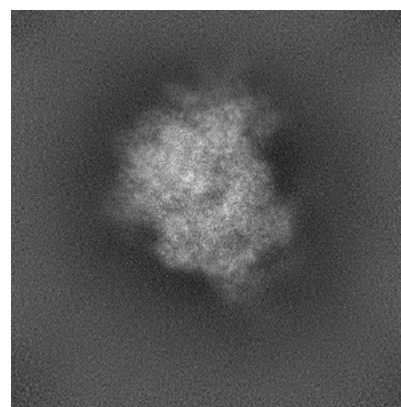
6.1.2 Raw map



X



Y

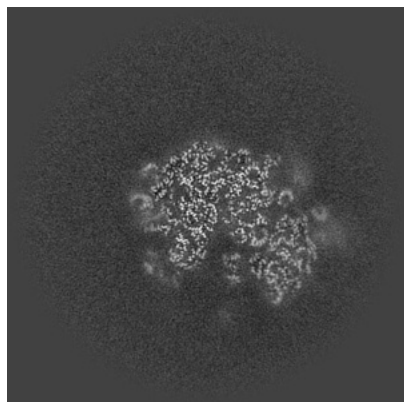


Z

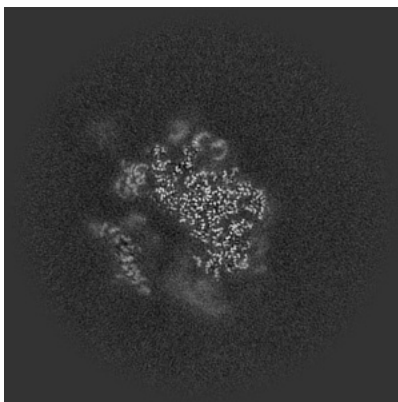
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

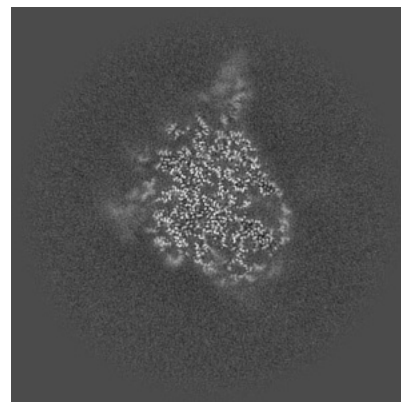
6.2.1 Primary map



X Index: 256

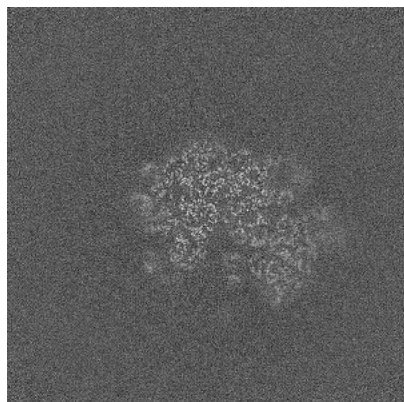


Y Index: 256

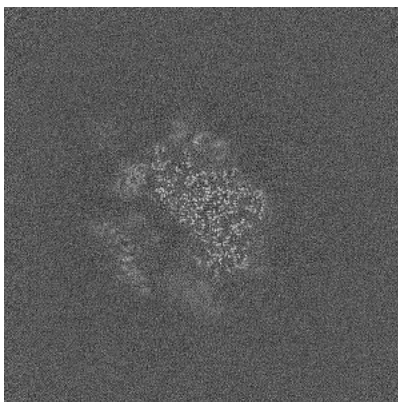


Z Index: 256

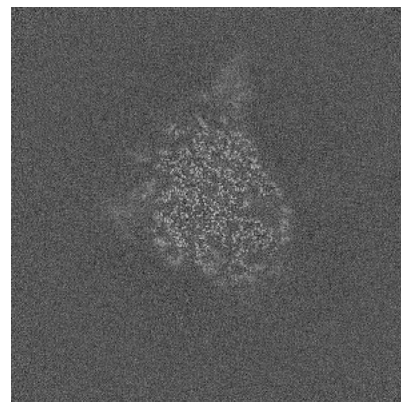
6.2.2 Raw map



X Index: 256



Y Index: 256

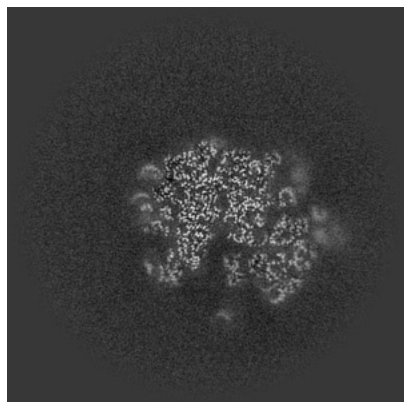


Z Index: 256

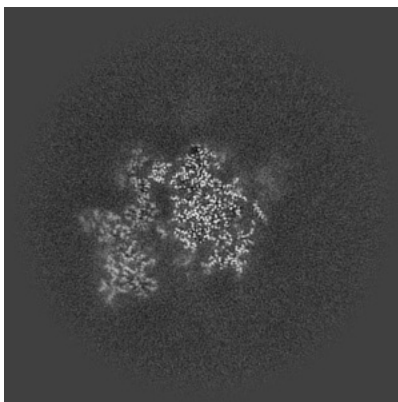
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

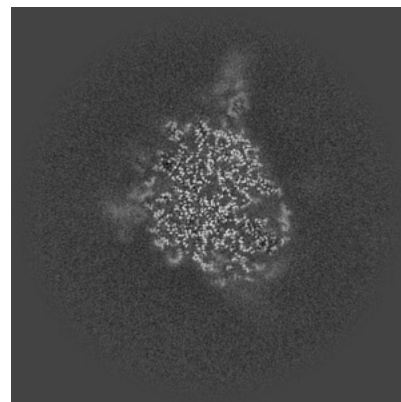
6.3.1 Primary map



X Index: 253

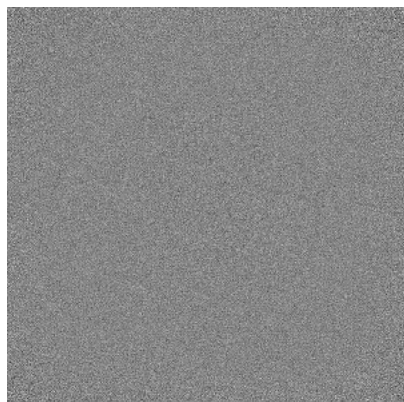


Y Index: 288

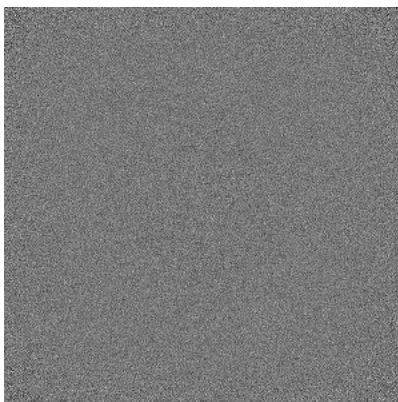


Z Index: 258

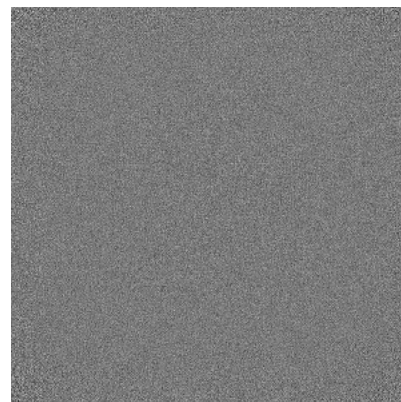
6.3.2 Raw map



X Index: 0



Y Index: 0

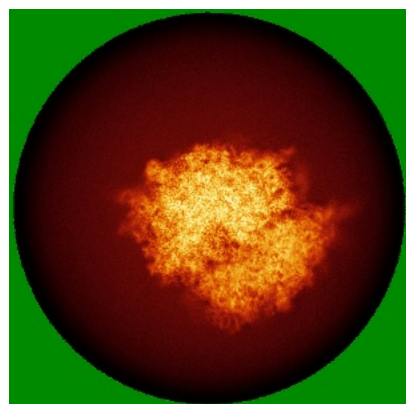


Z Index: 0

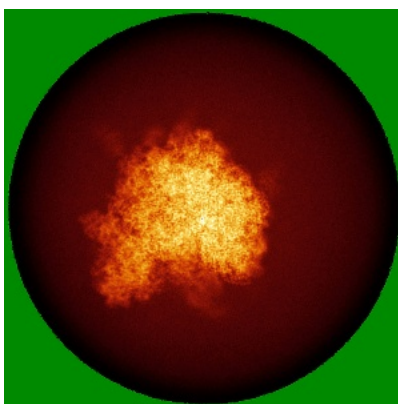
The images above show the largest variance slices of the map in three orthogonal directions.

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

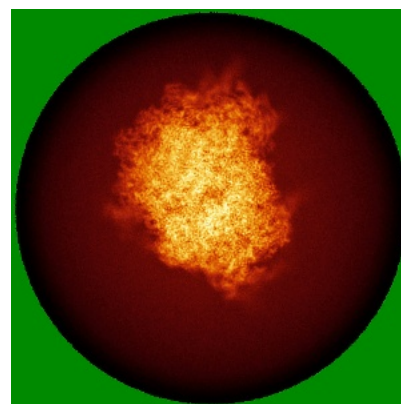
6.4.1 Primary map



X

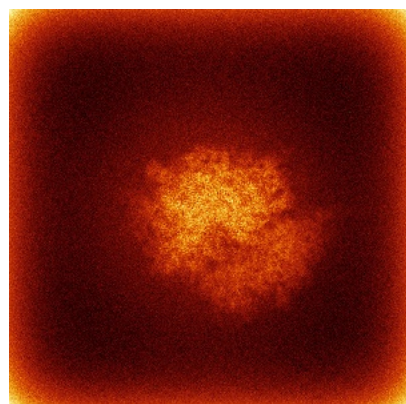


Y

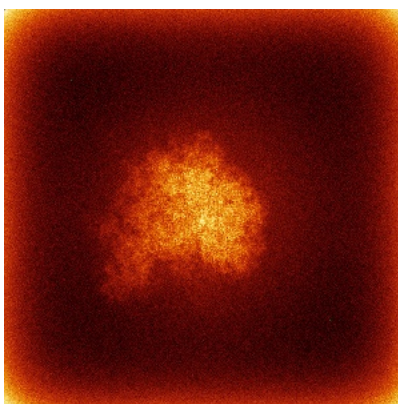


Z

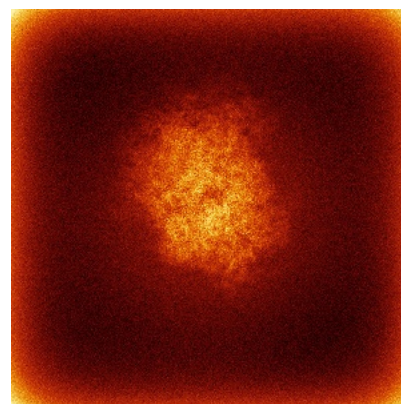
6.4.2 Raw map



X



Y

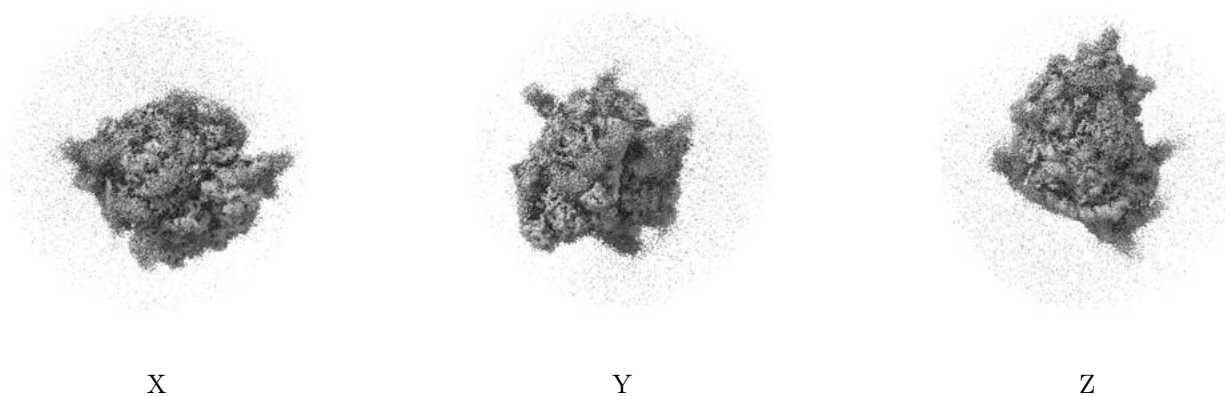


Z

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

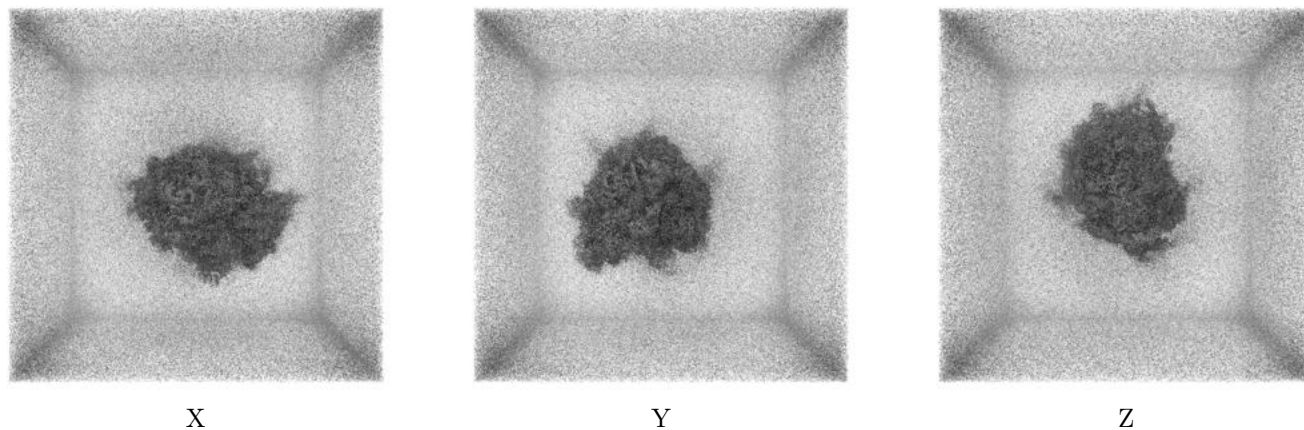
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0746. 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.

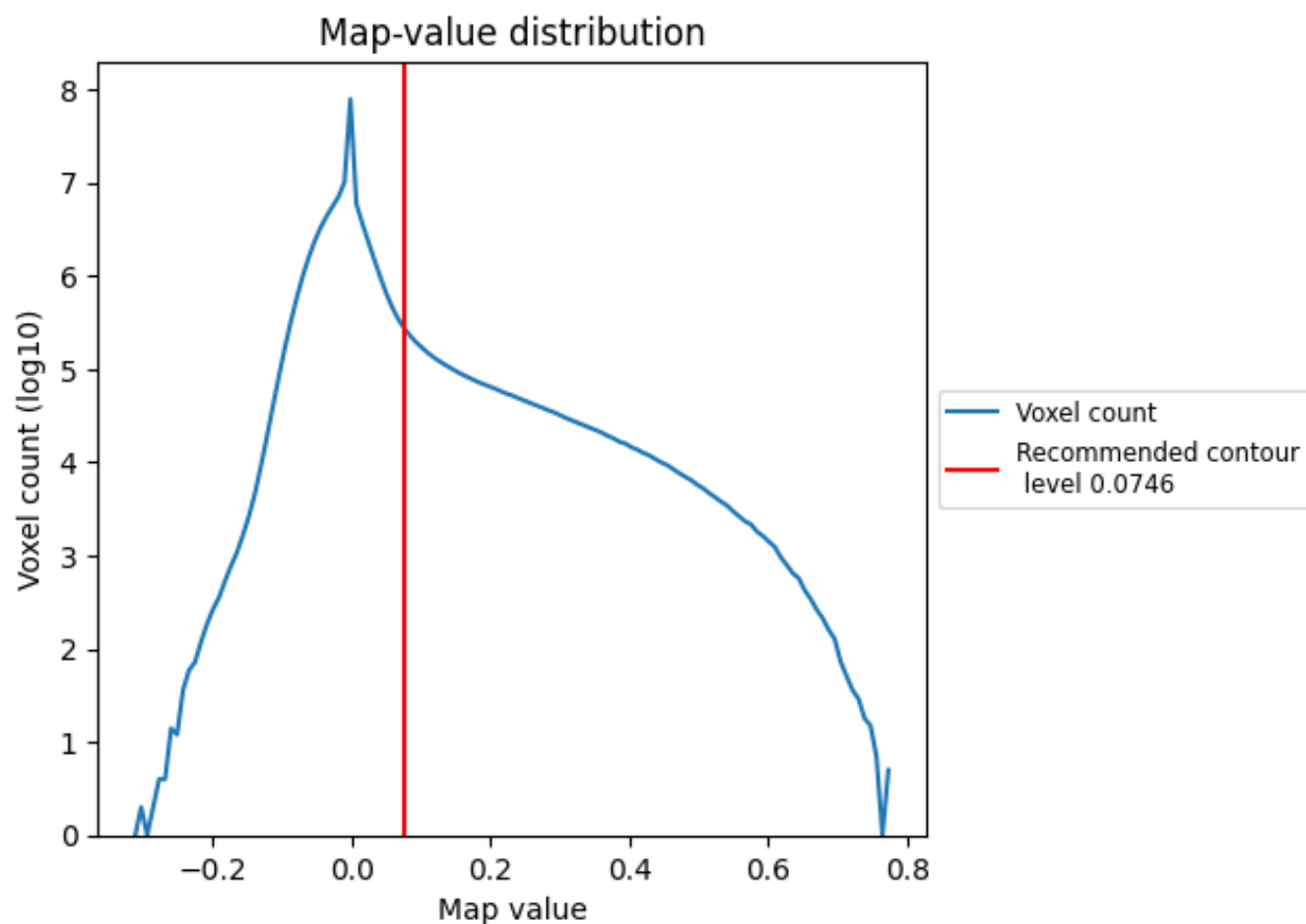
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

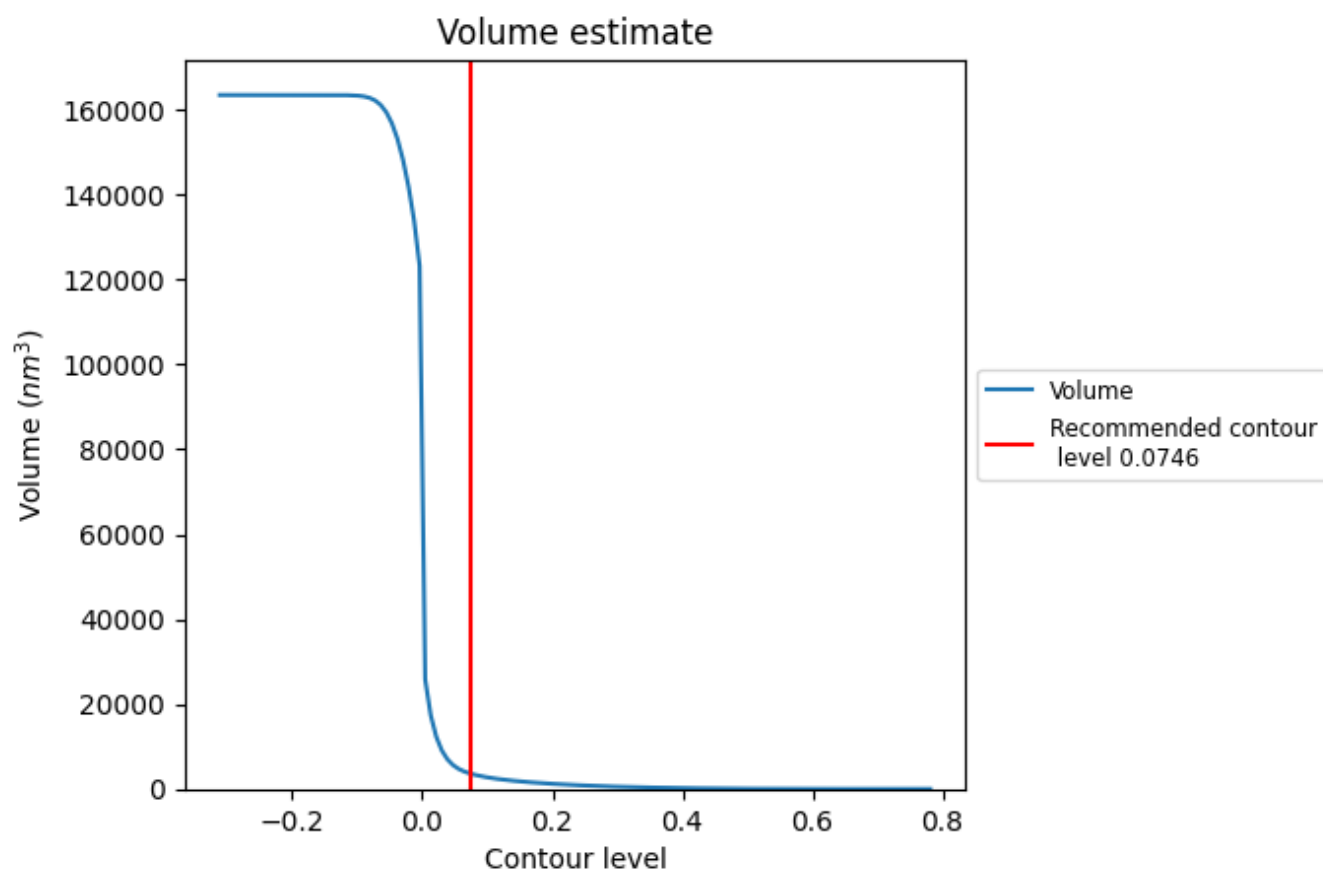
This section contains the results of statistical analysis of the map.

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.

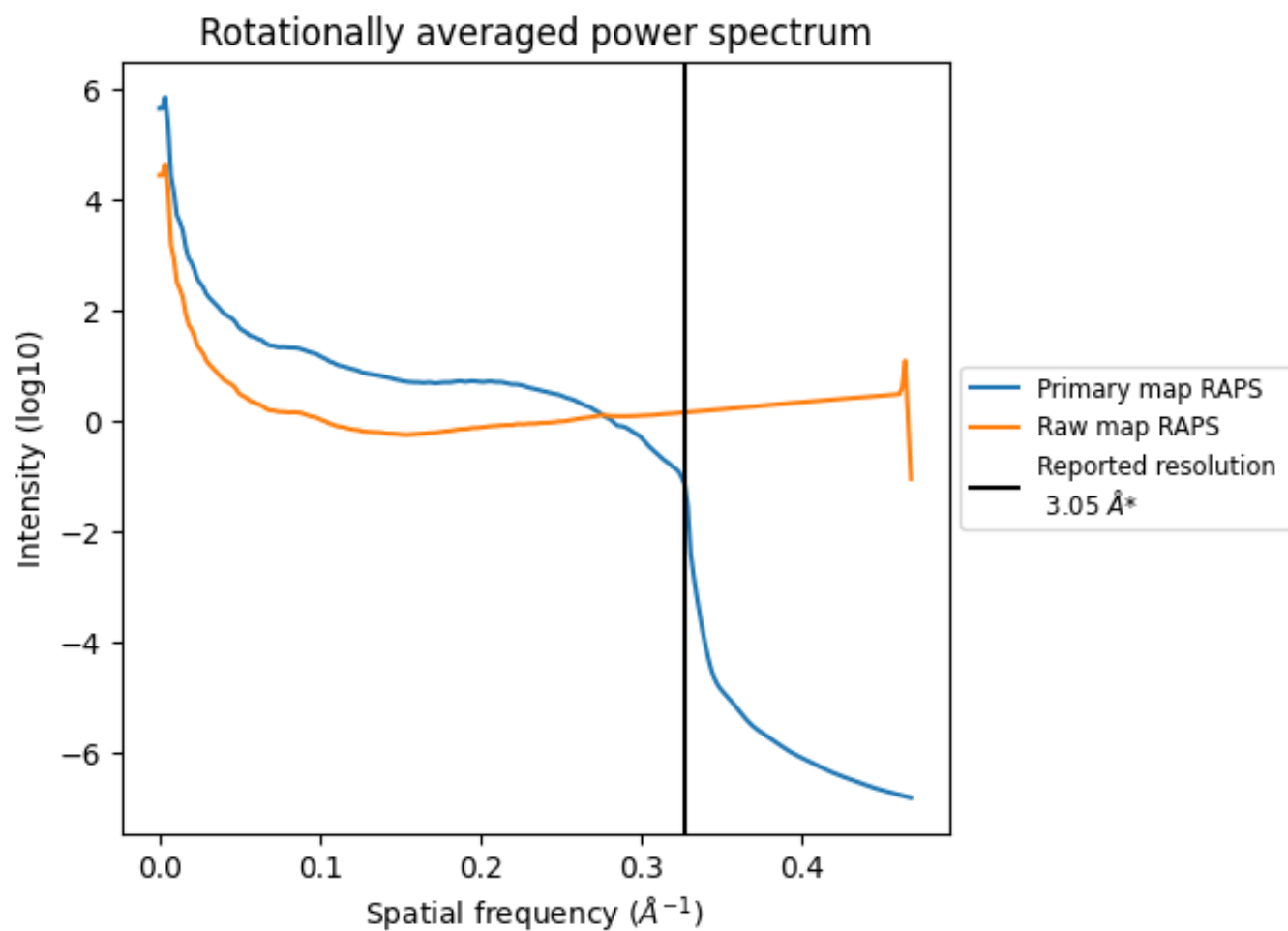
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3593 nm³; this corresponds to an approximate mass of 3246 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 ⓘ

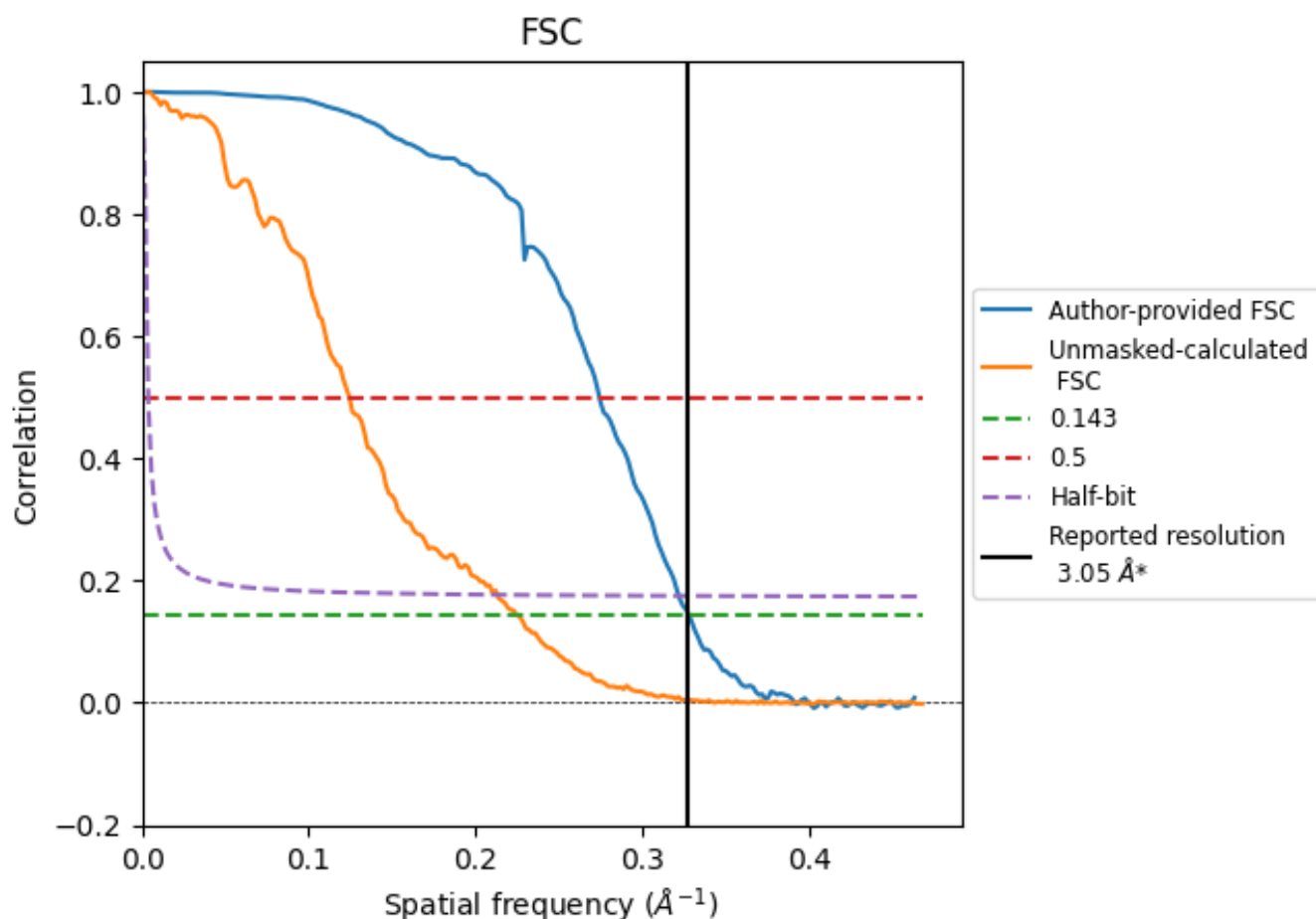


*Reported resolution corresponds to spatial frequency of 0.328 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.328 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

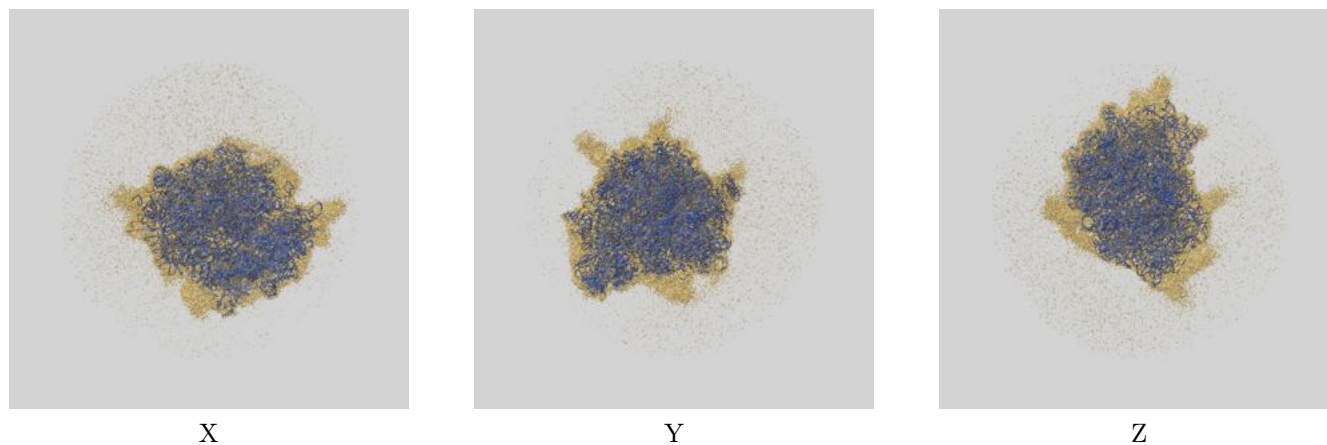
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	3.05	3.64	3.10
Unmasked-calculated*	4.44	8.05	4.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.44 differs from the reported value 3.05 by more than 10 %

9 Map-model fit [i](#)

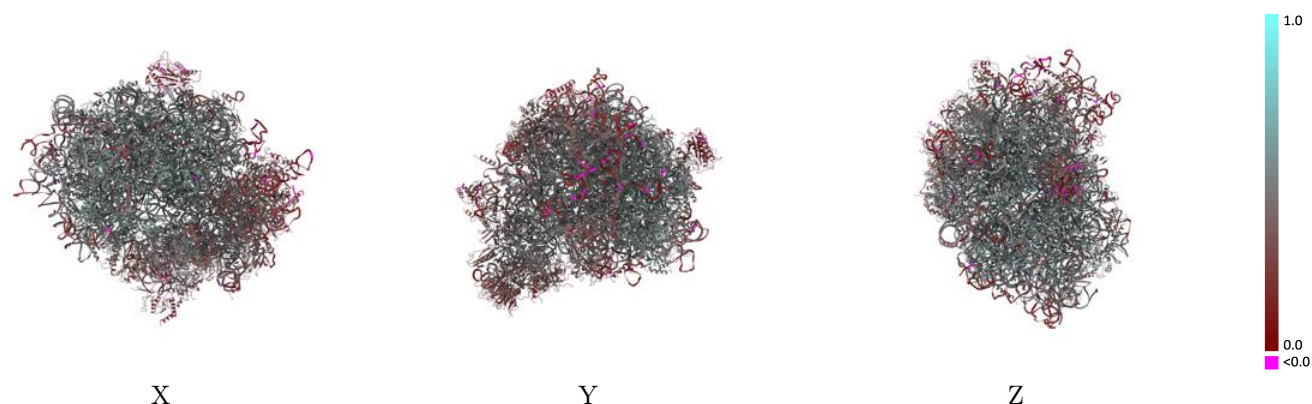
This section contains information regarding the fit between EMDB map EMD-71690 and PDB model 9PKB. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)



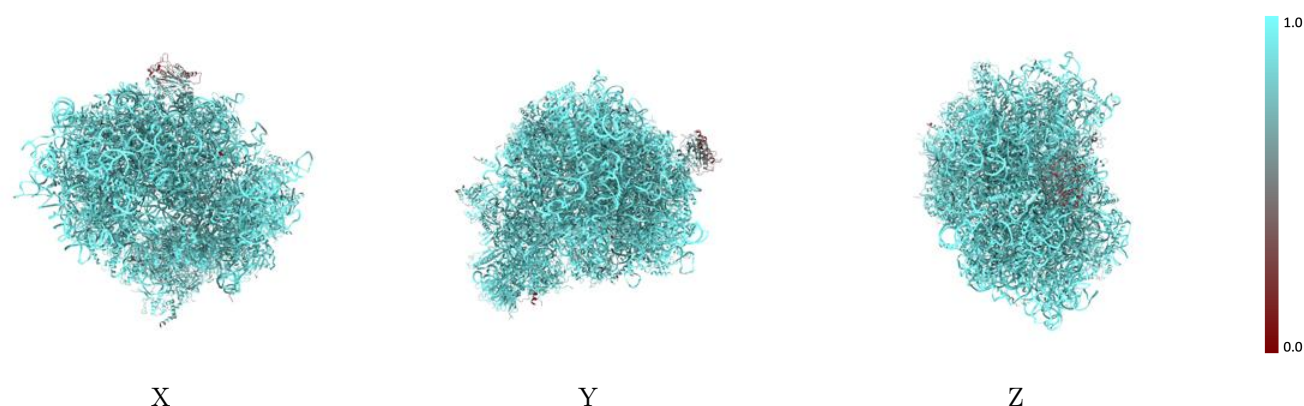
The images above show the 3D surface view of the map at the recommended contour level 0.0746 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



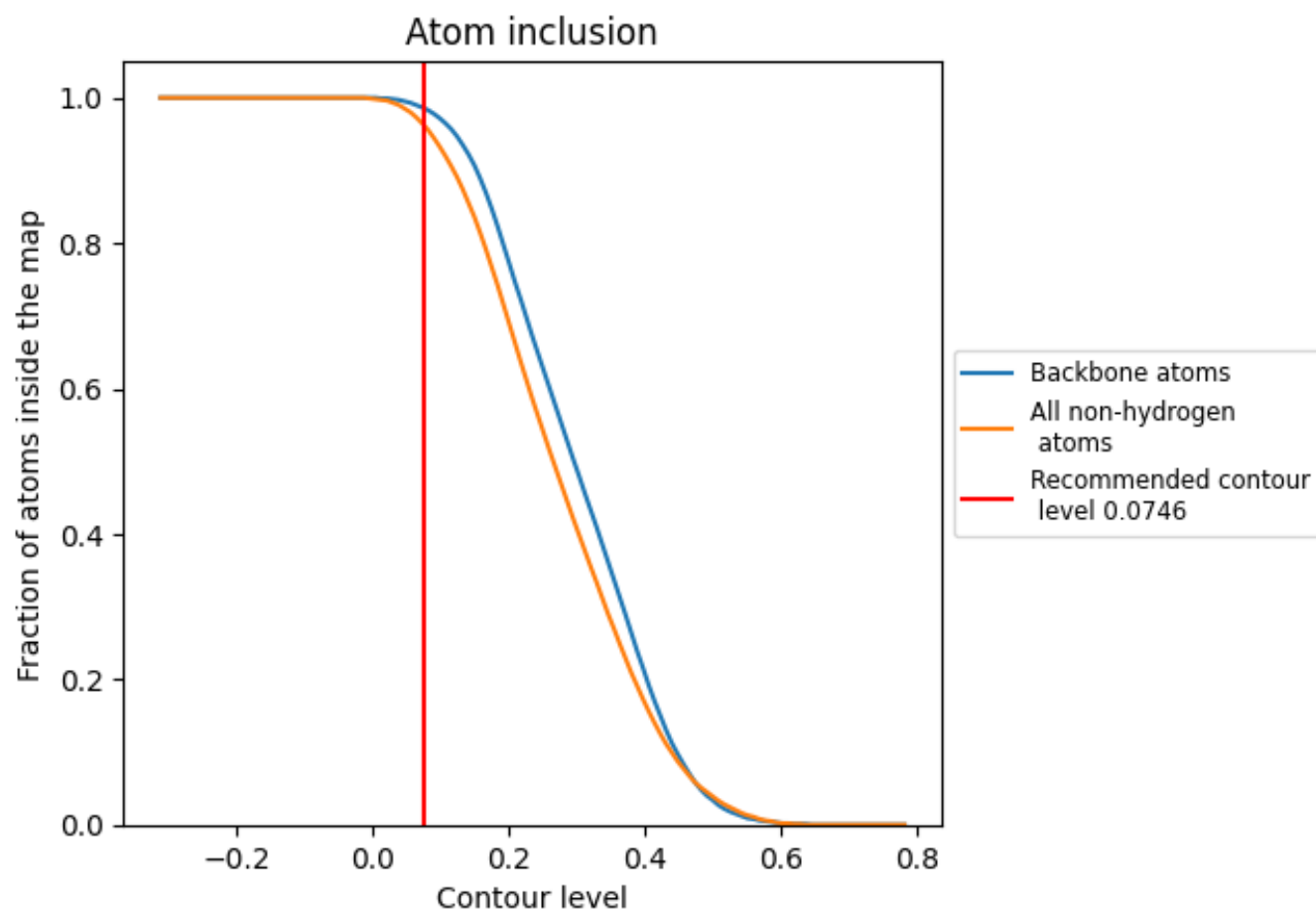
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0746).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% 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 (0.0746) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9630	 0.4510
CA	 0.5340	 0.2320
CB	 0.9040	 0.4200
CD	 0.9460	 0.4210
CI	 0.7950	 0.3940
L5	 0.9890	 0.4690
L7	 0.9990	 0.5010
L8	 0.9930	 0.4840
LA	 0.9840	 0.5430
LB	 0.9640	 0.5250
LC	 0.9700	 0.5300
LD	 0.9590	 0.4840
LE	 0.9520	 0.4770
LF	 0.9760	 0.5210
LG	 0.9480	 0.4790
LH	 0.9610	 0.5170
LI	 0.9680	 0.5270
LJ	 0.9520	 0.4680
LL	 0.9440	 0.5000
LM	 0.9770	 0.5140
LN	 0.9880	 0.5520
LO	 0.9740	 0.5250
LP	 0.9790	 0.5400
LQ	 0.9810	 0.5450
LR	 0.9530	 0.4790
LS	 0.9830	 0.5440
LT	 0.9620	 0.5180
LU	 0.9390	 0.4510
LV	 0.9750	 0.5340
LW	 0.9090	 0.3760
LX	 0.9710	 0.5110
LY	 0.9650	 0.5040
LZ	 0.9750	 0.5030
La	 0.9850	 0.5470
Lb	 0.9300	 0.4670



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Chain	Atom inclusion	Q-score
Lc	 0.9450	 0.4840
Ld	 0.9720	 0.5210
Le	 0.9830	 0.5430
Lf	 0.9830	 0.5470
Lg	 0.9740	 0.5230
Lh	 0.9670	 0.5090
Li	 0.9670	 0.4990
Lj	 0.9910	 0.5450
Lk	 0.9190	 0.4600
Ll	 0.9840	 0.5280
Lm	 0.9710	 0.5330
Ln	 0.9810	 0.5090
Lo	 0.9530	 0.5270
Lp	 0.9620	 0.5150
Lr	 0.9820	 0.5310
Ls	 0.9060	 0.3810
Lt	 0.7830	 0.2250
S2	 0.9930	 0.4130
SA	 0.9080	 0.4140
SB	 0.8940	 0.3620
SC	 0.9580	 0.4710
SD	 0.9260	 0.4110
SE	 0.9480	 0.4140
SF	 0.9190	 0.3640
SG	 0.9110	 0.3090
SH	 0.8930	 0.3480
SI	 0.9270	 0.3800
SJ	 0.9340	 0.4280
SK	 0.9290	 0.3900
SL	 0.9230	 0.4280
SM	 0.8180	 0.2440
SN	 0.9560	 0.4420
SO	 0.9390	 0.3860
SP	 0.9310	 0.4120
SQ	 0.9310	 0.3900
SR	 0.9060	 0.3790
SS	 0.9010	 0.3810
ST	 0.9450	 0.3810
SU	 0.9200	 0.3830
SV	 0.9450	 0.4400
SW	 0.9690	 0.4830
SX	 0.9520	 0.4920

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Chain	Atom inclusion	Q-score
SY	 0.8880	 0.3410
SZ	 0.8850	 0.3190
Sa	 0.9520	 0.4480
Sb	 0.9330	 0.3990
Sc	 0.8910	 0.3580
Sd	 0.9500	 0.4460
Se	 0.9010	 0.3920
Sf	 0.9020	 0.2860
Sg	 0.9120	 0.3190