



Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 08:26 PM EDT

PDB ID : 9P7L / pdb_00009p7l
EMDB ID : EMD-71346
Title : In situ human Post-eEF1A-AT-P state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 2.92 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

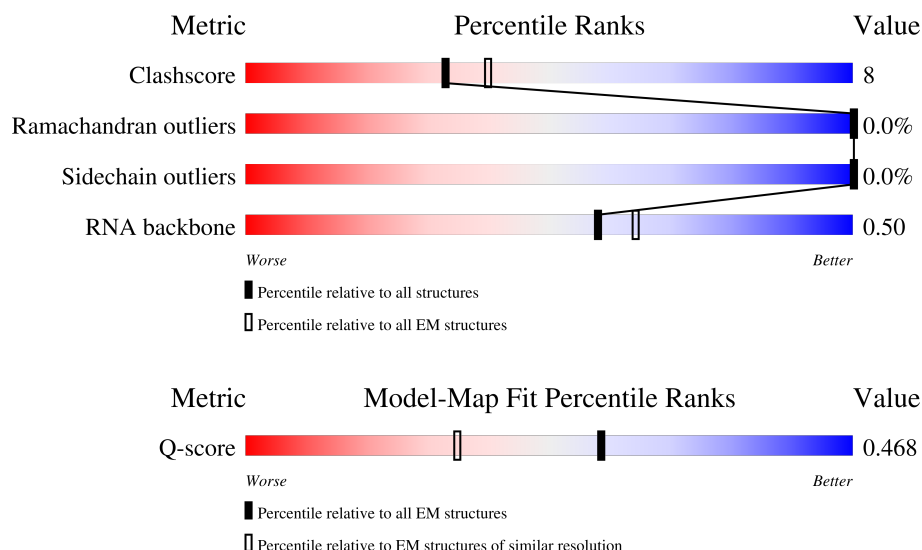
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.92 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	13007 (2.42 - 3.42)

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	CI	31	6% 77% 23%
2	Pt	74	59% 36% .
3	L5	3655	55% 37% 8%

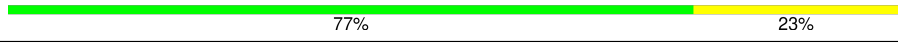
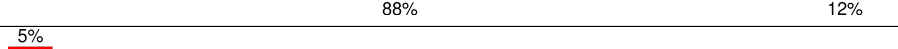
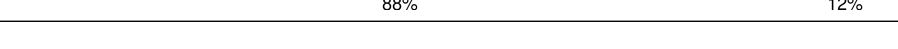
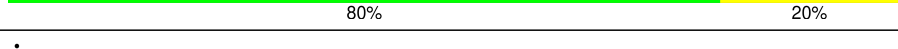
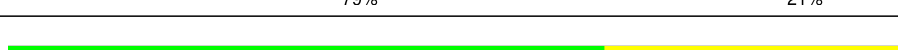
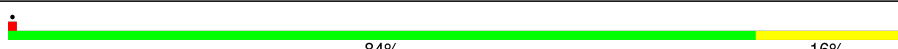
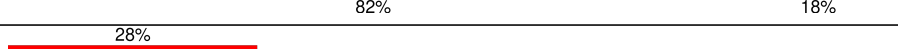
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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	156	
6	LA	248	
7	LB	402	
8	LC	368	
9	LD	293	
10	LE	250	
11	LF	225	
12	LG	241	
13	LH	190	
14	LI	213	
15	LJ	176	
16	LL	210	
17	LM	139	
18	LN	203	
19	LO	201	
20	LP	153	
21	LQ	187	
22	LR	187	
23	LS	175	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

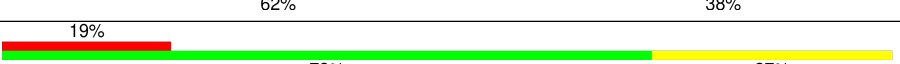
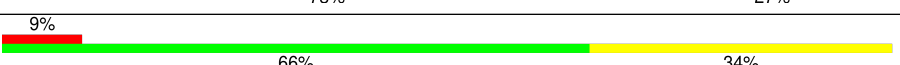
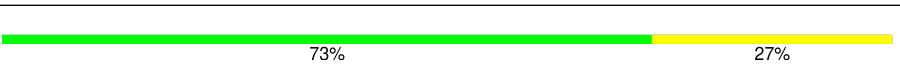
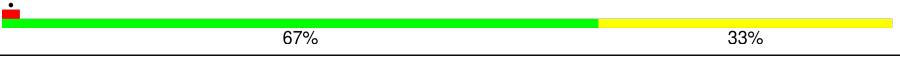
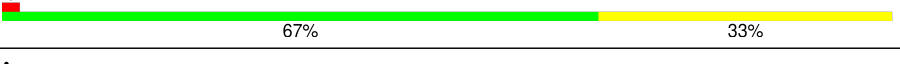
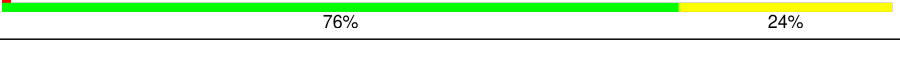
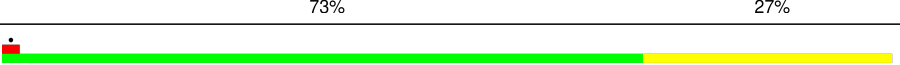
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Mol	Chain	Length	Quality of chain
29	LY	134	
30	LZ	135	
31	La	147	
32	Lb	121	
33	Lc	98	
34	Ld	107	
35	Le	128	
36	Lf	109	
37	Lg	114	
38	Lh	122	
39	Li	102	
40	Lj	86	
41	Lk	69	
42	Ll	50	
43	Lm	52	
44	Ln	24	
45	Lo	105	
46	Lp	91	
47	Lr	125	
48	Ls	196	
49	Lt	157	
50	SD	227	
51	SF	189	
52	SK	98	
53	SM	122	

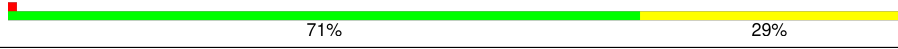
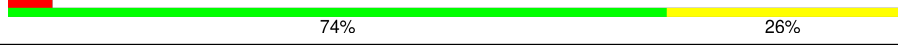
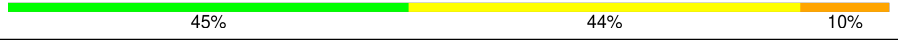
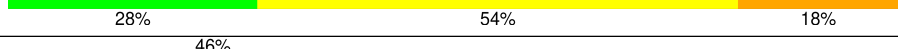
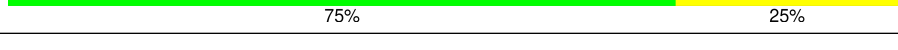
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Mol	Chain	Length	Quality of chain
54	SP	121	
55	SQ	144	
56	SR	135	
57	SS	145	
58	ST	143	
59	SU	104	
60	SZ	75	
61	Sc	64	
62	Sd	55	
63	Sf	67	
64	Sg	313	
65	SA	221	
66	SB	214	
67	SC	222	
68	SE	262	
69	SG	237	
70	SH	189	
71	SI	206	
72	SJ	185	
73	SL	153	
74	SN	150	
75	SO	140	
76	SV	83	
77	SW	129	
78	SX	141	

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Mol	Chain	Length	Quality of chain
79	SY	131	 72%28%
80	Sa	102	 72%28%
81	Sb	83	 71%29%
82	Se	58	 5%74%26%
83	S2	1740	 45%44%10%
84	AT	76	 28%54%18%
85	CF	441	 46%75%25%

2 Entry composition [i](#)

There are 89 unique types of molecules in this entry. The entry contains 223377 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 Transcription factor BTF3.

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

- Molecule 2 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Pt	74	Total	C	N	O	P	0	0
			1576	705	286	512	73		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Pt	3	C	U	conflict	GB X64278
Pt	?	-	U	deletion	GB X64278
Pt	?	-	G	deletion	GB X64278
Pt	19	G	U	conflict	GB X64278
Pt	50	U	-	insertion	GB X64278
Pt	74	C	-	insertion	GB X64278

- 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	213	Total	C	N	O	S	0	0
			1711	1082	329	285	15		

- 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 Small ribosomal subunit protein uS3.

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

- Molecule 51 is a protein called 40S ribosomal protein S5.

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

- Molecule 52 is a protein called 40S ribosomal protein S10.

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

- Molecule 53 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 54 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 55 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 56 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 57 is a protein called 40S ribosomal protein S18.

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

- Molecule 58 is a protein called 40S ribosomal protein S19.

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

- Molecule 59 is a protein called 40S ribosomal protein S20.

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

- Molecule 60 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 61 is a protein called 40S ribosomal protein S28.

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

- Molecule 62 is a protein called 40S ribosomal protein S29.

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

- Molecule 63 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 64 is a protein called Receptor of activated protein C kinase 1.

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

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

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

- Molecule 66 is a protein called 40S ribosomal protein S3a.

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

- Molecule 67 is a protein called 40S ribosomal protein S2.

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

- Molecule 68 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 69 is a protein called 40S ribosomal protein S6.

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

- Molecule 70 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 71 is a protein called 40S ribosomal protein S8.

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

- Molecule 72 is a protein called 40S ribosomal protein S9.

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

- Molecule 73 is a protein called 40S ribosomal protein S11.

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

- Molecule 74 is a protein called 40S ribosomal protein S13.

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

- Molecule 75 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 76 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 77 is a protein called 40S ribosomal protein S15a.

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

- Molecule 78 is a protein called 40S ribosomal protein S23.

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

- Molecule 79 is a protein called 40S ribosomal protein S24.

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

- Molecule 80 is a protein called 40S ribosomal protein S26.

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

- Molecule 81 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 82 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 83 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	S2	1740	Total	C	N	O	P	0	0
			36953	16508	6600	12106	1739		

- Molecule 84 is a RNA chain called A/T site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	AT	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 85 is a protein called Elongation factor 1-alpha 1.

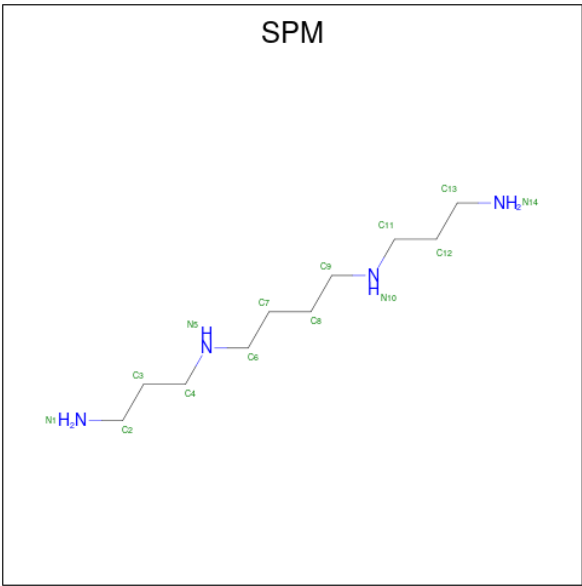
Mol	Chain	Residues	Atoms					AltConf	Trace	
85	CF	441	Total	C	N	O	P	S	0	0
			3383	2148	581	636	1	17		

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

Mol	Chain	Residues	Atoms		AltConf
86	L5	180	Total	Mg	0
			180	180	
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	
86	Le	1	Total	Mg	0
			1	1	
86	S2	28	Total	Mg	0
			28	28	

- Molecule 87 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by depositor).

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	

- Molecule 88 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃) (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	LN	1	Total	C	N	0
			10	7	3	

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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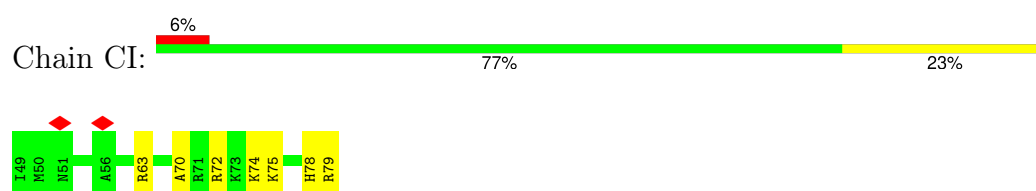
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Mol	Chain	Residues	Atoms		AltConf
89	Lj	1	Total 1	Zn 1	0
89	Lm	1	Total 1	Zn 1	0
89	Lo	1	Total 1	Zn 1	0
89	Lp	1	Total 1	Zn 1	0
89	Sa	1	Total 1	Zn 1	0

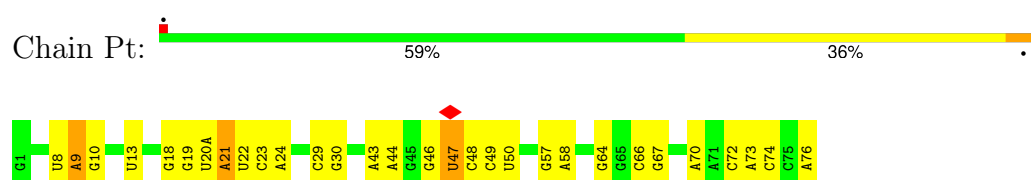
3 Residue-property plots

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.

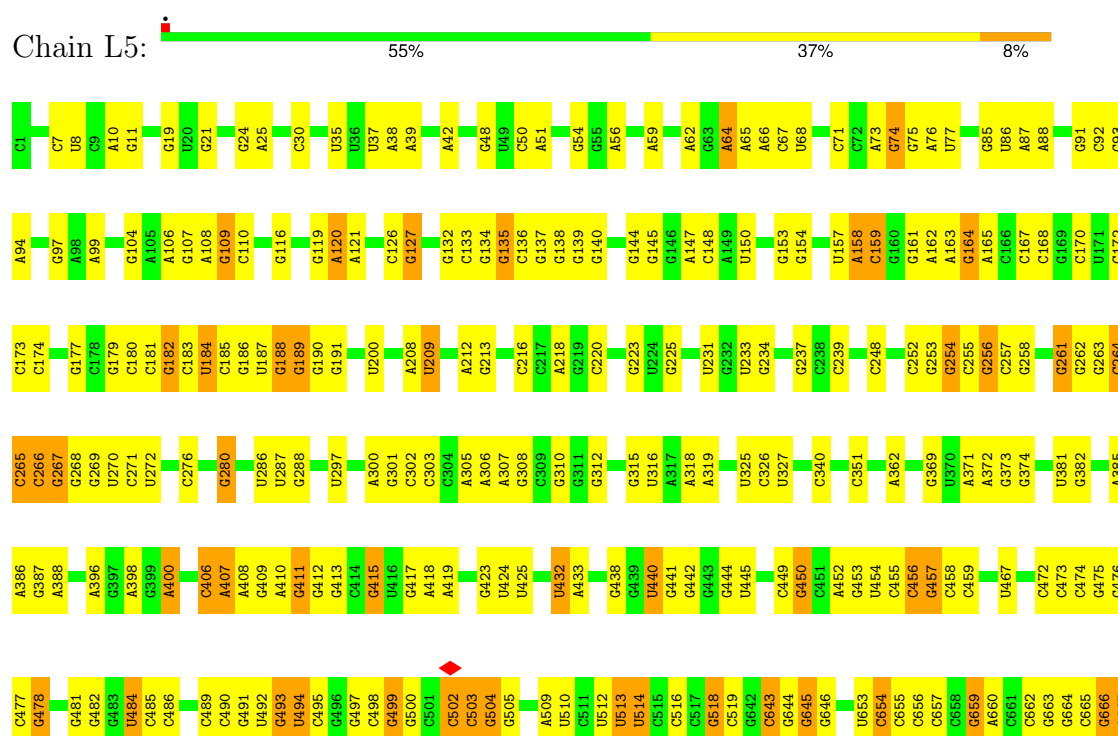
• Molecule 1: Transcription factor BTF3



• Molecule 2: P site tRNA

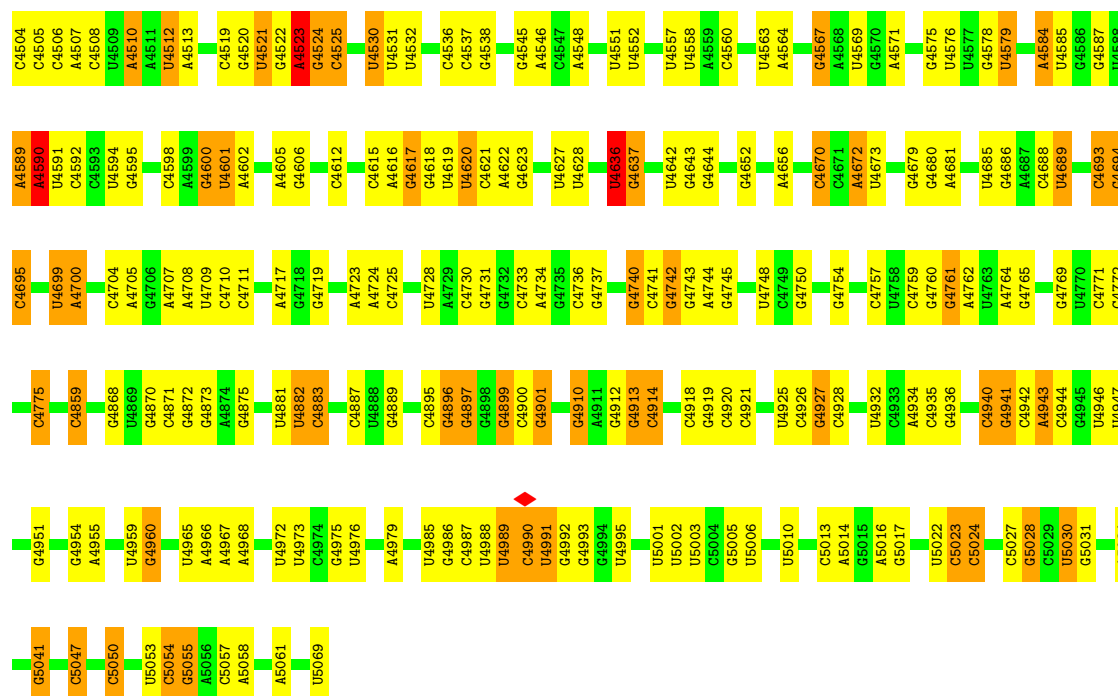


• Molecule 3: 28S rRNA



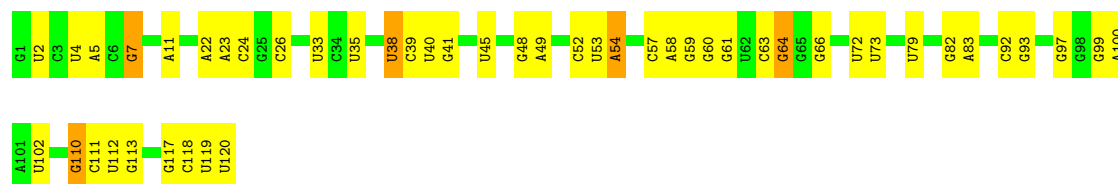






• Molecule 4: 5S rRNA

Chain L7: 60% 36%



• Molecule 5: 5.8S rRNA

Chain L8: 63% 31% 5%



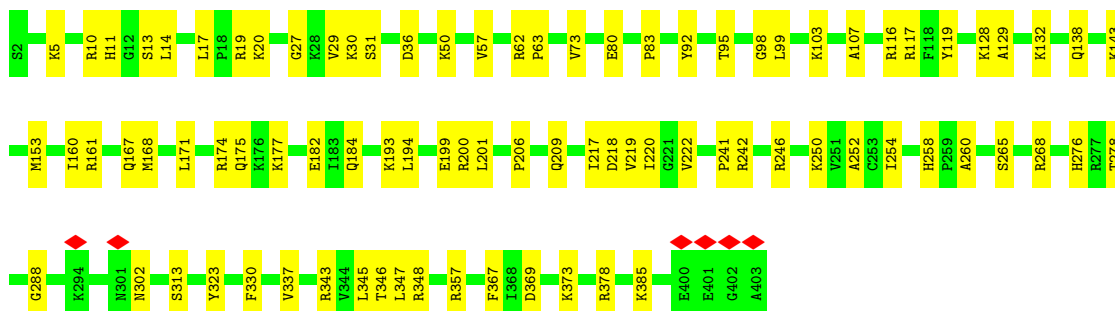
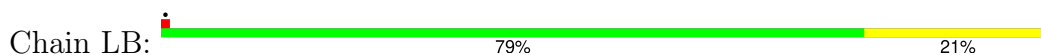
• Molecule 6: 60S ribosomal protein L8

Chain LA: 75% 25%

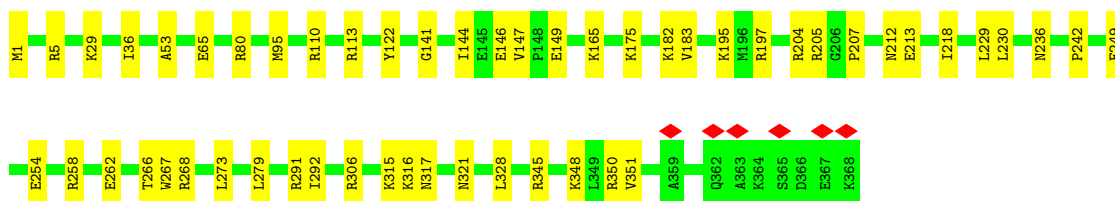




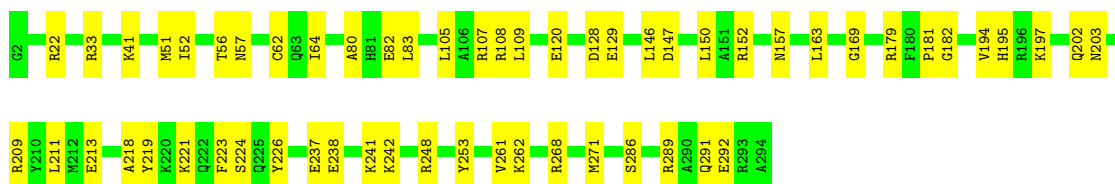
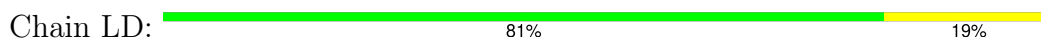
• Molecule 7: Large ribosomal subunit protein uL3



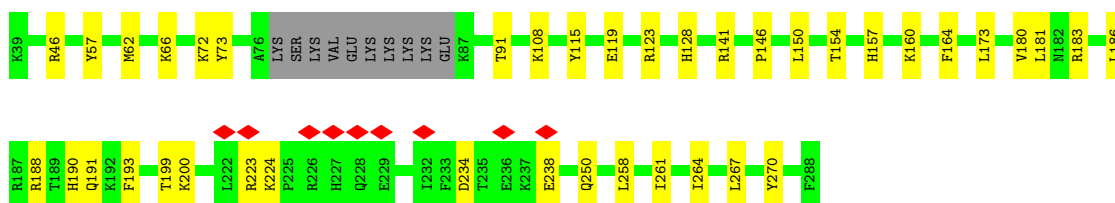
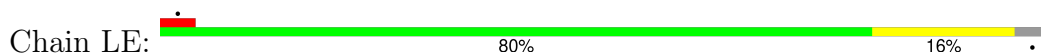
• Molecule 8: 60S ribosomal protein L4



• Molecule 9: Large ribosomal subunit protein uL18

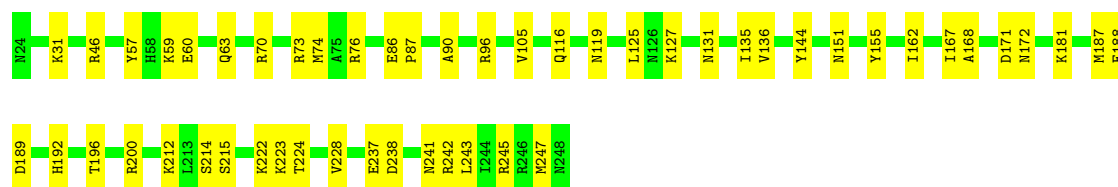


• Molecule 10: Large ribosomal subunit protein eL6



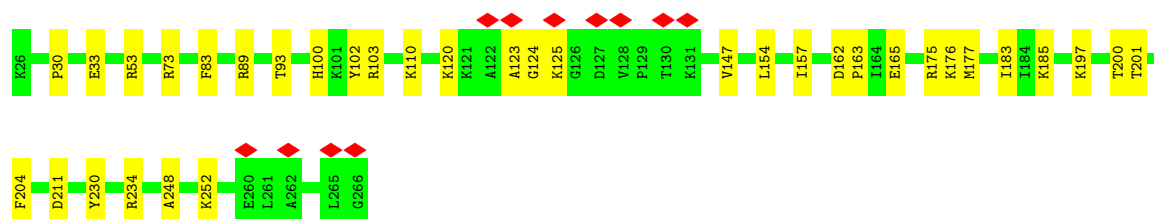
• Molecule 11: 60S ribosomal protein L7

Chain LF:  77% 23%



- Molecule 12: 60S ribosomal protein L7a

Chain LG:  5% 85% 15%



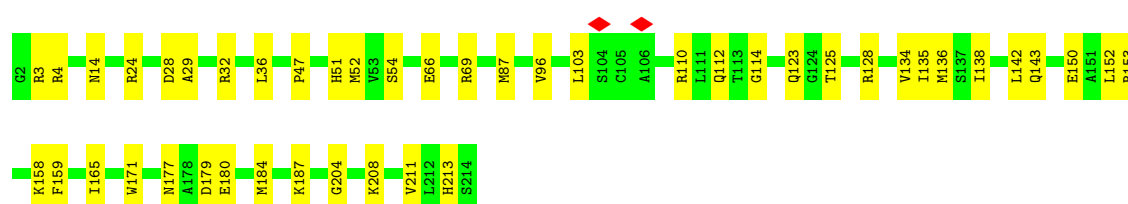
- Molecule 13: 60S ribosomal protein L9

Chain LH:  77% 23%



- Molecule 14: Ribosomal protein uL16-like

Chain LI:  79% 21%

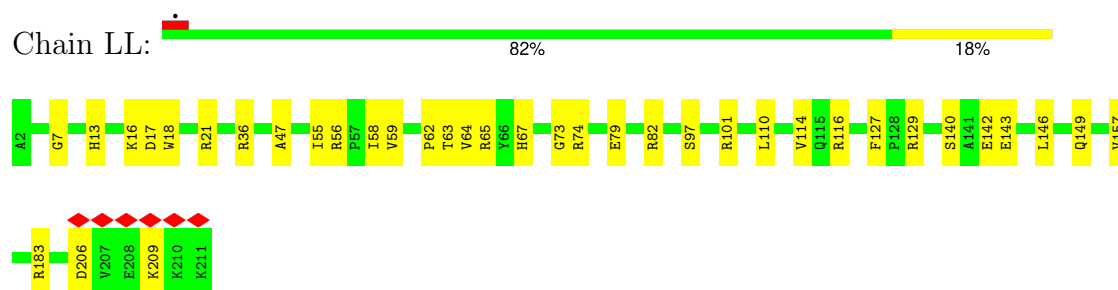


- Molecule 15: 60S ribosomal protein L11

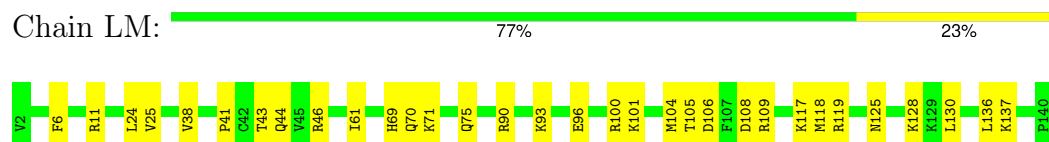
Chain LJ:  75% 22%



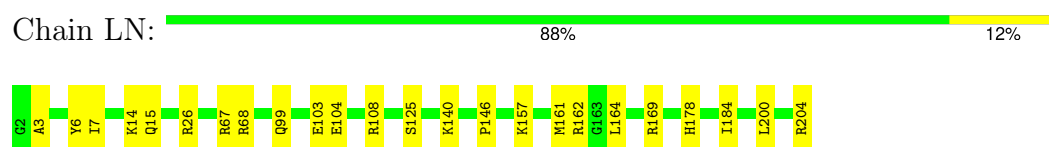
- Molecule 16: Large ribosomal subunit protein eL13



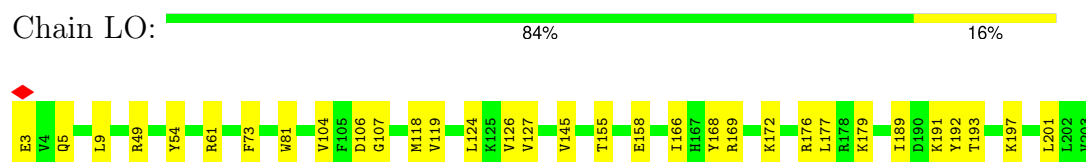
- Molecule 17: 60S ribosomal protein L14



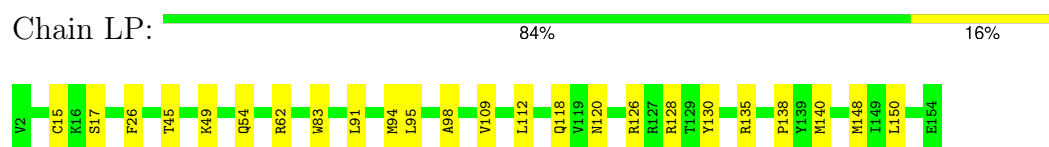
- Molecule 18: 60S ribosomal protein L15



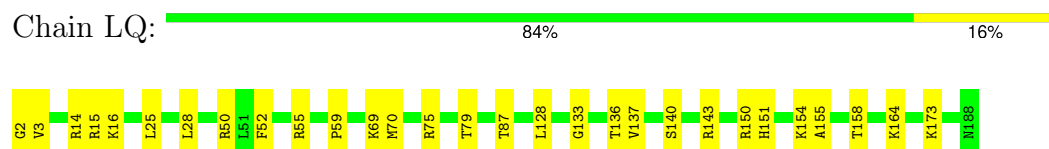
- Molecule 19: 60S ribosomal protein L13a



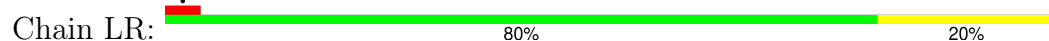
- Molecule 20: 60S ribosomal protein L17

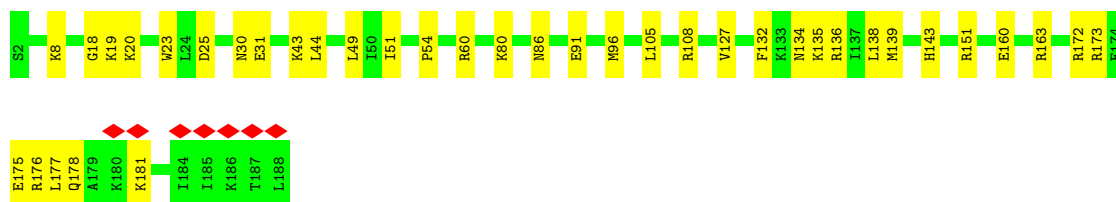


- Molecule 21: 60S ribosomal protein L18



- Molecule 22: 60S ribosomal protein L19





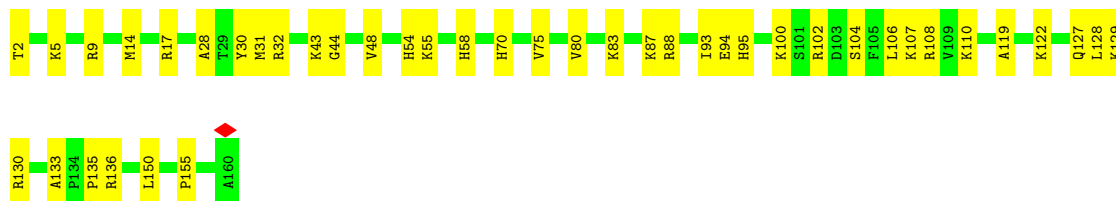
- Molecule 23: 60S ribosomal protein L18a

Chain LS: 83% 17%



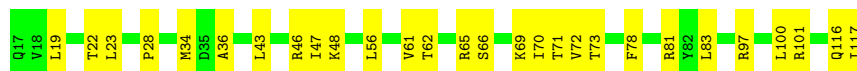
- Molecule 24: 60S ribosomal protein L21

Chain LT: 74% 26%



- Molecule 25: Heparin-binding protein HBp15

Chain LU: 72% 28%



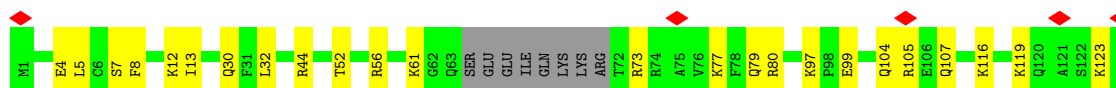
- Molecule 26: 60S ribosomal protein L23

Chain LV: 88% 12%



- Molecule 27: Ribosomal protein L24

Chain LW: 74% 19% 6%

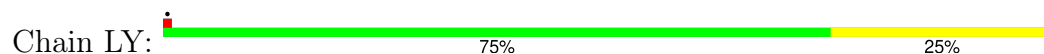


- Molecule 28: 60S ribosomal protein L23a

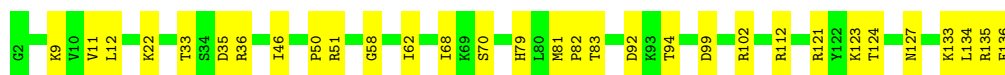
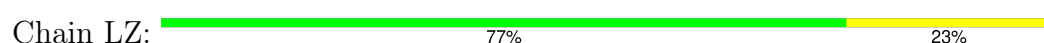
Chain LX: 92% 8%



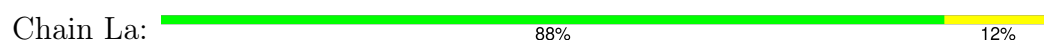
- Molecule 29: 60S ribosomal protein L26



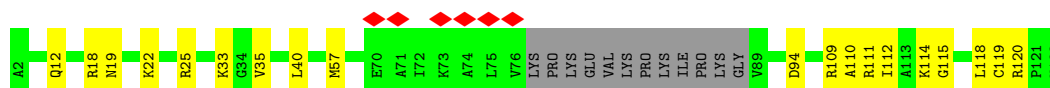
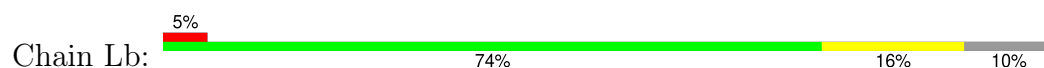
- Molecule 30: 60S ribosomal protein L27



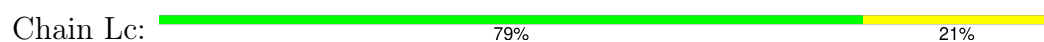
- Molecule 31: 60S ribosomal protein L27a



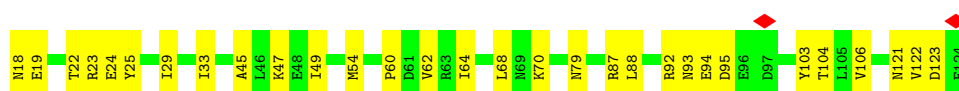
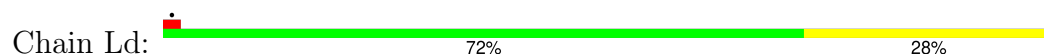
- Molecule 32: Large ribosomal subunit protein eL29



- Molecule 33: 60S ribosomal protein L30



- Molecule 34: 60S ribosomal protein L31



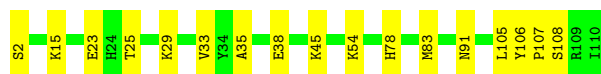
- Molecule 35: 60S ribosomal protein L32

Chain Le:  78% 22%



- Molecule 36: 60S ribosomal protein L35a

Chain Lf:  84% 16%



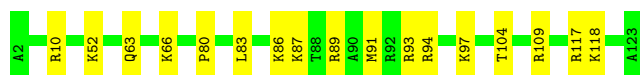
- Molecule 37: 60S ribosomal protein L34

Chain Lg:  88% 12%



- Molecule 38: 60S ribosomal protein L35

Chain Lh:  86% 14%



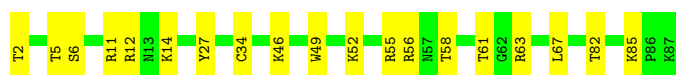
- Molecule 39: 60S ribosomal protein L36

Chain Li:  87% 13%



- Molecule 40: 60S ribosomal protein L37

Chain Lj:  78% 22%



- Molecule 41: 60S ribosomal protein L38

Chain Lk:  78% 22%



- Molecule 42: 60S ribosomal protein L39

Chain Ll:  80% 20%



- Molecule 43: Large ribosomal subunit protein eL40

Chain Lm:  79% 21%



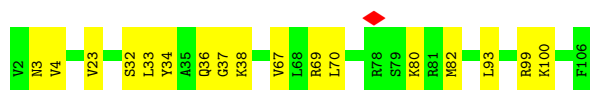
- Molecule 44: 60S ribosomal protein L41

Chain Ln:  67% 33%



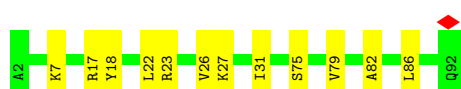
- Molecule 45: 60S ribosomal protein L36a

Chain Lo:  84% 16%



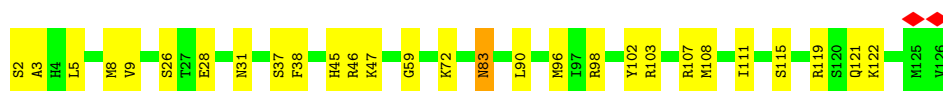
- Molecule 46: 60S ribosomal protein L37a

Chain Lp:  87% 13%



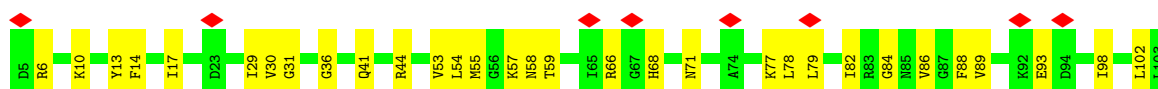
- Molecule 47: 60S ribosomal protein L28

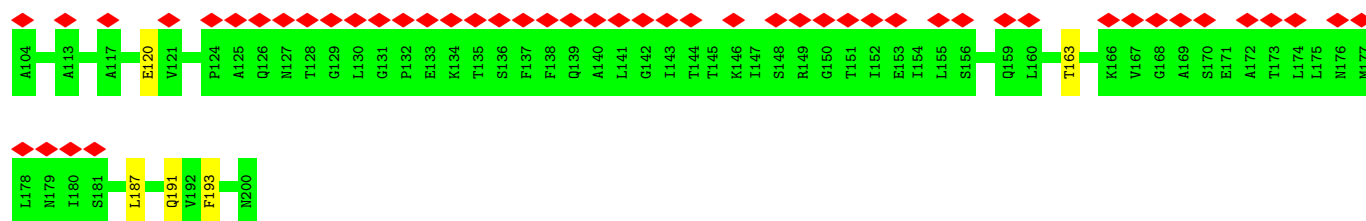
Chain Lr:  78% 22%



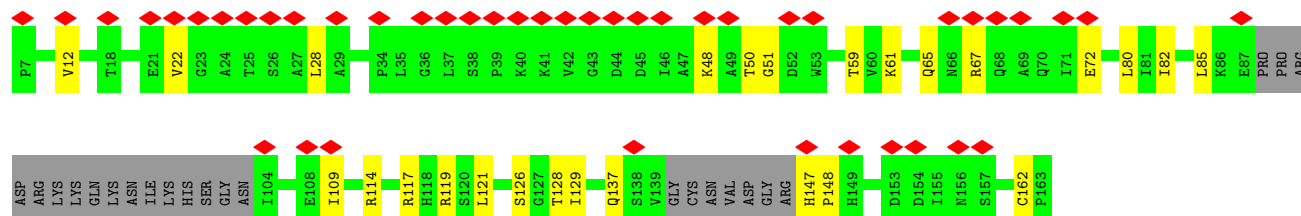
- Molecule 48: 60S acidic ribosomal protein P0

Chain Ls:  30% 82% 18%

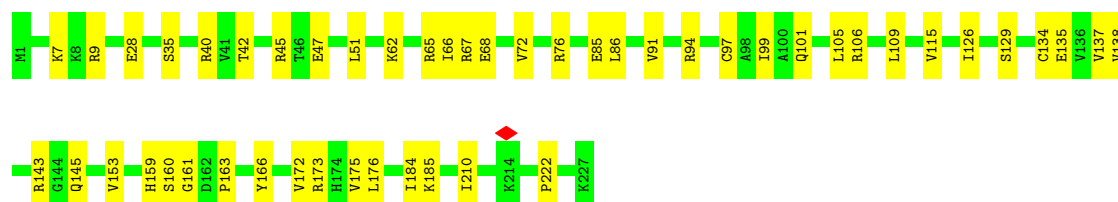
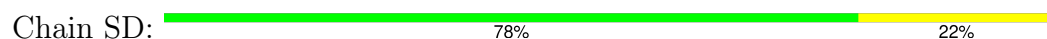




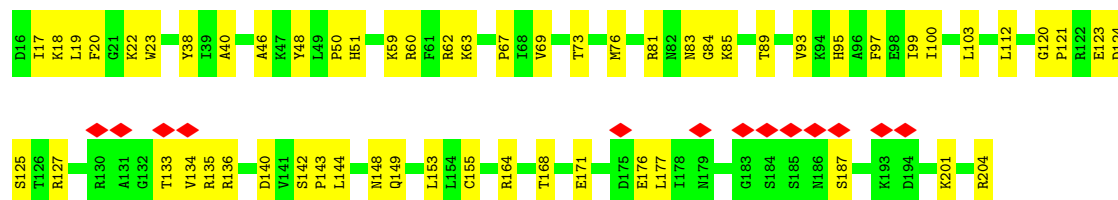
- Molecule 49: Large ribosomal subunit protein uL11



- Molecule 50: Small ribosomal subunit protein uS3



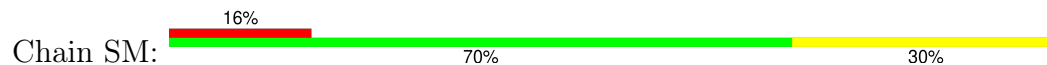
- Molecule 51: 40S ribosomal protein S5

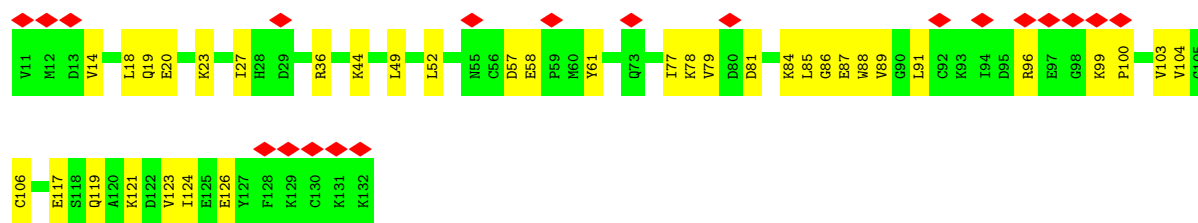


- Molecule 52: 40S ribosomal protein S10

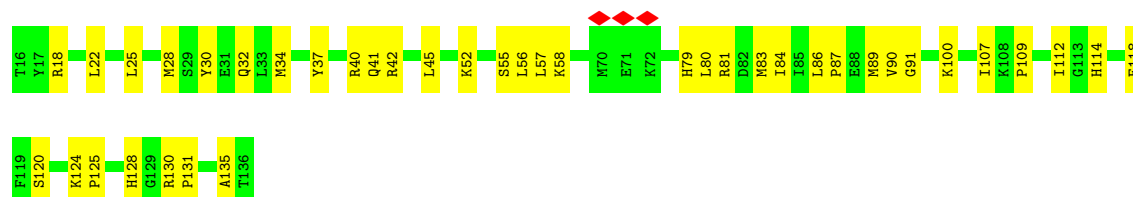


- Molecule 53: Small ribosomal subunit protein eS12

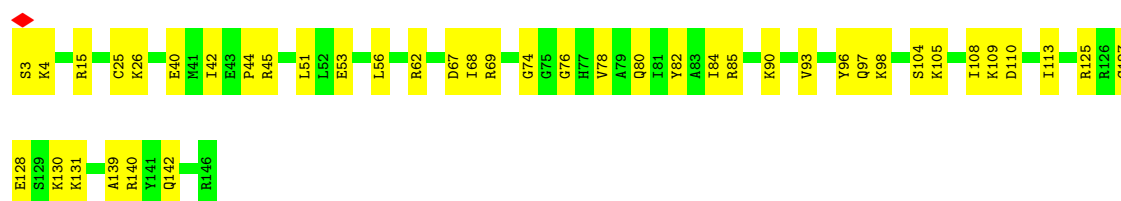




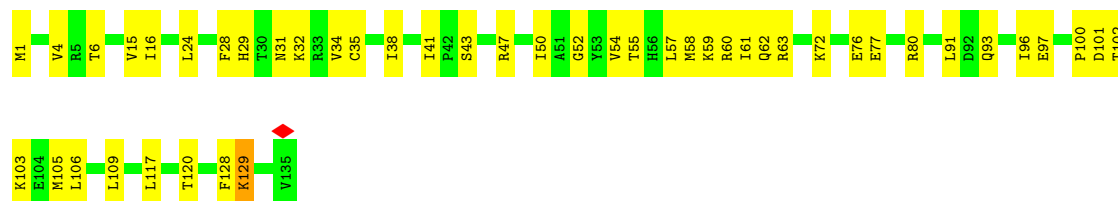
- Molecule 54: Small ribosomal subunit protein uS19



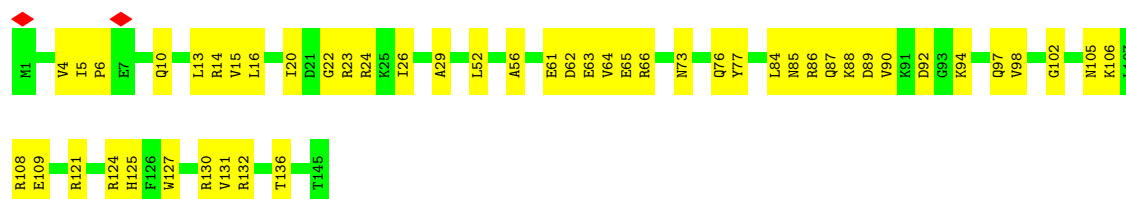
- Molecule 55: Small ribosomal subunit protein uS9



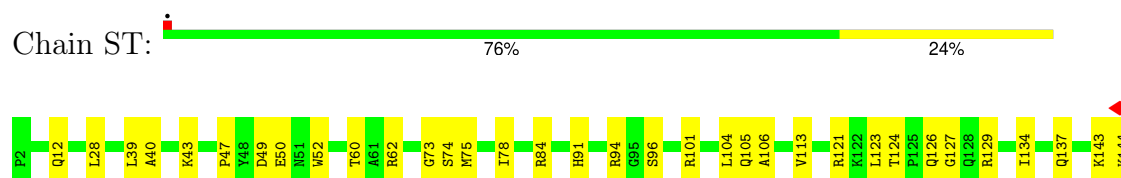
- Molecule 56: Small ribosomal subunit protein eS17



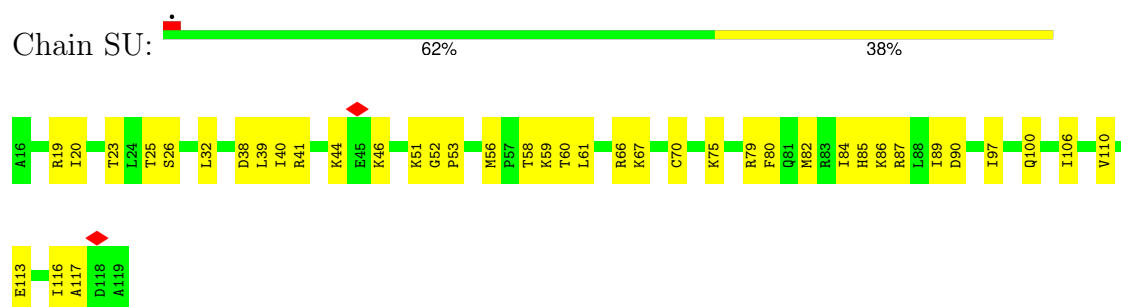
- Molecule 57: 40S ribosomal protein S18



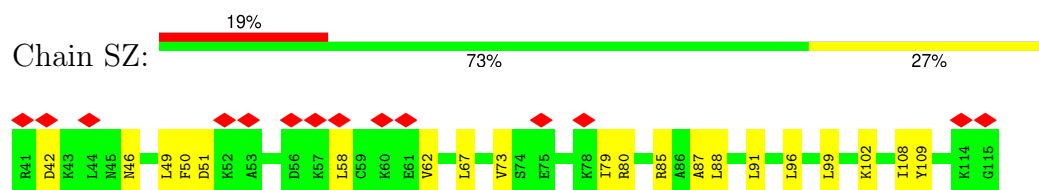
- Molecule 58: 40S ribosomal protein S19



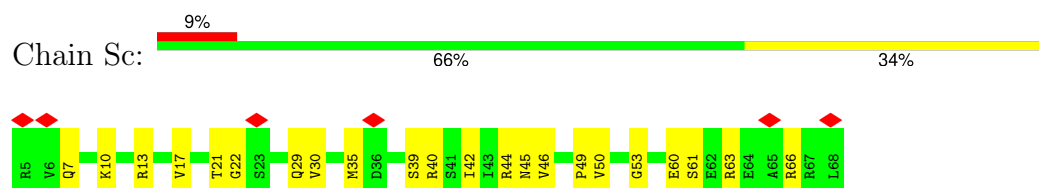
- Molecule 59: 40S ribosomal protein S20



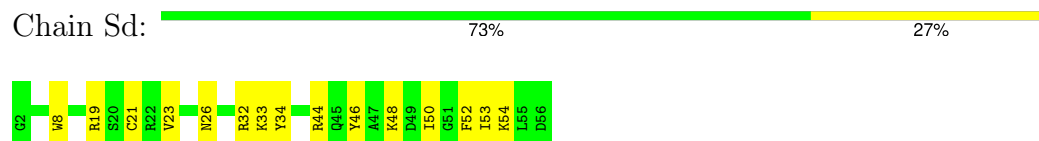
- Molecule 60: Small ribosomal subunit protein eS25



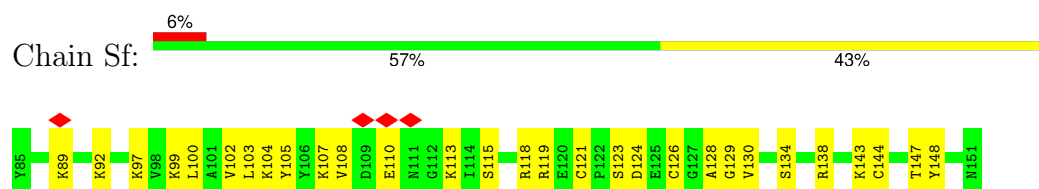
- Molecule 61: 40S ribosomal protein S28



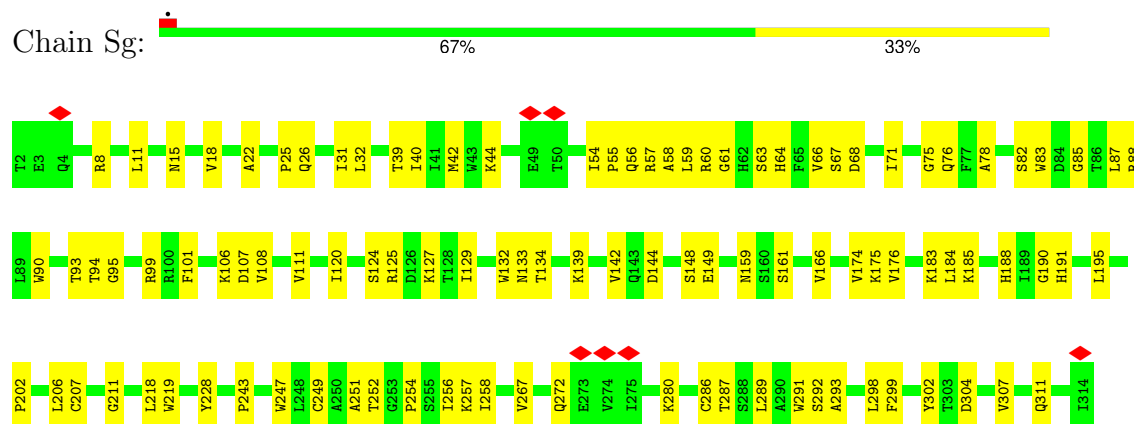
- Molecule 62: 40S ribosomal protein S29



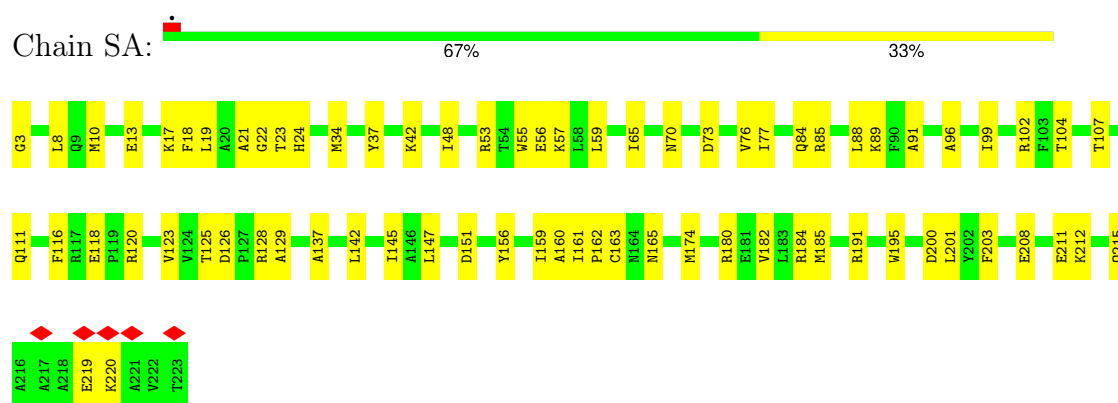
- Molecule 63: Ubiquitin-40S ribosomal protein S27a



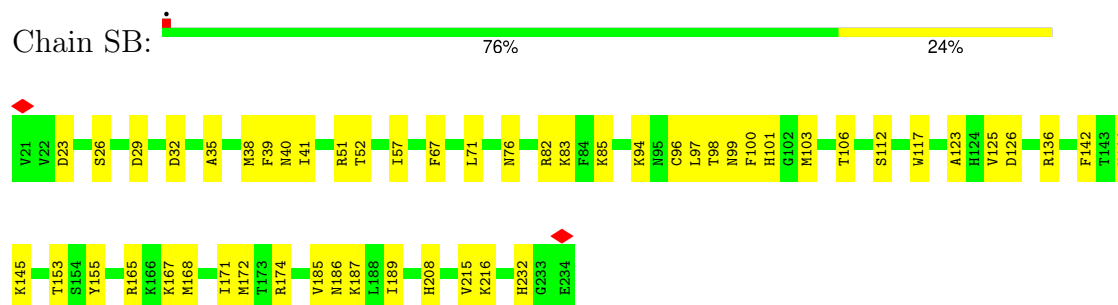
- Molecule 64: Receptor of activated protein C kinase 1



- Molecule 65: 40S ribosomal protein SA



- Molecule 66: 40S ribosomal protein S3a

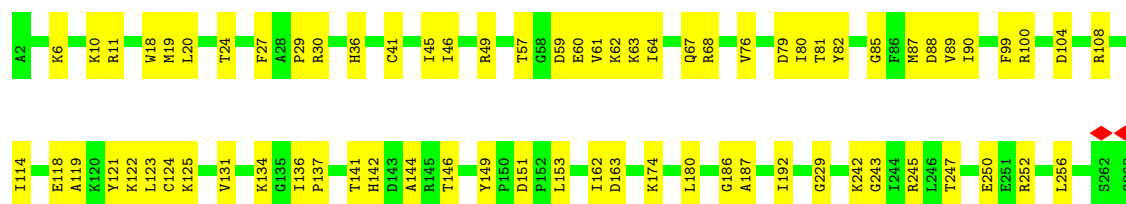


- Molecule 67: 40S ribosomal protein S2



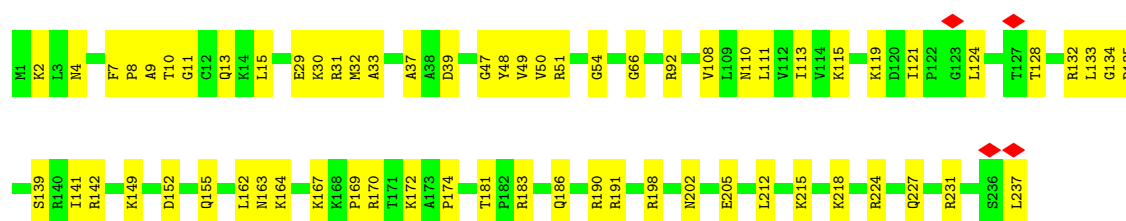
- Molecule 68: Small ribosomal subunit protein eS4, X isoform

Chain SE:  73% 27%



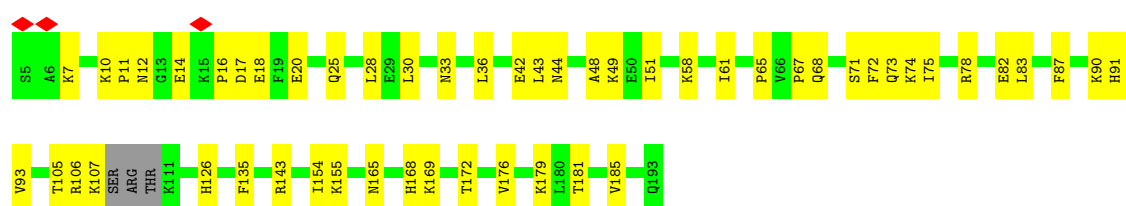
- Molecule 69: 40S ribosomal protein S6

Chain SG:  72% 28%



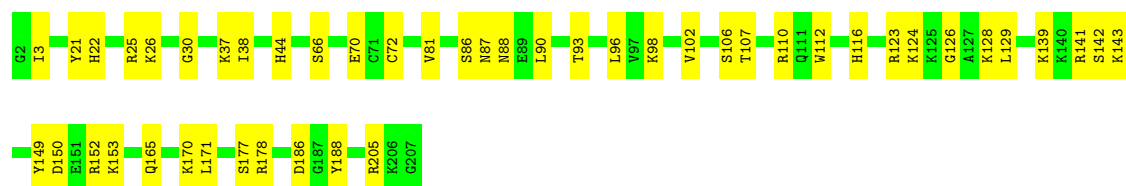
- Molecule 70: Small ribosomal subunit protein eS7

Chain SH:  70% 29%



- Molecule 71: 40S ribosomal protein S8

Chain SI:  77% 23%



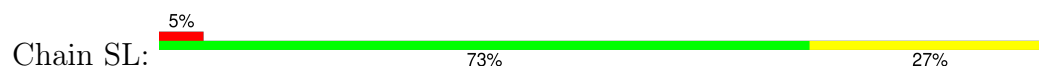
- Molecule 72: 40S ribosomal protein S9

Chain SJ:  75% 24%

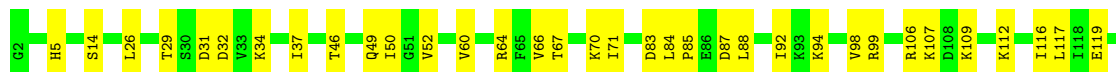
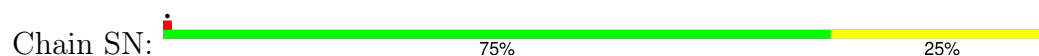




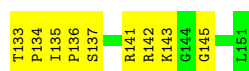
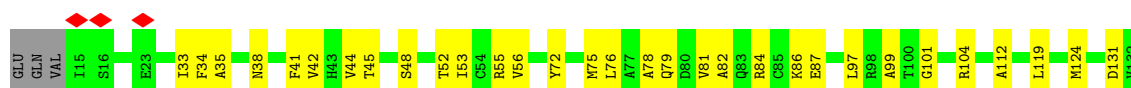
- Molecule 73: 40S ribosomal protein S11



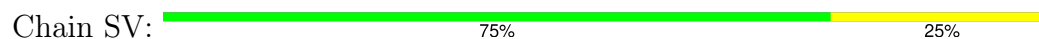
- Molecule 74: 40S ribosomal protein S13



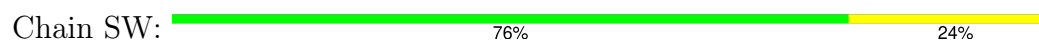
- Molecule 75: Small ribosomal subunit protein uS11



- Molecule 76: Small ribosomal subunit protein eS21



- Molecule 77: 40S ribosomal protein S15a



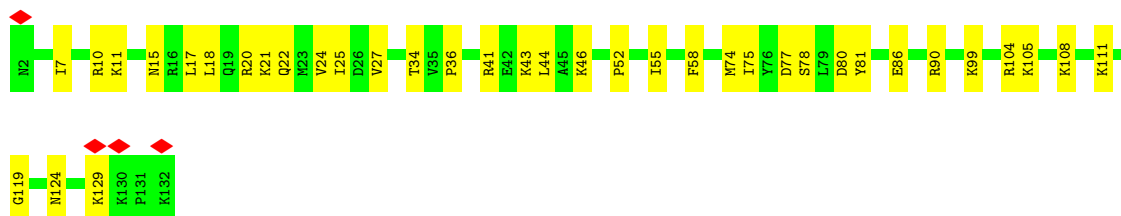
- Molecule 78: 40S ribosomal protein S23

Chain SX:  82% 18%



- Molecule 79: 40S ribosomal protein S24

Chain SY:  72% 28%



- Molecule 80: 40S ribosomal protein S26

Chain Sa:  72% 28%



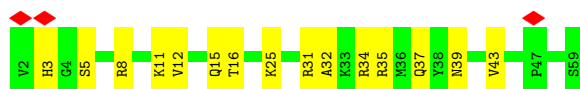
- Molecule 81: Small ribosomal subunit protein eS27

Chain Sb:  71% 29%

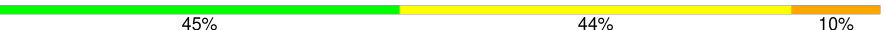


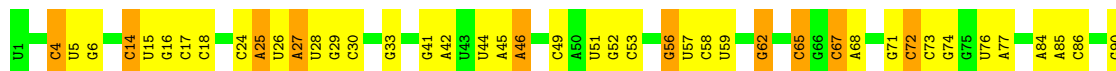
- Molecule 82: Small ribosomal subunit protein eS30

Chain Se:  5% 74% 26%

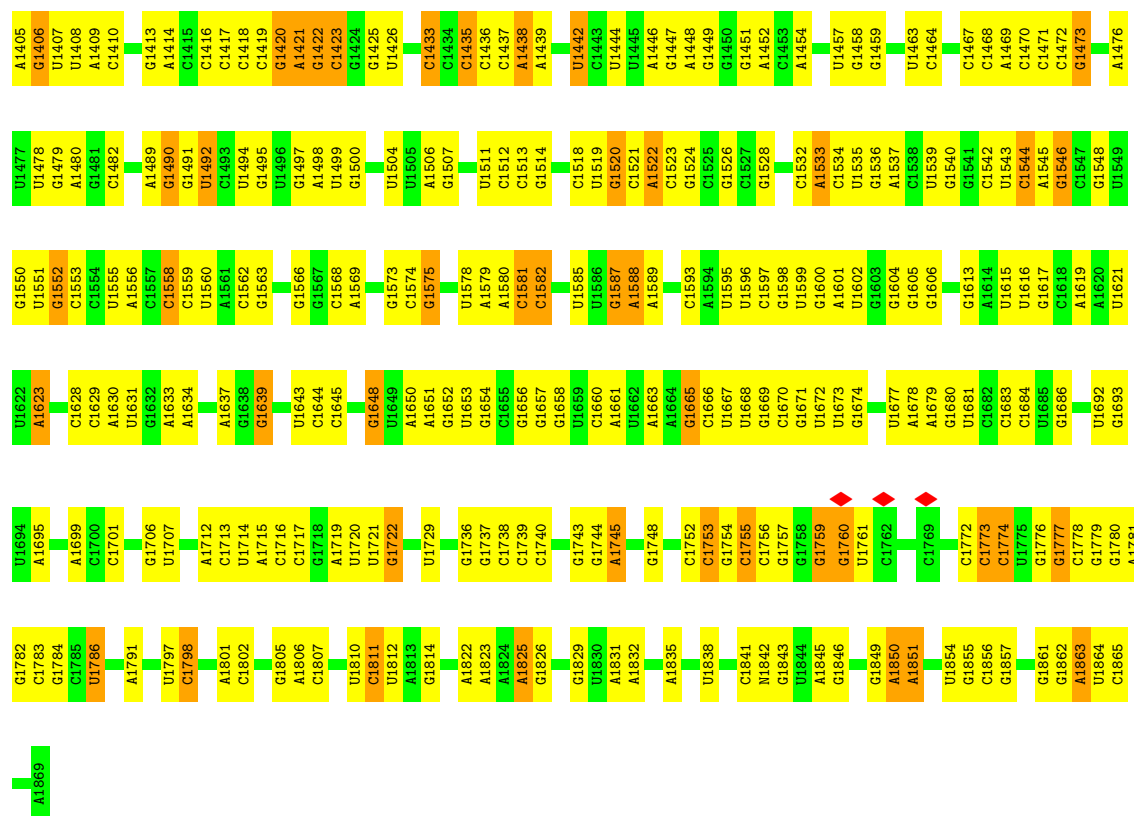


- Molecule 83: 18S rRNA

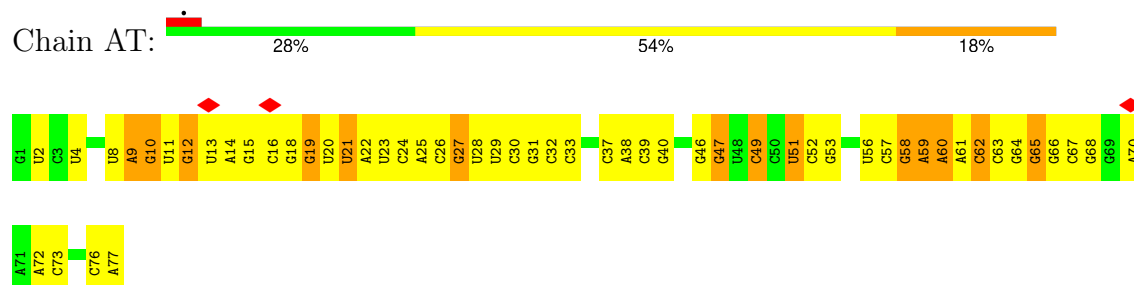
Chain S2:  45% 44% 10%



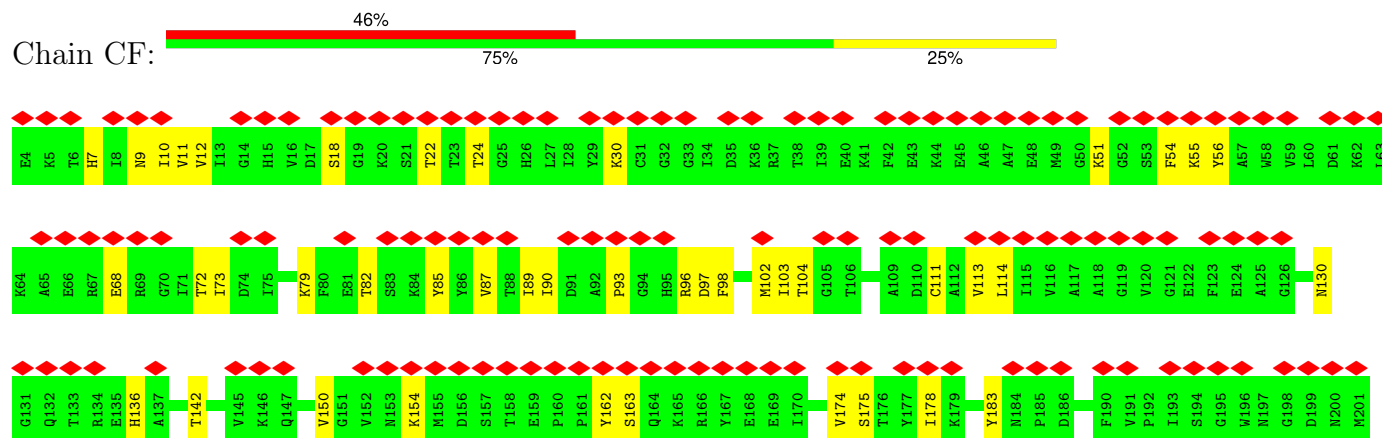
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U1172	A1173	U1174	G1175	G1176	G1177	U1178	G1179	A1182	G1187	A1188	A1189	A1190	A1191	A1192	U1193	U1194	U1195	U1196	U1197	U1198	U1199	U1200	U1201	U1202	G1203	A1204	G1205	G1206	G1207	G1208	A1209	C1210	C1211	C1212	C1213	C1214	C1215	C1216	A1217	C1218	G1222	A1223	G1224	U1225	G1226	G1227	A1228	G1229	C1230	C1231	U1232	C1233	G1234	G1235	U1236	C1237	U1238	U1239	A1240	A1241	U1242																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
C1094	C1095	G1096	G1097	G1098	G1099	A1100	U1101	G1102	G1103	G1104	C1105	C1106	C1107	C1108	C1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	C1117	C1118	G1119	A1120	A1121	A1122	A1123	G1124	G1125	G1126	C1127	C1128	C1129	C1130	C1131	C1132	A1133	U1134	U1135	U1136	U1137	C1138	C1139	G1140	G1141	G1142	A1143	A1144	A1145	C1146	C1147	A1148	A1149	A1150	G1151	U1152	C1153	U1154	U1155	U1156	G1165	G1171																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
U160	U161	C162	U163	A164	C165	A166	G167	C168	U169	A170	A171	U172	A173	A174	A175	C186	C187	C188	C189	C190	C191	C192	C193	C194	C195	C196	U197	U198	U199	G200	G201	G202	C203	G204	G205	G206	G207	G208	A209	U214	U219	A224	G225	G226	G227	G228	G229	G230	G231	G232	G233	G234	G235	G236	G237	G238	G239	G240	G241	G242	G243	G244	G245	G246	G247	G248	G249	G250	G251	G252	G253	G254	G255	G256	G257	G258	G259	G260	G261	G262	G263	G264	G265	G266	G267	G268	G269	G270	G271	G272	G273	G274	G275	G276	G277	G278	G279	G280	G281	G282	G283	G284	G285	G286	G287	G288	G289	G290	G291	G292	G293	G294	G295	G296	G297	G298	G299	G300	G301	G302	G303	G304	G305	G306	G307	G308	G309	G310	G311	G312	G313	G314	G315	G316	G317	G318	G319	G320	G321	G322	G323	G324	G325	G326	G327	G328	G329	G330	G331	G332	G333	G334	A335	A336	A337	A338	A339	A340	A341	A342	A343	A344	A345	A346	A347	A348	A349	C350	U351	C352	C353	U354	A355	A356	A357	A358	A359	A360	U361	C362	C363	A364	U365	U366	U367	U368	C369	G370	A371	U372	G373	A374	A375	A376	G377	U378	G379	G380	G381	G382	G383	U384	G385	C386	U387	A388	A389	A390	A391	A392	A393	A394	A395	A396	A397	A398	A399	A400	A401	A402	A403	A404	A405	A406	A407	A408	A409	A410	A411	A412	A413	A414	A415	A416	A417	A418	A419	A420	A421	A422	A423	A424	A425	A426	A427	A428	A429	A430	A431	A432	A433	A434	A435	A436	A437	A438	A439	A440	A441	A442	A443	A444	A445	A446	A447	A448	A449	A450	A451	A452	A453	A454	A455	A456	A457	A458	A459	A460	A461	A462	A463	A464	A465	A466	A467	A468	A469	A470	A471	A472	A473	A474	A475	A476	A477	A478	A479	A480	A481	A482	A483	A484	A485	A486	A487	A488	A489	A490	A491	A492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433

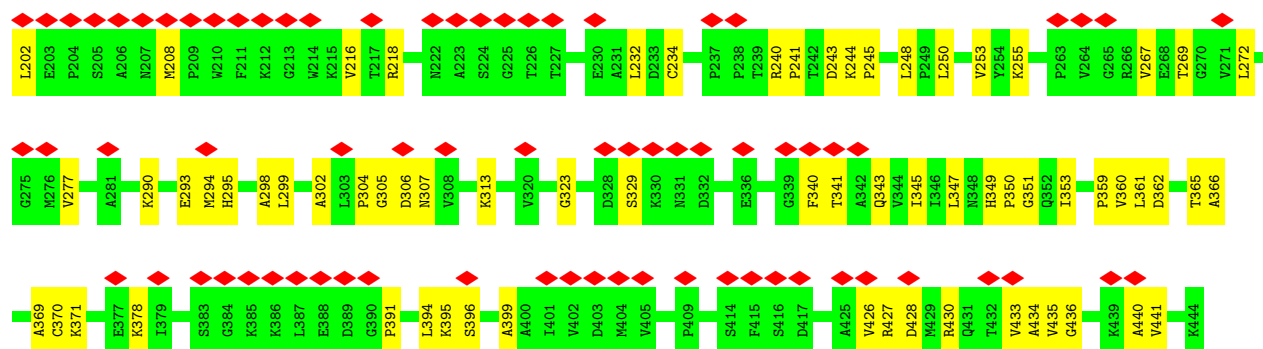


• Molecule 84: A/T site tRNA



• Molecule 85: Elongation factor 1-alpha 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60393	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	0.133	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0132	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: 5MC, OMC, 1MA, UY1, SPM, SEP, 6MZ, MA6, OMU, 4AC, OMG, B8N, G7M, A2M, MG, ZN, PSU, UR3, SPD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	CI	0.16	0/247	0.30	0/323
2	Pt	0.15	0/1761	0.26	0/2741
3	L5	0.27	0/85098	0.30	0/132762
4	L7	0.25	0/2861	0.26	0/4459
5	L8	0.27	0/3631	0.27	0/5657
6	LA	0.27	0/1936	0.42	0/2596
7	LB	0.24	0/3306	0.37	0/4424
8	LC	0.25	0/2981	0.39	0/4002
9	LD	0.21	0/2428	0.33	0/3252
10	LE	0.22	0/1973	0.41	0/2645
11	LF	0.27	0/1905	0.38	0/2539
12	LG	0.22	0/1960	0.38	0/2637
13	LH	0.23	0/1537	0.37	0/2066
14	LI	0.22	0/1751	0.36	0/2340
15	LJ	0.21	0/1385	0.43	0/1852
16	LL	0.22	0/1732	0.34	0/2315
17	LM	0.25	0/1161	0.42	0/1554
18	LN	0.26	0/1746	0.32	0/2338
19	LO	0.25	0/1682	0.36	0/2250
20	LP	0.25	0/1268	0.39	0/1701
21	LQ	0.26	0/1537	0.42	0/2052
22	LR	0.22	0/1582	0.38	0/2091
23	LS	0.27	0/1493	0.36	0/2003
24	LT	0.23	0/1326	0.33	0/1770
25	LU	0.22	0/839	0.50	0/1126
26	LV	0.24	0/993	0.38	0/1332
27	LW	0.20	0/959	0.38	0/1270
28	LX	0.22	0/1002	0.37	0/1345
29	LY	0.23	0/1132	0.39	0/1504
30	LZ	0.22	0/1130	0.36	0/1507
31	La	0.25	0/1191	0.32	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.20	0/889	0.41	0/1175
33	Lc	0.24	0/774	0.43	0/1038
34	Ld	0.24	0/903	0.38	0/1216
35	Le	0.25	0/1071	0.33	0/1429
36	Lf	0.26	0/895	0.34	0/1198
37	Lg	0.23	0/916	0.34	0/1220
38	Lh	0.21	0/1023	0.35	0/1351
39	Li	0.20	0/843	0.33	0/1115
40	Lj	0.26	0/720	0.37	0/952
41	Lk	0.21	0/575	0.40	0/761
42	Ll	0.24	0/454	0.32	0/599
43	Lm	0.21	0/435	0.37	0/575
44	Ln	0.20	0/231	0.30	0/294
45	Lo	0.21	0/876	0.34	0/1156
46	Lp	0.25	0/718	0.37	0/953
47	Lr	0.25	0/1017	0.36	0/1364
48	Ls	0.13	0/1519	0.36	0/2052
49	Lt	0.16	0/1009	0.48	0/1363
50	SD	0.16	0/1793	0.34	0/2414
51	SF	0.18	0/1516	0.37	0/2037
52	SK	0.21	0/851	0.55	0/1147
53	SM	0.13	0/950	0.36	0/1275
54	SP	0.16	0/1003	0.40	0/1342
55	SQ	0.18	0/1160	0.44	0/1553
56	SR	0.21	0/1105	0.55	2/1484 (0.1%)
57	SS	0.18	0/1216	0.43	0/1628
58	ST	0.15	0/1131	0.41	0/1515
59	SU	0.16	0/831	0.39	0/1115
60	SZ	0.16	0/604	0.45	0/810
61	Sc	0.15	0/508	0.37	0/680
62	Sd	0.17	0/470	0.37	0/623
63	Sf	0.16	0/560	0.45	0/745
64	Sg	0.13	0/2493	0.37	0/3394
65	SA	0.18	0/1778	0.41	0/2416
66	SB	0.18	0/1765	0.41	0/2362
67	SC	0.19	0/1744	0.39	0/2357
68	SE	0.16	0/2118	0.38	0/2849
69	SG	0.16	0/1946	0.37	0/2590
70	SH	0.19	0/1519	0.47	0/2033
71	SI	0.18	0/1715	0.38	0/2287
72	SJ	0.14	0/1550	0.33	0/2069
73	SL	0.19	0/1268	0.34	0/1696
74	SN	0.21	0/1232	0.35	0/1656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SO	0.21	0/1037	0.44	0/1391
76	SV	0.17	0/643	0.41	0/860
77	SW	0.20	0/1051	0.39	0/1406
78	SX	0.18	0/1116	0.41	0/1490
79	SY	0.16	0/1083	0.39	0/1438
80	Sa	0.21	0/836	0.37	0/1121
81	Sb	0.17	0/665	0.39	0/891
82	Se	0.14	0/465	0.36	0/612
83	S2	0.21	0/39756	0.28	0/61939
84	AT	0.13	0/1805	0.31	0/2809
85	CF	0.15	0/3442	0.40	0/4656
All	All	0.23	0/235126	0.33	2/344545 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
75	SO	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	SR	109	LEU	CA-C-N	5.02	133.76	124.82
56	SR	109	LEU	C-N-CA	5.02	133.76	124.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
75	SO	137	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CI	247	0	283	12	0
2	Pt	1576	0	803	17	0
3	L5	78444	0	39719	978	0
4	L7	2561	0	1295	32	0
5	L8	3315	0	1685	40	0
6	LA	1898	0	1993	45	0
7	LB	3238	0	3376	64	0
8	LC	2927	0	3104	43	0
9	LD	2382	0	2410	42	0
10	LE	1935	0	2096	31	0
11	LF	1870	0	1996	44	0
12	LG	1927	0	2074	24	0
13	LH	1518	0	1601	31	0
14	LI	1711	0	1749	30	0
15	LJ	1362	0	1399	25	0
16	LL	1701	0	1818	30	0
17	LM	1138	0	1204	24	0
18	LN	1701	0	1749	20	0
19	LO	1650	0	1794	24	0
20	LP	1242	0	1269	19	0
21	LQ	1513	0	1628	23	0
22	LR	1566	0	1729	31	0
23	LS	1453	0	1490	21	0
24	LT	1298	0	1366	35	0
25	LU	825	0	850	22	0
26	LV	979	0	1039	10	0
27	LW	945	0	1003	19	0
28	LX	985	0	1066	9	0
29	LY	1115	0	1205	24	0
30	LZ	1107	0	1182	21	0
31	La	1162	0	1213	12	0
32	Lb	876	0	948	15	0
33	Lc	764	0	804	13	0
34	Ld	888	0	930	19	0
35	Le	1053	0	1147	20	0
36	Lf	876	0	912	13	0
37	Lg	906	0	998	13	0
38	Lh	1015	0	1148	15	0
39	Li	832	0	917	12	0
40	Lj	705	0	737	16	0
41	Lk	569	0	637	10	0
42	Ll	444	0	483	8	0
43	Lm	429	0	465	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Ln	230	0	276	9	0
45	Lo	862	0	929	11	0
46	Lp	708	0	756	10	0
47	Lr	1002	0	1068	22	0
48	Ls	1496	0	1540	25	0
49	Lt	998	0	1032	16	0
50	SD	1765	0	1865	35	0
51	SF	1495	0	1549	44	0
52	SK	827	0	854	27	0
53	SM	940	0	965	24	0
54	SP	985	0	1031	29	0
55	SQ	1142	0	1213	33	0
56	SR	1090	0	1149	32	0
57	SS	1198	0	1261	42	0
58	ST	1112	0	1146	25	0
59	SU	821	0	883	33	0
60	SZ	598	0	656	19	0
61	Sc	506	0	536	18	0
62	Sd	459	0	452	11	0
63	Sf	548	0	551	25	0
64	Sg	2436	0	2393	68	0
65	SA	1741	0	1746	49	0
66	SB	1738	0	1809	33	0
67	SC	1707	0	1791	48	0
68	SE	2076	0	2177	47	0
69	SG	1923	0	2089	60	0
70	SH	1497	0	1590	37	0
71	SI	1686	0	1772	38	0
72	SJ	1525	0	1640	38	0
73	SL	1247	0	1323	31	0
74	SN	1208	0	1294	28	0
75	SO	1024	0	1050	31	0
76	SV	636	0	637	18	0
77	SW	1034	0	1080	26	0
78	SX	1098	0	1167	20	0
79	SY	1065	0	1142	29	0
80	Sa	821	0	870	23	0
81	Sb	651	0	672	15	0
82	Se	459	0	503	16	0
83	S2	36953	0	18679	641	0
84	AT	1616	0	824	35	0
85	CF	3383	0	3432	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	L5	180	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	S2	28	0	0	0	0
87	L5	98	0	182	4	0
88	L5	90	0	171	4	0
88	LN	10	0	19	0	0
89	Lg	1	0	0	0	0
89	Lj	1	0	0	0	0
89	Lm	1	0	0	0	0
89	Lo	1	0	0	0	0
89	Lp	1	0	0	0	0
89	Sa	1	0	0	0	0
All	All	223377	0	167078	3176	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 8.

All (3176) 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)
1:CI:79:ARG:NH1	3:L5:2708:U:O2'	1.62	1.32
3:L5:1996:C:H42	3:L5:2000:G:N2	1.51	1.05
3:L5:1996:C:N4	3:L5:2000:G:H22	1.61	0.99
83:S2:1652:G:H1	83:S2:1672:U:H3	1.08	0.98
1:CI:79:ARG:NH1	3:L5:2708:U:HO2'	1.58	0.91
3:L5:4946:U:HO2'	36:Lf:2:SER:N	1.69	0.91
3:L5:184:U:H3	3:L5:253:G:H1	1.20	0.90
3:L5:2557:G:H1	3:L5:2570:U:H3	1.13	0.90
83:S2:1656:G:H1	83:S2:1668:U:H3	0.97	0.90
3:L5:1095:A:H2	3:L5:1200:G:H1	1.06	0.89
11:LF:243:LEU:O	11:LF:247:MET:HB2	1.72	0.89
83:S2:1324:G:H1	83:S2:1504:U:H3	1.19	0.88
47:Lr:119:ARG:HD3	47:Lr:122:LYS:HZ3	1.38	0.87
3:L5:1996:C:H42	3:L5:2000:G:H22	0.91	0.86
83:S2:1033:G:H1	83:S2:1080:A:HO2'	1.15	0.85
75:SO:99:ALA:H	75:SO:133:THR:HG22	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1748:G:H1	83:S2:1786:U:H3	0.82	0.81
16:LL:64:VAL:HA	16:LL:67:HIS:HD2	1.44	0.81
83:S2:165:G:H2'	83:S2:166:A2M:H8	1.63	0.79
3:L5:2893:U:H5''	71:SI:205:ARG:HH22	1.47	0.79
65:SA:65:ILE:HD11	65:SA:182:VAL:HG11	1.64	0.78
83:S2:1288:OMU:HN3	83:S2:1311:C:H42	1.32	0.78
52:SK:53:LYS:HD3	52:SK:58:VAL:HG13	1.63	0.78
78:SX:107:ARG:HG3	78:SX:110:HIS:HB3	1.65	0.77
3:L5:2520:C:O2	3:L5:2640:G:N2	2.17	0.76
20:LP:126:ARG:HD3	20:LP:140:MET:HE1	1.67	0.76
27:LW:119:LYS:O	27:LW:123:LYS:HB2	1.86	0.76
74:SN:37:ILE:HG13	74:SN:50:ILE:HG21	1.68	0.76
3:L5:2416:G:N2	3:L5:2427:G:O6	2.18	0.76
70:SH:87:PHE:HB3	70:SH:90:LYS:HD2	1.68	0.76
3:L5:262:G:H2'	3:L5:263:G:H8	1.50	0.76
3:L5:1982:G:H5'	49:Lt:28:LEU:HD22	1.66	0.76
3:L5:664:G:N2	3:L5:666:G:O6	2.18	0.76
3:L5:4694:G:H4'	13:LH:71:ARG:HH12	1.49	0.76
3:L5:184:U:O2	3:L5:253:G:N2	2.19	0.76
51:SF:134:VAL:HG12	51:SF:135:ARG:HG2	1.68	0.76
63:Sf:126:CYS:SG	63:Sf:144:CYS:N	2.58	0.76
85:CF:360:VAL:HA	85:CF:369:ALA:HA	1.69	0.75
8:LC:149:GLU:OE2	47:Lr:72:LYS:NZ	2.19	0.75
74:SN:37:ILE:HD11	74:SN:71:ILE:HG23	1.68	0.75
3:L5:758:G:H4'	13:LH:51:LYS:HE3	1.68	0.75
78:SX:119:ARG:NH2	83:S2:1192:U:OP2	2.18	0.75
3:L5:3798:U:OP2	26:LV:74:LYS:NZ	2.18	0.75
3:L5:1095:A:N1	3:L5:1200:G:O6	2.20	0.75
71:SI:141:ARG:HE	71:SI:142:SER:H	1.34	0.74
55:SQ:74:GLY:O	55:SQ:80:GLN:NE2	2.20	0.74
3:L5:3937:C:H1'	18:LN:125:SER:HB3	1.70	0.74
59:SU:59:LYS:HB2	59:SU:84:ILE:HB	1.69	0.74
59:SU:38:ASP:HA	59:SU:41:ARG:HE	1.52	0.74
1:CI:74:LYS:HA	25:LU:116:GLN:O	1.88	0.73
3:L5:1732:C:H5''	24:LT:43:LYS:HE2	1.69	0.73
3:L5:2298:U:OP1	8:LC:204:ARG:NH1	2.22	0.73
1:CI:79:ARG:HH12	3:L5:2708:U:HO2'	1.18	0.73
3:L5:491:G:OP1	8:LC:5:ARG:NH1	2.22	0.73
3:L5:1480:C:O2'	3:L5:1482:G:OP2	2.07	0.73
3:L5:3641:U:OP2	3:L5:3646:A:N6	2.22	0.73
59:SU:26:SER:HB2	59:SU:32:LEU:HD11	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1095:A:C2	3:L5:1200:G:N1	2.50	0.73
4:L7:60:G:O2'	9:LD:268:ARG:NH1	2.22	0.72
58:ST:84:ARG:NH1	83:S2:1605:G:OP1	2.22	0.72
65:SA:42:LYS:HE3	65:SA:48:ILE:HD11	1.71	0.72
73:SL:97:ARG:NH2	83:S2:852:G:N3	2.37	0.72
3:L5:665:C:H4'	3:L5:666:G:H5'	1.71	0.72
25:LU:62:THR:HG1	25:LU:73:THR:HG1	1.34	0.72
66:SB:103:MET:HG3	66:SB:215:VAL:HG12	1.71	0.72
83:S2:928:G:H1	83:S2:1013:U:H3	1.36	0.72
67:SC:211:LYS:HG2	67:SC:215:MET:HE1	1.71	0.72
83:S2:851:C:H5''	83:S2:852:G:H5'	1.71	0.72
3:L5:2351:OMC:HM22	8:LC:95:MET:HG3	1.72	0.72
83:S2:488:U:OP2	85:CF:290:LYS:NZ	2.22	0.72
69:SG:152:ASP:OD1	69:SG:155:GLN:NE2	2.23	0.71
64:Sg:206:LEU:HD12	64:Sg:218:LEU:HD12	1.71	0.71
70:SH:44:ASN:OD1	70:SH:68:GLN:NE2	2.23	0.71
3:L5:2702:C:OP1	25:LU:101:ARG:NH2	2.24	0.71
53:SM:96:ARG:NH2	53:SM:100:PRO:O	2.23	0.71
73:SL:29:GLY:HA3	73:SL:30:LYS:HE2	1.71	0.71
3:L5:1095:A:H2	3:L5:1200:G:N1	1.86	0.71
52:SK:47:LYS:NZ	83:S2:1274:G:O4'	2.23	0.71
47:Lr:90:LEU:HD12	47:Lr:111:ILE:HG23	1.72	0.71
60:SZ:85:ARG:NH2	83:S2:1597:C:OP2	2.23	0.71
6:LA:137:ILE:HD11	6:LA:149:LYS:HB2	1.72	0.70
58:ST:101:ARG:HG2	58:ST:105:GLN:HE22	1.56	0.70
70:SH:154:ILE:HB	70:SH:185:VAL:HG22	1.73	0.70
3:L5:2103:G:N7	3:L5:2104:G:N2	2.38	0.70
13:LH:187:VAL:HG12	13:LH:188:GLN:HG3	1.73	0.70
3:L5:3701:OMC:H5	3:L5:3748:A:H62	1.39	0.70
65:SA:10:MET:HE2	65:SA:55:TRP:HB2	1.72	0.70
83:S2:1776:G:N2	83:S2:1777:G:N7	2.39	0.70
83:S2:888:U:H4'	83:S2:889:U:H5'	1.73	0.70
85:CF:79:LYS:HD3	85:CF:295:HIS:HB3	1.74	0.70
54:SP:114:HIS:ND1	54:SP:118:GLU:OE1	2.20	0.70
65:SA:102:ARG:HH12	83:S2:1377:U:H3'	1.57	0.70
57:SS:26:ILE:HD11	57:SS:52:LEU:HA	1.74	0.70
84:AT:15:G:N2	84:AT:49:C:O2	2.24	0.70
3:L5:1971:C:O2	48:Ls:41:GLN:NE2	2.25	0.69
22:LR:86:ASN:ND2	22:LR:91:GLU:OE1	2.22	0.69
51:SF:148:ASN:ND2	83:S2:1677:U:OP1	2.25	0.69
14:LI:150:GLU:OE2	14:LI:153:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:747:U:N3	83:S2:796:G:N1	2.40	0.69
64:Sg:8:ARG:HG3	64:Sg:311:GLN:HG2	1.74	0.69
3:L5:4305:G:N7	24:LT:87:LYS:NZ	2.39	0.69
79:SY:18:LEU:HD22	79:SY:20:ARG:HD3	1.73	0.69
26:LV:82:ILE:HB	26:LV:121:VAL:HG23	1.73	0.69
13:LH:48:LEU:HD21	13:LH:56:ARG:HE	1.56	0.69
25:LU:22:THR:OG1	25:LU:69:LYS:NZ	2.26	0.69
40:Lj:14:LYS:NZ	42:Ll:51:LEU:OXT	2.26	0.69
50:SD:106:ARG:HG3	50:SD:175:VAL:HG22	1.73	0.69
84:AT:18:G:H21	84:AT:59:A:H5'	1.56	0.69
6:LA:107:MET:HB3	6:LA:111:THR:HG21	1.75	0.69
3:L5:4873:G:N7	19:LO:179:LYS:NZ	2.41	0.69
25:LU:66:SER:HB3	25:LU:69:LYS:HB3	1.75	0.69
58:ST:12:GLN:NE2	83:S2:1593:C:O2	2.26	0.69
3:L5:2554:U:O2	3:L5:2764:A:N7	2.27	0.68
71:SI:98:LYS:HB3	83:S2:377:G:H5'	1.74	0.68
84:AT:21:U:H5'	84:AT:49:C:H42	1.57	0.68
22:LR:172:ARG:NH1	83:S2:909:G:OP1	2.26	0.68
72:SJ:162:ARG:NH1	83:S2:582:U:OP1	2.26	0.68
4:L7:23:A:N3	4:L7:118:C:O2'	2.26	0.68
37:Lg:89:ASP:OD2	37:Lg:93:ARG:NH1	2.26	0.68
51:SF:201:LYS:HG3	51:SF:204:ARG:HE	1.59	0.68
23:LS:76:LYS:NZ	23:LS:100:LEU:O	2.27	0.68
84:AT:64:G:O2'	85:CF:430:ARG:NH1	2.27	0.68
2:Pt:73:A:N3	14:LI:110:ARG:NH1	2.40	0.68
83:S2:1829:G:H1'	83:S2:1850:MA6:H2	1.76	0.68
84:AT:61:A:OP1	84:AT:63:C:N4	2.27	0.68
3:L5:1645:C:OP1	8:LC:80:ARG:NH2	2.26	0.68
48:Ls:58:ASN:ND2	48:Ls:84:GLY:O	2.23	0.68
75:SO:104:ARG:NH2	83:S2:959:G:OP1	2.26	0.67
48:Ls:68:HIS:O	48:Ls:71:ASN:ND2	2.28	0.67
76:SV:22:ARG:NH2	77:SW:18:GLU:O	2.27	0.67
83:S2:940:U:H3	83:S2:1002:U:H3	1.41	0.67
3:L5:2611:A:H5'	3:L5:2688:G:H4'	1.75	0.67
83:S2:925:G:H1	83:S2:1017:U:H3	1.43	0.67
64:Sg:175:LYS:HB3	64:Sg:184:LEU:HD11	1.75	0.67
1:CI:79:ARG:CZ	3:L5:2708:U:O2'	2.39	0.67
3:L5:2486:G:O6	3:L5:2493:G:O6	2.13	0.67
63:Sf:97:LYS:HD3	63:Sf:99:LYS:H	1.60	0.67
3:L5:188:G:N2	3:L5:190:G:O6	2.27	0.67
3:L5:1739:G:N3	3:L5:1742:A:N6	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2845:A:H61	3:L5:3843:C:H42	1.40	0.67
10:LE:180:VAL:HG21	10:LE:258:LEU:HD11	1.77	0.67
3:L5:2093:A:N3	3:L5:2094:G:N1	2.43	0.66
53:SM:91:LEU:HD12	53:SM:106:CYS:HB2	1.77	0.66
55:SQ:127:CYS:SG	55:SQ:128:GLU:N	2.68	0.66
57:SS:98:VAL:HG11	57:SS:106:LYS:HE2	1.76	0.66
22:LR:176:ARG:NH2	83:S2:910:G:OP1	2.28	0.66
83:S2:1422:G:H4'	83:S2:1423:C:H3'	1.78	0.66
1:CI:78:HIS:NE2	3:L5:2706:G:N7	2.44	0.66
51:SF:18:LYS:HE3	51:SF:22:LYS:HA	1.78	0.66
75:SO:86:LYS:HE3	75:SO:124:MET:HE1	1.78	0.66
79:SY:119:GLY:HA2	83:S2:85:A:H5'	1.76	0.66
33:Lc:40:GLN:OE1	33:Lc:42:LYS:NZ	2.28	0.66
50:SD:172:VAL:HG22	50:SD:185:LYS:HG2	1.77	0.66
58:ST:124:THR:HG23	58:ST:127:GLY:H	1.61	0.66
63:Sf:99:LYS:NZ	83:S2:1287:A:OP1	2.28	0.66
83:S2:1130:G:OP2	83:S2:1130:G:N2	2.27	0.66
57:SS:85:ASN:OD1	57:SS:97:GLN:NE2	2.28	0.66
3:L5:170:C:H42	3:L5:266:C:H42	1.44	0.66
7:LB:199:GLU:OE1	7:LB:200:ARG:NH1	2.28	0.66
57:SS:23:ARG:HD3	60:SZ:80:ARG:HH22	1.61	0.66
83:S2:1658:G:OP2	83:S2:1660:C:N4	2.28	0.66
3:L5:500:G:OP1	3:L5:504:G:N2	2.28	0.66
3:L5:3946:G:H1	3:L5:4067:U:H3	0.76	0.66
59:SU:46:LYS:NZ	59:SU:100:GLN:O	2.29	0.66
64:Sg:87:LEU:HB2	64:Sg:101:PHE:HB2	1.78	0.66
1:CI:75:LYS:O	25:LU:117:ILE:C	2.39	0.66
3:L5:1628:C:OP1	6:LA:14:SER:OG	2.13	0.66
3:L5:2389:A:H4'	34:Ld:70:LYS:HG3	1.76	0.66
3:L5:4546:A:N7	6:LA:215:ASN:ND2	2.44	0.66
23:LS:5:GLY:O	23:LS:111:ARG:NH2	2.29	0.66
27:LW:123:LYS:HD2	83:S2:320:G:H5''	1.78	0.66
69:SG:135:PRO:HG2	69:SG:141:ILE:HG13	1.78	0.66
3:L5:1175:A:H5''	9:LD:268:ARG:HE	1.61	0.65
49:Lt:117:ARG:HE	49:Lt:119:ARG:H	1.44	0.65
59:SU:51:LYS:HB3	59:SU:90:ASP:HB2	1.78	0.65
64:Sg:129:ILE:HB	64:Sg:142:VAL:HB	1.77	0.65
83:S2:830:A:OP2	83:S2:846:G:N2	2.28	0.65
69:SG:191:ARG:HH12	83:S2:312:G:H2'	1.60	0.65
33:Lc:48:LEU:HD23	33:Lc:57:LYS:HG3	1.78	0.65
58:ST:60:THR:HG23	58:ST:75:MET:HE2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1354:G:N2	83:S2:1357:A:OP2	2.28	0.65
51:SF:127:ARG:HG2	51:SF:136:ARG:HE	1.61	0.65
57:SS:22:GLY:HA2	57:SS:56:ALA:HB3	1.77	0.65
83:S2:159:A2M:H2'	83:S2:160:U:H6	1.61	0.65
53:SM:81:ASP:HB3	53:SM:84:LYS:HG2	1.76	0.65
72:SJ:164:PRO:HB3	72:SJ:170:PRO:HA	1.78	0.65
80:Sa:41:ILE:HG23	80:Sa:68:TYR:HE1	1.60	0.65
83:S2:1729:U:H3	83:S2:1805:G:H1	1.45	0.65
8:LC:254:GLU:OE2	8:LC:258:ARG:NH2	2.29	0.65
73:SL:22:ARG:NH1	73:SL:28:THR:OG1	2.30	0.65
83:S2:1417:C:O2	83:S2:1422:G:O6	2.15	0.65
3:L5:4092:G:N7	3:L5:4114:C:N4	2.45	0.65
3:L5:4094:G:N2	3:L5:4115:G:OP2	2.30	0.65
3:L5:1837:A:OP2	24:LT:130:ARG:NH1	2.28	0.65
65:SA:208:GLU:OE1	65:SA:212:LYS:NZ	2.30	0.65
8:LC:204:ARG:NH1	8:LC:205:ARG:O	2.30	0.64
29:LY:34:LEU:HD23	29:LY:38:LEU:HB3	1.78	0.64
84:AT:15:G:N2	84:AT:49:C:C2	2.65	0.64
3:L5:748:G:O6	23:LS:98:ARG:NH2	2.30	0.64
7:LB:10:ARG:NH2	7:LB:265:SER:O	2.29	0.64
10:LE:57:TYR:HB2	10:LE:62:MET:HE2	1.77	0.64
52:SK:14:LEU:HD13	52:SK:35:LEU:HD23	1.79	0.64
80:Sa:87:ARG:NH1	80:Sa:94:ASP:OD1	2.28	0.64
83:S2:28:U:H2'	83:S2:29:G:H8	1.62	0.64
3:L5:2516:G:O2'	37:Lg:62:LYS:NZ	2.31	0.64
33:Lc:37:MET:HE1	33:Lc:42:LYS:HE2	1.79	0.64
69:SG:183:ARG:NH2	83:S2:316:G:OP2	2.31	0.64
85:CF:97:ASP:OD1	85:CF:430:ARG:NH2	2.30	0.64
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.79	0.64
64:Sg:32:LEU:HA	64:Sg:42:MET:HA	1.79	0.64
30:LZ:99:ASP:HB2	30:LZ:102:ARG:HE	1.61	0.64
65:SA:102:ARG:NH1	83:S2:1378:A:OP2	2.31	0.64
7:LB:10:ARG:NH1	7:LB:11:HIS:O	2.31	0.64
67:SC:257:LYS:O	76:SV:16:LYS:NZ	2.31	0.64
3:L5:4887:C:H42	3:L5:4932:U:H3	1.45	0.64
3:L5:1726:U:H5'	11:LF:135:ILE:HD11	1.80	0.64
40:Lj:2:THR:HB	40:Lj:6:SER:HB2	1.80	0.64
23:LS:77:ASN:ND2	23:LS:137:CYS:SG	2.71	0.63
77:SW:71:LYS:NZ	83:S2:1156:U:OP1	2.30	0.63
3:L5:502:C:H3'	3:L5:503:C:H3'	1.80	0.63
3:L5:1982:G:H21	3:L5:2010:A:H5'	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2362:U:H2'	3:L5:2363:A2M:H8	1.80	0.63
61:Sc:29:GLN:HA	61:Sc:45:ASN:HA	1.80	0.63
3:L5:1669:A:OP1	32:Lb:18:ARG:NH2	2.27	0.63
3:L5:3594:C:O2	3:L5:3597:G:N2	2.31	0.63
85:CF:96:ARG:NH2	85:CF:430:ARG:O	2.32	0.63
3:L5:2764:A:H2'	3:L5:2765:A:H8	1.62	0.63
3:L5:4413:C:O2	14:LI:158:LYS:NZ	2.32	0.63
32:Lb:19:ASN:O	32:Lb:22:LYS:NZ	2.27	0.63
65:SA:37:TYR:HA	65:SA:53:ARG:HD3	1.80	0.63
78:SX:109:GLY:O	78:SX:119:ARG:NH1	2.32	0.63
83:S2:106:C:H2'	83:S2:107:A:H8	1.63	0.63
85:CF:51:LYS:HB3	85:CF:54:PHE:HB2	1.81	0.63
3:L5:2318:G:N2	3:L5:2321:G:OP2	2.27	0.63
16:LL:47:ALA:O	16:LL:149:GLN:NE2	2.32	0.63
83:S2:5:U:H2'	83:S2:6:G:H8	1.63	0.63
3:L5:137:G:H2'	3:L5:138:G:H8	1.63	0.63
3:L5:513:U:H3'	3:L5:514:U:H4'	1.80	0.63
3:L5:4242:U:H3	3:L5:4281:A:H2	1.46	0.63
51:SF:19:LEU:HD11	51:SF:50:PRO:HD3	1.81	0.63
64:Sg:254:PRO:O	64:Sg:272:GLN:NE2	2.31	0.63
83:S2:1528:G:O2'	83:S2:1666:C:OP1	2.17	0.63
85:CF:104:THR:HG23	85:CF:365:THR:HG23	1.78	0.63
3:L5:1866:U:OP1	14:LI:4:ARG:NH1	2.29	0.63
3:L5:62:A:N3	3:L5:77:U:O2'	2.29	0.63
3:L5:85:G:O2'	3:L5:97:G:O6	2.17	0.63
6:LA:29:LEU:O	6:LA:123:ARG:NH1	2.32	0.63
66:SB:26:SER:O	66:SB:51:ARG:NH2	2.32	0.63
67:SC:259:THR:HG23	76:SV:16:LYS:HZ3	1.63	0.63
2:Pt:50:U:H3	2:Pt:64:G:H1	0.75	0.63
13:LH:52:LYS:HB2	13:LH:54:ARG:HH11	1.64	0.63
45:Lo:33:LEU:HA	45:Lo:38:LYS:HG2	1.81	0.63
79:SY:111:LYS:NZ	83:S2:56:G:OP1	2.29	0.63
54:SP:18:ARG:HE	57:SS:88:LYS:HE2	1.63	0.62
3:L5:2458:C:H5''	18:LN:67:ARG:HD2	1.80	0.62
49:Lt:82:ILE:HG12	49:Lt:137:GLN:HG2	1.81	0.62
54:SP:135:ALA:HB2	83:S2:1235:G:H21	1.65	0.62
64:Sg:18:VAL:O	64:Sg:287:THR:OG1	2.17	0.62
65:SA:118:GLU:HG3	67:SC:65:LYS:HE2	1.81	0.62
85:CF:361:LEU:HD13	85:CF:370:CYS:HB3	1.81	0.62
3:L5:4251:A:H5''	15:LJ:108:GLY:HA3	1.81	0.62
68:SE:146:THR:HG21	83:S2:122:G:H21	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SG:13:GLN:NE2	83:S2:153:G:N3	2.46	0.62
85:CF:353:ILE:HB	85:CF:394:LEU:HB2	1.81	0.62
49:Lt:85:LEU:HD13	49:Lt:109:ILE:HD12	1.82	0.62
50:SD:62:LYS:O	50:SD:67:ARG:NH2	2.31	0.62
2:Pt:20(A):U:O4'	15:LJ:58:ARG:NH2	2.32	0.62
3:L5:2544:G:N1	5:L8:124:U:OP1	2.31	0.62
3:L5:4153:C:H5''	28:LX:38:LYS:HD2	1.80	0.62
49:Lt:65:GLN:HG3	49:Lt:67:ARG:H	1.64	0.62
69:SG:186:GLN:NE2	83:S2:332:G:O6	2.21	0.62
83:S2:508:A:H3'	83:S2:509:OMG:H8	1.62	0.62
3:L5:1499:C:OP1	21:LQ:150:ARG:NH2	2.33	0.62
3:L5:4162:C:H5	12:LG:73:ARG:HH12	1.47	0.62
3:L5:4897:G:OP1	17:LM:128:LYS:NZ	2.31	0.62
57:SS:15:VAL:HG12	57:SS:16:LEU:HG	1.81	0.62
69:SG:32:MET:HE2	69:SG:54:GLY:HA2	1.82	0.62
83:S2:94:G:O2'	83:S2:508:A:O2'	2.18	0.62
3:L5:3946:G:O6	3:L5:4067:U:O4	2.18	0.62
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.64	0.62
18:LN:164:LEU:O	18:LN:169:ARG:NH2	2.32	0.62
27:LW:116:LYS:NZ	83:S2:329:G:N7	2.47	0.62
51:SF:99:ILE:HD11	60:SZ:108:ILE:HG12	1.82	0.62
7:LB:107:ALA:HB2	7:LB:201:LEU:HD22	1.81	0.62
56:SR:60:ARG:HA	56:SR:63:ARG:HG2	1.81	0.62
68:SE:131:VAL:HA	68:SE:137:PRO:HA	1.81	0.62
77:SW:2:VAL:N	83:S2:1091:C:HO2'	1.97	0.62
79:SY:34:THR:O	83:S2:570:C:O2'	2.17	0.62
3:L5:4882:U:OP1	17:LM:117:LYS:NZ	2.33	0.62
5:L8:58:G:N7	40:Lj:63:ARG:NH2	2.38	0.62
26:LV:35:LYS:HB2	26:LV:67:LYS:HG3	1.81	0.62
39:Li:2:ALA:N	39:Li:5:TYR:HH	1.98	0.62
70:SH:51:ILE:HD11	70:SH:176:VAL:HG12	1.82	0.62
74:SN:70:LYS:NZ	83:S2:1020:A:N7	2.47	0.62
83:S2:588:G:OP2	83:S2:588:G:N2	2.31	0.62
3:L5:1591:U:OP2	3:L5:2856:C:O2'	2.14	0.62
72:SJ:18:ARG:HH22	83:S2:4:C:H1'	1.65	0.62
83:S2:1248:B8N:O36	83:S2:1701:C:N4	2.32	0.62
3:L5:3868:G:H22	3:L5:3900:G:H1'	1.65	0.61
19:LO:166:ILE:HD13	19:LO:169:ARG:HH21	1.65	0.61
19:LO:3:GLU:OE1	19:LO:5:GLN:NE2	2.32	0.61
23:LS:127:MET:HE1	24:LT:155:PRO:HG3	1.80	0.61
27:LW:80:ARG:NH2	69:SG:8:PRO:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:SE:134:LYS:NZ	83:S2:127:C:O2	2.32	0.61
3:L5:308:G:OP2	3:L5:308:G:N2	2.28	0.61
15:LJ:146:ARG:HG2	15:LJ:147:ARG:HG3	1.80	0.61
27:LW:77:LYS:NZ	27:LW:79:GLN:OE1	2.28	0.61
50:SD:45:ARG:NH2	50:SD:47:GLU:OE1	2.33	0.61
83:S2:1536:G:H2'	83:S2:1537:A:C8	2.36	0.61
8:LC:110:ARG:O	8:LC:113:ARG:NH1	2.30	0.61
50:SD:109:LEU:HD22	50:SD:175:VAL:HG11	1.82	0.61
65:SA:89:LYS:HD2	65:SA:201:LEU:HG	1.82	0.61
68:SE:153:LEU:O	68:SE:174:LYS:NZ	2.33	0.61
78:SX:128:VAL:HG23	78:SX:138:LYS:HE2	1.82	0.61
79:SY:119:GLY:O	83:S2:84:A:O2'	2.17	0.61
81:Sb:23:ARG:NH1	81:Sb:27:SER:O	2.34	0.61
3:L5:1187:G:OP2	3:L5:1187:G:N2	2.27	0.61
67:SC:196:ILE:HB	67:SC:223:TYR:HB2	1.82	0.61
3:L5:518:G:H1	3:L5:643:C:H2'	1.66	0.61
8:LC:65:GLU:HG3	8:LC:80:ARG:HD3	1.80	0.61
52:SK:80:ARG:NH2	52:SK:86:PRO:O	2.33	0.61
59:SU:56:MET:HB2	59:SU:86:LYS:HG3	1.82	0.61
69:SG:4:ASN:HB2	69:SG:110:ASN:HA	1.82	0.61
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.36	0.61
5:L8:62:A:OP1	38:Lh:52:LYS:NZ	2.33	0.61
26:LV:71:GLU:O	26:LV:75:LYS:NZ	2.31	0.61
31:La:72:THR:HG22	31:La:110:LYS:HB3	1.82	0.61
51:SF:127:ARG:HG2	51:SF:136:ARG:HB2	1.82	0.61
85:CF:378:LYS:HB2	85:CF:391:PRO:HG2	1.83	0.61
3:L5:173:C:H5''	16:LL:129:ARG:HH12	1.66	0.61
3:L5:665:C:O2	3:L5:668:C:N4	2.33	0.61
3:L5:4088:C:OP1	6:LA:37:ARG:NH1	2.33	0.61
13:LH:56:ARG:NH1	13:LH:58:ASP:OD2	2.32	0.61
51:SF:59:LYS:HB3	51:SF:62:ARG:HG3	1.82	0.61
83:S2:5:U:H2'	83:S2:6:G:C8	2.36	0.61
83:S2:1743:G:H21	83:S2:1791:A:H62	1.48	0.61
3:L5:1100:U:O3'	3:L5:1167:C:N4	2.34	0.61
3:L5:3615:G:H1'	27:LW:44:ARG:HD3	1.81	0.61
3:L5:4910:G:H4'	7:LB:95:THR:HG22	1.83	0.61
6:LA:114:CYS:HB3	6:LA:165:VAL:HB	1.81	0.61
35:Le:89:LEU:HD13	35:Le:118:LEU:HD22	1.82	0.61
69:SG:66:GLY:HA2	83:S2:1745:A:H1'	1.80	0.61
83:S2:71:G:H2'	83:S2:72:C:H4'	1.82	0.61
3:L5:438:G:N2	36:Lf:23:GLU:OE2	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LB:222:VAL:O	7:LB:343:ARG:NH1	2.33	0.61
65:SA:120:ARG:HD2	67:SC:266:TYR:HB3	1.81	0.61
83:S2:1536:G:H2'	83:S2:1537:A:H8	1.66	0.61
85:CF:10:ILE:HG12	85:CF:111:CYS:HB3	1.83	0.61
3:L5:67:C:OP2	3:L5:312:G:N2	2.33	0.60
3:L5:172:C:H4'	3:L5:173:C:H5'	1.81	0.60
3:L5:500:G:H1'	3:L5:504:G:H3'	1.81	0.60
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.36	0.60
3:L5:2092:G:O2'	3:L5:2262:G:N2	2.34	0.60
39:Li:62:LYS:HG2	39:Li:98:ARG:HH21	1.66	0.60
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.66	0.60
3:L5:2083:C:OP2	21:LQ:14:ARG:NH2	2.35	0.60
3:L5:4098:A:N1	3:L5:4112:C:N4	2.50	0.60
68:SE:79:ASP:HB3	68:SE:82:TYR:HB2	1.82	0.60
83:S2:928:G:H2'	83:S2:929:G:C8	2.37	0.60
85:CF:245:PRO:O	85:CF:269:THR:OG1	2.16	0.60
3:L5:505:G:H1	3:L5:653:U:H3	1.49	0.60
48:Ls:102:LEU:HD11	48:Ls:187:LEU:HD23	1.82	0.60
69:SG:172:LYS:NZ	83:S2:67:C:OP2	2.33	0.60
3:L5:966:A:H5''	3:L5:2092:G:H22	1.67	0.60
5:L8:75:OMG:OP2	29:LY:74:TYR:OH	2.19	0.60
70:SH:71:SER:HA	70:SH:74:LYS:HE3	1.83	0.60
72:SJ:93:LYS:HB2	72:SJ:96:TYR:HD2	1.67	0.60
73:SL:33:LEU:HD12	73:SL:34:PRO:HD2	1.84	0.60
75:SO:142:ARG:NH1	80:Sa:23:CYS:O	2.34	0.60
3:L5:1833:G:N2	3:L5:1835:G:O4'	2.34	0.60
3:L5:3619:G:H22	3:L5:3624:A:H1'	1.65	0.60
64:Sg:76:GLN:HE21	64:Sg:93:THR:HG23	1.67	0.60
77:SW:3:ARG:HH22	77:SW:28:ARG:HH21	1.48	0.60
83:S2:557:U:H2'	83:S2:558:G:C8	2.36	0.60
3:L5:1241:C:O2'	32:Lb:120:ARG:O	2.19	0.60
6:LA:112:ILE:HD11	46:Lp:79:VAL:HG22	1.82	0.60
13:LH:106:GLN:HB2	13:LH:111:LEU:HB3	1.84	0.60
54:SP:86:LEU:H	54:SP:89:MET:HE2	1.67	0.60
67:SC:187:ARG:NH2	83:S2:1143:A:OP2	2.28	0.60
67:SC:205:VAL:O	67:SC:224:THR:OG1	2.17	0.60
69:SG:162:LEU:O	69:SG:167:LYS:NZ	2.35	0.60
27:LW:7:SER:HB2	27:LW:13:ILE:HD11	1.84	0.60
65:SA:145:ILE:HG23	65:SA:159:ILE:HB	1.83	0.60
85:CF:24:THR:HG23	85:CF:89:ILE:HD13	1.82	0.60
29:LY:34:LEU:HD11	29:LY:47:MET:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Le:91:CYS:HB3	35:Le:95:TYR:HD2	1.65	0.60
67:SC:185:THR:OG1	83:S2:1155:U:OP1	2.16	0.60
73:SL:35:ARG:NH2	73:SL:55:TYR:O	2.35	0.60
3:L5:513:U:N3	3:L5:516:C:OP2	2.28	0.60
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.37	0.59
7:LB:83:PRO:O	7:LB:167:GLN:NE2	2.34	0.59
51:SF:124:ASP:OD1	51:SF:125:SER:N	2.31	0.59
58:ST:126:GLN:HB2	58:ST:129:ARG:HH21	1.67	0.59
59:SU:75:LYS:NZ	83:S2:1252:C:OP1	2.31	0.59
83:S2:1473:G:N1	83:S2:1476:A:OP2	2.32	0.59
83:S2:1748:G:O6	83:S2:1786:U:O4	2.20	0.59
3:L5:1811:G:H21	32:Lb:57:MET:HE3	1.66	0.59
3:L5:4340:U:O2	88:L5:5262:SPD:N10	2.34	0.59
34:Ld:22:THR:HG23	34:Ld:122:VAL:HG23	1.85	0.59
55:SQ:130:LYS:NZ	55:SQ:131:LYS:O	2.36	0.59
3:L5:3659:G:OP1	6:LA:241:ARG:NH1	2.35	0.59
14:LI:179:ASP:OD1	14:LI:180:GLU:N	2.35	0.59
32:Lb:109:ARG:HA	32:Lb:112:ILE:HG12	1.84	0.59
68:SE:121:TYR:HA	68:SE:163:ASP:HA	1.84	0.59
80:Sa:79:ILE:HD11	83:S2:1864:U:H5'	1.83	0.59
3:L5:2018:C:H2'	3:L5:2019:C:H6	1.66	0.59
7:LB:138:GLN:O	7:LB:143:LYS:NZ	2.36	0.59
71:SI:106:SER:HB3	71:SI:171:LEU:HG	1.84	0.59
3:L5:1094:G:O6	3:L5:1201:U:O2	2.21	0.59
3:L5:1500:A:H5''	3:L5:1501:C:H5''	1.85	0.59
3:L5:2101:C:H2'	3:L5:2102:G:C8	2.38	0.59
59:SU:85:HIS:ND1	83:S2:1447:G:OP1	2.35	0.59
65:SA:76:VAL:HG12	65:SA:123:VAL:HB	1.84	0.59
66:SB:99:ASN:OD1	66:SB:100:PHE:N	2.36	0.59
69:SG:183:ARG:HH12	83:S2:316:G:H5''	1.68	0.59
41:Lk:35:LYS:HB3	41:Lk:42:LEU:HD11	1.84	0.59
52:SK:35:LEU:HD13	52:SK:38:LYS:HB2	1.84	0.59
66:SB:125:VAL:HG12	66:SB:172:MET:HE3	1.83	0.59
3:L5:2572:C:O2'	30:LZ:112:ARG:NH2	2.35	0.59
3:L5:2658:G:N2	3:L5:2676:A:OP2	2.36	0.59
38:Lh:80:PRO:HD2	38:Lh:83:LEU:HD12	1.85	0.59
78:SX:37:LYS:NZ	83:S2:1811:C:OP1	2.27	0.59
3:L5:3732:A:H2'	3:L5:3733:A:H8	1.68	0.59
12:LG:157:ILE:HA	12:LG:201:THR:HG22	1.85	0.59
30:LZ:11:VAL:HG12	30:LZ:82:PRO:HA	1.85	0.59
51:SF:127:ARG:HH22	61:Sc:66:ARG:HH22	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:AT:2:U:H3	84:AT:72:A:H61	1.49	0.59
84:AT:59:A:O2'	84:AT:61:A:OP2	2.21	0.59
3:L5:3946:G:N2	3:L5:4067:U:O2	2.30	0.58
53:SM:36:ARG:NH1	83:S2:1310:U:OP1	2.36	0.58
58:ST:73:GLY:O	58:ST:94:ARG:NH2	2.35	0.58
77:SW:39:THR:HA	77:SW:42:MET:HG2	1.84	0.58
79:SY:36:PRO:HG3	83:S2:570:C:H4'	1.85	0.58
80:Sa:6:ARG:NH1	83:S2:1147:C:OP1	2.33	0.58
3:L5:1396:G:N7	31:La:110:LYS:NZ	2.42	0.58
45:Lo:69:ARG:HE	45:Lo:80:LYS:HG2	1.67	0.58
61:Sc:29:GLN:NE2	61:Sc:66:ARG:O	2.30	0.58
84:AT:67:C:H2'	84:AT:68:G:H8	1.66	0.58
34:Ld:64:ILE:HG23	34:Ld:68:LEU:HD23	1.85	0.58
48:Ls:29:ILE:HG22	48:Ls:88:PHE:HD1	1.68	0.58
74:SN:107:LYS:NZ	83:S2:1075:C:OP1	2.33	0.58
83:S2:186:C:H2'	83:S2:187:G:C8	2.38	0.58
3:L5:4266:G:O2'	3:L5:4267:G:N2	2.37	0.58
3:L5:4525:C:OP1	7:LB:246:ARG:NH2	2.34	0.58
64:Sg:99:ARG:NH1	64:Sg:134:THR:O	2.36	0.58
67:SC:167:ARG:NH1	67:SC:218:GLY:O	2.35	0.58
83:S2:420:G:O2'	83:S2:660:C:N3	2.36	0.58
52:SK:31:LYS:NZ	52:SK:39:ASN:H	2.02	0.58
79:SY:21:LYS:HE2	79:SY:75:ILE:HD11	1.85	0.58
83:S2:159:A2M:H2'	83:S2:160:U:C6	2.39	0.58
83:S2:556:U:H3'	83:S2:557:U:H4'	1.86	0.58
3:L5:4987:C:OP2	7:LB:116:ARG:NH2	2.36	0.58
4:L7:7:G:OP1	9:LD:33:ARG:NH1	2.35	0.58
27:LW:56:ARG:HH21	27:LW:61:LYS:HB3	1.68	0.58
48:Ls:54:LEU:HD23	48:Ls:88:PHE:HD2	1.67	0.58
57:SS:86:ARG:HE	57:SS:106:LYS:HD2	1.67	0.58
57:SS:86:ARG:NE	57:SS:106:LYS:HD2	2.17	0.58
72:SJ:136:ARG:HA	72:SJ:141:VAL:HA	1.86	0.58
73:SL:135:SER:O	73:SL:139:ARG:NH1	2.37	0.58
63:Sf:143:LYS:NZ	83:S2:1310:U:O3'	2.34	0.58
71:SI:116:HIS:O	71:SI:152:ARG:NH2	2.33	0.58
83:S2:1203:G:H2'	83:S2:1204:A:C8	2.38	0.58
85:CF:277:VAL:HG13	85:CF:329:SER:HB3	1.85	0.58
3:L5:4728:U:OP1	7:LB:132:LYS:NZ	2.36	0.58
9:LD:80:ALA:HA	9:LD:83:LEU:HD13	1.84	0.58
66:SB:98:THR:O	66:SB:232:HIS:NE2	2.35	0.58
67:SC:81:ILE:HG21	67:SC:88:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:639:C:H2'	83:S2:640:A:C8	2.39	0.58
83:S2:640:A:H2'	83:S2:641:A:C8	2.39	0.58
3:L5:4431:PSU:OP2	14:LI:3:ARG:NH2	2.35	0.58
9:LD:120:GLU:O	9:LD:248:ARG:NH1	2.36	0.58
54:SP:40:ARG:NH2	83:S2:1615:U:O4	2.37	0.58
76:SV:16:LYS:HG2	76:SV:23:ILE:HD13	1.86	0.58
83:S2:527:C:H2'	83:S2:528:A:C8	2.39	0.58
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.39	0.58
3:L5:4220:6MZ:OP2	24:LT:2:THR:OG1	2.18	0.58
41:Lk:8:ILE:HD11	41:Lk:56:LEU:HD13	1.86	0.58
81:Sb:20:LYS:NZ	83:S2:1016:U:OP2	2.33	0.58
3:L5:2299:G:OP1	8:LC:182:LYS:NZ	2.32	0.57
3:L5:2400:G:H21	37:Lg:6:THR:HG22	1.69	0.57
3:L5:2407:G:O6	42:Ll:2:SER:N	2.37	0.57
24:LT:119:ALA:HA	24:LT:122:LYS:HE3	1.85	0.57
36:Lf:33:VAL:HG13	36:Lf:38:GLU:HB2	1.85	0.57
67:SC:187:ARG:NH1	83:S2:1142:G:OP1	2.34	0.57
72:SJ:107:GLU:O	72:SJ:113:GLN:NE2	2.37	0.57
3:L5:2411:C:H2'	3:L5:2412:A:H8	1.70	0.57
64:Sg:78:ALA:HB3	64:Sg:90:TRP:HB2	1.85	0.57
74:SN:124:ARG:NH2	83:S2:1024:A:OP2	2.32	0.57
81:Sb:14:GLU:HA	81:Sb:17:ARG:HG2	1.86	0.57
83:S2:1098:C:H2'	83:S2:1099:G:C8	2.39	0.57
85:CF:22:THR:HG23	85:CF:56:TYR:HB2	1.85	0.57
3:L5:935:A:O2'	17:LM:44:GLN:O	2.18	0.57
6:LA:80:GLU:HB2	6:LA:170:ALA:HA	1.86	0.57
58:ST:91:HIS:NE2	83:S2:1665:G:OP1	2.34	0.57
83:S2:528:A:H2'	83:S2:529:A:C8	2.39	0.57
3:L5:305:A:OP2	18:LN:15:GLN:NE2	2.37	0.57
51:SF:81:ARG:O	51:SF:85:LYS:NZ	2.33	0.57
68:SE:27:PHE:O	83:S2:495:U:O2'	2.21	0.57
3:L5:327:U:O2'	39:Li:30:ARG:NH1	2.36	0.57
3:L5:1457:G:O2'	21:LQ:75:ARG:NH2	2.35	0.57
3:L5:2758:G:O2'	3:L5:2765:A:N3	2.33	0.57
3:L5:2809:G:O2'	3:L5:4644:G:OP1	2.22	0.57
3:L5:4523:A2M:H5''	3:L5:4524:G:H5'	1.86	0.57
27:LW:105:ARG:NH2	69:SG:149:LYS:O	2.37	0.57
77:SW:6:VAL:HG12	77:SW:34:ILE:HD11	1.86	0.57
84:AT:9:A:O2'	84:AT:10:G:N7	2.38	0.57
85:CF:350:PRO:O	85:CF:395:LYS:NZ	2.35	0.57
3:L5:1324:A:O2'	3:L5:1326:A2M:OP1	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L8:67:U:H2'	5:L8:68:G:H8	1.70	0.57
10:LE:141:ARG:NH1	10:LE:191:GLN:O	2.38	0.57
62:Sd:19:ARG:NH2	83:S2:1661:A:OP1	2.37	0.57
68:SE:57:THR:OG1	68:SE:60:GLU:OE1	2.20	0.57
69:SG:198:ARG:NH1	83:S2:126:G:OP2	2.38	0.57
71:SI:87:ASN:HB3	71:SI:90:LEU:HD13	1.86	0.57
83:S2:1255:G:OP1	83:S2:1256:G:O2'	2.15	0.57
3:L5:4612:C:C2	13:LH:120:GLU:HB2	2.39	0.57
3:L5:4618:OMG:H5'	26:LV:15:ARG:HB2	1.85	0.57
4:L7:26:C:O2'	15:LJ:147:ARG:NH1	2.26	0.57
25:LU:43:LEU:HD12	25:LU:47:ILE:HD11	1.86	0.57
57:SS:13:LEU:HD22	57:SS:20:ILE:HD11	1.85	0.57
58:ST:40:ALA:HB3	58:ST:43:LYS:HG2	1.86	0.57
83:S2:388:U:H2'	83:S2:389:A:H8	1.70	0.57
83:S2:436:OMG:OP2	83:S2:471:G:O2'	2.22	0.57
30:LZ:50:PRO:HD3	30:LZ:68:ILE:HG12	1.87	0.57
83:S2:1228:A:H2'	83:S2:1229:G:C8	2.40	0.57
3:L5:702:U:H2'	3:L5:703:G:O4'	2.05	0.57
3:L5:2296:G:O2'	8:LC:242:PRO:O	2.21	0.57
11:LF:171:ASP:OD1	11:LF:172:ASN:N	2.38	0.57
14:LI:28:ASP:OD1	14:LI:32:ARG:NH1	2.38	0.57
47:Lr:47:LYS:HB2	47:Lr:102:TYR:CZ	2.40	0.57
71:SI:72:CYS:HG	71:SI:112:TRP:CG	2.23	0.57
75:SO:145:GLY:O	80:Sa:22:ARG:NH2	2.38	0.57
84:AT:18:G:H1	84:AT:56:U:H1'	1.68	0.57
84:AT:39:C:H2'	84:AT:40:G:H8	1.70	0.57
3:L5:1700:G:OP1	8:LC:306:ARG:NH1	2.38	0.57
3:L5:2018:C:H2'	3:L5:2019:C:C6	2.40	0.57
3:L5:2335:C:H2'	3:L5:2336:G:H8	1.70	0.57
3:L5:2693:G:OP2	41:Lk:33:LYS:NZ	2.35	0.57
3:L5:2856:C:O2	7:LB:242:ARG:NH2	2.29	0.57
5:L8:90:C:H1'	29:LY:24:HIS:HB3	1.86	0.57
57:SS:130:ARG:NH2	83:S2:1230:C:OP1	2.38	0.57
63:Sf:119:ARG:HE	63:Sf:148:TYR:HD2	1.53	0.57
71:SI:150:ASP:HA	71:SI:153:LYS:HG2	1.86	0.57
73:SL:133:PRO:O	83:S2:383:G:O2'	2.23	0.57
13:LH:95:VAL:HG12	43:Lm:82:LEU:HD22	1.87	0.56
14:LI:177:ASN:HB2	14:LI:180:GLU:HG2	1.87	0.56
68:SE:90:ILE:HB	68:SE:99:PHE:HB2	1.85	0.56
71:SI:143:LYS:NZ	83:S2:202:G:OP1	2.38	0.56
81:Sb:54:VAL:HG13	81:Sb:63:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:CF:428:ASP:HB3	85:CF:433:VAL:HG11	1.86	0.56
3:L5:4097:G:O6	3:L5:4098:A:N6	2.38	0.56
3:L5:4279:A:H5'	3:L5:4281:A:H1'	1.87	0.56
7:LB:80:GLU:OE1	7:LB:323:TYR:OH	2.23	0.56
9:LD:128:ASP:OD1	9:LD:129:GLU:N	2.37	0.56
65:SA:57:LYS:NZ	65:SA:160:ALA:O	2.33	0.56
69:SG:11:GLY:HA2	83:S2:166:A2M:HM'1	1.87	0.56
75:SO:55:ARG:NH2	83:S2:954:U:O2	2.37	0.56
78:SX:9:THR:HG22	83:S2:681:PSU:H4'	1.88	0.56
83:S2:186:C:H2'	83:S2:187:G:H8	1.71	0.56
1:CI:75:LYS:O	25:LU:117:ILE:O	2.24	0.56
3:L5:158:A:N1	3:L5:276:C:O2'	2.32	0.56
3:L5:1646:A:O2'	40:Lj:49:TRP:O	2.18	0.56
3:L5:1667:G:N1	3:L5:2281:U:OP2	2.31	0.56
3:L5:3811:G:O2'	3:L5:3814:U:OP2	2.23	0.56
9:LD:223:PHE:HB3	9:LD:226:TYR:HB2	1.88	0.56
18:LN:157:LYS:O	18:LN:162:ARG:NH1	2.37	0.56
20:LP:94:MET:HG2	20:LP:148:MET:HE2	1.87	0.56
50:SD:9:ARG:NH1	83:S2:1551:U:OP1	2.38	0.56
56:SR:72:LYS:NZ	56:SR:76:GLU:OE2	2.38	0.56
64:Sg:82:SER:OG	64:Sg:83:TRP:N	2.38	0.56
70:SH:143:ARG:HB2	70:SH:155:LYS:HB2	1.88	0.56
81:Sb:49:HIS:ND1	81:Sb:69:GLY:O	2.38	0.56
83:S2:106:C:OP1	83:S2:431:G:O2'	2.23	0.56
83:S2:1560:U:O2	83:S2:1575:G:O6	2.22	0.56
25:LU:56:LEU:HD12	25:LU:61:VAL:HG23	1.87	0.56
27:LW:5:LEU:HB3	27:LW:30:GLN:HE21	1.69	0.56
50:SD:94:ARG:O	50:SD:101:GLN:NE2	2.38	0.56
59:SU:87:ARG:NH2	83:S2:1447:G:O5'	2.39	0.56
80:Sa:43:ASN:HA	80:Sa:66:LYS:HD3	1.88	0.56
83:S2:59:U:N3	83:S2:62:G:OP1	2.26	0.56
83:S2:795:A:H2'	83:S2:796:G:C8	2.40	0.56
83:S2:907:G:H2'	83:S2:908:A:C8	2.40	0.56
3:L5:1253:G:H2'	3:L5:1256:G:H5'	1.86	0.56
3:L5:3717:A:OP2	3:L5:3735:G:N2	2.37	0.56
14:LI:3:ARG:HG3	14:LI:123:GLN:HE22	1.70	0.56
19:LO:54:TYR:OH	19:LO:73:PHE:O	2.24	0.56
54:SP:52:LYS:NZ	83:S2:1299:A:O2'	2.37	0.56
71:SI:165:GLN:HB3	71:SI:171:LEU:HD23	1.86	0.56
75:SO:75:MET:SD	75:SO:79:GLN:NE2	2.79	0.56
2:Pt:50:U:O4	2:Pt:64:G:O6	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:97:G:OP1	16:LL:16:LYS:NZ	2.33	0.56
3:L5:147:A:OP1	12:LG:197:LYS:NZ	2.38	0.56
3:L5:2084:C:O2	21:LQ:16:LYS:NZ	2.39	0.56
3:L5:2630:U:OP1	25:LU:48:LYS:NZ	2.39	0.56
52:SK:24:LYS:O	52:SK:42:ASN:ND2	2.39	0.56
58:ST:47:PRO:HA	83:S2:1539:U:H4'	1.88	0.56
75:SO:33:ILE:HB	75:SO:97:LEU:HD23	1.88	0.56
3:L5:5030:U:H2'	3:L5:5031:G:H8	1.71	0.56
55:SQ:40:GLU:O	55:SQ:45:ARG:NH1	2.38	0.56
65:SA:85:ARG:NH1	65:SA:203:PHE:O	2.39	0.56
83:S2:300:U:H2'	83:S2:301:A:H8	1.71	0.56
83:S2:1822:A:H2'	83:S2:1823:A:C8	2.41	0.56
2:Pt:50:U:O2	2:Pt:64:G:N2	2.24	0.56
3:L5:3689:G:O2'	3:L5:3818:UY1:OP2	2.23	0.56
3:L5:3917:A:H2'	3:L5:3918:G:H8	1.70	0.56
6:LA:180:LEU:HD21	46:Lp:22:LEU:HB3	1.87	0.56
54:SP:124:LYS:HE3	83:S2:1239:U:H5'	1.88	0.56
63:Sf:126:CYS:HB3	63:Sf:130:VAL:HG11	1.88	0.56
83:S2:90:G:OP1	83:S2:445:A:N6	2.39	0.56
83:S2:1340:U:OP2	83:S2:1341:C:O2'	2.23	0.56
83:S2:1562:C:H2'	83:S2:1563:G:H8	1.71	0.56
2:Pt:64:G:O2'	14:LI:24:ARG:NH2	2.39	0.56
3:L5:2049:G:HO2'	3:L5:3884:PSU:HO2'	1.54	0.56
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.70	0.56
3:L5:4742:G:H2'	3:L5:4743:G:H8	1.71	0.56
35:Le:87:VAL:HG23	35:Le:88:LEU:HD12	1.88	0.56
82:Se:8:ARG:NH1	83:S2:615:C:O3'	2.38	0.56
3:L5:2745:A:H2'	3:L5:2746:A:H8	1.71	0.56
3:L5:4107:G:N2	3:L5:4108:G:O6	2.39	0.56
7:LB:95:THR:OG1	7:LB:98:GLY:O	2.21	0.56
67:SC:200:ARG:O	72:SJ:54:ARG:NH2	2.30	0.56
83:S2:399:C:H5	83:S2:680:G:H5''	1.71	0.56
84:AT:12:G:H2'	84:AT:13:U:O4'	2.06	0.56
3:L5:1734:G:N2	3:L5:1735:U:O4	2.33	0.55
3:L5:2521:G:H4'	37:Lg:26:PRO:HD2	1.88	0.55
8:LC:262:GLU:HB3	8:LC:273:LEU:HD13	1.88	0.55
22:LR:172:ARG:HA	22:LR:175:GLU:HG2	1.87	0.55
50:SD:45:ARG:NH2	50:SD:85:GLU:OE1	2.38	0.55
59:SU:79:ARG:NH2	83:S2:1669:G:OP1	2.38	0.55
63:Sf:92:LYS:NZ	83:S2:1271:C:OP1	2.32	0.55
3:L5:139:G:H2'	3:L5:140:G:H8	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:369:G:N2	3:L5:372:A:OP2	2.36	0.55
3:L5:956:A:H1'	3:L5:2076:G:H5''	1.88	0.55
3:L5:2484:A:H62	3:L5:2494:U:H3	1.54	0.55
13:LH:51:LYS:HE2	13:LH:54:ARG:HH12	1.71	0.55
18:LN:108:ARG:NH2	18:LN:161:MET:SD	2.79	0.55
44:Ln:1:MET:HG3	83:S2:1706:G:H5'	1.87	0.55
63:Sf:102:VAL:HG22	63:Sf:104:LYS:HG2	1.88	0.55
65:SA:125:THR:O	65:SA:165:ASN:ND2	2.38	0.55
69:SG:2:LYS:HB2	69:SG:108:VAL:HG12	1.87	0.55
74:SN:14:SER:HB3	83:S2:1016:U:H5''	1.88	0.55
83:S2:1206:G:O2'	83:S2:1208:A:OP1	2.19	0.55
84:AT:9:A:N6	84:AT:23:U:OP2	2.36	0.55
2:Pt:9:A:O2'	2:Pt:10:G:N7	2.34	0.55
3:L5:88:A:N7	21:LQ:173:LYS:NZ	2.54	0.55
3:L5:1266:G:N1	32:Lb:94:ASP:OD2	2.32	0.55
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.41	0.55
21:LQ:79:THR:HB	21:LQ:136:THR:HG22	1.88	0.55
54:SP:131:PRO:HA	83:S2:1237:C:H5'	1.88	0.55
75:SO:84:ARG:HA	75:SO:87:GLU:HG2	1.87	0.55
83:S2:1566:G:N2	83:S2:1569:A:OP2	2.30	0.55
84:AT:59:A:O2'	84:AT:62:C:N4	2.37	0.55
3:L5:24:G:N7	40:Lj:46:LYS:NZ	2.55	0.55
3:L5:679:C:H2'	3:L5:680:G:H8	1.71	0.55
3:L5:1283:G:N1	3:L5:2076:G:OP1	2.32	0.55
29:LY:47:MET:HE3	29:LY:48:PRO:HD2	1.89	0.55
57:SS:92:ASP:HB2	57:SS:94:LYS:HD3	1.89	0.55
64:Sg:61:GLY:O	64:Sg:88:ARG:NH1	2.39	0.55
79:SY:80:ASP:OD1	79:SY:81:TYR:N	2.39	0.55
83:S2:165:G:OP2	83:S2:165:G:N2	2.31	0.55
83:S2:1513:C:H2'	83:S2:1514:G:H8	1.72	0.55
2:Pt:43:A:H2'	2:Pt:44:A:C8	2.42	0.55
3:L5:1086:C:H2'	3:L5:1087:A:H8	1.72	0.55
3:L5:1095:A:N1	3:L5:1200:G:C6	2.73	0.55
3:L5:1172:C:H42	3:L5:1188:C:H42	1.55	0.55
3:L5:4567:G:H5'	7:LB:20:LYS:HB3	1.88	0.55
49:Lt:51:GLY:HA3	49:Lt:61:LYS:HE3	1.88	0.55
51:SF:164:ARG:NH1	83:S2:1533:A:OP2	2.40	0.55
61:Sc:44:ARG:NH1	61:Sc:61:SER:O	2.40	0.55
70:SH:11:PRO:HG2	70:SH:44:ASN:HD22	1.72	0.55
3:L5:2848:G:O2'	3:L5:3838:U:O4	2.22	0.55
6:LA:245:ARG:HG3	6:LA:247:ARG:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LJ:141:ILE:HA	15:LJ:144:LYS:HD2	1.88	0.55
22:LR:160:GLU:OE1	22:LR:163:ARG:NH2	2.39	0.55
83:S2:902:G:O2'	83:S2:903:A:O4'	2.25	0.55
83:S2:1171:G:O2'	83:S2:1187:G:O6	2.22	0.55
83:S2:1722:G:O6	83:S2:1812:U:O2	2.23	0.55
3:L5:74:G:H1'	16:LL:62:PRO:HG3	1.89	0.55
3:L5:1328:G:O2'	3:L5:2349:A:OP1	2.24	0.55
3:L5:2845:A:H61	3:L5:3843:C:N4	2.05	0.55
3:L5:4501:U:OP1	7:LB:5:LYS:NZ	2.40	0.55
3:L5:4636:PSU:N1	34:Ld:79:ASN:OD1	2.40	0.55
10:LE:264:ILE:HD11	10:LE:267:LEU:HD22	1.88	0.55
11:LF:155:TYR:OH	11:LF:188:GLU:OE2	2.24	0.55
14:LI:47:PRO:HG2	14:LI:142:LEU:HG	1.89	0.55
30:LZ:9:LYS:NZ	30:LZ:83:THR:O	2.31	0.55
37:Lg:44:SER:OG	37:Lg:46:CYS:SG	2.65	0.55
65:SA:147:LEU:HD13	65:SA:161:ILE:HB	1.89	0.55
3:L5:2480:G:H2'	3:L5:2481:G:H8	1.72	0.55
3:L5:4910:G:H22	19:LO:107:GLY:HA3	1.72	0.55
41:Lk:5:ILE:HG21	41:Lk:11:PHE:HB2	1.89	0.55
44:Ln:17:ARG:NH1	83:S2:1173:A:OP1	2.39	0.55
51:SF:142:SER:HB2	61:Sc:50:VAL:HG22	1.87	0.55
68:SE:80:ILE:HG23	68:SE:81:THR:HG23	1.89	0.55
83:S2:1259:A:N6	83:S2:1519:U:O5'	2.40	0.55
7:LB:92:TYR:HB3	7:LB:99:LEU:HD22	1.89	0.55
85:CF:241:PRO:HG2	85:CF:269:THR:HG22	1.88	0.55
3:L5:1258:G:H2'	3:L5:1259:G:C8	2.41	0.55
3:L5:4740:G:O6	3:L5:4959:U:O2	2.25	0.55
57:SS:62:ASP:OD1	57:SS:62:ASP:N	2.39	0.55
68:SE:122:LYS:N	68:SE:162:ILE:O	2.40	0.55
69:SG:50:VAL:HA	69:SG:113:ILE:HA	1.88	0.55
69:SG:139:SER:OG	69:SG:142:ARG:NH2	2.38	0.55
85:CF:175:SER:HA	85:CF:178:ILE:HG22	1.88	0.55
3:L5:4163:U:OP2	12:LG:53:ARG:NH2	2.39	0.54
3:L5:4992:G:H2'	3:L5:4993:G:C8	2.42	0.54
59:SU:23:THR:HB	59:SU:113:GLU:HB3	1.89	0.54
83:S2:1568:C:H2'	83:S2:1569:A:C8	2.41	0.54
85:CF:345:ILE:HA	85:CF:399:ALA:HA	1.89	0.54
3:L5:300:A:H2'	3:L5:301:G:H8	1.72	0.54
3:L5:423:G:H21	20:LP:118:GLN:NE2	2.05	0.54
3:L5:1100:U:O4	3:L5:1194:G:O6	2.25	0.54
3:L5:1718:C:OP2	11:LF:200:ARG:NH2	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2832:A:OP1	34:Ld:47:LYS:NZ	2.34	0.54
3:L5:3898:G:H5'	7:LB:254:ILE:HG13	1.89	0.54
50:SD:160:SER:OG	83:S2:1386:A:OP2	2.23	0.54
83:S2:391:C:H2'	83:S2:392:A:H8	1.72	0.54
17:LM:101:LYS:HD2	19:LO:201:LEU:HD22	1.88	0.54
20:LP:109:VAL:HA	20:LP:112:LEU:HD13	1.88	0.54
65:SA:22:GLY:O	65:SA:24:HIS:ND1	2.41	0.54
67:SC:94:ILE:HD11	67:SC:159:LYS:HG2	1.89	0.54
71:SI:177:SER:OG	83:S2:219:U:O2'	2.24	0.54
83:S2:1850:MA6:H8	83:S2:1850:MA6:O5'	2.06	0.54
3:L5:1326:A2M:OP2	3:L5:4445:U:O2'	2.22	0.54
3:L5:1404:G:N7	3:L5:1408:G:N1	2.56	0.54
3:L5:4239:A:H2'	3:L5:4240:G:C8	2.42	0.54
20:LP:118:GLN:OE1	20:LP:120:ASN:ND2	2.40	0.54
50:SD:99:ILE:HG23	50:SD:173:ARG:HH21	1.71	0.54
59:SU:60:THR:OG1	83:S2:1548:G:OP1	2.25	0.54
64:Sg:286:CYS:HA	64:Sg:302:TYR:HD1	1.72	0.54
66:SB:112:SER:HB3	80:Sa:68:TYR:HE2	1.73	0.54
75:SO:42:VAL:HG13	75:SO:81:VAL:HG21	1.88	0.54
3:L5:3823:G:OP2	3:L5:3823:G:N2	2.34	0.54
3:L5:4670:C:O2'	3:L5:4672:A:OP2	2.22	0.54
83:S2:207:G:H3'	83:S2:208:G:H8	1.72	0.54
83:S2:1286:G:N2	83:S2:1312:G:O2'	2.40	0.54
3:L5:2404:A:O2'	40:Lj:12:ARG:O	2.22	0.54
10:LE:146:PRO:O	10:LE:200:LYS:NZ	2.41	0.54
11:LF:60:GLU:OE2	11:LF:192:HIS:NE2	2.37	0.54
54:SP:130:ARG:HD3	54:SP:131:PRO:HD2	1.89	0.54
61:Sc:10:LYS:HZ1	61:Sc:35:MET:HB2	1.73	0.54
65:SA:128:ARG:NH2	65:SA:151:ASP:O	2.39	0.54
3:L5:2017:A:O2'	3:L5:2018:C:O5'	2.26	0.54
9:LD:152:ARG:O	9:LD:157:ASN:ND2	2.40	0.54
59:SU:66:ARG:HG2	83:S2:1256:G:H8	1.73	0.54
64:Sg:107:ASP:HB2	64:Sg:125:ARG:HG3	1.90	0.54
73:SL:82:MET:HE3	73:SL:85:THR:HG23	1.90	0.54
83:S2:1179:G:N2	83:S2:1182:A:OP2	2.39	0.54
3:L5:170:C:H42	3:L5:266:C:N4	2.06	0.54
3:L5:1298:C:H2'	3:L5:1299:G:C8	2.43	0.54
3:L5:1984:A:N6	3:L5:2010:A:O2'	2.39	0.54
55:SQ:97:GLN:HE21	64:Sg:58:ALA:HB3	1.72	0.54
56:SR:16:ILE:HD11	56:SR:54:VAL:HG21	1.90	0.54
64:Sg:15:ASN:ND2	83:S2:1472:C:O3'	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:SL:88:ILE:HG21	73:SL:126:VAL:HG11	1.89	0.54
81:Sb:62:VAL:HG13	81:Sb:74:THR:HG21	1.89	0.54
85:CF:7:HIS:CE1	85:CF:306:ASP:HA	2.42	0.54
2:Pt:18:G:O2'	2:Pt:57:G:N2	2.29	0.54
3:L5:261:G:H2'	3:L5:262:G:C8	2.43	0.54
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.89	0.54
3:L5:2495:U:H2'	3:L5:2496:G:H8	1.73	0.54
17:LM:104:MET:HE3	17:LM:109:ARG:HG2	1.89	0.54
70:SH:42:GLU:HG2	70:SH:43:LEU:HD22	1.90	0.54
72:SJ:143:ASN:OD1	83:S2:823:U:N3	2.37	0.54
76:SV:42:VAL:HG13	76:SV:43:THR:HG23	1.89	0.54
83:S2:149:A:N7	83:S2:169:U:O2	2.40	0.54
83:S2:1337:4AC:H2'	83:S2:1338:G:H8	1.73	0.54
83:S2:1616:U:O2'	83:S2:1661:A:N3	2.38	0.54
85:CF:240:ARG:HD2	85:CF:304:PRO:HB2	1.90	0.54
3:L5:153:G:H2'	3:L5:154:G:H8	1.73	0.54
3:L5:2459:G:N2	3:L5:2462:C:OP2	2.37	0.54
3:L5:2756:G:O6	30:LZ:51:ARG:NH2	2.35	0.54
3:L5:4695:C:O2	43:Lm:106:ARG:NH2	2.41	0.54
8:LC:183:VAL:HA	8:LC:204:ARG:HB3	1.90	0.54
53:SM:117:GLU:O	53:SM:121:LYS:NZ	2.41	0.54
68:SE:100:ARG:HB2	68:SE:114:ILE:HD13	1.90	0.54
83:S2:1417:C:H42	83:S2:1422:G:H22	1.56	0.54
3:L5:2588:C:OP1	3:L5:2768:C:O2'	2.22	0.53
3:L5:2639:U:O2'	3:L5:2694:G:O6	2.27	0.53
3:L5:5024:C:H41	3:L5:5028:G:H21	1.56	0.53
44:Ln:2:ARG:NE	83:S2:1842:4AC:OP2	2.31	0.53
55:SQ:67:ASP:OD2	55:SQ:69:ARG:NH1	2.41	0.53
64:Sg:57:ARG:NH2	64:Sg:94:THR:O	2.40	0.53
72:SJ:113:GLN:OE1	72:SJ:154:GLN:NE2	2.38	0.53
75:SO:141:ARG:NH2	83:S2:1856:C:OP1	2.39	0.53
3:L5:491:G:H2'	3:L5:492:U:C6	2.43	0.53
3:L5:707:C:O2'	3:L5:4943:A:N1	2.34	0.53
3:L5:1414:C:H2'	3:L5:1415:G:H8	1.72	0.53
58:ST:143:LYS:HD2	58:ST:144:LYS:HG2	1.89	0.53
83:S2:1112:U:O2	83:S2:1121:G:O6	2.26	0.53
83:S2:1587:G:OP1	83:S2:1587:G:N2	2.41	0.53
83:S2:1755:C:H2'	83:S2:1756:C:C6	2.43	0.53
84:AT:67:C:H2'	84:AT:68:G:C8	2.43	0.53
3:L5:68:U:OP1	18:LN:178:HIS:ND1	2.38	0.53
3:L5:325:U:H2'	3:L5:326:C:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:943:A:H62	11:LF:151:ASN:HD21	1.57	0.53
3:L5:4472:G:O2'	43:Lm:100:TYR:O	2.25	0.53
3:L5:4935:C:H2'	3:L5:4936:G:C8	2.44	0.53
5:L8:21:C:OP1	8:LC:195:LYS:NZ	2.41	0.53
26:LV:123:LYS:NZ	26:LV:127:ASP:OD1	2.39	0.53
27:LW:119:LYS:O	27:LW:123:LYS:CB	2.56	0.53
45:Lo:99:ARG:HH11	45:Lo:100:LYS:H	1.57	0.53
54:SP:22:LEU:HA	54:SP:25:LEU:HB2	1.90	0.53
68:SE:187:ALA:O	68:SE:245:ARG:NH1	2.36	0.53
74:SN:106:ARG:HH12	83:S2:1077:A:P	2.32	0.53
77:SW:107:SER:HB2	83:S2:860:G:H21	1.73	0.53
3:L5:2884:G:H2'	3:L5:2885:A:H8	1.73	0.53
15:LJ:114:ASP:HB3	57:SS:14:ARG:HE	1.73	0.53
51:SF:60:ARG:HE	83:S2:1679:A:P	2.31	0.53
53:SM:87:GLU:HG3	53:SM:103:VAL:HG11	1.89	0.53
56:SR:6:THR:HA	83:S2:1373:C:H5'	1.89	0.53
78:SX:28:LYS:HE2	78:SX:32:LEU:HD11	1.91	0.53
83:S2:1589:A:N3	83:S2:1653:U:O2'	2.42	0.53
84:AT:57:C:N4	84:AT:58:G:O6	2.42	0.53
3:L5:256:G:H2'	3:L5:257:C:C6	2.43	0.53
3:L5:699:C:N4	3:L5:700:G:O6	2.41	0.53
3:L5:1655:C:OP2	31:La:26:ARG:NH1	2.41	0.53
9:LD:41:LYS:NZ	24:LT:30:TYR:O	2.27	0.53
10:LE:186:LEU:N	10:LE:250:GLN:OE1	2.41	0.53
64:Sg:68:ASP:HB3	64:Sg:111:VAL:HG12	1.91	0.53
73:SL:133:PRO:HG2	83:S2:383:G:H21	1.74	0.53
79:SY:20:ARG:NH2	79:SY:22:GLN:OE1	2.33	0.53
83:S2:388:U:H2'	83:S2:389:A:C8	2.43	0.53
3:L5:184:U:O2'	3:L5:189:G:O4'	2.26	0.53
3:L5:2498:C:H2'	3:L5:2499:C:H6	1.74	0.53
3:L5:2624:G:OP2	25:LU:97:ARG:NH2	2.42	0.53
3:L5:4088:C:H2'	3:L5:4089:G:H8	1.74	0.53
3:L5:4163:U:H5'	3:L5:4164:C:H5''	1.91	0.53
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.43	0.53
21:LQ:50:ARG:HH21	21:LQ:140:SER:HB2	1.74	0.53
24:LT:28:ALA:HA	24:LT:31:MET:HE3	1.89	0.53
35:Le:4:LEU:HD23	35:Le:121:ARG:HB2	1.89	0.53
48:Ls:93:GLU:HB2	48:Ls:98:ILE:HD11	1.89	0.53
54:SP:100:LYS:HB2	83:S2:1240:A:C6	2.44	0.53
65:SA:184:ARG:HE	65:SA:191:ARG:HA	1.72	0.53
68:SE:49:ARG:NH2	83:S2:496:C:OP1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SG:191:ARG:HH22	83:S2:312:G:H2'	1.73	0.53
71:SI:22:HIS:HB3	83:S2:433:A:H5''	1.89	0.53
75:SO:78:ALA:HB1	75:SO:119:LEU:HD12	1.90	0.53
77:SW:53:ILE:HB	77:SW:60:LYS:HB2	1.90	0.53
81:Sb:37:CYS:HB3	81:Sb:40:CYS:HB2	1.89	0.53
83:S2:511:U:H2'	83:S2:512:A:H8	1.73	0.53
83:S2:1337:4AC:H2'	83:S2:1338:G:C8	2.43	0.53
2:Pt:23:C:H2'	2:Pt:24:A:C8	2.44	0.53
3:L5:2539:C:H2'	3:L5:2540:C:C6	2.44	0.53
3:L5:2739:C:O2	6:LA:188:LYS:NZ	2.40	0.53
3:L5:3697:U:H5''	3:L5:3698:G:H5'	1.89	0.53
12:LG:83:PHE:HA	12:LG:183:ILE:HD13	1.91	0.53
14:LI:152:LEU:HB3	14:LI:165:ILE:HD12	1.90	0.53
15:LJ:22:LEU:HD22	15:LJ:128:LEU:HD12	1.90	0.53
47:Lr:119:ARG:HD3	47:Lr:122:LYS:NZ	2.19	0.53
51:SF:20:PHE:HD2	51:SF:23:TRP:HZ3	1.56	0.53
55:SQ:131:LYS:HB2	55:SQ:140:ARG:HH22	1.74	0.53
59:SU:56:MET:HG3	59:SU:86:LYS:HE2	1.91	0.53
65:SA:3:GLY:N	65:SA:56:GLU:OE1	2.41	0.53
66:SB:83:LYS:HD3	66:SB:106:THR:HG22	1.90	0.53
70:SH:20:GLU:HG2	70:SH:48:ALA:HB3	1.91	0.53
83:S2:1228:A:H2'	83:S2:1229:G:H8	1.74	0.53
3:L5:1994:C:H2'	3:L5:1995:G:C8	2.44	0.53
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.44	0.53
3:L5:4467:A:O2'	3:L5:4510:A:N3	2.30	0.53
56:SR:60:ARG:NH1	83:S2:1464:C:O3'	2.41	0.53
69:SG:190:ARG:NH2	83:S2:334:C:OP2	2.37	0.53
83:S2:874:G:H2'	83:S2:875:A:H8	1.74	0.53
83:S2:1240:A:N3	83:S2:1267:C:O2'	2.37	0.53
83:S2:1468:C:H2'	83:S2:1469:A:H8	1.73	0.53
3:L5:126:C:H2'	3:L5:127:G:H8	1.74	0.53
13:LH:93:ARG:HG2	13:LH:182:SER:HB3	1.91	0.53
47:Lr:28:GLU:OE2	47:Lr:31:ASN:ND2	2.32	0.53
52:SK:31:LYS:HZ2	52:SK:39:ASN:H	1.55	0.53
66:SB:186:ASN:OD1	66:SB:187:LYS:N	2.41	0.53
71:SI:126:GLY:O	71:SI:128:LYS:NZ	2.42	0.53
72:SJ:124:HIS:HD2	82:Se:31:ARG:HE	1.57	0.53
83:S2:609:U:H2'	83:S2:610:G:H8	1.74	0.53
83:S2:1417:C:N3	83:S2:1422:G:N1	2.53	0.53
83:S2:1753:C:H5'	83:S2:1780:G:H1	1.74	0.53
84:AT:39:C:H2'	84:AT:40:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.43	0.53
3:L5:2568:C:H2'	3:L5:2569:G:H8	1.72	0.53
3:L5:4274:A:H2'	3:L5:4275:G:H8	1.74	0.53
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.91	0.53
25:LU:28:PRO:HG3	25:LU:100:LEU:HD11	1.92	0.53
53:SM:49:LEU:HD21	53:SM:123:VAL:HG11	1.90	0.53
54:SP:81:ARG:NH1	54:SP:120:SER:OG	2.42	0.53
64:Sg:247:TRP:HB3	64:Sg:258:ILE:HD11	1.91	0.53
72:SJ:82:VAL:HG11	72:SJ:92:MET:HE1	1.90	0.53
82:Se:12:VAL:HA	82:Se:15:GLN:HG3	1.91	0.53
83:S2:107:A:H2'	83:S2:108:G:C8	2.44	0.53
83:S2:140:C:O2'	83:S2:143:U:OP1	2.27	0.53
3:L5:3611:A:H2	3:L5:5016:A:H8	1.55	0.52
3:L5:4098:A:H2'	3:L5:4099:G:H4'	1.91	0.52
7:LB:17:LEU:O	7:LB:19:ARG:N	2.41	0.52
9:LD:181:PRO:HD2	9:LD:195:HIS:CD2	2.44	0.52
69:SG:237:LEU:O	83:S2:787:G:N1	2.42	0.52
83:S2:664:A:O2'	83:S2:670:A:N1	2.38	0.52
83:S2:942:G:H2'	83:S2:943:U:C6	2.45	0.52
6:LA:117:GLU:O	6:LA:162:ASN:ND2	2.34	0.52
55:SQ:78:VAL:HG12	83:S2:1673:U:H5''	1.92	0.52
68:SE:18:TRP:NE1	68:SE:41:CYS:O	2.42	0.52
83:S2:291:G:H2'	83:S2:292:A:C8	2.45	0.52
3:L5:1802:A:H5''	3:L5:1803:G:H5'	1.92	0.52
9:LD:291:GLN:NE2	14:LI:213:HIS:O	2.36	0.52
55:SQ:125:ARG:HB2	83:S2:1648:G:H5''	1.92	0.52
68:SE:89:VAL:HG11	68:SE:119:ALA:HB1	1.90	0.52
72:SJ:136:ARG:NH2	72:SJ:138:ARG:O	2.42	0.52
76:SV:62:MET:HE3	77:SW:20:ARG:HH12	1.74	0.52
80:Sa:7:ASN:ND2	80:Sa:10:ARG:O	2.42	0.52
83:S2:889:U:OP2	83:S2:896:U:N3	2.43	0.52
85:CF:218:ARG:NH1	85:CF:234:CYS:O	2.37	0.52
3:L5:2876:OMG:HM22	3:L5:2877:G:H5'	1.90	0.52
3:L5:5002:U:OP2	7:LB:385:LYS:NZ	2.42	0.52
5:L8:67:U:H2'	5:L8:68:G:C8	2.45	0.52
24:LT:102:ARG:O	24:LT:106:LEU:HG	2.09	0.52
34:Ld:23:ARG:HG2	34:Ld:121:ASN:HA	1.91	0.52
52:SK:8:ARG:NH2	83:S2:1314:U:O2'	2.42	0.52
68:SE:36:HIS:CG	68:SE:85:GLY:HA3	2.44	0.52
79:SY:25:ILE:HD13	79:SY:44:LEU:HD11	1.92	0.52
83:S2:1825:A:H61	84:AT:37:C:H42	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:659:G:H2'	3:L5:660:A:H8	1.75	0.52
3:L5:966:A:OP2	3:L5:2092:G:N2	2.42	0.52
31:La:87:ARG:HH12	31:La:118:PRO:HG3	1.73	0.52
65:SA:104:THR:O	65:SA:107:THR:OG1	2.27	0.52
67:SC:202:THR:HG23	72:SJ:54:ARG:HH22	1.74	0.52
72:SJ:60:LEU:HD11	72:SJ:73:GLU:HG3	1.92	0.52
75:SO:134:PRO:HB3	83:S2:944:A:H5''	1.92	0.52
76:SV:36:VAL:N	76:SV:51:LYS:O	2.40	0.52
83:S2:487:U:H5'	85:CF:313:LYS:HZ1	1.74	0.52
3:L5:1982:G:N2	3:L5:2009:A:O2'	2.43	0.52
3:L5:4598:C:O2'	13:LH:121:LYS:NZ	2.42	0.52
34:Ld:29:ILE:O	34:Ld:33:ILE:HG12	2.09	0.52
46:Lp:7:LYS:O	46:Lp:27:LYS:NZ	2.43	0.52
53:SM:52:LEU:HD22	53:SM:78:LYS:HE3	1.91	0.52
56:SR:101:ASP:OD1	56:SR:102:THR:N	2.43	0.52
57:SS:132:ARG:NH1	83:S2:1623:A:N1	2.57	0.52
70:SH:83:LEU:HB3	70:SH:92:VAL:HG21	1.90	0.52
70:SH:165:ASN:O	70:SH:169:LYS:NZ	2.38	0.52
3:L5:1857:C:H2'	3:L5:1858:A:H8	1.75	0.52
57:SS:4:VAL:HG13	60:SZ:51:ASP:HA	1.91	0.52
72:SJ:145:PRO:HD2	83:S2:522:A:H5''	1.92	0.52
79:SY:10:ARG:HA	83:S2:839:C:H41	1.75	0.52
80:Sa:12:LYS:NZ	83:S2:1086:G:OP2	2.36	0.52
83:S2:543:C:H3'	83:S2:544:G:H8	1.73	0.52
83:S2:1144:A:H2'	83:S2:1145:A:C8	2.45	0.52
3:L5:2000:G:O2'	3:L5:2001:G:N7	2.42	0.52
3:L5:2480:G:H2'	3:L5:2481:G:C8	2.44	0.52
27:LW:7:SER:OG	27:LW:8:PHE:N	2.42	0.52
60:SZ:80:ARG:O	83:S2:1598:G:O2'	2.19	0.52
65:SA:53:ARG:HG2	76:SV:83:PHE:CZ	2.45	0.52
70:SH:74:LYS:HG3	70:SH:75:ILE:HG23	1.90	0.52
70:SH:105:THR:HG23	70:SH:107:LYS:H	1.75	0.52
80:Sa:51:ARG:O	80:Sa:55:GLU:HG2	2.09	0.52
2:Pt:29:C:H2'	2:Pt:30:G:H8	1.73	0.52
3:L5:2059:C:O2	23:LS:118:ARG:NH2	2.43	0.52
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.44	0.52
18:LN:104:GLU:HG3	18:LN:161:MET:HG2	1.90	0.52
19:LO:126:VAL:HG13	19:LO:127:VAL:HG13	1.92	0.52
35:Le:108:ARG:HD2	35:Le:128:ARG:HB2	1.92	0.52
67:SC:72:ASP:OD2	67:SC:272:HIS:NE2	2.43	0.52
71:SI:123:ARG:HH21	71:SI:129:LEU:HD11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:SL:22:ARG:NH2	73:SL:23:VAL:O	2.40	0.52
83:S2:1546:G:H21	83:S2:1670:C:H1'	1.75	0.52
3:L5:1979:A:N6	3:L5:1984:A:OP1	2.38	0.52
3:L5:4088:C:H2'	3:L5:4089:G:C8	2.45	0.52
6:LA:40:TYR:HA	6:LA:91:GLY:HA3	1.91	0.52
15:LJ:29:SER:OG	15:LJ:30:GLY:N	2.42	0.52
44:Ln:21:ARG:HD3	83:S2:1717:C:H4'	1.92	0.52
49:Lt:50:THR:OG1	49:Lt:72:GLU:OE1	2.27	0.52
61:Sc:39:SER:O	80:Sa:51:ARG:NH1	2.42	0.52
69:SG:169:PRO:O	83:S2:72:C:N4	2.43	0.52
79:SY:124:ASN:HD22	83:S2:84:A:H5''	1.75	0.52
3:L5:4288:C:O2'	3:L5:4321:U:OP1	2.28	0.51
11:LF:86:GLU:OE2	24:LT:136:ARG:N	2.35	0.51
41:Lk:27:LYS:O	41:Lk:70:LYS:NZ	2.44	0.51
59:SU:26:SER:OG	59:SU:110:VAL:HA	2.09	0.51
60:SZ:91:LEU:HG	60:SZ:96:LEU:HD21	1.91	0.51
28:LX:148:ASP:OD1	28:LX:149:VAL:N	2.43	0.51
43:Lm:79:GLU:CD	43:Lm:81:SER:HG	2.16	0.51
50:SD:137:VAL:HB	50:SD:185:LYS:HB2	1.92	0.51
55:SQ:4:LYS:HE3	83:S2:1423:C:H41	1.76	0.51
58:ST:62:ARG:NH2	83:S2:1543:U:OP2	2.42	0.51
69:SG:162:LEU:HG	69:SG:167:LYS:HE3	1.90	0.51
83:S2:996:A:H2'	83:S2:997:A:C8	2.46	0.51
3:L5:1084:C:H2'	3:L5:1085:C:H6	1.75	0.51
3:L5:1696:C:H5'	3:L5:1719:A:H1'	1.93	0.51
3:L5:2415:U:H2'	3:L5:2416:G:C8	2.46	0.51
3:L5:4730:C:N4	3:L5:4731:G:O6	2.43	0.51
3:L5:5047:C:O2'	3:L5:5050:C:OP2	2.22	0.51
12:LG:176:LYS:HG2	39:Li:43:MET:HE1	1.92	0.51
16:LL:127:PHE:O	38:Lh:117:ARG:NH2	2.39	0.51
47:Lr:83:ASN:HD22	47:Lr:83:ASN:C	2.19	0.51
51:SF:112:LEU:HD13	51:SF:177:LEU:HD21	1.92	0.51
55:SQ:42:ILE:HG22	55:SQ:44:PRO:HD2	1.92	0.51
67:SC:85:SER:OG	76:SV:25:GLY:O	2.25	0.51
67:SC:248:TYR:OH	76:SV:10:ASP:OD1	2.24	0.51
3:L5:66:A:O2'	3:L5:326:C:O2	2.28	0.51
3:L5:382:G:N1	3:L5:385:A:OP2	2.35	0.51
3:L5:1281:G:N1	10:LE:128:HIS:HB2	2.25	0.51
3:L5:4327:C:OP1	24:LT:70:HIS:NE2	2.43	0.51
29:LY:2:LYS:HD2	29:LY:7:VAL:HG23	1.91	0.51
68:SE:125:LYS:O	68:SE:142:HIS:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:135:G:H22	38:Lh:94:ARG:HG3	1.74	0.51
3:L5:268:G:H2'	3:L5:269:G:H8	1.76	0.51
3:L5:1514:U:H2'	3:L5:1515:A:C8	2.46	0.51
3:L5:1704:C:O3'	11:LF:46:ARG:NH1	2.44	0.51
3:L5:2458:C:O2	3:L5:3671:G:N2	2.43	0.51
3:L5:2896:G:OP1	22:LR:136:ARG:NH1	2.43	0.51
3:L5:3796:U:HO2'	83:S2:1720:U:HO2'	1.54	0.51
3:L5:4472:G:H5''	43:Lm:102:ARG:HH21	1.75	0.51
3:L5:5023:C:H5''	71:SI:124:LYS:HE3	1.93	0.51
11:LF:238:ASP:O	11:LF:241:ASN:ND2	2.42	0.51
12:LG:100:HIS:CD2	12:LG:103:ARG:HD2	2.45	0.51
13:LH:48:LEU:HD11	13:LH:56:ARG:HD3	1.92	0.51
36:Lf:78:HIS:HB3	36:Lf:83:MET:HB3	1.92	0.51
64:Sg:127:LYS:HE2	64:Sg:149:GLU:HA	1.92	0.51
68:SE:68:ARG:HD3	68:SE:76:VAL:HG11	1.93	0.51
75:SO:135:ILE:O	83:S2:943:U:O2'	2.28	0.51
83:S2:587:A:H5'	83:S2:592:C:H41	1.75	0.51
3:L5:1100:U:H1'	3:L5:1167:C:H42	1.74	0.51
3:L5:1766:A:OP2	3:L5:1768:C:O2'	2.24	0.51
3:L5:2601:A:N6	3:L5:2744:A:OP2	2.35	0.51
3:L5:2745:A:H2'	3:L5:2746:A:C8	2.46	0.51
3:L5:3949:A:OP1	3:L5:4065:G:N2	2.41	0.51
6:LA:116:LEU:HD23	6:LA:164:ALA:HB2	1.90	0.51
47:Lr:38:PHE:O	47:Lr:45:HIS:NE2	2.26	0.51
62:Sd:32:ARG:NH2	83:S2:1660:C:O2	2.44	0.51
66:SB:123:ALA:HB2	66:SB:165:ARG:HG2	1.92	0.51
69:SG:170:ARG:NH1	83:S2:72:C:O2	2.44	0.51
71:SI:98:LYS:HG3	71:SI:178:ARG:HG2	1.92	0.51
77:SW:11:LEU:HD12	77:SW:74:VAL:HB	1.93	0.51
83:S2:1253:A:OP2	83:S2:1526:G:N2	2.40	0.51
83:S2:1277:C:H2'	83:S2:1278:A:C8	2.46	0.51
83:S2:1552:G:O2'	83:S2:1555:U:O2'	2.27	0.51
3:L5:419:A:N3	3:L5:1332:C:O2'	2.42	0.51
3:L5:1396:G:O2'	3:L5:1468:C:O2'	2.26	0.51
3:L5:2405:G:HO2'	3:L5:2791:C:HO2'	1.56	0.51
3:L5:2696:A:H62	41:Lk:35:LYS:NZ	2.09	0.51
3:L5:3736:A:H2'	3:L5:3737:A:H8	1.75	0.51
3:L5:4989:U:H1'	3:L5:4990:C:H5	1.75	0.51
5:L8:153:C:OP1	12:LG:185:LYS:NZ	2.42	0.51
6:LA:101:VAL:HG22	6:LA:165:VAL:HG22	1.93	0.51
9:LD:107:ARG:NH1	9:LD:169:GLY:O	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LJ:78:LYS:O	15:LJ:82:ILE:HG12	2.10	0.51
30:LZ:22:LYS:HE3	30:LZ:134:LEU:HB2	1.92	0.51
40:Lj:52:LYS:HG3	40:Lj:55:ARG:NH2	2.26	0.51
47:Lr:26:SER:OG	47:Lr:28:GLU:OE1	2.20	0.51
56:SR:35:CYS:SG	56:SR:47:ARG:HG3	2.51	0.51
78:SX:45:SER:OG	83:S2:648:A:N3	2.41	0.51
83:S2:300:U:H2'	83:S2:301:A:C8	2.46	0.51
3:L5:159:C:H5'	39:Li:25:ARG:HH11	1.76	0.51
3:L5:964:A:H2'	3:L5:965:G:H4'	1.93	0.51
3:L5:1494:U:H2'	3:L5:1495:G:H8	1.76	0.51
3:L5:2017:A:O2'	3:L5:2018:C:H6	1.94	0.51
3:L5:4301:U:OP2	3:L5:4303:C:N4	2.44	0.51
6:LA:181:LYS:HB2	6:LA:184:ARG:HG3	1.93	0.51
63:Sf:103:LEU:HD12	63:Sf:105:TYR:CE1	2.46	0.51
64:Sg:148:SER:OG	64:Sg:149:GLU:OE1	2.23	0.51
71:SI:70:GLU:OE2	73:SL:21:LYS:NZ	2.39	0.51
78:SX:95:GLU:OE1	78:SX:140:ARG:NH1	2.44	0.51
3:L5:1669:A:H4'	3:L5:1685:G:N2	2.26	0.51
3:L5:1857:C:H2'	3:L5:1858:A:C8	2.45	0.51
5:L8:26:C:O2'	8:LC:53:ALA:O	2.26	0.51
8:LC:218:ILE:HA	8:LC:229:LEU:HD22	1.93	0.51
21:LQ:133:GLY:O	21:LQ:136:THR:OG1	2.26	0.51
46:Lp:75:SER:O	46:Lp:79:VAL:HG23	2.11	0.51
64:Sg:63:SER:HB2	83:S2:1398:G:H1'	1.92	0.51
66:SB:40:ASN:ND2	66:SB:76:ASN:OD1	2.44	0.51
71:SI:141:ARG:HH12	83:S2:191:A:H5''	1.75	0.51
79:SY:41:ARG:HE	79:SY:55:ILE:HG23	1.76	0.51
83:S2:327:G:H5''	83:S2:328:U:C2	2.45	0.51
83:S2:941:C:H2'	83:S2:942:G:C8	2.45	0.51
83:S2:1037:G:H4'	83:S2:1845:A:H4'	1.93	0.51
83:S2:1226:G:N1	83:S2:1639:G7M:OP2	2.42	0.51
84:AT:29:U:H2'	84:AT:30:C:O4'	2.11	0.51
3:L5:248:C:O2	29:LY:121:ARG:NH2	2.44	0.51
3:L5:1333:A:H2'	3:L5:1334:A:H8	1.76	0.51
3:L5:2492:C:H2'	3:L5:2493:G:C8	2.46	0.51
3:L5:2580:U:O2'	30:LZ:79:HIS:ND1	2.44	0.51
3:L5:2764:A:H2'	3:L5:2765:A:C8	2.46	0.51
3:L5:3732:A:H2'	3:L5:3733:A:C8	2.46	0.51
3:L5:4492:U:O2'	3:L5:4512:U:O2	2.22	0.51
3:L5:4619:U:H2'	3:L5:4620:OMU:H6	1.93	0.51
3:L5:4942:C:H4'	10:LE:154:THR:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LE:91:THR:HA	10:LE:108:LYS:HA	1.93	0.51
12:LG:162:ASP:HB3	12:LG:163:PRO:HD3	1.93	0.51
16:LL:17:ASP:O	16:LL:21:ARG:NH2	2.44	0.51
33:Lc:82:GLY:HA2	33:Lc:91:VAL:HG12	1.92	0.51
83:S2:1854:U:H2'	83:S2:1855:G:H8	1.75	0.51
3:L5:209:U:OP1	29:LY:63:LYS:NZ	2.35	0.50
3:L5:1084:C:H2'	3:L5:1085:C:C6	2.46	0.50
3:L5:2568:C:H2'	3:L5:2569:G:C8	2.46	0.50
3:L5:4680:G:H2'	3:L5:4681:A:C8	2.47	0.50
4:L7:119:U:C2	9:LD:261:VAL:HG11	2.46	0.50
34:Ld:54:MET:HE3	34:Ld:60:PRO:HA	1.93	0.50
41:Lk:26:LYS:HB2	41:Lk:69:LEU:HD12	1.92	0.50
53:SM:18:LEU:HD12	53:SM:123:VAL:HG22	1.93	0.50
71:SI:66:SER:H	71:SI:188:TYR:HA	1.75	0.50
83:S2:24:C:HO2'	83:S2:25:A:H8	1.58	0.50
83:S2:28:U:H2'	83:S2:29:G:C8	2.43	0.50
83:S2:600:G:H2'	83:S2:601:OMG:H8	1.75	0.50
83:S2:1004:PSU:H2'	83:S2:1005:G:H8	1.77	0.50
83:S2:1096:G:H1	83:S2:1136:U:H3	1.59	0.50
3:L5:1306:C:H2'	3:L5:1307:A:H8	1.76	0.50
3:L5:3641:U:H5	3:L5:3646:A:N7	2.08	0.50
3:L5:4322:G:N2	3:L5:4325:A:OP2	2.33	0.50
7:LB:258:HIS:HA	7:LB:260:ALA:N	2.25	0.50
16:LL:55:ILE:O	16:LL:97:SER:OG	2.29	0.50
16:LL:56:ARG:NH1	16:LL:74:ARG:O	2.41	0.50
19:LO:119:VAL:N	23:LS:168:THR:O	2.41	0.50
21:LQ:15:ARG:NH1	21:LQ:52:PHE:O	2.43	0.50
48:Ls:120:GLU:HB3	48:Ls:163:THR:HG22	1.94	0.50
51:SF:84:GLY:O	83:S2:1673:U:O2'	2.24	0.50
69:SG:174:PRO:O	83:S2:77:A:O2'	2.27	0.50
78:SX:5:ARG:NH1	83:S2:661:U:OP1	2.42	0.50
83:S2:1030:A:H2'	83:S2:1031:A2M:H8	1.94	0.50
3:L5:1426:G:N1	3:L5:1458:C:OP2	2.33	0.50
3:L5:3633:C:OP1	87:L5:5293:SPM:N10	2.41	0.50
3:L5:4146:G:H2'	3:L5:4147:G:C8	2.46	0.50
3:L5:4615:C:O3'	7:LB:357:ARG:NH2	2.44	0.50
11:LF:127:LYS:HB2	24:LT:133:ALA:HB3	1.93	0.50
12:LG:30:PRO:HG2	30:LZ:124:THR:HA	1.92	0.50
50:SD:72:VAL:HG21	52:SK:70:TYR:HE1	1.75	0.50
51:SF:123:GLU:OE2	61:Sc:63:ARG:NH2	2.43	0.50
58:ST:134:ILE:HA	58:ST:137:GLN:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:SE:64:ILE:HG23	79:SY:17:LEU:HD12	1.92	0.50
70:SH:12:ASN:ND2	70:SH:14:GLU:OE2	2.45	0.50
74:SN:124:ARG:NH1	83:S2:677:G:OP1	2.39	0.50
83:S2:1435:C:O2'	83:S2:1436:C:O4'	2.24	0.50
83:S2:1562:C:H2'	83:S2:1563:G:C8	2.46	0.50
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.27	0.50
3:L5:2777:G:H5''	3:L5:2778:G:H5'	1.94	0.50
3:L5:2884:G:H2'	3:L5:2885:A:C8	2.47	0.50
7:LB:258:HIS:HA	7:LB:260:ALA:H	1.76	0.50
24:LT:48:VAL:HG21	24:LT:94:GLU:HG2	1.92	0.50
30:LZ:92:ASP:OD2	30:LZ:94:THR:OG1	2.23	0.50
51:SF:97:PHE:HA	51:SF:100:ILE:HG12	1.92	0.50
64:Sg:31:ILE:HG21	64:Sg:299:PHE:HE2	1.76	0.50
68:SE:29:PRO:HA	83:S2:496:C:H5'	1.93	0.50
68:SE:45:ILE:HG13	68:SE:61:VAL:HG11	1.92	0.50
69:SG:92:ARG:O	83:S2:453:C:O2'	2.22	0.50
76:SV:51:LYS:HE2	76:SV:76:ASP:HB2	1.94	0.50
79:SY:11:LYS:HB2	79:SY:24:VAL:HG12	1.93	0.50
83:S2:1240:A:H2'	83:S2:1241:A:C8	2.47	0.50
3:L5:450:G:H1	3:L5:1297:U:H3	1.58	0.50
3:L5:1070:G:O2'	3:L5:1071:C:O5'	2.26	0.50
3:L5:1195:G:H2'	3:L5:1196:G:C8	2.47	0.50
3:L5:2491:C:H2'	3:L5:2492:C:C6	2.47	0.50
3:L5:3661:G:H4'	3:L5:3662:A:H5'	1.94	0.50
3:L5:4084:G:O6	6:LA:72:ARG:NH2	2.42	0.50
3:L5:4725:C:OP1	7:LB:103:LYS:NZ	2.45	0.50
5:L8:60:G:OP1	28:LX:68:ARG:NH2	2.41	0.50
14:LI:14:ASN:O	14:LI:128:ARG:NH2	2.24	0.50
48:Ls:53:VAL:HG23	48:Ls:89:VAL:HB	1.93	0.50
67:SC:167:ARG:HB3	67:SC:177:PRO:HB2	1.93	0.50
82:Se:8:ARG:HG2	82:Se:11:LYS:HD3	1.93	0.50
83:S2:454:U:H2'	83:S2:455:A:H8	1.76	0.50
83:S2:482:G:N1	83:S2:485:A:OP2	2.44	0.50
3:L5:1333:A:H2'	3:L5:1334:A:C8	2.46	0.50
3:L5:2613:C:OP1	37:Lg:24:ARG:NH2	2.44	0.50
4:L7:92:C:H2'	4:L7:93:G:H8	1.75	0.50
56:SR:77:GLU:HA	56:SR:80:ARG:HG2	1.93	0.50
57:SS:121:ARG:HG3	57:SS:131:VAL:HB	1.93	0.50
65:SA:77:ILE:HG13	65:SA:99:ILE:HB	1.94	0.50
70:SH:51:ILE:HG21	70:SH:179:LYS:HG2	1.94	0.50
72:SJ:80:ARG:NH2	83:S2:818:A:OP1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:CF:150:VAL:HG11	85:CF:174:VAL:HG11	1.94	0.50
3:L5:137:G:H2'	3:L5:138:G:C8	2.46	0.50
3:L5:494:U:H2'	3:L5:495:C:C6	2.47	0.50
3:L5:691:C:H2'	3:L5:692:A:C8	2.47	0.50
3:L5:1942:A:H2'	3:L5:1943:A:H8	1.76	0.50
3:L5:3661:G:N7	6:LA:152:SER:OG	2.43	0.50
3:L5:3785:A2M:H2	3:L5:4551:U:O2	2.12	0.50
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.47	0.50
3:L5:4723:A:H2'	3:L5:4724:A:C8	2.46	0.50
5:L8:39:G:OP1	38:Lh:86:LYS:NZ	2.44	0.50
23:LS:99:ASP:OD1	23:LS:100:LEU:N	2.45	0.50
49:Lt:59:THR:HA	49:Lt:80:LEU:HD11	1.94	0.50
53:SM:79:VAL:HG11	53:SM:85:LEU:HD22	1.94	0.50
55:SQ:80:GLN:O	55:SQ:84:ILE:HD12	2.11	0.50
56:SR:31:ASN:HA	56:SR:34:VAL:HG22	1.93	0.50
74:SN:46:THR:HG22	74:SN:49:GLN:HG3	1.92	0.50
75:SO:34:PHE:HB3	75:SO:41:PHE:HB2	1.94	0.50
83:S2:1401:A:H2'	83:S2:1402:A:C8	2.46	0.50
83:S2:1801:A:H2'	83:S2:1802:C:C6	2.47	0.50
3:L5:1367:C:O2'	3:L5:1369:C:OP2	2.27	0.50
3:L5:1516:G:O2'	16:LL:18:TRP:NE1	2.42	0.50
3:L5:1916:G:N3	3:L5:2067:C:O2'	2.45	0.50
3:L5:3748:A:HO2'	6:LA:223:SER:HG	1.58	0.50
53:SM:58:GLU:OE1	53:SM:61:TYR:N	2.45	0.50
83:S2:84:A:N3	83:S2:150:A:O2'	2.41	0.50
83:S2:941:C:H2'	83:S2:942:G:H8	1.76	0.50
83:S2:1588:A:H2'	83:S2:1589:A:C8	2.46	0.50
85:CF:142:THR:HG23	85:CF:435:VAL:HG13	1.94	0.50
3:L5:120:A:N1	3:L5:148:C:O2'	2.42	0.50
3:L5:1989:G:H2'	3:L5:1990:A:C8	2.47	0.50
3:L5:2464:C:HO2'	3:L5:2465:C:H6	1.57	0.50
3:L5:2522:G:OP1	37:Lg:29:ARG:NH1	2.45	0.50
3:L5:4238:G:H2'	3:L5:4239:A:H8	1.77	0.50
9:LD:52:ILE:HA	9:LD:147:ASP:HB3	1.94	0.50
52:SK:53:LYS:NZ	52:SK:69:TRP:HD1	2.10	0.50
63:Sf:110:GLU:HG2	63:Sf:113:LYS:HD3	1.93	0.50
83:S2:323:C:H2'	83:S2:327:G:H1	1.77	0.50
83:S2:857:U:H2'	83:S2:858:A:C8	2.47	0.50
83:S2:1533:A:H2	83:S2:1536:G:N3	2.10	0.50
83:S2:1692:U:H2'	83:S2:1693:G:H8	1.76	0.50
3:L5:432:U:H1'	87:L5:5294:SPM:H82	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1171:G:O6	3:L5:1190:C:N4	2.39	0.49
3:L5:1270:A:H8	3:L5:2106:G:H21	1.59	0.49
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.46	0.49
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.47	0.49
3:L5:3599:A:H2'	3:L5:3600:G:C8	2.47	0.49
8:LC:315:LYS:HD2	11:LF:168:ALA:HB1	1.93	0.49
11:LF:237:GLU:OE2	23:LS:37:HIS:NE2	2.45	0.49
13:LH:24:THR:HA	13:LH:37:ASP:HA	1.94	0.49
42:LI:21:ARG:HG2	42:LI:22:PRO:HD2	1.94	0.49
48:Ls:13:TYR:O	48:Ls:17:ILE:HG12	2.11	0.49
68:SE:11:ARG:NH1	68:SE:24:THR:OG1	2.44	0.49
70:SH:30:LEU:HG	70:SH:33:ASN:HD22	1.77	0.49
77:SW:49:GLU:O	77:SW:64:ASN:ND2	2.43	0.49
78:SX:107:ARG:HG2	78:SX:112:VAL:HG22	1.94	0.49
83:S2:1083:A:N7	83:S2:1841:C:O2'	2.40	0.49
83:S2:1777:G:H2'	83:S2:1778:C:H6	1.75	0.49
3:L5:93:G:H2'	3:L5:94:A:C8	2.47	0.49
3:L5:180:C:H2'	3:L5:181:C:H6	1.78	0.49
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.48	0.49
3:L5:4457:PSU:H1'	7:LB:252:ALA:HB3	1.94	0.49
3:L5:4627:U:H4'	7:LB:373:LYS:HE2	1.94	0.49
6:LA:247:ARG:HH21	83:S2:1070:A:H5'	1.78	0.49
7:LB:29:VAL:HG12	7:LB:31:SER:H	1.77	0.49
14:LI:184:MET:HA	14:LI:187:LYS:HE3	1.93	0.49
56:SR:1:MET:HA	83:S2:1467:C:H5''	1.94	0.49
63:Sf:138:ARG:NH2	83:S2:1292:C:N3	2.43	0.49
64:Sg:258:ILE:HG23	64:Sg:267:VAL:HG23	1.93	0.49
67:SC:180:VAL:HG23	67:SC:197:PRO:HG3	1.94	0.49
83:S2:1457:U:H2'	83:S2:1458:G:H8	1.76	0.49
3:L5:305:A:P	18:LN:15:GLN:HE22	2.36	0.49
3:L5:1971:C:H2'	3:L5:1972:G:C8	2.47	0.49
3:L5:1974:U:H4'	3:L5:1975:G:H3'	1.94	0.49
3:L5:1992:U:H4'	3:L5:1993:C:H5''	1.94	0.49
3:L5:2257:C:O2'	3:L5:2259:G:OP2	2.22	0.49
3:L5:2638:G:H22	3:L5:2719:C:P	2.35	0.49
8:LC:146:GLU:HG2	8:LC:175:LYS:HB3	1.94	0.49
17:LM:24:LEU:HB2	17:LM:43:THR:HG21	1.95	0.49
24:LT:43:LYS:O	24:LT:58:HIS:ND1	2.45	0.49
67:SC:70:VAL:HG11	67:SC:93:ILE:HG12	1.95	0.49
67:SC:168:GLY:N	67:SC:179:THR:O	2.35	0.49
3:L5:1351:G:O6	21:LQ:55:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2492:C:H2'	3:L5:2493:G:H8	1.77	0.49
3:L5:4743:G:H2'	3:L5:4744:A:C8	2.47	0.49
7:LB:220:ILE:HG12	7:LB:278:THR:HG23	1.94	0.49
56:SR:47:ARG:O	56:SR:50:ILE:HG22	2.12	0.49
73:SL:103:GLU:HG3	78:SX:11:ARG:HB2	1.94	0.49
82:Se:32:ALA:HB2	83:S2:525:A:H5''	1.93	0.49
83:S2:102:A:H4'	83:S2:104:A:C8	2.48	0.49
3:L5:418:A:C2	5:L8:17:A:H1'	2.47	0.49
3:L5:1366:G:H5''	16:LL:36:ARG:HH12	1.77	0.49
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.41	0.49
3:L5:4742:G:H2'	3:L5:4743:G:C8	2.47	0.49
6:LA:206:PRO:HG3	6:LA:213:GLY:HA3	1.93	0.49
7:LB:218:ASP:OD2	7:LB:348:ARG:NH2	2.33	0.49
10:LE:190:HIS:HB3	10:LE:193:PHE:HD2	1.78	0.49
31:La:100:ILE:HG12	31:La:123:ILE:HD12	1.95	0.49
47:Lr:2:SER:OG	47:Lr:3:ALA:N	2.45	0.49
50:SD:7:LYS:HD2	59:SU:25:THR:HG21	1.95	0.49
64:Sg:106:LYS:HB3	64:Sg:125:ARG:HB2	1.94	0.49
68:SE:87:MET:HE1	68:SE:123:LEU:H	1.76	0.49
69:SG:92:ARG:NH1	83:S2:1738:C:OP1	2.40	0.49
74:SN:99:ARG:NH2	74:SN:119:GLU:OE2	2.44	0.49
81:Sb:11:SER:OG	81:Sb:14:GLU:OE1	2.26	0.49
83:S2:1103:C:H2'	83:S2:1104:G:H8	1.77	0.49
83:S2:1372:U:OP1	83:S2:1385:G:N2	2.44	0.49
84:AT:21:U:C4	84:AT:47:G:H1'	2.47	0.49
85:CF:10:ILE:HD12	85:CF:87:VAL:HG21	1.94	0.49
85:CF:349:HIS:H	85:CF:396:SER:HB2	1.78	0.49
3:L5:3723:A:H2'	3:L5:3724:A:H8	1.77	0.49
6:LA:7:GLY:HA2	6:LA:10:LYS:HG3	1.94	0.49
17:LM:71:LYS:O	17:LM:75:GLN:HG3	2.13	0.49
34:Ld:62:VAL:HG22	34:Ld:104:THR:HB	1.95	0.49
43:Lm:109:ASN:ND2	43:Lm:119:ASN:HB3	2.27	0.49
52:SK:49:MET:O	52:SK:53:LYS:HG2	2.13	0.49
52:SK:76:ILE:O	52:SK:80:ARG:HG2	2.12	0.49
57:SS:136:THR:HG22	83:S2:1520:G:H5''	1.93	0.49
63:Sf:107:LYS:NZ	63:Sf:108:VAL:O	2.38	0.49
64:Sg:8:ARG:HE	64:Sg:311:GLN:HB2	1.78	0.49
65:SA:180:ARG:HD3	65:SA:195:TRP:HB2	1.93	0.49
68:SE:62:LYS:HB2	68:SE:80:ILE:HD12	1.95	0.49
72:SJ:40:LYS:HG2	82:Se:34:ARG:HH12	1.77	0.49
74:SN:92:ILE:HD13	74:SN:122:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1215:C:O2'	83:S2:1645:C:OP2	2.24	0.49
83:S2:1417:C:O2	83:S2:1422:G:C6	2.66	0.49
85:CF:114:LEU:HD23	85:CF:150:VAL:HG22	1.94	0.49
2:Pt:23:C:H2'	2:Pt:24:A:H8	1.77	0.49
3:L5:54:G:O2'	18:LN:108:ARG:NH2	2.37	0.49
3:L5:444:G:H2'	3:L5:445:U:C6	2.48	0.49
3:L5:959:G:O2'	3:L5:2263:A:N6	2.45	0.49
3:L5:2622:G:O6	25:LU:81:ARG:NH2	2.46	0.49
3:L5:3680:U:OP1	6:LA:54:ARG:NH2	2.34	0.49
3:L5:3718:A2M:H2'	3:L5:3719:A:O4'	2.13	0.49
3:L5:3944:G:H1	3:L5:4069:U:H3	1.61	0.49
3:L5:4967:A:H2'	3:L5:4968:A:H8	1.77	0.49
13:LH:41:ILE:HG22	13:LH:43:VAL:HG13	1.94	0.49
17:LM:6:PHE:H	17:LM:11:ARG:NH2	2.11	0.49
24:LT:9:ARG:O	24:LT:55:LYS:NZ	2.39	0.49
29:LY:10:ASP:HB3	29:LY:13:LYS:HB2	1.93	0.49
55:SQ:90:LYS:HA	55:SQ:93:VAL:HG22	1.94	0.49
69:SG:133:LEU:HD12	83:S2:65:C:C4	2.47	0.49
83:S2:27:A2M:H2'	83:S2:28:U:O4'	2.12	0.49
83:S2:525:A:H2'	83:S2:526:A:H8	1.77	0.49
83:S2:880:G:H3'	83:S2:881:G:H8	1.76	0.49
83:S2:1467:C:H2'	83:S2:1468:C:H6	1.77	0.49
3:L5:139:G:H2'	3:L5:140:G:C8	2.47	0.49
3:L5:2083:C:P	21:LQ:14:ARG:HH22	2.35	0.49
3:L5:2657:G:OP2	33:Lc:36:LYS:NZ	2.33	0.49
3:L5:2896:G:H5''	22:LR:134:ASN:HD22	1.78	0.49
3:L5:4954:G:H2'	3:L5:4955:A:H8	1.78	0.49
5:L8:111:U:OP2	42:Ll:8:ARG:NH1	2.46	0.49
7:LB:63:PRO:O	7:LB:357:ARG:NH2	2.45	0.49
51:SF:103:LEU:HD11	60:SZ:67:LEU:HD22	1.94	0.49
60:SZ:99:LEU:HD11	60:SZ:102:LYS:HB2	1.94	0.49
64:Sg:40:ILE:HD11	64:Sg:66:VAL:HG11	1.93	0.49
64:Sg:159:ASN:OD1	64:Sg:161:SER:OG	2.27	0.49
64:Sg:195:LEU:HD23	64:Sg:211:GLY:HA3	1.94	0.49
67:SC:123:ARG:HG2	67:SC:145:LYS:HD3	1.95	0.49
67:SC:191:VAL:HG11	67:SC:236:PHE:HA	1.94	0.49
71:SI:86:SER:OG	83:S2:376:A:N3	2.43	0.49
83:S2:527:C:H2'	83:S2:528:A:H8	1.78	0.49
83:S2:563:G:O2'	83:S2:564:A:OP1	2.30	0.49
83:S2:1004:PSU:H2'	83:S2:1005:G:C8	2.47	0.49
83:S2:1438:A:H2'	83:S2:1439:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1777:G:H2'	83:S2:1778:C:C6	2.48	0.49
83:S2:1779:G:H2'	83:S2:1780:G:C8	2.47	0.49
1:CI:70:ALA:HB2	22:LR:54:PRO:HG3	1.95	0.49
3:L5:729:G:H5''	11:LF:76:ARG:HD2	1.94	0.49
3:L5:734:G:H22	3:L5:929:A:H2	1.61	0.49
3:L5:1279:A:O2'	3:L5:1281:G:N7	2.39	0.49
3:L5:2675:G:N1	33:Lc:33:GLN:OE1	2.36	0.49
3:L5:3910:C:H2'	3:L5:3911:C:H6	1.77	0.49
3:L5:4685:U:H2'	3:L5:4686:G:C8	2.47	0.49
14:LI:36:LEU:HD11	14:LI:69:ARG:HH11	1.78	0.49
17:LM:119:ARG:HG3	19:LO:189:ILE:HG23	1.93	0.49
34:Ld:45:ALA:O	34:Ld:49:ILE:HD12	2.13	0.49
62:Sd:48:LYS:HZ3	62:Sd:53:ILE:HG22	1.78	0.49
63:Sf:134:SER:H	83:S2:1308:U:HO2'	1.54	0.49
63:Sf:147:THR:OG1	83:S2:1292:C:O2'	2.29	0.49
64:Sg:280:LYS:NZ	83:S2:1459:G:OP2	2.42	0.49
79:SY:105:LYS:NZ	83:S2:507:G:O6	2.46	0.49
80:Sa:59:PHE:HB2	80:Sa:62:TYR:HB2	1.94	0.49
83:S2:162:C:H2'	83:S2:163:U:O4'	2.13	0.49
3:L5:97:G:N7	16:LL:13:HIS:NE2	2.53	0.49
3:L5:239:C:OP1	29:LY:46:SER:OG	2.27	0.49
3:L5:2899:C:OP1	22:LR:108:ARG:NH2	2.35	0.49
16:LL:64:VAL:HA	16:LL:67:HIS:CD2	2.35	0.49
42:LI:12:PHE:HE2	42:LI:51:LEU:HD22	1.78	0.49
49:Lt:114:ARG:NH1	49:Lt:126:SER:O	2.46	0.49
50:SD:51:LEU:HD12	50:SD:91:VAL:HG12	1.94	0.49
59:SU:61:LEU:HD12	59:SU:82:MET:HB3	1.94	0.49
60:SZ:42:ASP:OD1	60:SZ:42:ASP:N	2.44	0.49
64:Sg:40:ILE:HB	64:Sg:59:LEU:HB2	1.93	0.49
64:Sg:207:CYS:SG	64:Sg:219:TRP:HB2	2.53	0.49
70:SH:7:LYS:HD3	70:SH:10:LYS:HB3	1.94	0.49
72:SJ:111:GLN:HE21	72:SJ:123:ILE:HG13	1.76	0.49
83:S2:1010:G:H2'	83:S2:1011:A:C8	2.48	0.49
3:L5:262:G:H2'	3:L5:263:G:C8	2.39	0.48
3:L5:679:C:H2'	3:L5:680:G:C8	2.48	0.48
7:LB:36:ASP:N	7:LB:36:ASP:OD1	2.46	0.48
7:LB:119:TYR:OH	7:LB:129:ALA:N	2.42	0.48
22:LR:30:ASN:OD1	22:LR:31:GLU:N	2.45	0.48
22:LR:91:GLU:OE1	22:LR:91:GLU:N	2.44	0.48
31:La:95:THR:HG23	31:La:97:ALA:H	1.78	0.48
44:Ln:10:MET:HE2	83:S2:1172:U:H4'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SG:181:THR:HG22	69:SG:183:ARG:H	1.77	0.48
73:SL:68:ILE:HD13	73:SL:131:CYS:HB3	1.94	0.48
76:SV:17:CYS:HB2	76:SV:56:CYS:HB3	1.94	0.48
77:SW:115:GLU:HA	77:SW:118:ARG:HB2	1.94	0.48
83:S2:511:U:H2'	83:S2:512:A:C8	2.48	0.48
3:L5:386:A:O2'	29:LY:87:ARG:NH1	2.46	0.48
3:L5:1697:G:H22	3:L5:2084:C:P	2.36	0.48
3:L5:4195:G:O2'	3:L5:4442:PSU:OP1	2.24	0.48
3:L5:4260:U:H2'	3:L5:4261:C:C6	2.48	0.48
4:L7:48:G:OP1	9:LD:226:TYR:OH	2.29	0.48
6:LA:229:ALA:HB3	6:LA:234:LYS:HB3	1.95	0.48
19:LO:168:TYR:CE2	19:LO:172:LYS:HD2	2.47	0.48
73:SL:49:GLU:OE1	73:SL:116:CYS:HA	2.13	0.48
83:S2:993:G:OP1	83:S2:1131:G:N2	2.39	0.48
83:S2:1656:G:O6	83:S2:1668:U:O4	2.31	0.48
3:L5:711:A:H2'	3:L5:712:C:C6	2.48	0.48
3:L5:4966:A:H5''	7:LB:128:LYS:HG3	1.95	0.48
34:Ld:18:ASN:OD1	34:Ld:19:GLU:N	2.47	0.48
69:SG:7:PHE:HB3	69:SG:10:THR:HG22	1.95	0.48
83:S2:1405:A:H2'	83:S2:1406:G:O4'	2.13	0.48
85:CF:294:MET:HE2	85:CF:299:LEU:HD21	1.95	0.48
3:L5:907:C:H2'	3:L5:908:G:H8	1.79	0.48
3:L5:978:G:H2'	3:L5:979:C:C6	2.48	0.48
3:L5:1601:A:OP1	40:Lj:5:THR:OG1	2.25	0.48
3:L5:2878:G:OP2	3:L5:2879:A:O2'	2.29	0.48
15:LJ:38:LYS:HG3	15:LJ:42:GLN:HE22	1.78	0.48
18:LN:99:GLN:O	18:LN:103:GLU:HG3	2.11	0.48
30:LZ:33:THR:OG1	30:LZ:35:ASP:OD1	2.31	0.48
50:SD:126:ILE:O	50:SD:129:SER:OG	2.25	0.48
64:Sg:120:ILE:HB	64:Sg:132:TRP:HB2	1.96	0.48
67:SC:227:ARG:NH2	83:S2:663:C:O2'	2.46	0.48
69:SG:33:ALA:HA	69:SG:51:ARG:HD2	1.96	0.48
70:SH:10:LYS:NZ	70:SH:16:PRO:O	2.45	0.48
73:SL:78:THR:HG22	73:SL:79:LYS:HG3	1.94	0.48
83:S2:16:G:H2'	83:S2:17:C:C6	2.49	0.48
83:S2:145:G:H2'	83:S2:146:G:C8	2.48	0.48
83:S2:1010:G:H2'	83:S2:1011:A:H8	1.79	0.48
85:CF:349:HIS:ND1	85:CF:351:GLY:O	2.45	0.48
1:CI:72:ARG:NH2	22:LR:25:ASP:OD2	2.46	0.48
3:L5:1969:G:H4'	48:Ls:36:GLY:HA2	1.95	0.48
3:L5:2407:G:OP2	3:L5:2407:G:N2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4523:A2M:H1'	3:L5:4558:U:C4	2.48	0.48
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.49	0.48
12:LG:175:ARG:HG2	12:LG:230:TYR:CD2	2.48	0.48
17:LM:93:LYS:HA	17:LM:96:GLU:HG3	1.95	0.48
29:LY:4:ASN:HB3	29:LY:7:VAL:HG22	1.93	0.48
33:Lc:38:ILE:HD11	33:Lc:46:VAL:HG21	1.95	0.48
36:Lf:35:ALA:HB3	36:Lf:38:GLU:HG3	1.96	0.48
50:SD:161:GLY:HA3	83:S2:1388:A:H61	1.78	0.48
54:SP:125:PRO:HG3	57:SS:127:TRP:CZ2	2.49	0.48
63:Sf:103:LEU:HD12	63:Sf:105:TYR:HE1	1.78	0.48
71:SI:141:ARG:NH2	83:S2:192:C:OP2	2.47	0.48
85:CF:73:ILE:HG23	85:CF:98:PHE:CE1	2.48	0.48
85:CF:370:CYS:SG	85:CF:371:LYS:N	2.86	0.48
3:L5:705:G:H2'	3:L5:706:C:C6	2.48	0.48
3:L5:2870:A:H2'	3:L5:2871:A:C8	2.48	0.48
3:L5:5054:C:H4'	3:L5:5055:G:H8	1.79	0.48
7:LB:217:ILE:HD12	7:LB:347:LEU:HB3	1.93	0.48
13:LH:115:ARG:HD3	13:LH:123:ILE:HD12	1.96	0.48
56:SR:32:LYS:NZ	83:S2:1452:A:OP2	2.46	0.48
57:SS:102:GLY:HA2	57:SS:105:ASN:HD21	1.78	0.48
79:SY:78:SER:OG	79:SY:80:ASP:OD1	2.23	0.48
83:S2:487:U:H5'	85:CF:313:LYS:NZ	2.28	0.48
83:S2:549:C:H2'	83:S2:550:C:C6	2.48	0.48
83:S2:804:U:H2'	83:S2:805:U:C6	2.49	0.48
83:S2:1324:G:N2	83:S2:1504:U:O2	2.38	0.48
85:CF:243:ASP:OD1	85:CF:244:LYS:NZ	2.39	0.48
3:L5:181:C:H2'	3:L5:182:G:C8	2.48	0.48
3:L5:381:U:H4'	3:L5:415:G:H5'	1.94	0.48
3:L5:705:G:OP2	35:Le:5:ARG:NH1	2.45	0.48
3:L5:1438:U:H4'	11:LF:31:LYS:HE3	1.96	0.48
3:L5:2468:U:O2'	3:L5:2506:G:N2	2.47	0.48
3:L5:3664:G:H2'	3:L5:3665:G:H8	1.79	0.48
3:L5:4070:U:H2'	3:L5:4071:U:C6	2.49	0.48
7:LB:220:ILE:HB	7:LB:346:THR:HB	1.96	0.48
57:SS:26:ILE:HG22	57:SS:56:ALA:HA	1.95	0.48
67:SC:169:TYR:OH	67:SC:175:GLY:O	2.30	0.48
74:SN:5:HIS:HB3	74:SN:117:LEU:HD13	1.95	0.48
83:S2:516:A:N1	83:S2:643:A:O2'	2.42	0.48
83:S2:1348:G:H2'	83:S2:1349:G:H8	1.78	0.48
3:L5:318:A:H2'	3:L5:319:A:C8	2.49	0.48
3:L5:4064:C:H2'	3:L5:4065:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4095:G:N7	3:L5:4096:C:N4	2.61	0.48
9:LD:62:CYS:HB3	9:LD:105:LEU:HD22	1.95	0.48
16:LL:59:VAL:HG21	16:LL:73:GLY:HA3	1.94	0.48
33:Lc:48:LEU:HD11	33:Lc:60:ILE:HG21	1.94	0.48
56:SR:91:LEU:HD11	65:SA:21:ALA:HB2	1.95	0.48
58:ST:104:LEU:HD22	58:ST:121:ARG:HD2	1.96	0.48
74:SN:88:LEU:O	74:SN:92:ILE:HG12	2.14	0.48
83:S2:17:C:O2'	83:S2:1194:A:N1	2.46	0.48
83:S2:352:U:H2'	83:S2:353:C:C6	2.49	0.48
3:L5:10:A:H2'	3:L5:11:G:C8	2.49	0.48
3:L5:1175:A:H4'	9:LD:268:ARG:HH21	1.79	0.48
3:L5:1756:U:O2'	3:L5:1758:G:OP2	2.25	0.48
3:L5:4941:G:OP2	10:LE:188:ARG:NH2	2.38	0.48
6:LA:117:GLU:OE2	6:LA:163:ARG:NE	2.47	0.48
7:LB:369:ASP:OD1	7:LB:373:LYS:NZ	2.44	0.48
11:LF:105:VAL:HG13	11:LF:136:VAL:HG12	1.96	0.48
49:Lt:22:VAL:HA	49:Lt:48:LYS:HG2	1.96	0.48
50:SD:159:HIS:N	83:S2:1385:G:OP1	2.41	0.48
52:SK:27:VAL:HG23	52:SK:28:HIS:CD2	2.49	0.48
56:SR:59:LYS:HD3	56:SR:62:GLN:HE22	1.77	0.48
69:SG:39:ASP:OD1	69:SG:47:GLY:N	2.46	0.48
69:SG:202:ASN:ND2	83:S2:125:C:OP1	2.41	0.48
77:SW:53:ILE:N	77:SW:60:LYS:O	2.46	0.48
83:S2:329:G:H2'	83:S2:330:G:C8	2.48	0.48
83:S2:677:G:H21	83:S2:1028:A:H62	1.61	0.48
83:S2:1643:U:H2'	83:S2:1644:C:C6	2.48	0.48
3:L5:438:G:OP1	35:Le:16:ARG:NH1	2.44	0.48
3:L5:716:C:OP1	8:LC:317:ASN:HB2	2.14	0.48
3:L5:4868:G:O2'	3:L5:4872:G:OP1	2.31	0.48
3:L5:4959:U:H2'	3:L5:4960:G:C8	2.49	0.48
7:LB:27:GLY:HA2	7:LB:276:HIS:CD2	2.49	0.48
8:LC:1:MET:O	8:LC:29:LYS:NZ	2.45	0.48
14:LI:66:GLU:OE2	14:LI:69:ARG:NH2	2.35	0.48
33:Lc:45:LEU:HB2	33:Lc:104:ILE:HD11	1.95	0.48
38:Lh:89:ARG:O	38:Lh:93:ARG:HG2	2.14	0.48
50:SD:145:GLN:O	83:S2:1332:A:O2'	2.29	0.48
50:SD:163:PRO:HA	50:SD:166:TYR:CZ	2.49	0.48
54:SP:55:SER:HA	54:SP:58:LYS:HE3	1.96	0.48
62:Sd:54:LYS:NZ	83:S2:1482:C:OP1	2.41	0.48
63:Sf:121:CYS:HB3	63:Sf:130:VAL:HG13	1.95	0.48
69:SG:132:ARG:NH2	83:S2:152:U:O4'	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:SJ:121:LYS:HD3	83:S2:527:C:H4'	1.95	0.48
77:SW:25:VAL:HG12	77:SW:65:LEU:HD21	1.96	0.48
81:Sb:45:THR:OG1	81:Sb:82:LYS:NZ	2.47	0.48
83:S2:1797:U:H2'	83:S2:1798:C:C6	2.48	0.48
85:CF:359:PRO:HB3	85:CF:428:ASP:HB2	1.95	0.48
3:L5:327:U:HO2'	39:Li:30:ARG:HH11	1.59	0.47
3:L5:440:U:O2'	36:Lf:91:ASN:O	2.28	0.47
3:L5:1294:A:H1'	3:L5:1296:G:N1	2.29	0.47
3:L5:1390:G:N2	3:L5:1393:G:OP2	2.40	0.47
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.14	0.47
3:L5:1699:A:H4'	8:LC:306:ARG:HH22	1.78	0.47
3:L5:2007:G:H21	3:L5:2012:A:H62	1.61	0.47
3:L5:2570:U:H2'	3:L5:2571:C:C6	2.49	0.47
3:L5:2706:G:H1	22:LR:43:LYS:HE2	1.79	0.47
3:L5:3945:A:H2'	3:L5:3946:G:C8	2.48	0.47
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.46	0.47
5:L8:60:G:O6	5:L8:96:C:O2'	2.29	0.47
6:LA:20:VAL:HA	6:LA:23:ARG:HG3	1.95	0.47
23:LS:15:ARG:HD2	23:LS:25:PRO:HG2	1.96	0.47
57:SS:24:ARG:HG3	57:SS:29:ALA:HB2	1.95	0.47
83:S2:628:A:N6	83:S2:1500:G:O2'	2.47	0.47
3:L5:223:G:OP2	8:LC:165:LYS:NZ	2.46	0.47
3:L5:705:G:P	35:Le:5:ARG:HH22	2.37	0.47
3:L5:1897:A:O5'	21:LQ:2:GLY:N	2.47	0.47
4:L7:99:G:N7	23:LS:55:LYS:NZ	2.48	0.47
9:LD:146:LEU:HB2	9:LD:163:LEU:HD12	1.96	0.47
11:LF:57:TYR:OH	11:LF:189:ASP:OD1	2.28	0.47
34:Ld:93:ASN:O	34:Ld:95:ASP:N	2.47	0.47
40:Lj:27:TYR:HA	40:Lj:34:CYS:HA	1.95	0.47
54:SP:79:HIS:HD2	83:S2:1298:G:C4	2.32	0.47
59:SU:38:ASP:HA	59:SU:41:ARG:NE	2.26	0.47
60:SZ:46:ASN:O	60:SZ:80:ARG:NH2	2.48	0.47
64:Sg:85:GLY:HA2	64:Sg:108:VAL:HG23	1.96	0.47
66:SB:23:ASP:N	66:SB:23:ASP:OD1	2.46	0.47
68:SE:180:LEU:HB3	68:SE:229:GLY:HA3	1.96	0.47
70:SH:143:ARG:HH21	77:SW:54:ASP:H	1.61	0.47
83:S2:980:A:H2'	83:S2:981:A:C8	2.50	0.47
83:S2:1467:C:H2'	83:S2:1468:C:C6	2.50	0.47
3:L5:1268:G:N7	32:Lb:111:ARG:NH2	2.62	0.47
3:L5:1411:C:H2'	3:L5:1412:G:C8	2.50	0.47
3:L5:4302:U:H4'	24:LT:5:LYS:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4622:A:H4'	7:LB:13:SER:HB2	1.96	0.47
11:LF:192:HIS:O	11:LF:196:THR:OG1	2.29	0.47
17:LM:11:ARG:CZ	17:LM:61:ILE:HD11	2.45	0.47
52:SK:64:TRP:HB3	62:Sd:23:VAL:HA	1.95	0.47
74:SN:83:ASP:OD1	74:SN:84:LEU:N	2.46	0.47
75:SO:38:ASN:ND2	83:S2:960:U:OP2	2.46	0.47
83:S2:692:G:N7	83:S2:693:A:N6	2.62	0.47
83:S2:1103:C:H2'	83:S2:1104:G:C8	2.48	0.47
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.97	0.47
3:L5:1996:C:H4'	48:Ls:44:ARG:HG2	1.96	0.47
3:L5:2898:G:OP2	22:LR:135:LYS:NZ	2.42	0.47
3:L5:3870:C:H2'	3:L5:3871:A:H8	1.78	0.47
5:L8:155:C:OP1	12:LG:89:ARG:NH1	2.44	0.47
10:LE:223:ARG:HH22	10:LE:238:GLU:HG3	1.78	0.47
14:LI:103:LEU:H	14:LI:112:GLN:HE22	1.62	0.47
27:LW:97:LYS:O	27:LW:99:GLU:N	2.46	0.47
55:SQ:82:TYR:O	55:SQ:85:ARG:HG2	2.14	0.47
64:Sg:218:LEU:HB2	64:Sg:228:TYR:HB3	1.94	0.47
68:SE:88:ASP:OD1	68:SE:122:LYS:NZ	2.32	0.47
69:SG:163:ASN:HA	69:SG:167:LYS:HD3	1.95	0.47
83:S2:15:U:H2'	83:S2:16:G:O4'	2.14	0.47
83:S2:120:U:H2'	83:S2:121:OMU:H6	1.95	0.47
83:S2:520:A:O2'	83:S2:825:A:N3	2.45	0.47
83:S2:1243:U:OP2	83:S2:1518:C:O2'	2.27	0.47
83:S2:1692:U:H2'	83:S2:1693:G:C8	2.49	0.47
83:S2:1743:G:N2	83:S2:1791:A:H62	2.13	0.47
83:S2:1825:A:N6	84:AT:37:C:H42	2.12	0.47
3:L5:4122:G:O2'	30:LZ:136:PHE:OXT	2.26	0.47
3:L5:4991:U:H2'	3:L5:4992:G:C8	2.49	0.47
3:L5:5027:C:H41	71:SI:170:LYS:HD3	1.78	0.47
5:L8:119:C:H2'	5:L8:120:G:H8	1.78	0.47
8:LC:345:ARG:O	8:LC:348:LYS:HG3	2.14	0.47
20:LP:45:THR:HG22	20:LP:49:LYS:HE2	1.96	0.47
20:LP:138:PRO:HB3	20:LP:140:MET:HE3	1.95	0.47
21:LQ:155:ALA:O	21:LQ:158:THR:OG1	2.29	0.47
26:LV:131:ARG:NH2	85:CF:68:GLU:OE1	2.47	0.47
48:Ls:53:VAL:HA	48:Ls:89:VAL:HA	1.96	0.47
51:SF:73:THR:HG22	51:SF:93:VAL:HG21	1.96	0.47
53:SM:44:LYS:HE3	63:Sf:129:GLY:H	1.77	0.47
62:Sd:33:LYS:HE2	62:Sd:34:TYR:CZ	2.50	0.47
75:SO:131:ASP:OD1	75:SO:133:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2111:G:N2	3:L5:2251:G:O2'	2.47	0.47
3:L5:2808:G:O3'	22:LR:60:ARG:NH1	2.48	0.47
3:L5:3720:G:H22	3:L5:3733:A:H2	1.63	0.47
3:L5:3841:OMC:HM23	3:L5:3841:OMC:H1'	1.77	0.47
3:L5:4887:C:N4	3:L5:4932:U:H3	2.11	0.47
16:LL:110:LEU:O	16:LL:114:VAL:HG13	2.15	0.47
16:LL:140:SER:HA	16:LL:143:GLU:HG2	1.96	0.47
18:LN:140:LYS:HD3	18:LN:140:LYS:HA	1.68	0.47
23:LS:83:ARG:HG3	23:LS:125:GLN:HB2	1.95	0.47
52:SK:55:ARG:HG3	52:SK:57:TYR:HD2	1.79	0.47
57:SS:63:GLU:HA	57:SS:66:ARG:HE	1.79	0.47
64:Sg:124:SER:OG	64:Sg:125:ARG:N	2.47	0.47
83:S2:1117:C:H2'	83:S2:1118:C:C6	2.49	0.47
83:S2:1217:A:H2'	83:S2:1218:C:C6	2.48	0.47
83:S2:1532:C:O2'	83:S2:1601:A:N1	2.48	0.47
83:S2:1748:G:N2	83:S2:1786:U:O2	2.35	0.47
3:L5:109:G:OP2	16:LL:74:ARG:NH2	2.44	0.47
3:L5:667:A:H5'	47:Lr:46:ARG:NH2	2.29	0.47
3:L5:725:G:P	8:LC:350:ARG:HH22	2.37	0.47
3:L5:959:G:C8	10:LE:123:ARG:HG2	2.49	0.47
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.50	0.47
3:L5:1973:G:O2'	49:Lt:117:ARG:NH1	2.39	0.47
3:L5:2845:A:N6	3:L5:3843:C:H42	2.10	0.47
3:L5:3867:A2M:HM'3	3:L5:3867:A2M:H1'	1.56	0.47
3:L5:4954:G:H2'	3:L5:4955:A:C8	2.49	0.47
3:L5:4965:U:H4'	3:L5:4966:A:H5'	1.96	0.47
4:L7:2:U:H3	4:L7:117:G:H1	1.63	0.47
5:L8:39:G:H1'	5:L8:103:A:N6	2.30	0.47
6:LA:131:GLY:H	6:LA:169:VAL:HG13	1.79	0.47
9:LD:41:LYS:NZ	24:LT:32:ARG:O	2.48	0.47
9:LD:51:MET:HE1	9:LD:163:LEU:HA	1.97	0.47
11:LF:116:GLN:HB2	21:LQ:3:VAL:HG23	1.95	0.47
12:LG:120:LYS:HE2	12:LG:125:LYS:HB2	1.97	0.47
29:LY:30:MET:HB3	29:LY:101:PRO:HG3	1.97	0.47
33:Lc:51:ASN:HB2	33:Lc:77:ASN:HB2	1.97	0.47
57:SS:89:ASP:OD1	57:SS:90:VAL:N	2.48	0.47
57:SS:106:LYS:HA	57:SS:109:GLU:HG2	1.96	0.47
69:SG:121:ILE:HD13	69:SG:124:LEU:HD22	1.95	0.47
69:SG:134:GLY:O	83:S2:65:C:N4	2.36	0.47
83:S2:955:A:N1	83:S2:968:U:O2'	2.46	0.47
83:S2:1468:C:H2'	83:S2:1469:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1478:U:H2'	83:S2:1479:G:C8	2.50	0.47
85:CF:341:THR:HB	85:CF:440:ALA:HB3	1.97	0.47
3:L5:7:C:H2'	3:L5:8:U:C6	2.50	0.47
3:L5:667:A:H5''	3:L5:668:C:H5''	1.97	0.47
3:L5:1179:U:H3'	3:L5:1180:C:H5''	1.96	0.47
3:L5:4761:G:H2'	3:L5:4762:A:H8	1.80	0.47
3:L5:4910:G:N2	19:LO:106:ASP:O	2.48	0.47
26:LV:42:VAL:HB	26:LV:45:ILE:HG13	1.97	0.47
36:Lf:45:LYS:HD2	36:Lf:105:LEU:HA	1.97	0.47
56:SR:35:CYS:HA	56:SR:38:ILE:HG12	1.96	0.47
66:SB:82:ARG:NH1	66:SB:189:ILE:O	2.48	0.47
69:SG:164:LYS:H	69:SG:167:LYS:HB3	1.79	0.47
79:SY:104:ARG:HG2	79:SY:108:LYS:HE2	1.97	0.47
80:Sa:44:ILE:HG23	80:Sa:45:VAL:HG13	1.95	0.47
81:Sb:34:ASP:HB3	81:Sb:82:LYS:HE3	1.95	0.47
83:S2:534:G:H2'	83:S2:535:G:H8	1.80	0.47
83:S2:834:C:H42	83:S2:839:C:H42	1.63	0.47
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.50	0.47
3:L5:1983:A:O2'	3:L5:2011:C:OP1	2.32	0.47
3:L5:2279:A:O2'	35:Le:48:ARG:NH2	2.48	0.47
3:L5:4239:A:H2'	3:L5:4240:G:H8	1.80	0.47
3:L5:4617:G:OP1	7:LB:62:ARG:NH1	2.41	0.47
4:L7:39:C:H4'	15:LJ:47:THR:HG23	1.97	0.47
4:L7:110:G:H2'	4:L7:111:C:C6	2.50	0.47
5:L8:47:C:H1'	5:L8:61:A:H2'	1.96	0.47
9:LD:289:ARG:O	9:LD:292:GLU:HG3	2.15	0.47
24:LT:88:ARG:NH1	32:Lb:33:LYS:O	2.47	0.47
29:LY:114:ASP:O	29:LY:118:ILE:HD12	2.15	0.47
63:Sf:97:LYS:NZ	63:Sf:100:LEU:H	2.13	0.47
67:SC:84:PHE:CE2	67:SC:264:SER:HA	2.50	0.47
73:SL:85:THR:HG21	83:S2:373:G:H4'	1.96	0.47
80:Sa:4:LYS:NZ	83:S2:1863:A:OP2	2.41	0.47
83:S2:455:A:H2'	83:S2:456:C:C6	2.49	0.47
83:S2:603:C:N4	83:S2:620:G:O6	2.44	0.47
3:L5:965:G:H21	3:L5:2092:G:H1'	1.80	0.47
3:L5:3723:A:H2'	3:L5:3724:A:C8	2.50	0.47
3:L5:4091:G:H2'	3:L5:4092:G:H8	1.79	0.47
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.50	0.47
3:L5:4748:U:H5''	36:Lf:54:LYS:HE3	1.97	0.47
5:L8:90:C:H2'	5:L8:91:A:C8	2.50	0.47
7:LB:288:GLY:HA3	7:LB:330:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LD:209:ARG:O	9:LD:213:GLU:HG2	2.15	0.47
9:LD:211:LEU:HB3	9:LD:219:TYR:HB2	1.96	0.47
20:LP:17:SER:HB2	20:LP:98:ALA:HB2	1.96	0.47
48:Ls:30:VAL:HG21	48:Ls:187:LEU:HG	1.96	0.47
60:SZ:58:LEU:HD12	60:SZ:62:VAL:HG21	1.97	0.47
67:SC:194:ARG:HD3	67:SC:196:ILE:HD11	1.97	0.47
76:SV:30:ALA:O	76:SV:60:ARG:HD3	2.15	0.47
83:S2:1845:A:H2'	83:S2:1846:G:C8	2.50	0.47
3:L5:3911:C:H2'	3:L5:3912:U:H6	1.79	0.46
3:L5:4238:G:H2'	3:L5:4239:A:C8	2.49	0.46
12:LG:89:ARG:O	12:LG:93:THR:OG1	2.26	0.46
15:LJ:102:THR:OG1	15:LJ:104:ASN:OD1	2.32	0.46
24:LT:127:GLN:NE2	24:LT:129:LYS:O	2.48	0.46
51:SF:51:HIS:NE2	83:S2:1674:G:OP1	2.36	0.46
53:SM:57:ASP:OD1	83:S2:1285:G:N1	2.31	0.46
58:ST:39:LEU:HD21	58:ST:52:TRP:CZ3	2.50	0.46
71:SI:25:ARG:HA	83:S2:448:A:H5''	1.98	0.46
71:SI:25:ARG:HH22	83:S2:434:G:P	2.38	0.46
71:SI:139:LYS:HE3	71:SI:149:TYR:CE2	2.51	0.46
72:SJ:59:GLU:O	72:SJ:62:THR:OG1	2.32	0.46
80:Sa:12:LYS:HG3	80:Sa:15:ARG:HB2	1.98	0.46
83:S2:517:OMC:H2'	83:S2:518:G:O4'	2.16	0.46
83:S2:1201:U:H2'	83:S2:1202:U:C6	2.50	0.46
3:L5:75:G:O2'	16:LL:101:ARG:NH1	2.43	0.46
3:L5:3867:A2M:H2'	3:L5:3868:G:O4'	2.15	0.46
3:L5:4761:G:H2'	3:L5:4762:A:C8	2.50	0.46
10:LE:223:ARG:HB3	10:LE:224:LYS:HB2	1.95	0.46
56:SR:29:HIS:HA	56:SR:32:LYS:HG2	1.97	0.46
61:Sc:17:VAL:HA	61:Sc:30:VAL:HG12	1.97	0.46
62:Sd:8:TRP:HZ3	83:S2:1512:C:H5''	1.79	0.46
64:Sg:292:SER:OG	64:Sg:293:ALA:N	2.48	0.46
69:SG:37:ALA:HA	69:SG:49:VAL:HA	1.96	0.46
72:SJ:38:ARG:N	72:SJ:42:GLU:OE2	2.48	0.46
83:S2:1393:G:H2'	83:S2:1394:G:C8	2.50	0.46
83:S2:1713:C:H2'	83:S2:1714:U:C6	2.50	0.46
85:CF:103:ILE:HD13	85:CF:362:ASP:OD2	2.16	0.46
3:L5:1613:A:H5''	6:LA:183:GLY:HA2	1.97	0.46
3:L5:2540:C:H2'	3:L5:2541:G:H8	1.80	0.46
3:L5:4077:A:N1	3:L5:4171:C:N4	2.61	0.46
3:L5:4605:A:H4'	85:CF:130:ASN:HD21	1.81	0.46
3:L5:4991:U:H2'	3:L5:4992:G:H8	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L7:40:U:O2	15:LJ:75:ARG:NE	2.35	0.46
7:LB:73:VAL:O	26:LV:89:ARG:NH2	2.46	0.46
50:SD:40:ARG:NH2	59:SU:106:ILE:O	2.48	0.46
53:SM:14:VAL:HG21	53:SM:126:GLU:HG3	1.96	0.46
55:SQ:140:ARG:HB2	83:S2:1644:C:H4'	1.97	0.46
70:SH:73:GLN:HB3	70:SH:135:PHE:CZ	2.50	0.46
71:SI:37:LYS:NZ	71:SI:93:THR:OG1	2.48	0.46
74:SN:26:LEU:HD21	74:SN:60:VAL:HG12	1.98	0.46
79:SY:7:ILE:HG22	79:SY:27:VAL:HG12	1.96	0.46
83:S2:1277:C:H2'	83:S2:1278:A:H8	1.79	0.46
83:S2:1523:C:H2'	83:S2:1524:G:H8	1.80	0.46
83:S2:1534:C:H4'	83:S2:1535:U:H5''	1.97	0.46
3:L5:264:C:H2'	3:L5:265:C:C4	2.50	0.46
3:L5:2579:G:N2	3:L5:2582:A:OP2	2.40	0.46
3:L5:2822:G:H5''	22:LR:18:GLY:HA3	1.96	0.46
3:L5:3690:U:H2'	3:L5:3691:G:O4'	2.16	0.46
3:L5:4524:G:N3	7:LB:252:ALA:HB1	2.31	0.46
8:LC:207:PRO:HB3	8:LC:249:PHE:CD2	2.50	0.46
13:LH:92:MET:HE2	13:LH:179:ILE:HG22	1.97	0.46
21:LQ:15:ARG:HB3	21:LQ:52:PHE:HB3	1.97	0.46
38:Lh:87:LYS:HB3	38:Lh:91:MET:HE2	1.97	0.46
46:Lp:82:ALA:O	46:Lp:86:LEU:HG	2.14	0.46
51:SF:83:ASN:OD1	83:S2:1651:A:O2'	2.31	0.46
57:SS:105:ASN:HA	57:SS:108:ARG:CD	2.45	0.46
64:Sg:107:ASP:OD2	64:Sg:125:ARG:NH1	2.48	0.46
65:SA:34:MET:HE1	65:SA:162:PRO:HB3	1.98	0.46
78:SX:129:SER:HB2	83:S2:29:G:H4'	1.97	0.46
82:Se:3:HIS:O	84:AT:27:G:O2'	2.25	0.46
83:S2:495:U:H2'	83:S2:496:C:O4'	2.16	0.46
83:S2:1420:G:O2'	83:S2:1421:A:N3	2.48	0.46
83:S2:1825:A:OP1	84:AT:38:A:O2'	2.27	0.46
85:CF:323:GLY:HA3	85:CF:366:ALA:HB2	1.98	0.46
3:L5:180:C:H2'	3:L5:181:C:C6	2.50	0.46
3:L5:257:C:H2'	3:L5:258:G:C8	2.51	0.46
3:L5:1091:C:H2'	3:L5:1092:G:H8	1.81	0.46
3:L5:1241:C:H5	32:Lb:118:LEU:HD23	1.81	0.46
3:L5:1399:G:H2'	3:L5:1400:G:H8	1.80	0.46
3:L5:1563:A:H2'	3:L5:1564:A:C8	2.50	0.46
3:L5:1683:PSU:H2'	3:L5:1684:A:C8	2.50	0.46
3:L5:3654:G:O2'	3:L5:3693:U:OP1	2.30	0.46
3:L5:3856:A:H5''	20:LP:83:TRP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L7:57:C:H2'	4:L7:58:A:H8	1.80	0.46
14:LI:87:MET:HG3	14:LI:138:ILE:HG12	1.96	0.46
17:LM:25:VAL:HB	17:LM:38:VAL:HG13	1.97	0.46
19:LO:9:LEU:HD23	19:LO:118:MET:HB2	1.97	0.46
25:LU:23:LEU:HB3	25:LU:70:ILE:HG23	1.96	0.46
34:Ld:92:ARG:HG3	34:Ld:94:GLU:HB2	1.98	0.46
51:SF:63:LYS:NZ	83:S2:1678:A:OP2	2.34	0.46
52:SK:29:MET:SD	52:SK:42:ASN:HB2	2.56	0.46
54:SP:87:PRO:HD3	54:SP:112:ILE:HD11	1.98	0.46
64:Sg:22:ALA:HB1	64:Sg:71:ILE:HG23	1.98	0.46
65:SA:147:LEU:HD12	65:SA:163:CYS:SG	2.56	0.46
74:SN:29:THR:OG1	74:SN:32:ASP:OD2	2.22	0.46
83:S2:737:G:H2'	83:S2:738:C:H4'	1.97	0.46
83:S2:1579:A:H4'	83:S2:1581:C:H5	1.80	0.46
3:L5:92:C:OP1	88:L5:5262:SPD:N10	2.49	0.46
3:L5:150:U:OP2	12:LG:200:THR:OG1	2.26	0.46
3:L5:2458:C:O2'	3:L5:3671:G:N3	2.45	0.46
3:L5:3606:U:H2'	3:L5:3607:U:C6	2.50	0.46
3:L5:4688:C:H2'	3:L5:4689:PSU:C6	2.51	0.46
5:L8:148:A:H2'	5:L8:149:G:C8	2.51	0.46
16:LL:206:ASP:HA	16:LL:209:LYS:HD3	1.97	0.46
34:Ld:24:GLU:OE2	34:Ld:87:ARG:NH2	2.41	0.46
49:Lt:12:VAL:HG11	49:Lt:65:GLN:H	1.79	0.46
67:SC:114:LYS:HE2	83:S2:1202:U:H4'	1.96	0.46
69:SG:2:LYS:HB3	69:SG:15:LEU:HD11	1.98	0.46
72:SJ:40:LYS:NZ	83:S2:641:A:OP1	2.32	0.46
73:SL:111:VAL:HG12	73:SL:140:PHE:HB2	1.97	0.46
83:S2:27:A2M:HM'3	83:S2:27:A2M:H1'	1.69	0.46
2:Pt:22:U:H2'	2:Pt:23:C:H6	1.81	0.46
3:L5:267:G:H2'	3:L5:268:G:H8	1.80	0.46
3:L5:1733:G:N3	3:L5:4214:A:H2'	2.30	0.46
3:L5:1995:G:H2'	3:L5:1996:C:C6	2.51	0.46
3:L5:2079:G:H2'	3:L5:2080:U:C6	2.51	0.46
3:L5:2611:A:H2'	3:L5:2612:G:C8	2.51	0.46
3:L5:3595:U:H5''	3:L5:3597:G:OP2	2.16	0.46
3:L5:4775:C:H41	3:L5:4859:C:N4	2.14	0.46
5:L8:5:U:H2'	5:L8:6:C:H6	1.81	0.46
10:LE:72:LYS:HD3	32:Lb:119:CYS:HB3	1.97	0.46
13:LH:41:ILE:HD12	13:LH:73:ILE:HD11	1.96	0.46
50:SD:66:ILE:HD11	50:SD:86:LEU:HB3	1.98	0.46
53:SM:20:GLU:HG2	53:SM:119:GLN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SQ:53:GLU:HG3	55:SQ:85:ARG:HH21	1.81	0.46
70:SH:126:HIS:CE1	70:SH:181:THR:HG23	2.51	0.46
83:S2:656:G:H5'	83:S2:662:G:N2	2.31	0.46
83:S2:1203:G:H2'	83:S2:1204:A:H8	1.79	0.46
83:S2:1806:A:H2'	83:S2:1807:C:C6	2.51	0.46
3:L5:1431:C:H2'	3:L5:1432:G:O4'	2.15	0.46
3:L5:1875:C:H2'	3:L5:1876:U:C6	2.51	0.46
3:L5:4899:G:HO2'	3:L5:4901:G:H8	1.61	0.46
9:LD:203:ASN:N	9:LD:203:ASN:OD1	2.48	0.46
15:LJ:12:MET:HG3	15:LJ:137:PRO:HB2	1.97	0.46
22:LR:8:LYS:HG2	22:LR:19:LYS:HG3	1.98	0.46
24:LT:104:SER:O	24:LT:107:LYS:HG3	2.16	0.46
29:LY:127:GLN:O	29:LY:130:LYS:HG3	2.15	0.46
30:LZ:58:GLY:O	30:LZ:62:ILE:HG12	2.16	0.46
39:Li:94:LEU:O	39:Li:98:ARG:HG2	2.16	0.46
51:SF:76:MET:SD	51:SF:89:THR:HG23	2.56	0.46
55:SQ:62:ARG:O	55:SQ:96:TYR:OH	2.33	0.46
67:SC:84:PHE:HE2	67:SC:264:SER:HA	1.80	0.46
79:SY:86:GLU:OE2	79:SY:90:ARG:HD2	2.15	0.46
83:S2:945:U:H2'	83:S2:946:U:C6	2.51	0.46
85:CF:87:VAL:HG11	85:CF:232:LEU:HD21	1.97	0.46
3:L5:2763:U:H4'	3:L5:2764:A:H5''	1.98	0.46
3:L5:3712:A:N7	3:L5:3713:U:H1'	2.31	0.46
3:L5:4153:C:H2'	3:L5:4154:G:C8	2.50	0.46
3:L5:4623:OMG:HM23	3:L5:4623:OMG:H1'	1.80	0.46
3:L5:4693:C:OP1	13:LH:64:ARG:NH1	2.47	0.46
29:LY:23:SER:HA	29:LY:26:ARG:HB2	1.97	0.46
45:Lo:23:VAL:HG22	45:Lo:70:LEU:HD22	1.98	0.46
48:Ls:78:LEU:O	48:Ls:82:ILE:HG12	2.15	0.46
55:SQ:142:GLN:HE22	83:S2:1225:U:H1'	1.80	0.46
57:SS:10:GLN:HE21	57:SS:13:LEU:HG	1.81	0.46
64:Sg:191:HIS:ND1	64:Sg:195:LEU:HD21	2.31	0.46
68:SE:144:ALA:HB3	83:S2:121:OMU:HM23	1.97	0.46
73:SL:28:THR:HA	73:SL:29:GLY:HA2	1.51	0.46
74:SN:112:LYS:O	74:SN:116:ILE:HG12	2.16	0.46
83:S2:671:A:H4'	83:S2:672:A:H5''	1.97	0.46
83:S2:746:C:H2'	83:S2:747:U:C6	2.51	0.46
83:S2:1425:G:H2'	83:S2:1426:U:C6	2.51	0.46
83:S2:1595:U:H2'	83:S2:1596:U:C6	2.51	0.46
85:CF:72:THR:OG1	85:CF:93:PRO:O	2.27	0.46
3:L5:302:C:H2'	3:L5:303:C:H6	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2095:A:H4'	3:L5:2096:G:H5'	1.98	0.46
3:L5:2765:A:H2'	3:L5:2766:A:C8	2.51	0.46
3:L5:3951:G:H1'	3:L5:4062:A:H61	1.80	0.46
3:L5:4095:G:H2'	3:L5:4096:C:C6	2.50	0.46
3:L5:4220:6MZ:O5'	3:L5:4220:6MZ:H8	2.16	0.46
3:L5:4305:G:C6	24:LT:80:VAL:HG21	2.51	0.46
6:LA:225:ILE:HG12	6:LA:234:LYS:HA	1.98	0.46
7:LB:117:ARG:HA	7:LB:177:LYS:HD2	1.98	0.46
14:LI:135:ILE:HG22	14:LI:136:MET:HG3	1.97	0.46
16:LL:79:GLU:HA	16:LL:82:ARG:HG2	1.98	0.46
17:LM:90:ARG:HA	17:LM:93:LYS:HG2	1.97	0.46
43:Lm:79:GLU:OE2	43:Lm:81:SER:OG	2.24	0.46
51:SF:40:ALA:HB3	51:SF:67:PRO:HA	1.98	0.46
54:SP:28:MET:HG2	54:SP:32:GLN:HG2	1.98	0.46
54:SP:41:GLN:HG3	54:SP:84:ILE:HD13	1.98	0.46
58:ST:28:LEU:HD12	58:ST:106:ALA:HB1	1.98	0.46
66:SB:145:LYS:HB2	66:SB:145:LYS:HE3	1.71	0.46
83:S2:115:U:H2'	83:S2:116:OMU:C6	2.46	0.46
83:S2:475:C:H1'	83:S2:507:G:H1'	1.97	0.46
83:S2:479:C:H5''	85:CF:255:LYS:HD2	1.98	0.46
83:S2:946:U:H2'	83:S2:947:G:C8	2.51	0.46
83:S2:1031:A2M:H1'	83:S2:1031:A2M:HM'3	1.58	0.46
83:S2:1447:G:H2'	83:S2:1448:A:H8	1.81	0.46
3:L5:4456:OMC:HM21	7:LB:241:PRO:HD3	1.97	0.45
35:Le:69:MET:HE3	35:Le:73:GLY:HA2	1.97	0.45
47:Lr:5:LEU:O	47:Lr:9:VAL:HG23	2.16	0.45
55:SQ:139:ALA:HB2	83:S2:1650:A:H5''	1.96	0.45
59:SU:19:ARG:HB2	59:SU:117:ALA:HB2	1.98	0.45
59:SU:58:THR:HG23	83:S2:1446:A:H5''	1.98	0.45
64:Sg:166:VAL:HG12	64:Sg:176:VAL:HG12	1.98	0.45
66:SB:71:LEU:HD11	66:SB:189:ILE:HG23	1.98	0.45
69:SG:7:PHE:CE2	69:SG:9:ALA:HB3	2.51	0.45
71:SI:26:LYS:HE3	83:S2:444:G:O6	2.16	0.45
83:S2:901:G:H2'	83:S2:902:G:C8	2.51	0.45
83:S2:1112:U:H2'	83:S2:1113:A:C8	2.51	0.45
83:S2:1550:G:O2'	83:S2:1558:C:O2	2.24	0.45
83:S2:1759:G:N2	83:S2:1760:G:O6	2.45	0.45
3:L5:71:C:H1'	16:LL:62:PRO:O	2.16	0.45
3:L5:92:C:OP2	3:L5:4341:C:O2'	2.22	0.45
3:L5:424:U:H2'	3:L5:425:U:C6	2.51	0.45
3:L5:4281:A:H2'	3:L5:4282:A:H2'	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4473:A:O2'	43:Lm:122:ARG:NH2	2.49	0.45
8:LC:230:LEU:HD21	8:LC:236:ASN:H	1.82	0.45
28:LX:119:ILE:HD13	28:LX:149:VAL:HG11	1.98	0.45
36:Lf:15:LYS:HB3	36:Lf:25:THR:HG23	1.97	0.45
54:SP:37:TYR:O	57:SS:88:LYS:NZ	2.49	0.45
57:SS:62:ASP:O	57:SS:65:GLU:HG3	2.17	0.45
63:Sf:118:ARG:CZ	63:Sf:134:SER:HB3	2.46	0.45
68:SE:192:ILE:HG12	68:SE:243:GLY:HA3	1.99	0.45
72:SJ:114:VAL:HG23	72:SJ:126:ALA:HB1	1.97	0.45
83:S2:929:G:H2'	83:S2:930:C:O4'	2.17	0.45
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.50	0.45
13:LH:27:VAL:HG12	13:LH:84:VAL:HG21	1.98	0.45
25:LU:46:ARG:HA	25:LU:46:ARG:HD2	1.82	0.45
59:SU:67:LYS:HB3	83:S2:1337:4AC:H5''	1.99	0.45
69:SG:133:LEU:HB2	83:S2:65:C:N3	2.31	0.45
70:SH:165:ASN:HA	70:SH:168:HIS:HE1	1.81	0.45
83:S2:17:C:H2'	83:S2:18:C:H6	1.81	0.45
83:S2:534:G:H2'	83:S2:535:G:C8	2.51	0.45
85:CF:340:PHE:HB3	85:CF:441:VAL:HG23	1.99	0.45
3:L5:1743:A:N1	3:L5:1789:C:O2'	2.45	0.45
3:L5:1952:G:OP1	23:LS:139:ARG:NE	2.50	0.45
3:L5:4363:A:H5''	45:Lo:36:GLN:HG2	1.97	0.45
3:L5:4896:G:H2'	3:L5:4897:G:C8	2.51	0.45
8:LC:36:ILE:HD12	8:LC:122:TYR:CE2	2.51	0.45
15:LJ:77:ALA:O	15:LJ:80:GLU:HG2	2.16	0.45
18:LN:146:PRO:HB2	38:Lh:104:THR:HG23	1.98	0.45
52:SK:52:LEU:HA	52:SK:55:ARG:HG2	1.99	0.45
58:ST:49:ASP:OD1	58:ST:50:GLU:N	2.49	0.45
68:SE:151:ASP:HA	69:SG:212:LEU:HD21	1.98	0.45
83:S2:24:C:O2'	83:S2:25:A:O5'	2.35	0.45
83:S2:525:A:H2'	83:S2:526:A:C8	2.51	0.45
83:S2:1275:G:N2	83:S2:1506:A:OP2	2.49	0.45
3:L5:960:A:H2'	3:L5:970:G:N7	2.32	0.45
3:L5:1188:C:H2'	3:L5:1189:G:H8	1.82	0.45
3:L5:1802:A:N3	24:LT:130:ARG:NH2	2.56	0.45
3:L5:1993:C:H2'	3:L5:1994:C:C6	2.51	0.45
3:L5:2870:A:H2'	3:L5:2871:A:H8	1.81	0.45
3:L5:3598:C:H2'	3:L5:3599:A:H8	1.82	0.45
3:L5:4113:U:H4'	3:L5:4115:G:C5	2.50	0.45
3:L5:4935:C:H2'	3:L5:4936:G:H8	1.81	0.45
5:L8:58:G:O6	40:Lj:63:ARG:NH1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LB:206:PRO:HG2	7:LB:209:GLN:HG3	1.97	0.45
15:LJ:56:THR:OG1	15:LJ:64:ARG:N	2.49	0.45
21:LQ:70:MET:HE1	21:LQ:137:VAL:HB	1.99	0.45
35:Le:8:VAL:HG23	35:Le:10:PRO:HD3	1.99	0.45
51:SF:140:ASP:OD1	51:SF:140:ASP:N	2.50	0.45
59:SU:80:PHE:HB3	62:Sd:52:PHE:HB3	1.99	0.45
61:Sc:44:ARG:HH22	61:Sc:63:ARG:HH11	1.64	0.45
64:Sg:67:SER:HG	64:Sg:83:TRP:CD1	2.35	0.45
64:Sg:133:ASN:HB3	64:Sg:139:LYS:HD2	1.99	0.45
69:SG:49:VAL:HB	69:SG:115:LYS:HG2	1.98	0.45
74:SN:64:ARG:NH2	83:S2:919:A:OP2	2.43	0.45
83:S2:981:A:H2'	83:S2:982:G:C8	2.52	0.45
83:S2:1337:4AC:O5'	83:S2:1337:4AC:H6	2.16	0.45
83:S2:1383:A2M:HM'3	83:S2:1383:A2M:H1'	1.59	0.45
83:S2:1438:A:H2'	83:S2:1439:A:H8	1.81	0.45
83:S2:1518:C:H5''	83:S2:1519:U:H5''	1.99	0.45
85:CF:11:VAL:HA	85:CF:90:ILE:HB	1.99	0.45
3:L5:362:A:N6	42:Ll:37:TYR:O	2.45	0.45
3:L5:371:A:N3	3:L5:1531:U:O2'	2.41	0.45
3:L5:1100:U:H3	3:L5:1194:G:H1	1.63	0.45
3:L5:2693:G:OP1	41:Lk:35:LYS:HE2	2.16	0.45
3:L5:3861:A:H2'	3:L5:3862:A:H8	1.81	0.45
11:LF:90:ALA:HB2	11:LF:125:LEU:HD11	1.98	0.45
22:LR:139:MET:HG2	22:LR:143:HIS:CE1	2.51	0.45
31:La:63:LEU:HD21	31:La:65:ARG:HE	1.82	0.45
39:Li:59:GLU:HA	39:Li:62:LYS:HE3	1.99	0.45
57:SS:61:GLU:HA	57:SS:64:VAL:HG12	1.99	0.45
64:Sg:25:PRO:HA	64:Sg:293:ALA:HB2	1.98	0.45
72:SJ:40:LYS:HG2	82:Se:34:ARG:NH1	2.32	0.45
79:SY:77:ASP:OD1	79:SY:77:ASP:N	2.49	0.45
83:S2:116:OMU:HM23	83:S2:116:OMU:H1'	1.73	0.45
83:S2:1856:C:H2'	83:S2:1857:G:H8	1.81	0.45
3:L5:473:C:H2'	3:L5:474:C:C6	2.52	0.45
3:L5:1091:C:H2'	3:L5:1092:G:C8	2.52	0.45
3:L5:1392:A:H2'	3:L5:1393:G:C8	2.51	0.45
3:L5:1908:A:H2'	3:L5:1909:G:O4'	2.17	0.45
3:L5:3910:C:H2'	3:L5:3911:C:C6	2.51	0.45
3:L5:4113:U:H4'	3:L5:4115:G:C6	2.52	0.45
3:L5:4946:U:O2'	36:Lf:2:SER:N	2.43	0.45
6:LA:114:CYS:N	6:LA:165:VAL:O	2.48	0.45
6:LA:132:ASN:O	6:LA:169:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LF:96:ARG:HH12	11:LF:224:THR:HG22	1.81	0.45
20:LP:54:GLN:HA	20:LP:83:TRP:CD1	2.51	0.45
22:LR:177:LEU:O	22:LR:181:LYS:HG2	2.17	0.45
57:SS:102:GLY:HA2	57:SS:105:ASN:ND2	2.32	0.45
66:SB:32:ASP:O	66:SB:96:CYS:N	2.45	0.45
67:SC:193:VAL:HG11	67:SC:240:THR:HG22	1.99	0.45
77:SW:30:CYS:SG	77:SW:31:SER:N	2.90	0.45
83:S2:59:U:H5''	83:S2:503:C:N4	2.31	0.45
83:S2:683:OMG:N1	83:S2:1022:U:OP2	2.39	0.45
83:S2:698:G:H8	83:S2:733:C:C2	2.35	0.45
3:L5:1461:C:H2'	3:L5:1462:A:C8	2.51	0.45
3:L5:1764:G:H4'	3:L5:1769:G:C6	2.52	0.45
3:L5:1899:G:O2'	35:Le:57:ASN:OD1	2.34	0.45
3:L5:2554:U:C2	3:L5:2764:A:N7	2.85	0.45
3:L5:2565:A:H3'	3:L5:2566:G:H8	1.82	0.45
3:L5:3916:G:H2'	3:L5:3917:A:C8	2.51	0.45
3:L5:4128:A:O2'	12:LG:33:GLU:O	2.30	0.45
3:L5:4459:U:H2'	3:L5:4460:U:C6	2.51	0.45
7:LB:161:ARG:HG2	7:LB:184:GLN:HA	1.99	0.45
8:LC:292:ILE:HG12	21:LQ:128:LEU:HD21	1.99	0.45
24:LT:44:GLY:HA2	24:LT:95:HIS:CD2	2.52	0.45
52:SK:63:ALA:HB3	52:SK:68:TYR:HE2	1.82	0.45
53:SM:23:LYS:O	53:SM:27:ILE:HG12	2.16	0.45
55:SQ:104:SER:O	55:SQ:108:ILE:HG12	2.16	0.45
59:SU:23:THR:O	59:SU:113:GLU:N	2.49	0.45
67:SC:81:ILE:HG23	67:SC:86:LEU:HB2	1.99	0.45
68:SE:247:THR:OG1	68:SE:250:GLU:OE1	2.33	0.45
78:SX:52:LEU:HD11	78:SX:73:GLN:HB2	1.98	0.45
83:S2:57:U:OP1	83:S2:504:G:O2'	2.34	0.45
83:S2:344:U:H2'	83:S2:345:U:H6	1.80	0.45
83:S2:659:G:HO2'	83:S2:662:G:HO2'	1.61	0.45
83:S2:808:A:H2	83:S2:855:G:H22	1.63	0.45
83:S2:900:C:H3'	83:S2:901:G:H8	1.81	0.45
83:S2:1348:G:OP2	83:S2:1348:G:N2	2.46	0.45
85:CF:272:LEU:HB3	85:CF:302:ALA:HB3	1.98	0.45
3:L5:659:G:H2'	3:L5:660:A:C8	2.51	0.45
3:L5:1086:C:H2'	3:L5:1087:A:C8	2.50	0.45
3:L5:1548:G:O2'	3:L5:2812:A:N3	2.42	0.45
3:L5:1806:G:H2'	3:L5:1807:C:H6	1.80	0.45
3:L5:2364:OMG:HM23	3:L5:2364:OMG:H1'	1.65	0.45
3:L5:2495:U:H2'	3:L5:2496:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2520:C:H2'	3:L5:2521:G:H8	1.82	0.45
3:L5:3867:A2M:H8	3:L5:3867:A2M:H5''	1.98	0.45
7:LB:92:TYR:OH	7:LB:182:GLU:OE1	2.35	0.45
11:LF:162:ILE:HD12	11:LF:167:ILE:HB	1.99	0.45
15:LJ:40:LEU:HD23	15:LJ:40:LEU:HA	1.83	0.45
17:LM:41:PRO:HB3	17:LM:70:GLN:OE1	2.17	0.45
18:LN:6:TYR:CZ	39:Li:40:VAL:HG22	2.52	0.45
19:LO:193:THR:HG22	19:LO:197:LYS:HE3	1.99	0.45
24:LT:75:VAL:HG22	24:LT:88:ARG:HG2	1.99	0.45
51:SF:22:LYS:HG3	51:SF:23:TRP:CD2	2.52	0.45
53:SM:19:GLN:HE22	53:SM:88:TRP:CG	2.35	0.45
64:Sg:174:VAL:HG23	64:Sg:188:HIS:HB2	1.99	0.45
64:Sg:249:CYS:HB3	64:Sg:258:ILE:HD13	1.99	0.45
66:SB:67:PHE:CE2	75:SO:48:SER:HB3	2.52	0.45
68:SE:104:ASP:OD1	68:SE:108:ARG:N	2.37	0.45
78:SX:93:PHE:O	78:SX:140:ARG:NH1	2.50	0.45
83:S2:118:C:H2'	83:S2:119:U:O4'	2.17	0.45
83:S2:1232:PSU:H2'	83:S2:1233:G:C8	2.52	0.45
3:L5:161:G:H2'	3:L5:162:A:H8	1.82	0.45
3:L5:189:G:H2'	3:L5:190:G:H8	1.81	0.45
3:L5:267:G:OP1	38:Lh:109:ARG:NH2	2.46	0.45
3:L5:270:U:H2'	3:L5:271:C:C6	2.52	0.45
3:L5:287:U:H2'	3:L5:288:G:C8	2.52	0.45
3:L5:1340:OMC:HM23	3:L5:1340:OMC:H1'	1.71	0.45
3:L5:2824:OMC:HM23	3:L5:2824:OMC:H1'	1.67	0.45
3:L5:4769:G:H5''	19:LO:176:ARG:HD3	1.99	0.45
4:L7:49:A:H5''	9:LD:224:SER:HB2	1.99	0.45
4:L7:73:U:O2'	4:L7:102:U:O4	2.29	0.45
19:LO:124:LEU:HD23	19:LO:124:LEU:HA	1.84	0.45
28:LX:110:LYS:HE3	28:LX:114:LYS:NZ	2.32	0.45
50:SD:134:CYS:SG	50:SD:135:GLU:N	2.89	0.45
56:SR:41:ILE:HG22	56:SR:43:SER:H	1.82	0.45
64:Sg:57:ARG:HE	64:Sg:95:GLY:HA3	1.82	0.45
67:SC:74:LYS:HD3	67:SC:74:LYS:HA	1.79	0.45
67:SC:130:ILE:HG13	67:SC:162:ILE:HD11	1.98	0.45
67:SC:256:TRP:CD2	77:SW:68:ARG:HD3	2.52	0.45
70:SH:65:PRO:HB2	70:SH:67:PRO:HD2	1.99	0.45
71:SI:107:THR:HG23	71:SI:110:ARG:HH21	1.81	0.45
73:SL:80:MET:HE2	73:SL:122:ILE:HG13	1.99	0.45
77:SW:10:ALA:O	77:SW:14:ILE:HG13	2.17	0.45
83:S2:98:C:H2'	83:S2:426:A:H4'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:158:A:H2'	83:S2:159:A2M:O4'	2.16	0.45
83:S2:329:G:H2'	83:S2:330:G:H8	1.82	0.45
83:S2:674:C:H2'	83:S2:675:U:C6	2.51	0.45
83:S2:1457:U:H2'	83:S2:1458:G:C8	2.52	0.45
83:S2:1773:C:H2'	83:S2:1774:C:H5''	1.98	0.45
84:AT:28:U:H2'	84:AT:29:U:C6	2.52	0.45
85:CF:360:VAL:HG13	85:CF:427:ARG:HB2	1.99	0.45
3:L5:135:G:N7	38:Lh:97:LYS:HE3	2.32	0.44
3:L5:163:A:H2'	3:L5:164:G:H8	1.81	0.44
3:L5:271:C:H2'	3:L5:272:U:C6	2.52	0.44
3:L5:1195:G:H2'	3:L5:1196:G:H8	1.81	0.44
3:L5:1588:U:H2'	3:L5:1589:C:C6	2.52	0.44
3:L5:1795:A:N3	4:L7:79:U:O2'	2.48	0.44
3:L5:2756:G:H2'	3:L5:2757:A:C8	2.52	0.44
3:L5:3799:A:N3	3:L5:4506:C:O2'	2.40	0.44
3:L5:4066:U:H2'	3:L5:4067:U:H6	1.82	0.44
3:L5:4590:A2M:HM'3	3:L5:4590:A2M:H1'	1.59	0.44
3:L5:4620:OMU:HM23	3:L5:4620:OMU:H1'	1.68	0.44
3:L5:4642:U:H2'	3:L5:4643:G:H8	1.82	0.44
3:L5:5057:C:H2'	3:L5:5058:A:C8	2.52	0.44
67:SC:166:ARG:HB3	67:SC:247:THR:HB	1.99	0.44
69:SG:48:TYR:OH	69:SG:119:LYS:O	2.27	0.44
69:SG:215:LYS:O	69:SG:218:LYS:HG3	2.17	0.44
83:S2:96:C:H2'	83:S2:97:U:C6	2.52	0.44
83:S2:109:PSU:H2'	83:S2:110:U:C6	2.51	0.44
83:S2:349:A:H2'	83:S2:350:C:C6	2.51	0.44
83:S2:432:G:H2'	83:S2:433:A:C8	2.53	0.44
83:S2:897:U:C4	83:S2:898:U:H1'	2.52	0.44
83:S2:1447:G:H2'	83:S2:1448:A:C8	2.52	0.44
83:S2:1845:A:H2'	83:S2:1846:G:H8	1.82	0.44
3:L5:408:A:O2'	3:L5:411:G:OP2	2.27	0.44
3:L5:717:U:H2'	3:L5:718:C:C6	2.52	0.44
3:L5:1317:U:H2'	3:L5:1318:C:C6	2.52	0.44
3:L5:1645:C:H2'	3:L5:1646:A:C8	2.52	0.44
3:L5:2706:G:N2	3:L5:2710:C:OP2	2.51	0.44
7:LB:201:LEU:HD23	7:LB:201:LEU:HA	1.82	0.44
10:LE:119:GLU:HG2	35:Le:7:LEU:HD22	1.99	0.44
13:LH:107:GLU:N	13:LH:107:GLU:OE1	2.49	0.44
25:LU:36:ALA:HB3	25:LU:65:ARG:HH21	1.82	0.44
57:SS:84:LEU:O	57:SS:87:GLN:NE2	2.50	0.44
71:SI:44:HIS:ND1	83:S2:1740:C:OP1	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:SO:44:VAL:HG12	75:SO:53:ILE:HB	2.00	0.44
79:SY:58:PHE:HE2	79:SY:74:MET:HE1	1.82	0.44
83:S2:17:C:H2'	83:S2:18:C:C6	2.51	0.44
3:L5:162:A:H2'	3:L5:163:A:C8	2.53	0.44
3:L5:730:G:OP2	11:LF:76:ARG:NE	2.47	0.44
3:L5:943:A:H62	11:LF:151:ASN:ND2	2.16	0.44
3:L5:1802:A:O2'	24:LT:108:ARG:NH2	2.47	0.44
3:L5:2347:A:C4	35:Le:31:ILE:HD11	2.53	0.44
3:L5:3825:A2M:HM'3	3:L5:3825:A2M:H1'	1.66	0.44
3:L5:4111:U:H2'	3:L5:4112:C:C5	2.53	0.44
3:L5:4587:G:OP1	19:LO:61:ARG:NH1	2.43	0.44
3:L5:4600:G:H4'	3:L5:4601:U:O5'	2.17	0.44
3:L5:4717:A:OP2	7:LB:30:LYS:NZ	2.37	0.44
11:LF:241:ASN:O	11:LF:245:ARG:HG2	2.18	0.44
13:LH:63:ASN:OD1	13:LH:66:GLU:HG2	2.17	0.44
33:Lc:47:ILE:HD12	33:Lc:94:LEU:HD11	1.98	0.44
40:Lj:85:LYS:HE3	40:Lj:85:LYS:HB3	1.79	0.44
46:Lp:27:LYS:O	46:Lp:31:ILE:HD12	2.16	0.44
65:SA:220:LYS:HA	65:SA:220:LYS:HD3	1.82	0.44
66:SB:38:MET:HE3	66:SB:185:VAL:HG21	1.99	0.44
69:SG:135:PRO:HA	83:S2:169:U:H5''	2.00	0.44
71:SI:110:ARG:HH11	71:SI:123:ARG:NH1	2.15	0.44
83:S2:106:C:H2'	83:S2:107:A:C8	2.48	0.44
83:S2:166:A2M:HM'3	83:S2:166:A2M:H1'	1.61	0.44
85:CF:82:THR:OG1	85:CF:85:TYR:O	2.31	0.44
3:L5:212:A:H2'	3:L5:213:G:H8	1.82	0.44
3:L5:400:A2M:HM'3	3:L5:400:A2M:H1'	1.59	0.44
3:L5:1354:A:N1	3:L5:1385:G:O2'	2.44	0.44
3:L5:2385:U:H2'	3:L5:2386:U:H6	1.82	0.44
3:L5:2521:G:H5'	3:L5:2640:G:H1'	1.98	0.44
3:L5:2634:C:H2'	3:L5:2635:U:H6	1.83	0.44
3:L5:3598:C:H2'	3:L5:3599:A:C8	2.53	0.44
4:L7:11:A:N1	4:L7:66:G:O2'	2.44	0.44
6:LA:180:LEU:HD22	46:Lp:18:TYR:HB3	2.00	0.44
7:LB:153:MET:HB3	7:LB:194:LEU:HD11	1.99	0.44
47:Lr:107:ARG:HH11	47:Lr:108:MET:HE3	1.82	0.44
50:SD:42:THR:OG1	50:SD:45:ARG:O	2.27	0.44
50:SD:65:ARG:HA	50:SD:68:GLU:HG2	1.99	0.44
50:SD:115:VAL:HG21	50:SD:138:VAL:HG11	2.00	0.44
57:SS:5:ILE:HD12	57:SS:6:PRO:HD2	1.99	0.44
59:SU:20:ILE:HA	59:SU:116:ILE:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SU:52:GLY:HA3	83:S2:1401:A:H4'	1.99	0.44
66:SB:97:LEU:HD23	66:SB:232:HIS:CG	2.52	0.44
69:SG:142:ARG:NH2	83:S2:144:U:OP1	2.50	0.44
79:SY:41:ARG:NH2	79:SY:52:PRO:O	2.50	0.44
83:S2:1093:A:H2'	83:S2:1094:C:C6	2.52	0.44
85:CF:248:LEU:HD23	85:CF:267:VAL:HA	1.98	0.44
2:Pt:8:U:O2'	2:Pt:21:A:N1	2.45	0.44
3:L5:252:C:H2'	3:L5:253:G:C8	2.53	0.44
3:L5:441:G:H2'	3:L5:442:G:H8	1.81	0.44
3:L5:481:G:H2'	3:L5:482:G:C8	2.52	0.44
3:L5:750:U:H1'	3:L5:917:A:C8	2.52	0.44
3:L5:1348:U:H2'	3:L5:1349:G:H8	1.82	0.44
3:L5:1444:G:H22	3:L5:2104:G:N2	2.16	0.44
3:L5:4913:G:H4'	3:L5:4914:C:O5'	2.18	0.44
7:LB:50:LYS:HB2	7:LB:345:LEU:HD11	2.00	0.44
9:LD:197:LYS:HB3	9:LD:202:GLN:HB2	1.98	0.44
10:LE:183:ARG:HA	10:LE:183:ARG:HD2	1.86	0.44
22:LR:173:ARG:O	22:LR:176:ARG:NH1	2.50	0.44
28:LX:110:LYS:HE3	28:LX:114:LYS:HZ3	1.82	0.44
45:Lo:67:VAL:HG11	45:Lo:82:MET:HE3	1.99	0.44
51:SF:127:ARG:H	51:SF:135:ARG:HD2	1.82	0.44
54:SP:120:SER:OG	54:SP:120:SER:O	2.30	0.44
61:Sc:7:GLN:OE1	61:Sc:61:SER:OG	2.22	0.44
61:Sc:46:VAL:HG23	61:Sc:50:VAL:HG21	1.99	0.44
63:Sf:107:LYS:O	63:Sf:115:SER:OG	2.26	0.44
68:SE:67:GLN:NE2	79:SY:17:LEU:O	2.44	0.44
69:SG:31:ARG:NH1	83:S2:1745:A:O3'	2.50	0.44
74:SN:87:ASP:OD1	74:SN:88:LEU:N	2.50	0.44
75:SO:143:LYS:NZ	83:S2:1066:U:OP1	2.50	0.44
83:S2:85:A:H2'	83:S2:86:C:H6	1.83	0.44
83:S2:1347:U:H2'	83:S2:1348:G:N3	2.33	0.44
83:S2:1712:A:H2'	83:S2:1713:C:C6	2.53	0.44
84:AT:26:C:H2'	84:AT:27:G:H8	1.83	0.44
3:L5:458:C:H2'	3:L5:459:C:H6	1.82	0.44
3:L5:1846:G:H2'	3:L5:1847:C:H6	1.83	0.44
6:LA:140:ASN:HB2	6:LA:142:GLU:CD	2.43	0.44
34:Ld:93:ASN:HB2	34:Ld:103:TYR:HD1	1.83	0.44
37:Lg:60:ARG:HA	37:Lg:60:ARG:HD2	1.84	0.44
41:Lk:12:LEU:O	41:Lk:16:ARG:HG3	2.18	0.44
41:Lk:17:ARG:NH2	41:Lk:38:CYS:SG	2.90	0.44
54:SP:30:TYR:O	54:SP:34:MET:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SS:5:ILE:N	60:SZ:50:PHE:O	2.50	0.44
59:SU:70:CYS:SG	83:S2:1491:G:O2'	2.60	0.44
64:Sg:202:PRO:HG2	64:Sg:243:PRO:HA	1.98	0.44
83:S2:159:A2M:HM'3	83:S2:159:A2M:H1'	1.43	0.44
83:S2:886:A:H62	83:S2:901:G:N2	2.16	0.44
83:S2:1683:C:H2'	83:S2:1684:C:H6	1.83	0.44
83:S2:1759:G:O2'	83:S2:1760:G:O4'	2.28	0.44
84:AT:49:C:H2'	84:AT:60:A:H1'	1.99	0.44
3:L5:268:G:H2'	3:L5:269:G:C8	2.53	0.44
3:L5:280:G:H5''	18:LN:14:LYS:HE2	1.99	0.44
3:L5:382:G:O2'	3:L5:407:A:N6	2.46	0.44
3:L5:4441:A:H5''	14:LI:114:GLY:HA2	2.00	0.44
3:L5:4508:C:N3	3:L5:4512:U:H5	2.15	0.44
3:L5:4524:G:C2	7:LB:252:ALA:HB1	2.53	0.44
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.17	0.44
3:L5:4591:U:H2'	3:L5:4592:C:C6	2.52	0.44
5:L8:65:A:O2'	38:Lh:10:ARG:NH2	2.51	0.44
19:LO:155:THR:O	19:LO:158:GLU:HG3	2.17	0.44
27:LW:73:ARG:NH2	83:S2:1748:G:O6	2.50	0.44
29:LY:22:PRO:HD2	29:LY:25:ILE:HD11	2.00	0.44
40:Lj:67:LEU:HD23	40:Lj:67:LEU:HA	1.83	0.44
54:SP:91:GLY:H	54:SP:107:ILE:HB	1.82	0.44
55:SQ:76:GLY:O	83:S2:1544:C:O2'	2.28	0.44
56:SR:24:LEU:HA	56:SR:24:LEU:HD23	1.82	0.44
62:Sd:21:CYS:HB3	62:Sd:26:ASN:H	1.82	0.44
66:SB:29:ASP:OD1	66:SB:29:ASP:N	2.51	0.44
66:SB:94:LYS:HA	66:SB:94:LYS:HD2	1.78	0.44
68:SE:124:CYS:HB3	68:SE:141:THR:HB	1.99	0.44
70:SH:49:LYS:O	70:SH:61:ILE:HG22	2.18	0.44
81:Sb:36:LYS:HB3	81:Sb:78:SER:HB3	1.99	0.44
82:Se:31:ARG:NH2	83:S2:525:A:O3'	2.50	0.44
83:S2:799:OMU:HM23	83:S2:799:OMU:H1'	1.81	0.44
83:S2:1304:U:H2'	83:S2:1305:C:C6	2.53	0.44
83:S2:1736:G:H2'	83:S2:1737:G:C8	2.53	0.44
3:L5:318:A:H2'	3:L5:319:A:H8	1.82	0.44
3:L5:1199:G:H2'	3:L5:1200:G:H8	1.83	0.44
3:L5:2020:U:H2'	3:L5:2021:G:H8	1.83	0.44
3:L5:2249:C:H2'	3:L5:2250:C:H5	1.82	0.44
3:L5:2558:C:H2'	3:L5:2559:G:H8	1.82	0.44
3:L5:4926:C:H5''	3:L5:4927:G:H21	1.83	0.44
3:L5:5005:G:N2	3:L5:5041:G:O2'	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LF:119:ASN:ND2	11:LF:212:LYS:HD3	2.33	0.44
19:LO:124:LEU:HB3	19:LO:126:VAL:HG12	1.98	0.44
51:SF:38:TYR:HE2	51:SF:143:PRO:HG2	1.82	0.44
51:SF:51:HIS:CE1	55:SQ:78:VAL:HG21	2.53	0.44
51:SF:69:VAL:O	51:SF:73:THR:HG23	2.17	0.44
56:SR:28:PHE:HA	56:SR:55:THR:HG21	1.99	0.44
64:Sg:11:LEU:HB2	64:Sg:307:VAL:HG13	2.00	0.44
66:SB:52:THR:HG23	66:SB:57:ILE:HA	2.00	0.44
68:SE:134:LYS:N	83:S2:298:G:OP1	2.47	0.44
75:SO:42:VAL:HG12	75:SO:56:VAL:O	2.18	0.44
83:S2:51:U:H2'	83:S2:52:G:H8	1.82	0.44
83:S2:328:U:O2'	83:S2:329:G:O5'	2.30	0.44
83:S2:484:A2M:H8	83:S2:484:A2M:O5'	2.17	0.44
83:S2:1013:U:OP1	83:S2:1129:G:O2'	2.31	0.44
83:S2:1360:U:O2'	83:S2:1379:A:OP2	2.33	0.44
83:S2:1801:A:H2'	83:S2:1802:C:H6	1.83	0.44
3:L5:423:G:OP1	20:LP:62:ARG:NH1	2.48	0.44
3:L5:662:C:H2'	3:L5:663:G:C8	2.53	0.44
3:L5:1398:A:OP1	31:La:136:LYS:NZ	2.50	0.44
3:L5:2376:A:H2'	3:L5:2377:C:C6	2.53	0.44
3:L5:2875:C:OP1	46:Lp:23:ARG:NH2	2.51	0.44
3:L5:4139:G:H1'	3:L5:4146:G:N1	2.32	0.44
3:L5:4232:U:H5'	45:Lo:3:ASN:HB3	2.00	0.44
9:LD:179:ARG:HA	9:LD:179:ARG:HD3	1.69	0.44
10:LE:150:LEU:HD11	10:LE:164:PHE:HB2	1.99	0.44
27:LW:104:GLN:O	27:LW:107:GLN:HG3	2.18	0.44
51:SF:95:HIS:O	51:SF:99:ILE:HG12	2.18	0.44
57:SS:73:ASN:HB3	57:SS:76:GLN:HE22	1.83	0.44
66:SB:40:ASN:OD1	66:SB:41:ILE:HD12	2.18	0.44
72:SJ:40:LYS:HA	72:SJ:43:VAL:HG12	2.00	0.44
73:SL:4:ILE:HD12	73:SL:55:TYR:HA	2.00	0.44
74:SN:34:LYS:HA	74:SN:37:ILE:HG22	1.99	0.44
74:SN:109:LYS:NZ	83:S2:1033:G:OP1	2.38	0.44
78:SX:138:LYS:NZ	83:S2:30:C:OP1	2.50	0.44
83:S2:576:A2M:HM'3	83:S2:576:A2M:H1'	1.64	0.44
83:S2:1117:C:H2'	83:S2:1118:C:H6	1.83	0.44
83:S2:1222:G:H2'	83:S2:1223:A:C8	2.53	0.44
83:S2:1713:C:H2'	83:S2:1714:U:H6	1.82	0.44
3:L5:455:C:O2'	3:L5:456:C:H5'	2.18	0.43
3:L5:1581:G:OP1	88:L5:5286:SPD:N10	2.47	0.43
3:L5:2861:OMC:HM23	3:L5:2861:OMC:H1'	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3606:U:H2'	3:L5:3607:U:H6	1.82	0.43
3:L5:3866:C:H2'	3:L5:3867:A2M:O4'	2.18	0.43
3:L5:4153:C:H2'	3:L5:4154:G:H8	1.82	0.43
3:L5:4589:A:N1	3:L5:4621:C:O2'	2.45	0.43
3:L5:4896:G:H2'	3:L5:4897:G:H8	1.83	0.43
12:LG:248:ALA:O	12:LG:252:LYS:HG2	2.17	0.43
30:LZ:46:ILE:HA	30:LZ:70:SER:HA	1.99	0.43
63:Sf:89:LYS:O	83:S2:1507:G:N2	2.47	0.43
65:SA:19:LEU:HD13	65:SA:24:HIS:CE1	2.53	0.43
65:SA:91:ALA:HA	65:SA:96:ALA:HB3	2.00	0.43
72:SJ:150:ARG:HG3	83:S2:821:G:C6	2.53	0.43
83:S2:172:OMU:H6	83:S2:314:U:H1'	2.00	0.43
83:S2:601:OMG:H1'	83:S2:601:OMG:HM23	1.64	0.43
83:S2:1199:A:H2'	83:S2:1200:A:C8	2.53	0.43
85:CF:218:ARG:NH2	85:CF:234:CYS:SG	2.87	0.43
85:CF:343:GLN:O	85:CF:436:GLY:HA2	2.17	0.43
85:CF:347:LEU:O	85:CF:396:SER:OG	2.36	0.43
3:L5:162:A:H2'	3:L5:163:A:H8	1.82	0.43
3:L5:1278:C:H2'	3:L5:1279:A:O4'	2.18	0.43
3:L5:1281:G:OP1	8:LC:316:LYS:NZ	2.48	0.43
3:L5:1346:C:H2'	3:L5:1347:G:H8	1.83	0.43
3:L5:1510:G:H2'	3:L5:1511:U:C6	2.53	0.43
3:L5:1677:PSU:H4'	3:L5:1680:G:C2	2.52	0.43
3:L5:1869:G:C6	88:L5:5287:SPD:H32	2.53	0.43
3:L5:2522:G:OP2	37:Lg:29:ARG:NH2	2.52	0.43
3:L5:2633:U:H2'	3:L5:2634:C:H6	1.83	0.43
3:L5:3877:A:N3	3:L5:4401:G:O2'	2.47	0.43
3:L5:4156:G:H5''	3:L5:4157:A:H2'	1.99	0.43
4:L7:4:U:H2'	4:L7:5:A:H8	1.83	0.43
4:L7:35:U:O2	4:L7:45:U:O2'	2.34	0.43
8:LC:212:ASN:ND2	8:LC:213:GLU:OE1	2.51	0.43
21:LQ:151:HIS:ND1	21:LQ:164:LYS:O	2.49	0.43
45:Lo:4:VAL:HG23	45:Lo:93:LEU:HD23	1.99	0.43
52:SK:3:MET:HG3	52:SK:44:HIS:HB3	1.99	0.43
53:SM:52:LEU:N	53:SM:77:ILE:O	2.50	0.43
55:SQ:26:LYS:O	55:SQ:67:ASP:N	2.36	0.43
55:SQ:69:ARG:HH21	83:S2:1426:U:P	2.41	0.43
60:SZ:80:ARG:HG3	83:S2:1598:G:H2'	2.00	0.43
64:Sg:291:TRP:CE2	64:Sg:298:LEU:HD13	2.53	0.43
65:SA:48:ILE:HD13	65:SA:48:ILE:HA	1.80	0.43
65:SA:185:MET:HB3	65:SA:191:ARG:HH21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:SB:117:TRP:HB3	66:SB:153:THR:HG22	2.00	0.43
71:SI:150:ASP:HA	71:SI:153:LYS:CG	2.49	0.43
74:SN:49:GLN:HA	74:SN:52:VAL:HG22	2.00	0.43
83:S2:468:A2M:HM'3	83:S2:468:A2M:H1'	1.61	0.43
83:S2:647:U:H2'	83:S2:648:A:C8	2.53	0.43
83:S2:1232:PSU:H2'	83:S2:1233:G:H8	1.82	0.43
83:S2:1523:C:H2'	83:S2:1524:G:C8	2.53	0.43
2:Pt:22:U:H2'	2:Pt:23:C:C6	2.52	0.43
3:L5:667:A:N1	8:LC:291:ARG:NH2	2.66	0.43
3:L5:705:G:H2'	3:L5:706:C:H6	1.83	0.43
3:L5:1807:C:O3'	24:LT:110:LYS:NZ	2.51	0.43
3:L5:2250:C:H2'	3:L5:2251:G:C8	2.54	0.43
3:L5:2754:G:OP2	30:LZ:133:LYS:NZ	2.39	0.43
3:L5:4111:U:H2'	3:L5:4112:C:H5	1.84	0.43
3:L5:4458:C:H2'	3:L5:4459:U:C6	2.52	0.43
3:L5:4736:C:H2'	3:L5:4737:G:H8	1.83	0.43
3:L5:4986:G:H1'	7:LB:174:ARG:NH2	2.32	0.43
4:L7:61:G:H5''	9:LD:271:MET:HE2	2.00	0.43
6:LA:28:ARG:HD2	6:LA:123:ARG:HG3	2.01	0.43
19:LO:191:LYS:HE3	19:LO:192:TYR:CZ	2.53	0.43
30:LZ:12:LEU:HB2	30:LZ:81:MET:HB3	1.99	0.43
53:SM:86:GLY:HA2	53:SM:89:VAL:HG12	1.99	0.43
56:SR:93:GLN:NE2	56:SR:96:ILE:HG22	2.33	0.43
57:SS:124:ARG:HB2	57:SS:131:VAL:HG12	1.99	0.43
58:ST:39:LEU:HA	58:ST:39:LEU:HD23	1.70	0.43
64:Sg:183:LYS:HD2	64:Sg:183:LYS:HA	1.81	0.43
65:SA:200:ASP:HA	65:SA:203:PHE:CD2	2.53	0.43
66:SB:167:LYS:O	66:SB:171:ILE:HG12	2.18	0.43
68:SE:149:TYR:CD2	69:SG:205:GLU:HB3	2.53	0.43
73:SL:85:THR:HA	73:SL:113:LEU:H	1.82	0.43
75:SO:142:ARG:HH12	80:Sa:24:THR:HA	1.84	0.43
78:SX:88:ASP:OD2	78:SX:134:TYR:OH	2.34	0.43
2:Pt:47:U:O2'	2:Pt:50:U:OP1	2.34	0.43
3:L5:208:A:H2	3:L5:233:U:H5''	1.82	0.43
3:L5:737:C:C4	3:L5:739:G:H5''	2.54	0.43
3:L5:940:C:OP1	11:LF:242:ARG:NH2	2.49	0.43
3:L5:979:C:OP2	10:LE:66:LYS:HD3	2.18	0.43
3:L5:1298:C:H2'	3:L5:1299:G:H8	1.81	0.43
3:L5:1316:OMG:P	35:Le:43:ASN:HD22	2.41	0.43
3:L5:1718:C:O2'	11:LF:181:LYS:NZ	2.52	0.43
3:L5:3870:C:H2'	3:L5:3871:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4342:C:O3'	45:Lo:37:GLY:HA3	2.18	0.43
4:L7:120:U:H4'	9:LD:262:LYS:HG2	2.00	0.43
7:LB:168:MET:HE3	7:LB:175:GLN:HG2	2.00	0.43
9:LD:182:GLY:HA2	9:LD:194:VAL:HG13	1.99	0.43
13:LH:92:MET:HG2	13:LH:181:VAL:HA	2.01	0.43
14:LI:96:VAL:HG22	14:LI:125:THR:HG22	2.01	0.43
21:LQ:154:LYS:HE2	21:LQ:158:THR:HB	2.00	0.43
53:SM:58:GLU:HB3	53:SM:61:TYR:HB2	2.00	0.43
63:Sf:124:ASP:OD1	63:Sf:124:ASP:N	2.41	0.43
64:Sg:39:THR:HG22	64:Sg:60:ARG:HG2	2.00	0.43
65:SA:70:ASN:HB3	65:SA:73:ASP:OD1	2.19	0.43
65:SA:137:ALA:HB1	65:SA:142:LEU:HB3	1.99	0.43
68:SE:6:LYS:O	68:SE:30:ARG:NH2	2.51	0.43
83:S2:367:U:H4'	83:S2:371:A:C8	2.54	0.43
83:S2:454:U:H2'	83:S2:455:A:C8	2.52	0.43
83:S2:1539:U:H2'	83:S2:1540:G:C8	2.53	0.43
3:L5:267:G:H2'	3:L5:268:G:C8	2.53	0.43
3:L5:1294:A:H1'	3:L5:1296:G:C2	2.54	0.43
3:L5:1705:G:H2'	3:L5:1706:A:O4'	2.18	0.43
3:L5:2474:G:H2'	3:L5:2502:G:N2	2.33	0.43
3:L5:2517:A:N3	3:L5:2539:C:O2'	2.52	0.43
3:L5:2632:PSU:H2'	3:L5:2633:U:C6	2.53	0.43
3:L5:4126:C:H5''	3:L5:4127:A:H5''	2.00	0.43
5:L8:144:U:H2'	5:L8:145:C:C6	2.53	0.43
11:LF:119:ASN:HD21	11:LF:212:LYS:HD3	1.83	0.43
15:LJ:62:ILE:HD12	15:LJ:68:ILE:HD11	2.00	0.43
36:Lf:29:LYS:HB2	36:Lf:83:MET:HE1	2.01	0.43
58:ST:74:SER:O	58:ST:78:ILE:HG12	2.18	0.43
59:SU:51:LYS:HD3	83:S2:1433:C:N4	2.34	0.43
64:Sg:191:HIS:CD2	64:Sg:195:LEU:HD11	2.52	0.43
78:SX:17:ARG:O	78:SX:21:LYS:HG3	2.18	0.43
79:SY:15:ASN:OD1	79:SY:20:ARG:HG2	2.18	0.43
3:L5:441:G:H2'	3:L5:442:G:C8	2.54	0.43
3:L5:1175:A:H2	3:L5:1185:G:H1	1.66	0.43
3:L5:1818:G:O2'	3:L5:1820:C:OP2	2.24	0.43
3:L5:3709:U:H2'	3:L5:3710:G:C8	2.53	0.43
3:L5:3893:C:O2'	3:L5:4979:A:N1	2.48	0.43
3:L5:3923:A:H2'	3:L5:3924:C:C6	2.54	0.43
3:L5:4147:G:H2'	3:L5:4148:C:C6	2.54	0.43
3:L5:4620:OMU:OP2	3:L5:4670:C:N4	2.35	0.43
5:L8:119:C:H2'	5:L8:120:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LB:57:VAL:HB	7:LB:367:PHE:HB3	2.01	0.43
11:LF:214:SER:OG	11:LF:215:SER:N	2.50	0.43
12:LG:230:TYR:CE2	12:LG:234:ARG:HD2	2.54	0.43
15:LJ:35:ARG:O	15:LJ:39:VAL:HG23	2.19	0.43
17:LM:118:MET:HG2	19:LO:192:TYR:CZ	2.54	0.43
20:LP:94:MET:HE3	20:LP:94:MET:HB2	1.92	0.43
22:LR:175:GLU:O	22:LR:178:GLN:HG3	2.19	0.43
23:LS:77:ASN:HD21	23:LS:146:HIS:CE1	2.35	0.43
25:LU:22:THR:HA	25:LU:71:THR:HA	1.99	0.43
29:LY:54:GLU:HB2	29:LY:108:ARG:HB3	1.99	0.43
55:SQ:25:CYS:HA	55:SQ:68:ILE:HD13	2.01	0.43
63:Sf:103:LEU:HG	63:Sf:104:LYS:H	1.83	0.43
83:S2:155:G:C6	83:S2:164:A:C6	3.06	0.43
85:CF:30:LYS:HD3	85:CF:202:LEU:HB2	2.01	0.43
3:L5:271:C:H2'	3:L5:272:U:H6	1.84	0.43
3:L5:475:G:H2'	3:L5:476:G:C8	2.53	0.43
3:L5:499:G:H2'	3:L5:499:G:N3	2.34	0.43
3:L5:1234:G:H2'	3:L5:1235:G:H8	1.83	0.43
3:L5:1257:A:H3'	3:L5:1258:G:C8	2.54	0.43
3:L5:1751:A:H2'	3:L5:1752:G:C8	2.54	0.43
3:L5:2020:U:O3'	48:Ls:57:LYS:HA	2.19	0.43
3:L5:2903:G:H1'	3:L5:2904:U:C5	2.53	0.43
3:L5:4069:U:H2'	3:L5:4070:U:C6	2.53	0.43
3:L5:4419:U:H1'	84:AT:19:G:O6	2.19	0.43
12:LG:165:GLU:OE2	18:LN:26:ARG:NH1	2.46	0.43
14:LI:52:MET:HE1	14:LI:159:PHE:HE2	1.83	0.43
21:LQ:25:LEU:HA	21:LQ:28:LEU:HD23	2.01	0.43
27:LW:4:GLU:HG2	27:LW:12:LYS:HE3	2.01	0.43
27:LW:52:THR:O	27:LW:56:ARG:HG2	2.18	0.43
66:SB:144:LYS:HD3	66:SB:208:HIS:HB3	2.01	0.43
67:SC:176:LYS:O	67:SC:200:ARG:NH2	2.52	0.43
74:SN:94:LYS:O	74:SN:98:VAL:HG23	2.18	0.43
77:SW:28:ARG:HD3	83:S2:921:G:C5	2.53	0.43
83:S2:293:C:O2'	83:S2:294:U:H3'	2.18	0.43
83:S2:342:C:H2'	83:S2:343:A:H8	1.84	0.43
83:S2:508:A:H3'	83:S2:509:OMG:C8	2.49	0.43
83:S2:696:G:H21	83:S2:737:G:N2	2.16	0.43
85:CF:18:SER:HA	85:CF:154:LYS:HE3	2.01	0.43
3:L5:303:C:OP2	18:LN:68:ARG:NH2	2.46	0.43
3:L5:490:C:N4	3:L5:491:G:O6	2.51	0.43
3:L5:935:A:N7	17:LM:46:ARG:NH2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1562:G:H5'	3:L5:1563:A:OP2	2.18	0.43
3:L5:1790:U:C5	87:L5:5259:SPM:H91	2.54	0.43
3:L5:1867:A:H2'	3:L5:1868:A:C8	2.54	0.43
5:L8:96:C:H5''	38:Lh:66:LYS:HG2	2.01	0.43
8:LC:348:LYS:HA	8:LC:351:VAL:HG12	1.99	0.43
9:LD:64:ILE:HD13	9:LD:109:LEU:HD22	2.00	0.43
9:LD:150:LEU:HD12	15:LJ:146:ARG:HG3	2.01	0.43
14:LI:47:PRO:HB3	14:LI:171:TRP:CZ2	2.53	0.43
22:LR:127:VAL:HG12	22:LR:132:PHE:HD2	1.82	0.43
48:Ls:31:GLY:HA2	48:Ls:86:VAL:HG12	2.00	0.43
64:Sg:176:VAL:HG23	64:Sg:185:LYS:HB2	2.01	0.43
66:SB:171:ILE:HG22	66:SB:174:ARG:HE	1.83	0.43
75:SO:135:ILE:HG21	83:S2:986:G:N2	2.33	0.43
83:S2:696:G:H8	83:S2:733:C:H41	1.65	0.43
83:S2:1491:G:H2'	83:S2:1492:U:C6	2.54	0.43
83:S2:1511:U:H2'	83:S2:1512:C:C6	2.53	0.43
83:S2:1680:G:H2'	83:S2:1681:U:C6	2.53	0.43
85:CF:250:LEU:HD21	85:CF:253:VAL:HG13	2.01	0.43
2:Pt:29:C:H2'	2:Pt:30:G:C8	2.54	0.43
3:L5:351:C:OP2	8:LC:197:ARG:NH1	2.39	0.43
3:L5:664:G:H2'	3:L5:665:C:C6	2.53	0.43
3:L5:1494:U:H2'	3:L5:1495:G:C8	2.54	0.43
3:L5:1947:U:H2'	43:Lm:109:ASN:OD1	2.18	0.43
3:L5:2515:G:OP1	37:Lg:37:LYS:NZ	2.39	0.43
5:L8:153:C:H2'	5:L8:154:G:H8	1.84	0.43
6:LA:116:LEU:HB2	6:LA:126:LEU:HB2	1.99	0.43
12:LG:147:VAL:O	12:LG:177:MET:HG2	2.19	0.43
18:LN:200:LEU:HD22	18:LN:204:ARG:NH1	2.33	0.43
54:SP:125:PRO:HG3	57:SS:127:TRP:CH2	2.53	0.43
65:SA:111:GLN:HA	65:SA:116:PHE:CG	2.54	0.43
65:SA:215:GLN:O	65:SA:219:GLU:HG2	2.19	0.43
68:SE:100:ARG:NH2	68:SE:118:GLU:OE2	2.51	0.43
74:SN:29:THR:OG1	74:SN:31:ASP:OD1	2.37	0.43
75:SO:136:PRO:HB3	83:S2:944:A:H1'	2.00	0.43
83:S2:116:OMU:O5'	83:S2:116:OMU:H6	2.18	0.43
83:S2:943:U:C2	83:S2:944:A:C8	3.06	0.43
83:S2:1317:C:H2'	83:S2:1318:G:H8	1.84	0.43
83:S2:1581:C:H5'	83:S2:1582:C:H5	1.82	0.43
3:L5:173:C:H2'	3:L5:174:C:C6	2.54	0.43
3:L5:223:G:H4'	3:L5:225:G:C8	2.54	0.43
3:L5:1186:U:H2'	3:L5:1187:G:N3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1700:G:H5''	3:L5:1704:C:H42	1.83	0.43
3:L5:2413:U:H2'	3:L5:2414:G:H8	1.84	0.43
3:L5:2475:G:H5''	3:L5:2476:G:C8	2.54	0.43
4:L7:26:C:H5''	9:LD:56:THR:HG21	2.01	0.43
7:LB:14:LEU:HD22	7:LB:17:LEU:HD11	2.01	0.43
51:SF:168:THR:HG23	51:SF:171:GLU:H	1.84	0.43
56:SR:102:THR:HA	56:SR:105:MET:HG3	2.01	0.43
60:SZ:80:ARG:HD3	83:S2:1598:G:H3'	2.01	0.43
72:SJ:93:LYS:HB2	72:SJ:96:TYR:CD2	2.50	0.43
82:Se:12:VAL:HG13	83:S2:616:A:H1'	2.01	0.43
83:S2:1025:U:OP1	83:S2:1090:C:O2'	2.35	0.43
83:S2:1208:A:H2'	83:S2:1209:A:H8	1.84	0.43
85:CF:12:VAL:HG12	85:CF:113:VAL:HB	2.01	0.43
85:CF:178:ILE:HG12	85:CF:183:TYR:HB2	2.00	0.43
3:L5:286:U:H2'	3:L5:287:U:C6	2.54	0.42
3:L5:1326:A2M:HM'3	3:L5:1326:A2M:H1'	1.52	0.42
3:L5:1730:U:H4'	24:LT:100:LYS:HB2	2.01	0.42
3:L5:2351:OMC:H1'	3:L5:2351:OMC:HM23	1.65	0.42
3:L5:2608:G:H2'	3:L5:2609:G:H8	1.84	0.42
3:L5:2610:G:H2'	3:L5:2611:A:C8	2.54	0.42
3:L5:2743:A:H2'	3:L5:2744:A:C8	2.54	0.42
3:L5:3722:G:H2'	3:L5:3723:A:H8	1.83	0.42
3:L5:3925:OMU:H1'	3:L5:3925:OMU:HM23	1.77	0.42
3:L5:4192:A:H2'	3:L5:4193:C:H6	1.83	0.42
3:L5:4364:G:H2'	3:L5:4365:C:H6	1.83	0.42
3:L5:4530:UR3:H2'	3:L5:4531:U:H2'	2.00	0.42
3:L5:4775:C:H41	3:L5:4859:C:H42	1.67	0.42
3:L5:5030:U:H2'	3:L5:5031:G:C8	2.53	0.42
6:LA:115:CYS:SG	6:LA:124:GLY:HA3	2.59	0.42
7:LB:160:ILE:HG12	7:LB:193:LYS:HD3	2.01	0.42
11:LF:59:LYS:HE2	11:LF:63:GLN:NE2	2.34	0.42
15:LJ:43:LEU:HB2	15:LJ:117:ILE:HD11	2.00	0.42
22:LR:80:LYS:HA	22:LR:80:LYS:HD2	1.89	0.42
22:LR:105:LEU:HD23	22:LR:138:LEU:HD23	2.01	0.42
24:LT:14:MET:HE2	24:LT:14:MET:HB3	1.83	0.42
35:Le:35:TRP:CZ2	35:Le:56:PRO:HD2	2.54	0.42
54:SP:90:VAL:HG11	54:SP:109:PRO:HG3	2.01	0.42
61:Sc:7:GLN:HE22	61:Sc:60:GLU:HG2	1.84	0.42
65:SA:18:PHE:HB3	65:SA:23:THR:OG1	2.18	0.42
68:SE:252:ARG:O	68:SE:256:LEU:HG	2.19	0.42
75:SO:101:GLY:HA3	75:SO:134:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:167:C:H2'	3:L5:168:C:C6	2.54	0.42
3:L5:184:U:O4'	3:L5:254:G:N2	2.51	0.42
3:L5:674:G:H2'	3:L5:675:C:C6	2.53	0.42
3:L5:1194:G:H2'	3:L5:1195:G:C8	2.54	0.42
3:L5:1751:A:H2'	3:L5:1752:G:H8	1.84	0.42
3:L5:1806:G:H2'	3:L5:1807:C:C6	2.53	0.42
3:L5:2864:A:H2'	3:L5:2865:U:H6	1.84	0.42
5:L8:82:A:N7	5:L8:84:A:H3'	2.33	0.42
6:LA:66:PRO:HG2	6:LA:67:TYR:CE2	2.54	0.42
9:LD:56:THR:HG22	9:LD:57:ASN:H	1.84	0.42
16:LL:7:GLY:O	31:La:49:HIS:NE2	2.48	0.42
20:LP:15:CYS:SG	20:LP:150:LEU:HB2	2.60	0.42
50:SD:222:PRO:HB3	64:Sg:190:GLY:HA3	2.02	0.42
58:ST:129:ARG:HG3	83:S2:1416:C:OP1	2.18	0.42
64:Sg:251:ALA:HA	64:Sg:256:ILE:HD13	2.02	0.42
66:SB:126:ASP:OD2	66:SB:136:ARG:NH2	2.47	0.42
67:SC:169:TYR:CG	67:SC:173:LYS:HG2	2.54	0.42
68:SE:59:ASP:O	68:SE:63:LYS:HG3	2.19	0.42
70:SH:78:ARG:HH22	70:SH:82:GLU:CD	2.28	0.42
71:SI:3:ILE:O	71:SI:30:GLY:N	2.50	0.42
73:SL:111:VAL:HG11	73:SL:128:VAL:HG11	2.00	0.42
75:SO:82:ALA:HB1	75:SO:124:MET:HE3	2.01	0.42
77:SW:50:PHE:HB3	77:SW:63:VAL:HG13	2.01	0.42
83:S2:1409:A:H2'	83:S2:1410:C:C6	2.53	0.42
83:S2:1780:G:H3'	83:S2:1781:A:C8	2.54	0.42
85:CF:7:HIS:ND1	85:CF:305:GLY:O	2.51	0.42
3:L5:423:G:H5'	20:LP:26:PHE:HZ	1.84	0.42
3:L5:1206:C:H2'	3:L5:1207:C:H6	1.84	0.42
3:L5:1834:U:C2	24:LT:128:LEU:HD13	2.55	0.42
3:L5:4389:C:H2'	3:L5:4390:A:C8	2.54	0.42
4:L7:63:C:H5'	4:L7:64:G:H5''	2.01	0.42
8:LC:328:LEU:HB3	11:LF:187:MET:HG3	2.00	0.42
10:LE:261:ILE:HG23	10:LE:267:LEU:HD23	2.00	0.42
12:LG:102:TYR:OH	12:LG:211:ASP:OD2	2.27	0.42
48:Ls:6:ARG:O	48:Ls:10:LYS:HG2	2.19	0.42
51:SF:48:TYR:HE2	55:SQ:56:LEU:HD13	1.84	0.42
56:SR:100:PRO:HA	56:SR:103:LYS:HB3	2.01	0.42
56:SR:106:LEU:HD21	65:SA:19:LEU:HD21	2.00	0.42
61:Sc:40:ARG:NH2	61:Sc:42:ILE:HD11	2.34	0.42
67:SC:64:THR:HG22	67:SC:66:LEU:H	1.85	0.42
70:SH:30:LEU:O	70:SH:33:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:SJ:138:ARG:HA	72:SJ:156:HIS:HB3	2.00	0.42
83:S2:321:C:H2'	83:S2:322:C:C6	2.53	0.42
83:S2:379:C:H2'	83:S2:380:G:C8	2.54	0.42
83:S2:569:A:H2'	83:S2:570:C:O4'	2.19	0.42
83:S2:898:U:H2'	83:S2:900:C:O4'	2.19	0.42
83:S2:1227:G:C2	83:S2:1228:A:C8	3.07	0.42
83:S2:1657:G:H2'	83:S2:1658:G:H8	1.84	0.42
83:S2:1760:G:N1	83:S2:1774:C:OP1	2.52	0.42
3:L5:302:C:H2'	3:L5:303:C:C6	2.54	0.42
3:L5:1199:G:H2'	3:L5:1200:G:C8	2.54	0.42
3:L5:1302:U:H3'	3:L5:1303:A:H8	1.84	0.42
3:L5:1534:A2M:N3	40:Lj:11:ARG:HB2	2.34	0.42
3:L5:1847:C:H2'	3:L5:1848:C:C6	2.55	0.42
3:L5:2041:A:N7	3:L5:4434:C:O2'	2.49	0.42
3:L5:2412:A:H2'	3:L5:2413:U:C6	2.54	0.42
3:L5:2634:C:H2'	3:L5:2635:U:C6	2.55	0.42
3:L5:2667:C:O4'	22:LR:96:MET:HG2	2.19	0.42
3:L5:4277:G:H5''	24:LT:17:ARG:HG2	2.01	0.42
3:L5:4347:G:H2'	3:L5:4348:A:C8	2.54	0.42
4:L7:72:U:H2'	4:L7:73:U:O4'	2.19	0.42
7:LB:168:MET:SD	7:LB:171:LEU:HD12	2.59	0.42
32:Lb:35:VAL:HB	32:Lb:40:LEU:HD21	2.02	0.42
48:Ls:66:ARG:HB2	48:Ls:79:LEU:HD11	2.00	0.42
51:SF:133:THR:HG22	51:SF:134:VAL:HG23	2.02	0.42
54:SP:128:HIS:HB3	83:S2:1522:A:C5	2.55	0.42
55:SQ:105:LYS:NZ	55:SQ:109:LYS:HD2	2.35	0.42
57:SS:125:HIS:CD2	57:SS:131:VAL:HG11	2.55	0.42
69:SG:10:THR:HA	69:SG:128:THR:HG23	2.01	0.42
83:S2:128:U:O2'	83:S2:130:G:N7	2.52	0.42
83:S2:382:C:H2'	83:S2:383:G:C8	2.54	0.42
83:S2:647:U:H2'	83:S2:648:A:H8	1.84	0.42
83:S2:1189:A:H2'	83:S2:1190:A:H8	1.84	0.42
83:S2:1588:A:H2'	83:S2:1589:A:H8	1.85	0.42
83:S2:1719:A:N6	83:S2:1814:G:O2'	2.52	0.42
3:L5:64:A:H1'	3:L5:76:A:H1'	2.00	0.42
3:L5:689:U:H2'	3:L5:690:C:C6	2.55	0.42
3:L5:1079:C:H2'	3:L5:1080:C:H6	1.85	0.42
3:L5:1504:G:H2'	3:L5:1505:C:C6	2.54	0.42
4:L7:38:U:N3	4:L7:41:G:OP2	2.34	0.42
12:LG:154:LEU:HB3	12:LG:204:PHE:HB2	2.01	0.42
16:LL:142:GLU:O	16:LL:146:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LM:125:ASN:C	17:LM:125:ASN:HD22	2.27	0.42
20:LP:91:LEU:HD23	20:LP:91:LEU:HA	1.90	0.42
25:LU:72:VAL:HG21	25:LU:83:LEU:HD21	2.02	0.42
30:LZ:121:ARG:NH1	30:LZ:127:ASN:OD1	2.46	0.42
34:Ld:25:TYR:CE1	34:Ld:88:LEU:HD12	2.54	0.42
36:Lf:106:TYR:HB2	36:Lf:107:PRO:HD3	2.01	0.42
49:Lt:121:LEU:HD13	49:Lt:129:ILE:HG13	2.01	0.42
54:SP:42:ARG:HH22	83:S2:1613:G:P	2.43	0.42
59:SU:38:ASP:OD1	59:SU:39:LEU:N	2.52	0.42
67:SC:144:SER:HB3	67:SC:150:ALA:HB2	2.02	0.42
69:SG:191:ARG:NH1	83:S2:312:G:H2'	2.32	0.42
70:SH:43:LEU:HD12	70:SH:72:PHE:CE1	2.54	0.42
70:SH:106:ARG:NH1	83:S2:861:A:O2'	2.52	0.42
72:SJ:86:VAL:HG11	72:SJ:105:PHE:HD1	1.84	0.42
83:S2:26:U:H2'	83:S2:27:A2M:H8	2.01	0.42
83:S2:1617:G:N2	83:S2:1619:A:H3'	2.35	0.42
3:L5:106:A:H2'	3:L5:107:G:O4'	2.19	0.42
3:L5:179:G:H2'	3:L5:180:C:C6	2.55	0.42
3:L5:231:U:H4'	29:LY:100:HIS:CD2	2.54	0.42
3:L5:433:A:C2	3:L5:3867:A2M:H4'	2.54	0.42
3:L5:457:G:H2'	3:L5:458:C:H6	1.83	0.42
3:L5:1401:C:H2'	3:L5:1402:C:C6	2.54	0.42
3:L5:1539:G:H2'	3:L5:1540:C:H6	1.84	0.42
3:L5:2256:C:H2'	3:L5:2257:C:O4'	2.19	0.42
3:L5:2385:U:H2'	3:L5:2386:U:C6	2.55	0.42
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.55	0.42
3:L5:2749:C:H2'	3:L5:2750:G:C8	2.55	0.42
3:L5:4253:A:H5'	3:L5:4254:G:C8	2.55	0.42
4:L7:52:C:O2'	4:L7:54:A:N7	2.52	0.42
9:LD:218:ALA:HA	9:LD:221:LYS:HG2	2.02	0.42
13:LH:114:ILE:HB	13:LH:124:ARG:HB2	2.01	0.42
20:LP:128:ARG:NH1	20:LP:130:TYR:OH	2.52	0.42
25:LU:19:LEU:HD12	25:LU:78:PHE:HB3	2.02	0.42
55:SQ:110:ASP:HA	55:SQ:113:ILE:HG12	2.01	0.42
63:Sf:123:SER:HG	63:Sf:126:CYS:H	1.67	0.42
71:SI:81:VAL:HG22	71:SI:102:VAL:HG12	2.01	0.42
73:SL:18:GLN:HG3	73:SL:33:LEU:HD11	2.01	0.42
74:SN:85:PRO:HG2	74:SN:129:TYR:CE2	2.55	0.42
83:S2:1140:G:O2'	83:S2:1151:G:O2'	2.38	0.42
83:S2:1198:G:H2'	83:S2:1199:A:C8	2.55	0.42
3:L5:319:A:H1'	3:L5:3726:A:N3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1364:U:OP2	16:LL:36:ARG:NH2	2.36	0.42
3:L5:1730:U:H2'	3:L5:1731:C:C6	2.55	0.42
3:L5:1998:A:H5'	48:Ls:55:MET:O	2.19	0.42
3:L5:2019:C:H2'	3:L5:2020:U:H6	1.85	0.42
3:L5:2293:U:H2'	3:L5:2294:G:C8	2.55	0.42
3:L5:2538:U:H2'	3:L5:2539:C:C6	2.55	0.42
3:L5:2778:G:N2	5:L8:113:C:OP2	2.50	0.42
3:L5:3718:A2M:HM'3	3:L5:3718:A2M:H1'	1.64	0.42
3:L5:3917:A:H2'	3:L5:3918:G:C8	2.54	0.42
3:L5:4419:U:H6	3:L5:4419:U:H2'	1.71	0.42
8:LC:141:GLY:O	8:LC:204:ARG:NH2	2.49	0.42
10:LE:157:HIS:HA	10:LE:160:LYS:HE3	2.01	0.42
19:LO:54:TYR:CD1	19:LO:145:VAL:HG21	2.55	0.42
23:LS:29:ARG:NH1	24:LT:150:LEU:HD12	2.35	0.42
25:LU:28:PRO:HB2	25:LU:34:MET:HG2	2.02	0.42
36:Lf:45:LYS:NZ	36:Lf:108:SER:HA	2.35	0.42
45:Lo:32:SER:C	45:Lo:34:TYR:H	2.27	0.42
50:SD:35:SER:HB2	50:SD:97:CYS:SG	2.59	0.42
56:SR:52:GLY:O	56:SR:55:THR:OG1	2.35	0.42
59:SU:53:PRO:HB3	59:SU:89:ILE:HG12	2.02	0.42
64:Sg:44:LYS:HG2	64:Sg:56:GLN:HB2	2.02	0.42
64:Sg:107:ASP:C	64:Sg:124:SER:HG	2.22	0.42
65:SA:208:GLU:HA	65:SA:211:GLU:HG2	2.00	0.42
67:SC:194:ARG:HB3	67:SC:225:SER:HB3	2.01	0.42
67:SC:264:SER:H	67:SC:267:GLN:HE21	1.67	0.42
69:SG:149:LYS:HA	69:SG:149:LYS:HD2	1.89	0.42
70:SH:58:LYS:HA	70:SH:58:LYS:HD2	1.80	0.42
72:SJ:81:LEU:HD23	72:SJ:81:LEU:HA	1.90	0.42
72:SJ:87:LEU:HD13	72:SJ:100:LEU:HD21	2.01	0.42
73:SL:22:ARG:NH1	73:SL:31:GLU:OE2	2.45	0.42
73:SL:57:ASP:OD1	73:SL:60:CYS:N	2.52	0.42
75:SO:45:THR:HA	75:SO:52:THR:HA	2.01	0.42
76:SV:32:ILE:HG12	76:SV:60:ARG:HD2	2.02	0.42
76:SV:74:LYS:HE2	76:SV:83:PHE:HB3	2.00	0.42
80:Sa:36:ILE:HD13	80:Sa:84:VAL:HG11	2.01	0.42
80:Sa:79:ILE:HD13	80:Sa:84:VAL:HG23	2.02	0.42
81:Sb:53:VAL:HG13	81:Sb:62:VAL:HG23	2.01	0.42
83:S2:46:A:H61	83:S2:433:A:H2	1.66	0.42
83:S2:693:A:H2'	83:S2:694:G:C8	2.54	0.42
83:S2:1533:A:H62	83:S2:1602:U:H3	1.66	0.42
83:S2:1856:C:H2'	83:S2:1857:G:C8	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:678:C:H4'	47:Lr:96:MET:HE2	2.01	0.42
3:L5:1241:C:N3	32:Lb:115:GLY:HA2	2.34	0.42
3:L5:1503:A:H62	21:LQ:87:THR:HG21	1.84	0.42
3:L5:1577:G:OP1	46:Lp:17:ARG:NH2	2.48	0.42
3:L5:2021:G:OP1	48:Ls:58:ASN:N	2.50	0.42
3:L5:3758:U:H2'	3:L5:3765:G:N2	2.35	0.42
3:L5:3765:G:H21	3:L5:3766:A:N6	2.16	0.42
3:L5:4093:G:N2	3:L5:4114:C:N3	2.61	0.42
3:L5:4232:U:H5''	45:Lo:3:ASN:O	2.20	0.42
3:L5:4504:C:H2'	3:L5:4505:C:C6	2.55	0.42
4:L7:112:U:H2'	4:L7:113:G:H8	1.85	0.42
5:L8:60:G:P	28:LX:68:ARG:HH22	2.42	0.42
22:LR:23:TRP:CE3	22:LR:51:ILE:HG12	2.55	0.42
26:LV:43:LYS:HG3	26:LV:60:MET:HG2	2.02	0.42
34:Ld:88:LEU:HD23	34:Ld:106:VAL:HG22	2.02	0.42
39:Li:68:ARG:NH2	39:Li:71:LYS:HG3	2.35	0.42
48:Ls:77:LYS:HE2	48:Ls:193:PHE:HE1	1.85	0.42
50:SD:76:ARG:HB2	52:SK:22:VAL:HG11	2.01	0.42
50:SD:135:GLU:HG2	50:SD:153:VAL:HB	2.02	0.42
52:SK:27:VAL:HB	52:SK:43:LEU:HD12	2.02	0.42
55:SQ:3:SER:OG	55:SQ:4:LYS:N	2.53	0.42
56:SR:57:LEU:O	56:SR:61:ILE:HG13	2.20	0.42
65:SA:160:ALA:HB3	76:SV:66:ASP:OD2	2.20	0.42
65:SA:163:CYS:SG	65:SA:174:MET:HG3	2.60	0.42
68:SE:19:MET:HE3	68:SE:108:ARG:HD2	2.00	0.42
80:Sa:14:GLY:H	80:Sa:15:ARG:HH11	1.66	0.42
83:S2:1165:G:OP2	83:S2:1165:G:N2	2.34	0.42
1:CI:63:ARG:HD2	1:CI:63:ARG:HA	1.85	0.42
3:L5:424:U:H2'	3:L5:425:U:H6	1.84	0.42
3:L5:727:C:OP1	11:LF:73:ARG:NH2	2.40	0.42
3:L5:919:C:OP1	17:LM:69:HIS:ND1	2.31	0.42
3:L5:1197:C:H2'	3:L5:1198:G:C8	2.54	0.42
3:L5:1210:C:OP1	11:LF:70:ARG:HD3	2.20	0.42
3:L5:1341:U:H2'	3:L5:1342:A:H8	1.84	0.42
3:L5:1369:C:OP2	3:L5:1370:G:O2'	2.25	0.42
3:L5:1473:U:H2'	3:L5:1474:C:C6	2.55	0.42
3:L5:1824:G:H2'	3:L5:1825:A:C8	2.55	0.42
3:L5:1844:G:O3'	32:Lb:25:ARG:NH1	2.53	0.42
3:L5:2401:A2M:H5''	3:L5:2401:A2M:H8	2.01	0.42
3:L5:2897:G:H2'	3:L5:2898:G:H8	1.84	0.42
3:L5:4760:G:H2'	3:L5:4761:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4989:U:H1'	3:L5:4990:C:C5	2.55	0.42
3:L5:5002:U:H2'	3:L5:5003:U:C6	2.54	0.42
18:LN:3:ALA:O	18:LN:7:ILE:HD12	2.20	0.42
43:Lm:99:CYS:HB2	43:Lm:114:LYS:HE3	2.01	0.42
52:SK:46:MET:SD	52:SK:47:LYS:HG3	2.60	0.42
67:SC:256:TRP:CE2	77:SW:68:ARG:HD3	2.55	0.42
72:SJ:39:ASN:HB2	83:S2:642:U:P	2.60	0.42
72:SJ:124:HIS:CD2	82:Se:35:ARG:HD2	2.54	0.42
80:Sa:98:PRO:HA	80:Sa:99:PRO:HD3	1.95	0.42
83:S2:339:A:H2'	83:S2:340:C:H5	1.84	0.42
83:S2:672:A:N6	83:S2:1027:A:OP1	2.52	0.42
83:S2:1144:A:H5'	83:S2:1355:C:H5	1.84	0.42
3:L5:1427:A:OP2	3:L5:1457:G:N1	2.48	0.42
3:L5:2262:G:OP2	47:Lr:98:ARG:NH2	2.40	0.42
3:L5:2490:U:H3'	3:L5:2491:C:C6	2.54	0.42
3:L5:3897:G:OP1	7:LB:250:LYS:HD2	2.18	0.42
3:L5:4132:C:H2'	3:L5:4133:C:O4'	2.20	0.42
3:L5:4392:OMG:HM21	3:L5:4394:A:H2'	2.02	0.42
3:L5:4478:G:O2'	3:L5:4602:A:N1	2.45	0.42
5:L8:83:C:H42	29:LY:50:ARG:NH2	2.18	0.42
8:LC:279:LEU:HD23	8:LC:279:LEU:HA	1.89	0.42
10:LE:46:ARG:O	10:LE:62:MET:HE1	2.19	0.42
16:LL:18:TRP:CD1	16:LL:18:TRP:H	2.36	0.42
17:LM:96:GLU:O	17:LM:100:ARG:HG2	2.20	0.42
46:Lp:23:ARG:HA	46:Lp:26:VAL:HG12	2.02	0.42
53:SM:44:LYS:HE2	63:Sf:128:ALA:H	1.84	0.42
56:SR:54:VAL:O	56:SR:58:MET:HG2	2.20	0.42
59:SU:97:ILE:O	59:SU:100:GLN:HG3	2.20	0.42
60:SZ:50:PHE:HE2	60:SZ:87:ALA:HB2	1.85	0.42
64:Sg:144:ASP:OD1	64:Sg:144:ASP:N	2.45	0.42
65:SA:8:LEU:HD22	65:SA:59:LEU:HD11	2.02	0.42
65:SA:84:GLN:O	65:SA:88:LEU:HD23	2.20	0.42
65:SA:126:ASP:HB3	65:SA:129:ALA:HB3	2.02	0.42
68:SE:247:THR:N	68:SE:250:GLU:OE2	2.50	0.42
72:SJ:149:VAL:HG11	72:SJ:157:ILE:HD11	2.02	0.42
79:SY:11:LYS:NZ	83:S2:832:G:O6	2.53	0.42
81:Sb:34:ASP:O	81:Sb:79:PHE:HA	2.20	0.42
83:S2:588:G:H4'	83:S2:589:G:H5'	2.02	0.42
83:S2:909:G:H2'	83:S2:910:G:C8	2.55	0.42
83:S2:1039:C:H2'	83:S2:1040:G:H8	1.85	0.42
83:S2:1060:A:H1'	83:S2:1062:A:N7	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1266:C:H2'	83:S2:1267:C:H6	1.85	0.42
83:S2:1545:A:C2	83:S2:1671:G:H1'	2.54	0.42
85:CF:162:TYR:HB3	85:CF:208:MET:HB3	2.02	0.42
1:CI:78:HIS:CD2	3:L5:2706:G:N7	2.88	0.41
3:L5:121:A:OP1	12:LG:110:LYS:NZ	2.33	0.41
3:L5:475:G:H2'	3:L5:476:G:H8	1.84	0.41
3:L5:1074:G:H3'	3:L5:1075:G:H8	1.84	0.41
3:L5:1545:G:H2'	3:L5:1546:C:C6	2.55	0.41
3:L5:1758:G:H2'	3:L5:1759:G:C8	2.55	0.41
3:L5:4606:G:N2	84:AT:63:C:O2'	2.52	0.41
4:L7:7:G:H5''	9:LD:22:ARG:HD3	2.01	0.41
6:LA:57:PRO:HD2	6:LA:170:ALA:HB3	2.01	0.41
6:LA:58:LEU:HD13	6:LA:75:LEU:HG	2.02	0.41
13:LH:91:LYS:HE3	13:LH:143:GLU:OE2	2.20	0.41
29:LY:31:SER:HA	29:LY:48:PRO:HA	2.02	0.41
50:SD:105:LEU:HD23	50:SD:184:ILE:HD11	2.00	0.41
54:SP:41:GLN:O	54:SP:45:LEU:HG	2.19	0.41
58:ST:121:ARG:HH21	83:S2:1563:G:H5''	1.85	0.41
59:SU:40:ILE:O	59:SU:44:LYS:HG2	2.19	0.41
64:Sg:64:HIS:NE2	83:S2:1451:G:OP1	2.50	0.41
73:SL:21:LYS:HD2	73:SL:21:LYS:HA	1.81	0.41
74:SN:66:VAL:HG13	74:SN:67:THR:HG23	2.02	0.41
83:S2:224:A:H2'	83:S2:225:G:C8	2.55	0.41
83:S2:953:C:H2'	83:S2:954:U:C6	2.55	0.41
83:S2:1288:OMU:HM23	83:S2:1288:OMU:H1'	1.89	0.41
83:S2:1490:OMG:HM23	83:S2:1490:OMG:H1'	1.85	0.41
83:S2:1545:A:H2'	83:S2:1546:G:C8	2.55	0.41
83:S2:1716:C:H2'	83:S2:1717:C:H6	1.85	0.41
84:AT:24:C:H2'	84:AT:25:A:C8	2.54	0.41
84:AT:65:G:H2'	84:AT:66:G:C8	2.55	0.41
3:L5:1896:A:OP1	11:LF:223:LYS:NZ	2.46	0.41
3:L5:2424:OMG:H1'	3:L5:2424:OMG:HM23	1.78	0.41
3:L5:2749:C:H2'	3:L5:2750:G:H8	1.84	0.41
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.55	0.41
3:L5:4392:OMG:N3	3:L5:4447:5MC:HM52	2.36	0.41
5:L8:120:G:H2'	5:L8:121:G:H8	1.85	0.41
8:LC:266:THR:HG22	8:LC:267:TRP:H	1.85	0.41
9:LD:41:LYS:HD2	24:LT:93:ILE:HG21	2.01	0.41
10:LE:223:ARG:NH2	10:LE:238:GLU:HG3	2.35	0.41
19:LO:81:TRP:HB2	19:LO:104:VAL:HG21	2.02	0.41
22:LR:44:LEU:HD22	22:LR:49:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SF:149:GLN:HE21	51:SF:153:LEU:HG	1.85	0.41
55:SQ:98:LYS:O	64:Sg:57:ARG:NH1	2.43	0.41
58:ST:62:ARG:CZ	83:S2:1542:C:H5''	2.49	0.41
60:SZ:96:LEU:H	60:SZ:96:LEU:HD23	1.85	0.41
62:Sd:46:TYR:O	62:Sd:50:ILE:HG12	2.20	0.41
67:SC:74:LYS:HB3	67:SC:269:PHE:CE2	2.54	0.41
69:SG:224:ARG:HH21	69:SG:227:GLN:HG3	1.85	0.41
80:Sa:13:LYS:HD3	80:Sa:13:LYS:HA	1.70	0.41
83:S2:156:G:H2'	83:S2:157:U:C6	2.55	0.41
83:S2:323:C:O2'	83:S2:325:C:N4	2.54	0.41
83:S2:920:A:O2'	83:S2:922:A:O5'	2.38	0.41
83:S2:964:A:H2'	83:S2:965:U:H6	1.84	0.41
83:S2:1101:U:H2'	83:S2:1102:G:H8	1.85	0.41
83:S2:1643:U:H2'	83:S2:1644:C:H6	1.85	0.41
85:CF:102:MET:HG3	85:CF:136:HIS:CE1	2.54	0.41
3:L5:654:C:O3'	8:LC:268:ARG:NH1	2.47	0.41
3:L5:1309:C:H2'	3:L5:1310:C:C6	2.55	0.41
3:L5:1537:A:H2'	3:L5:1538:U:C6	2.54	0.41
3:L5:1996:C:N4	3:L5:2000:G:N2	2.34	0.41
3:L5:2249:C:H2'	3:L5:2250:C:C5	2.56	0.41
3:L5:2407:G:H2'	42:Ll:13:LEU:HD22	2.02	0.41
3:L5:2811:G:N1	3:L5:2814:C:OP2	2.46	0.41
3:L5:3945:A:H2'	3:L5:3946:G:H8	1.85	0.41
3:L5:4452:U:OP2	3:L5:4522:G:N1	2.28	0.41
3:L5:4710:C:H2'	3:L5:4711:C:C6	2.56	0.41
5:L8:94:G:H21	40:Lj:82:THR:HB	1.85	0.41
13:LH:128:MET:SD	13:LH:157:SER:HB3	2.60	0.41
14:Li:28:ASP:OD1	14:Li:29:ALA:N	2.53	0.41
22:LR:173:ARG:O	22:LR:176:ARG:HD3	2.20	0.41
25:LU:97:ARG:HA	25:LU:97:ARG:HD2	1.77	0.41
27:LW:56:ARG:HE	27:LW:61:LYS:CB	2.33	0.41
60:SZ:73:VAL:HG12	60:SZ:79:ILE:HD11	2.02	0.41
61:Sc:13:ARG:HD3	61:Sc:53:GLY:HA2	2.01	0.41
64:Sg:26:GLN:NE2	64:Sg:75:GLY:HA3	2.35	0.41
68:SE:20:LEU:HD11	68:SE:46:ILE:HG21	2.02	0.41
69:SG:2:LYS:HD3	69:SG:15:LEU:HD21	2.02	0.41
69:SG:50:VAL:CG2	69:SG:111:LEU:HB3	2.50	0.41
69:SG:227:GLN:HB3	69:SG:231:ARG:HH21	1.85	0.41
70:SH:18:GLU:C	70:SH:20:GLU:H	2.29	0.41
75:SO:75:MET:O	75:SO:79:GLN:HG3	2.21	0.41
80:Sa:5:ARG:NH2	83:S2:1864:U:OP2	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:96:C:H2'	83:S2:97:U:H6	1.85	0.41
83:S2:376:A:H2'	83:S2:377:G:O4'	2.21	0.41
83:S2:1270:G:O2'	83:S2:1301:A:N7	2.49	0.41
83:S2:1739:C:H2'	83:S2:1740:C:C6	2.55	0.41
3:L5:86:U:H2'	3:L5:87:A:C8	2.56	0.41
3:L5:159:C:OP2	39:Li:25:ARG:HG2	2.20	0.41
3:L5:749:G:C6	3:L5:912:G:C8	3.08	0.41
3:L5:1178:G:H2'	9:LD:286:SER:HB3	2.03	0.41
3:L5:1565:A:C5	3:L5:1566:C:H1'	2.55	0.41
3:L5:2021:G:H2'	3:L5:2022:C:C6	2.56	0.41
3:L5:2306:G:H1'	3:L5:2332:A:N6	2.35	0.41
3:L5:3648:A:H1'	3:L5:3785:A2M:N6	2.35	0.41
3:L5:3687:A:O2'	6:LA:236:GLY:N	2.52	0.41
3:L5:4246:G:H2'	3:L5:4247:G:H8	1.85	0.41
3:L5:4280:A:C8	15:LJ:145:LYS:HE3	2.55	0.41
3:L5:4431:PSU:P	14:LI:3:ARG:HH22	2.42	0.41
3:L5:4536:OMC:HM22	3:L5:4537:C:O4'	2.20	0.41
3:L5:4704:C:H2'	3:L5:4705:A:C8	2.55	0.41
3:L5:4918:C:H2'	3:L5:4919:G:C8	2.55	0.41
7:LB:302:ASN:HB2	7:LB:313:SER:HA	2.03	0.41
10:LE:224:LYS:NZ	10:LE:234:ASP:OD2	2.53	0.41
12:LG:123:ALA:HA	12:LG:124:GLY:HA2	1.75	0.41
16:LL:58:ILE:HG12	16:LL:116:ARG:HD2	2.02	0.41
20:LP:95:LEU:HD23	20:LP:148:MET:HE1	2.02	0.41
40:Lj:58:THR:O	40:Lj:61:THR:OG1	2.33	0.41
47:Lr:8:MET:HE3	47:Lr:8:MET:HB3	1.81	0.41
51:SF:120:GLY:HA2	51:SF:121:PRO:HD3	1.95	0.41
59:SU:67:LYS:HA	62:Sd:44:ARG:NH1	2.36	0.41
61:Sc:40:ARG:HH21	61:Sc:42:ILE:HD11	1.84	0.41
68:SE:136:ILE:HD12	68:SE:149:TYR:CE1	2.55	0.41
69:SG:29:GLU:OE2	69:SG:30:LYS:NZ	2.54	0.41
72:SJ:136:ARG:HB3	72:SJ:141:VAL:HG12	2.03	0.41
75:SO:34:PHE:O	75:SO:41:PHE:N	2.51	0.41
83:S2:14:C:H2'	83:S2:15:U:C6	2.55	0.41
83:S2:52:G:H2'	83:S2:53:C:C6	2.55	0.41
83:S2:834:C:N4	83:S2:839:C:H42	2.18	0.41
83:S2:1739:C:H2'	83:S2:1740:C:H6	1.85	0.41
3:L5:1280:C:O2'	8:LC:321:ASN:OD1	2.21	0.41
3:L5:1558:A:H2'	3:L5:1559:G:H8	1.86	0.41
3:L5:1558:A:H2'	3:L5:1559:G:C8	2.55	0.41
3:L5:1881:C:H5'	3:L5:2281:U:H1'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2079:G:H2'	3:L5:2080:U:H6	1.85	0.41
3:L5:2275:G:H2'	3:L5:2276:A:C8	2.55	0.41
3:L5:3607:U:H2'	3:L5:3608:A:C8	2.56	0.41
3:L5:4305:G:O5'	24:LT:83:LYS:NZ	2.54	0.41
6:LA:22:HIS:O	6:LA:24:LYS:NZ	2.51	0.41
6:LA:242:ARG:NH2	6:LA:243:THR:O	2.53	0.41
6:LA:245:ARG:HG2	6:LA:247:ARG:HH11	1.85	0.41
10:LE:115:TYR:CE1	47:Lr:119:ARG:HG3	2.56	0.41
11:LF:144:TYR:CE2	11:LF:237:GLU:HB2	2.56	0.41
22:LR:151:ARG:HH21	73:SL:118:ARG:NE	2.18	0.41
23:LS:84:TYR:HE1	23:LS:93:MET:HE3	1.86	0.41
42:Ll:23:ILE:HG23	42:Ll:38:ASN:HB2	2.02	0.41
47:Lr:107:ARG:O	47:Lr:111:ILE:HG12	2.21	0.41
50:SD:76:ARG:O	50:SD:76:ARG:NH1	2.53	0.41
50:SD:176:LEU:HD13	83:S2:1499:U:H4'	2.02	0.41
68:SE:242:LYS:HD3	68:SE:242:LYS:HA	1.78	0.41
70:SH:91:HIS:CE1	70:SH:169:LYS:HG2	2.56	0.41
82:Se:34:ARG:HD3	82:Se:37:GLN:HE21	1.85	0.41
82:Se:39:ASN:HA	82:Se:43:VAL:HG12	2.02	0.41
83:S2:1189:A:H2'	83:S2:1190:A:C8	2.56	0.41
3:L5:86:U:H2'	3:L5:87:A:H8	1.85	0.41
3:L5:190:G:H2'	3:L5:191:G:H8	1.86	0.41
3:L5:754:U:H2'	3:L5:755:C:C6	2.55	0.41
3:L5:1503:A:H1'	3:L5:1504:G:C8	2.55	0.41
3:L5:1977:C:O2'	3:L5:1978:C:OP1	2.37	0.41
3:L5:4278:C:HO2'	3:L5:4281:A:H8	1.62	0.41
4:L7:58:A:H2'	4:L7:59:G:H8	1.84	0.41
5:L8:95:A:N3	38:Lh:63:GLN:NE2	2.68	0.41
8:LC:144:ILE:HG22	8:LC:147:VAL:HG21	2.03	0.41
9:LD:237:GLU:HG2	9:LD:241:LYS:NZ	2.36	0.41
11:LF:86:GLU:HG2	24:LT:135:PRO:HB3	2.03	0.41
13:LH:4:ILE:HG12	13:LH:61:TRP:CH2	2.56	0.41
20:LP:95:LEU:HA	20:LP:148:MET:HE1	2.03	0.41
30:LZ:35:ASP:OD1	30:LZ:36:ARG:N	2.53	0.41
47:Lr:47:LYS:O	47:Lr:103:ARG:HD2	2.21	0.41
47:Lr:59:GLY:O	47:Lr:121:GLN:NE2	2.36	0.41
58:ST:91:HIS:HE2	83:S2:1665:G:P	2.40	0.41
64:Sg:302:TYR:HB2	64:Sg:304:ASP:OD1	2.21	0.41
66:SB:142:PHE:HB2	66:SB:208:HIS:CE1	2.55	0.41
69:SG:133:LEU:H	69:SG:133:LEU:HD23	1.86	0.41
73:SL:5:GLN:NE2	73:SL:11:GLN:O	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:SY:99:LYS:O	79:SY:99:LYS:HD3	2.20	0.41
83:S2:1128:C:H2'	83:S2:1129:G:C8	2.56	0.41
83:S2:1174:PSU:H2'	83:S2:1175:G:H8	1.86	0.41
83:S2:1628:C:H2'	83:S2:1629:C:C6	2.55	0.41
3:L5:406:C:O2'	3:L5:407:A:OP1	2.37	0.41
3:L5:1511:U:H2'	3:L5:1512:G:H8	1.86	0.41
3:L5:1735:U:OP2	87:L5:5259:SPM:N10	2.54	0.41
3:L5:2869:U:O2'	3:L5:2881:A:N7	2.53	0.41
3:L5:2893:U:O2'	71:SI:88:ASN:ND2	2.52	0.41
3:L5:4301:U:H4'	24:LT:54:HIS:CD2	2.56	0.41
3:L5:4578:G:H2'	3:L5:4579:PSU:C6	2.55	0.41
3:L5:5002:U:H2'	3:L5:5003:U:H6	1.86	0.41
10:LE:173:LEU:HD21	10:LE:191:GLN:HB3	2.02	0.41
39:Li:76:ARG:HA	39:Li:76:ARG:HD3	1.79	0.41
51:SF:73:THR:O	51:SF:89:THR:HG21	2.21	0.41
51:SF:76:MET:HA	51:SF:155:CYS:HB3	2.02	0.41
51:SF:144:LEU:HD23	61:Sc:49:PRO:HB2	2.03	0.41
66:SB:123:ALA:HB3	66:SB:168:MET:HE2	2.02	0.41
70:SH:61:ILE:HD12	70:SH:93:VAL:HG23	2.02	0.41
74:SN:34:LYS:O	74:SN:37:ILE:HG22	2.21	0.41
77:SW:16:ASN:ND2	83:S2:1094:C:O2	2.53	0.41
83:S2:568:C:H2'	83:S2:569:A:O4'	2.21	0.41
83:S2:737:G:H8	83:S2:738:C:H4'	1.86	0.41
83:S2:1093:A:H2'	83:S2:1094:C:H6	1.86	0.41
83:S2:1190:A:N3	83:S2:1714:U:O2'	2.53	0.41
85:CF:9:ASN:ND2	85:CF:307:ASN:OD1	2.50	0.41
3:L5:484:U:O4	3:L5:665:C:H2'	2.20	0.41
3:L5:1187:G:H2'	3:L5:1188:C:C6	2.56	0.41
3:L5:1670:G:OP1	32:Lb:12:GLN:NE2	2.41	0.41
3:L5:1727:U:OP1	11:LF:131:ASN:ND2	2.51	0.41
3:L5:1895:G:OP1	11:LF:96:ARG:NH2	2.53	0.41
3:L5:1960:A:C4	48:Ls:14:PHE:HE2	2.39	0.41
3:L5:1961:G:OP2	48:Ls:59:THR:OG1	2.32	0.41
3:L5:2436:U:C4	28:LX:130:PRO:HG3	2.56	0.41
3:L5:2497:C:H2'	3:L5:2498:C:C6	2.55	0.41
3:L5:3910:C:O2'	3:L5:4196:OMG:N2	2.54	0.41
3:L5:4743:G:H2'	3:L5:4744:A:H8	1.85	0.41
3:L5:4883:C:N4	10:LE:181:LEU:O	2.46	0.41
3:L5:4920:C:H2'	3:L5:4921:C:C6	2.56	0.41
4:L7:82:G:H2'	4:L7:83:A:C8	2.55	0.41
5:L8:121:G:H2'	5:L8:122:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LE:270:TYR:OH	17:LM:106:ASP:OD2	2.32	0.41
11:LF:87:PRO:HG3	11:LF:144:TYR:CG	2.56	0.41
16:LL:183:ARG:HA	16:LL:183:ARG:HD2	1.86	0.41
17:LM:136:LEU:O	17:LM:137:LYS:HE2	2.21	0.41
23:LS:76:LYS:HD3	23:LS:131:GLU:HG3	2.02	0.41
30:LZ:123:LYS:O	30:LZ:124:THR:OG1	2.34	0.41
33:Lc:44:LYS:HD3	33:Lc:97:ILE:O	2.21	0.41
37:Lg:33:LEU:HD23	37:Lg:33:LEU:HA	1.88	0.41
50:SD:28:GLU:HB2	52:SK:61:GLN:HG2	2.01	0.41
55:SQ:51:LEU:HD23	55:SQ:51:LEU:HA	1.86	0.41
71:SI:21:TYR:CE2	71:SI:22:HIS:HD2	2.38	0.41
71:SI:186:ASP:OD2	83:S2:219:U:O2'	2.35	0.41
78:SX:17:ARG:HH12	83:S2:659:G:N2	2.19	0.41
81:Sb:67:THR:OG1	81:Sb:70:LYS:O	2.28	0.41
83:S2:605:A:N3	83:S2:639:C:H1'	2.35	0.41
83:S2:696:G:N2	83:S2:730:C:OP2	2.53	0.41
83:S2:835:C:H5'	83:S2:836:G:H5'	2.02	0.41
83:S2:1244:PSU:H2'	83:S2:1245:G:C8	2.55	0.41
83:S2:1470:C:H2'	83:S2:1471:C:H6	1.85	0.41
84:AT:25:A:H2'	84:AT:26:C:O4'	2.21	0.41
85:CF:82:THR:HG21	85:CF:232:LEU:HD22	2.03	0.41
3:L5:21:G:H1'	5:L8:103:A:N3	2.35	0.41
3:L5:493:G:O2'	3:L5:494:U:OP1	2.38	0.41
3:L5:742:G:H2'	3:L5:743:G:H8	1.86	0.41
3:L5:978:G:H2'	3:L5:979:C:H6	1.83	0.41
3:L5:1189:G:H2'	3:L5:1190:C:C6	2.56	0.41
3:L5:1725:U:H2'	3:L5:1726:U:H6	1.86	0.41
3:L5:2823:G:N7	22:LR:20:LYS:HD3	2.35	0.41
3:L5:3896:C:H1'	7:LB:268:ARG:NH2	2.35	0.41
3:L5:3922[A]:G:H4'	3:L5:3923:A:OP2	2.20	0.41
9:LD:108:ARG:CZ	9:LD:253:TYR:HB2	2.50	0.41
11:LF:222:LYS:HE3	11:LF:224:THR:OG1	2.21	0.41
13:LH:34:LEU:HD23	13:LH:34:LEU:HA	1.88	0.41
14:LI:51:HIS:HB3	14:LI:134:VAL:HG13	2.03	0.41
15:LJ:17:ILE:HG23	15:LJ:132:VAL:HG23	2.02	0.41
17:LM:130:LEU:HB3	19:LO:177:LEU:HD11	2.02	0.41
21:LQ:59:PRO:HG3	21:LQ:143:ARG:HA	2.02	0.41
23:LS:20:PRO:C	23:LS:21:LYS:HD3	2.46	0.41
31:La:36:GLY:HA3	31:La:40:HIS:CE1	2.56	0.41
34:Ld:70:LYS:HE3	34:Ld:70:LYS:HB2	1.80	0.41
34:Ld:123:ASP:N	34:Ld:123:ASP:OD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Le:35:TRP:O	35:Le:36:ARG:NH1	2.49	0.41
49:Lt:121:LEU:HD22	49:Lt:128:THR:HG23	2.03	0.41
52:SK:2:LEU:HD22	83:S2:1315:U:H4'	2.02	0.41
54:SP:57:LEU:HD11	54:SP:83:MET:HE2	2.03	0.41
56:SR:76:GLU:HB3	56:SR:80:ARG:HH21	1.85	0.41
56:SR:96:ILE:HD11	56:SR:117:LEU:HD23	2.03	0.41
56:SR:128:PHE:CD2	56:SR:129:LYS:HG3	2.56	0.41
57:SS:76:GLN:HG2	57:SS:77:TYR:CD1	2.55	0.41
57:SS:132:ARG:HD3	83:S2:1623:A:C6	2.56	0.41
58:ST:96:SER:OG	83:S2:1568:C:OP1	2.36	0.41
60:SZ:88:LEU:HD13	60:SZ:109:TYR:HD2	1.86	0.41
61:Sc:21:THR:OG1	61:Sc:22:GLY:N	2.52	0.41
65:SA:185:MET:HE1	76:SV:46:PHE:HB2	2.03	0.41
66:SB:35:ALA:HB1	66:SB:39:PHE:HD2	1.86	0.41
66:SB:85:LYS:HB2	66:SB:101:HIS:HB3	2.03	0.41
71:SI:139:LYS:HE2	71:SI:139:LYS:HB2	1.67	0.41
73:SL:112:HIS:CD2	73:SL:141:ASN:HD21	2.39	0.41
77:SW:55:ASP:HB3	81:Sb:25:VAL:HG13	2.03	0.41
82:Se:5:SER:HB3	82:Se:8:ARG:NH2	2.36	0.41
83:S2:130:G:H4'	83:S2:132:U:H5''	2.03	0.41
83:S2:344:U:H2'	83:S2:345:U:C6	2.55	0.41
83:S2:428:OMU:H6	83:S2:428:OMU:H2'	1.82	0.41
83:S2:544:G:H2'	83:S2:545:A:C8	2.55	0.41
83:S2:596:U:H1'	83:S2:645:C:H1'	2.03	0.41
83:S2:896:U:N3	83:S2:897:U:H5	2.19	0.41
83:S2:926:A:H61	83:S2:1015:U:H3	1.67	0.41
84:AT:12:G:H22	84:AT:23:U:H3	1.69	0.41
3:L5:153:G:H2'	3:L5:154:G:C8	2.54	0.41
3:L5:1307:A:H2'	3:L5:1308:C:C6	2.55	0.41
3:L5:1596:U:O2'	20:LP:135:ARG:NH1	2.42	0.41
3:L5:1932:A:P	19:LO:49:ARG:HH12	2.42	0.41
3:L5:2517:A:H5'	37:Lg:62:LYS:HD3	2.02	0.41
3:L5:3807:A:OP1	44:Ln:23:ARG:HD3	2.21	0.41
5:L8:87:G:O6	29:LY:113:LYS:NZ	2.39	0.41
9:LD:82:GLU:OE2	9:LD:108:ARG:NH2	2.34	0.41
13:LH:26:ILE:HG13	13:LH:35:ARG:HG3	2.02	0.41
17:LM:105:THR:HG22	17:LM:108:ASP:OD2	2.21	0.41
44:Ln:2:ARG:HB3	44:Ln:5:TRP:CD1	2.56	0.41
65:SA:156:TYR:HE1	76:SV:61:ARG:HG3	1.85	0.41
70:SH:17:ASP:HB2	70:SH:20:GLU:HB2	2.03	0.41
79:SY:43:LYS:HA	79:SY:46:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:Se:12:VAL:O	82:Se:16:THR:OG1	2.34	0.41
83:S2:99:A2M:H1'	83:S2:99:A2M:HM'3	1.85	0.41
83:S2:194:C:H2'	83:S2:195:C:H6	1.87	0.41
83:S2:1007:C:H2'	83:S2:1008:A:C8	2.56	0.41
83:S2:1115:U:O2'	83:S2:1117:C:OP2	2.26	0.41
83:S2:1407:U:H2'	83:S2:1408:U:C6	2.56	0.41
85:CF:216:VAL:HG21	85:CF:218:ARG:NH2	2.36	0.41
85:CF:426:VAL:HB	85:CF:434:ALA:HB3	2.01	0.41
3:L5:19:G:P	38:Lh:93:ARG:HE	2.44	0.40
3:L5:724:C:OP1	8:LC:350:ARG:HD2	2.21	0.40
3:L5:1079:C:H2'	3:L5:1080:C:C6	2.55	0.40
3:L5:2436:U:OP2	28:LX:135:LYS:NZ	2.49	0.40
3:L5:2864:A:H2'	3:L5:2865:U:C6	2.56	0.40
3:L5:4064:C:H2'	3:L5:4065:G:H8	1.86	0.40
3:L5:4460:U:H2'	3:L5:4461:C:C6	2.56	0.40
3:L5:4507:A:H2'	3:L5:4508:C:C6	2.55	0.40
3:L5:4563:U:C2	3:L5:4564:A:C8	3.09	0.40
3:L5:4627:U:H5''	7:LB:373:LYS:HG2	2.03	0.40
3:L5:5023:C:C4	3:L5:5024:C:H1'	2.56	0.40
5:L8:5:U:H2'	5:L8:6:C:C6	2.56	0.40
5:L8:39:G:H1'	5:L8:103:A:H61	1.86	0.40
11:LF:70:ARG:O	11:LF:74:MET:HG2	2.21	0.40
15:LJ:81:GLU:O	15:LJ:84:GLU:HG3	2.21	0.40
16:LL:63:THR:HG23	16:LL:65:ARG:H	1.86	0.40
30:LZ:33:THR:C	30:LZ:35:ASP:H	2.29	0.40
32:Lb:110:ALA:O	32:Lb:114:LYS:HG3	2.21	0.40
48:Ls:29:ILE:HD11	48:Ls:191:GLN:HG2	2.03	0.40
56:SR:4:VAL:HG11	83:S2:1372:U:O2	2.21	0.40
57:SS:85:ASN:ND2	83:S2:1629:C:O2'	2.54	0.40
68:SE:186:GLY:HA3	83:S2:809:A:OP1	2.21	0.40
71:SI:38:ILE:HD11	71:SI:96:LEU:HD21	2.03	0.40
75:SO:72:TYR:CZ	75:SO:76:LEU:HD11	2.56	0.40
83:S2:90:G:H2'	83:S2:91:A:O4'	2.20	0.40
83:S2:129:C:H4'	83:S2:130:G:H5'	2.04	0.40
83:S2:1598:G:N2	83:S2:1599:U:O4	2.43	0.40
84:AT:51:U:H2'	84:AT:52:C:C6	2.56	0.40
85:CF:294:MET:SD	85:CF:299:LEU:HD11	2.61	0.40
3:L5:99:A:H5''	18:LN:184:ILE:HD12	2.03	0.40
3:L5:477:C:H2'	3:L5:478:G:H8	1.87	0.40
3:L5:644:G:H2'	3:L5:645:G:C8	2.55	0.40
3:L5:1907:A:H2'	3:L5:1908:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4080:C:H2'	3:L5:4081:G:H8	1.86	0.40
3:L5:4300:U:H2'	3:L5:4301:U:C6	2.57	0.40
3:L5:4616:A:H2'	3:L5:4617:G:O4'	2.21	0.40
7:LB:378:ARG:HE	27:LW:32:LEU:HD21	1.87	0.40
9:LD:238:GLU:C	9:LD:242:LYS:HZ2	2.29	0.40
10:LE:199:THR:HG21	10:LE:270:TYR:HE2	1.86	0.40
13:LH:102:ASN:HB2	13:LH:115:ARG:HB2	2.03	0.40
16:LL:58:ILE:HD13	16:LL:157:VAL:HG22	2.03	0.40
23:LS:69:GLU:OE1	23:LS:70:LYS:N	2.54	0.40
44:Ln:2:ARG:NH2	83:S2:1842:4AC:H5	2.36	0.40
49:Lt:114:ARG:NH2	49:Lt:162:CYS:SG	2.94	0.40
49:Lt:147:HIS:HA	49:Lt:148:PRO:HD3	1.89	0.40
50:SD:45:ARG:HH21	50:SD:85:GLU:CD	2.27	0.40
51:SF:17:ILE:HG13	51:SF:46:ALA:HB3	2.02	0.40
53:SM:124:ILE:HD13	53:SM:124:ILE:HA	1.96	0.40
54:SP:56:LEU:HD22	54:SP:80:LEU:HD11	2.04	0.40
64:Sg:54:ILE:HD12	64:Sg:55:PRO:HD2	2.04	0.40
70:SH:36:LEU:HD11	70:SH:78:ARG:CZ	2.52	0.40
70:SH:143:ARG:HE	77:SW:53:ILE:HA	1.86	0.40
75:SO:35:ALA:HB3	75:SO:112:ALA:HB2	2.03	0.40
83:S2:1177:PSU:H2'	83:S2:1178:U:C6	2.56	0.40
84:AT:49:C:H5''	84:AT:51:U:OP2	2.20	0.40
85:CF:293:GLU:HG2	85:CF:298:ALA:HA	2.02	0.40
3:L5:35:U:H4'	3:L5:1525:A:C2	2.56	0.40
3:L5:50:C:C2	3:L5:51:A:C8	3.09	0.40
3:L5:374:G:OP2	40:Lj:56:ARG:NH1	2.46	0.40
3:L5:701:G:H2'	3:L5:702:U:C2	2.57	0.40
3:L5:950:G:H2'	3:L5:951:G:H8	1.85	0.40
3:L5:1273:G:C6	10:LE:73:TYR:HB2	2.56	0.40
3:L5:1786:A:H2'	3:L5:1789:C:C5	2.56	0.40
3:L5:2267:U:OP1	47:Lr:37:SER:HB2	2.22	0.40
3:L5:2540:C:H2'	3:L5:2541:G:C8	2.56	0.40
3:L5:2542:G:H2'	3:L5:2543:A:C8	2.56	0.40
3:L5:2899:C:P	22:LR:108:ARG:HH22	2.44	0.40
3:L5:3928:A:H2'	3:L5:3929:G:O4'	2.21	0.40
3:L5:4563:U:H2'	3:L5:4564:A:H8	1.86	0.40
3:L5:4940:C:H5'	3:L5:4941:G:H5''	2.02	0.40
3:L5:5053:U:H5'	3:L5:5054:C:C5	2.56	0.40
7:LB:219:VAL:HG11	7:LB:337:VAL:HG13	2.04	0.40
8:LC:141:GLY:C	8:LC:204:ARG:HH21	2.27	0.40
10:LE:115:TYR:CD1	47:Lr:115:SER:HB3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LF:237:GLU:HG3	23:LS:38:VAL:HG22	2.04	0.40
29:LY:115:ARG:O	29:LY:119:LEU:HG	2.21	0.40
30:LZ:135:ARG:HD2	30:LZ:135:ARG:HA	1.77	0.40
31:La:75:LEU:HD23	31:La:75:LEU:HA	1.89	0.40
52:SK:7:ASN:ND2	52:SK:40:VAL:HB	2.36	0.40
56:SR:97:GLU:OE1	56:SR:120:THR:OG1	2.36	0.40
64:Sg:252:THR:HG21	64:Sg:257:LYS:HD2	2.02	0.40
66:SB:136:ARG:HB3	66:SB:216:LYS:HG3	2.03	0.40
67:SC:64:THR:HG22	67:SC:66:LEU:N	2.36	0.40
67:SC:207:ALA:HB3	67:SC:210:PRO:HG2	2.02	0.40
74:SN:140:LYS:HA	74:SN:140:LYS:HD3	1.93	0.40
77:SW:20:ARG:HA	77:SW:20:ARG:HD2	1.95	0.40
78:SX:3:LYS:NZ	83:S2:663:C:OP2	2.33	0.40
82:Se:25:LYS:HB3	82:Se:25:LYS:HE2	1.84	0.40
83:S2:51:U:H2'	83:S2:52:G:C8	2.56	0.40
83:S2:900:C:H5'	83:S2:901:G:N7	2.36	0.40
83:S2:1177:PSU:H2'	83:S2:1178:U:H6	1.87	0.40
85:CF:55:LYS:HE3	85:CF:56:TYR:CE2	2.56	0.40
3:L5:37:U:H2'	3:L5:38:A:O4'	2.21	0.40
3:L5:307:A:N3	3:L5:310:G:O2'	2.53	0.40
3:L5:417:G:OP1	3:L5:2329:U:O2'	2.33	0.40
3:L5:457:G:H2'	3:L5:458:C:C6	2.55	0.40
3:L5:458:C:H2'	3:L5:459:C:C6	2.57	0.40
3:L5:1348:U:H2'	3:L5:1349:G:C8	2.56	0.40
3:L5:1509:C:H5''	31:La:2:PRO:HD3	2.04	0.40
3:L5:2413:U:H2'	3:L5:2414:G:C8	2.57	0.40
3:L5:4344:U:H2'	3:L5:4345:C:C6	2.56	0.40
3:L5:4637:OMG:HM23	3:L5:4637:OMG:H1'	1.78	0.40
11:LF:228:VAL:HA	23:LS:39:VAL:HG22	2.03	0.40
13:LH:91:LYS:HB3	13:LH:143:GLU:OE2	2.20	0.40
14:LI:54:SER:HB3	14:LI:135:ILE:HD11	2.03	0.40
16:LL:127:PHE:HB2	38:Lh:118:LYS:HB3	2.03	0.40
29:LY:116:LYS:HA	29:LY:119:LEU:HD12	2.03	0.40
33:Lc:78:ASN:N	33:Lc:78:ASN:OD1	2.53	0.40
35:Le:12:ILE:HD11	35:Le:69:MET:HE2	2.04	0.40
35:Le:19:LYS:HE3	35:Le:19:LYS:HB3	1.89	0.40
53:SM:104:VAL:HG21	83:S2:1284:A:C2	2.56	0.40
55:SQ:15:ARG:HH22	83:S2:1444:U:P	2.44	0.40
55:SQ:90:LYS:HE2	55:SQ:90:LYS:HB3	1.86	0.40
57:SS:5:ILE:HD13	60:SZ:49:LEU:HB2	2.03	0.40
58:ST:113:VAL:HG22	58:ST:123:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:SB:155:TYR:OH	83:S2:989:C:OP2	2.32	0.40
67:SC:212:LYS:HE2	67:SC:212:LYS:HB3	1.93	0.40
70:SH:169:LYS:O	70:SH:172:THR:OG1	2.30	0.40
73:SL:39:ASN:O	83:S2:292:A:O2'	2.29	0.40
77:SW:60:LYS:NZ	83:S2:921:G:O6	2.53	0.40
83:S2:348:A:H2'	83:S2:349:A:C8	2.57	0.40
83:S2:455:A:H2'	83:S2:456:C:H6	1.85	0.40
83:S2:595:U:H2'	83:S2:596:U:C6	2.56	0.40
83:S2:1279:C:H2'	83:S2:1280:G:H8	1.86	0.40
83:S2:1558:C:H2'	83:S2:1559:C:C6	2.57	0.40
3:L5:735:G:H5''	17:LM:70:GLN:HG2	2.04	0.40
3:L5:1080:C:N3	3:L5:1220:G:N1	2.69	0.40
3:L5:1768:C:H2'	3:L5:1770:A:N7	2.37	0.40
3:L5:4520:G:H2'	3:L5:4521:PSU:O4'	2.21	0.40
4:L7:40:U:O4'	15:LJ:46:GLN:NE2	2.55	0.40
4:L7:58:A:H2'	4:L7:59:G:C8	2.57	0.40
14:LI:204:GLY:HA3	14:LI:208:LYS:HE3	2.04	0.40
14:LI:208:LYS:HA	14:LI:211:VAL:HG22	2.03	0.40
21:LQ:69:LYS:HA	21:LQ:69:LYS:HD3	1.85	0.40
25:LU:19:LEU:HA	25:LU:19:LEU:HD23	1.86	0.40
35:Le:122:VAL:HG12	35:Le:124:ASN:H	1.87	0.40
37:Lg:69:LYS:HG3	37:Lg:73:HIS:CD2	2.57	0.40
44:Ln:4:LYS:NZ	83:S2:1843:G:N7	2.62	0.40
50:SD:210:ILE:HD13	56:SR:15:VAL:HG11	2.04	0.40
51:SF:176:GLU:OE2	51:SF:187:SER:HB2	2.21	0.40
52:SK:54:SER:OG	83:S2:1277:C:O4'	2.29	0.40
53:SM:99:LYS:HG2	53:SM:100:PRO:HD2	2.03	0.40
64:Sg:42:MET:HE1	64:Sg:44:LYS:HZ2	1.87	0.40
64:Sg:289:LEU:HD12	64:Sg:289:LEU:HA	1.88	0.40
65:SA:13:GLU:O	65:SA:17:LYS:HG2	2.21	0.40
65:SA:185:MET:HE2	65:SA:185:MET:HB2	2.02	0.40
67:SC:103:LYS:HG3	67:SC:133:TYR:HE1	1.85	0.40
68:SE:10:LYS:NZ	83:S2:95:G:OP1	2.30	0.40
70:SH:25:GLN:O	70:SH:28:LEU:HG	2.21	0.40
72:SJ:41:ARG:HE	83:S2:642:U:H5''	1.86	0.40
72:SJ:79:ARG:NH1	72:SJ:83:ARG:HD2	2.37	0.40
72:SJ:136:ARG:HH21	72:SJ:139:LYS:HA	1.87	0.40
79:SY:129:LYS:HA	79:SY:129:LYS:HD3	1.92	0.40
83:S2:639:C:H2'	83:S2:640:A:H8	1.82	0.40
83:S2:680:G:H2'	83:S2:681:PSU:C6	2.57	0.40
83:S2:931:C:H2'	83:S2:932:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1216:C:H4'	83:S2:1644:C:OP1	2.22	0.40
83:S2:1667:U:H2'	83:S2:1668:U:C6	2.57	0.40
83:S2:1706:G:H2'	83:S2:1707:U:H6	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CI	29/31 (94%)	29 (100%)	0	0	100	100
6	LA	246/248 (99%)	226 (92%)	20 (8%)	0	100	100
7	LB	400/402 (100%)	382 (96%)	18 (4%)	0	100	100
8	LC	366/368 (100%)	347 (95%)	19 (5%)	0	100	100
9	LD	291/293 (99%)	280 (96%)	11 (4%)	0	100	100
10	LE	236/250 (94%)	223 (94%)	13 (6%)	0	100	100
11	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
12	LG	239/241 (99%)	227 (95%)	12 (5%)	0	100	100
13	LH	188/190 (99%)	183 (97%)	5 (3%)	0	100	100
14	LI	211/213 (99%)	200 (95%)	11 (5%)	0	100	100
15	LJ	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
16	LL	208/210 (99%)	199 (96%)	9 (4%)	0	100	100
17	LM	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
18	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
19	LO	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
20	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
21	LQ	185/187 (99%)	180 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	LR	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
23	LS	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
24	LT	157/159 (99%)	154 (98%)	3 (2%)	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%)	107 (96%)	5 (4%)	0	100	100
28	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
29	LY	132/134 (98%)	129 (98%)	3 (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%)	100 (95%)	5 (5%)	0	100	100
33	Lc	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
34	Ld	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
35	Le	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
36	Lf	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
37	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
38	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
39	Li	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
40	Lj	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
41	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
42	Ll	48/50 (96%)	48 (100%)	0	0	100	100
43	Lm	50/52 (96%)	50 (100%)	0	0	100	100
44	Ln	22/24 (92%)	22 (100%)	0	0	100	100
45	Lo	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
46	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
47	Lr	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
48	Ls	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
49	Lt	128/157 (82%)	109 (85%)	19 (15%)	0	100	100
50	SD	225/227 (99%)	212 (94%)	12 (5%)	1 (0%)	30	58
51	SF	187/189 (99%)	176 (94%)	11 (6%)	0	100	100
52	SK	96/98 (98%)	88 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	SM	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
54	SP	119/121 (98%)	118 (99%)	1 (1%)	0	100	100
55	SQ	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
56	SR	133/135 (98%)	123 (92%)	9 (7%)	1 (1%)	16	43
57	SS	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
58	ST	141/143 (99%)	140 (99%)	1 (1%)	0	100	100
59	SU	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
60	SZ	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
61	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
62	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
63	Sf	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
64	Sg	311/313 (99%)	289 (93%)	22 (7%)	0	100	100
65	SA	219/221 (99%)	208 (95%)	11 (5%)	0	100	100
66	SB	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
67	SC	218/222 (98%)	202 (93%)	16 (7%)	0	100	100
68	SE	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
69	SG	235/237 (99%)	222 (94%)	13 (6%)	0	100	100
70	SH	182/189 (96%)	163 (90%)	19 (10%)	0	100	100
71	SI	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
72	SJ	183/185 (99%)	176 (96%)	6 (3%)	1 (0%)	24	53
73	SL	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
74	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
75	SO	135/140 (96%)	123 (91%)	12 (9%)	0	100	100
76	SV	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
77	SW	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
78	SX	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
79	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
80	Sa	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
81	Sb	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
82	Se	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
85	CF	438/441 (99%)	422 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	12110/12348 (98%)	11559 (96%)	548 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
56	SR	129	LYS
50	SD	143	ARG
72	SJ	138	ARG

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CI	25/25 (100%)	25 (100%)	0	100	100
6	LA	190/190 (100%)	190 (100%)	0	100	100
7	LB	348/348 (100%)	348 (100%)	0	100	100
8	LC	306/306 (100%)	306 (100%)	0	100	100
9	LD	246/247 (100%)	246 (100%)	0	100	100
10	LE	212/222 (96%)	212 (100%)	0	100	100
11	LF	194/194 (100%)	194 (100%)	0	100	100
12	LG	203/205 (99%)	203 (100%)	0	100	100
13	LH	169/169 (100%)	169 (100%)	0	100	100
14	LI	180/180 (100%)	179 (99%)	1 (1%)	78	92
15	LJ	143/148 (97%)	143 (100%)	0	100	100
16	LL	176/176 (100%)	176 (100%)	0	100	100
17	LM	118/118 (100%)	118 (100%)	0	100	100
18	LN	171/171 (100%)	171 (100%)	0	100	100
19	LO	173/173 (100%)	173 (100%)	0	100	100
20	LP	134/134 (100%)	134 (100%)	0	100	100
21	LQ	164/164 (100%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	LR	166/166 (100%)	166 (100%)	0	100	100
23	LS	156/156 (100%)	156 (100%)	0	100	100
24	LT	139/139 (100%)	139 (100%)	0	100	100
25	LU	91/91 (100%)	91 (100%)	0	100	100
26	LV	101/101 (100%)	101 (100%)	0	100	100
27	LW	95/103 (92%)	95 (100%)	0	100	100
28	LX	108/108 (100%)	108 (100%)	0	100	100
29	LY	124/124 (100%)	124 (100%)	0	100	100
30	LZ	117/117 (100%)	117 (100%)	0	100	100
31	La	120/120 (100%)	120 (100%)	0	100	100
32	Lb	88/101 (87%)	88 (100%)	0	100	100
33	Lc	83/83 (100%)	83 (100%)	0	100	100
34	Ld	98/98 (100%)	98 (100%)	0	100	100
35	Le	114/114 (100%)	114 (100%)	0	100	100
36	Lf	88/88 (100%)	88 (100%)	0	100	100
37	Lg	98/98 (100%)	98 (100%)	0	100	100
38	Lh	109/109 (100%)	109 (100%)	0	100	100
39	Li	86/86 (100%)	86 (100%)	0	100	100
40	Lj	73/73 (100%)	73 (100%)	0	100	100
41	Lk	64/64 (100%)	64 (100%)	0	100	100
42	Ll	47/47 (100%)	47 (100%)	0	100	100
43	Lm	48/48 (100%)	48 (100%)	0	100	100
44	Ln	23/23 (100%)	23 (100%)	0	100	100
45	Lo	93/93 (100%)	93 (100%)	0	100	100
46	Lp	74/74 (100%)	74 (100%)	0	100	100
47	Lr	109/109 (100%)	108 (99%)	1 (1%)	70	88
48	Ls	162/164 (99%)	162 (100%)	0	100	100
49	Lt	107/130 (82%)	107 (100%)	0	100	100
50	SD	190/190 (100%)	190 (100%)	0	100	100
51	SF	159/159 (100%)	159 (100%)	0	100	100
52	SK	89/89 (100%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	SM	102/104 (98%)	102 (100%)	0	100	100
54	SP	107/107 (100%)	107 (100%)	0	100	100
55	SQ	119/119 (100%)	119 (100%)	0	100	100
56	SR	122/122 (100%)	122 (100%)	0	100	100
57	SS	126/126 (100%)	126 (100%)	0	100	100
58	ST	113/113 (100%)	113 (100%)	0	100	100
59	SU	94/94 (100%)	94 (100%)	0	100	100
60	SZ	66/66 (100%)	66 (100%)	0	100	100
61	Sc	57/57 (100%)	57 (100%)	0	100	100
62	Sd	48/48 (100%)	48 (100%)	0	100	100
63	Sf	60/60 (100%)	60 (100%)	0	100	100
64	Sg	272/272 (100%)	272 (100%)	0	100	100
65	SA	183/183 (100%)	183 (100%)	0	100	100
66	SB	195/195 (100%)	195 (100%)	0	100	100
67	SC	186/188 (99%)	186 (100%)	0	100	100
68	SE	224/224 (100%)	224 (100%)	0	100	100
69	SG	207/207 (100%)	207 (100%)	0	100	100
70	SH	166/169 (98%)	166 (100%)	0	100	100
71	SI	178/178 (100%)	178 (100%)	0	100	100
72	SJ	161/161 (100%)	161 (100%)	0	100	100
73	SL	137/137 (100%)	137 (100%)	0	100	100
74	SN	130/130 (100%)	130 (100%)	0	100	100
75	SO	107/110 (97%)	107 (100%)	0	100	100
76	SV	67/67 (100%)	67 (100%)	0	100	100
77	SW	112/112 (100%)	112 (100%)	0	100	100
78	SX	113/113 (100%)	113 (100%)	0	100	100
79	SY	113/113 (100%)	113 (100%)	0	100	100
80	Sa	89/89 (100%)	89 (100%)	0	100	100
81	Sb	75/75 (100%)	75 (100%)	0	100	100
82	Se	47/47 (100%)	47 (100%)	0	100	100
85	CF	365/366 (100%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	10512/10587 (99%)	10510 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
14	LI	143	GLN
47	Lr	83	ASN

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

Mol	Chain	Res	Type
6	LA	97	ASN
7	LB	109	HIS
7	LB	184	GLN
8	LC	187	GLN
8	LC	215	ASN
8	LC	329	ASN
9	LD	202	GLN
11	LF	151	ASN
11	LF	235	ASN
12	LG	64	GLN
12	LG	100	HIS
12	LG	112	GLN
12	LG	141	ASN
13	LH	39	ASN
13	LH	78	GLN
14	LI	59	GLN
14	LI	73	ASN
14	LI	123	GLN
14	LI	166	HIS
14	LI	177	ASN
16	LL	175	ASN
17	LM	34	ASN
18	LN	87	HIS
18	LN	109	HIS
18	LN	199	GLN
20	LP	75	GLN
20	LP	133	HIS
20	LP	137	ASN
21	LQ	93	GLN
22	LR	36	ASN

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Mol	Chain	Res	Type
23	LS	77	ASN
23	LS	108	GLN
23	LS	173	ASN
24	LT	98	HIS
24	LT	131	GLN
25	LU	27	HIS
25	LU	41	GLN
26	LV	77	HIS
27	LW	50	ASN
29	LY	43	ASN
31	La	34	ASN
34	Ld	30	HIS
35	Le	52	GLN
36	Lf	99	HIS
39	Li	26	HIS
40	Lj	66	HIS
47	Lr	23	GLN
48	Ls	71	ASN
48	Ls	179	ASN
48	Ls	195	ASN
49	Lt	65	GLN
50	SD	74	GLN
50	SD	145	GLN
51	SF	29	GLN
51	SF	79	HIS
52	SK	84	HIS
54	SP	54	HIS
55	SQ	97	GLN
55	SQ	142	GLN
56	SR	83	ASN
58	ST	63	HIS
60	SZ	112	ASN
64	Sg	76	GLN
64	Sg	196	ASN
65	SA	84	GLN
66	SB	101	HIS
66	SB	118	GLN
68	SE	50	ASN
70	SH	39	GLN
70	SH	76	GLN
71	SI	99	ASN
71	SI	167	GLN

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Mol	Chain	Res	Type
71	SI	181	GLN
72	SJ	27	GLN
73	SL	11	GLN
73	SL	100	ASN
73	SL	141	ASN
74	SN	13	GLN
74	SN	105	ASN
77	SW	15	ASN
77	SW	70	ASN
78	SX	16	HIS
78	SX	31	HIS
78	SX	92	ASN
82	Se	37	GLN
85	CF	9	ASN
85	CF	15	HIS
85	CF	132	GLN
85	CF	296	HIS
85	CF	352	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Pt	72/74 (97%)	15 (20%)	0
3	L5	3643/3655 (99%)	743 (20%)	15 (0%)
4	L7	119/120 (99%)	11 (9%)	0
5	L8	155/156 (99%)	24 (15%)	0
83	S2	1714/1740 (98%)	375 (21%)	3 (0%)
84	AT	74/76 (97%)	29 (39%)	1 (1%)
All	All	5777/5821 (99%)	1197 (20%)	19 (0%)

All (1197) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Pt	9	A
2	Pt	13	U
2	Pt	19	G
2	Pt	21	A
2	Pt	46	G
2	Pt	47	U
2	Pt	48	C
2	Pt	49	C

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Mol	Chain	Res	Type
2	Pt	58	A
2	Pt	66	C
2	Pt	67	G
2	Pt	70	A
2	Pt	72	C
2	Pt	74	C
2	Pt	76	A
3	L5	25	A
3	L5	30	C
3	L5	39	A
3	L5	42	A
3	L5	48	G
3	L5	56	A
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	73	A
3	L5	74	G
3	L5	91	G
3	L5	104	G
3	L5	108	A
3	L5	109	G
3	L5	110	C
3	L5	116	G
3	L5	119	G
3	L5	120	A
3	L5	127	G
3	L5	132	G
3	L5	133	C
3	L5	134	G
3	L5	135	G
3	L5	136	C
3	L5	144	G
3	L5	145	G
3	L5	157	U
3	L5	158	A
3	L5	159	C
3	L5	164	G
3	L5	165	A
3	L5	177	G
3	L5	182	G
3	L5	183	C

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Mol	Chain	Res	Type
3	L5	184	U
3	L5	185	C
3	L5	186	G
3	L5	187	U
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	220	C
3	L5	234	G
3	L5	237	G
3	L5	255	C
3	L5	256	G
3	L5	261	G
3	L5	264	C
3	L5	265	C
3	L5	266	C
3	L5	267	G
3	L5	280	G
3	L5	297	U
3	L5	306	A
3	L5	315	G
3	L5	316	U
3	L5	340	C
3	L5	373	G
3	L5	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	432	U
3	L5	440	U
3	L5	449	C
3	L5	450	G
3	L5	452	A

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Mol	Chain	Res	Type
3	L5	453	G
3	L5	454	U
3	L5	456	C
3	L5	457	G
3	L5	467	U
3	L5	472	C
3	L5	478	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	497	G
3	L5	498	C
3	L5	499	G
3	L5	502	C
3	L5	503	C
3	L5	504	G
3	L5	509	A
3	L5	510	U
3	L5	512	U
3	L5	513	U
3	L5	514	U
3	L5	518	G
3	L5	519	C
3	L5	643	C
3	L5	645	G
3	L5	646	G
3	L5	654	C
3	L5	655	C
3	L5	656	C
3	L5	657	C
3	L5	659	G
3	L5	666	G
3	L5	667	A
3	L5	668	C
3	L5	669	C
3	L5	673	C
3	L5	674	G
3	L5	685	C
3	L5	686	A

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Mol	Chain	Res	Type
3	L5	687	U
3	L5	697	G
3	L5	703	G
3	L5	704	C
3	L5	708	G
3	L5	729	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	906	C
3	L5	910	G
3	L5	913	U
3	L5	914	U
3	L5	915	A
3	L5	917	A
3	L5	923	C
3	L5	924	C
3	L5	926	G
3	L5	932	A
3	L5	933	G
3	L5	935	A
3	L5	936	C
3	L5	941	C
3	L5	943	A
3	L5	944	A
3	L5	945	U
3	L5	956	A
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	965	G
3	L5	966	A
3	L5	967	C
3	L5	969	C

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Mol	Chain	Res	Type
3	L5	970	G
3	L5	982	U
3	L5	985	C
3	L5	989	U
3	L5	1070	G
3	L5	1071	C
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	1179	U
3	L5	1180	C
3	L5	1181	C
3	L5	1182	C
3	L5	1183	C
3	L5	1184	A
3	L5	1202	C
3	L5	1203	G
3	L5	1210	C
3	L5	1211	G
3	L5	1214	C
3	L5	1215	C
3	L5	1218	G
3	L5	1219	G
3	L5	1221	G
3	L5	1222	A
3	L5	1241	C
3	L5	1246	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	1271	G
3	L5	1272	C
3	L5	1273	G
3	L5	1275	G

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Mol	Chain	Res	Type
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
3	L5	1367	C
3	L5	1379	C
3	L5	1387	A
3	L5	1394	G
3	L5	1397	A
3	L5	1403	G
3	L5	1404	G
3	L5	1407	C
3	L5	1409	C
3	L5	1410	U
3	L5	1411	C
3	L5	1416	G
3	L5	1417	C
3	L5	1420	A
3	L5	1425	G
3	L5	1437	C
3	L5	1438	U
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	1457	G
3	L5	1482	G
3	L5	1483	C
3	L5	1497	A

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Mol	Chain	Res	Type
3	L5	1498	G
3	L5	1502	G
3	L5	1517	G
3	L5	1524	A2M
3	L5	1534	A2M
3	L5	1537	A
3	L5	1547	A
3	L5	1566	C
3	L5	1578	U
3	L5	1591	U
3	L5	1596	U
3	L5	1624	G
3	L5	1625	OMG
3	L5	1631	A
3	L5	1633	G
3	L5	1634	A
3	L5	1638	A
3	L5	1640	C
3	L5	1641	G
3	L5	1642	A
3	L5	1654	G
3	L5	1661	C
3	L5	1676	C
3	L5	1677	PSU
3	L5	1678	C
3	L5	1691	G
3	L5	1697	G
3	L5	1699	A
3	L5	1700	G
3	L5	1701	A
3	L5	1702	C
3	L5	1704	C
3	L5	1705	G
3	L5	1717	C
3	L5	1718	C
3	L5	1719	A
3	L5	1726	U
3	L5	1731	C
3	L5	1734	G
3	L5	1742	A
3	L5	1750	G
3	L5	1753	G

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Mol	Chain	Res	Type
3	L5	1755	C
3	L5	1757	U
3	L5	1758	G
3	L5	1760	G
3	L5	1761	G
3	L5	1762	C
3	L5	1763	C
3	L5	1764	G
3	L5	1765	A
3	L5	1766	A
3	L5	1767	A
3	L5	1768	C
3	L5	1770	A
3	L5	1775	A
3	L5	1785	C
3	L5	1787	A
3	L5	1803	G
3	L5	1804	A
3	L5	1806	G
3	L5	1810	G
3	L5	1815	G
3	L5	1821	G
3	L5	1822	U
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1855	G
3	L5	1869	G
3	L5	1882	U
3	L5	1888	A
3	L5	1892	A
3	L5	1893	C
3	L5	1897	A
3	L5	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

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Mol	Chain	Res	Type
3	L5	1940	G
3	L5	1951	G
3	L5	1959	U
3	L5	1961	G
3	L5	1962	A
3	L5	1965	G
3	L5	1974	U
3	L5	1975	G
3	L5	1978	C
3	L5	1980	U
3	L5	1981	G
3	L5	1982	G
3	L5	1984	A
3	L5	1985	G
3	L5	1986	U
3	L5	1989	G
3	L5	1991	A
3	L5	1993	C
3	L5	1997	U
3	L5	1998	A
3	L5	1999	A
3	L5	2001	G
3	L5	2002	A
3	L5	2003	G
3	L5	2004	U
3	L5	2005	G
3	L5	2011	C
3	L5	2017	A
3	L5	2018	C
3	L5	2024	G
3	L5	2026	A
3	L5	2046	G
3	L5	2048	U
3	L5	2055	G
3	L5	2056	G
3	L5	2069	A
3	L5	2084	C
3	L5	2085	G
3	L5	2092	G
3	L5	2093	A
3	L5	2095	A
3	L5	2096	G

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Mol	Chain	Res	Type
3	L5	2097	U
3	L5	2098	G
3	L5	2101	C
3	L5	2102	G
3	L5	2107	C
3	L5	2110	C
3	L5	2112	G
3	L5	2250	C
3	L5	2252	G
3	L5	2256	C
3	L5	2258	C
3	L5	2263	A
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2313	A
3	L5	2322	G
3	L5	2333	G
3	L5	2348	G
3	L5	2351	OMC
3	L5	2360	A
3	L5	2364	OMG
3	L5	2383	C
3	L5	2395	A
3	L5	2397	G
3	L5	2398	U
3	L5	2401	A2M
3	L5	2417	A
3	L5	2425	U
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

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Mol	Chain	Res	Type
3	L5	2489	C
3	L5	2490	U
3	L5	2494	U
3	L5	2504	C
3	L5	2505	C
3	L5	2506	G
3	L5	2513	A
3	L5	2519	U
3	L5	2520	C
3	L5	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
3	L5	2556	G
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	2618	G
3	L5	2627	C
3	L5	2653	C
3	L5	2662	G
3	L5	2669	C
3	L5	2676	A
3	L5	2687	U
3	L5	2694	G
3	L5	2695	A
3	L5	2696	A
3	L5	2706	G
3	L5	2707	U
3	L5	2708	U
3	L5	2710	C
3	L5	2711	G
3	L5	2712	G
3	L5	2719	C

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Mol	Chain	Res	Type
3	L5	2721	G
3	L5	2724	G
3	L5	2726	G
3	L5	2729	C
3	L5	2739	C
3	L5	2742	G
3	L5	2743	A
3	L5	2759	G
3	L5	2761	U
3	L5	2763	U
3	L5	2769	U
3	L5	2770	C
3	L5	2788	U
3	L5	2790	U
3	L5	2806	A
3	L5	2814	C
3	L5	2815	A2M
3	L5	2826	U
3	L5	2827	G
3	L5	2855	G
3	L5	2867	C
3	L5	2877	G
3	L5	2900	U
3	L5	2902	G
3	L5	2903	G
3	L5	2904	U
3	L5	2905	C
3	L5	2907	G
3	L5	2908	U
3	L5	3588	C
3	L5	3590	G
3	L5	3591	C
3	L5	3592	G
3	L5	3594	C
3	L5	3595	U
3	L5	3596	A
3	L5	3597	G
3	L5	3604	A
3	L5	3605	C
3	L5	3626	G
3	L5	3630	A
3	L5	3635	A

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Mol	Chain	Res	Type
3	L5	3644	U
3	L5	3646	A
3	L5	3648	A
3	L5	3662	A
3	L5	3664	G
3	L5	3670	C
3	L5	3673	C
3	L5	3674	G
3	L5	3691	G
3	L5	3701	OMC
3	L5	3710	G
3	L5	3711	A
3	L5	3713	U
3	L5	3727	A
3	L5	3753	G
3	L5	3764	U
3	L5	3770	U
3	L5	3774	A
3	L5	3775	A
3	L5	3776	G
3	L5	3777	G
3	L5	3785	A2M
3	L5	3786	U
3	L5	3792	OMG
3	L5	3811	G
3	L5	3814	U
3	L5	3817	A
3	L5	3819	G
3	L5	3824	A
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3867	A2M
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3885	G
3	L5	3892	U
3	L5	3897	G
3	L5	3899	OMG
3	L5	3901	A
3	L5	3906	A

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Mol	Chain	Res	Type
3	L5	3907	G
3	L5	3908	A
3	L5	3915	U
3	L5	3923	A
3	L5	3938	G
3	L5	3939	G
3	L5	3942	A
3	L5	3944	G
3	L5	3947	A
3	L5	3949	A
3	L5	3950	U
3	L5	3951	G
3	L5	3953	G
3	L5	4057	C
3	L5	4058	U
3	L5	4059	C
3	L5	4061	G
3	L5	4062	A
3	L5	4064	C
3	L5	4068	U
3	L5	4076	G
3	L5	4084	G
3	L5	4093	G
3	L5	4095	G
3	L5	4097	G
3	L5	4099	G
3	L5	4101	C
3	L5	4104	G
3	L5	4108	G
3	L5	4111	U
3	L5	4114	C
3	L5	4115	G
3	L5	4116	C
3	L5	4119	C
3	L5	4121	G
3	L5	4122	G
3	L5	4127	A
3	L5	4133	C
3	L5	4141	G
3	L5	4142	C
3	L5	4143	G
3	L5	4144	C

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Mol	Chain	Res	Type
3	L5	4146	G
3	L5	4149	C
3	L5	4150	G
3	L5	4162	C
3	L5	4163	U
3	L5	4168	G
3	L5	4170	A
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4212	A
3	L5	4222	G
3	L5	4228	OMG
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	4304	A
3	L5	4305	G
3	L5	4306	OMU
3	L5	4314	C
3	L5	4319	C
3	L5	4329	G
3	L5	4330	G
3	L5	4332	C
3	L5	4339	A
3	L5	4349	C
3	L5	4350	C
3	L5	4354	U
3	L5	4371	G
3	L5	4373	G
3	L5	4377	G

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Mol	Chain	Res	Type
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
3	L5	4438	U
3	L5	4448	G
3	L5	4449	A
3	L5	4452	U
3	L5	4464	A
3	L5	4466	C
3	L5	4475	G
3	L5	4488	A
3	L5	4500	PSU
3	L5	4510	A
3	L5	4512	U
3	L5	4513	A
3	L5	4519	C
3	L5	4523	A2M
3	L5	4524	G
3	L5	4525	C
3	L5	4545	G
3	L5	4548	A
3	L5	4557	U
3	L5	4560	C
3	L5	4567	G
3	L5	4569	U
3	L5	4575	G
3	L5	4584	A
3	L5	4589	A
3	L5	4590	A2M
3	L5	4600	G
3	L5	4601	U
3	L5	4617	G
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4652	G
3	L5	4656	A
3	L5	4670	C
3	L5	4672	A

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Mol	Chain	Res	Type
3	L5	4679	G
3	L5	4693	C
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
3	L5	4734	A
3	L5	4740	G
3	L5	4741	C
3	L5	4742	G
3	L5	4745	G
3	L5	4750	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4764	A
3	L5	4765	G
3	L5	4771	C
3	L5	4772	C
3	L5	4775	C
3	L5	4859	C
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	4897	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

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Mol	Chain	Res	Type
3	L5	4925	U
3	L5	4927	G
3	L5	4928	C
3	L5	4934	A
3	L5	4940	C
3	L5	4941	G
3	L5	4943	A
3	L5	4944	C
3	L5	4947	U
3	L5	4951	G
3	L5	4960	G
3	L5	4975	G
3	L5	4976	U
3	L5	4985	U
3	L5	4988	U
3	L5	4989	U
3	L5	4990	C
3	L5	4991	U
3	L5	4995	U
3	L5	5006	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	7	G
4	L7	22	A
4	L7	24	C
4	L7	33	U
4	L7	38	U
4	L7	53	U

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Mol	Chain	Res	Type
4	L7	54	A
4	L7	64	G
4	L7	97	G
4	L7	100	A
4	L7	110	G
5	L8	25	G
5	L8	34	U
5	L8	35	C
5	L8	38	U
5	L8	59	A
5	L8	62	A
5	L8	63	U
5	L8	80	A
5	L8	82	A
5	L8	84	A
5	L8	85	U
5	L8	87	G
5	L8	94	G
5	L8	103	A
5	L8	105	C
5	L8	111	U
5	L8	114	G
5	L8	123	U
5	L8	124	U
5	L8	125	C
5	L8	126	C
5	L8	127	U
5	L8	147	G
5	L8	150	C
83	S2	4	C
83	S2	14	C
83	S2	25	A
83	S2	33	G
83	S2	41	G
83	S2	42	A
83	S2	44	U
83	S2	45	A
83	S2	46	A
83	S2	49	C
83	S2	56	G
83	S2	58	C
83	S2	62	G

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Mol	Chain	Res	Type
83	S2	65	C
83	S2	67	C
83	S2	68	A
83	S2	72	C
83	S2	73	C
83	S2	74	G
83	S2	76	U
83	S2	103	A
83	S2	113	G
83	S2	115	U
83	S2	130	G
83	S2	143	U
83	S2	149	A
83	S2	158	A
83	S2	159	A2M
83	S2	160	U
83	S2	168	C
83	S2	170	A
83	S2	171	A
83	S2	175	A
83	S2	190	G
83	S2	191	A
83	S2	196	C
83	S2	197	U
83	S2	198	U
83	S2	200	G
83	S2	203	G
83	S2	204	G
83	S2	206	G
83	S2	207	G
83	S2	208	G
83	S2	209	A
83	S2	214	U
83	S2	291	G
83	S2	292	A
83	S2	295	C
83	S2	302	A
83	S2	306	C
83	S2	307	G
83	S2	308	G
83	S2	309	G
83	S2	311	C

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Mol	Chain	Res	Type
83	S2	312	G
83	S2	313	A
83	S2	318	A
83	S2	319	C
83	S2	323	C
83	S2	324	C
83	S2	325	C
83	S2	326	C
83	S2	328	U
83	S2	329	G
83	S2	332	G
83	S2	339	A
83	S2	340	C
83	S2	351	G
83	S2	360	A
83	S2	362	C
83	S2	364	A
83	S2	368	U
83	S2	370	G
83	S2	381	C
83	S2	383	G
83	S2	385	G
83	S2	386	C
83	S2	398	A
83	S2	407	G
83	S2	408	A
83	S2	409	C
83	S2	436	OMG
83	S2	438	G
83	S2	448	A
83	S2	449	A
83	S2	450	C
83	S2	452	G
83	S2	464	A
83	S2	465	A
83	S2	471	G
83	S2	472	C
83	S2	473	A
83	S2	474	G
83	S2	476	A
83	S2	478	G
83	S2	482	G

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Mol	Chain	Res	Type
83	S2	487	U
83	S2	488	U
83	S2	492	C
83	S2	493	A
83	S2	502	C
83	S2	517	OMC
83	S2	531	A
83	S2	532	C
83	S2	536	A
83	S2	537	C
83	S2	540	U
83	S2	542	U
83	S2	544	G
83	S2	546	G
83	S2	547	G
83	S2	557	U
83	S2	558	G
83	S2	559	G
83	S2	563	G
83	S2	564	A
83	S2	576	A2M
83	S2	583	A
83	S2	587	A
83	S2	589	G
83	S2	590	A
83	S2	591	U
83	S2	603	C
83	S2	604	A
83	S2	606	G
83	S2	614	C
83	S2	617	G
83	S2	622	C
83	S2	623	G
83	S2	627	OMU
83	S2	628	A
83	S2	631	U
83	S2	643	A
83	S2	644	OMG
83	S2	655	A
83	S2	660	C
83	S2	668	A2M
83	S2	669	A

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Mol	Chain	Res	Type
83	S2	671	A
83	S2	672	A
83	S2	673	G
83	S2	683	OMG
83	S2	688	U
83	S2	689	U
83	S2	692	G
83	S2	695	C
83	S2	696	G
83	S2	697	G
83	S2	698	G
83	S2	732	U
83	S2	733	C
83	S2	737	G
83	S2	738	C
83	S2	749	U
83	S2	750	C
83	S2	751	G
83	S2	752	G
83	S2	753	C
83	S2	788	G
83	S2	791	C
83	S2	792	C
83	S2	798	G
83	S2	799	OMU
83	S2	801	PSU
83	S2	821	G
83	S2	822	U
83	S2	823	U
83	S2	824	C
83	S2	827	A
83	S2	830	A
83	S2	834	C
83	S2	835	C
83	S2	836	G
83	S2	837	A
83	S2	838	G
83	S2	839	C
83	S2	842	C
83	S2	844	U
83	S2	847	A
83	S2	861	A

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Mol	Chain	Res	Type
83	S2	867	OMG
83	S2	870	A
83	S2	874	G
83	S2	877	C
83	S2	878	G
83	S2	880	G
83	S2	888	U
83	S2	889	U
83	S2	891	G
83	S2	893	U
83	S2	894	G
83	S2	896	U
83	S2	897	U
83	S2	898	U
83	S2	899	U
83	S2	900	C
83	S2	901	G
83	S2	903	A
83	S2	904	A
83	S2	913	A
83	S2	920	A
83	S2	930	C
83	S2	933	G
83	S2	934	G
83	S2	963	A
83	S2	969	U
83	S2	970	G
83	S2	971	G
83	S2	972	A
83	S2	990	A
83	S2	992	A
83	S2	997	A
83	S2	999	G
83	S2	1008	A
83	S2	1017	U
83	S2	1023	A
83	S2	1027	A
83	S2	1045	PSU
83	S2	1060	A
83	S2	1061	U
83	S2	1062	A
83	S2	1083	A

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Mol	Chain	Res	Type
83	S2	1085	C
83	S2	1109	C
83	S2	1113	A
83	S2	1116	C
83	S2	1121	G
83	S2	1123	C
83	S2	1126	G
83	S2	1133	A
83	S2	1138	C
83	S2	1148	A
83	S2	1150	A
83	S2	1153	C
83	S2	1154	U
83	S2	1195	A
83	S2	1207	G
83	S2	1208	A
83	S2	1215	C
83	S2	1216	C
83	S2	1217	A
83	S2	1224	G
83	S2	1227	G
83	S2	1240	A
83	S2	1242	U
83	S2	1243	U
83	S2	1248	B8N
83	S2	1251	A
83	S2	1253	A
83	S2	1256	G
83	S2	1257	G
83	S2	1259	A
83	S2	1264	C
83	S2	1271	C
83	S2	1274	G
83	S2	1275	G
83	S2	1283	C
83	S2	1285	G
83	S2	1286	G
83	S2	1288	OMU
83	S2	1290	G
83	S2	1294	G
83	S2	1295	A
83	S2	1301	A

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Mol	Chain	Res	Type
83	S2	1302	G
83	S2	1303	C
83	S2	1308	U
83	S2	1333	U
83	S2	1342	U
83	S2	1357	A
83	S2	1358	U
83	S2	1371	U
83	S2	1373	C
83	S2	1376	A
83	S2	1378	A
83	S2	1402	A
83	S2	1406	G
83	S2	1413	G
83	S2	1414	A
83	S2	1418	C
83	S2	1419	C
83	S2	1420	G
83	S2	1421	A
83	S2	1422	G
83	S2	1423	C
83	S2	1433	C
83	S2	1435	C
83	S2	1437	C
83	S2	1438	A
83	S2	1442	OMU
83	S2	1449	G
83	S2	1454	A
83	S2	1463	U
83	S2	1473	G
83	S2	1480	A
83	S2	1489	A
83	S2	1490	OMG
83	S2	1492	U
83	S2	1494	U
83	S2	1495	G
83	S2	1497	G
83	S2	1498	A
83	S2	1520	G
83	S2	1521	C
83	S2	1522	A
83	S2	1533	A

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Mol	Chain	Res	Type
83	S2	1544	C
83	S2	1546	G
83	S2	1552	G
83	S2	1553	C
83	S2	1556	A
83	S2	1558	C
83	S2	1573	G
83	S2	1574	C
83	S2	1575	G
83	S2	1578	U
83	S2	1580	A
83	S2	1581	C
83	S2	1582	C
83	S2	1585	U
83	S2	1587	G
83	S2	1588	A
83	S2	1600	G
83	S2	1604	G
83	S2	1606	G
83	S2	1621	U
83	S2	1623	A
83	S2	1630	A
83	S2	1631	U
83	S2	1633	A
83	S2	1634	A
83	S2	1637	A
83	S2	1648	G
83	S2	1654	G
83	S2	1663	A
83	S2	1665	G
83	S2	1686	G
83	S2	1695	A
83	S2	1699	A
83	S2	1715	A
83	S2	1721	U
83	S2	1722	G
83	S2	1744	G
83	S2	1745	A
83	S2	1752	C
83	S2	1753	C
83	S2	1754	G
83	S2	1755	C

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Mol	Chain	Res	Type
83	S2	1757	G
83	S2	1759	G
83	S2	1760	G
83	S2	1761	U
83	S2	1772	C
83	S2	1773	C
83	S2	1774	C
83	S2	1777	G
83	S2	1782	G
83	S2	1783	C
83	S2	1784	G
83	S2	1786	U
83	S2	1798	C
83	S2	1810	U
83	S2	1811	C
83	S2	1825	A
83	S2	1826	G
83	S2	1831	A
83	S2	1835	A
83	S2	1838	U
83	S2	1849	G
83	S2	1851	MA6
83	S2	1861	G
83	S2	1862	G
83	S2	1863	A
83	S2	1865	C
84	AT	4	U
84	AT	8	U
84	AT	9	A
84	AT	10	G
84	AT	12	G
84	AT	14	A
84	AT	16	C
84	AT	19	G
84	AT	20	U
84	AT	21	U
84	AT	22	A
84	AT	27	G
84	AT	31	G
84	AT	32	C
84	AT	33	C
84	AT	46	G

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Mol	Chain	Res	Type
84	AT	47	G
84	AT	49	C
84	AT	51	U
84	AT	53	G
84	AT	58	G
84	AT	59	A
84	AT	60	A
84	AT	62	C
84	AT	65	G
84	AT	70	A
84	AT	73	C
84	AT	76	C
84	AT	77	A

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	254	G
3	L5	406	C
3	L5	493	G
3	L5	912	G
3	L5	914	U
3	L5	1082	C
3	L5	1633	G
3	L5	1977	C
3	L5	2416	G
3	L5	2675	G
3	L5	2760	G
3	L5	3673	C
3	L5	4600	G
3	L5	4699	U
3	L5	4913	G
83	S2	291	G
83	S2	563	G
83	S2	688	U
84	AT	11	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

179 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	3899	3	23,26,27	0.61	0	32,38,41	0.53	0
3	PSU	L5	4628	3	18,21,22	0.99	1 (5%)	21,30,33	1.99	6 (28%)
3	OMC	L5	2824	3	19,22,23	0.62	0	25,31,34	0.69	0
83	B8N	S2	1248	83	25,29,30	3.28	6 (24%)	28,42,45	1.99	8 (28%)
83	PSU	S2	109	83	18,21,22	1.10	1 (5%)	21,30,33	1.98	5 (23%)
83	G7M	S2	1639	2,83	23,26,27	2.67	9 (39%)	34,39,42	2.62	11 (32%)
83	OMG	S2	509	83	23,26,27	0.50	0	32,38,41	0.46	0
83	PSU	S2	93	83	18,21,22	1.09	1 (5%)	21,30,33	1.75	4 (19%)
83	PSU	S2	1056	83	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
3	A2M	L5	1326	3	22,25,26	1.20	2 (9%)	30,36,39	1.52	9 (30%)
3	A2M	L5	1871	3,86	22,25,26	1.24	2 (9%)	30,36,39	1.64	6 (20%)
3	OMG	L5	2364	3,86	23,26,27	0.53	0	32,38,41	0.48	0
83	OMC	S2	1703	83	19,22,23	0.57	0	25,31,34	0.72	0
83	OMU	S2	172	83	19,22,23	3.35	7 (36%)	25,31,34	1.79	4 (16%)
3	PSU	L5	1860	3	18,21,22	1.12	2 (11%)	21,30,33	2.00	4 (19%)
3	A2M	L5	4523	3,86	22,25,26	1.26	2 (9%)	30,36,39	1.63	9 (30%)
3	OMC	L5	3869	3	19,22,23	0.60	0	25,31,34	0.74	0
83	OMU	S2	116	83	19,22,23	3.34	7 (36%)	25,31,34	1.74	5 (20%)
83	A2M	S2	484	83	22,25,26	1.16	1 (4%)	30,36,39	1.49	7 (23%)
3	PSU	L5	4299	3	18,21,22	1.01	1 (5%)	21,30,33	1.83	4 (19%)
83	PSU	S2	1367	83	18,21,22	1.07	1 (5%)	21,30,33	1.99	5 (23%)
3	PSU	L5	1862	3	18,21,22	1.07	1 (5%)	21,30,33	1.95	4 (19%)
83	OMU	S2	428	83	19,22,23	3.36	7 (36%)	25,31,34	1.84	5 (20%)
3	A2M	L5	3785	3,86	22,25,26	1.15	1 (4%)	30,36,39	1.65	9 (30%)
3	OMU	L5	4227	3	19,22,23	3.27	7 (36%)	25,31,34	1.85	5 (20%)
3	OMG	L5	4392	3	23,26,27	0.54	0	32,38,41	0.48	0
83	PSU	S2	651	83	18,21,22	1.13	2 (11%)	21,30,33	1.96	4 (19%)
3	PSU	L5	4471	3	18,21,22	1.11	1 (5%)	21,30,33	1.94	4 (19%)
3	OMG	L5	4637	3	23,26,27	0.54	0	32,38,41	0.51	0
3	OMC	L5	2422	3,86	19,22,23	0.62	0	25,31,34	0.75	1 (4%)
83	OMG	S2	867	83	23,26,27	0.49	0	32,38,41	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4552	3	18,21,22	1.03	1 (5%)	21,30,33	1.95	4 (19%)
83	PSU	S2	814	83	18,21,22	1.07	1 (5%)	21,30,33	1.84	4 (19%)
83	A2M	S2	159	83	22,25,26	1.27	1 (4%)	30,36,39	1.55	10 (33%)
3	PSU	L5	5010	3	18,21,22	1.12	1 (5%)	21,30,33	1.94	4 (19%)
83	PSU	S2	1045	83	18,21,22	1.09	1 (5%)	21,30,33	1.87	4 (19%)
3	A2M	L5	3718	3	22,25,26	1.15	1 (4%)	30,36,39	1.49	5 (16%)
3	A2M	L5	400	3	22,25,26	1.23	2 (9%)	30,36,39	1.58	9 (30%)
3	PSU	L5	4576	3	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L5	3822	3	18,21,22	1.10	1 (5%)	21,30,33	1.96	6 (28%)
5	PSU	L8	69	5	18,21,22	1.09	1 (5%)	21,30,33	1.93	5 (23%)
3	PSU	L5	4293	3	18,21,22	1.10	2 (11%)	21,30,33	2.00	4 (19%)
83	A2M	S2	1383	83	22,25,26	1.19	1 (4%)	30,36,39	1.66	6 (20%)
3	PSU	L5	1744	3,86	18,21,22	1.10	2 (11%)	21,30,33	1.95	4 (19%)
3	5MC	L5	4447	3	19,22,23	0.91	2 (10%)	26,32,35	0.68	0
83	A2M	S2	99	83,86	22,25,26	1.21	1 (4%)	30,36,39	1.57	6 (20%)
3	OMG	L5	4370	3	23,26,27	0.54	0	32,38,41	0.51	0
3	A2M	L5	1534	3,86	22,25,26	1.18	1 (4%)	30,36,39	1.51	9 (30%)
3	PSU	L5	3851	3	18,21,22	1.08	1 (5%)	21,30,33	1.92	4 (19%)
3	A2M	L5	398	3	22,25,26	1.15	1 (4%)	30,36,39	1.59	6 (20%)
3	PSU	L5	3844	3	18,21,22	1.08	1 (5%)	21,30,33	1.85	4 (19%)
3	PSU	L5	2839	3	18,21,22	1.05	1 (5%)	21,30,33	1.95	4 (19%)
3	A2M	L5	4590	3	22,25,26	1.20	1 (4%)	30,36,39	1.58	6 (20%)
83	PSU	S2	1081	83	18,21,22	1.05	1 (5%)	21,30,33	1.93	5 (23%)
83	OMU	S2	1326	83	19,22,23	3.37	7 (36%)	25,31,34	1.81	5 (20%)
3	A2M	L5	3825	3	22,25,26	1.17	1 (4%)	30,36,39	1.56	7 (23%)
85	SEP	CF	163	85	8,9,10	1.61	1 (12%)	7,12,14	1.43	1 (14%)
3	OMG	L5	1522	3	23,26,27	0.54	0	32,38,41	0.60	0
3	OMC	L5	3841	3	19,22,23	0.64	0	25,31,34	0.65	0
3	OMU	L5	2837	3	19,22,23	3.30	7 (36%)	25,31,34	1.86	4 (16%)
3	PSU	L5	3884	3	18,21,22	1.09	2 (11%)	21,30,33	1.99	4 (19%)
3	PSU	L5	4361	3	18,21,22	1.08	2 (11%)	21,30,33	1.95	4 (19%)
3	PSU	L5	3920	3,86	18,21,22	1.07	2 (11%)	21,30,33	1.94	4 (19%)
83	PSU	S2	105	83	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
83	PSU	S2	863	83	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
3	A2M	L5	3830	3	22,25,26	1.18	1 (4%)	30,36,39	1.60	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	5MC	L5	3782	3,86	19,22,23	0.68	0	26,32,35	0.68	0
83	OMC	S2	174	83	19,22,23	0.54	0	25,31,34	0.72	1 (4%)
3	6MZ	L5	4220	3	22,25,26	3.93	12 (54%)	29,36,39	2.46	11 (37%)
3	A2M	L5	2401	3	22,25,26	1.19	1 (4%)	30,36,39	1.60	7 (23%)
3	OMU	L5	4620	3	19,22,23	3.22	7 (36%)	25,31,34	1.75	5 (20%)
3	PSU	L5	4442	3	18,21,22	1.05	1 (5%)	21,30,33	1.99	6 (28%)
83	PSU	S2	801	83	18,21,22	1.09	1 (5%)	21,30,33	1.95	5 (23%)
83	PSU	S2	866	83	18,21,22	1.06	1 (5%)	21,30,33	1.94	5 (23%)
3	OMG	L5	4196	3,2	23,26,27	0.55	0	32,38,41	0.44	0
3	OMC	L5	2365	3	19,22,23	0.59	0	25,31,34	0.61	0
3	PSU	L5	2632	3	18,21,22	1.07	1 (5%)	21,30,33	1.94	4 (19%)
83	OMU	S2	1442	83	19,22,23	3.39	7 (36%)	25,31,34	1.80	5 (20%)
3	OMU	L5	4306	3	19,22,23	3.23	7 (36%)	25,31,34	1.81	4 (16%)
83	PSU	S2	966	83,86	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
3	OMC	L5	2351	3,86	19,22,23	0.68	0	25,31,34	1.24	2 (8%)
3	PSU	L5	4673	3,86	18,21,22	1.09	2 (11%)	21,30,33	1.87	4 (19%)
83	OMG	S2	1328	83	23,26,27	0.46	0	32,38,41	0.43	0
3	A2M	L5	2815	3	22,25,26	1.18	2 (9%)	30,36,39	1.54	9 (30%)
83	OMC	S2	1391	83	19,22,23	0.50	0	25,31,34	0.69	0
3	PSU	L5	4973	3	18,21,22	1.07	2 (11%)	21,30,33	1.96	4 (19%)
3	PSU	L5	1781	3	18,21,22	1.02	1 (5%)	21,30,33	1.86	4 (19%)
3	UR3	L5	4530	3	19,22,23	2.68	7 (36%)	26,32,35	1.59	3 (11%)
83	PSU	S2	686	83	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)
83	PSU	S2	1177	83	18,21,22	1.03	2 (11%)	21,30,33	1.89	4 (19%)
3	PSU	L5	4493	3	18,21,22	1.04	1 (5%)	21,30,33	1.86	4 (19%)
3	OMC	L5	2804	3	19,22,23	0.62	0	25,31,34	0.68	0
83	A2M	S2	1031	83	22,25,26	1.18	1 (4%)	30,36,39	1.60	7 (23%)
83	MA6	S2	1851	83	23,26,27	1.26	2 (8%)	33,38,41	3.37	12 (36%)
83	PSU	S2	1046	83	18,21,22	1.07	1 (5%)	21,30,33	1.97	5 (23%)
83	PSU	S2	1004	83	18,21,22	1.12	1 (5%)	21,30,33	2.02	5 (23%)
3	A2M	L5	4571	3	22,25,26	1.23	2 (9%)	30,36,39	1.58	6 (20%)
83	PSU	S2	1232	83	18,21,22	1.11	1 (5%)	21,30,33	1.94	4 (19%)
3	OMC	L5	4536	3	19,22,23	0.62	0	25,31,34	0.76	0
3	OMG	L5	1316	3	23,26,27	0.57	0	32,38,41	0.53	0
83	OMU	S2	121	83	19,22,23	3.37	7 (36%)	25,31,34	1.83	5 (20%)
3	OMC	L5	3701	3	19,22,23	0.67	0	25,31,34	1.70	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4312	3	18,21,22	1.06	1 (5%)	21,30,33	1.97	4 (19%)
83	OMC	S2	517	83	19,22,23	0.52	0	25,31,34	0.61	0
83	OMU	S2	799	83	19,22,23	3.35	7 (36%)	25,31,34	1.83	5 (20%)
83	4AC	S2	1842	83	21,24,25	0.37	0	28,34,37	0.45	0
3	OMG	L5	4494	3	23,26,27	0.57	0	32,38,41	0.52	0
83	PSU	S2	1174	83	18,21,22	1.10	1 (5%)	21,30,33	1.94	4 (19%)
83	PSU	S2	681	83	18,21,22	1.03	1 (5%)	21,30,33	1.97	4 (19%)
3	A2M	L5	2787	3	22,25,26	1.15	1 (4%)	30,36,39	1.47	6 (20%)
3	OMG	L5	3627	3	23,26,27	0.55	0	32,38,41	0.57	0
3	PSU	L5	4353	3	18,21,22	1.07	2 (11%)	21,30,33	2.11	5 (23%)
83	OMU	S2	1288	83	19,22,23	3.41	7 (36%)	25,31,34	1.80	5 (20%)
3	PSU	L5	4500	3	18,21,22	1.12	2 (11%)	21,30,33	1.99	5 (23%)
3	A2M	L5	3867	3	22,25,26	1.26	2 (9%)	30,36,39	1.48	7 (23%)
3	OMC	L5	2861	3	19,22,23	0.61	0	25,31,34	0.77	1 (4%)
3	OMG	L5	4499	3	23,26,27	0.55	0	32,38,41	0.50	0
3	OMG	L5	2876	3	23,26,27	0.52	0	32,38,41	0.52	0
3	PSU	L5	1782	3	18,21,22	1.04	1 (5%)	21,30,33	1.95	4 (19%)
83	OMG	S2	601	83	23,26,27	0.50	0	32,38,41	0.47	0
3	PSU	L5	3853	3,86	18,21,22	1.03	1 (5%)	21,30,33	1.90	4 (19%)
3	PSU	L5	4689	3	18,21,22	1.06	2 (11%)	21,30,33	2.05	4 (19%)
83	A2M	S2	166	83	22,25,26	1.28	1 (4%)	30,36,39	1.56	6 (20%)
3	PSU	L5	1677	3	18,21,22	1.01	2 (11%)	21,30,33	1.90	4 (19%)
83	OMG	S2	1490	83	23,26,27	0.52	0	32,38,41	0.47	0
3	A2M	L5	1524	3	22,25,26	1.27	2 (9%)	30,36,39	1.52	6 (20%)
3	PSU	L5	4296	3	18,21,22	1.11	1 (5%)	21,30,33	1.95	4 (19%)
3	PSU	L5	3695	3	18,21,22	1.05	2 (11%)	21,30,33	1.96	4 (19%)
3	PSU	L5	4636	3	18,21,22	1.08	2 (11%)	21,30,33	2.03	6 (28%)
5	OMG	L8	75	5	23,26,27	0.54	0	32,38,41	0.51	0
3	PSU	L5	4431	3	18,21,22	1.05	1 (5%)	21,30,33	1.94	4 (19%)
3	PSU	L5	5001	3	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
83	PSU	S2	649	83	18,21,22	1.08	1 (5%)	21,30,33	2.01	5 (23%)
83	OMC	S2	462	83	19,22,23	0.53	0	25,31,34	0.69	0
3	OMG	L5	4228	3	23,26,27	0.54	0	32,38,41	0.63	0
83	6MZ	S2	1832	83,86	26,26,26	2.80	5 (19%)	36,39,39	2.07	9 (25%)
3	PSU	L5	4579	3	18,21,22	1.06	2 (11%)	21,30,33	1.94	4 (19%)
83	OMU	S2	354	83	19,22,23	3.31	7 (36%)	25,31,34	1.87	5 (20%)
3	1MA	L5	1322	3,86	21,25,26	0.60	0	30,37,40	0.80	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMU	L5	3925	3	19,22,23	3.26	7 (36%)	25,31,34	1.88	5 (20%)
3	A2M	L5	2363	3,86	22,25,26	1.22	2 (9%)	30,36,39	1.52	9 (30%)
3	UY1	L5	3818	3	19,22,23	4.87	8 (42%)	21,31,34	1.94	5 (23%)
83	OMG	S2	436	83	23,26,27	0.50	0	32,38,41	0.54	0
83	OMC	S2	1272	83	19,22,23	0.50	0	25,31,34	0.78	1 (4%)
3	PSU	L5	4532	3	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
3	PSU	L5	4521	3,86	18,21,22	1.09	2 (11%)	21,30,33	1.99	4 (19%)
3	PSU	L5	1536	3	18,21,22	1.09	1 (5%)	21,30,33	2.04	4 (19%)
3	A2M	L5	1323	3	22,25,26	1.21	2 (9%)	30,36,39	1.62	9 (30%)
3	OMG	L5	1625	3	23,26,27	0.53	0	32,38,41	0.45	0
3	PSU	L5	3637	3	18,21,22	1.09	1 (5%)	21,30,33	2.05	4 (19%)
3	OMG	L5	3744	3	23,26,27	0.54	0	32,38,41	0.50	0
3	OMG	L5	4623	3	23,26,27	0.57	0	32,38,41	0.56	0
3	PSU	L5	1792	3	18,21,22	1.02	1 (5%)	21,30,33	1.92	4 (19%)
83	OMG	S2	644	83	23,26,27	0.48	0	32,38,41	0.52	0
83	OMU	S2	627	83	19,22,23	3.39	7 (36%)	25,31,34	1.81	4 (16%)
83	PSU	S2	1244	83	18,21,22	1.10	1 (5%)	21,30,33	1.93	4 (19%)
83	PSU	S2	406	83	18,21,22	1.10	1 (5%)	21,30,33	1.96	5 (23%)
83	OMG	S2	683	83	23,26,27	0.51	0	32,38,41	0.48	0
3	OMG	L5	4618	3	23,26,27	0.55	0	32,38,41	0.51	0
3	PSU	L5	4972	3	18,21,22	1.08	1 (5%)	21,30,33	1.94	5 (23%)
3	PSU	L5	3639	3	18,21,22	1.07	2 (11%)	21,30,33	2.00	5 (23%)
83	A2M	S2	27	83	22,25,26	1.21	1 (4%)	30,36,39	1.54	7 (23%)
3	OMC	L5	1340	3	19,22,23	0.61	0	25,31,34	0.80	0
83	A2M	S2	576	83	22,25,26	1.19	1 (4%)	30,36,39	1.55	5 (16%)
83	A2M	S2	668	83,86	22,25,26	1.35	2 (9%)	30,36,39	1.57	9 (30%)
3	OMG	L5	3792	3	23,26,27	0.51	0	32,38,41	0.53	0
83	4AC	S2	1337	83	21,24,25	0.39	0	28,34,37	0.69	1 (3%)
3	PSU	L5	4403	3	18,21,22	1.07	2 (11%)	21,30,33	2.07	6 (28%)
3	PSU	L5	1582	3	18,21,22	1.09	2 (11%)	21,30,33	1.98	5 (23%)
3	OMG	L5	2424	3	23,26,27	0.57	0	32,38,41	0.49	0
83	A2M	S2	468	83	22,25,26	1.24	1 (4%)	30,36,39	1.60	6 (20%)
3	OMC	L5	4456	3	19,22,23	0.69	0	25,31,34	0.85	1 (4%)
3	PSU	L5	4457	3	18,21,22	1.03	2 (11%)	21,30,33	1.94	4 (19%)
3	OMU	L5	4498	3	19,22,23	3.25	7 (36%)	25,31,34	1.87	5 (20%)
3	OMC	L5	3887	3	19,22,23	0.61	0	25,31,34	0.71	0
5	PSU	L8	55	5	18,21,22	1.05	1 (5%)	21,30,33	1.84	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
83	MA6	S2	1850	83	23,26,27	1.29	2 (8%)	33,38,41	3.33	12 (36%)
3	OMC	L5	3808	3	19,22,23	0.66	0	25,31,34	0.76	1 (4%)
3	PSU	L5	1683	3	18,21,22	1.05	1 (5%)	21,30,33	1.95	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	3899	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
83	B8N	S2	1248	83	-	6/16/34/35	0/2/2/2
83	PSU	S2	109	83	-	0/7/25/26	0/2/2/2
83	G7M	S2	1639	2,83	-	0/7/25/26	0/3/3/3
83	OMG	S2	509	83	-	0/9/27/28	0/3/3/3
83	PSU	S2	93	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	1056	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	3/9/27/28	0/3/3/3
3	A2M	L5	1871	3,86	-	0/9/27/28	0/3/3/3
3	OMG	L5	2364	3,86	-	3/9/27/28	0/3/3/3
83	OMC	S2	1703	83	-	0/9/27/28	0/2/2/2
83	OMU	S2	172	83	-	1/9/27/28	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4523	3,86	-	0/9/27/28	0/3/3/3
3	OMC	L5	3869	3	-	1/9/27/28	0/2/2/2
83	OMU	S2	116	83	-	1/9/27/28	0/2/2/2
83	A2M	S2	484	83	-	0/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1367	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	428	83	-	6/9/27/28	0/2/2/2
3	A2M	L5	3785	3,86	-	0/9/27/28	0/3/3/3
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
83	PSU	S2	651	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	4637	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	2422	3,86	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	OMG	S2	867	83	-	2/9/27/28	0/3/3/3
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	814	83	-	0/7/25/26	0/2/2/2
83	A2M	S2	159	83	-	3/9/27/28	0/3/3/3
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1045	83	-	2/7/25/26	0/2/2/2
3	A2M	L5	3718	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
83	A2M	S2	1383	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	1744	3,86	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
83	A2M	S2	99	83,86	-	2/9/27/28	0/3/3/3
3	OMG	L5	4370	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	1534	3,86	-	1/9/27/28	0/3/3/3
3	PSU	L5	3851	3	-	1/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4590	3	-	4/9/27/28	0/3/3/3
83	PSU	S2	1081	83	-	1/7/25/26	0/2/2/2
83	OMU	S2	1326	83	-	0/9/27/28	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
85	SEP	CF	163	85	-	6/6/8/10	-
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	3,86	-	0/7/25/26	0/2/2/2
83	PSU	S2	105	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	863	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
3	5MC	L5	3782	3,86	-	0/7/25/26	0/2/2/2
83	OMC	S2	174	83	-	0/9/27/28	0/2/2/2
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2401	3	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	L5	4620	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	801	83	-	2/7/25/26	0/2/2/2
83	PSU	S2	866	83	-	0/7/25/26	0/2/2/2
3	OMG	L5	4196	3,2	-	1/9/27/28	0/3/3/3
3	OMC	L5	2365	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	1442	83	-	2/9/27/28	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
83	PSU	S2	966	83,86	-	0/7/25/26	0/2/2/2
3	OMC	L5	2351	3,86	-	4/9/27/28	0/2/2/2
3	PSU	L5	4673	3,86	-	0/7/25/26	0/2/2/2
83	OMG	S2	1328	83	-	1/9/27/28	0/3/3/3
3	A2M	L5	2815	3	-	3/9/27/28	0/3/3/3
83	OMC	S2	1391	83	-	0/9/27/28	0/2/2/2
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	2/7/25/26	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	686	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	1177	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
83	A2M	S2	1031	83	-	1/9/27/28	0/3/3/3
83	MA6	S2	1851	83	-	1/11/29/30	0/3/3/3
83	PSU	S2	1046	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	1004	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
83	PSU	S2	1232	83	-	0/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
83	OMU	S2	121	83	-	0/9/27/28	0/2/2/2
3	OMC	L5	3701	3	-	6/9/27/28	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
83	OMC	S2	517	83	-	2/9/27/28	0/2/2/2
83	OMU	S2	799	83	-	2/9/27/28	0/2/2/2
83	4AC	S2	1842	83	-	0/11/29/30	0/2/2/2
3	OMG	L5	4494	3	-	1/9/27/28	0/3/3/3
83	PSU	S2	1174	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	681	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	3	-	5/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	3627	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	1288	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	3/9/27/28	0/3/3/3
3	OMC	L5	2861	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
83	OMG	S2	601	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	3853	3,86	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
83	A2M	S2	166	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	1677	3	-	3/7/25/26	0/2/2/2
83	OMG	S2	1490	83	-	1/9/27/28	0/3/3/3
3	A2M	L5	1524	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4296	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4636	3	-	2/7/25/26	0/2/2/2
5	OMG	L8	75	5	-	1/9/27/28	0/3/3/3
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	649	83	-	0/7/25/26	0/2/2/2
83	OMC	S2	462	83	-	0/9/27/28	0/2/2/2
3	OMG	L5	4228	3	-	2/9/27/28	0/3/3/3
83	6MZ	S2	1832	83,86	-	7/12/28/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	354	83	-	0/9/27/28	0/2/2/2
3	1MA	L5	1322	3,86	-	0/7/25/26	0/3/3/3
3	OMU	L5	3925	3	-	1/9/27/28	0/2/2/2
3	A2M	L5	2363	3,86	-	1/9/27/28	0/3/3/3
3	UY1	L5	3818	3	-	2/9/27/28	0/2/2/2
83	OMG	S2	436	83	-	2/9/27/28	0/3/3/3
83	OMC	S2	1272	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4521	3,86	-	0/7/25/26	0/2/2/2
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	1323	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	1625	3	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4623	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
83	OMG	S2	644	83	-	3/9/27/28	0/3/3/3
83	OMU	S2	627	83	-	2/9/27/28	0/2/2/2
83	PSU	S2	1244	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	406	83	-	0/7/25/26	0/2/2/2
83	OMG	S2	683	83	-	2/9/27/28	0/3/3/3
3	OMG	L5	4618	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
83	A2M	S2	27	83	-	0/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
83	A2M	S2	576	83	-	4/9/27/28	0/3/3/3
83	A2M	S2	668	83,86	-	2/9/27/28	0/3/3/3
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
83	4AC	S2	1337	83	-	1/11/29/30	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	1/9/27/28	0/3/3/3
83	A2M	S2	468	83	-	1/9/27/28	0/3/3/3
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	1/9/27/28	0/2/2/2
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
83	MA6	S2	1850	83	-	0/11/29/30	0/3/3/3
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2

All (300) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	C6-C5	12.63	1.49	1.35
83	S2	1832	6MZ	C6-N6	12.51	1.48	1.34
3	L5	4220	6MZ	C6-N6	11.91	1.47	1.34
3	L5	3818	UY1	C2-N1	11.72	1.51	1.36
83	S2	1288	OMU	C2-N1	8.65	1.52	1.38
83	S2	1442	OMU	C2-N1	8.40	1.51	1.38
83	S2	799	OMU	C2-N1	8.33	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	172	OMU	C2-N1	8.31	1.51	1.38
3	L5	4220	6MZ	C3'-C2'	-8.30	1.30	1.53
83	S2	627	OMU	C2-N1	8.27	1.51	1.38
83	S2	1326	OMU	C2-N1	8.21	1.51	1.38
83	S2	121	OMU	C2-N1	8.20	1.51	1.38
83	S2	428	OMU	C2-N1	8.14	1.51	1.38
83	S2	116	OMU	C2-N1	8.12	1.51	1.38
83	S2	354	OMU	C2-N1	8.09	1.51	1.38
3	L5	2837	OMU	C2-N1	8.05	1.51	1.38
3	L5	4227	OMU	C2-N1	7.94	1.50	1.38
83	S2	1248	B8N	C6-N1	7.93	1.55	1.36
3	L5	3925	OMU	C2-N1	7.86	1.50	1.38
3	L5	4306	OMU	C2-N1	7.84	1.50	1.38
3	L5	4498	OMU	C2-N1	7.81	1.50	1.38
3	L5	4620	OMU	C2-N1	7.74	1.50	1.38
3	L5	3818	UY1	C2-N3	7.70	1.50	1.37
83	S2	1248	B8N	C4-N3	-7.70	1.26	1.40
83	S2	1248	B8N	C4-C5	7.20	1.63	1.47
83	S2	1442	OMU	C2-N3	7.02	1.50	1.38
83	S2	121	OMU	C2-N3	7.00	1.50	1.38
83	S2	116	OMU	C2-N3	6.97	1.50	1.38
83	S2	627	OMU	C2-N3	6.97	1.50	1.38
83	S2	1326	OMU	C2-N3	6.96	1.50	1.38
83	S2	1288	OMU	C2-N3	6.90	1.50	1.38
83	S2	428	OMU	C2-N3	6.89	1.50	1.38
83	S2	799	OMU	C2-N3	6.83	1.49	1.38
83	S2	172	OMU	C2-N3	6.81	1.49	1.38
83	S2	354	OMU	C2-N3	6.76	1.49	1.38
3	L5	2837	OMU	C2-N3	6.73	1.49	1.38
3	L5	3925	OMU	C2-N3	6.71	1.49	1.38
3	L5	4227	OMU	C2-N3	6.66	1.49	1.38
3	L5	4498	OMU	C2-N3	6.63	1.49	1.38
3	L5	4620	OMU	C2-N3	6.61	1.49	1.38
83	S2	1639	G7M	C4-N3	6.56	1.49	1.34
3	L5	4306	OMU	C2-N3	6.53	1.49	1.38
3	L5	4530	UR3	C6-C5	6.29	1.49	1.35
3	L5	4530	UR3	C2-N1	6.07	1.46	1.38
83	S2	428	OMU	C6-C5	5.91	1.48	1.35
83	S2	1326	OMU	C6-C5	5.90	1.48	1.35
83	S2	121	OMU	C6-C5	5.87	1.48	1.35
83	S2	1288	OMU	C6-C5	5.87	1.48	1.35
83	S2	1442	OMU	C6-C5	5.85	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	627	OMU	C6-C5	5.82	1.48	1.35
83	S2	172	OMU	C6-C5	5.82	1.48	1.35
83	S2	1248	B8N	C2-N1	5.81	1.56	1.39
83	S2	799	OMU	C6-C5	5.76	1.48	1.35
3	L5	2837	OMU	C6-C5	5.75	1.48	1.35
83	S2	116	OMU	C6-C5	5.75	1.48	1.35
83	S2	354	OMU	C6-C5	5.75	1.48	1.35
3	L5	4227	OMU	C6-C5	5.74	1.48	1.35
3	L5	4498	OMU	C6-C5	5.68	1.48	1.35
3	L5	4620	OMU	C6-C5	5.68	1.48	1.35
3	L5	4530	UR3	C2-N3	5.67	1.50	1.39
3	L5	3925	OMU	O4-C4	-5.67	1.13	1.24
3	L5	4306	OMU	C6-C5	5.66	1.48	1.35
3	L5	3925	OMU	C6-C5	5.64	1.48	1.35
3	L5	4306	OMU	O4-C4	-5.58	1.13	1.24
3	L5	4620	OMU	O4-C4	-5.57	1.13	1.24
3	L5	2837	OMU	O4-C4	-5.57	1.13	1.24
3	L5	4227	OMU	O4-C4	-5.57	1.13	1.24
83	S2	1639	G7M	C2-N3	5.51	1.46	1.33
3	L5	4498	OMU	O4-C4	-5.50	1.13	1.24
83	S2	627	OMU	O4-C4	-5.48	1.13	1.24
83	S2	354	OMU	O4-C4	-5.47	1.13	1.24
83	S2	1248	B8N	C6-C5	5.46	1.42	1.35
83	S2	121	OMU	O4-C4	-5.46	1.13	1.24
3	L5	3818	UY1	C6-N1	5.45	1.45	1.36
83	S2	116	OMU	O4-C4	-5.44	1.13	1.24
83	S2	428	OMU	O4-C4	-5.42	1.13	1.24
83	S2	799	OMU	O4-C4	-5.42	1.13	1.24
83	S2	1326	OMU	O4-C4	-5.41	1.13	1.24
83	S2	1288	OMU	O4-C4	-5.38	1.14	1.24
83	S2	1442	OMU	O4-C4	-5.35	1.14	1.24
83	S2	172	OMU	O4-C4	-5.32	1.14	1.24
83	S2	1639	G7M	C2-N2	4.95	1.45	1.34
3	L5	4220	6MZ	O4'-C1'	-4.88	1.30	1.42
83	S2	1639	G7M	C5-N7	-4.87	1.33	1.39
3	L5	4220	6MZ	O4'-C4'	4.69	1.55	1.45
3	L5	3818	UY1	C4-N3	4.52	1.47	1.38
83	S2	627	OMU	C4-N3	4.51	1.46	1.38
83	S2	428	OMU	C4-N3	4.47	1.46	1.38
83	S2	116	OMU	C4-N3	4.46	1.46	1.38
83	S2	1442	OMU	C4-N3	4.40	1.46	1.38
83	S2	1326	OMU	C4-N3	4.39	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	1288	OMU	C4-N3	4.38	1.46	1.38
83	S2	172	OMU	C4-N3	4.36	1.46	1.38
83	S2	121	OMU	C4-N3	4.35	1.46	1.38
3	L5	4220	6MZ	C5'-C4'	-4.32	1.38	1.51
83	S2	799	OMU	C4-N3	4.27	1.45	1.38
83	S2	354	OMU	C4-N3	4.25	1.45	1.38
3	L5	4498	OMU	C4-N3	4.18	1.45	1.38
3	L5	2837	OMU	C4-N3	4.15	1.45	1.38
3	L5	4227	OMU	C4-N3	4.12	1.45	1.38
3	L5	3925	OMU	C4-N3	4.05	1.45	1.38
3	L5	4306	OMU	C4-N3	4.01	1.45	1.38
3	L5	4620	OMU	C4-N3	3.95	1.45	1.38
83	S2	1639	G7M	C5-C6	3.90	1.54	1.43
83	S2	1248	B8N	C1'-C5	3.72	1.58	1.50
3	L5	3818	UY1	O4-C4	-3.70	1.16	1.23
83	S2	93	PSU	C6-C5	3.61	1.39	1.35
83	S2	1232	PSU	C6-C5	3.60	1.39	1.35
83	S2	1004	PSU	C6-C5	3.59	1.39	1.35
83	S2	105	PSU	C6-C5	3.59	1.39	1.35
83	S2	651	PSU	C6-C5	3.57	1.39	1.35
83	S2	966	PSU	C6-C5	3.56	1.39	1.35
3	L5	2401	A2M	O5'-C5'	-3.56	1.33	1.44
83	S2	863	PSU	C6-C5	3.55	1.39	1.35
3	L5	3825	A2M	O5'-C5'	-3.55	1.33	1.44
3	L5	4296	PSU	C6-C5	3.55	1.39	1.35
3	L5	1871	A2M	O5'-C5'	-3.55	1.33	1.44
3	L5	5010	PSU	C6-C5	3.54	1.39	1.35
83	S2	668	A2M	O5'-C5'	-3.52	1.33	1.44
85	CF	163	SEP	P-O1P	3.51	1.61	1.50
83	S2	406	PSU	C6-C5	3.51	1.39	1.35
83	S2	1174	PSU	C6-C5	3.51	1.39	1.35
83	S2	1244	PSU	C6-C5	3.51	1.39	1.35
83	S2	1045	PSU	C6-C5	3.50	1.39	1.35
3	L5	4220	6MZ	C5-C4	-3.48	1.32	1.39
3	L5	1860	PSU	C6-C5	3.48	1.39	1.35
83	S2	99	A2M	O5'-C5'	-3.47	1.34	1.44
3	L5	1323	A2M	O5'-C5'	-3.46	1.34	1.44
83	S2	109	PSU	C6-C5	3.45	1.39	1.35
83	S2	801	PSU	C6-C5	3.45	1.39	1.35
83	S2	814	PSU	C6-C5	3.44	1.39	1.35
3	L5	4523	A2M	O5'-C5'	-3.44	1.34	1.44
3	L5	3822	PSU	C6-C5	3.43	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3830	A2M	O5'-C5'	-3.43	1.34	1.44
3	L5	2815	A2M	O5'-C5'	-3.42	1.34	1.44
3	L5	3785	A2M	O5'-C5'	-3.42	1.34	1.44
83	S2	686	PSU	C6-C5	3.41	1.39	1.35
83	S2	468	A2M	O5'-C5'	-3.40	1.34	1.44
3	L5	1524	A2M	O5'-C5'	-3.40	1.34	1.44
3	L5	1326	A2M	O5'-C5'	-3.40	1.34	1.44
83	S2	1056	PSU	C6-C5	3.40	1.39	1.35
83	S2	1367	PSU	C6-C5	3.39	1.39	1.35
83	S2	1031	A2M	O5'-C5'	-3.39	1.34	1.44
3	L5	400	A2M	O5'-C5'	-3.39	1.34	1.44
83	S2	649	PSU	C6-C5	3.39	1.39	1.35
3	L5	2787	A2M	O5'-C5'	-3.39	1.34	1.44
3	L5	1744	PSU	C6-C5	3.38	1.39	1.35
3	L5	4471	PSU	C6-C5	3.38	1.39	1.35
5	L8	69	PSU	C6-C5	3.36	1.39	1.35
3	L5	4500	PSU	C6-C5	3.35	1.39	1.35
3	L5	4571	A2M	O5'-C5'	-3.35	1.34	1.44
3	L5	3844	PSU	C6-C5	3.35	1.39	1.35
3	L5	2632	PSU	C6-C5	3.34	1.39	1.35
3	L5	3851	PSU	C6-C5	3.34	1.39	1.35
3	L5	5001	PSU	C6-C5	3.34	1.39	1.35
3	L5	3718	A2M	O5'-C5'	-3.34	1.34	1.44
3	L5	4590	A2M	O5'-C5'	-3.34	1.34	1.44
83	S2	866	PSU	C6-C5	3.33	1.39	1.35
83	S2	1383	A2M	O5'-C5'	-3.33	1.34	1.44
3	L5	4532	PSU	C6-C5	3.33	1.39	1.35
3	L5	398	A2M	O5'-C5'	-3.32	1.34	1.44
3	L5	4220	6MZ	C5-N7	-3.32	1.33	1.39
83	S2	576	A2M	O5'-C5'	-3.32	1.34	1.44
83	S2	1046	PSU	C6-C5	3.31	1.39	1.35
83	S2	27	A2M	O5'-C5'	-3.31	1.34	1.44
3	L5	1534	A2M	O5'-C5'	-3.31	1.34	1.44
5	L8	55	PSU	C6-C5	3.31	1.39	1.35
3	L5	2363	A2M	O5'-C5'	-3.30	1.34	1.44
3	L5	4972	PSU	C6-C5	3.30	1.38	1.35
3	L5	4673	PSU	C6-C5	3.29	1.38	1.35
3	L5	4293	PSU	C6-C5	3.27	1.38	1.35
3	L5	3637	PSU	C6-C5	3.25	1.38	1.35
3	L5	1782	PSU	C6-C5	3.25	1.38	1.35
3	L5	1862	PSU	C6-C5	3.25	1.38	1.35
3	L5	4576	PSU	C6-C5	3.24	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4312	PSU	C6-C5	3.24	1.38	1.35
3	L5	3818	UY1	C1'-C5	3.24	1.57	1.50
3	L5	3867	A2M	O5'-C5'	-3.24	1.34	1.44
3	L5	4636	PSU	C6-C5	3.23	1.38	1.35
3	L5	1781	PSU	C6-C5	3.23	1.38	1.35
3	L5	3818	UY1	O2-C2	-3.22	1.16	1.23
3	L5	4431	PSU	C6-C5	3.22	1.38	1.35
3	L5	1536	PSU	C6-C5	3.22	1.38	1.35
83	S2	166	A2M	O5'-C5'	-3.20	1.34	1.44
3	L5	4521	PSU	C6-C5	3.20	1.38	1.35
3	L5	4973	PSU	C6-C5	3.20	1.38	1.35
3	L5	4361	PSU	C6-C5	3.18	1.38	1.35
3	L5	3920	PSU	C6-C5	3.18	1.38	1.35
3	L5	4579	PSU	C6-C5	3.18	1.38	1.35
3	L5	1582	PSU	C6-C5	3.18	1.38	1.35
83	S2	1832	6MZ	C5-N7	-3.16	1.33	1.39
3	L5	4353	PSU	C6-C5	3.16	1.38	1.35
83	S2	1081	PSU	C6-C5	3.15	1.38	1.35
83	S2	484	A2M	O5'-C5'	-3.15	1.35	1.44
3	L5	1683	PSU	C6-C5	3.14	1.38	1.35
3	L5	4493	PSU	C6-C5	3.14	1.38	1.35
3	L5	3695	PSU	C6-C5	3.14	1.38	1.35
3	L5	2839	PSU	C6-C5	3.14	1.38	1.35
83	S2	159	A2M	O5'-C5'	-3.09	1.35	1.44
83	S2	1850	MA6	C6-N6	3.08	1.45	1.36
3	L5	4220	6MZ	C2'-C1'	3.06	1.63	1.53
3	L5	3639	PSU	C6-C5	3.05	1.38	1.35
3	L5	3884	PSU	C6-C5	3.04	1.38	1.35
3	L5	4552	PSU	C6-C5	3.03	1.38	1.35
83	S2	681	PSU	C6-C5	3.02	1.38	1.35
3	L5	4442	PSU	C6-C5	3.02	1.38	1.35
83	S2	1851	MA6	C6-N6	3.01	1.45	1.36
83	S2	1832	6MZ	C5-C4	-3.01	1.33	1.39
3	L5	1792	PSU	C6-C5	3.00	1.38	1.35
3	L5	4403	PSU	C6-C5	3.00	1.38	1.35
3	L5	3853	PSU	C6-C5	2.99	1.38	1.35
83	S2	1177	PSU	C6-C5	2.98	1.38	1.35
3	L5	4689	PSU	C6-C5	2.95	1.38	1.35
3	L5	4220	6MZ	C8-N9	-2.94	1.32	1.37
3	L5	4457	PSU	C6-C5	2.93	1.38	1.35
3	L5	4299	PSU	C6-C5	2.90	1.38	1.35
83	S2	668	A2M	O4'-C4'	-2.90	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	627	OMU	C5-C4	2.90	1.50	1.43
83	S2	172	OMU	C5-C4	2.87	1.49	1.43
83	S2	1832	6MZ	C8-N9	-2.87	1.32	1.37
83	S2	1326	OMU	C5-C4	2.85	1.49	1.43
83	S2	1639	G7M	C2-N1	2.83	1.44	1.37
83	S2	799	OMU	C5-C4	2.82	1.49	1.43
83	S2	428	OMU	C5-C4	2.82	1.49	1.43
83	S2	1288	OMU	C5-C4	2.81	1.49	1.43
83	S2	1442	OMU	C5-C4	2.81	1.49	1.43
83	S2	121	OMU	C5-C4	2.79	1.49	1.43
3	L5	4530	UR3	O2-C2	-2.76	1.17	1.22
83	S2	354	OMU	C5-C4	2.74	1.49	1.43
3	L5	4628	PSU	C6-C5	2.74	1.38	1.35
3	L5	4498	OMU	C5-C4	2.71	1.49	1.43
83	S2	627	OMU	C6-N1	2.70	1.44	1.38
3	L5	4220	6MZ	O3'-C3'	2.70	1.49	1.43
3	L5	1677	PSU	C6-C5	2.67	1.38	1.35
3	L5	4227	OMU	C5-C4	2.67	1.49	1.43
83	S2	121	OMU	C6-N1	2.67	1.44	1.38
83	S2	1326	OMU	C6-N1	2.66	1.44	1.38
83	S2	116	OMU	C5-C4	2.65	1.49	1.43
3	L5	1524	A2M	O4'-C4'	-2.64	1.39	1.45
3	L5	2837	OMU	C5-C4	2.64	1.49	1.43
83	S2	1442	OMU	C6-N1	2.63	1.44	1.38
3	L5	3925	OMU	C5-C4	2.63	1.49	1.43
83	S2	1288	OMU	C6-N1	2.62	1.44	1.38
83	S2	354	OMU	C6-N1	2.61	1.44	1.38
83	S2	799	OMU	C6-N1	2.60	1.44	1.38
3	L5	4306	OMU	C5-C4	2.59	1.49	1.43
83	S2	116	OMU	C6-N1	2.58	1.44	1.38
83	S2	172	OMU	C6-N1	2.55	1.44	1.38
3	L5	4498	OMU	C6-N1	2.54	1.44	1.38
83	S2	428	OMU	C6-N1	2.54	1.44	1.38
3	L5	4620	OMU	C5-C4	2.53	1.49	1.43
3	L5	2837	OMU	C6-N1	2.53	1.44	1.38
83	S2	1639	G7M	O6-C6	-2.52	1.18	1.23
83	S2	1850	MA6	C5-C4	-2.51	1.34	1.39
3	L5	4227	OMU	C6-N1	2.50	1.44	1.38
3	L5	4530	UR3	C6-N1	2.48	1.44	1.38
3	L5	4620	OMU	C6-N1	2.47	1.44	1.38
3	L5	4306	OMU	C6-N1	2.45	1.43	1.38
83	S2	1639	G7M	C6-N1	2.43	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1323	A2M	O4'-C4'	-2.42	1.39	1.45
3	L5	3925	OMU	C6-N1	2.41	1.43	1.38
3	L5	4523	A2M	O4'-C4'	-2.40	1.39	1.45
83	S2	1851	MA6	C5-C4	-2.39	1.34	1.39
3	L5	2363	A2M	O4'-C4'	-2.38	1.39	1.45
3	L5	4220	6MZ	C6-N1	-2.34	1.31	1.35
3	L5	3867	A2M	O4'-C4'	-2.34	1.39	1.45
83	S2	1832	6MZ	C6-N1	-2.30	1.31	1.35
3	L5	3884	PSU	C4-C5	-2.24	1.38	1.44
3	L5	400	A2M	O4'-C4'	-2.22	1.40	1.45
3	L5	3639	PSU	C4-C5	-2.20	1.38	1.44
3	L5	1326	A2M	O4'-C4'	-2.19	1.40	1.45
3	L5	4530	UR3	C5-C4	2.18	1.49	1.43
3	L5	1871	A2M	O4'-C4'	-2.15	1.40	1.45
3	L5	4500	PSU	C4-C5	-2.15	1.38	1.44
3	L5	4353	PSU	C4-C5	-2.13	1.38	1.44
3	L5	4293	PSU	C4-C5	-2.13	1.38	1.44
3	L5	4689	PSU	C4-C5	-2.11	1.38	1.44
3	L5	1744	PSU	C4-C5	-2.11	1.38	1.44
3	L5	2815	A2M	O4'-C4'	-2.10	1.40	1.45
3	L5	4403	PSU	C4-C5	-2.10	1.38	1.44
3	L5	1860	PSU	C4-C5	-2.09	1.38	1.44
3	L5	4521	PSU	C4-C5	-2.08	1.38	1.44
3	L5	4571	A2M	O4'-C4'	-2.08	1.40	1.45
83	S2	1177	PSU	C4-C5	-2.07	1.38	1.44
3	L5	4530	UR3	C3U-N3	2.07	1.50	1.47
83	S2	1639	G7M	C4-N9	-2.07	1.32	1.38
3	L5	4447	5MC	C4-N3	-2.06	1.30	1.34
3	L5	3695	PSU	C4-C5	-2.06	1.38	1.44
3	L5	4673	PSU	C4-C5	-2.04	1.38	1.44
3	L5	4973	PSU	C4-C5	-2.04	1.38	1.44
3	L5	4447	5MC	C5-C4	-2.03	1.42	1.44
3	L5	4361	PSU	C4-C5	-2.03	1.38	1.44
3	L5	4579	PSU	C4-C5	-2.02	1.38	1.44
3	L5	1677	PSU	C4-C5	-2.02	1.38	1.44
3	L5	3920	PSU	C4-C5	-2.02	1.38	1.44
3	L5	4636	PSU	C4-C5	-2.02	1.38	1.44
3	L5	4457	PSU	C4-C5	-2.02	1.38	1.44
3	L5	4220	6MZ	C4-N9	-2.01	1.33	1.37
83	S2	651	PSU	C4-C5	-2.00	1.38	1.44
3	L5	1582	PSU	C4-C5	-2.00	1.38	1.44

All (686) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1851	MA6	N1-C6-N6	-11.99	102.25	116.86
83	S2	1850	MA6	N1-C6-N6	-11.70	102.60	116.86
83	S2	1850	MA6	C5-C6-N6	7.87	137.79	125.33
83	S2	1851	MA6	C5-C6-N6	7.86	137.77	125.33
83	S2	1639	G7M	C1'-N9-C4	7.71	149.26	126.49
83	S2	1639	G7M	C1'-N9-C8	-7.57	101.19	126.74
3	L5	3925	OMU	C4-N3-C2	-5.94	119.24	126.61
3	L5	4498	OMU	C4-N3-C2	-5.85	119.35	126.61
3	L5	4220	6MZ	N1-C2-N3	-5.85	119.72	128.58
83	S2	1832	6MZ	N1-C2-N3	-5.78	119.83	128.58
3	L5	4227	OMU	C4-N3-C2	-5.75	119.47	126.61
83	S2	354	OMU	C4-N3-C2	-5.71	119.52	126.61
83	S2	428	OMU	C4-N3-C2	-5.65	119.60	126.61
3	L5	2837	OMU	C4-N3-C2	-5.65	119.60	126.61
83	S2	1850	MA6	N1-C2-N3	-5.64	120.04	128.58
83	S2	627	OMU	C4-N3-C2	-5.64	119.61	126.61
83	S2	799	OMU	C4-N3-C2	-5.62	119.64	126.61
3	L5	4306	OMU	C4-N3-C2	-5.60	119.67	126.61
3	L5	4530	UR3	C4-N3-C2	-5.59	120.08	124.58
83	S2	1851	MA6	N1-C2-N3	-5.58	120.14	128.58
83	S2	1326	OMU	C4-N3-C2	-5.55	119.72	126.61
83	S2	121	OMU	C4-N3-C2	-5.50	119.78	126.61
3	L5	3637	PSU	N1-C2-N3	5.49	120.96	115.17
83	S2	1288	OMU	C4-N3-C2	-5.45	119.85	126.61
83	S2	172	OMU	C4-N3-C2	-5.43	119.86	126.61
83	S2	1442	OMU	C4-N3-C2	-5.43	119.88	126.61
3	L5	4353	PSU	N1-C2-N3	5.29	120.74	115.17
83	S2	1851	MA6	N9-C8-N7	-5.28	106.44	113.94
3	L5	4689	PSU	N1-C2-N3	5.28	120.74	115.17
3	L5	4636	PSU	C4-N3-C2	-5.26	119.13	126.37
3	L5	1536	PSU	N1-C2-N3	5.25	120.71	115.17
83	S2	1850	MA6	N9-C8-N7	-5.24	106.51	113.94
83	S2	1248	B8N	C5-C4-N3	5.22	125.63	116.15
3	L5	4220	6MZ	C9-N6-C6	-5.21	118.02	122.85
83	S2	649	PSU	C4-N3-C2	-5.21	119.20	126.37
3	L5	1677	PSU	C4-N3-C2	-5.17	119.25	126.37
3	L5	3701	OMC	C1'-N1-C2	5.15	129.83	118.44
83	S2	1004	PSU	N1-C2-N3	5.13	120.58	115.17
83	S2	116	OMU	C4-N3-C2	-5.12	120.25	126.61
3	L5	4403	PSU	C4-N3-C2	-5.12	119.32	126.37
3	L5	4521	PSU	C4-N3-C2	-5.10	119.34	126.37
3	L5	3637	PSU	C4-N3-C2	-5.09	119.36	126.37
3	L5	4293	PSU	C4-N3-C2	-5.09	119.36	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4312	PSU	N1-C2-N3	5.06	120.51	115.17
3	L5	3639	PSU	N1-C2-N3	5.06	120.51	115.17
3	L5	4620	OMU	C4-N3-C2	-5.05	120.35	126.61
3	L5	1860	PSU	C4-N3-C2	-5.04	119.43	126.37
3	L5	4353	PSU	C4-N3-C2	-5.03	119.44	126.37
3	L5	1860	PSU	N1-C2-N3	5.03	120.47	115.17
3	L5	1582	PSU	N1-C2-N3	5.02	120.47	115.17
3	L5	4403	PSU	N1-C2-N3	5.02	120.46	115.17
83	S2	1081	PSU	C4-N3-C2	-5.01	119.47	126.37
83	S2	681	PSU	N1-C2-N3	5.01	120.45	115.17
3	L5	4457	PSU	C4-N3-C2	-5.01	119.47	126.37
3	L5	4973	PSU	C4-N3-C2	-4.99	119.49	126.37
3	L5	1862	PSU	N1-C2-N3	4.98	120.43	115.17
83	S2	109	PSU	C4-N3-C2	-4.97	119.52	126.37
83	S2	1367	PSU	N1-C2-N3	4.97	120.41	115.17
83	S2	1046	PSU	N1-C2-N3	4.97	120.41	115.17
3	L5	4471	PSU	N1-C2-N3	4.97	120.41	115.17
83	S2	109	PSU	N1-C2-N3	4.96	120.40	115.17
3	L5	1536	PSU	C4-N3-C2	-4.96	119.55	126.37
3	L5	4442	PSU	C4-N3-C2	-4.95	119.55	126.37
83	S2	863	PSU	C4-N3-C2	-4.95	119.55	126.37
83	S2	681	PSU	C4-N3-C2	-4.95	119.55	126.37
3	L5	4293	PSU	N1-C2-N3	4.95	120.39	115.17
3	L5	4521	PSU	N1-C2-N3	4.95	120.39	115.17
3	L5	4296	PSU	N1-C2-N3	4.94	120.38	115.17
83	S2	649	PSU	N1-C2-N3	4.94	120.38	115.17
3	L5	5010	PSU	N1-C2-N3	4.94	120.38	115.17
3	L5	1782	PSU	N1-C2-N3	4.94	120.38	115.17
83	S2	866	PSU	C4-N3-C2	-4.94	119.56	126.37
3	L5	4628	PSU	N1-C2-N3	4.94	120.38	115.17
3	L5	4361	PSU	N1-C2-N3	4.94	120.38	115.17
83	S2	651	PSU	N1-C2-N3	4.93	120.37	115.17
3	L5	4442	PSU	N1-C2-N3	4.93	120.37	115.17
3	L5	1782	PSU	C4-N3-C2	-4.93	119.58	126.37
3	L5	2632	PSU	N1-C2-N3	4.93	120.37	115.17
3	L5	3920	PSU	N1-C2-N3	4.93	120.36	115.17
3	L5	4579	PSU	N1-C2-N3	4.93	120.36	115.17
3	L5	1582	PSU	C4-N3-C2	-4.93	119.59	126.37
83	S2	801	PSU	C4-N3-C2	-4.93	119.59	126.37
3	L5	2839	PSU	N1-C2-N3	4.92	120.36	115.17
3	L5	4552	PSU	N1-C2-N3	4.92	120.36	115.17
83	S2	105	PSU	N1-C2-N3	4.92	120.36	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	406	PSU	N1-C2-N3	4.92	120.36	115.17
3	L5	1683	PSU	C4-N3-C2	-4.92	119.60	126.37
3	L5	4552	PSU	C4-N3-C2	-4.92	119.60	126.37
83	S2	406	PSU	C4-N3-C2	-4.91	119.60	126.37
83	S2	1232	PSU	N1-C2-N3	4.91	120.35	115.17
3	L5	2839	PSU	C4-N3-C2	-4.91	119.61	126.37
3	L5	3822	PSU	N1-C2-N3	4.91	120.34	115.17
3	L5	4636	PSU	N1-C2-N3	4.91	120.34	115.17
3	L5	4973	PSU	N1-C2-N3	4.91	120.34	115.17
3	L5	3920	PSU	C4-N3-C2	-4.90	119.62	126.37
3	L5	4628	PSU	C4-N3-C2	-4.90	119.62	126.37
3	L5	3884	PSU	N1-C2-N3	4.90	120.33	115.17
83	S2	1367	PSU	C4-N3-C2	-4.90	119.63	126.37
3	L5	4431	PSU	N1-C2-N3	4.90	120.33	115.17
83	S2	801	PSU	N1-C2-N3	4.89	120.33	115.17
3	L5	3822	PSU	C4-N3-C2	-4.88	119.64	126.37
3	L5	3695	PSU	C4-N3-C2	-4.88	119.65	126.37
83	S2	686	PSU	N1-C2-N3	4.88	120.31	115.17
3	L5	5010	PSU	C4-N3-C2	-4.88	119.65	126.37
83	S2	1177	PSU	C4-N3-C2	-4.87	119.66	126.37
3	L5	2632	PSU	C4-N3-C2	-4.87	119.66	126.37
3	L5	4500	PSU	C4-N3-C2	-4.87	119.66	126.37
3	L5	1744	PSU	C4-N3-C2	-4.87	119.66	126.37
3	L5	4431	PSU	C4-N3-C2	-4.87	119.67	126.37
83	S2	1174	PSU	N1-C2-N3	4.87	120.30	115.17
3	L5	4361	PSU	C4-N3-C2	-4.86	119.67	126.37
3	L5	1792	PSU	N1-C2-N3	4.86	120.30	115.17
3	L5	4500	PSU	N1-C2-N3	4.86	120.30	115.17
3	L5	4296	PSU	C4-N3-C2	-4.86	119.67	126.37
3	L5	4972	PSU	N1-C2-N3	4.86	120.30	115.17
83	S2	1081	PSU	N1-C2-N3	4.86	120.29	115.17
3	L5	4493	PSU	C4-N3-C2	-4.86	119.68	126.37
3	L5	3884	PSU	C4-N3-C2	-4.86	119.68	126.37
83	S2	1056	PSU	C4-N3-C2	-4.85	119.69	126.37
83	S2	1244	PSU	C4-N3-C2	-4.84	119.70	126.37
3	L5	1862	PSU	C4-N3-C2	-4.84	119.70	126.37
3	L5	3695	PSU	N1-C2-N3	4.84	120.28	115.17
83	S2	1046	PSU	C4-N3-C2	-4.84	119.71	126.37
3	L5	3851	PSU	N1-C2-N3	4.84	120.27	115.17
3	L5	4312	PSU	C4-N3-C2	-4.83	119.72	126.37
3	L5	3818	UY1	C4-N3-C2	-4.83	119.72	126.37
83	S2	863	PSU	N1-C2-N3	4.83	120.26	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L8	69	PSU	N1-C2-N3	4.83	120.26	115.17
3	L5	1744	PSU	N1-C2-N3	4.83	120.26	115.17
3	L5	4457	PSU	N1-C2-N3	4.83	120.26	115.17
3	L5	3853	PSU	N1-C2-N3	4.82	120.25	115.17
3	L5	1792	PSU	C4-N3-C2	-4.82	119.73	126.37
3	L5	4532	PSU	C4-N3-C2	-4.81	119.74	126.37
3	L5	3639	PSU	C4-N3-C2	-4.81	119.75	126.37
83	S2	1174	PSU	C4-N3-C2	-4.81	119.75	126.37
83	S2	1244	PSU	N1-C2-N3	4.80	120.23	115.17
3	L5	1683	PSU	N1-C2-N3	4.80	120.23	115.17
3	L5	5001	PSU	N1-C2-N3	4.80	120.23	115.17
83	S2	686	PSU	C4-N3-C2	-4.80	119.76	126.37
3	L5	1781	PSU	N1-C2-N3	4.80	120.23	115.17
83	S2	966	PSU	N1-C2-N3	4.79	120.22	115.17
5	L8	69	PSU	C4-N3-C2	-4.79	119.77	126.37
3	L5	4471	PSU	C4-N3-C2	-4.79	119.77	126.37
3	L5	5001	PSU	C4-N3-C2	-4.78	119.79	126.37
83	S2	1232	PSU	C4-N3-C2	-4.77	119.79	126.37
3	L5	4299	PSU	C4-N3-C2	-4.77	119.80	126.37
83	S2	1004	PSU	C4-N3-C2	-4.77	119.80	126.37
3	L5	4689	PSU	C4-N3-C2	-4.77	119.80	126.37
3	L5	4532	PSU	N1-C2-N3	4.76	120.19	115.17
83	S2	1045	PSU	N1-C2-N3	4.76	120.19	115.17
83	S2	866	PSU	N1-C2-N3	4.76	120.19	115.17
3	L5	3851	PSU	C4-N3-C2	-4.76	119.82	126.37
3	L5	4576	PSU	C4-N3-C2	-4.76	119.82	126.37
83	S2	651	PSU	C4-N3-C2	-4.76	119.82	126.37
83	S2	966	PSU	C4-N3-C2	-4.74	119.84	126.37
3	L5	3853	PSU	C4-N3-C2	-4.73	119.85	126.37
3	L5	4493	PSU	N1-C2-N3	4.73	120.16	115.17
3	L5	1677	PSU	N1-C2-N3	4.73	120.15	115.17
3	L5	4972	PSU	C4-N3-C2	-4.73	119.86	126.37
3	L5	4673	PSU	C4-N3-C2	-4.72	119.88	126.37
83	S2	1832	6MZ	C5-C4-N3	-4.71	120.24	126.72
83	S2	105	PSU	C4-N3-C2	-4.71	119.89	126.37
3	L5	4673	PSU	N1-C2-N3	4.71	120.13	115.17
3	L5	1781	PSU	C4-N3-C2	-4.70	119.89	126.37
83	S2	1832	6MZ	N9-C8-N7	-4.69	107.28	113.94
83	S2	1248	B8N	C4-N3-C2	-4.69	119.84	125.62
3	L5	4220	6MZ	N9-C8-N7	-4.69	107.28	113.94
3	L5	3844	PSU	N1-C2-N3	4.69	120.12	115.17
5	L8	55	PSU	N1-C2-N3	4.69	120.11	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1177	PSU	N1-C2-N3	4.66	120.08	115.17
3	L5	4576	PSU	N1-C2-N3	4.65	120.07	115.17
83	S2	1056	PSU	N1-C2-N3	4.65	120.07	115.17
83	S2	1045	PSU	C4-N3-C2	-4.63	119.99	126.37
3	L5	4579	PSU	C4-N3-C2	-4.63	119.99	126.37
5	L8	55	PSU	C4-N3-C2	-4.62	120.01	126.37
83	S2	1851	MA6	C5-C4-N3	-4.61	120.38	126.72
83	S2	814	PSU	N1-C2-N3	4.60	120.02	115.17
3	L5	4299	PSU	N1-C2-N3	4.56	119.98	115.17
83	S2	814	PSU	C4-N3-C2	-4.55	120.11	126.37
83	S2	1639	G7M	C2-N3-C4	4.53	120.10	112.30
3	L5	3844	PSU	C4-N3-C2	-4.52	120.14	126.37
83	S2	93	PSU	N1-C2-N3	4.50	119.91	115.17
3	L5	4220	6MZ	C5-C4-N3	-4.46	120.57	126.72
83	S2	1850	MA6	C5-C4-N3	-4.43	120.61	126.72
83	S2	93	PSU	C4-N3-C2	-4.43	120.27	126.37
3	L5	1871	A2M	C3'-C2'-C1'	-4.33	94.52	102.81
3	L5	3818	UY1	N1-C2-N3	4.14	119.53	115.17
83	S2	1851	MA6	C4-N9-C8	4.12	110.06	105.74
83	S2	1639	G7M	C5-C4-N3	-4.08	120.43	128.15
83	S2	1850	MA6	C4-N9-C8	4.08	110.02	105.74
83	S2	354	OMU	N3-C2-N1	4.05	120.16	114.89
3	L5	4498	OMU	N3-C2-N1	4.04	120.15	114.89
83	S2	1383	A2M	C3'-C2'-C1'	-4.04	95.07	102.81
83	S2	121	OMU	N3-C2-N1	4.00	120.10	114.89
3	L5	3925	OMU	N3-C2-N1	3.99	120.08	114.89
3	L5	2837	OMU	N3-C2-N1	3.96	120.05	114.89
83	S2	1639	G7M	C5-C6-N1	3.96	120.02	111.84
3	L5	3701	OMC	C1'-N1-C6	-3.95	112.33	120.78
3	L5	4306	OMU	N3-C2-N1	3.94	120.03	114.89
83	S2	428	OMU	N3-C2-N1	3.94	120.02	114.89
83	S2	799	OMU	N3-C2-N1	3.92	120.00	114.89
3	L5	4227	OMU	N3-C2-N1	3.91	119.98	114.89
3	L5	3925	OMU	C5-C4-N3	3.87	120.22	114.80
3	L5	3830	A2M	C3'-C2'-C1'	-3.86	95.41	102.81
3	L5	398	A2M	C3'-C2'-C1'	-3.86	95.42	102.81
83	S2	172	OMU	N3-C2-N1	3.85	119.90	114.89
83	S2	1326	OMU	N3-C2-N1	3.83	119.87	114.89
3	L5	4620	OMU	N3-C2-N1	3.81	119.85	114.89
3	L5	4498	OMU	C5-C4-N3	3.80	120.12	114.80
3	L5	2351	OMC	C1'-N1-C2	3.79	126.82	118.44
83	S2	627	OMU	C5-C4-N3	3.76	120.07	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1442	OMU	N3-C2-N1	3.76	119.78	114.89
83	S2	1288	OMU	N3-C2-N1	3.76	119.78	114.89
83	S2	1248	B8N	C1'-C5-C4	3.73	123.27	117.61
3	L5	4227	OMU	C5-C4-N3	3.73	120.02	114.80
3	L5	4523	A2M	C3'-C2'-C1'	-3.70	95.72	102.81
3	L5	2837	OMU	C5-C4-N3	3.70	119.98	114.80
83	S2	116	OMU	N3-C2-N1	3.68	119.68	114.89
83	S2	1031	A2M	C3'-C2'-C1'	-3.68	95.76	102.81
83	S2	1850	MA6	C4-C5-C6	3.67	119.70	115.91
3	L5	1534	A2M	C3'-C2'-C1'	-3.64	95.84	102.81
3	L5	4530	UR3	C5-C4-N3	3.63	119.81	115.04
3	L5	4306	OMU	C5-C4-N3	3.62	119.86	114.80
83	S2	354	OMU	C5-C4-N3	3.61	119.86	114.80
83	S2	1383	A2M	O3'-C3'-C2'	3.59	121.22	111.19
83	S2	1850	MA6	C2-N1-C6	3.58	120.57	111.83
83	S2	1851	MA6	C4-C5-C6	3.57	119.60	115.91
83	S2	627	OMU	N3-C2-N1	3.57	119.54	114.89
3	L5	4590	A2M	C3'-C2'-C1'	-3.56	96.00	102.81
83	S2	1248	B8N	N3-C2-N1	3.55	121.06	116.72
83	S2	799	OMU	C5-C4-N3	3.54	119.77	114.80
3	L5	1536	PSU	O2-C2-N1	-3.53	119.15	122.79
83	S2	468	A2M	C3'-C2'-C1'	-3.51	96.09	102.81
83	S2	576	A2M	C3'-C2'-C1'	-3.50	96.10	102.81
83	S2	1326	OMU	C5-C4-N3	3.50	119.71	114.80
83	S2	1288	OMU	C5-C4-N3	3.50	119.70	114.80
83	S2	428	OMU	C5-C4-N3	3.49	119.69	114.80
83	S2	1442	OMU	C5-C4-N3	3.49	119.69	114.80
83	S2	121	OMU	C5-C4-N3	3.47	119.66	114.80
83	S2	166	A2M	O3'-C3'-C2'	3.46	120.86	111.19
3	L5	4689	PSU	C6-N1-C2	-3.46	119.48	122.69
83	S2	1851	MA6	C2-N1-C6	3.46	120.28	111.83
3	L5	2401	A2M	C3'-C2'-C1'	-3.44	96.21	102.81
3	L5	398	A2M	O3'-C3'-C2'	3.44	120.80	111.19
3	L5	4571	A2M	C3'-C2'-C1'	-3.42	96.26	102.81
83	S2	1851	MA6	N3-C4-N9	3.42	132.98	127.17
3	L5	4220	6MZ	C2-N3-C4	3.41	120.16	111.83
83	S2	1832	6MZ	C2-N3-C4	3.40	120.14	111.83
3	L5	2401	A2M	O3'-C3'-C2'	3.40	120.70	111.19
83	S2	172	OMU	C5-C4-N3	3.40	119.56	114.80
3	L5	4689	PSU	O2-C2-N1	-3.39	119.29	122.79
3	L5	3718	A2M	C3'-C2'-C1'	-3.39	96.32	102.81
83	S2	576	A2M	O3'-C3'-C2'	3.38	120.65	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4571	A2M	O3'-C3'-C2'	3.36	120.59	111.19
3	L5	4620	OMU	C5-C4-N3	3.35	119.49	114.80
83	S2	116	OMU	C5-C4-N3	3.35	119.49	114.80
3	L5	1683	PSU	O2-C2-N1	-3.34	119.34	122.79
83	S2	99	A2M	O3'-C3'-C2'	3.33	120.50	111.19
83	S2	99	A2M	C3'-C2'-C1'	-3.32	96.45	102.81
83	S2	468	A2M	O3'-C3'-C2'	3.31	120.46	111.19
83	S2	1850	MA6	N3-C4-N9	3.30	132.77	127.17
83	S2	1639	G7M	O6-C6-C5	-3.29	120.67	128.01
3	L5	1323	A2M	O3'-C3'-C2'	3.29	120.38	111.19
3	L5	4353	PSU	O2-C2-N1	-3.28	119.41	122.79
83	S2	1832	6MZ	N3-C4-N9	3.27	132.73	127.17
3	L5	2815	A2M	C2'-C1'-N9	3.26	119.12	113.75
3	L5	1323	A2M	C2'-C1'-N9	3.25	119.11	113.75
83	S2	1639	G7M	N9-C4-N3	3.24	132.44	125.95
3	L5	4628	PSU	O2-C2-N1	-3.24	119.45	122.79
3	L5	2787	A2M	O3'-C3'-C2'	3.24	120.25	111.19
83	S2	1832	6MZ	C4-N9-C8	3.22	109.12	105.74
3	L5	1524	A2M	O3'-C3'-C2'	3.22	120.19	111.19
83	S2	1031	A2M	O3'-C3'-C2'	3.21	120.17	111.19
3	L5	4220	6MZ	C4-N9-C8	3.19	109.09	105.74
83	S2	1851	MA6	C2-N3-C4	3.19	119.62	111.83
85	CF	163	SEP	OG-CB-CA	3.18	111.24	108.14
83	S2	1004	PSU	C6-N1-C2	-3.17	119.75	122.69
3	L5	3830	A2M	O3'-C3'-C2'	3.13	119.95	111.19
3	L5	2815	A2M	O3'-C3'-C2'	3.13	119.94	111.19
83	S2	27	A2M	O3'-C3'-C2'	3.13	119.94	111.19
83	S2	1850	MA6	C2-N3-C4	3.12	119.46	111.83
3	L5	3718	A2M	O3'-C3'-C2'	3.12	119.92	111.19
83	S2	651	PSU	O2-C2-N1	-3.12	119.57	122.79
3	L5	3825	A2M	O3'-C3'-C2'	3.12	119.92	111.19
83	S2	1004	PSU	O2-C2-N1	-3.11	119.58	122.79
3	L5	3884	PSU	O2-C2-N1	-3.11	119.58	122.79
83	S2	1850	MA6	C5-N7-C8	3.11	108.33	103.45
83	S2	1046	PSU	O2-C2-N1	-3.10	119.59	122.79
83	S2	1639	G7M	CN7-N7-C5	3.09	130.65	126.80
3	L5	1871	A2M	C4-N9-C1'	-3.09	119.41	126.63
3	L5	3825	A2M	C3'-C2'-C1'	-3.09	96.90	102.81
83	S2	1851	MA6	C5-N7-C8	3.09	108.30	103.45
83	S2	1174	PSU	O2-C2-N1	-3.09	119.61	122.79
83	S2	1383	A2M	C4-N9-C1'	-3.09	119.42	126.63
3	L5	4523	A2M	O3'-C3'-C2'	3.08	119.82	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	627	OMU	O4-C4-C5	-3.08	119.86	125.16
83	S2	428	OMU	O4-C4-C5	-3.07	119.86	125.16
3	L5	1792	PSU	O2-C2-N1	-3.07	119.62	122.79
83	S2	668	A2M	C4-N9-C1'	-3.06	119.48	126.63
83	S2	1442	OMU	O4-C4-C5	-3.05	119.90	125.16
3	L5	400	A2M	O3'-C3'-C2'	3.04	119.70	111.19
83	S2	116	OMU	O4-C4-C5	-3.03	119.93	125.16
3	L5	4220	6MZ	N3-C4-N9	3.03	132.33	127.17
3	L5	1536	PSU	C6-N1-C2	-3.02	119.88	122.69
83	S2	1832	6MZ	C5-N7-C8	3.02	108.19	103.45
3	L5	4523	A2M	C4-N9-C1'	-3.02	119.57	126.63
3	L5	2401	A2M	C4-N9-C1'	-3.02	119.57	126.63
3	L5	3853	PSU	O2-C2-N1	-3.01	119.68	122.79
3	L5	5001	PSU	O2-C2-N1	-3.01	119.69	122.79
3	L5	4498	OMU	O4-C4-C5	-3.00	119.98	125.16
83	S2	1639	G7M	C2-N1-C6	-3.00	119.67	125.11
3	L5	3695	PSU	O2-C2-N1	-3.00	119.70	122.79
3	L5	4500	PSU	O2-C2-N1	-3.00	119.70	122.79
3	L5	4227	OMU	O4-C4-C5	-3.00	119.99	125.16
83	S2	121	OMU	O4-C4-C5	-3.00	120.00	125.16
3	L5	3639	PSU	C6-N1-C2	-2.99	119.91	122.69
3	L5	4552	PSU	O2-C2-N1	-2.99	119.70	122.79
83	S2	159	A2M	O3'-C3'-C2'	2.99	119.55	111.19
83	S2	1031	A2M	C4-N9-C1'	-2.99	119.65	126.63
5	L8	69	PSU	O2-C2-N1	-2.98	119.72	122.79
3	L5	4579	PSU	C6-N1-C2	-2.98	119.93	122.69
3	L5	3844	PSU	O2-C2-N1	-2.98	119.72	122.79
83	S2	27	A2M	C3'-C2'-C1'	-2.97	97.11	102.81
3	L5	4579	PSU	O2-C2-N1	-2.97	119.72	122.79
83	S2	1326	OMU	O4-C4-C5	-2.97	120.04	125.16
3	L5	400	A2M	C3'-C2'-C1'	-2.97	97.12	102.81
83	S2	99	A2M	C4-N9-C1'	-2.97	119.69	126.63
3	L5	3830	A2M	C4-N9-C1'	-2.96	119.71	126.63
83	S2	468	A2M	C4-N9-C1'	-2.96	119.72	126.63
83	S2	799	OMU	O4-C4-C5	-2.94	120.08	125.16
3	L5	4403	PSU	O2-C2-N1	-2.94	119.75	122.79
3	L5	4636	PSU	O2-C2-N1	-2.93	119.76	122.79
3	L5	3785	A2M	O3'-C3'-C2'	2.93	119.40	111.19
3	L5	4312	PSU	O2-C2-N1	-2.93	119.77	122.79
3	L5	3701	OMC	O2-C2-N3	-2.93	117.71	122.33
3	L5	4312	PSU	C6-N1-C2	-2.93	119.97	122.69
3	L5	3818	UY1	C6-N1-C2	-2.93	119.97	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1871	A2M	O3'-C3'-C2'	2.93	119.38	111.19
3	L5	2839	PSU	O2-C2-N1	-2.93	119.77	122.79
83	S2	1832	6MZ	C4-C5-C6	2.92	119.21	116.78
3	L5	2837	OMU	O4-C4-C5	-2.92	120.12	125.16
83	S2	1288	OMU	O4-C4-C5	-2.92	120.12	125.16
83	S2	406	PSU	O2-C2-N1	-2.92	119.77	122.79
83	S2	1244	PSU	O2-C2-N1	-2.92	119.78	122.79
3	L5	4590	A2M	C4-N9-C1'	-2.92	119.81	126.63
3	L5	4431	PSU	O2-C2-N1	-2.91	119.78	122.79
3	L5	1782	PSU	O2-C2-N1	-2.91	119.79	122.79
3	L5	1860	PSU	O2-C2-N1	-2.90	119.80	122.79
3	L5	3785	A2M	C4'-O4'-C1'	-2.90	103.07	109.47
3	L5	398	A2M	C4-N9-C1'	-2.90	119.86	126.63
3	L5	2351	OMC	C1'-N1-C6	-2.89	114.60	120.78
83	S2	1177	PSU	O2-C2-N1	-2.89	119.81	122.79
3	L5	5010	PSU	O2-C2-N1	-2.89	119.81	122.79
3	L5	2632	PSU	O2-C2-N1	-2.88	119.82	122.79
3	L5	4442	PSU	O2-C2-N1	-2.88	119.82	122.79
3	L5	3639	PSU	O2-C2-N1	-2.88	119.82	122.79
83	S2	1232	PSU	O2-C2-N1	-2.88	119.82	122.79
3	L5	3925	OMU	O4-C4-C5	-2.87	120.20	125.16
3	L5	4576	PSU	O2-C2-N1	-2.87	119.83	122.79
83	S2	814	PSU	O2-C2-N1	-2.87	119.83	122.79
3	L5	3785	A2M	C4-N9-C1'	-2.87	119.93	126.63
83	S2	166	A2M	C3'-C2'-C1'	-2.86	97.32	102.81
3	L5	3884	PSU	C6-N1-C2	-2.86	120.04	122.69
83	S2	484	A2M	C4-N9-C1'	-2.85	119.96	126.63
3	L5	3637	PSU	C6-N1-C2	-2.85	120.05	122.69
3	L5	3844	PSU	C6-N1-C2	-2.85	120.05	122.69
3	L5	4972	PSU	O2-C2-N1	-2.85	119.85	122.79
83	S2	354	OMU	O4-C4-C5	-2.85	120.25	125.16
3	L5	4620	OMU	O4-C4-C5	-2.85	120.25	125.16
3	L5	4471	PSU	O2-C2-N1	-2.85	119.85	122.79
83	S2	1383	A2M	C1'-N9-C8	2.84	133.40	127.09
3	L5	4353	PSU	C6-N1-C2	-2.84	120.06	122.69
3	L5	3920	PSU	O2-C2-N1	-2.84	119.86	122.79
83	S2	681	PSU	O2-C2-N1	-2.84	119.86	122.79
3	L5	4590	A2M	O3'-C3'-C2'	2.84	119.12	111.19
83	S2	484	A2M	O3'-C3'-C2'	2.84	119.12	111.19
83	S2	651	PSU	C6-N1-C2	-2.84	120.06	122.69
3	L5	1871	A2M	C1'-N9-C8	2.83	133.38	127.09
3	L5	4532	PSU	O2-C2-N1	-2.83	119.87	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1367	PSU	O2-C2-N1	-2.83	119.87	122.79
3	L5	3818	UY1	C6-C5-C4	2.82	120.08	118.17
3	L5	3851	PSU	O2-C2-N1	-2.82	119.88	122.79
3	L5	4361	PSU	O2-C2-N1	-2.82	119.88	122.79
83	S2	966	PSU	O2-C2-N1	-2.82	119.88	122.79
83	S2	27	A2M	C4-N9-C1'	-2.81	120.05	126.63
3	L5	4306	OMU	O4-C4-C5	-2.81	120.32	125.16
3	L5	1744	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L5	2839	PSU	C6-N1-C2	-2.81	120.08	122.69
83	S2	159	A2M	C4-N9-C1'	-2.81	120.07	126.63
83	S2	668	A2M	C1'-N9-C8	2.80	133.31	127.09
83	S2	99	A2M	C1'-N9-C8	2.80	133.31	127.09
3	L5	3867	A2M	C4-N9-C1'	-2.79	120.11	126.63
3	L5	4973	PSU	O2-C2-N1	-2.79	119.91	122.79
3	L5	3830	A2M	C1'-N9-C8	2.79	133.28	127.09
3	L5	1326	A2M	C4-N9-C1'	-2.78	120.12	126.63
3	L5	4220	6MZ	C5-N7-C8	2.78	107.82	103.45
3	L5	4521	PSU	O2-C2-N1	-2.78	119.92	122.79
3	L5	3825	A2M	C4-N9-C1'	-2.78	120.13	126.63
3	L5	4296	PSU	O2-C2-N1	-2.78	119.92	122.79
3	L5	2401	A2M	C1'-N9-C8	2.77	133.24	127.09
83	S2	1232	PSU	C6-N1-C2	-2.77	120.12	122.69
3	L5	4457	PSU	O2-C2-N1	-2.77	119.94	122.79
3	L5	1582	PSU	O2-C2-N1	-2.76	119.94	122.79
3	L5	398	A2M	C1'-N9-C8	2.76	133.22	127.09
83	S2	1045	PSU	O2-C2-N1	-2.76	119.94	122.79
83	S2	1248	B8N	O4-C4-N3	-2.76	115.51	119.99
83	S2	1031	A2M	C1'-N9-C8	2.75	133.21	127.09
3	L5	4673	PSU	O2-C2-N1	-2.75	119.95	122.79
83	S2	109	PSU	O2-C2-N1	-2.75	119.95	122.79
3	L5	1524	A2M	C4'-O4'-C1'	-2.74	103.41	109.47
3	L5	2363	A2M	C4-N9-C1'	-2.74	120.22	126.63
3	L5	4500	PSU	C6-N1-C2	-2.74	120.15	122.69
3	L5	4471	PSU	C6-N1-C2	-2.73	120.16	122.69
83	S2	668	A2M	O4'-C1'-C2'	2.73	111.29	106.59
83	S2	484	A2M	C1'-N9-C8	2.73	133.15	127.09
83	S2	686	PSU	O2-C2-N1	-2.73	119.98	122.79
3	L5	1862	PSU	C6-N1-C2	-2.73	120.16	122.69
3	L5	400	A2M	C4-N9-C1'	-2.73	120.26	126.63
3	L5	4293	PSU	O2-C2-N1	-2.72	119.98	122.79
3	L5	1326	A2M	O3'-C3'-C2'	2.72	118.80	111.19
3	L5	4590	A2M	C1'-N9-C8	2.72	133.12	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4571	A2M	C4-N9-C1'	-2.71	120.29	126.63
3	L5	3867	A2M	C1'-N9-C8	2.71	133.11	127.09
3	L5	4523	A2M	C1'-N9-C8	2.71	133.10	127.09
83	S2	468	A2M	C1'-N9-C8	2.70	133.09	127.09
3	L5	4220	6MZ	C5-C6-N1	2.70	121.05	118.15
3	L5	1781	PSU	O2-C2-N1	-2.70	120.00	122.79
3	L5	3701	OMC	O2-C2-N1	2.70	124.19	118.90
3	L5	1323	A2M	C3'-C2'-C1'	-2.70	97.64	102.81
3	L5	4972	PSU	C6-N1-C2	-2.70	120.19	122.69
83	S2	866	PSU	O2-C2-N1	-2.69	120.01	122.79
3	L5	1677	PSU	O2-C2-N1	-2.69	120.02	122.79
83	S2	1174	PSU	C6-N1-C2	-2.69	120.20	122.69
3	L5	3822	PSU	O2-C2-N1	-2.68	120.03	122.79
83	S2	801	PSU	O2-C2-N1	-2.67	120.03	122.79
3	L5	1860	PSU	C6-N1-C2	-2.67	120.21	122.69
83	S2	172	OMU	O4-C4-C5	-2.67	120.56	125.16
3	L5	4673	PSU	C6-N1-C2	-2.66	120.22	122.69
3	L5	2363	A2M	C1'-N9-C8	2.65	132.98	127.09
83	S2	1046	PSU	C6-N1-C2	-2.65	120.23	122.69
83	S2	105	PSU	O2-C2-N1	-2.65	120.06	122.79
3	L5	4361	PSU	C6-N1-C2	-2.65	120.24	122.69
3	L5	3825	A2M	C1'-N9-C8	2.65	132.97	127.09
83	S2	576	A2M	C4-N9-C1'	-2.64	120.45	126.63
3	L5	4628	PSU	C6-N1-C2	-2.64	120.24	122.69
3	L5	1862	PSU	O2-C2-N1	-2.64	120.06	122.79
83	S2	686	PSU	C6-N1-C2	-2.64	120.24	122.69
83	S2	814	PSU	C6-N1-C2	-2.64	120.24	122.69
3	L5	3867	A2M	C2'-C1'-N9	2.63	118.08	113.75
3	L5	3818	UY1	O2-C2-N1	-2.62	120.08	122.79
3	L5	4296	PSU	C6-N1-C2	-2.62	120.26	122.69
83	S2	1056	PSU	O2-C2-N1	-2.62	120.09	122.79
3	L5	1792	PSU	C6-N1-C2	-2.62	120.26	122.69
3	L5	400	A2M	C1'-N9-C8	2.61	132.90	127.09
3	L5	1326	A2M	C1'-N9-C8	2.61	132.90	127.09
3	L5	5001	PSU	C6-N1-C2	-2.61	120.27	122.69
83	S2	27	A2M	C1'-N9-C8	2.61	132.89	127.09
3	L5	1524	A2M	O4'-C1'-C2'	2.60	111.07	106.59
83	S2	159	A2M	C1'-N9-C8	2.60	132.87	127.09
3	L5	1582	PSU	C6-N1-C2	-2.60	120.28	122.69
3	L5	2632	PSU	C6-N1-C2	-2.60	120.28	122.69
3	L5	3920	PSU	C6-N1-C2	-2.60	120.28	122.69
83	S2	681	PSU	C6-N1-C2	-2.59	120.28	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4353	PSU	C6-C5-C4	2.59	119.92	118.17
83	S2	105	PSU	C6-N1-C2	-2.59	120.29	122.69
83	S2	1639	G7M	CN7-N7-C8	-2.58	120.88	124.79
3	L5	2787	A2M	O4'-C1'-C2'	2.58	111.03	106.59
3	L5	3695	PSU	C6-N1-C2	-2.58	120.30	122.69
3	L5	5010	PSU	C6-N1-C2	-2.57	120.31	122.69
3	L5	1744	PSU	C6-N1-C2	-2.57	120.31	122.69
3	L5	3718	A2M	C1'-N9-C8	2.57	132.79	127.09
3	L5	4431	PSU	C6-N1-C2	-2.57	120.31	122.69
3	L5	2363	A2M	O3'-C3'-C2'	2.57	118.37	111.19
3	L5	4552	PSU	C6-N1-C2	-2.56	120.31	122.69
3	L5	4973	PSU	C6-N1-C2	-2.56	120.31	122.69
83	S2	1045	PSU	C6-N1-C2	-2.56	120.31	122.69
3	L5	3785	A2M	C1'-N9-C8	2.56	132.78	127.09
3	L5	3851	PSU	C6-N1-C2	-2.56	120.32	122.69
3	L5	1683	PSU	C6-N1-C2	-2.56	120.32	122.69
3	L5	4403	PSU	C6-C5-C4	2.55	119.90	118.17
3	L5	3853	PSU	C6-N1-C2	-2.55	120.32	122.69
3	L5	4299	PSU	O2-C2-N1	-2.54	120.17	122.79
3	L5	1323	A2M	C4-N9-C1'	-2.54	120.69	126.63
83	S2	93	PSU	C6-N1-C2	-2.54	120.33	122.69
3	L5	1323	A2M	O4'-C1'-C2'	2.54	110.96	106.59
5	L8	55	PSU	C6-N1-C2	-2.54	120.34	122.69
83	S2	484	A2M	O4'-C1'-C2'	2.53	110.95	106.59
83	S2	166	A2M	C4-N9-C1'	-2.52	120.73	126.63
5	L8	69	PSU	C6-N1-C2	-2.52	120.35	122.69
3	L5	4576	PSU	C6-N1-C2	-2.52	120.35	122.69
83	S2	1367	PSU	C6-N1-C2	-2.51	120.36	122.69
83	S2	93	PSU	O2-C2-N1	-2.51	120.20	122.79
3	L5	3718	A2M	C4-N9-C1'	-2.51	120.76	126.63
3	L5	3785	A2M	C3'-C2'-C1'	-2.51	98.00	102.81
83	S2	863	PSU	O2-C2-N1	-2.50	120.20	122.79
83	S2	406	PSU	C6-N1-C2	-2.50	120.37	122.69
83	S2	1177	PSU	C6-N1-C2	-2.50	120.37	122.69
83	S2	109	PSU	C6-N1-C2	-2.50	120.38	122.69
83	S2	1244	PSU	C6-N1-C2	-2.49	120.38	122.69
83	S2	649	PSU	O2-C2-N1	-2.49	120.22	122.79
3	L5	1781	PSU	C6-N1-C2	-2.48	120.39	122.69
83	S2	966	PSU	C6-N1-C2	-2.48	120.39	122.69
83	S2	1851	MA6	C1'-N9-C8	-2.48	121.59	127.09
3	L5	1782	PSU	C6-N1-C2	-2.48	120.39	122.69
3	L5	4293	PSU	C6-N1-C2	-2.47	120.40	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2363	A2M	O4'-C1'-C2'	2.45	110.81	106.59
3	L5	1323	A2M	C1'-N9-C8	2.45	132.54	127.09
3	L5	2787	A2M	C4-N9-C1'	-2.45	120.90	126.63
3	L5	1326	A2M	C3'-C2'-C1'	-2.45	98.12	102.81
3	L5	4571	A2M	C1'-N9-C8	2.44	132.52	127.09
83	S2	576	A2M	C1'-N9-C8	2.44	132.52	127.09
3	L5	4456	OMC	C1'-N1-C2	2.44	123.83	118.44
83	S2	166	A2M	C1'-N9-C8	2.44	132.51	127.09
83	S2	1367	PSU	C6-C5-C4	2.44	119.82	118.17
3	L5	1534	A2M	C4-N9-C1'	-2.44	120.93	126.63
5	L8	55	PSU	O2-C2-N1	-2.43	120.28	122.79
3	L5	4532	PSU	C6-N1-C2	-2.42	120.44	122.69
83	S2	668	A2M	O3'-C3'-C2'	2.42	117.96	111.19
3	L5	2815	A2M	O4'-C1'-C2'	2.42	110.75	106.59
83	S2	1337	4AC	N4-C4-N3	2.41	117.78	113.87
3	L5	4457	PSU	C6-N1-C2	-2.41	120.45	122.69
83	S2	1081	PSU	O2-C2-N1	-2.41	120.31	122.79
3	L5	4220	6MZ	C4-C5-C6	2.40	118.78	116.78
3	L5	4493	PSU	O2-C2-N1	-2.40	120.31	122.79
3	L5	2363	A2M	C3'-C2'-C1'	-2.40	98.22	102.81
3	L5	4442	PSU	C6-N1-C2	-2.37	120.49	122.69
83	S2	159	A2M	O3'-C3'-C4'	-2.37	104.28	111.08
3	L5	3785	A2M	C2-N1-C6	-2.37	114.84	118.73
3	L5	2815	A2M	C3'-C2'-C1'	-2.36	98.28	102.81
83	S2	1850	MA6	C1'-N9-C8	-2.36	121.85	127.09
3	L5	1326	A2M	C2'-C1'-N9	2.36	117.64	113.75
3	L5	4521	PSU	C6-N1-C2	-2.36	120.50	122.69
83	S2	801	PSU	C6-N1-C2	-2.36	120.50	122.69
3	L5	2861	OMC	C1'-N1-C2	2.35	123.64	118.44
3	L5	1326	A2M	O4'-C1'-C2'	2.35	110.64	106.59
83	S2	1442	OMU	C1'-N1-C2	2.34	121.79	117.59
3	L5	3867	A2M	O3'-C3'-C2'	2.34	117.73	111.19
3	L5	4220	6MZ	C3'-C2'-C1'	2.34	105.88	101.46
3	L5	1534	A2M	C1'-N9-C8	2.34	132.28	127.09
83	S2	863	PSU	C6-N1-C2	-2.33	120.53	122.69
83	S2	1081	PSU	C6-N1-C2	-2.33	120.53	122.69
3	L5	3822	PSU	C6-N1-C2	-2.33	120.53	122.69
3	L5	4299	PSU	C6-N1-C2	-2.33	120.53	122.69
3	L5	4530	UR3	C6-N1-C2	-2.32	119.90	121.80
83	S2	159	A2M	O4'-C1'-C2'	2.32	110.58	106.59
3	L5	2787	A2M	C1'-N9-C8	2.32	132.24	127.09
3	L5	3925	OMU	O2-C2-N1	-2.31	119.79	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4403	PSU	C6-N1-C2	-2.31	120.55	122.69
3	L5	1534	A2M	O3'-C3'-C4'	-2.31	104.46	111.08
3	L5	4403	PSU	O4'-C1'-C2'	2.31	108.34	105.15
3	L5	1871	A2M	C6-C5-C4	-2.30	114.04	117.18
3	L5	3808	OMC	C1'-N1-C2	2.29	123.50	118.44
3	L5	3785	A2M	C5-C6-N1	2.28	123.31	117.51
83	S2	1639	G7M	N9-C8-N7	-2.28	106.95	112.48
3	L5	2815	A2M	C1'-N9-C8	2.27	132.14	127.09
3	L5	4500	PSU	C6-C5-C4	2.27	119.71	118.17
3	L5	4442	PSU	O4'-C1'-C2'	2.27	108.29	105.15
3	L5	4498	OMU	O2-C2-N1	-2.27	119.84	122.80
3	L5	1677	PSU	C6-N1-C2	-2.27	120.59	122.69
83	S2	668	A2M	C2'-C1'-N9	2.26	117.47	113.75
3	L5	4523	A2M	C6-C5-C4	-2.26	114.09	117.18
3	L5	4493	PSU	C6-N1-C2	-2.26	120.59	122.69
3	L5	4590	A2M	C6-C5-C4	-2.26	114.09	117.18
3	L5	2815	A2M	C4-N9-C1'	-2.25	121.38	126.63
3	L5	1582	PSU	C6-C5-C4	2.25	119.69	118.17
3	L5	3822	PSU	O4'-C1'-C2'	2.24	108.25	105.15
83	S2	159	A2M	C2'-C1'-N9	2.24	117.44	113.75
3	L5	3785	A2M	C6-C5-C4	-2.24	114.12	117.18
83	S2	1288	OMU	C1'-N1-C2	2.23	121.59	117.59
83	S2	121	OMU	O2-C2-N1	-2.23	119.90	122.80
3	L5	400	A2M	O4'-C1'-C2'	2.22	110.41	106.59
3	L5	1322	1MA	N1-C6-N6	2.22	125.29	119.71
3	L5	3867	A2M	C3'-C2'-C1'	-2.22	98.56	102.81
3	L5	398	A2M	C6-C5-C4	-2.22	114.15	117.18
83	S2	1056	PSU	C6-N1-C2	-2.22	120.64	122.69
3	L5	1524	A2M	C4-N9-C1'	-2.21	121.45	126.63
83	S2	668	A2M	C6-C5-C4	-2.21	114.15	117.18
83	S2	468	A2M	C6-C5-C4	-2.21	114.16	117.18
3	L5	4972	PSU	C6-C5-C4	2.21	119.67	118.17
83	S2	1383	A2M	C6-C5-C4	-2.21	114.17	117.18
83	S2	27	A2M	C6-C5-C4	-2.21	114.17	117.18
3	L5	3867	A2M	C6-C5-C4	-2.20	114.17	117.18
83	S2	866	PSU	C6-N1-C2	-2.20	120.65	122.69
83	S2	866	PSU	C6-C5-C4	2.20	119.66	118.17
83	S2	99	A2M	C6-C5-C4	-2.20	114.18	117.18
3	L5	2401	A2M	C6-C5-C4	-2.20	114.18	117.18
3	L5	3830	A2M	C6-C5-C4	-2.19	114.18	117.18
3	L5	2363	A2M	C6-C5-C4	-2.19	114.18	117.18
83	S2	799	OMU	C1'-N1-C2	2.19	121.53	117.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2363	A2M	C2'-C1'-N9	2.19	117.36	113.75
3	L5	3825	A2M	C6-C5-C4	-2.19	114.19	117.18
5	L8	69	PSU	O4'-C1'-C2'	2.19	108.18	105.15
83	S2	649	PSU	C6-C5-C4	2.19	119.65	118.17
3	L5	400	A2M	C2'-C1'-N9	2.18	117.33	113.75
3	L5	1524	A2M	C1'-N9-C8	2.17	131.92	127.09
3	L5	4636	PSU	C6-C5-C4	2.17	119.64	118.17
83	S2	1031	A2M	C6-C5-C4	-2.17	114.21	117.18
3	L5	3637	PSU	O2-C2-N1	-2.17	120.55	122.79
3	L5	3639	PSU	C6-C5-C4	2.17	119.64	118.17
3	L5	1326	A2M	C6-C5-C4	-2.17	114.22	117.18
3	L5	2422	OMC	C1'-N1-C2	2.16	123.22	118.44
83	S2	801	PSU	C6-C5-C4	2.16	119.63	118.17
83	S2	468	A2M	O4'-C1'-C2'	2.16	110.30	106.59
3	L5	1871	A2M	C4'-O4'-C1'	-2.16	104.71	109.47
83	S2	1248	B8N	O4-C4-C5	-2.15	118.85	122.58
83	S2	27	A2M	O4'-C1'-C2'	2.15	110.30	106.59
83	S2	159	A2M	O4'-C4'-C3'	2.14	109.40	105.15
3	L5	4227	OMU	O2-C2-N1	-2.14	120.01	122.80
83	S2	428	OMU	O2-C2-N1	-2.14	120.01	122.80
3	L5	4628	PSU	C6-C5-C4	2.14	119.62	118.17
3	L5	3825	A2M	C5-C6-N1	2.13	122.93	117.51
83	S2	1272	OMC	C1'-N1-C2	2.13	123.14	118.44
83	S2	109	PSU	C6-C5-C4	2.12	119.61	118.17
3	L5	1534	A2M	O3'-C3'-C2'	2.12	117.11	111.19
83	S2	166	A2M	O4'-C1'-C2'	2.11	110.22	106.59
83	S2	1248	B8N	O4'-C1'-C2'	2.11	108.07	105.15
83	S2	166	A2M	C6-C5-C4	-2.11	114.30	117.18
83	S2	649	PSU	C6-N1-C2	-2.11	120.74	122.69
83	S2	354	OMU	O2-C2-N1	-2.11	120.06	122.80
83	S2	1326	OMU	O2-C2-N1	-2.10	120.06	122.80
3	L5	1323	A2M	C2-N1-C6	-2.10	115.27	118.73
3	L5	4636	PSU	O4'-C1'-C2'	2.10	108.06	105.15
3	L5	1524	A2M	C2-N1-C6	-2.10	115.27	118.73
83	S2	576	A2M	C6-C5-C4	-2.10	114.31	117.18
3	L5	3825	A2M	C2-N1-C6	-2.10	115.28	118.73
83	S2	159	A2M	C6-C5-C4	-2.10	114.31	117.18
83	S2	484	A2M	C6-C5-C4	-2.10	114.31	117.18
3	L5	4571	A2M	C6-C5-C4	-2.10	114.32	117.18
3	L5	3785	A2M	O4'-C4'-C3'	2.09	109.31	105.15
83	S2	1832	6MZ	C5-C6-N1	2.09	120.40	118.15
3	L5	1534	A2M	C2-N1-C6	-2.09	115.30	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2401	A2M	C5-C6-N1	2.09	122.82	117.51
83	S2	484	A2M	O4'-C4'-C3'	2.09	109.30	105.15
3	L5	4636	PSU	C6-N1-C2	-2.09	120.75	122.69
3	L5	400	A2M	C6-C5-C4	-2.09	114.33	117.18
3	L5	1322	1MA	CM1-N1-C6	-2.09	116.92	120.15
83	S2	1081	PSU	O4'-C1'-C2'	2.08	108.03	105.15
3	L5	4523	A2M	C4'-O4'-C1'	-2.08	104.87	109.47
83	S2	159	A2M	C5-C6-N1	2.08	122.80	117.51
3	L5	2787	A2M	C6-C5-C4	-2.08	114.34	117.18
3	L5	4523	A2M	C5-C6-N1	2.08	122.80	117.51
3	L5	398	A2M	C5-C6-N1	2.08	122.79	117.51
3	L5	2363	A2M	C5-C6-N1	2.08	122.78	117.51
3	L5	1326	A2M	C5-C6-N1	2.08	122.78	117.51
3	L5	4442	PSU	C6-C5-C4	2.07	119.57	118.17
3	L5	3822	PSU	C6-C5-C4	2.07	119.57	118.17
3	L5	2815	A2M	C5-C6-N1	2.07	122.76	117.51
83	S2	1031	A2M	C5-C6-N1	2.06	122.75	117.51
83	S2	1031	A2M	C2-N1-C6	-2.06	115.35	118.73
3	L5	3718	A2M	C2-N1-C6	-2.06	115.35	118.73
83	S2	668	A2M	C2-N1-C6	-2.06	115.35	118.73
3	L5	2401	A2M	C2-N1-C6	-2.06	115.35	118.73
83	S2	159	A2M	C2-N1-C6	-2.06	115.35	118.73
83	S2	99	A2M	C5-C6-N1	2.06	122.73	117.51
3	L5	400	A2M	C5-C6-N1	2.06	122.73	117.51
3	L5	4523	A2M	C2-N1-C6	-2.05	115.36	118.73
3	L5	4628	PSU	O4'-C1'-C2'	2.05	107.99	105.15
83	S2	406	PSU	C6-C5-C4	2.05	119.56	118.17
3	L5	1534	A2M	C5-C6-N1	2.05	122.71	117.51
3	L5	1323	A2M	C5-C6-N1	2.05	122.71	117.51
83	S2	27	A2M	C5-C6-N1	2.04	122.70	117.51
3	L5	2363	A2M	C2-N1-C6	-2.04	115.37	118.73
3	L5	1323	A2M	C6-C5-C4	-2.04	114.39	117.18
83	S2	1383	A2M	C5-C6-N1	2.04	122.69	117.51
3	L5	3830	A2M	C5-C6-N1	2.04	122.69	117.51
3	L5	4523	A2M	O4'-C1'-C2'	2.04	110.10	106.59
83	S2	1248	B8N	C31-N3-C4	2.04	120.06	117.18
3	L5	2787	A2M	C5-C6-N1	2.04	122.68	117.51
3	L5	2815	A2M	C2-N1-C6	-2.02	115.41	118.73
3	L5	1326	A2M	C2-N1-C6	-2.02	115.41	118.73
83	S2	686	PSU	C6-C5-C4	2.02	119.54	118.17
3	L5	4590	A2M	C5-C6-N1	2.02	122.64	117.51
3	L5	4571	A2M	O4'-C1'-C2'	2.02	110.06	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1534	A2M	C6-C5-C4	-2.02	114.42	117.18
3	L5	3867	A2M	C2-N1-C6	-2.02	115.42	118.73
83	S2	116	OMU	C1'-N1-C2	2.02	121.21	117.59
83	S2	1046	PSU	O4'-C1'-C2'	2.01	107.94	105.15
83	S2	484	A2M	C5-C6-N1	2.01	122.63	117.51
3	L5	1534	A2M	C2'-C1'-N9	2.01	117.07	113.75
3	L5	400	A2M	C2-N1-C6	-2.01	115.42	118.73
83	S2	668	A2M	O3'-C3'-C4'	-2.01	105.30	111.08
83	S2	668	A2M	C5-C6-N1	2.01	122.61	117.51
83	S2	174	OMC	C1'-N1-C2	2.00	122.87	118.44
3	L5	4620	OMU	O2-C2-N1	-2.00	120.19	122.80
3	L5	2815	A2M	C6-C5-C4	-2.00	114.44	117.18
83	S2	1004	PSU	C6-C5-C4	2.00	119.53	118.17

There are no chirality outliers.

All (167) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L8	75	OMG	C1'-C2'-O2'-CM2
85	CF	163	SEP	C-CA-CB-OG
85	CF	163	SEP	CB-OG-P-O1P
85	CF	163	SEP	CB-OG-P-O2P
85	CF	163	SEP	CB-OG-P-O3P
3	L5	400	A2M	C1'-C2'-O2'-CM'
3	L5	1326	A2M	O4'-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	2351	OMC	C1'-C2'-O2'-CM2
3	L5	2364	OMG	C1'-C2'-O2'-CM2
3	L5	2787	A2M	C1'-C2'-O2'-CM'
3	L5	2815	A2M	O4'-C4'-C5'-O5'
3	L5	2815	A2M	C1'-C2'-O2'-CM'
3	L5	2824	OMC	C1'-C2'-O2'-CM2
3	L5	2861	OMC	C1'-C2'-O2'-CM2
3	L5	3701	OMC	O4'-C4'-C5'-O5'
3	L5	3718	A2M	C1'-C2'-O2'-CM'
3	L5	3792	OMG	O4'-C4'-C5'-O5'
3	L5	3867	A2M	C1'-C2'-O2'-CM'
3	L5	4196	OMG	C1'-C2'-O2'-CM2
3	L5	4500	PSU	O4'-C4'-C5'-O5'
3	L5	4590	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	L5	4590	A2M	C1'-C2'-O2'-CM'
3	L5	4620	OMU	C1'-C2'-O2'-CM2
3	L5	4637	OMG	O4'-C4'-C5'-O5'
83	S2	116	OMU	C1'-C2'-O2'-CM2
83	S2	159	A2M	C1'-C2'-O2'-CM'
83	S2	166	A2M	C1'-C2'-O2'-CM'
83	S2	428	OMU	C2'-C1'-N1-C6
83	S2	468	A2M	C1'-C2'-O2'-CM'
83	S2	576	A2M	C1'-C2'-O2'-CM'
83	S2	601	OMG	C1'-C2'-O2'-CM2
83	S2	644	OMG	O4'-C4'-C5'-O5'
83	S2	1031	A2M	C1'-C2'-O2'-CM'
83	S2	1248	B8N	O4'-C4'-C5'-O5'
83	S2	1288	OMU	O4'-C4'-C5'-O5'
83	S2	1328	OMG	C1'-C2'-O2'-CM2
83	S2	1337	4AC	N3-C4-N4-C7
83	S2	1383	A2M	C1'-C2'-O2'-CM'
83	S2	1832	6MZ	C5-C6-N6-C9
83	S2	1832	6MZ	N1-C6-N6-C9
83	S2	1832	6MZ	C5'-O5'-P-OP2
83	S2	1832	6MZ	C5'-O5'-P-OP3
3	L5	3701	OMC	C2'-C1'-N1-C2
83	S2	428	OMU	C2'-C1'-N1-C2
3	L5	1323	A2M	O4'-C4'-C5'-O5'
3	L5	1326	A2M	C3'-C4'-C5'-O5'
3	L5	2364	OMG	O4'-C4'-C5'-O5'
3	L5	2401	A2M	C3'-C4'-C5'-O5'
3	L5	3867	A2M	C3'-C4'-C5'-O5'
3	L5	3899	OMG	O4'-C4'-C5'-O5'
3	L5	3899	OMG	C3'-C4'-C5'-O5'
3	L5	4500	PSU	C3'-C4'-C5'-O5'
3	L5	4590	A2M	C3'-C4'-C5'-O5'
83	S2	159	A2M	O4'-C4'-C5'-O5'
83	S2	576	A2M	O4'-C4'-C5'-O5'
83	S2	576	A2M	C3'-C4'-C5'-O5'
83	S2	683	OMG	C3'-C4'-C5'-O5'
83	S2	799	OMU	C3'-C4'-C5'-O5'
83	S2	799	OMU	O4'-C4'-C5'-O5'
83	S2	801	PSU	C3'-C4'-C5'-O5'
83	S2	867	OMG	C3'-C4'-C5'-O5'
3	L5	1536	PSU	C3'-C4'-C5'-O5'
3	L5	1536	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	L5	2401	A2M	O4'-C4'-C5'-O5'
3	L5	3701	OMC	C3'-C4'-C5'-O5'
3	L5	3867	A2M	O4'-C4'-C5'-O5'
83	S2	436	OMG	O4'-C4'-C5'-O5'
83	S2	517	OMC	C3'-C4'-C5'-O5'
83	S2	517	OMC	O4'-C4'-C5'-O5'
83	S2	627	OMU	O4'-C4'-C5'-O5'
83	S2	683	OMG	O4'-C4'-C5'-O5'
83	S2	867	OMG	O4'-C4'-C5'-O5'
83	S2	1272	OMC	C3'-C4'-C5'-O5'
83	S2	1272	OMC	O4'-C4'-C5'-O5'
83	S2	1442	OMU	O4'-C4'-C5'-O5'
83	S2	1832	6MZ	O4'-C4'-C5'-O5'
3	L5	3701	OMC	C2'-C1'-N1-C6
3	L5	4447	5MC	C2'-C1'-N1-C6
3	L5	1625	OMG	C3'-C4'-C5'-O5'
3	L5	2815	A2M	C3'-C4'-C5'-O5'
3	L5	3792	OMG	C3'-C4'-C5'-O5'
83	S2	159	A2M	C3'-C4'-C5'-O5'
83	S2	644	OMG	C3'-C4'-C5'-O5'
83	S2	1288	OMU	C3'-C4'-C5'-O5'
3	L5	4637	OMG	C3'-C4'-C5'-O5'
83	S2	668	A2M	O4'-C4'-C5'-O5'
83	S2	668	A2M	C3'-C4'-C5'-O5'
83	S2	1045	PSU	C3'-C4'-C5'-O5'
83	S2	1248	B8N	C3'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C2
3	L5	398	A2M	O4'-C4'-C5'-O5'
3	L5	1524	A2M	O4'-C4'-C5'-O5'
3	L5	1677	PSU	O4'-C4'-C5'-O5'
3	L5	4228	OMG	O4'-C4'-C5'-O5'
3	L5	4471	PSU	C3'-C4'-C5'-O5'
83	S2	801	PSU	O4'-C4'-C5'-O5'
83	S2	1045	PSU	O4'-C4'-C5'-O5'
3	L5	1323	A2M	C3'-C4'-C5'-O5'
3	L5	1524	A2M	C3'-C4'-C5'-O5'
3	L5	1677	PSU	C3'-C4'-C5'-O5'
3	L5	1781	PSU	C3'-C4'-C5'-O5'
3	L5	4228	OMG	C3'-C4'-C5'-O5'
83	S2	99	A2M	O4'-C4'-C5'-O5'
83	S2	1442	OMU	C3'-C4'-C5'-O5'
83	S2	1248	B8N	N34-C33-C34-O36

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Mol	Chain	Res	Type	Atoms
3	L5	2787	A2M	C2'-C1'-N9-C8
3	L5	2364	OMG	C3'-C4'-C5'-O5'
3	L5	2787	A2M	C3'-C4'-C5'-O5'
83	S2	627	OMU	C3'-C4'-C5'-O5'
83	S2	1832	6MZ	C3'-C4'-C5'-O5'
3	L5	3925	OMU	C1'-C2'-O2'-CM2
83	S2	428	OMU	O4'-C4'-C5'-O5'
3	L5	2422	OMC	C3'-C4'-C5'-O5'
85	CF	163	SEP	CA-CB-OG-P
3	L5	4447	5MC	O4'-C1'-N1-C2
3	L5	2422	OMC	O4'-C4'-C5'-O5'
83	S2	1832	6MZ	C5'-O5'-P-OP1
3	L5	4447	5MC	O4'-C1'-N1-C6
83	S2	576	A2M	C4'-C5'-O5'-P
85	CF	163	SEP	N-CA-CB-OG
3	L5	3701	OMC	O4'-C1'-N1-C6
3	L5	2363	A2M	C3'-C2'-O2'-CM'
3	L5	4498	OMU	C3'-C2'-O2'-CM2
3	L5	3818	UY1	C4'-C5'-O5'-P
3	L5	4500	PSU	C4'-C5'-O5'-P
3	L5	4590	A2M	C4'-C5'-O5'-P
83	S2	644	OMG	C4'-C5'-O5'-P
83	S2	1851	MA6	C4'-C5'-O5'-P
3	L5	1677	PSU	O4'-C1'-C5-C4
3	L5	3818	UY1	O4'-C1'-C5-C4
83	S2	1248	B8N	O4'-C1'-C5-C4
3	L5	2787	A2M	C2'-C1'-N9-C4
83	S2	428	OMU	O4'-C1'-N1-C2
83	S2	428	OMU	C3'-C4'-C5'-O5'
83	S2	436	OMG	C3'-C4'-C5'-O5'
83	S2	428	OMU	O4'-C1'-N1-C6
83	S2	1490	OMG	C4'-C5'-O5'-P
3	L5	1524	A2M	C3'-C2'-O2'-CM'
3	L5	3869	OMC	C3'-C2'-O2'-CM2
3	L5	4370	OMG	C3'-C2'-O2'-CM2
3	L5	3887	OMC	C4'-C5'-O5'-P
3	L5	3627	OMG	O4'-C4'-C5'-O5'
3	L5	3701	OMC	O4'-C1'-N1-C2
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	3844	PSU	C4'-C5'-O5'-P
3	L5	4471	PSU	O4'-C4'-C5'-O5'
83	S2	172	OMU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	L5	2424	OMG	C1'-C2'-O2'-CM2
3	L5	3841	OMC	C1'-C2'-O2'-CM2
83	S2	1081	PSU	C4'-C5'-O5'-P
3	L5	398	A2M	C3'-C4'-C5'-O5'
3	L5	1781	PSU	O4'-C4'-C5'-O5'
83	S2	99	A2M	C3'-C4'-C5'-O5'
3	L5	4636	PSU	O4'-C1'-C5-C6
83	S2	1248	B8N	O4'-C1'-C5-C6
3	L5	4494	OMG	C3'-C2'-O2'-CM2
3	L5	2351	OMC	C2'-C1'-N1-C6
3	L5	3851	PSU	C3'-C4'-C5'-O5'
3	L5	4636	PSU	C2'-C1'-C5-C6
3	L5	2351	OMC	O4'-C4'-C5'-O5'
3	L5	2787	A2M	O4'-C1'-N9-C8
83	S2	1248	B8N	N3-C31-C32-C33
3	L5	2351	OMC	C2'-C1'-N1-C2
3	L5	4623	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

80 monomers are involved in 120 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2824	OMC	1	0
83	S2	1248	B8N	1	0
83	S2	109	PSU	1	0
83	S2	1639	G7M	1	0
83	S2	509	OMG	2	0
3	L5	1326	A2M	3	0
3	L5	1871	A2M	1	0
3	L5	2364	OMG	1	0
83	S2	172	OMU	1	0
3	L5	4523	A2M	2	0
83	S2	116	OMU	3	0
83	S2	484	A2M	1	0
83	S2	428	OMU	1	0
3	L5	3785	A2M	2	0
3	L5	4392	OMG	2	0
3	L5	4637	OMG	1	0
83	S2	159	A2M	4	0
3	L5	3718	A2M	4	0
3	L5	400	A2M	1	0
83	S2	1383	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4447	5MC	1	0
83	S2	99	A2M	1	0
3	L5	1534	A2M	1	0
3	L5	4590	A2M	1	0
3	L5	3825	A2M	1	0
3	L5	3841	OMC	1	0
3	L5	3884	PSU	1	0
3	L5	4220	6MZ	2	0
3	L5	2401	A2M	1	0
3	L5	4620	OMU	3	0
3	L5	4442	PSU	1	0
3	L5	4196	OMG	1	0
3	L5	2632	PSU	1	0
3	L5	2351	OMC	2	0
3	L5	4530	UR3	1	0
83	S2	1177	PSU	2	0
83	S2	1031	A2M	2	0
83	S2	1004	PSU	2	0
83	S2	1232	PSU	2	0
3	L5	4536	OMC	1	0
3	L5	1316	OMG	1	0
83	S2	121	OMU	2	0
3	L5	3701	OMC	1	0
83	S2	517	OMC	1	0
83	S2	799	OMU	1	0
83	S2	1842	4AC	2	0
83	S2	1174	PSU	1	0
83	S2	681	PSU	2	0
83	S2	1288	OMU	2	0
3	L5	3867	A2M	5	0
3	L5	2861	OMC	1	0
3	L5	2876	OMG	1	0
83	S2	601	OMG	2	0
3	L5	4689	PSU	1	0
83	S2	166	A2M	3	0
3	L5	1677	PSU	1	0
83	S2	1490	OMG	1	0
3	L5	4636	PSU	1	0
5	L8	75	OMG	1	0
3	L5	4431	PSU	2	0
3	L5	4579	PSU	1	0
3	L5	3925	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2363	A2M	1	0
3	L5	3818	UY1	1	0
83	S2	436	OMG	1	0
3	L5	4521	PSU	1	0
3	L5	4623	OMG	1	0
83	S2	1244	PSU	1	0
83	S2	683	OMG	1	0
3	L5	4618	OMG	1	0
83	S2	27	A2M	3	0
3	L5	1340	OMC	2	0
83	S2	576	A2M	1	0
83	S2	1337	4AC	4	0
3	L5	2424	OMG	1	0
83	S2	468	A2M	1	0
3	L5	4456	OMC	1	0
3	L5	4457	PSU	1	0
83	S2	1850	MA6	2	0
3	L5	1683	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 242 ligands modelled in this entry, 225 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
88	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.82	0
88	SPD	L5	5285	-	9,9,9	0.30	0	8,8,8	0.84	0
88	SPD	LN	301	-	9,9,9	0.32	0	8,8,8	0.86	0
87	SPM	L5	5264	-	13,13,13	0.36	0	12,12,12	0.95	0
88	SPD	L5	5292	-	9,9,9	0.34	0	8,8,8	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	SPD	L5	5289	-	9,9,9	0.32	0	8,8,8	0.86	0
87	SPM	L5	5290	-	13,13,13	0.38	0	12,12,12	0.95	0
87	SPM	L5	5259	-	13,13,13	0.35	0	12,12,12	0.96	0
87	SPM	L5	5265	-	13,13,13	0.35	0	12,12,12	0.94	0
87	SPM	L5	5268	-	13,13,13	0.36	0	12,12,12	1.07	0
88	SPD	L5	5262	-	9,9,9	0.31	0	8,8,8	0.97	0
88	SPD	L5	5284	-	9,9,9	0.33	0	8,8,8	0.86	0
88	SPD	L5	5288	-	9,9,9	0.32	0	8,8,8	0.88	0
87	SPM	L5	5293	-	13,13,13	0.35	0	12,12,12	0.92	0
88	SPD	L5	5291	-	9,9,9	0.32	0	8,8,8	0.90	0
88	SPD	L5	5286	-	9,9,9	0.34	0	8,8,8	0.86	0
87	SPM	L5	5294	-	13,13,13	0.36	0	12,12,12	0.87	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
88	SPD	L5	5287	-	-	0/7/7/7	-
88	SPD	L5	5285	-	-	1/7/7/7	-
88	SPD	LN	301	-	-	1/7/7/7	-
87	SPM	L5	5264	-	-	5/11/11/11	-
88	SPD	L5	5292	-	-	5/7/7/7	-
88	SPD	L5	5289	-	-	3/7/7/7	-
87	SPM	L5	5290	-	-	5/11/11/11	-
87	SPM	L5	5259	-	-	5/11/11/11	-
87	SPM	L5	5265	-	-	5/11/11/11	-
87	SPM	L5	5268	-	-	2/11/11/11	-
88	SPD	L5	5262	-	-	1/7/7/7	-
88	SPD	L5	5284	-	-	1/7/7/7	-
88	SPD	L5	5288	-	-	4/7/7/7	-
87	SPM	L5	5293	-	-	3/11/11/11	-
88	SPD	L5	5291	-	-	1/7/7/7	-
88	SPD	L5	5286	-	-	2/7/7/7	-
87	SPM	L5	5294	-	-	3/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	L5	5294	SPM	N10-C11-C12-C13
88	L5	5289	SPD	N6-C7-C8-C9
87	L5	5293	SPM	C7-C8-C9-N10
87	L5	5264	SPM	C7-C8-C9-N10
87	L5	5264	SPM	C8-C9-N10-C11
87	L5	5290	SPM	C12-C11-N10-C9
87	L5	5264	SPM	N10-C11-C12-C13
87	L5	5265	SPM	N5-C6-C7-C8
87	L5	5265	SPM	C7-C8-C9-N10
88	L5	5288	SPD	C4-C5-N6-C7
87	L5	5259	SPM	C2-C3-C4-N5
88	L5	5288	SPD	C8-C7-N6-C5
88	L5	5292	SPD	C4-C5-N6-C7
88	L5	5285	SPD	C3-C4-C5-N6
87	L5	5290	SPM	C8-C9-N10-C11
87	L5	5293	SPM	N5-C6-C7-C8
88	L5	5289	SPD	C2-C3-C4-C5
88	L5	5262	SPD	N6-C7-C8-C9
88	L5	5286	SPD	C2-C3-C4-C5
88	L5	5284	SPD	C2-C3-C4-C5
87	L5	5265	SPM	N10-C11-C12-C13
88	L5	5292	SPD	C8-C7-N6-C5
87	L5	5259	SPM	N5-C6-C7-C8
88	L5	5286	SPD	C3-C4-C5-N6
87	L5	5290	SPM	C7-C6-N5-C4
87	L5	5290	SPM	C2-C3-C4-N5
87	L5	5290	SPM	N1-C2-C3-C4
87	L5	5293	SPM	C7-C6-N5-C4
88	L5	5292	SPD	C3-C4-C5-N6
88	L5	5292	SPD	N1-C2-C3-C4
87	L5	5265	SPM	C12-C11-N10-C9
87	L5	5259	SPM	C6-C7-C8-C9
87	L5	5268	SPM	N10-C11-C12-C13
88	L5	5289	SPD	C8-C7-N6-C5
88	LN	301	SPD	C4-C5-N6-C7
87	L5	5294	SPM	C2-C3-C4-N5
87	L5	5264	SPM	C3-C4-N5-C6
87	L5	5268	SPM	C7-C6-N5-C4
88	L5	5288	SPD	C3-C4-C5-N6
87	L5	5265	SPM	C7-C6-N5-C4

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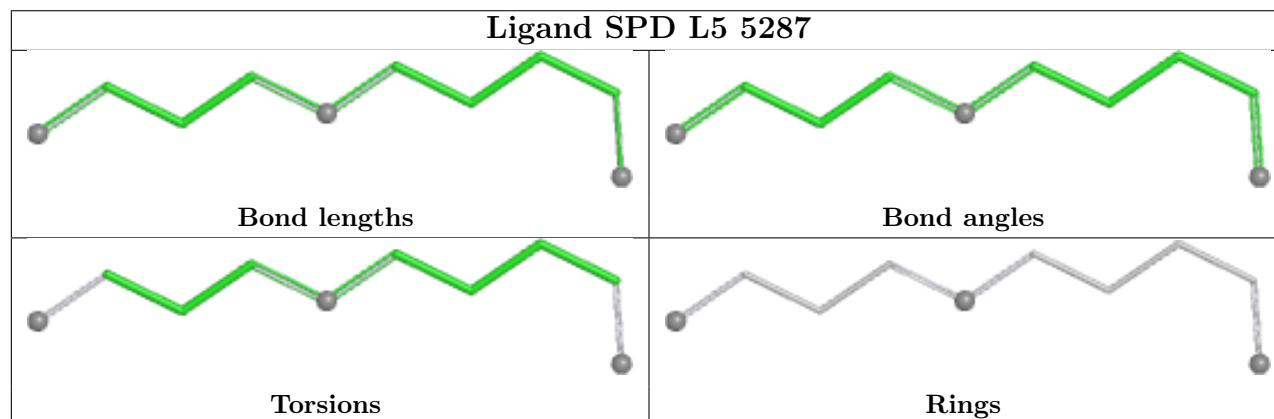
Mol	Chain	Res	Type	Atoms
88	L5	5288	SPD	C2-C3-C4-C5
87	L5	5259	SPM	N1-C2-C3-C4
87	L5	5259	SPM	C11-C12-C13-N14
87	L5	5264	SPM	N1-C2-C3-C4
88	L5	5291	SPD	N6-C7-C8-C9
87	L5	5294	SPM	C6-C7-C8-C9
88	L5	5292	SPD	C2-C3-C4-C5

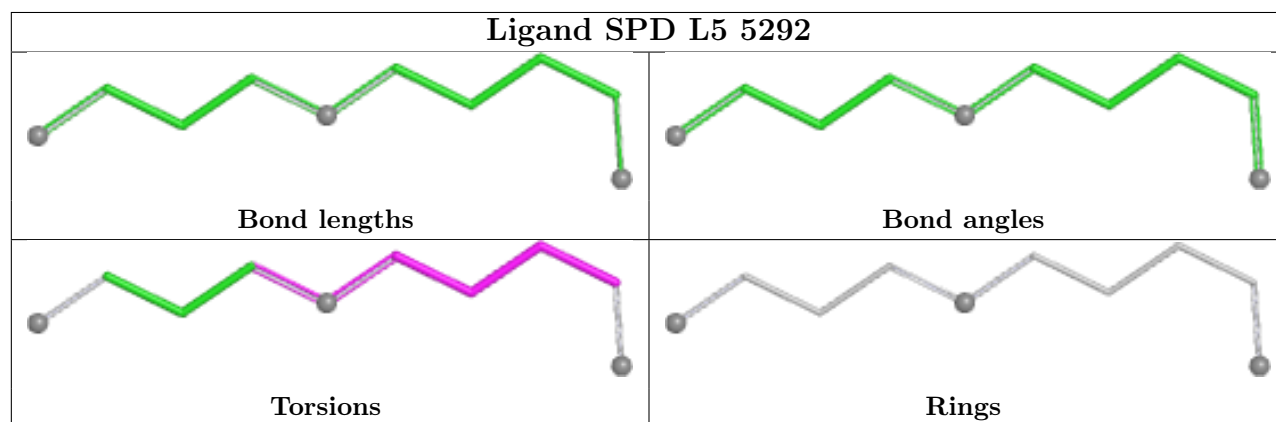
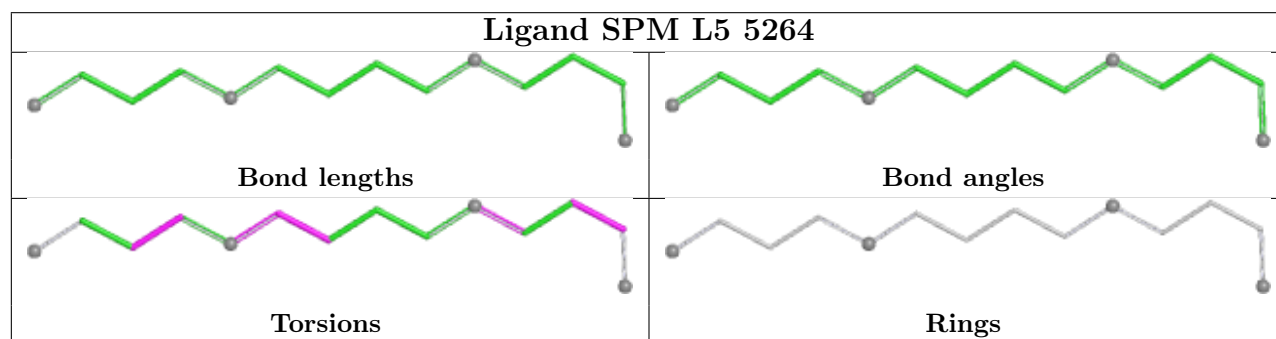
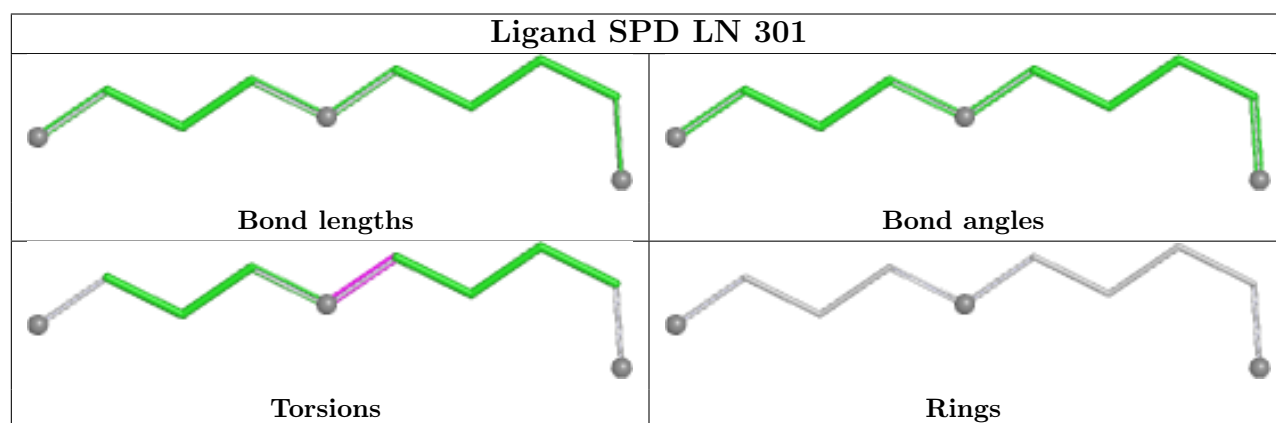
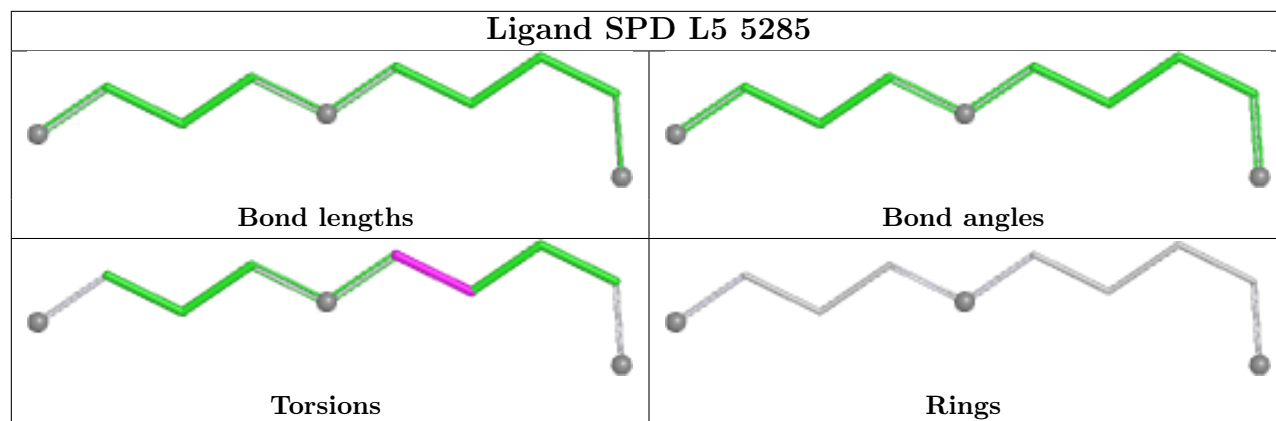
There are no ring outliers.

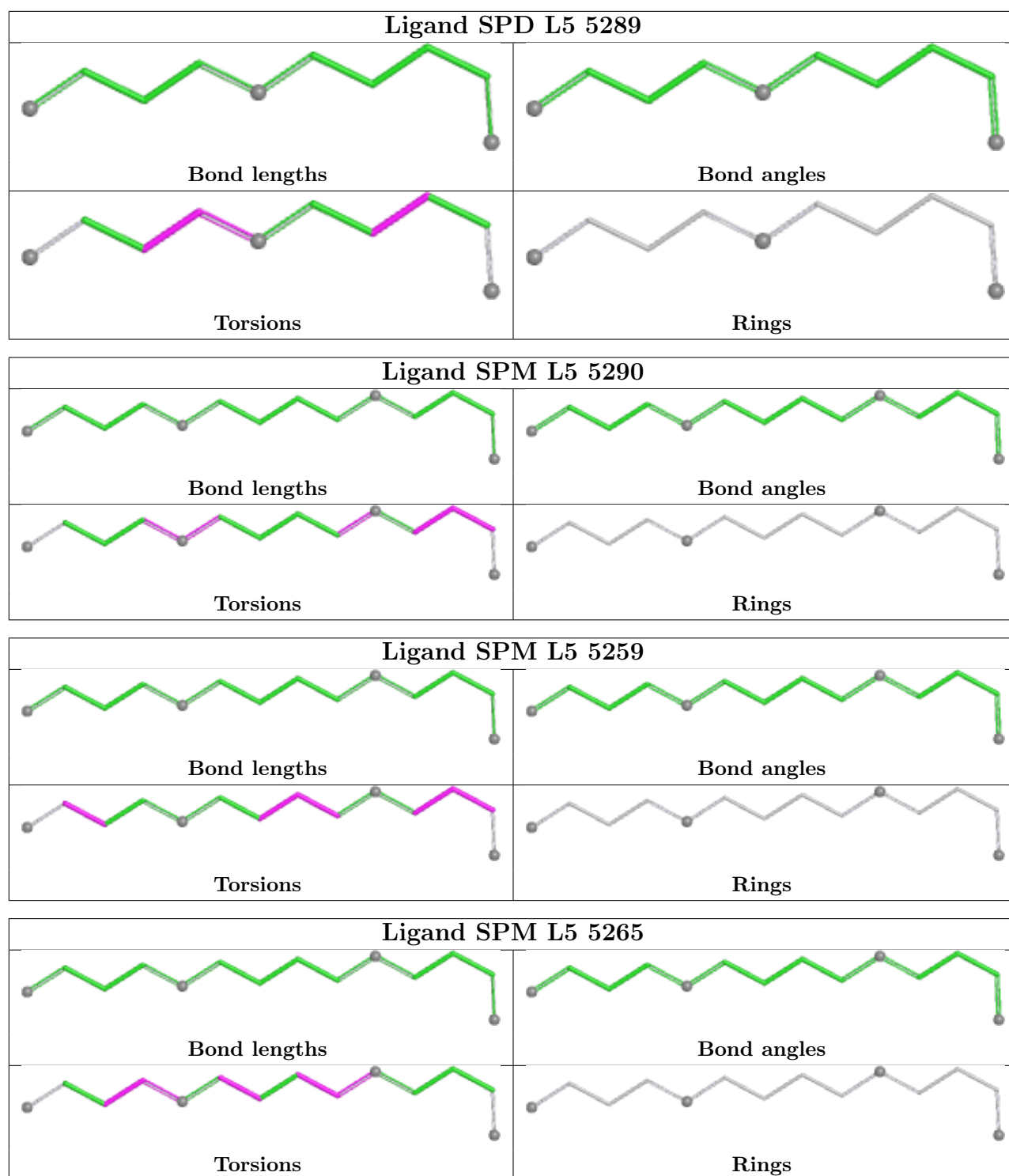
6 monomers are involved in 8 short contacts:

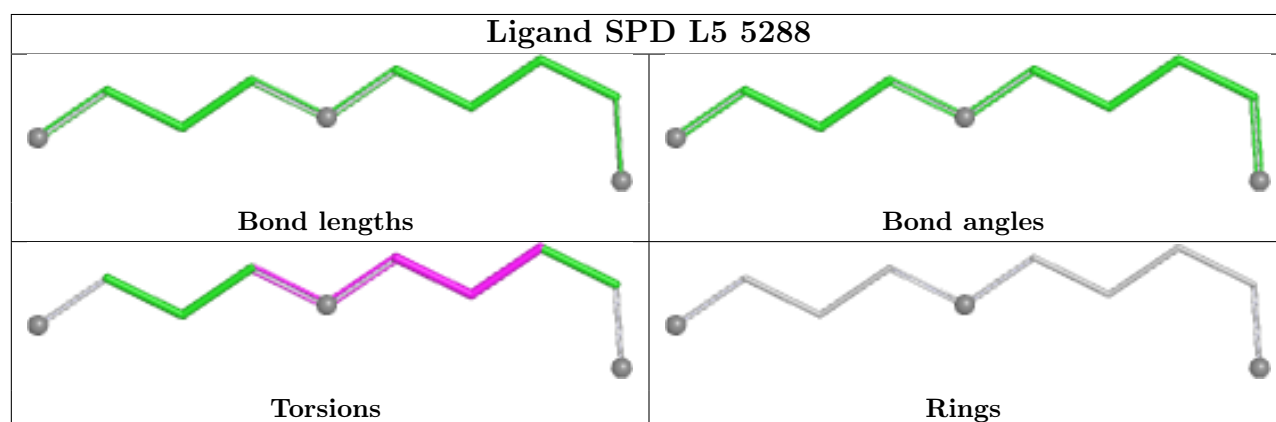
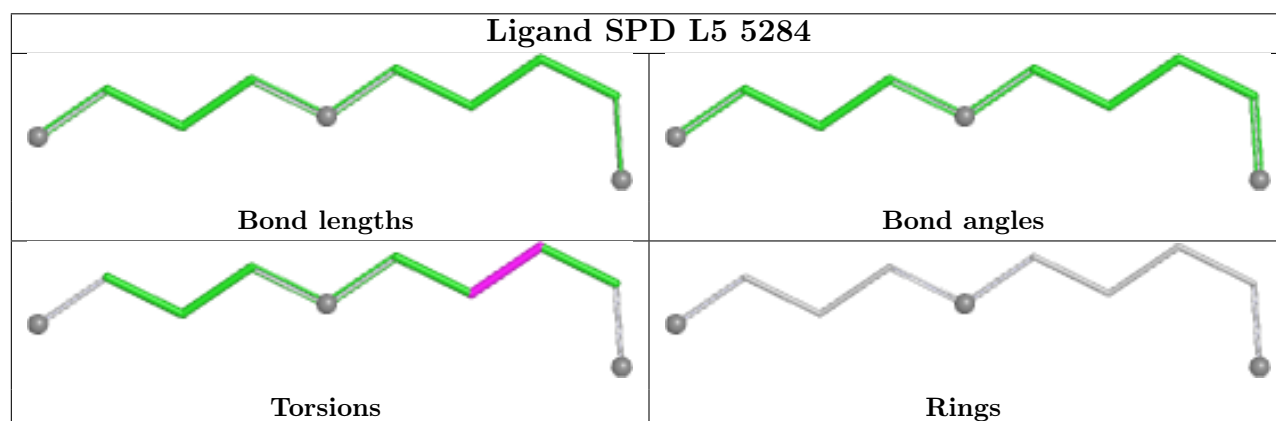
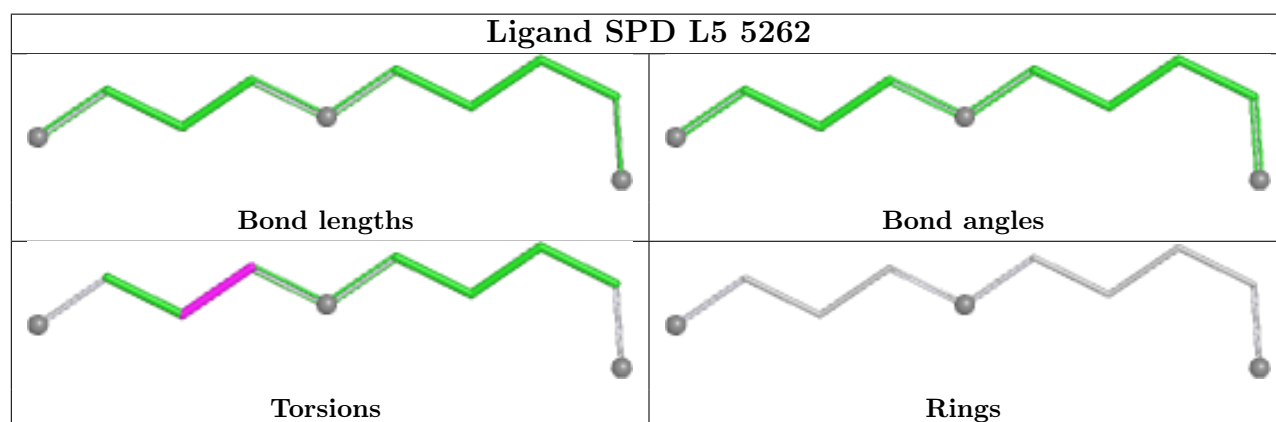
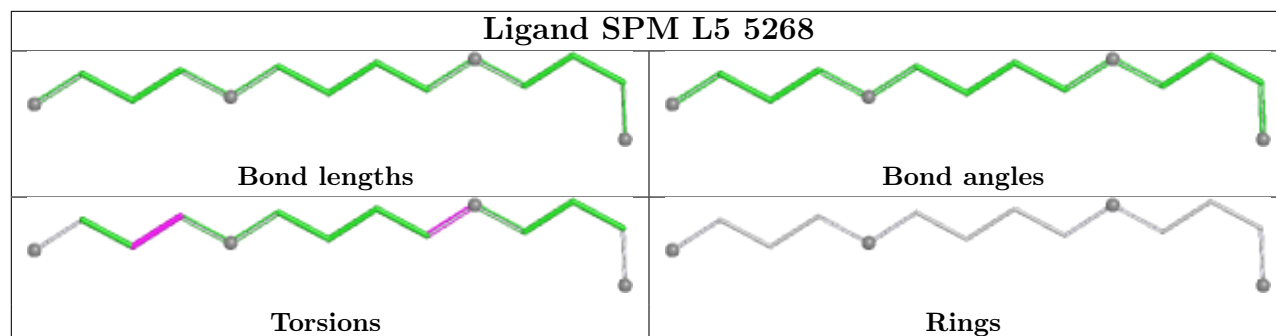
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5287	SPD	1	0
87	L5	5259	SPM	2	0
88	L5	5262	SPD	2	0
87	L5	5293	SPM	1	0
88	L5	5286	SPD	1	0
87	L5	5294	SPM	1	0

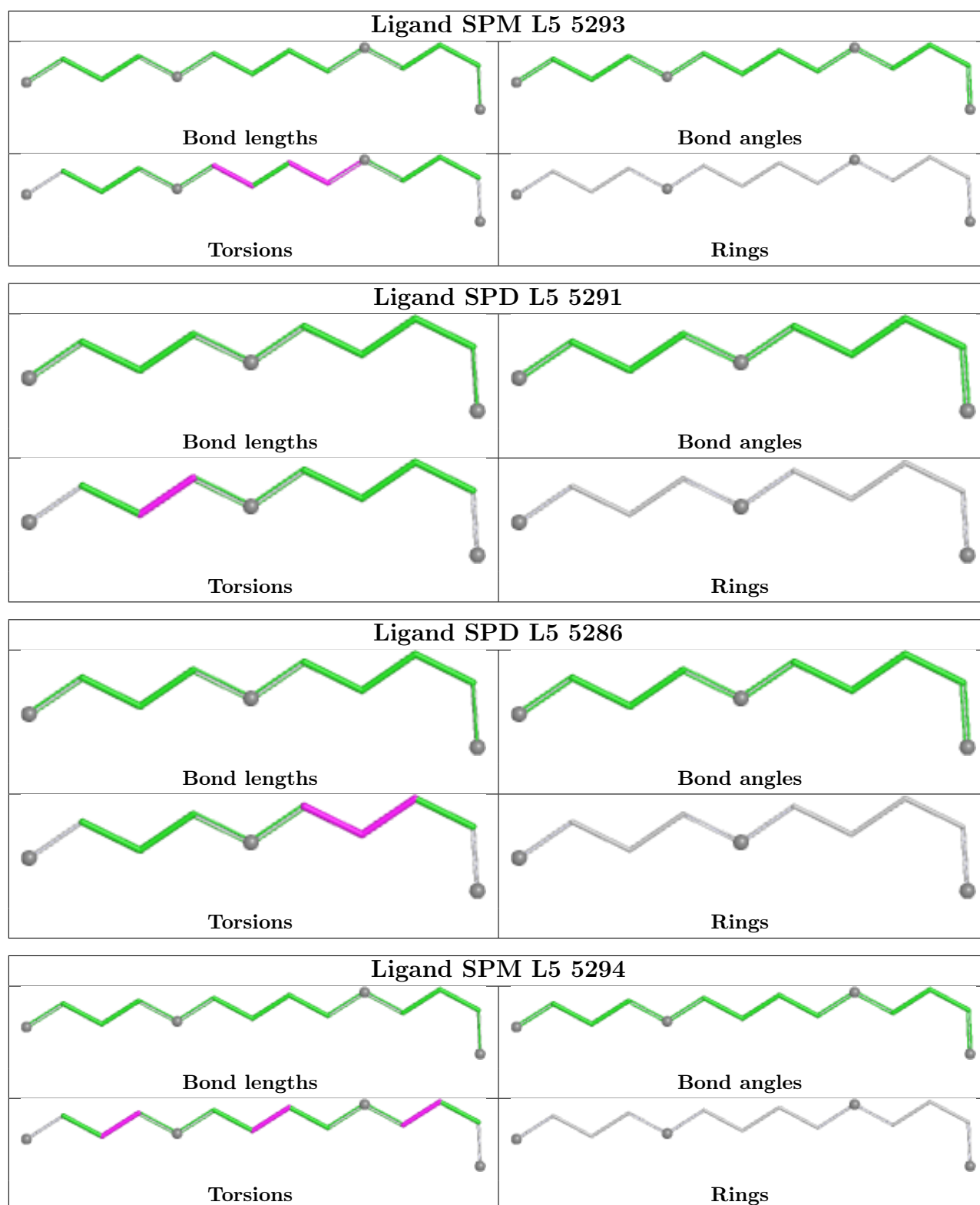
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	L5	10
83	S2	5
2	Pt	1
84	AT	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	28.78
1	L5	1706:A	O3'	1716:G	P	21.02
1	L5	2910:G	O3'	3584:C	P	20.91
1	L5	760:G	O3'	903:C	P	16.91
1	S2	698:G	O3'	730:C	P	15.51
1	L5	519:C	O3'	642:G	P	15.12
1	L5	4776:G	O3'	4858:C	P	14.46
1	L5	2112:G	O3'	2249:C	P	14.33
1	L5	3954:A	O3'	4056:A	P	14.19
1	L5	990:C	O3'	1064:G	P	12.73
1	S2	739:C	O3'	746:C	P	12.57
1	L5	1222:A	O3'	1234:G	P	10.96
1	Pt	15:G	O3'	18:G	P	9.83
1	S2	225:G	O3'	287:U	P	7.46
1	L5	1100:U	O3'	1167:C	P	6.66
1	AT	16:C	O3'	18:G	P	4.99
1	S2	1831:A	O3'	1832:6MZ	P	4.21

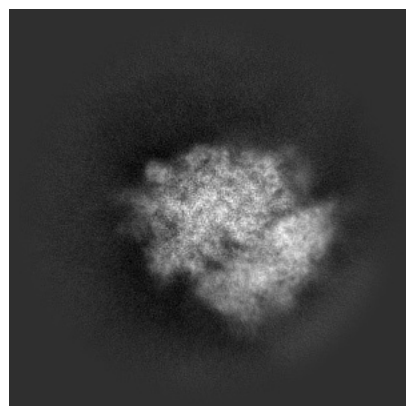
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71346. These allow visual inspection of the internal detail of the map and identification of artifacts.

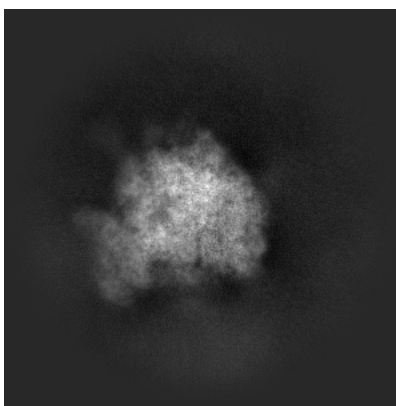
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

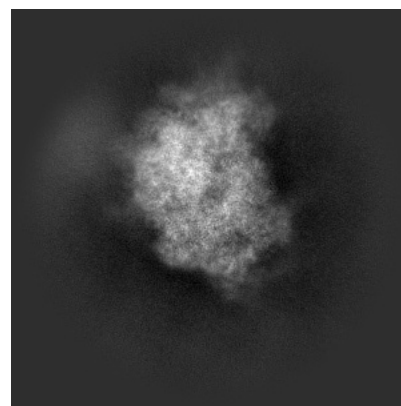
6.1.1 Primary map



X

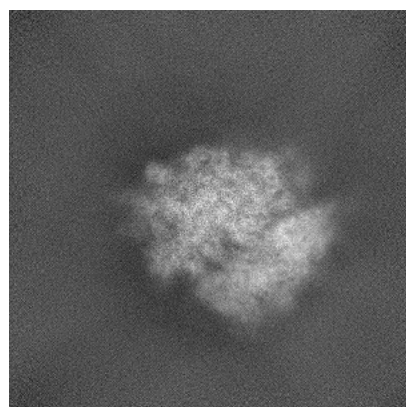


Y

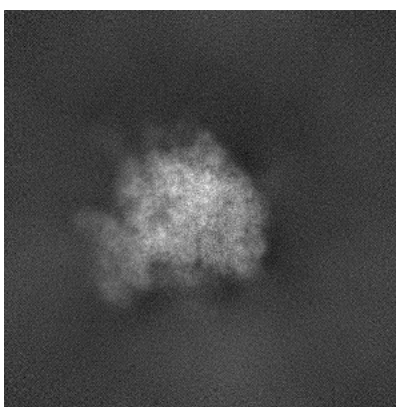


Z

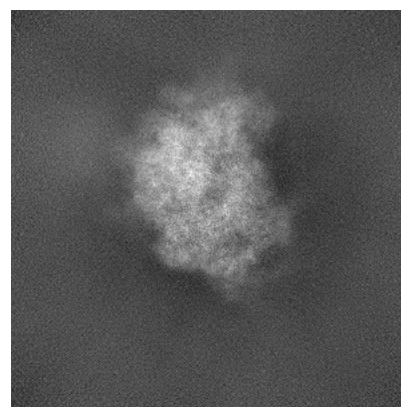
6.1.2 Raw map



X



Y

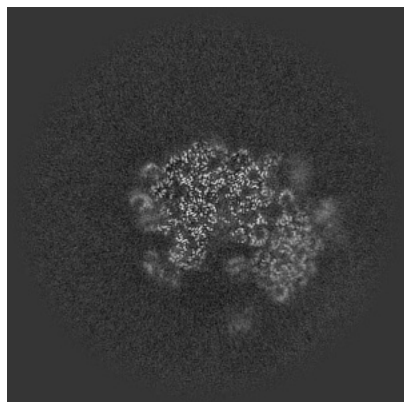


Z

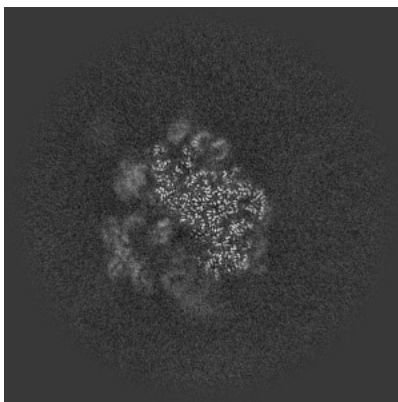
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

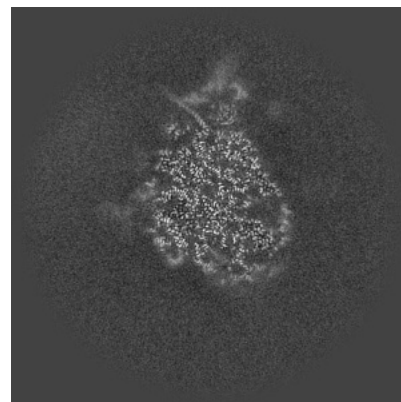
6.2.1 Primary map



X Index: 256

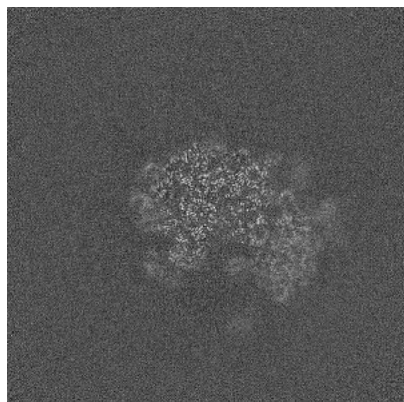


Y Index: 256

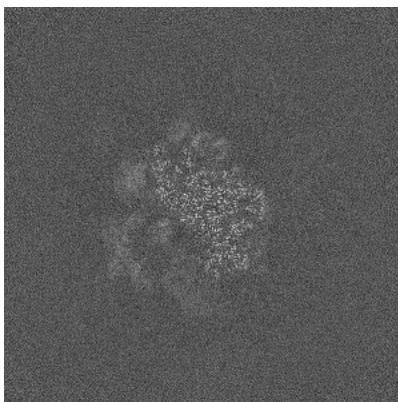


Z Index: 256

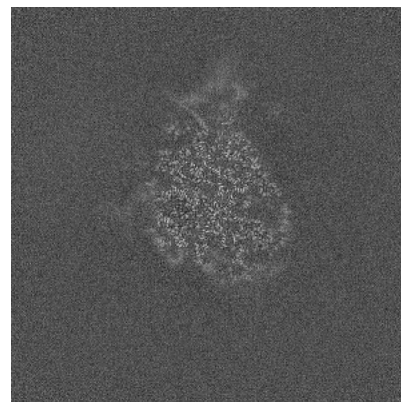
6.2.2 Raw map



X Index: 256



Y Index: 256

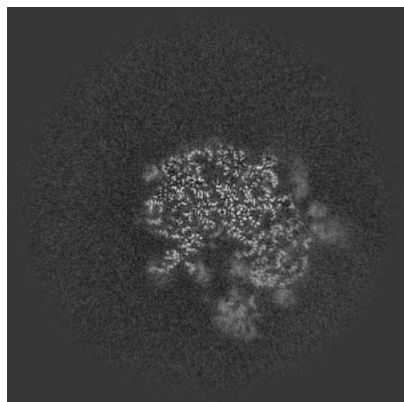


Z Index: 256

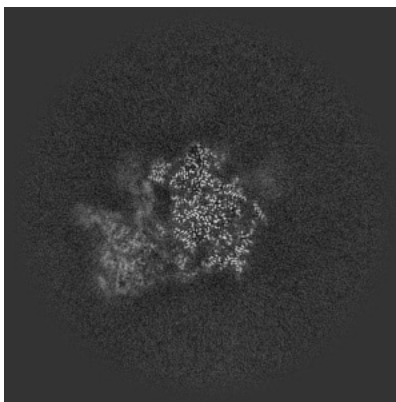
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

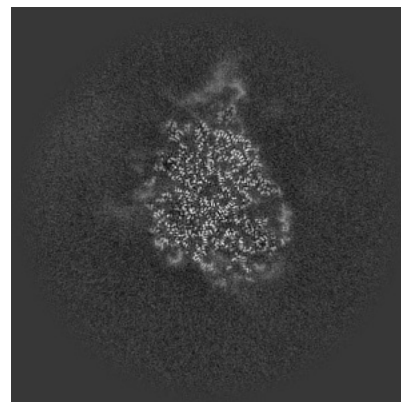
6.3.1 Primary map



X Index: 243

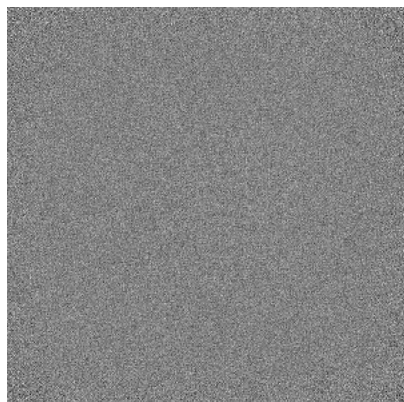


Y Index: 288

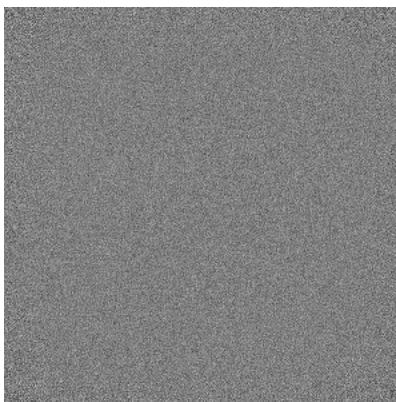


Z Index: 258

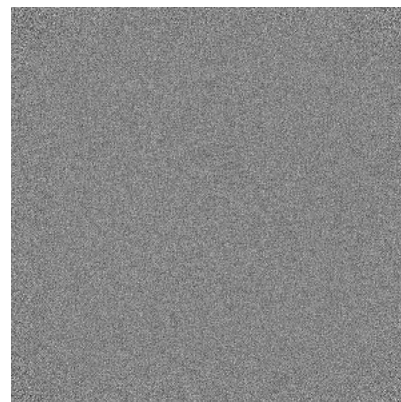
6.3.2 Raw map



X Index: 0



Y Index: 0

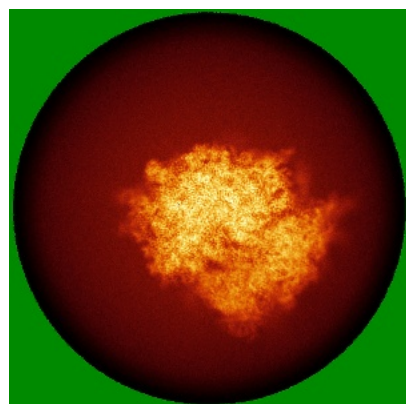


Z Index: 0

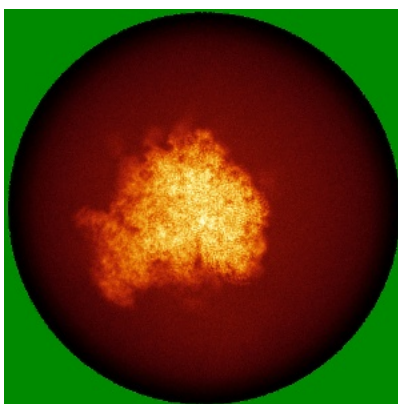
The images above show the largest variance slices of the map in three orthogonal directions.

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

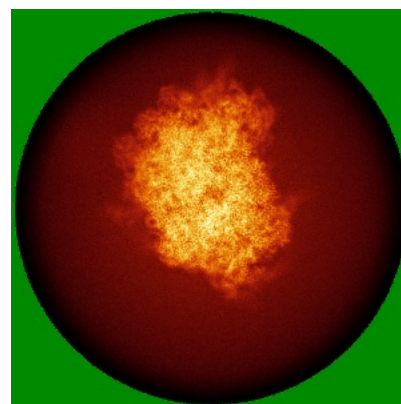
6.4.1 Primary map



X

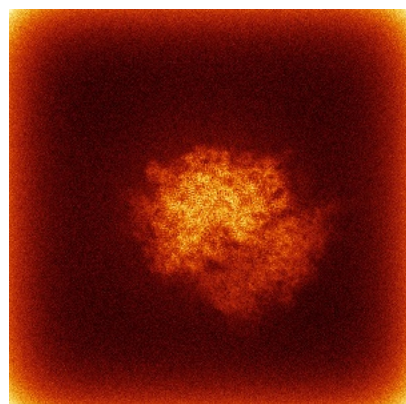


Y

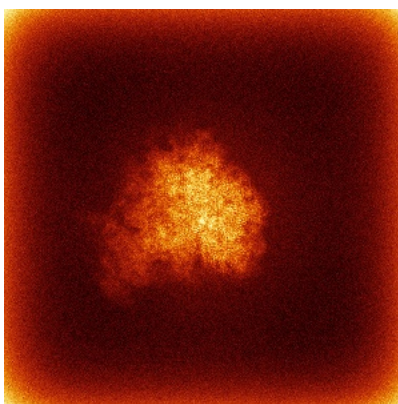


Z

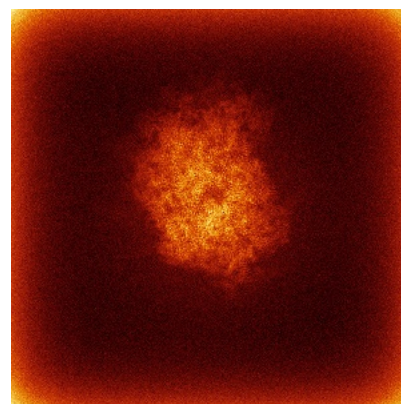
6.4.2 Raw map



X



Y

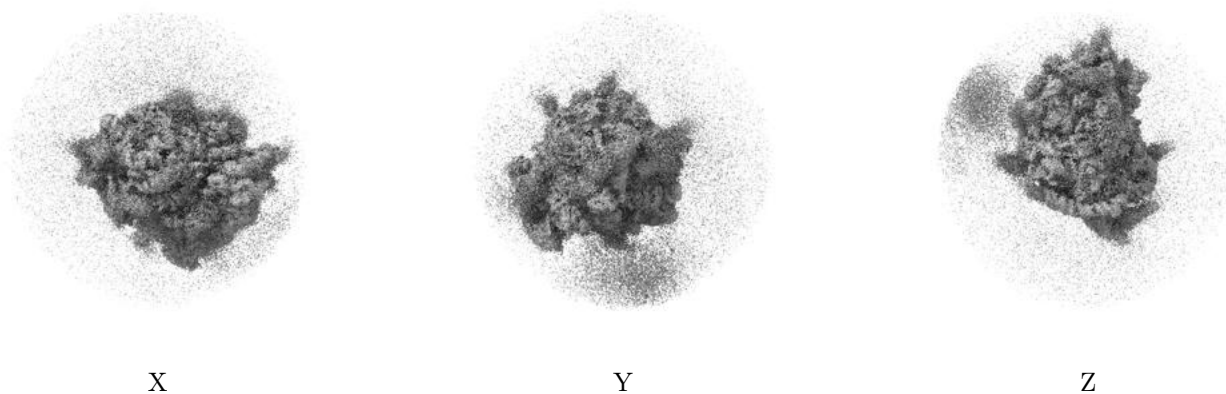


Z

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.

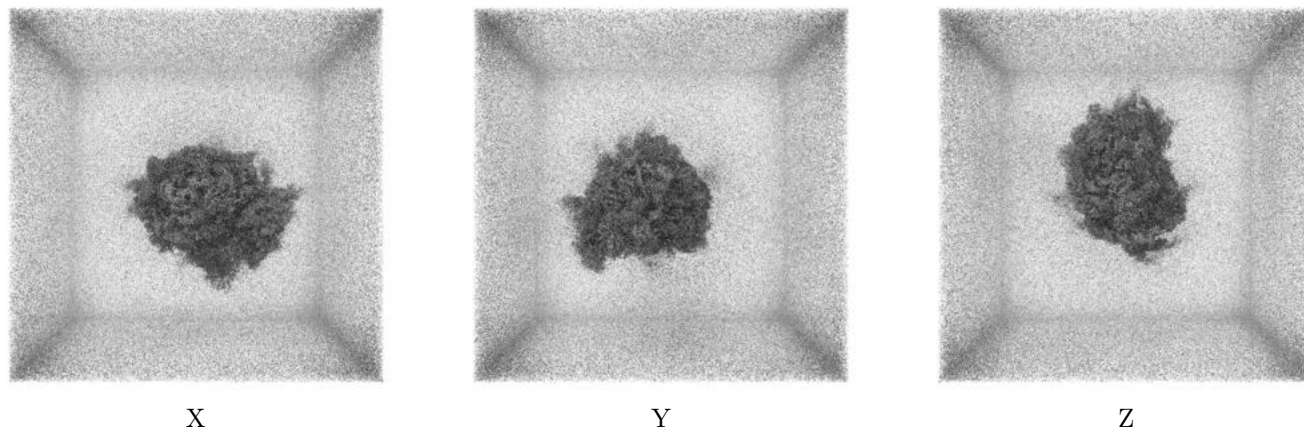
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0132. 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.

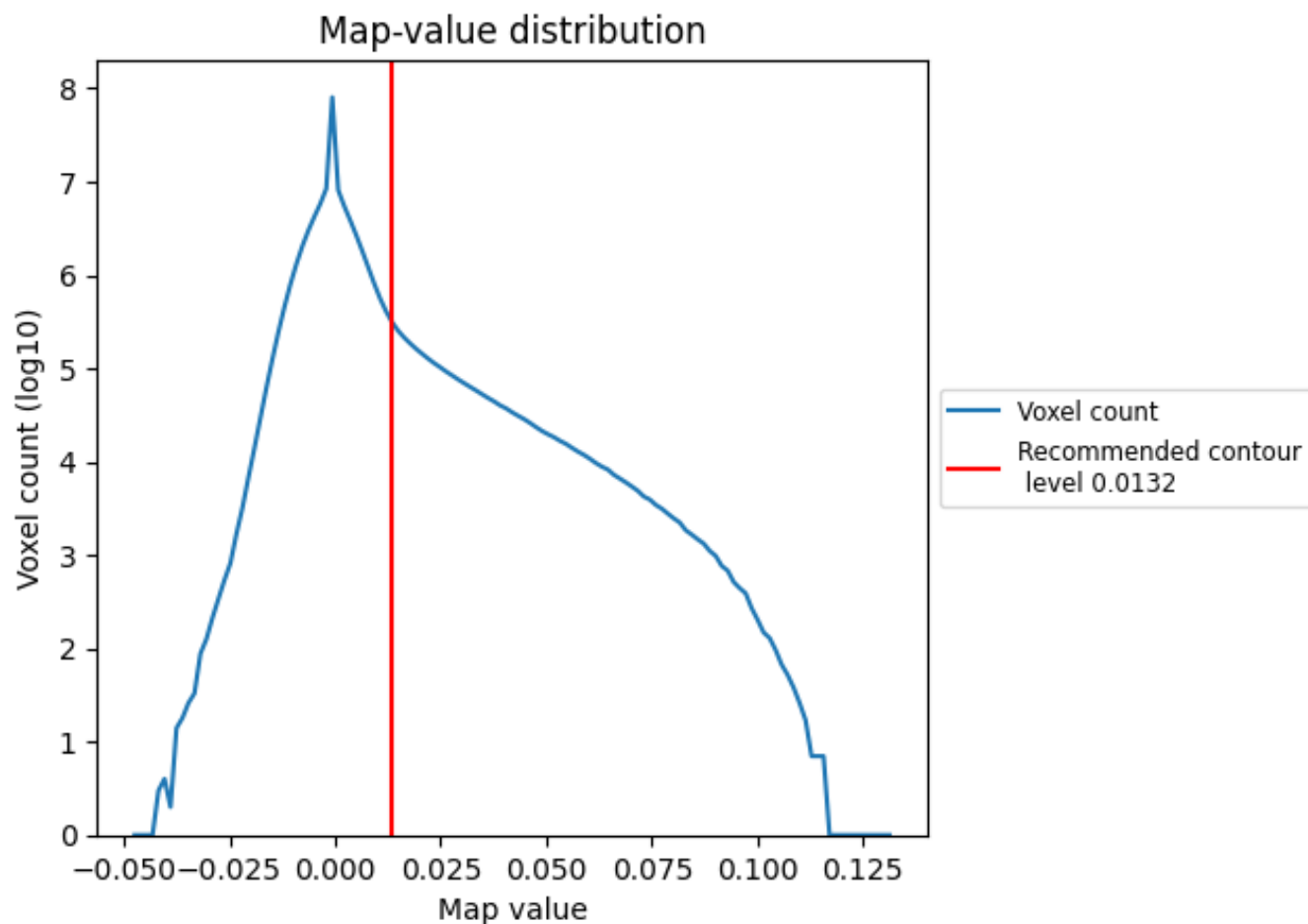
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

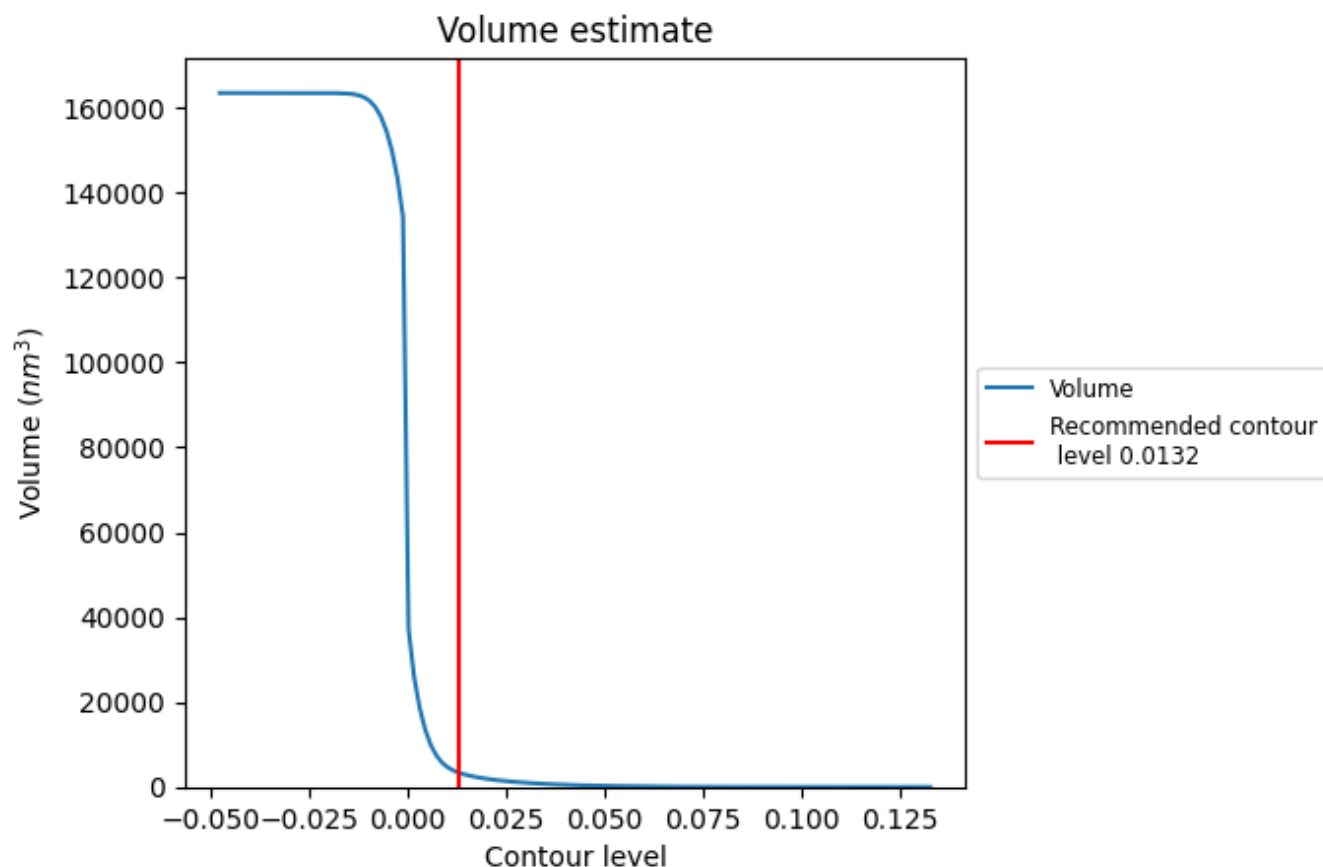
This section contains the results of statistical analysis of the map.

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.

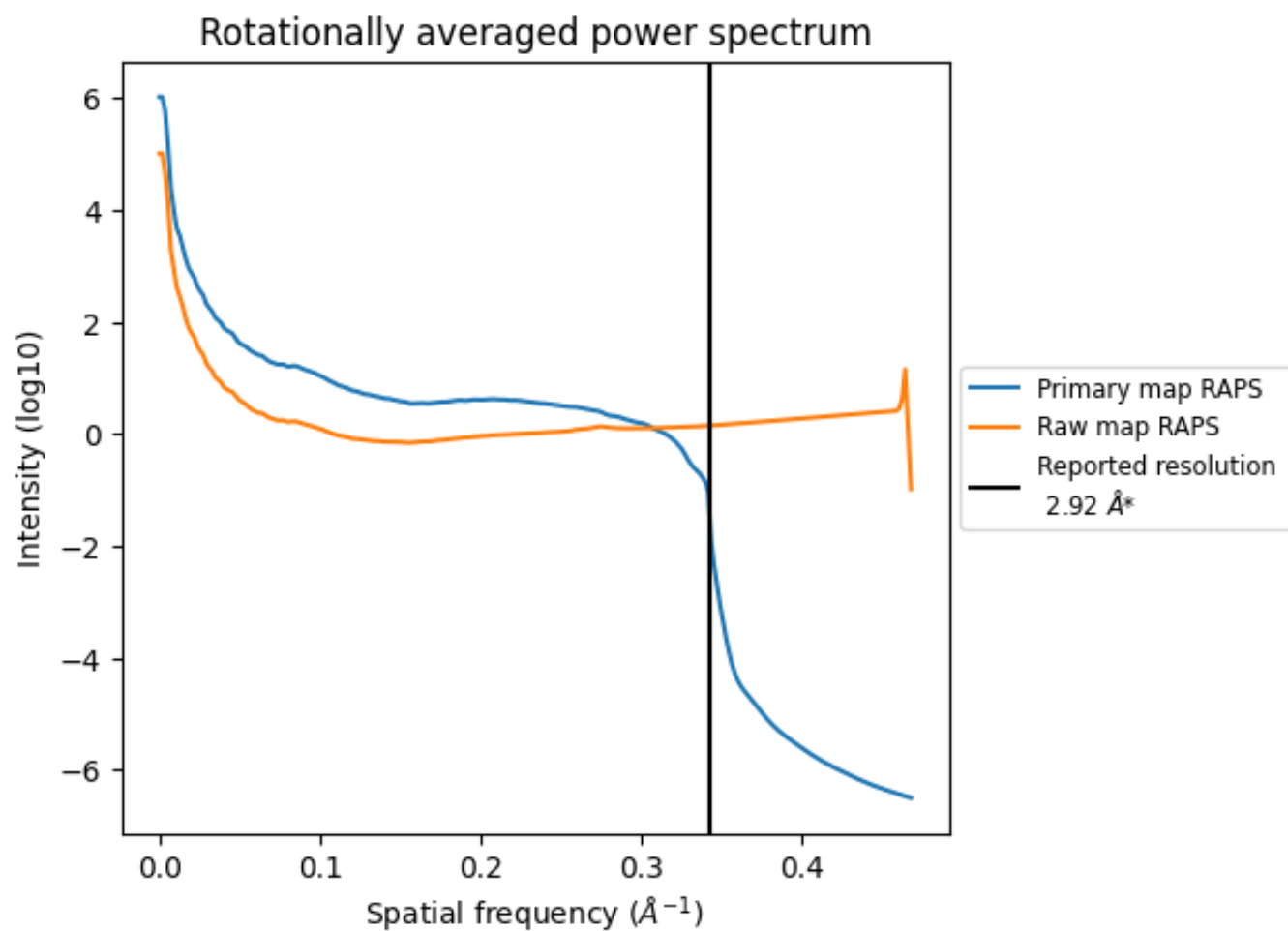
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3341 nm^3 ; this corresponds to an approximate mass of 3018 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 ⓘ

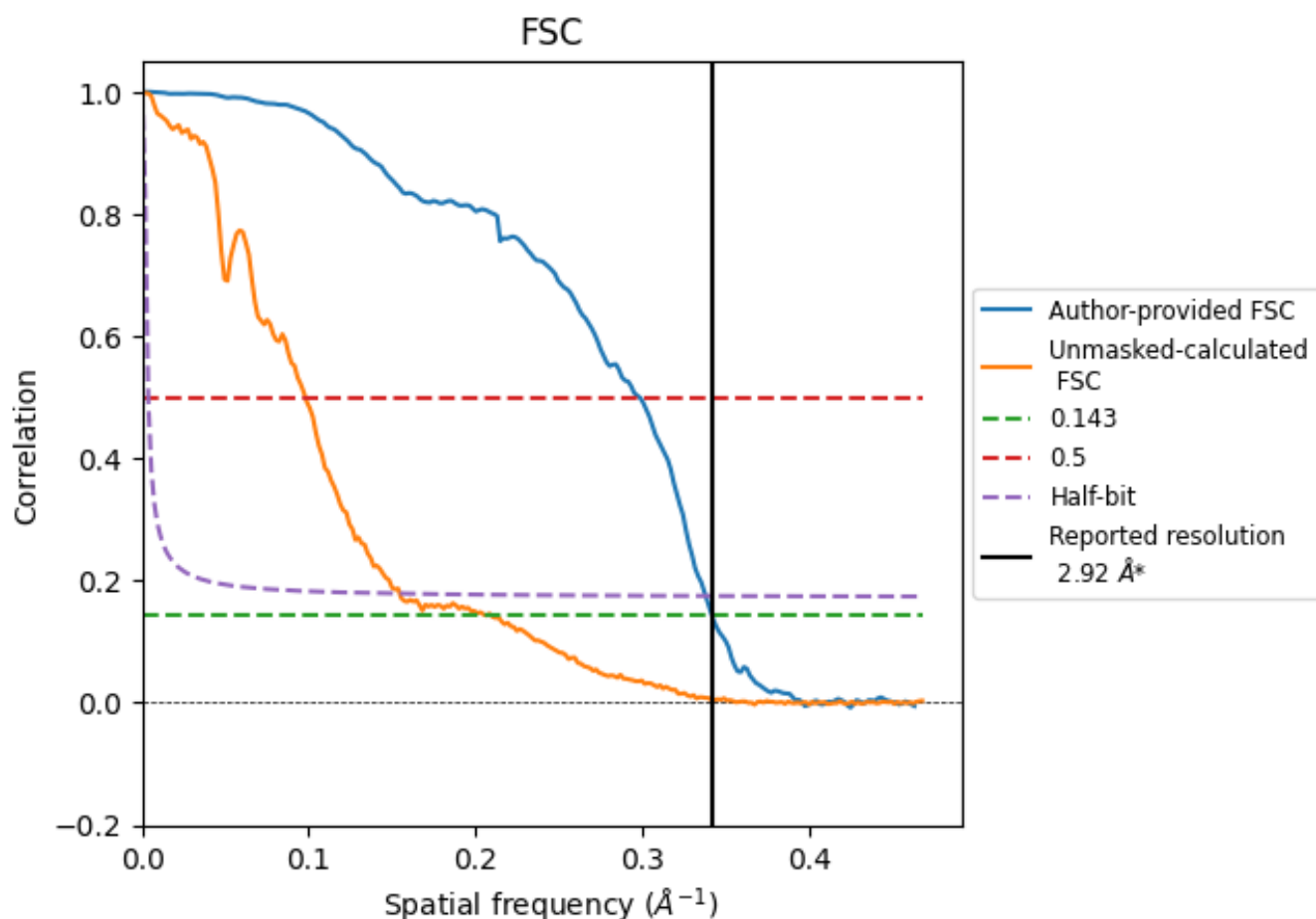


*Reported resolution corresponds to spatial frequency of 0.342 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.342 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

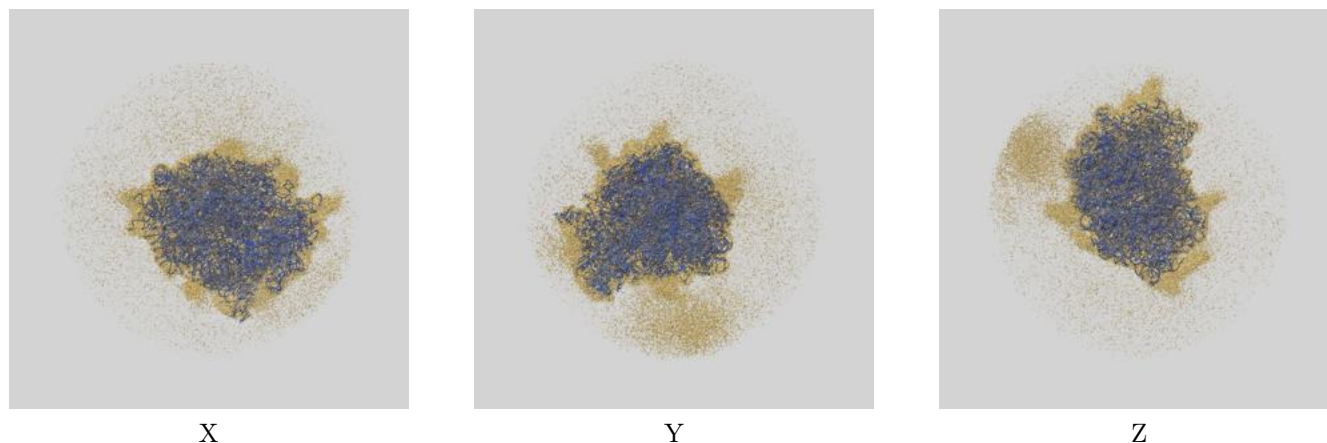
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.92	3.35	2.96
Unmasked-calculated*	4.85	10.21	6.47

*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 4.85 differs from the reported value 2.92 by more than 10 %

9 Map-model fit [i](#)

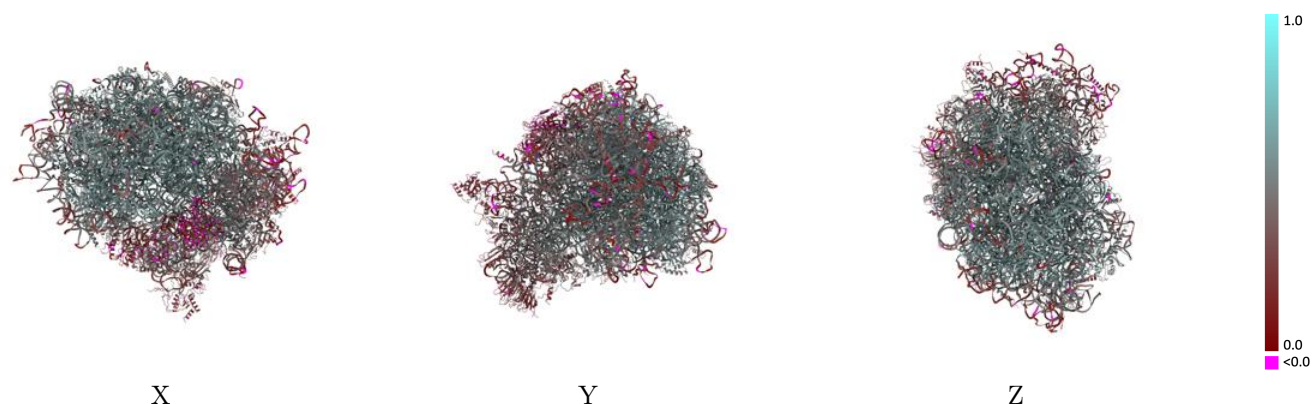
This section contains information regarding the fit between EMDB map EMD-71346 and PDB model 9P7L. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



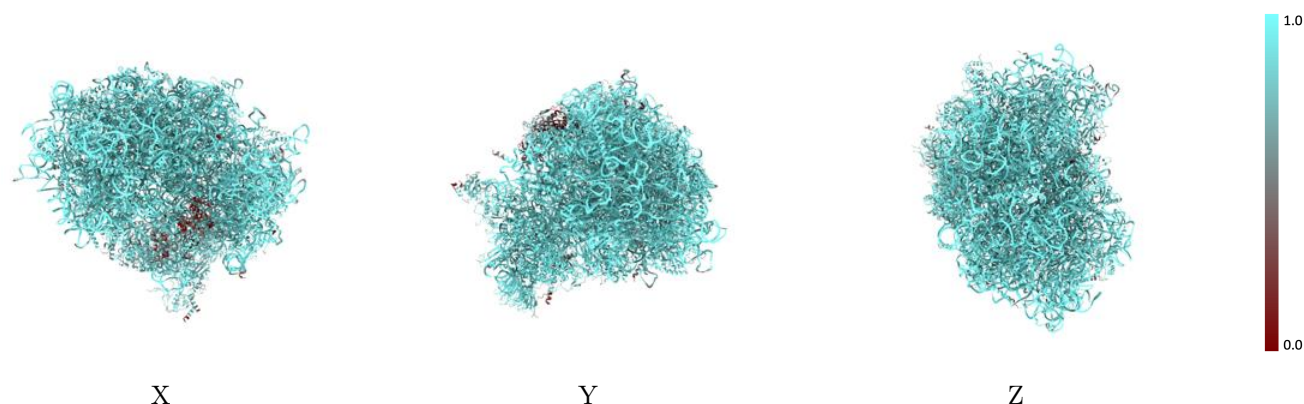
The images above show the 3D surface view of the map at the recommended contour level 0.0132 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



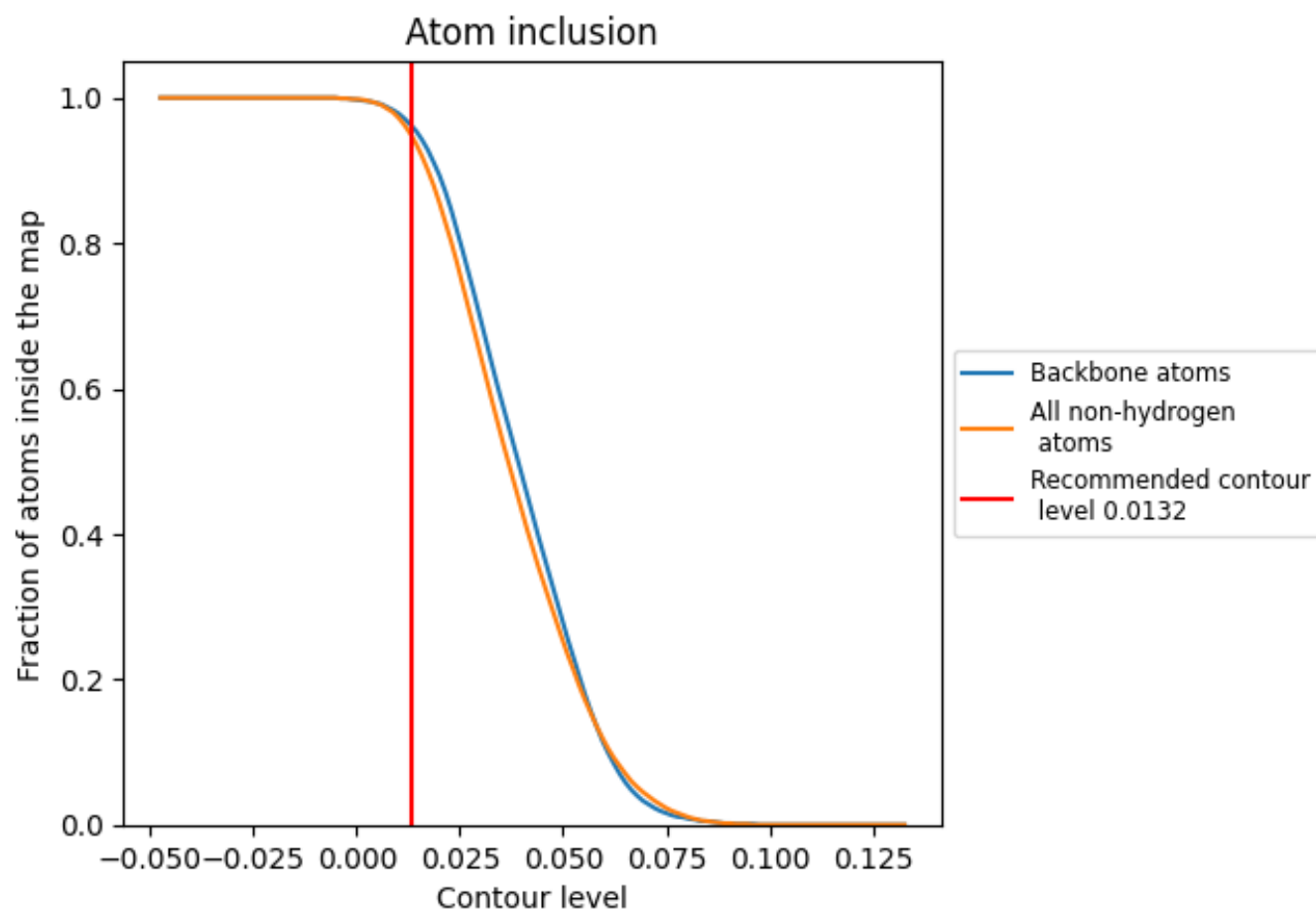
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0132).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.0132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.4680
AT	 0.8550	 0.1640
CF	 0.4840	 0.1320
CI	 0.7740	 0.3780
L5	 0.9790	 0.5070
L7	 0.9970	 0.5480
L8	 0.9880	 0.5300
LA	 0.9780	 0.5750
LB	 0.9470	 0.5570
LC	 0.9490	 0.5490
LD	 0.9550	 0.5070
LE	 0.9140	 0.4870
LF	 0.9720	 0.5530
LG	 0.9100	 0.4930
LH	 0.9570	 0.5330
LI	 0.9490	 0.5430
LJ	 0.9420	 0.4890
LL	 0.9270	 0.5220
LM	 0.9680	 0.5380
LN	 0.9920	 0.5880
LO	 0.9660	 0.5550
LP	 0.9660	 0.5640
LQ	 0.9700	 0.5720
LR	 0.9230	 0.5020
LS	 0.9740	 0.5700
LT	 0.9460	 0.5340
LU	 0.9530	 0.4690
LV	 0.9570	 0.5610
LW	 0.9010	 0.4040
LX	 0.9500	 0.5360
LY	 0.9500	 0.5400
LZ	 0.9720	 0.5230
La	 0.9800	 0.5790
Lb	 0.9100	 0.4820
Lc	 0.9550	 0.5160



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Chain	Atom inclusion	Q-score
Ld	 0.9310	 0.5370
Le	 0.9720	 0.5810
Lf	 0.9760	 0.5790
Lg	 0.9540	 0.5480
Lh	 0.9440	 0.5310
Li	 0.9320	 0.5250
Lj	 0.9840	 0.5750
Lk	 0.9160	 0.4770
Ll	 0.9600	 0.5610
Lm	 0.9470	 0.5570
Ln	 0.9620	 0.5520
Lo	 0.8530	 0.5490
Lp	 0.9460	 0.5520
Lr	 0.9620	 0.5550
Ls	 0.6280	 0.1900
Lt	 0.5590	 0.1340
Pt	 0.9680	 0.4120
S2	 0.9860	 0.4300
SA	 0.9180	 0.4200
SB	 0.9240	 0.4590
SC	 0.9650	 0.4630
SD	 0.9200	 0.3490
SE	 0.9580	 0.4170
SF	 0.8180	 0.3690
SG	 0.8980	 0.3200
SH	 0.9090	 0.3620
SI	 0.9190	 0.4400
SJ	 0.9320	 0.4000
SK	 0.9120	 0.2970
SL	 0.9030	 0.4730
SM	 0.6860	 0.1750
SN	 0.9540	 0.4900
SO	 0.9090	 0.4700
SP	 0.9020	 0.3500
SQ	 0.9210	 0.3650
SR	 0.9120	 0.3580
SS	 0.8770	 0.3600
ST	 0.9230	 0.3640
SU	 0.9150	 0.3250
SV	 0.9580	 0.4220
SW	 0.9780	 0.4900
SX	 0.9480	 0.4770

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Chain	Atom inclusion	Q-score
SY	 0.9230	 0.3340
SZ	 0.6760	 0.3160
Sa	 0.9490	 0.4850
Sb	 0.9440	 0.4580
Sc	 0.8350	 0.3920
Sd	 0.9710	 0.4150
Se	 0.8870	 0.3580
Sf	 0.8220	 0.2180
Sg	 0.8860	 0.2590