



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 05:16 AM EDT

PDB ID : 9P76 / pdb_00009p76
EMDB ID : EMD-71333
Title : In situ human eEF1A-A/T-P state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 2.83 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

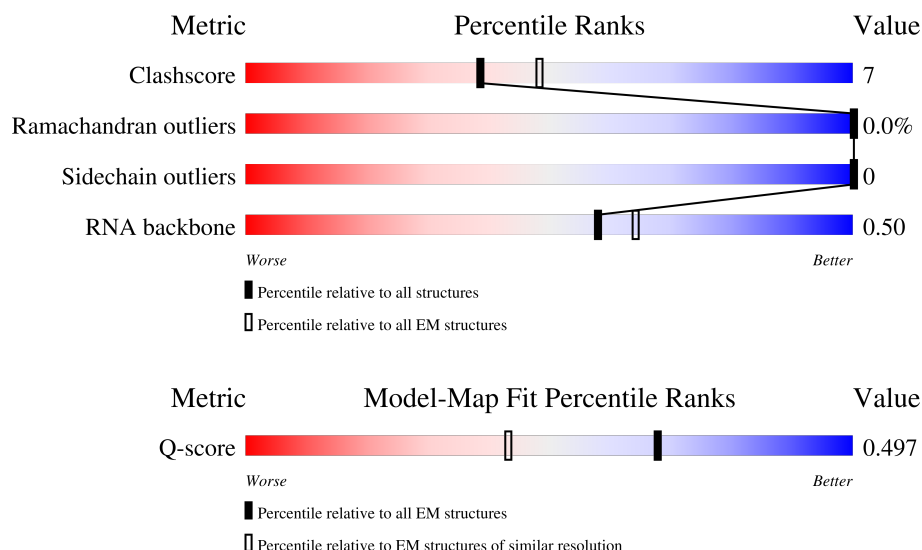
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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.



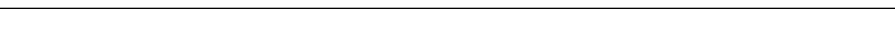
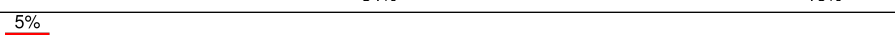
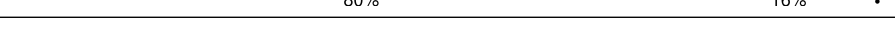
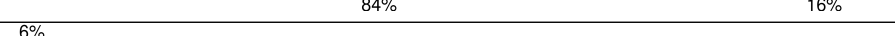
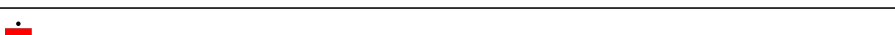
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11847 (2.33 - 3.33)

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	
2	Pt	74	
3	CF	441	

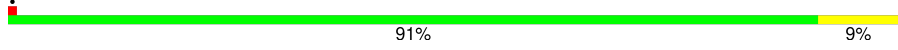
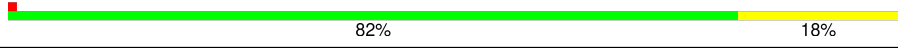
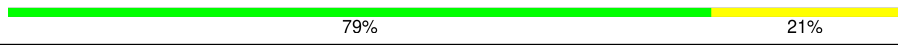
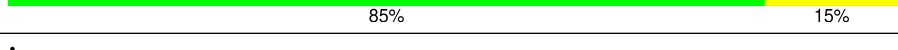
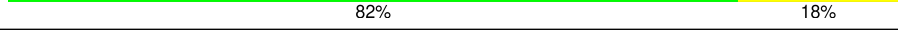
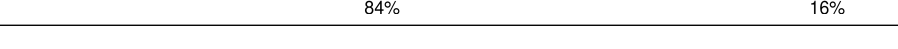
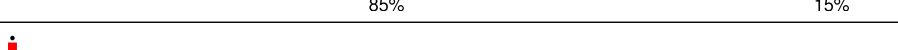
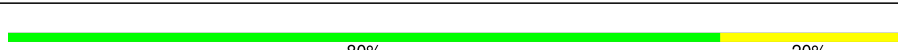
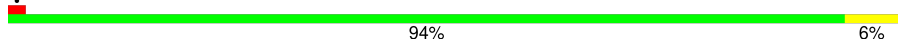
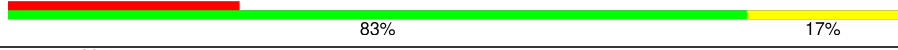
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Mol	Chain	Length	Quality of chain
4	AT	76	
5	L5	3655	
6	L7	120	
7	L8	156	
8	LA	248	
9	LB	402	
10	LC	368	
11	LD	293	
12	LE	250	
13	LF	225	
14	LG	241	
15	LH	190	
16	LI	213	
17	LJ	176	
18	LL	210	
19	LM	139	
20	LN	203	
21	LO	201	
22	LP	153	
23	LQ	187	
24	LR	187	
25	LS	175	
26	LT	159	
27	LU	101	
28	LV	131	

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Mol	Chain	Length	Quality of chain
29	LW	124	
30	LX	120	
31	LY	134	
32	LZ	135	
33	La	147	
34	Lb	121	
35	Lc	98	
36	Ld	107	
37	Le	128	
38	Lf	109	
39	Lg	114	
40	Lh	122	
41	Li	102	
42	Lj	86	
43	Lk	69	
44	Ll	50	
45	Lm	52	
46	Ln	24	
47	Lo	105	
48	Lp	91	
49	Lr	125	
50	Ls	196	
51	Lt	157	
52	SD	227	
53	SF	189	

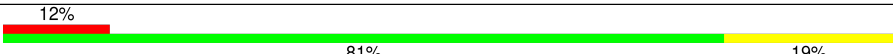
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Mol	Chain	Length	Quality of chain
54	SK	98	
55	SM	122	
56	SP	121	
57	SQ	144	
58	SR	135	
59	SS	145	
60	ST	143	
61	SU	104	
62	SZ	75	
63	Sc	64	
64	Sd	55	
65	Sf	67	
66	Sg	313	
67	SA	221	
68	SB	214	
69	SC	220	
70	SE	262	
71	SG	237	
72	SH	189	
73	SI	206	
74	SJ	185	
75	SL	153	
76	SN	150	
77	SO	137	
78	SV	83	

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Mol	Chain	Length	Quality of chain
79	SW	129	 81% 19%
80	SX	141	 82% 18%
81	SY	131	 5% 76% 24%
82	Sa	102	 83% 17%
83	Sb	83	 82% 18%
84	Se	58	 12% 81% 19%
85	S2	1740	 49% 42% 9%

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 protein called Elongation factor 1-alpha 1.

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

- Molecule 4 is a RNA chain called AT site tRNA.

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

- Molecule 5 is a RNA chain called 28S rRNA.

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

- Molecule 6 is a RNA chain called 5S rRNA.

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

- Molecule 7 is a RNA chain called 5.8S rRNA.

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

- Molecule 8 is a protein called 60S ribosomal protein L8.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 12 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 13 is a protein called 60S ribosomal protein L7.

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

- Molecule 14 is a protein called 60S ribosomal protein L7a.

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

- Molecule 15 is a protein called 60S ribosomal protein L9.

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

- Molecule 16 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LI	213	Total	C	N	O	S	0	0
			1711	1082	329	285	15		

- Molecule 17 is a protein called 60S ribosomal protein L11.

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

- Molecule 18 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 19 is a protein called 60S ribosomal protein L14.

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

- Molecule 20 is a protein called 60S ribosomal protein L15.

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

- Molecule 21 is a protein called 60S ribosomal protein L13a.

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

- Molecule 22 is a protein called 60S ribosomal protein L17.

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

- Molecule 23 is a protein called 60S ribosomal protein L18.

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

- Molecule 24 is a protein called 60S ribosomal protein L19.

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

- Molecule 25 is a protein called 60S ribosomal protein L18a.

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

- Molecule 26 is a protein called 60S ribosomal protein L21.

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

- Molecule 27 is a protein called Heparin-binding protein HBp15.

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

- Molecule 28 is a protein called 60S ribosomal protein L23.

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

- Molecule 29 is a protein called Ribosomal protein L24.

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

- Molecule 30 is a protein called 60S ribosomal protein L23a.

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

- Molecule 31 is a protein called 60S ribosomal protein L26.

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

- Molecule 32 is a protein called 60S ribosomal protein L27.

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

- Molecule 33 is a protein called 60S ribosomal protein L27a.

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

- Molecule 34 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 35 is a protein called 60S ribosomal protein L30.

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

- Molecule 36 is a protein called 60S ribosomal protein L31.

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

- Molecule 37 is a protein called 60S ribosomal protein L32.

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

- Molecule 38 is a protein called 60S ribosomal protein L35a.

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

- Molecule 39 is a protein called 60S ribosomal protein L34.

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

- Molecule 40 is a protein called 60S ribosomal protein L35.

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

- Molecule 41 is a protein called 60S ribosomal protein L36.

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

- Molecule 42 is a protein called 60S ribosomal protein L37.

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

- Molecule 43 is a protein called 60S ribosomal protein L38.

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

- Molecule 44 is a protein called 60S ribosomal protein L39.

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

- Molecule 45 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 46 is a protein called 60S ribosomal protein L41.

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

- Molecule 47 is a protein called 60S ribosomal protein L36a.

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

- Molecule 48 is a protein called 60S ribosomal protein L37a.

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

- Molecule 49 is a protein called 60S ribosomal protein L28.

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

- Molecule 50 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 51 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 52 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 53 is a protein called 40S ribosomal protein S5.

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

- Molecule 54 is a protein called 40S ribosomal protein S10.

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

- Molecule 55 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 56 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 57 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 58 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 59 is a protein called 40S ribosomal protein S18.

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

- Molecule 60 is a protein called 40S ribosomal protein S19.

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

- Molecule 61 is a protein called 40S ribosomal protein S20.

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

- Molecule 62 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 63 is a protein called 40S ribosomal protein S28.

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

- Molecule 64 is a protein called 40S ribosomal protein S29.

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

- Molecule 65 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 66 is a protein called Receptor of activated protein C kinase 1.

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

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

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

- Molecule 68 is a protein called 40S ribosomal protein S3a.

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

- Molecule 69 is a protein called 40S ribosomal protein S2.

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

- Molecule 70 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 71 is a protein called 40S ribosomal protein S6.

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

- Molecule 72 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 73 is a protein called 40S ribosomal protein S8.

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

- Molecule 74 is a protein called 40S ribosomal protein S9.

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

- Molecule 75 is a protein called 40S ribosomal protein S11.

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

- Molecule 76 is a protein called 40S ribosomal protein S13.

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

- Molecule 77 is a protein called 40S ribosomal protein S14.

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

- Molecule 78 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 79 is a protein called 40S ribosomal protein S15a.

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

- Molecule 80 is a protein called 40S ribosomal protein S23.

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

- Molecule 81 is a protein called 40S ribosomal protein S24.

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

- Molecule 82 is a protein called 40S ribosomal protein S26.

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

- Molecule 83 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 84 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 85 is a RNA chain called 18S rRNA.

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

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

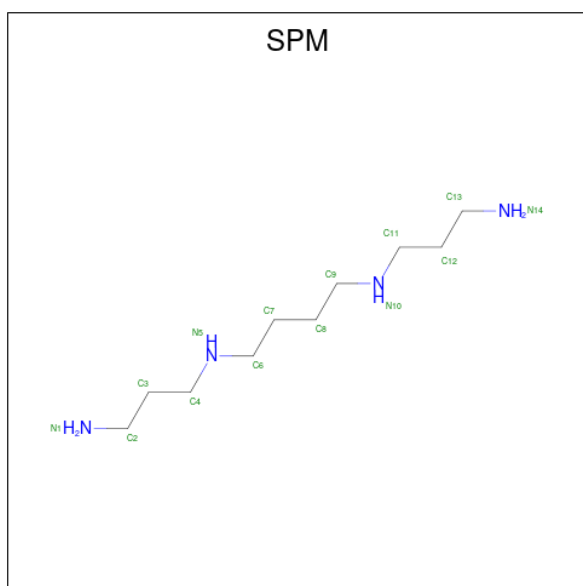
Mol	Chain	Residues	Atoms		AltConf
86	L5	178	Total	Mg	0
			178	178	
86	L7	3	Total	Mg	0
			3	3	
86	L8	4	Total	Mg	0
			4	4	
86	LA	1	Total	Mg	0
			1	1	
86	LB	1	Total	Mg	0
			1	1	
86	LP	1	Total	Mg	0
			1	1	
86	LV	1	Total	Mg	0
			1	1	
86	Le	1	Total	Mg	0
			1	1	
86	Lj	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
86	SS	1	Total	Mg	0
			1	1	
86	SG	1	Total	Mg	0
			1	1	
86	S2	26	Total	Mg	0
			26	26	

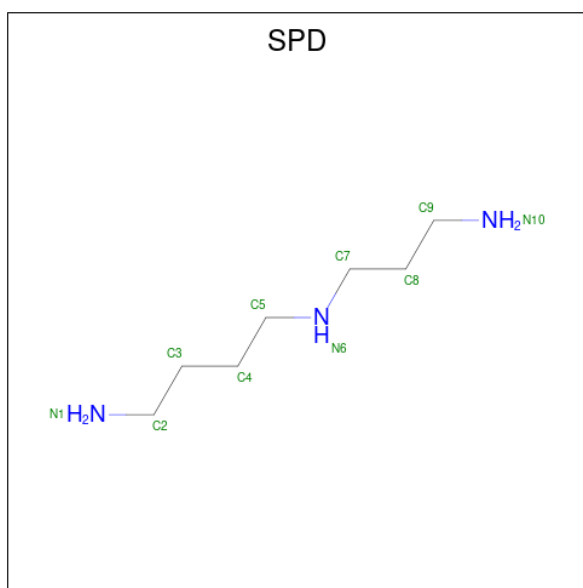
- Molecule 87 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



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

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

Interest" by depositor).



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

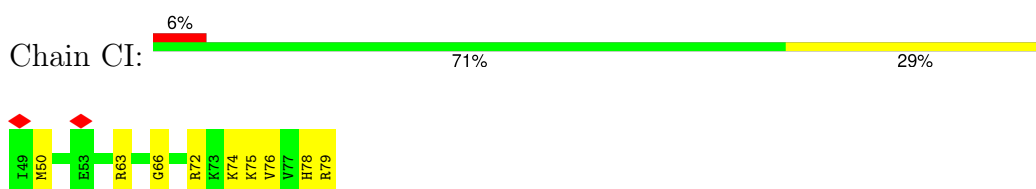
- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

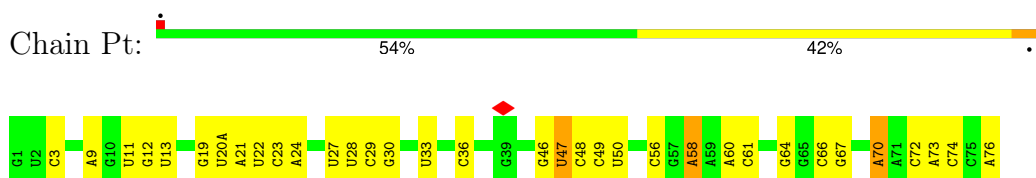
3 Residue-property plots [i](#)

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.

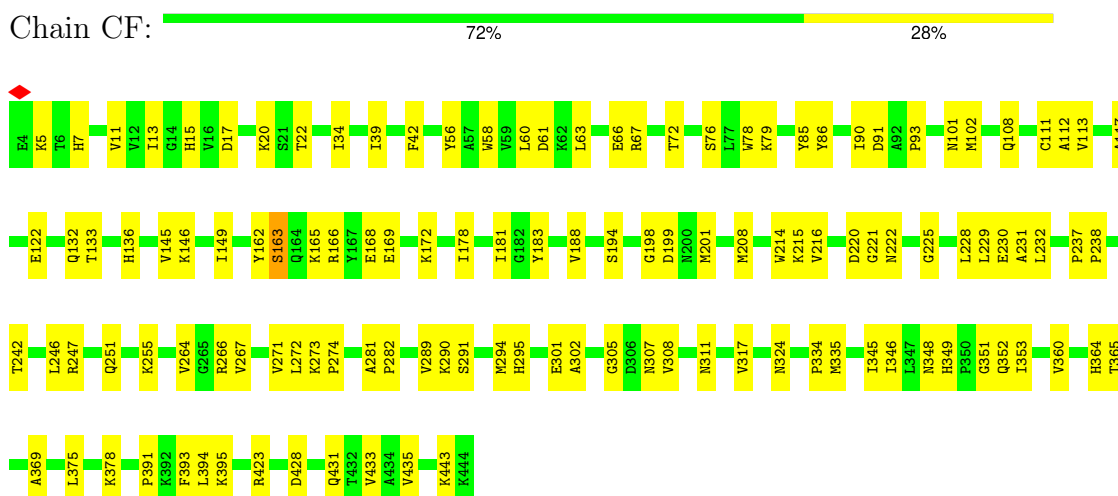
- Molecule 1: Transcription factor BTF3



- Molecule 2: P site tRNA



- Molecule 3: Elongation factor 1-alpha 1



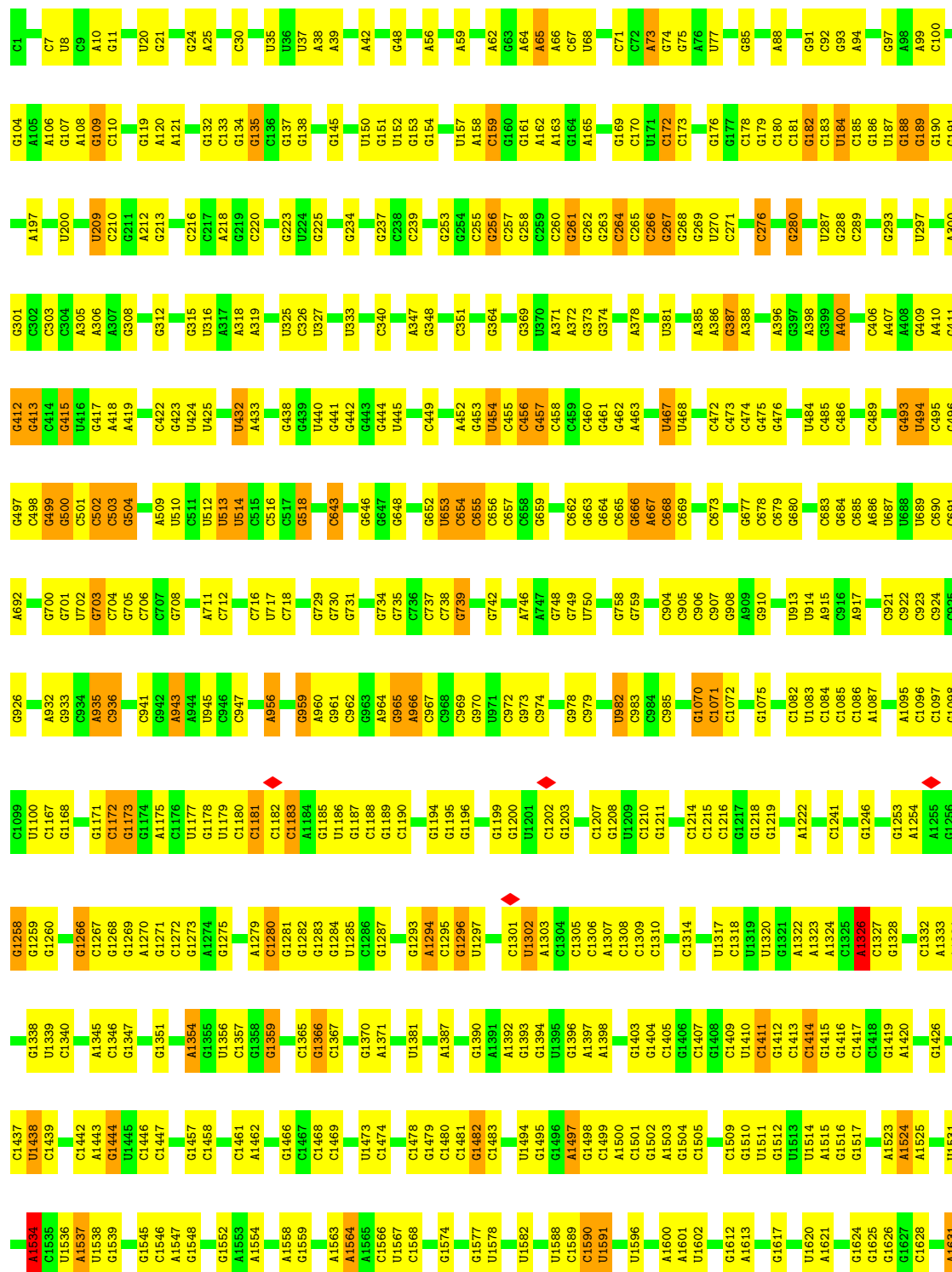
- Molecule 4: AT site tRNA



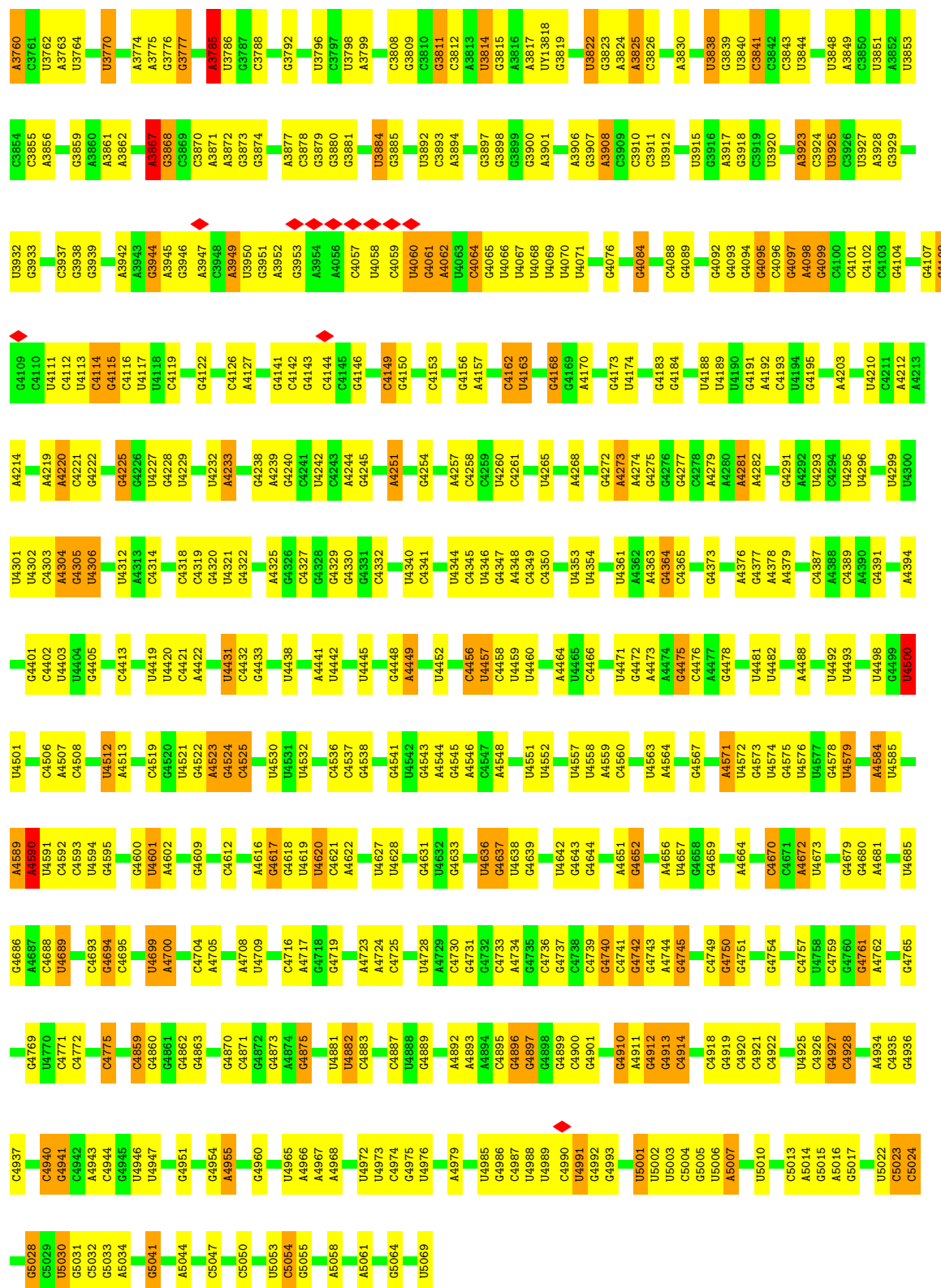


● Molecule 5: 28S rRNA

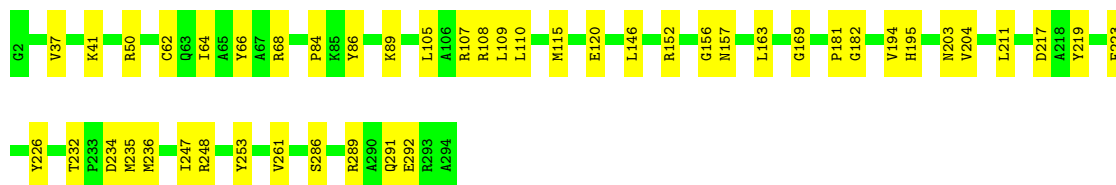
Chain L5: 55% 38% 7%



G3659	C2909	C2814	C2719	C2627	A2537	U2436	U2329	G2094	U1992	C1913	G1811	A1632
C3660	G2910	A2815	C2720	C2627	U2538	C2437	G2330	A2095	C1993	G1912	G1815	G1633
G3661	C3584	G2816	G2721	U2632	C2539	G2438	G2331	G2096	C1994	C1913	G1815	A1634
A3662	G3585			U2633	C2540	G2449	G2332	G2097	G1995	C1732	G1818	C1732
A3663	C3588	G2822	G2724	U2634	A2543	A2448	G2333	G2098	G1996	G1733	G1819	A1637
A3664	G2823	G2823	A2725	U2635	G2544	A2449	G2334	C2101	A1998	G1734	G1820	A1638
A3665	G3589	C2824	G2726	U2636	U2545	A2453	G2335	G2102	U1999	G1735	G1821	U1639
C3666	G3590	A2825		U2637	G2546	A2458	G2336	G2103	A2000		G1822	C1640
	C3591	U2826	G2732	U2638	G2547	C2458	G2337	G2104	G2001	G1739	G1823	G1641
	G3592	G2827	C2733	U2639	G2547	C2459	G2338	G2105	A2002	G1740	G1824	A1642
	C3593	U2828		U2640	G2550	C2464	G2339	G2106	G2003	A1742	A1825	C1645
	C3594	U2829	C2739	A2641	G2550	C2465	G2340	G2107	G2004	A1743	A1825	A1646
	U3595						G2341			U1744		U1647
	A3596	A2832	G2742				G2342		G2005		U1834	
	G3597	A2743	A2743	G2648	U2554	U2468	G2343	C2110	U2006	C1931	G1835	G1654
	C3598	A2744	A2744	G2649	G2555	C2469	G2344	G2111	G2007	A1932	G1836	C1655
	A3599	A2745		U2556	G2556	G2470	G2345	G2112	U2008	G1933	A1837	
	G3600	A2746		G2557	G2557	G2471	G2346	G2113	A2009	A1934	G1838	
							G2347	G2114	G2010	C1935	G1839	C1661
	A3604	G2838		C2653	A2573	G2472	U2362	G2115	A2010	C1936	G1842	C1662
	U3605	U2839	C2749	C2654	C2579	G2473	G2363	G2116	G2011		G1843	C1663
	G3606		G2750	C2655		G2474	G2364	G2117	A2012		G1844	
	A3607	A2844			A2565	G2475		G2118	G2017		G1845	G1667
	G3608	A2845	G2756	G2658	C2568	C2478	A2368	G2119	C2018		G1846	A1668
	A3609	G2846	A2757	G2659	G2569	G2479	A2369	G2120	G2019		G1847	A1669
	A3610	G2847	G2758	G2660	U2570	G2480	A2370	G2121	C2020		G1848	
	A3611	G2848	G2759	G2661	G2571	G2481	C2377	G2122	U2020		G1849	
				U2662	G2572	G2482	G2378	G2123	G2021		G1850	
	G3615	G2855	U2761	U2663	C2573	G2483	A2379	G2124	C2022		G1851	U1672
		C2856	G2762	U2664	A2573	G2484	G2380	G2125	G2023		G1852	U1673
	G3619	G2861	U2763	U2665		G2485	A2381	G2126	C2024		G1853	
	A3624	G2862	U2764	G2666	G2579	G2486	U2382	G2127	A2025		G1854	U1676
	G3625	U2863	A2765	G2667	U2580	G2487	U2383	G2128	G2026		G1855	U1677
	G3626	A2864	G2766	C2670	A2581	G2488	U2384	G2129	U2027		G1856	C1678
	G3627	U2865	U2767	C2671	C2582	G2489	A2385	G2130	G2028		G1857	A1679
		G2866	U2768	C2672		G2490	A2386	G2131	G2029		G1858	G1690
	A3630	C2867	C2770	G2675	G2586	G2491	G2387	G2132	G2030		G1859	
		A2870		A2676	A2587	G2492	U2388	G2133	G2031		G1860	U1683
	C3633	A2871	G2773	G2677	C2588	G2493	G2389	G2134	G2032		G1861	A1684
	G3634			U2678	C2589	G2494	G2400	G2135	G2033		G1862	G1685
	A3635	G2876	G2777	U2679	G2590	G2495	A2401	G2136	U2034		G1863	C1686
	C3636	G2877	G2778	G2687	A2591	G2496	G2402	G2137	G2035		G1864	U1687
	U3637			G2688	G2592	G2497	A2403	G2138	G2036		G1865	G1688
	G3638	C2890	A2783	G2689	A2601	G2498	G2404	G2139	G2037		G1866	
	U3639	U2891	G2784	G2690	G2602	G2499	G2405	G2140	U2038		G1867	C1696
	U3640	A2894	U2785	A2696	C2603		U2406	G2141	G2039		G1868	
	U3641		G2786	C2702	C2607		C2411	G2142	G2040		G1869	U1775
			U2790		G2610		A2412	G2143	A2041		G1870	
	U3644	G2898	U2803	G2706	A2611	A2513	U2413	G2144	G2042		G1871	
	U3645	C2899	C2804	U2707	G2612	G2514	U2414	G2145	G2043		G1872	
	A3646	U2900	G2805	U2708	C2613	G2515	U2415	G2146	G2044		G1873	U1779
	A3647	G2901	C2806	G2709	G2614	G2516	A2417	G2147	G2045		G1874	A1780
	A3648	G2902	A2806	G2710	G2615	G2517	G2418	G2148	G2046		G1875	U1781
		G2903		G2711	G2616	G2518	G2419	G2149	G2047		G1876	U1782
	G3654	U2904	G2809	G2712	A2621	G2519	G2420	G2150	G2048		G1877	
	C3655	C2905	U2810		G2622	U2520	G2421	G2151	U2049		G1878	C1785
	U3656	G2906	G2811	C2716	A2623	C2521	G2422	G2152	G2050		G1879	A1786
	G3657	U2907	A2812	G2717	G2624	G2522	G2423	G2153	G2051		G1880	A1787
				U2718		A2529	G2424	G2154	G2052		G1881	A1788
							G2425	G2155	G2053		G1882	C1789
								G2156	A2054		G1883	
								G2157	G2055		G1884	G1705
								G2158	G2056		G1885	
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								G2160	G2058		G1887	G1704
								G2161	G2059		G1888	C1705
								G2162	G2060		G1889	
								G2163	G2061		G1890	
								G2164	G2062		G1891	
								G2165	G2063		G1892	
								G2166	G2064		G1893	
								G2167	G2065		G1894	
								G2168	G2066		G1895	
								G2169	G2067		G1896	C1717
								G2170	G2068		G1897	G1718
								G2171	G2069		G1898	A1804
								G2172	G2070		G1899	A1719
								G2173	G2071		G1900	
								G2174	G2072		G1901	
								G2175	G2073		G1902	
								G2176	G2074		G1903	
								G2177	G2075		G1904	
								G2178	G2076		G1905	
								G2179	G2077		G1906	
								G2180	G2078		G1907	
								G2181	G2079		G1908	
								G2182	G2080		G1909	
								G2183	G2081		G1910	
								G2184	G2082		G1911	
								G2185	G2083		G1912	
								G2186	G2084		G1913	
								G2187	G2085		G1914	
								G2188	G2086		G1915	
								G2189	G2087		G1916	
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								G2195	G2093		G1922	
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								G2199	G2097		G1926	
								G2200	G2098		G1927	
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								G2202	G2100		G1929	
								G2203	G2101		G1930	
								G2204	G2102		G1931	
								G2205	G2103		G1932	
								G2206	G2104		G1933	
								G2207	G2105		G1934	
								G2208	G2106		G1935	
								G2209	G2107		G1936	
								G2210	G2108		G1937	
								G2211	G2109		G1938	
								G2212	G2110		G1939	
								G2213	G2111		G1940	
								G2214	G2112		G1941	
								G2215	G2113		G1942	
								G2216	G2114		G1943	
								G2217	G2115		G1944	
								G2218	G2116		G1945	
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								G2220	G2118		G1947	
								G2221	G2119		G1948	
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								G2225	G2123		G1952	
								G2226	G2124		G1953	
								G2227	G2125		G1954	
								G2228	G2126		G1955	
								G2229	G2127		G1956	
								G2230	G2128		G1957	
								G2231	G2129		G1958	
								G2232	G2130		G1959	
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								G2234	G2132		G1961	
								G2235	G2133		G1962	
								G22				

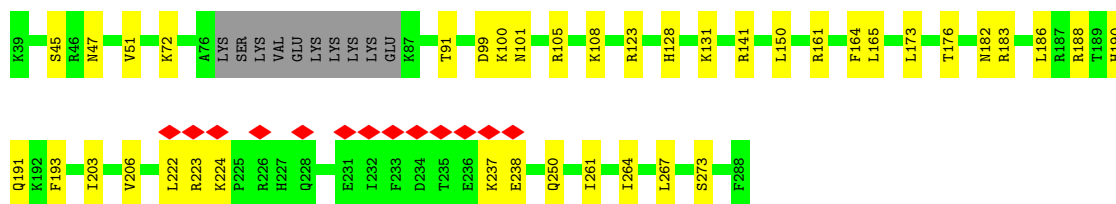


Chain LD:  84% 16%



- Molecule 12: Large ribosomal subunit protein eL6

Chain LE:  5% 80% 16%



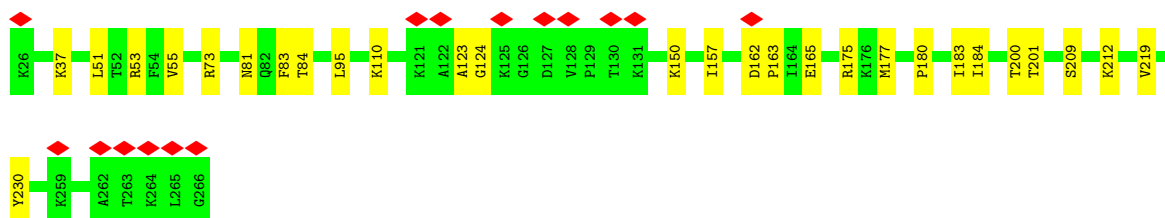
- Molecule 13: 60S ribosomal protein L7

Chain LF:  84% 16%



- Molecule 14: 60S ribosomal protein L7a

Chain LG:  6% 88% 12%



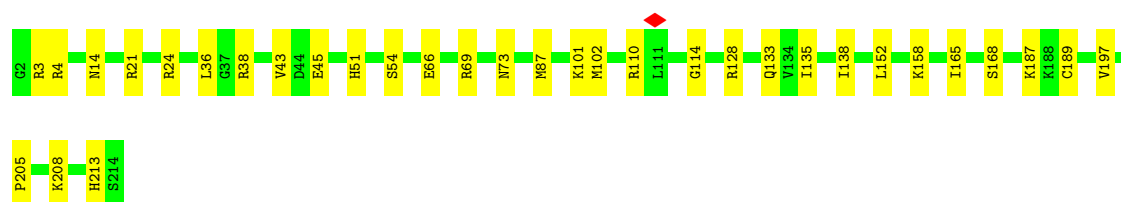
- Molecule 15: 60S ribosomal protein L9

Chain LH:  86% 14%



- Molecule 16: Ribosomal protein uL16-like

Chain LI:  85% 15%



- Molecule 17: 60S ribosomal protein L11

Chain LJ: 80% 17%



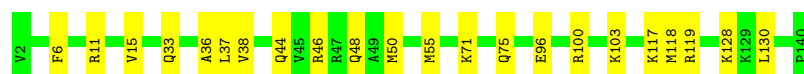
- Molecule 18: Large ribosomal subunit protein eL13

Chain LL: 90% 10%



- Molecule 19: 60S ribosomal protein L14

Chain LM: 84% 16%



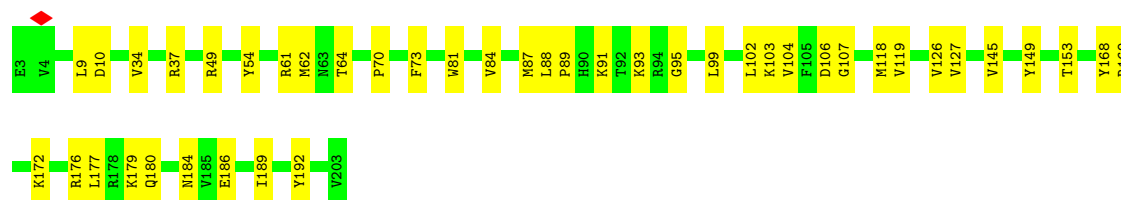
- Molecule 20: 60S ribosomal protein L15

Chain LN: 89% 11%



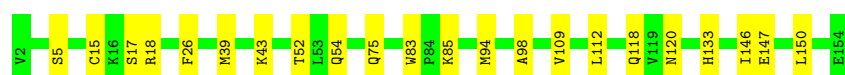
- Molecule 21: 60S ribosomal protein L13a

Chain LO: 79% 21%



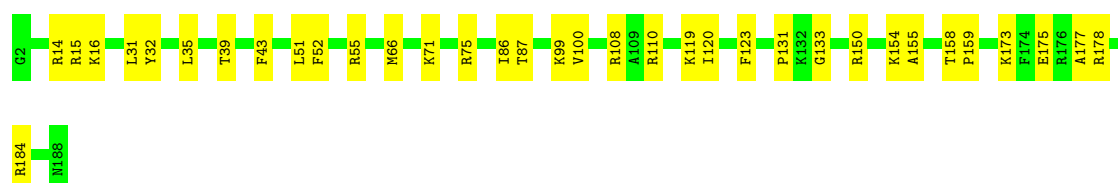
- Molecule 22: 60S ribosomal protein L17

Chain LP:  86% 14%



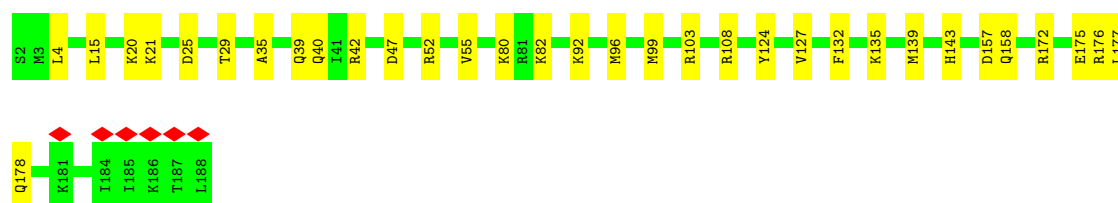
- Molecule 23: 60S ribosomal protein L18

Chain LQ:  81% 19%



- Molecule 24: 60S ribosomal protein L19

Chain LR:  82% 18%



- Molecule 25: 60S ribosomal protein L18a

Chain LS:  83% 17%



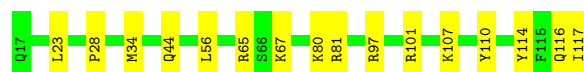
- Molecule 26: 60S ribosomal protein L21

Chain LT:  82% 18%



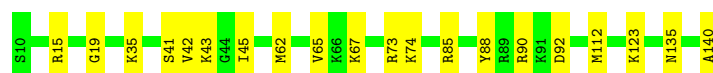
- Molecule 27: Heparin-binding protein HBp15

Chain LU:  84% 16%



- Molecule 28: 60S ribosomal protein L23

Chain LV:  85% 15%

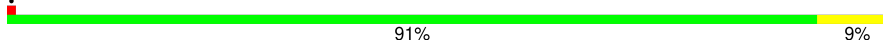


- Molecule 29: Ribosomal protein L24

Chain LW:  77% 17% 6%



- Molecule 30: 60S ribosomal protein L23a

Chain LX:  91% 9%



- Molecule 31: 60S ribosomal protein L26

Chain LY:  82% 18%



- Molecule 32: 60S ribosomal protein L27

Chain LZ:  79% 21%



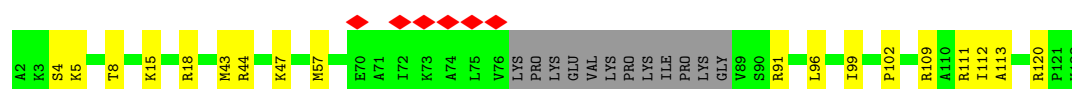
- Molecule 33: 60S ribosomal protein L27a

Chain La:  89% 11%



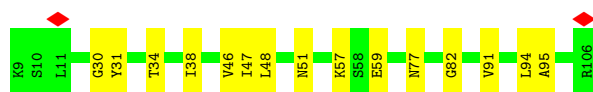
- Molecule 34: Large ribosomal subunit protein eL29

Chain Lb:  5% 75% 15% 10%



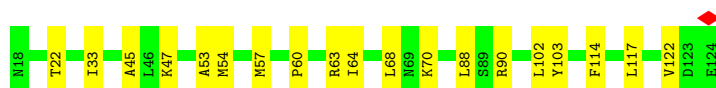
- Molecule 35: 60S ribosomal protein L30

Chain Lc:  85% 15%



- Molecule 36: 60S ribosomal protein L31

Chain Ld:  82% 18%



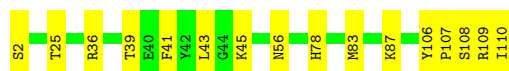
- Molecule 37: 60S ribosomal protein L32

Chain Le:  84% 16%



- Molecule 38: 60S ribosomal protein L35a

Chain Lf:  85% 15%



- Molecule 39: 60S ribosomal protein L34

Chain Lg:  85% 15%



- Molecule 40: 60S ribosomal protein L35

Chain Lh:  83% 17%



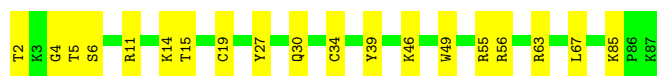
- Molecule 41: 60S ribosomal protein L36

Chain Li:  90% 10%



- Molecule 42: 60S ribosomal protein L37

Chain Lj:  78% 22%



- Molecule 43: 60S ribosomal protein L38

Chain Lk:  75% 25%



- Molecule 44: 60S ribosomal protein L39

Chain Ll:  80% 20%



- Molecule 45: Large ribosomal subunit protein eL40

Chain Lm:  88% 12%



- Molecule 46: 60S ribosomal protein L41

Chain Ln:  79% 21%



- Molecule 47: 60S ribosomal protein L36a

Chain Lo:  5% 87% 13%



- Molecule 48: 60S ribosomal protein L37a

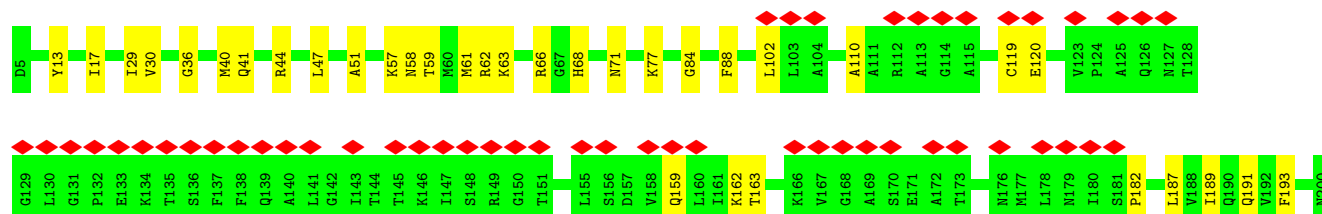
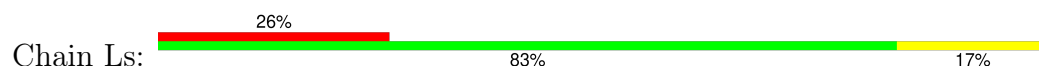
Chain Lp:  89% 11%



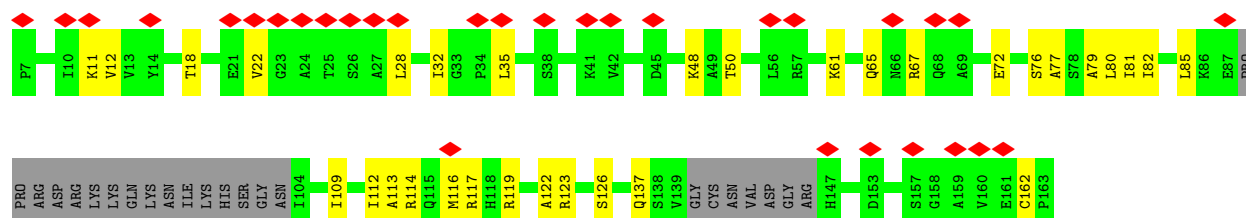
- Molecule 49: 60S ribosomal protein L28



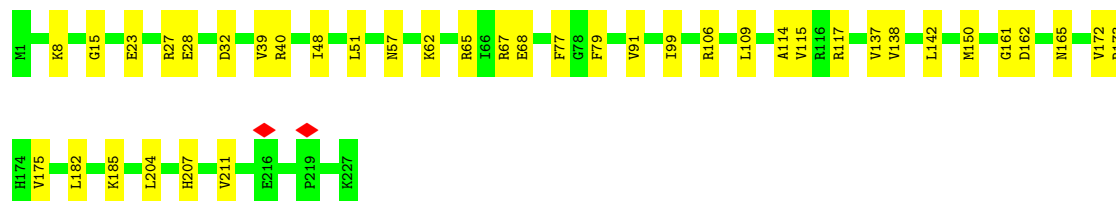
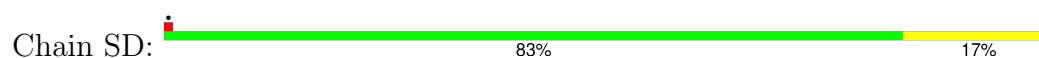
- Molecule 50: 60S acidic ribosomal protein P0



- Molecule 51: Large ribosomal subunit protein uL11

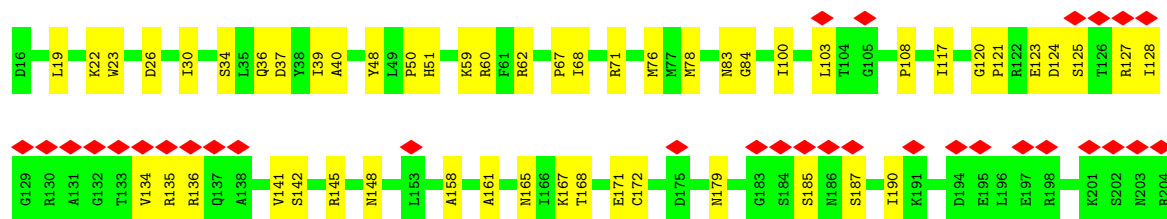


- Molecule 52: Small ribosomal subunit protein uS3



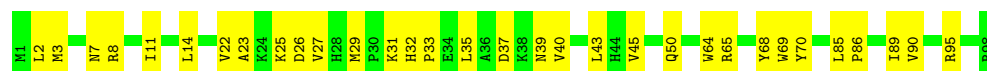
- Molecule 53: 40S ribosomal protein S5





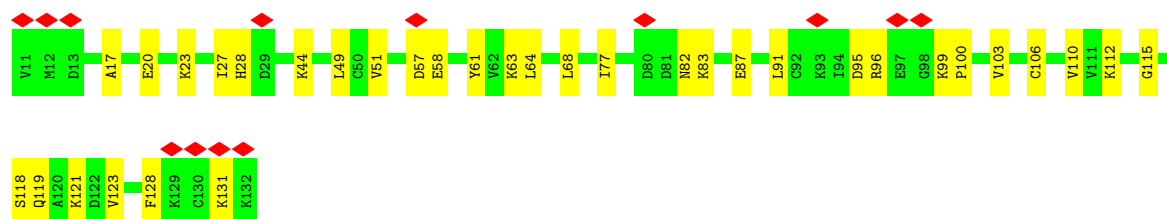
- Molecule 54: 40S ribosomal protein S10

Chain SK: 67% 33%



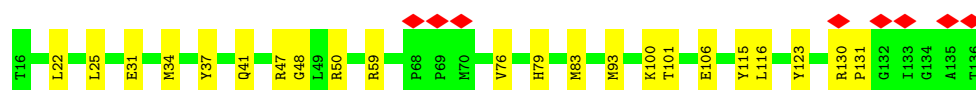
- Molecule 55: Small ribosomal subunit protein eS12

Chain SM: 11% 72% 28%



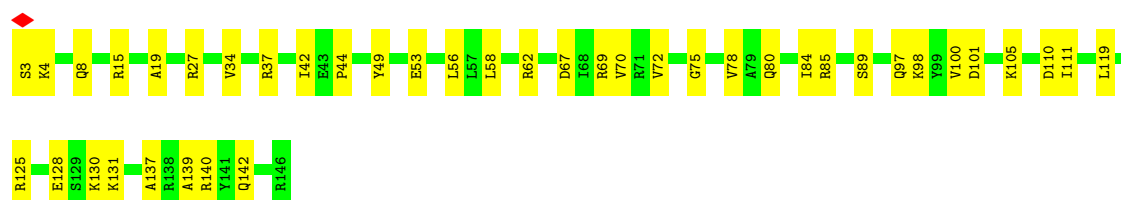
- Molecule 56: Small ribosomal subunit protein uS19

Chain SP: 7% 82% 18%



- Molecule 57: Small ribosomal subunit protein uS9

Chain SQ: 72% 28%



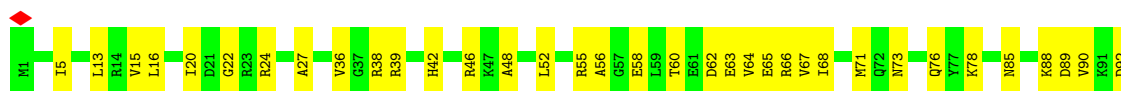
- Molecule 58: Small ribosomal subunit protein eS17

Chain SR: 87% 12%



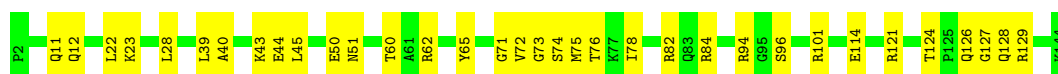
- Molecule 59: 40S ribosomal protein S18

Chain SS: 68% 32%



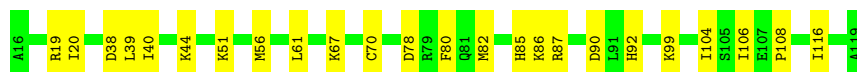
- Molecule 60: 40S ribosomal protein S19

Chain ST: 76% 24%



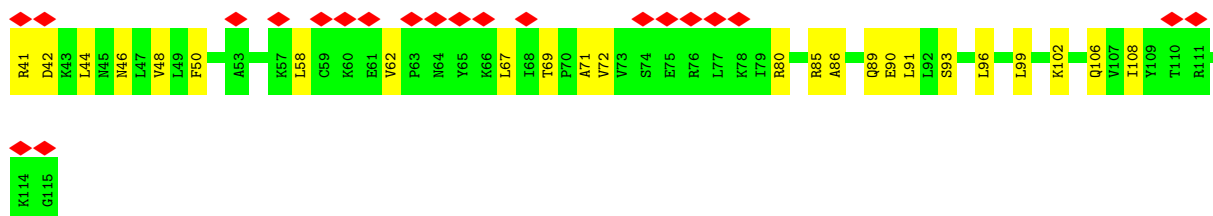
- Molecule 61: 40S ribosomal protein S20

Chain SU: 77% 23%



- Molecule 62: Small ribosomal subunit protein eS25

Chain SZ: 28% 68% 32%



- Molecule 63: 40S ribosomal protein S28

Chain Sc: 9% 69% 31%



- Molecule 64: 40S ribosomal protein S29

Chain Sd:  82% 18%



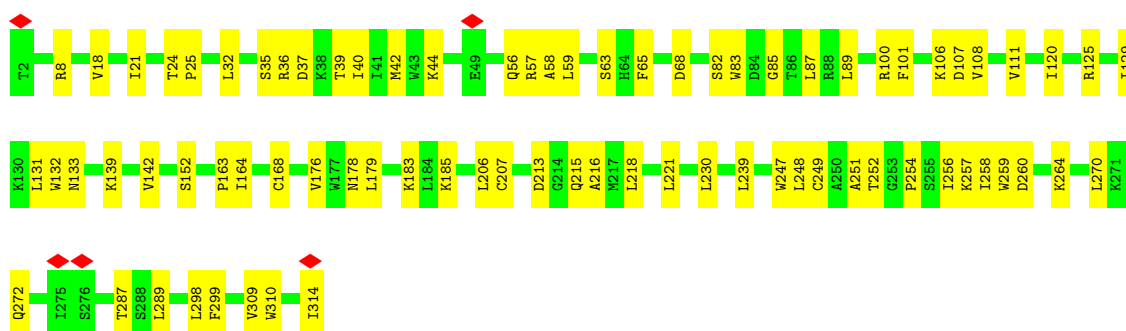
- Molecule 65: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  12% 67% 33%



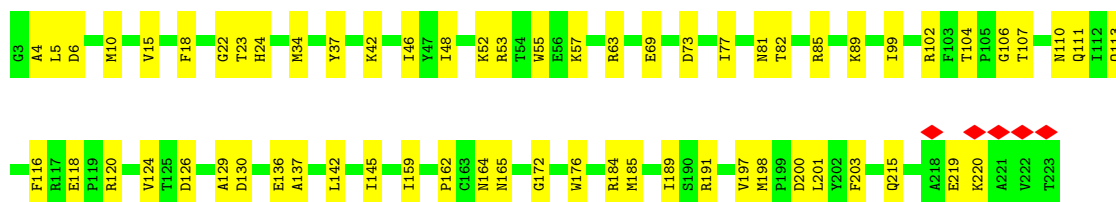
- Molecule 66: Receptor of activated protein C kinase 1

Chain Sg:  75% 25%



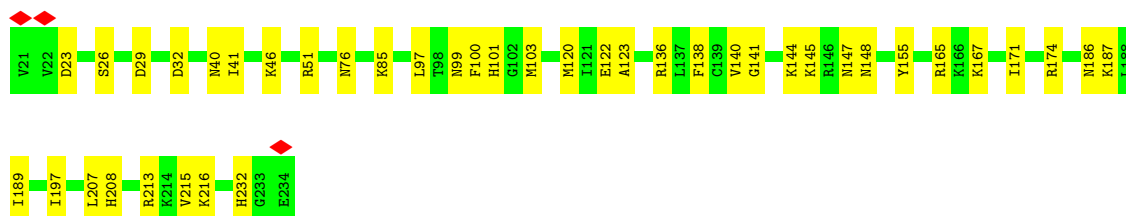
- Molecule 67: 40S ribosomal protein SA

Chain SA:  71% 29%



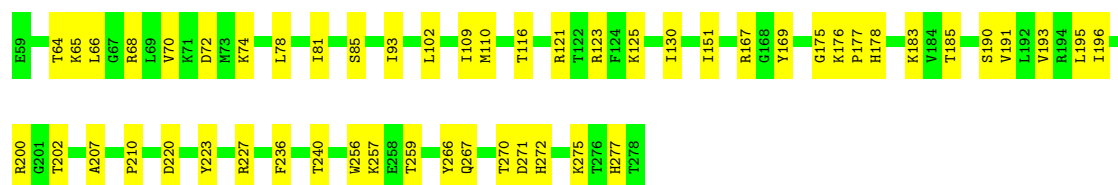
- Molecule 68: 40S ribosomal protein S3a

Chain SB:  81% 19%



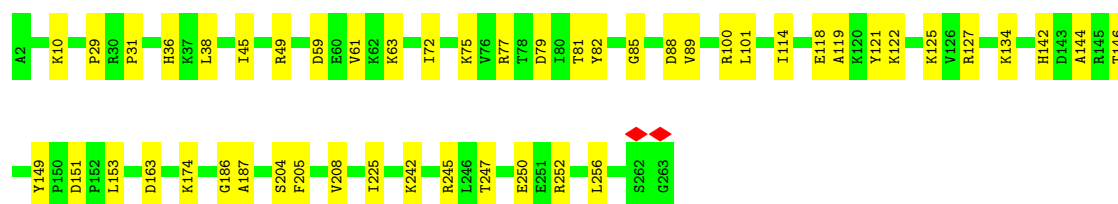
- Molecule 69: 40S ribosomal protein S2

Chain SC:  76% 24%



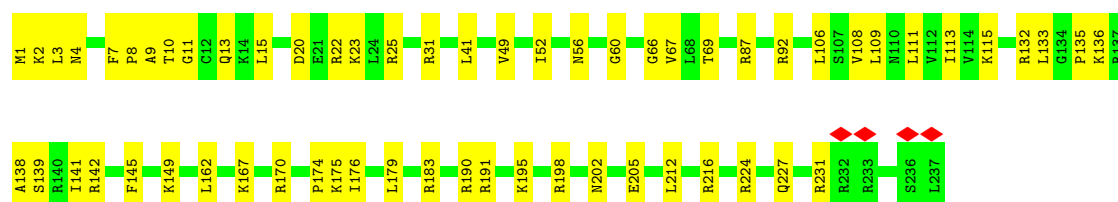
- Molecule 70: Small ribosomal subunit protein eS4, X isoform

Chain SE:  81% 19%



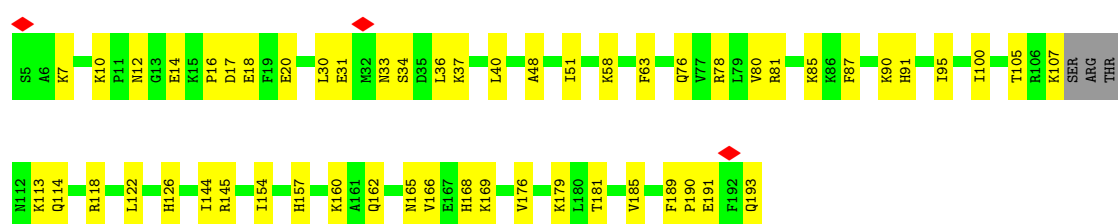
- Molecule 71: 40S ribosomal protein S6

Chain SG:  74% 26%



- Molecule 72: Small ribosomal subunit protein eS7

Chain SH:  69% 29%



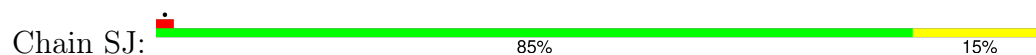
- Molecule 73: 40S ribosomal protein S8

Chain SI:  79% 21%

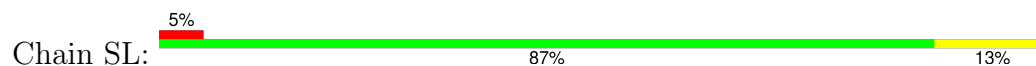




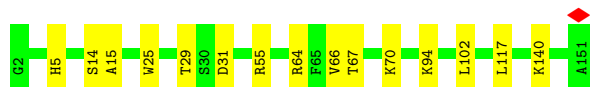
- Molecule 74: 40S ribosomal protein S9



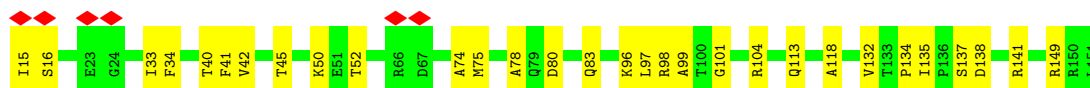
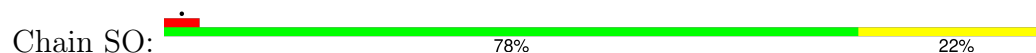
- Molecule 75: 40S ribosomal protein S11



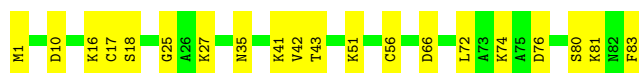
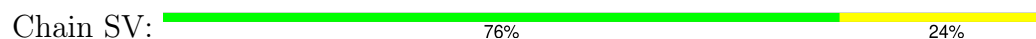
- Molecule 76: 40S ribosomal protein S13



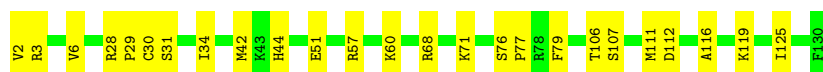
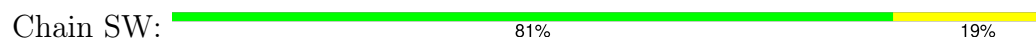
- Molecule 77: 40S ribosomal protein S14



- Molecule 78: Small ribosomal subunit protein eS21



- Molecule 79: 40S ribosomal protein S15a



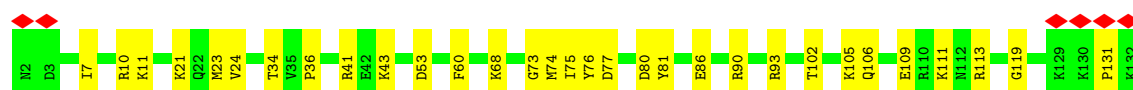
- Molecule 80: 40S ribosomal protein S23

Chain SX:  82% 18%



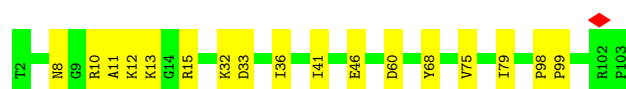
- Molecule 81: 40S ribosomal protein S24

Chain SY:  5% 76% 24%



- Molecule 82: 40S ribosomal protein S26

Chain Sa:  83% 17%



- Molecule 83: Small ribosomal subunit protein eS27

Chain Sb:  82% 18%



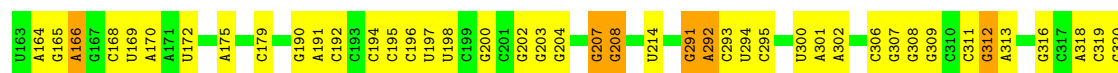
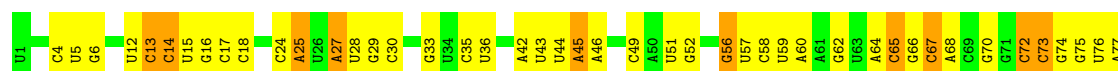
- Molecule 84: Small ribosomal subunit protein eS30

Chain Se:  12% 81% 19%



- Molecule 85: 18S rRNA

Chain S2:  49% 42% 9%





U1631	G1632	A1633	A1634	A1637	G1638	G1639	U1643	C1644	G1648	U1649	A1650	A1651	G1652	U1653	G1654	G1655	C1656	G1657	G1658	U1659	C1660	A1661	U1662	A1663	G1664	G1665	C1666	U1667	U1668	G1671	U1672	U1673	G1674	U1677	A1678	A1679	G1680	U1681	G1682	C1683	C1684	U1685	G1686	C1687	C1688	U1692	G1693	U1694	A1695	C1698	A1699		
C1705	G1706	U1707	A1715	C1716	C1717	G1718	A1719	U1720	U1721	G1722	U1729	U1730	A1731	G1732	G1736	G1737	C1738	G1744	A1745	G1748	G1749	C1750	A1751	G1752	C1753	G1754	C1755	C1756	G1757	G1758	G1759	G1760	U1761	C1762	G1763	G1764	C1767	A1768	C1769	G1770	G1771	C1772	C1773	C1774	U1775	G1776	G1777	C1778	G1779	G1780	A1781	G1782	C1783
G1784	C1785	U1786	U1797	C1798	A1801	C1802	U1803	U1804	G1805	U1808	A1809	U1810	G1814	U1821	A1825	G1826	G1829	U1830	A1831	A1832	C1833	A1834	A1835	U1838	N1842	G1843	U1844	A1845	G1846	G1849	A1850	A1851	U1854	G1855	C1856	G1857	G1858	A1859	A1860	G1861	G1862	A1863	U1864	C1865	A1869								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119172	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	0.140	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.011	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, 4AC, 6MZ, OMG, OMU, G7M, UR3, OMC, SPM, 1MA, MA6, MG, PSU, ZN, B8N, UY1, SEP, A2M, 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	0.13	0/1761	0.26	0/2741
3	CF	0.14	0/3442	0.40	0/4656
4	AT	0.12	0/1805	0.25	0/2809
5	L5	0.21	0/85098	0.30	1/132762 (0.0%)
6	L7	0.19	0/2861	0.25	0/4459
7	L8	0.20	0/3631	0.28	0/5657
8	LA	0.21	0/1936	0.42	0/2596
9	LB	0.20	0/3306	0.37	0/4424
10	LC	0.19	0/2981	0.36	0/4002
11	LD	0.16	0/2428	0.33	0/3252
12	LE	0.17	0/1973	0.41	0/2645
13	LF	0.18	0/1905	0.31	0/2539
14	LG	0.18	0/1960	0.39	0/2637
15	LH	0.18	0/1537	0.35	0/2066
16	LI	0.17	0/1751	0.33	0/2340
17	LJ	0.16	0/1385	0.38	0/1852
18	LL	0.17	0/1732	0.33	0/2315
19	LM	0.18	0/1161	0.37	0/1554
20	LN	0.19	0/1746	0.34	0/2338
21	LO	0.20	0/1682	0.35	0/2250
22	LP	0.20	0/1268	0.40	0/1701
23	LQ	0.20	0/1537	0.37	0/2052
24	LR	0.17	0/1582	0.35	0/2091
25	LS	0.19	0/1493	0.36	0/2003
26	LT	0.18	0/1326	0.33	0/1770
27	LU	0.18	0/839	0.45	0/1126
28	LV	0.18	0/993	0.35	0/1332
29	LW	0.17	0/959	0.38	0/1270
30	LX	0.16	0/1002	0.32	0/1345
31	LY	0.19	0/1132	0.38	0/1504

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LZ	0.17	0/1130	0.35	0/1507
33	La	0.18	0/1191	0.31	0/1591
34	Lb	0.16	0/889	0.41	0/1175
35	Lc	0.18	0/774	0.38	0/1038
36	Ld	0.18	0/903	0.34	0/1216
37	Le	0.21	0/1071	0.38	0/1429
38	Lf	0.20	0/895	0.37	0/1198
39	Lg	0.18	0/916	0.34	0/1220
40	Lh	0.16	0/1023	0.32	0/1351
41	Li	0.16	0/843	0.35	0/1115
42	Lj	0.19	0/720	0.36	0/952
43	Lk	0.19	0/575	0.47	0/761
44	Ll	0.17	0/454	0.29	0/599
45	Lm	0.17	0/435	0.36	0/575
46	Ln	0.16	0/231	0.31	0/294
47	Lo	0.17	0/876	0.35	0/1156
48	Lp	0.17	0/718	0.32	0/953
49	Lr	0.17	0/1017	0.33	0/1364
50	Ls	0.12	0/1519	0.34	0/2052
51	Lt	0.16	0/1009	0.50	0/1363
52	SD	0.13	0/1793	0.30	0/2414
53	SF	0.15	0/1516	0.36	0/2037
54	SK	0.16	0/851	0.43	0/1147
55	SM	0.14	0/950	0.40	0/1275
56	SP	0.17	0/1003	0.40	0/1342
57	SQ	0.15	0/1160	0.39	0/1553
58	SR	0.16	0/1105	0.45	0/1484
59	SS	0.14	0/1216	0.37	0/1628
60	ST	0.15	0/1131	0.40	0/1515
61	SU	0.17	0/831	0.47	0/1115
62	SZ	0.17	0/604	0.48	0/810
63	Sc	0.16	0/508	0.40	0/680
64	Sd	0.14	0/470	0.37	0/623
65	Sf	0.16	0/560	0.48	0/745
66	Sg	0.13	0/2493	0.38	0/3394
67	SA	0.15	0/1778	0.35	0/2416
68	SB	0.14	0/1765	0.37	0/2362
69	SC	0.15	0/1744	0.34	0/2357
70	SE	0.14	0/2118	0.37	0/2849
71	SG	0.15	0/1946	0.37	0/2590
72	SH	0.16	0/1519	0.41	0/2033
73	SI	0.16	0/1715	0.37	0/2287
74	SJ	0.13	0/1550	0.32	0/2069

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SL	0.15	0/1268	0.34	0/1696
76	SN	0.13	0/1232	0.29	0/1656
77	SO	0.17	0/1037	0.39	0/1391
78	SV	0.16	0/643	0.39	0/860
79	SW	0.18	0/1051	0.38	0/1406
80	SX	0.15	0/1116	0.35	0/1490
81	SY	0.15	0/1083	0.40	0/1438
82	Sa	0.15	0/836	0.33	0/1121
83	Sb	0.16	0/665	0.37	0/891
84	Se	0.14	0/465	0.38	0/612
85	S2	0.18	0/39756	0.28	0/61939
All	All	0.19	0/235126	0.32	1/344545 (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
77	SO	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L5	1703	C	C2'-C3'-O3'	5.16	117.24	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
77	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	14	0
2	Pt	1576	0	803	20	0
3	CF	3383	0	3431	80	0
4	AT	1616	0	824	30	0
5	L5	78444	0	39718	961	0
6	L7	2561	0	1295	16	0
7	L8	3315	0	1685	36	0
8	LA	1898	0	1993	44	0
9	LB	3238	0	3376	67	0
10	LC	2927	0	3104	28	0
11	LD	2382	0	2410	31	0
12	LE	1935	0	2096	29	0
13	LF	1870	0	1996	28	0
14	LG	1927	0	2074	17	0
15	LH	1518	0	1601	19	0
16	LI	1711	0	1749	22	0
17	LJ	1362	0	1399	18	0
18	LL	1701	0	1818	22	0
19	LM	1138	0	1204	16	0
20	LN	1701	0	1749	21	0
21	LO	1650	0	1794	32	0
22	LP	1242	0	1269	16	0
23	LQ	1513	0	1628	26	0
24	LR	1566	0	1729	26	0
25	LS	1453	0	1490	20	0
26	LT	1298	0	1366	23	0
27	LU	825	0	850	14	0
28	LV	979	0	1039	14	0
29	LW	945	0	1003	18	0
30	LX	985	0	1066	8	0
31	LY	1115	0	1205	16	0
32	LZ	1107	0	1182	17	0
33	La	1162	0	1213	12	0
34	Lb	876	0	948	16	0
35	Lc	764	0	804	8	0
36	Ld	888	0	930	11	0
37	Le	1053	0	1147	16	0
38	Lf	876	0	912	10	0
39	Lg	906	0	998	16	0
40	Lh	1015	0	1148	19	0
41	Li	832	0	917	7	0
42	Lj	705	0	737	19	0
43	Lk	569	0	637	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Ll	444	0	483	11	0
45	Lm	429	0	465	5	0
46	Ln	230	0	276	4	0
47	Lo	862	0	929	10	0
48	Lp	708	0	756	9	0
49	Lr	1002	0	1068	4	0
50	Ls	1496	0	1540	22	0
51	Lt	998	0	1032	26	0
52	SD	1765	0	1865	27	0
53	SF	1495	0	1549	38	0
54	SK	827	0	854	23	0
55	SM	940	0	965	21	0
56	SP	985	0	1031	17	0
57	SQ	1142	0	1213	31	0
58	SR	1090	0	1149	13	0
59	SS	1198	0	1261	33	0
60	ST	1112	0	1146	24	0
61	SU	821	0	883	17	0
62	SZ	598	0	656	19	0
63	Sc	506	0	536	14	0
64	Sd	459	0	452	10	0
65	Sf	548	0	551	17	0
66	Sg	2436	0	2393	50	0
67	SA	1741	0	1746	48	0
68	SB	1738	0	1809	25	0
69	SC	1707	0	1791	39	0
70	SE	2076	0	2177	33	0
71	SG	1923	0	2089	60	0
72	SH	1497	0	1590	40	0
73	SI	1686	0	1772	34	0
74	SJ	1525	0	1640	22	0
75	SL	1247	0	1323	13	0
76	SN	1208	0	1294	14	0
77	SO	1024	0	1050	19	0
78	SV	636	0	637	16	0
79	SW	1034	0	1080	24	0
80	SX	1098	0	1167	22	0
81	SY	1065	0	1142	22	0
82	Sa	821	0	870	12	0
83	Sb	651	0	672	13	0
84	Se	459	0	503	11	0
85	S2	36953	0	18678	537	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	L5	178	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	LB	1	0	0	0	0
86	LP	1	0	0	0	0
86	LV	1	0	0	0	0
86	Le	1	0	0	0	0
86	Lj	1	0	0	0	0
86	S2	26	0	0	0	0
86	SG	1	0	0	0	0
86	SS	1	0	0	0	0
87	L5	98	0	182	4	0
88	L5	90	0	171	3	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	167075	2774	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 7.

All (2774) 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	5:L5:2708:U:O2'	1.64	1.29
5:L5:1996:C:H42	5:L5:2000:G:H22	1.10	0.98
5:L5:1996:C:H42	5:L5:2000:G:N2	1.66	0.93
5:L5:4946:U:HO2'	38:Lf:2:SER:N	1.67	0.92
1:CI:74:LYS:HA	27:LU:116:GLN:O	1.68	0.91
4:AT:51:U:H3	4:AT:65:G:H1	1.12	0.89
85:S2:1652:G:H1	85:S2:1672:U:H3	1.20	0.87
85:S2:1748:G:H1	85:S2:1786:U:H3	0.87	0.86
85:S2:928:G:H1	85:S2:1013:U:H3	1.21	0.86
85:S2:925:G:H1	85:S2:1017:U:H3	1.24	0.84
5:L5:1996:C:N4	5:L5:2000:G:H22	1.77	0.82
18:LL:64:VAL:HA	18:LL:67:HIS:HD2	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:S2:1656:G:H1	85:S2:1668:U:H3	1.27	0.81
57:SQ:72:VAL:HG11	57:SQ:80:GLN:HG3	1.62	0.80
3:CF:13:ILE:HD12	3:CF:136:HIS:HB3	1.65	0.79
5:L5:3946:G:H1	5:L5:4067:U:H3	0.80	0.79
1:CI:79:ARG:NH1	5:L5:2708:U:HO2'	1.77	0.78
85:S2:940:U:H3	85:S2:1002:U:H3	1.30	0.78
85:S2:1776:G:N2	85:S2:1777:G:N7	2.33	0.77
5:L5:2049:G:HO2'	5:L5:3884:PSU:HO2'	1.31	0.77
68:SB:103:MET:HG3	68:SB:215:VAL:HG12	1.66	0.77
85:S2:1033:G:H1	85:S2:1080:A:HO2'	1.32	0.77
5:L5:2702:C:OP1	27:LU:101:ARG:NH2	2.19	0.76
3:CF:15:HIS:HE2	3:CF:133:THR:HG1	1.30	0.76
5:L5:664:G:N2	5:L5:666:G:O6	2.19	0.76
5:L5:4242:U:H3	5:L5:4281:A:H2	1.35	0.75
5:L5:2557:G:H1	5:L5:2570:U:H3	1.34	0.74
65:Sf:126:CYS:SG	65:Sf:144:CYS:N	2.57	0.74
69:SC:210:PRO:HB3	69:SC:240:THR:HG21	1.68	0.74
5:L5:3717:A:H2'	5:L5:3718:A2M:H8	1.68	0.73
5:L5:2611:A:H5'	5:L5:2688:G:H4'	1.70	0.73
5:L5:184:U:O2	5:L5:253:G:N2	2.21	0.73
5:L5:665:C:H4'	5:L5:666:G:H5'	1.70	0.73
5:L5:1702:C:H4'	10:LC:308:LYS:HD2	1.71	0.73
5:L5:3641:U:OP2	5:L5:3646:A:N6	2.22	0.72
5:L5:2458:C:H5''	20:LN:67:ARG:HD2	1.70	0.72
5:L5:4910:G:H4'	9:LB:95:THR:HG22	1.72	0.72
66:Sg:87:LEU:HB2	66:Sg:101:PHE:HB2	1.71	0.72
4:AT:61:A:OP1	4:AT:63:C:N4	2.22	0.71
60:ST:12:GLN:NE2	85:S2:1593:C:O2	2.23	0.71
5:L5:2300:A:N7	10:LC:143:ARG:NH1	2.38	0.71
70:SE:79:ASP:HB3	70:SE:82:TYR:HB2	1.72	0.71
53:SF:134:VAL:HG12	53:SF:135:ARG:HG2	1.73	0.71
85:S2:851:C:H5''	85:S2:852:G:H5'	1.73	0.71
5:L5:1172:C:H42	5:L5:1188:C:H42	1.37	0.70
5:L5:1366:G:H5''	18:LL:36:ARG:HH12	1.56	0.70
66:Sg:247:TRP:HB3	66:Sg:258:ILE:HD11	1.71	0.70
65:Sf:99:LYS:NZ	85:S2:1287:A:OP1	2.24	0.70
85:S2:94:G:HO2'	85:S2:508:A:HO2'	1.40	0.70
5:L5:4098:A:N1	5:L5:4112:C:N4	2.40	0.70
25:LS:76:LYS:NZ	25:LS:100:LEU:O	2.25	0.70
19:LM:15:VAL:HG22	19:LM:50:MET:HE1	1.73	0.69
4:AT:24:C:N3	4:AT:25:A:N6	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SQ:131:LYS:HB2	57:SQ:140:ARG:HH22	1.57	0.69
3:CF:93:PRO:HD2	3:CF:102:MET:HB3	1.73	0.69
77:SO:104:ARG:NH2	85:S2:959:G:OP1	2.24	0.69
85:S2:628:A:N6	85:S2:1500:G:O2'	2.25	0.69
5:L5:172:C:H4'	5:L5:173:C:H5'	1.74	0.69
15:LH:106:GLN:HB2	15:LH:111:LEU:HB3	1.73	0.69
27:LU:65:ARG:HG2	27:LU:67:LYS:H	1.57	0.69
5:L5:4546:A:N7	8:LA:215:ASN:ND2	2.40	0.69
8:LA:114:CYS:HB3	8:LA:165:VAL:HB	1.75	0.69
5:L5:3946:G:N2	5:L5:4067:U:O2	2.24	0.69
8:LA:107:MET:HB3	8:LA:111:THR:HG21	1.74	0.69
1:CI:72:ARG:NH2	24:LR:25:ASP:OD2	2.26	0.68
28:LV:35:LYS:HB2	28:LV:67:LYS:HG3	1.74	0.68
71:SG:198:ARG:NH1	85:S2:126:G:OP2	2.25	0.68
9:LB:289:GLN:HE22	9:LB:292:LEU:HD11	1.58	0.68
85:S2:838:G:H1	85:S2:840:C:HO2'	1.42	0.68
3:CF:360:VAL:HA	3:CF:369:ALA:HA	1.74	0.68
73:SI:88:ASN:OD1	73:SI:205:ARG:NH2	2.27	0.68
75:SL:85:THR:HG21	85:S2:373:G:H4'	1.76	0.68
85:S2:1754:G:N7	85:S2:1779:G:N2	2.41	0.68
53:SF:127:ARG:HG2	53:SF:136:ARG:HE	1.59	0.68
13:LF:243:LEU:O	13:LF:247:MET:HB2	1.94	0.68
59:SS:22:GLY:HA2	59:SS:56:ALA:HB3	1.76	0.68
57:SQ:4:LYS:HE3	85:S2:1423:C:H41	1.58	0.68
56:SP:130:ARG:HD3	56:SP:131:PRO:HD2	1.75	0.67
59:SS:85:ASN:OD1	59:SS:97:GLN:NE2	2.26	0.67
5:L5:500:G:H1'	5:L5:504:G:H3'	1.74	0.67
71:SG:11:GLY:HA2	85:S2:166:A2M:HM'1	1.76	0.67
66:Sg:152:SER:HG	66:Sg:168:CYS:HG	1.41	0.67
5:L5:4594:U:H2'	5:L5:4595:G:H8	1.60	0.67
5:L5:748:G:O6	25:LS:98:ARG:NH2	2.27	0.67
5:L5:2486:G:O6	5:L5:2493:G:O6	2.13	0.67
22:LP:39:MET:HG2	22:LP:43:LYS:HD3	1.75	0.67
5:L5:2093:A:N3	5:L5:2094:G:N1	2.43	0.67
9:LB:10:ARG:NH1	9:LB:11:HIS:O	2.27	0.67
5:L5:4162:C:H5	14:LG:73:ARG:HH12	1.43	0.67
85:S2:1417:C:O2	85:S2:1422:G:O6	2.13	0.67
61:SU:51:LYS:HB3	61:SU:90:ASP:HB2	1.77	0.67
85:S2:751:G:H1'	85:S2:793:G:H21	1.59	0.66
5:L5:3701:OMC:H5	5:L5:3748:A:H62	1.43	0.66
34:Lb:109:ARG:HA	34:Lb:112:ILE:HG12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SU:19:ARG:HH11	61:SU:92:HIS:HB3	1.59	0.66
57:SQ:58:LEU:HB3	57:SQ:62:ARG:HD2	1.76	0.66
66:Sg:206:LEU:HD12	66:Sg:218:LEU:HD12	1.77	0.66
69:SC:193:VAL:HG11	69:SC:240:THR:HG22	1.77	0.66
66:Sg:252:THR:HG21	66:Sg:257:LYS:HD2	1.78	0.66
72:SH:154:ILE:HB	72:SH:185:VAL:HG22	1.76	0.66
43:Lk:54:GLU:OE2	43:Lk:58:GLN:NE2	2.29	0.66
56:SP:37:TYR:O	59:SS:88:LYS:NZ	2.28	0.66
5:L5:3937:C:H1'	20:LN:125:SER:HB3	1.78	0.66
85:S2:1277:C:H2'	85:S2:1278:A:H8	1.61	0.66
3:CF:163:SEP:O2P	3:CF:165:LYS:NZ	2.28	0.66
5:L5:2092:G:O2'	5:L5:2262:G:N2	2.29	0.66
5:L5:2601:A:N6	5:L5:2744:A:OP2	2.28	0.66
5:L5:2758:G:O2'	5:L5:2765:A:N3	2.25	0.65
13:LF:105:VAL:HG13	13:LF:136:VAL:HG12	1.79	0.65
85:S2:1228:A:H2'	85:S2:1229:G:H8	1.60	0.65
53:SF:84:GLY:O	85:S2:1673:U:O2'	2.13	0.65
5:L5:1973:G:O2'	51:Lt:117:ARG:NH1	2.28	0.65
5:L5:4525:C:OP1	9:LB:246:ARG:NH2	2.28	0.65
8:LA:29:LEU:O	8:LA:123:ARG:NH1	2.30	0.65
9:LB:90:VAL:HG23	9:LB:163:ILE:HD11	1.78	0.65
15:LH:106:GLN:NE2	15:LH:113:GLU:OE2	2.30	0.65
50:Ls:58:ASN:ND2	50:Ls:84:GLY:O	2.22	0.65
84:Se:41:ARG:NH2	85:S2:639:C:OP1	2.29	0.65
3:CF:246:LEU:O	3:CF:247:ARG:NH1	2.29	0.65
5:L5:4992:G:H2'	5:L5:4993:G:C8	2.32	0.65
80:SX:107:ARG:HG3	80:SX:110:HIS:HB3	1.77	0.65
5:L5:188:G:N2	5:L5:190:G:O6	2.30	0.65
67:SA:102:ARG:HH12	85:S2:1377:U:H3'	1.61	0.65
71:SG:135:PRO:HG2	71:SG:141:ILE:HG22	1.76	0.65
72:SH:7:LYS:HD3	72:SH:10:LYS:HB3	1.79	0.65
1:CI:66:GLY:HA3	36:Ld:70:LYS:NZ	2.12	0.65
5:L5:1563:A:N6	85:S2:1028:A:N1	2.45	0.65
67:SA:102:ARG:NH1	85:S2:1378:A:OP2	2.30	0.65
74:SJ:162:ARG:NH1	85:S2:582:U:OP1	2.29	0.65
85:S2:1658:G:OP2	85:S2:1660:C:N4	2.30	0.65
5:L5:2351:OMC:HM22	10:LC:95:MET:HG3	1.79	0.65
22:LP:109:VAL:HA	22:LP:112:LEU:HD13	1.78	0.65
54:SK:50:GLN:HE22	85:S2:1276:A:H1'	1.62	0.65
65:Sf:97:LYS:NZ	85:S2:1289:U:OP2	2.30	0.65
85:S2:106:C:H2'	85:S2:107:A:H8	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:S2:864:A:H2'	85:S2:865:A:H8	1.62	0.64
5:L5:1172:C:HO2'	5:L5:1173:G:H8	1.45	0.64
5:L5:1669:A:OP1	34:Lb:18:ARG:NH2	2.30	0.64
5:L5:4305:G:N7	26:LT:87:LYS:NZ	2.43	0.64
51:Lt:117:ARG:HE	51:Lt:119:ARG:H	1.45	0.64
5:L5:109:G:OP2	18:LL:74:ARG:NH2	2.30	0.64
5:L5:4092:G:N7	5:L5:4114:C:N4	2.45	0.64
8:LA:137:ILE:HD11	8:LA:149:LYS:HB2	1.79	0.64
24:LR:172:ARG:NH1	85:S2:909:G:OP1	2.29	0.64
71:SG:183:ARG:NH2	85:S2:316:G:OP2	2.31	0.64
72:SH:105:THR:HG23	72:SH:107:LYS:H	1.61	0.64
85:S2:1562:C:H2'	85:S2:1563:G:H8	1.62	0.64
5:L5:1095:A:H2	5:L5:1200:G:H1	1.43	0.64
9:LB:222:VAL:O	9:LB:343:ARG:NH1	2.30	0.64
29:LW:105:ARG:NH2	71:SG:149:LYS:O	2.30	0.64
71:SG:202:ASN:ND2	85:S2:125:C:OP1	2.31	0.64
85:S2:928:G:H2'	85:S2:929:G:C8	2.33	0.64
3:CF:353:ILE:HB	3:CF:394:LEU:HB2	1.80	0.64
57:SQ:140:ARG:HB2	85:S2:1644:C:H4'	1.78	0.64
5:L5:1995:G:O2'	51:Lt:122:ALA:O	2.12	0.64
5:L5:2554:U:O2	5:L5:2764:A:N7	2.30	0.64
61:SU:61:LEU:HB2	61:SU:82:MET:HB3	1.80	0.64
85:S2:747:U:N3	85:S2:796:G:N1	2.46	0.64
5:L5:1994:C:H2'	5:L5:1995:G:C8	2.33	0.64
5:L5:2083:C:OP2	23:LQ:14:ARG:NH2	2.29	0.64
81:SY:74:MET:SD	81:SY:90:ARG:NH1	2.71	0.64
5:L5:1982:G:N2	5:L5:2009:A:O2'	2.31	0.63
5:L5:4225:G:OP1	16:LI:24:ARG:NH2	2.30	0.63
3:CF:294:MET:HB2	3:CF:308:VAL:HG12	1.81	0.63
5:L5:67:C:OP2	5:L5:312:G:N2	2.30	0.63
52:SD:8:LYS:HG2	61:SU:61:LEU:HD11	1.78	0.63
71:SG:22:ARG:HG3	71:SG:25:ARG:HH12	1.63	0.63
71:SG:190:ARG:NH2	85:S2:334:C:OP2	2.31	0.63
5:L5:1414:C:H2'	5:L5:1415:G:H8	1.62	0.63
49:Lr:28:GLU:OE2	49:Lr:31:ASN:ND2	2.30	0.63
85:S2:1203:G:H2'	85:S2:1204:A:C8	2.33	0.63
5:L5:3659:G:OP1	8:LA:241:ARG:NH1	2.32	0.63
5:L5:4431:PSU:OP2	16:LI:3:ARG:NH2	2.29	0.63
85:S2:948:C:H2'	85:S2:949:G:H8	1.63	0.63
5:L5:500:G:OP1	5:L5:504:G:N2	2.31	0.63
7:L8:62:A:OP1	40:Lh:52:LYS:NZ	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:SI:133:GLU:HA	73:SI:136:ILE:HG12	1.80	0.63
71:SG:132:ARG:NH2	85:S2:152:U:O4'	2.32	0.63
85:S2:1228:A:H2'	85:S2:1229:G:C8	2.34	0.63
5:L5:2658:G:N2	5:L5:2676:A:OP2	2.31	0.63
16:LI:205:PRO:HD2	16:LI:208:LYS:HE2	1.79	0.63
83:Sb:20:LYS:NZ	85:S2:1016:U:OP2	2.32	0.63
85:S2:165:G:OP2	85:S2:165:G:N2	2.28	0.63
5:L5:262:G:H2'	5:L5:263:G:H8	1.63	0.63
17:LJ:146:ARG:HG2	17:LJ:147:ARG:HG3	1.81	0.63
60:ST:124:THR:HG23	60:ST:127:GLY:H	1.64	0.63
85:S2:1129:G:H3'	85:S2:1130:G:H21	1.64	0.63
5:L5:1405:C:N3	5:L5:1413:C:N4	2.46	0.62
5:L5:1726:U:H5'	13:LF:135:ILE:HD11	1.81	0.62
5:L5:4873:G:N7	21:LO:179:LYS:NZ	2.43	0.62
33:La:84:GLU:OE1	33:La:87:ARG:NH2	2.33	0.62
71:SG:92:ARG:NH1	85:S2:1738:C:OP1	2.29	0.62
5:L5:387:G:HO2'	5:L5:412:G:H1	1.45	0.62
58:SR:32:LYS:NZ	85:S2:1452:A:OP2	2.33	0.62
32:LZ:9:LYS:NZ	32:LZ:83:THR:O	2.28	0.62
53:SF:34:SER:HA	63:Sc:55:VAL:HG23	1.80	0.62
72:SH:114:GLN:HE22	85:S2:874:G:H21	1.47	0.62
5:L5:62:A:N3	5:L5:77:U:O2'	2.30	0.62
17:LJ:38:LYS:HD2	17:LJ:123:ILE:HD11	1.82	0.62
5:L5:3811:G:O2'	5:L5:3814:U:OP2	2.17	0.62
52:SD:106:ARG:HG3	52:SD:175:VAL:HG22	1.82	0.62
73:SI:22:HIS:HB3	85:S2:433:A:H5''	1.81	0.62
80:SX:68:LYS:HB3	80:SX:91:LEU:HD13	1.81	0.62
9:LB:107:ALA:HB2	9:LB:201:LEU:HD22	1.82	0.62
53:SF:36:GLN:NE2	53:SF:37:ASP:OD1	2.33	0.62
5:L5:1785:C:OP1	16:LI:133:GLN:NE2	2.32	0.62
5:L5:4717:A:OP2	9:LB:30:LYS:NZ	2.28	0.62
83:Sb:14:GLU:HA	83:Sb:17:ARG:HG2	1.81	0.62
3:CF:272:LEU:HB3	3:CF:302:ALA:HB3	1.82	0.62
21:LO:34:VAL:HG22	21:LO:103:LYS:HB2	1.82	0.62
36:Ld:90:ARG:HD3	36:Ld:102:LEU:HD13	1.82	0.62
40:Lh:80:PRO:HD2	40:Lh:83:LEU:HD12	1.82	0.62
85:S2:993:G:OP1	85:S2:1131:G:N2	2.28	0.62
3:CF:194:SER:HB3	3:CF:199:ASP:HB2	1.81	0.61
22:LP:17:SER:HB2	22:LP:98:ALA:HB2	1.82	0.61
36:Ld:64:ILE:HG23	36:Ld:68:LEU:HD23	1.82	0.61
57:SQ:89:SER:OG	57:SQ:119:LEU:O	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:SB:26:SER:O	68:SB:51:ARG:NH2	2.33	0.61
5:L5:2845:A:H61	5:L5:3843:C:H42	1.46	0.61
54:SK:25:LYS:NZ	85:S2:1497:G:N7	2.48	0.61
67:SA:126:ASP:OD1	67:SA:165:ASN:ND2	2.33	0.61
73:SI:70:GLU:OE2	75:SL:21:LYS:NZ	2.31	0.61
5:L5:1499:C:OP1	23:LQ:150:ARG:NH2	2.33	0.61
8:LA:104:VAL:HA	8:LA:107:MET:HE3	1.82	0.61
70:SE:153:LEU:O	70:SE:174:LYS:NZ	2.33	0.61
2:Pt:50:U:H3	2:Pt:64:G:H1	0.77	0.61
5:L5:679:C:H2'	5:L5:680:G:H8	1.65	0.61
5:L5:2624:G:OP2	27:LU:97:ARG:NH2	2.32	0.61
5:L5:1739:G:N3	5:L5:1742:A:N6	2.48	0.61
66:Sg:107:ASP:HB2	66:Sg:125:ARG:HG3	1.82	0.61
82:Sa:8:ASN:ND2	85:S2:1861:G:OP1	2.33	0.61
85:S2:1536:G:H2'	85:S2:1537:A:H8	1.65	0.61
5:L5:1734:G:N2	5:L5:1735:U:O4	2.27	0.61
5:L5:2832:A:OP1	36:Ld:47:LYS:NZ	2.28	0.61
7:L8:58:G:N7	42:Lj:63:ARG:NH2	2.37	0.61
43:Lk:8:ILE:HD11	43:Lk:56:LEU:HD13	1.83	0.61
46:Ln:1:MET:HG3	85:S2:1706:G:H5'	1.81	0.61
66:Sg:32:LEU:HA	66:Sg:42:MET:HA	1.83	0.61
69:SC:72:ASP:OD2	69:SC:272:HIS:NE2	2.28	0.61
70:SE:146:THR:HG21	85:S2:122:G:H21	1.65	0.61
85:S2:1729:U:H3	85:S2:1805:G:H1	1.45	0.61
5:L5:99:A:H5''	20:LN:184:ILE:HD12	1.82	0.61
5:L5:4097:G:O6	5:L5:4098:A:N6	2.34	0.61
70:SE:125:LYS:O	70:SE:142:HIS:N	2.33	0.61
72:SH:160:LYS:HD3	72:SH:189:PHE:HB3	1.81	0.61
81:SY:34:THR:O	85:S2:570:C:O2'	2.17	0.61
1:CI:75:LYS:H	27:LU:117:ILE:C	2.09	0.61
5:L5:513:U:N3	5:L5:516:C:OP2	2.30	0.61
5:L5:1320:U:O2'	5:L5:1891:A:N1	2.32	0.61
53:SF:168:THR:OG1	53:SF:171:GLU:OE1	2.19	0.61
85:S2:557:U:H2'	85:S2:558:G:C8	2.36	0.61
4:AT:12:G:H22	4:AT:23:U:H3	1.49	0.61
71:SG:2:LYS:HB2	71:SG:108:VAL:HG12	1.83	0.61
71:SG:66:GLY:HA2	85:S2:1745:A:H1'	1.82	0.61
5:L5:1332:C:H2'	5:L5:1333:A:H8	1.66	0.61
5:L5:2484:A:H62	5:L5:2494:U:H3	1.49	0.61
5:L5:4618:OMG:H5'	28:LV:15:ARG:HB2	1.83	0.61
70:SE:88:ASP:OD1	70:SE:122:LYS:NZ	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:SI:25:ARG:HA	85:S2:448:A:H5''	1.81	0.61
3:CF:201:MET:HG3	3:CF:228:LEU:HD12	1.83	0.60
5:L5:3949:A:N1	5:L5:4064:C:N4	2.34	0.60
29:LW:80:ARG:NH2	71:SG:8:PRO:O	2.33	0.60
55:SM:96:ARG:NH2	55:SM:100:PRO:O	2.34	0.60
5:L5:2613:C:OP1	39:Lg:24:ARG:NH2	2.34	0.60
71:SG:176:ILE:HG12	71:SG:179:LEU:HD11	1.83	0.60
71:SG:183:ARG:HH12	85:S2:316:G:H5''	1.66	0.60
71:SG:191:ARG:HH12	85:S2:312:G:H2'	1.66	0.60
5:L5:137:G:H2'	5:L5:138:G:H8	1.66	0.60
5:L5:1326:A2M:H2'	5:L5:1327:C:C6	2.36	0.60
64:Sd:2:GLY:N	85:S2:1271:C:O2	2.33	0.60
81:SY:76:TYR:OH	81:SY:86:GLU:OE1	2.18	0.60
85:S2:70:G:H21	85:S2:79:A:H62	1.49	0.60
5:L5:170:C:H42	5:L5:266:C:H42	1.49	0.60
5:L5:1942:A:H2'	5:L5:1943:A:C8	2.37	0.60
66:Sg:68:ASP:HB3	66:Sg:111:VAL:HG22	1.83	0.60
68:SB:171:ILE:HG22	68:SB:174:ARG:HE	1.66	0.60
74:SJ:11:LYS:NZ	85:S2:24:C:OP1	2.29	0.60
5:L5:1548:G:O2'	5:L5:2812:A:N3	2.32	0.60
6:L7:6:C:O2'	11:LD:50:ARG:NH2	2.35	0.60
85:S2:609:U:H2'	85:S2:610:G:H8	1.66	0.60
85:S2:1748:G:O6	85:S2:1786:U:O4	2.20	0.60
16:LI:87:MET:HG2	16:LI:138:ILE:HG12	1.83	0.60
69:SC:200:ARG:O	74:SJ:54:ARG:NH2	2.32	0.60
85:S2:1337:4AC:H2'	85:S2:1338:G:H8	1.66	0.60
85:S2:1550:G:H3'	85:S2:1579:A:H61	1.67	0.60
57:SQ:78:VAL:HG12	85:S2:1673:U:H5''	1.84	0.60
72:SH:51:ILE:HG21	72:SH:179:LYS:HG2	1.82	0.60
73:SI:106:SER:HB3	73:SI:171:LEU:HG	1.83	0.60
79:SW:2:VAL:N	85:S2:1091:C:HO2'	2.00	0.60
5:L5:2756:G:O6	32:LZ:51:ARG:NH2	2.29	0.60
9:LB:147:GLU:OE2	9:LB:198:ARG:NH2	2.34	0.60
67:SA:37:TYR:OH	78:SV:66:ASP:OD2	2.19	0.60
72:SH:165:ASN:O	72:SH:169:LYS:NZ	2.28	0.60
85:S2:1759:G:N2	85:S2:1760:G:O6	2.33	0.60
5:L5:158:A:N1	5:L5:276:C:O2'	2.32	0.60
7:L8:111:U:OP2	44:LI:8:ARG:NH1	2.35	0.60
10:LC:141:GLY:O	10:LC:204:ARG:NH1	2.30	0.60
57:SQ:19:ALA:HB2	57:SQ:75:GLY:HA3	1.84	0.60
85:S2:1013:U:OP1	85:S2:1129:G:O2'	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:1100:U:O3'	5:L5:1167:C:N4	2.35	0.60
5:L5:3717:A:H2'	5:L5:3718:A2M:C8	2.31	0.60
5:L5:4279:A:H5'	5:L5:4281:A:H1'	1.84	0.60
51:Lt:18:THR:O	51:Lt:61:LYS:NZ	2.35	0.60
5:L5:4897:G:OP1	19:LM:128:LYS:NZ	2.35	0.59
10:LC:110:ARG:O	10:LC:113:ARG:NH1	2.32	0.59
11:LD:120:GLU:O	11:LD:248:ARG:NH1	2.35	0.59
70:SE:49:ARG:NH2	85:S2:496:C:OP1	2.32	0.59
75:SL:133:PRO:O	85:S2:383:G:O2'	2.20	0.59
9:LB:113:GLU:OE2	9:LB:169:ARG:NH1	2.34	0.59
52:SD:40:ARG:NH2	61:SU:106:ILE:O	2.35	0.59
65:Sf:89:LYS:NZ	65:Sf:90:LYS:O	2.33	0.59
66:Sg:40:ILE:HB	66:Sg:59:LEU:HB2	1.83	0.59
69:SC:267:GLN:OE1	78:SV:35:ASN:ND2	2.35	0.59
72:SH:162:GLN:HE22	72:SH:166:VAL:HB	1.66	0.59
5:L5:758:G:H4'	15:LH:51:LYS:HE3	1.84	0.59
20:LN:146:PRO:HB2	40:Lh:104:THR:HG23	1.83	0.59
44:Ll:28:ARG:HA	44:Ll:33:ASN:HD22	1.66	0.59
5:L5:4274:A:H2'	5:L5:4275:G:C8	2.37	0.59
5:L5:4537:C:H2'	5:L5:4538:G:H8	1.66	0.59
53:SF:30:ILE:HG23	53:SF:117:ILE:HD11	1.84	0.59
5:L5:88:A:N7	23:LQ:173:LYS:NZ	2.50	0.59
5:L5:1759:G:H1	5:L5:1773:U:H3	1.50	0.59
11:LD:223:PHE:HB3	11:LD:226:TYR:HB2	1.85	0.59
49:Lr:26:SER:OG	49:Lr:28:GLU:OE1	2.17	0.59
50:Ls:68:HIS:O	50:Ls:71:ASN:ND2	2.36	0.59
70:SE:144:ALA:HB3	85:S2:121:OMU:HM23	1.85	0.59
85:S2:508:A:H3'	85:S2:509:OMG:H8	1.65	0.59
85:S2:1854:U:H2'	85:S2:1855:G:H8	1.66	0.59
5:L5:378:A:O2'	5:L5:413:G:N2	2.35	0.59
7:L8:93:C:HO2'	7:L8:94:G:H8	1.49	0.59
17:LJ:136:ARG:NH2	17:LJ:161:GLU:OE2	2.32	0.59
26:LT:43:LYS:O	26:LT:58:HIS:ND1	2.35	0.59
59:SS:5:ILE:N	62:SZ:50:PHE:O	2.35	0.59
69:SC:227:ARG:NH2	85:S2:663:C:O2'	2.35	0.59
85:S2:695:C:N4	85:S2:736:C:O2'	2.36	0.59
3:CF:108:GLN:HE22	3:CF:251:GLN:HG3	1.66	0.59
5:L5:267:G:OP1	40:Lh:109:ARG:NH2	2.36	0.59
5:L5:4910:G:N2	21:LO:106:ASP:O	2.36	0.59
54:SK:8:ARG:NH2	85:S2:1314:U:O2'	2.36	0.59
70:SE:45:ILE:HG13	70:SE:61:VAL:HG11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:SW:107:SER:HB2	85:S2:860:G:H21	1.66	0.59
5:L5:1933:G:H2'	5:L5:1934:A:C8	2.38	0.59
5:L5:3664:G:H2'	5:L5:3665:G:H8	1.68	0.59
5:L5:4725:C:OP1	9:LB:103:LYS:NZ	2.34	0.59
16:LI:14:ASN:O	16:LI:128:ARG:NH2	2.26	0.59
51:Lt:114:ARG:NH2	51:Lt:126:SER:OG	2.36	0.59
52:SD:161:GLY:HA3	85:S2:1388:A:H61	1.68	0.59
55:SM:51:VAL:HG12	55:SM:77:ILE:HB	1.84	0.59
63:Sc:66:ARG:HH12	63:Sc:68:LEU:HD23	1.68	0.59
67:SA:22:GLY:O	67:SA:24:HIS:ND1	2.36	0.59
1:CI:50:MET:HG3	27:LU:114:TYR:CE2	2.37	0.59
5:L5:1866:U:OP1	16:LI:4:ARG:NH1	2.35	0.59
17:LJ:141:ILE:HA	17:LJ:144:LYS:HD2	1.84	0.59
25:LS:95:ARG:NH2	25:LS:112:ASP:OD2	2.36	0.59
85:S2:482:G:N1	85:S2:485:A:OP2	2.34	0.59
2:Pt:20(A):U:O4'	17:LJ:58:ARG:NH2	2.36	0.58
5:L5:966:A:OP2	5:L5:2092:G:N2	2.34	0.58
69:SC:176:LYS:O	69:SC:200:ARG:NH2	2.35	0.58
5:L5:1704:C:O3'	13:LF:46:ARG:NH1	2.36	0.58
5:L5:3666:C:OP1	8:LA:234:LYS:NZ	2.29	0.58
85:S2:1829:G:H1'	85:S2:1850:MA6:H2	1.84	0.58
71:SG:170:ARG:NH1	85:S2:72:C:O2	2.36	0.58
5:L5:1500:A:H5''	5:L5:1501:C:H5''	1.85	0.58
5:L5:2899:C:OP1	24:LR:108:ARG:NH2	2.36	0.58
5:L5:3822:PSU:OP1	87:L5:5291:SPM:N5	2.29	0.58
61:SU:85:HIS:ND1	85:S2:1447:G:OP1	2.36	0.58
85:S2:874:G:H2'	85:S2:875:A:H8	1.68	0.58
85:S2:981:A:H2'	85:S2:982:G:C8	2.38	0.58
5:L5:3732:A:H2'	5:L5:3733:A:H8	1.69	0.58
49:Lr:38:PHE:O	49:Lr:45:HIS:NE2	2.30	0.58
51:Lt:77:ALA:HB3	51:Lt:80:LEU:HB2	1.85	0.58
3:CF:11:VAL:HG12	3:CF:90:ILE:HB	1.85	0.58
5:L5:1979:A:N6	5:L5:1984:A:OP1	2.36	0.58
51:Lt:12:VAL:HG11	51:Lt:65:GLN:H	1.67	0.58
60:ST:65:TYR:HE1	60:ST:128:GLN:HG3	1.69	0.58
85:S2:795:A:H2'	85:S2:796:G:C8	2.39	0.58
5:L5:3799:A:N3	5:L5:4506:C:O2'	2.32	0.58
5:L5:4088:C:OP1	8:LA:37:ARG:NH1	2.36	0.58
5:L5:4098:A:H2'	5:L5:4099:G:H4'	1.85	0.58
11:LD:41:LYS:NZ	26:LT:32:ARG:O	2.35	0.58
29:LW:56:ARG:HH21	29:LW:61:LYS:HB3	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:S2:49:C:H2'	85:S2:472:C:H41	1.68	0.58
85:S2:1240:A:N3	85:S2:1267:C:O2'	2.33	0.58
5:L5:1741:G:O6	6:L7:103:A:O2'	2.19	0.58
5:L5:1857:C:H2'	5:L5:1858:A:H8	1.68	0.58
5:L5:4986:G:H1'	9:LB:174:ARG:HH21	1.68	0.58
8:LA:101:VAL:HG22	8:LA:165:VAL:HG22	1.85	0.58
16:LI:21:ARG:O	16:LI:24:ARG:NH1	2.37	0.58
69:SC:121:ARG:HH12	69:SC:123:ARG:HE	1.52	0.58
14:LG:180:PRO:HG3	14:LG:219:VAL:HG13	1.85	0.58
60:ST:126:GLN:HB2	60:ST:129:ARG:HH21	1.68	0.58
77:SO:134:PRO:HB3	85:S2:944:A:H5''	1.85	0.58
5:L5:4472:G:O2'	45:Lm:100:TYR:O	2.21	0.57
61:SU:20:ILE:HG22	61:SU:116:ILE:HG22	1.85	0.57
62:SZ:99:LEU:HD21	62:SZ:102:LYS:HB2	1.86	0.57
79:SW:71:LYS:NZ	85:S2:1156:U:OP1	2.37	0.57
85:S2:1096:G:H1	85:S2:1136:U:H3	1.50	0.57
85:S2:1286:G:N2	85:S2:1312:G:O2'	2.36	0.57
10:LC:218:ILE:HA	10:LC:229:LEU:HD22	1.86	0.57
52:SD:15:GLY:HA3	64:Sd:50:ILE:HG23	1.86	0.57
57:SQ:3:SER:OG	57:SQ:4:LYS:N	2.36	0.57
67:SA:89:LYS:HD2	67:SA:201:LEU:HG	1.84	0.57
4:AT:51:U:O4	4:AT:65:G:O6	2.21	0.57
5:L5:4094:G:N2	5:L5:4115:G:OP2	2.37	0.57
5:L5:4413:C:O2	16:LI:158:LYS:NZ	2.37	0.57
66:Sg:63:SER:HB2	85:S2:1398:G:H1'	1.86	0.57
71:SG:2:LYS:HD3	71:SG:15:LEU:HD21	1.86	0.57
85:S2:1528:G:O2'	85:S2:1666:C:OP1	2.22	0.57
5:L5:4301:U:OP2	5:L5:4303:C:N4	2.37	0.57
7:L8:67:U:H2'	7:L8:68:G:H8	1.70	0.57
9:LB:378:ARG:HE	29:LW:32:LEU:HD21	1.68	0.57
22:LP:18:ARG:NH2	22:LP:147:GLU:OE1	2.37	0.57
72:SH:20:GLU:HG2	72:SH:48:ALA:HB3	1.86	0.57
80:SX:68:LYS:NZ	85:S2:616:A:OP1	2.37	0.57
5:L5:4153:C:H5''	30:LX:38:LYS:HD2	1.87	0.57
45:Lm:99:CYS:HB2	45:Lm:114:LYS:HE3	1.86	0.57
72:SH:34:SER:OG	72:SH:78:ARG:NH2	2.36	0.57
75:SL:35:ARG:NH2	75:SL:55:TYR:O	2.37	0.57
4:AT:67:C:H2'	4:AT:68:G:H8	1.69	0.57
5:L5:1339:U:H2'	5:L5:1340:OMC:C6	2.39	0.57
5:L5:4095:G:N7	5:L5:4096:C:N4	2.52	0.57
18:LL:64:VAL:HA	18:LL:67:HIS:CD2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SS:46:ARG:NH1	60:ST:50:GLU:OE2	2.38	0.57
85:S2:84:A:N3	85:S2:150:A:O2'	2.37	0.57
85:S2:888:U:H4'	85:S2:889:U:H5'	1.86	0.57
5:L5:1932:A:OP1	21:LO:49:ARG:NH2	2.26	0.57
5:L5:3611:A:H2	5:L5:5016:A:H8	1.52	0.57
5:L5:4274:A:H2'	5:L5:4275:G:H8	1.70	0.57
5:L5:4775:C:H41	5:L5:4859:C:H42	1.52	0.57
51:Lt:65:GLN:HG3	51:Lt:67:ARG:H	1.68	0.57
85:S2:533:A:H61	85:S2:550:C:H42	1.52	0.57
2:Pt:33:U:N3	2:Pt:36:C:OP2	2.33	0.57
3:CF:72:THR:HB	3:CF:93:PRO:HA	1.86	0.57
5:L5:2516:G:O2'	39:Lg:62:LYS:NZ	2.38	0.57
5:L5:5064:G:H21	22:LP:75:GLN:HE22	1.52	0.57
10:LC:298:ILE:HD13	23:LQ:131:PRO:HB3	1.87	0.57
21:LO:9:LEU:HD23	21:LO:118:MET:HB2	1.87	0.57
57:SQ:97:GLN:HE21	66:Sg:58:ALA:HB3	1.69	0.57
60:ST:22:LEU:HG	60:ST:28:LEU:HD21	1.87	0.57
66:Sg:176:VAL:HG23	66:Sg:185:LYS:HB2	1.86	0.57
85:S2:1589:A:N3	85:S2:1653:U:O2'	2.38	0.57
3:CF:132:GLN:O	3:CF:136:HIS:ND1	2.29	0.57
5:L5:513:U:H3'	5:L5:514:U:H4'	1.87	0.57
5:L5:4107:G:N2	5:L5:4108:G:O6	2.36	0.57
66:Sg:216:ALA:N	66:Sg:230:LEU:O	2.37	0.57
75:SL:33:LEU:HD12	75:SL:34:PRO:HD2	1.87	0.57
85:S2:1354:G:N2	85:S2:1357:A:OP2	2.29	0.57
3:CF:273:LYS:HE2	3:CF:301:GLU:HG2	1.87	0.57
9:LB:17:LEU:O	9:LB:19:ARG:N	2.37	0.57
11:LD:152:ARG:O	11:LD:157:ASN:ND2	2.38	0.57
15:LH:187:VAL:HG12	15:LH:188:GLN:HG3	1.87	0.57
55:SM:63:LYS:HD3	55:SM:64:LEU:HD22	1.86	0.57
65:Sf:144:CYS:HB2	65:Sf:146:LEU:HD23	1.87	0.57
85:S2:1536:G:H2'	85:S2:1537:A:C8	2.40	0.57
5:L5:1727:U:OP1	13:LF:131:ASN:ND2	2.37	0.56
29:LW:7:SER:HB2	29:LW:13:ILE:HD11	1.86	0.56
45:Lm:79:GLU:OE2	45:Lm:81:SER:OG	2.23	0.56
5:L5:1628:C:OP1	8:LA:14:SER:OG	2.23	0.56
9:LB:10:ARG:NH2	9:LB:265:SER:O	2.38	0.56
24:LR:92:LYS:HG2	24:LR:96:MET:HE3	1.87	0.56
66:Sg:129:ILE:HB	66:Sg:142:VAL:HB	1.87	0.56
72:SH:157:HIS:HB3	72:SH:190:PRO:HG3	1.87	0.56
85:S2:1144:A:H5'	85:S2:1355:C:H41	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:184:U:O2'	5:L5:189:G:O4'	2.23	0.56
5:L5:2568:C:H2'	5:L5:2569:G:H8	1.71	0.56
5:L5:4238:G:H2'	5:L5:4239:A:H8	1.71	0.56
64:Sd:12:ARG:NH1	85:S2:1513:C:OP1	2.27	0.56
66:Sg:120:ILE:HB	66:Sg:132:TRP:HB2	1.86	0.56
68:SB:40:ASN:HD21	68:SB:76:ASN:HB2	1.69	0.56
71:SG:162:LEU:HG	71:SG:167:LYS:HE3	1.86	0.56
71:SG:191:ARG:HH22	85:S2:312:G:H2'	1.70	0.56
72:SH:111:LYS:HE3	85:S2:796:G:H21	1.69	0.56
74:SJ:145:PRO:HD2	85:S2:522:A:H5''	1.87	0.56
85:S2:1606:G:N1	85:S2:1632:G:O2'	2.32	0.56
5:L5:2007:G:H21	5:L5:2012:A:H62	1.52	0.56
55:SM:91:LEU:HD12	55:SM:106:CYS:HB2	1.88	0.56
62:SZ:58:LEU:HD12	62:SZ:62:VAL:HG21	1.85	0.56
66:Sg:164:ILE:HG22	66:Sg:178:ASN:HA	1.86	0.56
85:S2:368:U:H3'	85:S2:369:C:H2'	1.88	0.56
85:S2:1277:C:H2'	85:S2:1278:A:C8	2.39	0.56
85:S2:1581:C:H5'	85:S2:1582:C:H5	1.71	0.56
4:AT:67:C:H2'	4:AT:68:G:C8	2.40	0.56
5:L5:327:U:O2'	41:Li:30:ARG:NH1	2.38	0.56
5:L5:1279:A:OP1	12:LE:131:LYS:NZ	2.38	0.56
5:L5:1969:G:H4'	50:Ls:36:GLY:HA2	1.87	0.56
5:L5:2411:C:H2'	5:L5:2412:A:C8	2.41	0.56
5:L5:2745:A:H2'	5:L5:2746:A:H8	1.71	0.56
5:L5:3736:A:H2'	5:L5:3737:A:C8	2.40	0.56
5:L5:4340:U:O2	88:L5:5261:SPD:N10	2.39	0.56
26:LT:44:GLY:HA2	26:LT:95:HIS:HB3	1.88	0.56
52:SD:162:ASP:OD1	52:SD:165:ASN:ND2	2.35	0.56
68:SB:99:ASN:OD1	68:SB:100:PHE:N	2.39	0.56
68:SB:122:GLU:HG2	68:SB:140:VAL:HG12	1.87	0.56
85:S2:436:OMG:OP2	85:S2:471:G:O2'	2.23	0.56
2:Pt:50:U:O2	2:Pt:64:G:N2	2.21	0.56
5:L5:1283:G:N1	5:L5:2076:G:OP1	2.30	0.56
5:L5:4347:G:H2'	5:L5:4348:A:C8	2.41	0.56
9:LB:161:ARG:HG2	9:LB:184:GLN:HA	1.88	0.56
73:SI:150:ASP:HA	73:SI:153:LYS:HG2	1.88	0.56
79:SW:3:ARG:HH22	79:SW:28:ARG:HH21	1.54	0.56
85:S2:1010:G:H2'	85:S2:1011:A:C8	2.41	0.56
85:S2:1513:C:H2'	85:S2:1514:G:H8	1.69	0.56
85:S2:1736:G:H2'	85:S2:1737:G:H8	1.71	0.56
55:SM:28:HIS:CE1	55:SM:115:GLY:HA3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:Sg:21:ILE:HG21	66:Sg:299:PHE:HB2	1.88	0.56
66:Sg:213:ASP:OD2	66:Sg:215:GLN:NE2	2.39	0.56
77:SO:15:ILE:HG23	77:SO:16:SER:H	1.71	0.56
5:L5:1095:A:N1	5:L5:1200:G:O6	2.39	0.56
5:L5:1703:C:O2'	5:L5:1704:C:O4'	2.20	0.56
5:L5:2580:U:OP1	32:LZ:36:ARG:NH1	2.33	0.56
42:Lj:2:THR:HB	42:Lj:6:SER:HB2	1.88	0.56
42:Lj:14:LYS:NZ	44:Ll:51:LEU:OXT	2.38	0.56
81:SY:119:GLY:HA2	85:S2:85:A:H5'	1.88	0.56
85:S2:159:A2M:H2	85:S2:467:G:H21	1.71	0.56
5:L5:2910:G:N2	5:L5:3585:G:O2'	2.38	0.56
11:LD:232:THR:OG1	11:LD:234:ASP:OD1	2.22	0.56
17:LJ:83:LEU:HD22	17:LJ:132:VAL:HG11	1.87	0.56
18:LL:111:GLN:HA	18:LL:114:VAL:HG22	1.88	0.56
3:CF:58:TRP:HA	3:CF:61:ASP:HB2	1.86	0.56
4:AT:63:C:H2'	4:AT:64:G:H8	1.71	0.56
5:L5:3633:C:OP1	87:L5:5291:SPM:N10	2.39	0.56
5:L5:5023:C:OP2	73:SI:124:LYS:NZ	2.39	0.56
17:LJ:17:ILE:HD12	17:LJ:80:GLU:HG2	1.88	0.56
52:SD:99:ILE:HG23	52:SD:173:ARG:HH21	1.70	0.56
59:SS:109:GLU:HA	59:SS:112:GLU:HG2	1.88	0.56
85:S2:1347:U:H2'	85:S2:1348:G:N3	2.21	0.56
1:CI:50:MET:HG3	27:LU:114:TYR:CD2	2.41	0.55
5:L5:1346:C:H2'	5:L5:1347:G:H8	1.71	0.55
5:L5:4537:C:H2'	5:L5:4538:G:C8	2.40	0.55
5:L5:268:G:H2'	5:L5:269:G:H8	1.70	0.55
5:L5:2362:U:H2'	5:L5:2363:A2M:H8	1.87	0.55
5:L5:4302:U:H4'	26:LT:5:LYS:HD3	1.86	0.55
85:S2:28:U:H2'	85:S2:29:G:H8	1.72	0.55
5:L5:239:C:OP1	31:LY:46:SER:OG	2.24	0.55
5:L5:1241:C:O2'	34:Lb:120:ARG:O	2.23	0.55
21:LO:54:TYR:CD1	21:LO:145:VAL:HG21	2.42	0.55
25:LS:68:PHE:O	25:LS:70:LYS:NZ	2.40	0.55
15:LH:120:GLU:OE2	15:LH:124:ARG:NH1	2.31	0.55
50:Ls:120:GLU:HB3	50:Ls:163:THR:HG22	1.87	0.55
81:SY:41:ARG:HH21	81:SY:53:ASP:HA	1.72	0.55
5:L5:1480:C:O2'	5:L5:1482:G:OP2	2.24	0.55
5:L5:3615:G:H1'	29:LW:44:ARG:HD3	1.89	0.55
5:L5:4281:A:H2'	5:L5:4282:A:H2'	1.88	0.55
21:LO:62:MET:HE2	21:LO:64:THR:HB	1.88	0.55
38:Lf:43:LEU:O	38:Lf:109:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SA:37:TYR:OH	67:SA:57:LYS:NZ	2.39	0.55
71:SG:133:LEU:HD12	85:S2:65:C:C4	2.42	0.55
74:SJ:124:HIS:HD2	84:Se:31:ARG:HE	1.55	0.55
5:L5:667:A:H5''	5:L5:668:C:H5''	1.88	0.55
5:L5:2876:OMG:HM22	5:L5:2877:G:H5'	1.88	0.55
5:L5:4670:C:O2'	5:L5:4672:A:OP2	2.22	0.55
85:S2:1101:U:H2'	85:S2:1102:G:C8	2.42	0.55
85:S2:1422:G:H4'	85:S2:1423:C:H3'	1.88	0.55
4:AT:14:A:H3'	4:AT:15:G:H8	1.72	0.55
5:L5:2744:A:H2'	5:L5:2745:A:C8	2.41	0.55
8:LA:118:GLU:OE2	8:LA:156:LYS:NZ	2.40	0.55
9:LB:165:HIS:HB3	9:LB:180:LEU:HD23	1.88	0.55
13:LF:127:LYS:HB2	26:LT:133:ALA:HB3	1.88	0.55
17:LJ:84:GLU:OE2	17:LJ:92:TYR:OH	2.22	0.55
72:SH:31:GLU:HA	72:SH:37:LYS:HG3	1.89	0.55
81:SY:80:ASP:OD1	81:SY:81:TYR:N	2.40	0.55
81:SY:119:GLY:O	85:S2:84:A:O2'	2.23	0.55
83:Sb:62:VAL:HG23	83:Sb:74:THR:HG21	1.89	0.55
85:S2:1171:G:O2'	85:S2:1187:G:O6	2.21	0.55
85:S2:1203:G:H2'	85:S2:1204:A:H8	1.72	0.55
3:CF:281:ALA:HB2	3:CF:334:PRO:HB2	1.89	0.55
4:AT:15:G:N2	4:AT:49:C:C2	2.75	0.55
5:L5:502:C:H3'	5:L5:503:C:H3'	1.89	0.55
5:L5:2324:C:O2'	37:Le:98:GLU:OE1	2.24	0.55
16:LI:66:GLU:OE2	16:LI:69:ARG:NH2	2.27	0.55
38:Lf:78:HIS:HB3	38:Lf:83:MET:HB3	1.89	0.55
55:SM:118:SER:O	55:SM:121:LYS:NZ	2.39	0.55
68:SB:186:ASN:HA	68:SB:189:ILE:HD12	1.89	0.55
5:L5:1281:G:N1	12:LE:128:HIS:HB2	2.21	0.55
5:L5:1294:A:H1'	5:L5:1296:G:C2	2.42	0.55
5:L5:4419:U:OP1	5:L5:4475:G:N2	2.38	0.55
39:Lg:41:ALA:O	39:Lg:52:ARG:NH1	2.37	0.55
60:ST:121:ARG:HH21	85:S2:1563:G:H5''	1.72	0.55
67:SA:10:MET:HE3	67:SA:55:TRP:HB2	1.89	0.55
71:SG:7:PHE:HD2	71:SG:10:THR:HG22	1.71	0.55
3:CF:162:TYR:HB3	3:CF:208:MET:HB3	1.89	0.54
4:AT:16:C:O2'	4:AT:19:G:OP1	2.24	0.54
5:L5:2000:G:O2'	5:L5:2001:G:N7	2.40	0.54
5:L5:3654:G:O2'	5:L5:3693:U:OP1	2.25	0.54
11:LD:41:LYS:NZ	26:LT:30:TYR:O	2.30	0.54
47:Lo:78:ARG:O	47:Lo:80:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SQ:142:GLN:NE2	85:S2:1527:C:OP1	2.30	0.54
71:SG:20:ASP:HB3	71:SG:23:LYS:HB2	1.89	0.54
71:SG:31:ARG:NH1	85:S2:1745:A:O3'	2.40	0.54
76:SN:70:LYS:NZ	85:S2:1020:A:N7	2.55	0.54
85:S2:604:A:N3	85:S2:639:C:O2'	2.38	0.54
85:S2:1259:A:H1'	85:S2:1264:C:H42	1.70	0.54
5:L5:1669:A:H4'	5:L5:1685:G:N2	2.22	0.54
59:SS:105:ASN:HB2	59:SS:108:ARG:HH21	1.72	0.54
59:SS:121:ARG:HG3	59:SS:131:VAL:HB	1.88	0.54
67:SA:118:GLU:HG3	69:SC:65:LYS:HE2	1.88	0.54
85:S2:878:G:H22	85:S2:908:A:H2	1.55	0.54
85:S2:1337:4AC:H2'	85:S2:1338:G:C8	2.42	0.54
2:Pt:23:C:H2'	2:Pt:24:A:C8	2.43	0.54
5:L5:4775:C:H41	5:L5:4859:C:N4	2.06	0.54
26:LT:119:ALA:HA	26:LT:122:LYS:HE3	1.88	0.54
47:Lo:33:LEU:HA	47:Lo:38:LYS:HG2	1.89	0.54
5:L5:965:G:H21	5:L5:2092:G:H1'	1.72	0.54
5:L5:3688:U:OP2	8:LA:198:ARG:NH2	2.39	0.54
5:L5:3861:A:H2'	5:L5:3862:A:C8	2.42	0.54
5:L5:3868:G:H22	5:L5:3900:G:H1'	1.73	0.54
5:L5:3946:G:O6	5:L5:4067:U:O4	2.25	0.54
5:L5:4126:C:OP1	14:LG:37:LYS:NZ	2.40	0.54
7:L8:75:OMG:OP2	31:LY:74:TYR:OH	2.22	0.54
9:LB:92:TYR:HB3	9:LB:99:LEU:HD22	1.90	0.54
52:SD:28:GLU:OE2	52:SD:65:ARG:NH2	2.41	0.54
52:SD:32:ASP:OD1	52:SD:57:ASN:ND2	2.40	0.54
68:SB:32:ASP:OD1	68:SB:46:LYS:NZ	2.38	0.54
77:SO:135:ILE:O	85:S2:943:U:O2'	2.26	0.54
85:S2:145:G:H2'	85:S2:146:G:C8	2.42	0.54
5:L5:935:A:O2'	19:LM:44:GLN:O	2.26	0.54
5:L5:1324:A:O2'	5:L5:1326:A2M:OP1	2.24	0.54
5:L5:2017:A:O2'	5:L5:2018:C:O5'	2.24	0.54
5:L5:2637:U:OP1	39:Lg:28:ASN:ND2	2.37	0.54
5:L5:4239:A:H2'	5:L5:4240:G:C8	2.42	0.54
53:SF:124:ASP:OD1	53:SF:125:SER:N	2.30	0.54
85:S2:1677:U:H2'	85:S2:1678:A:H8	1.73	0.54
4:AT:18:G:H21	4:AT:59:A:H5'	1.73	0.54
5:L5:417:G:OP1	5:L5:2329:U:O2'	2.25	0.54
5:L5:1396:G:N7	33:La:110:LYS:NZ	2.51	0.54
5:L5:3798:U:OP2	28:LV:74:LYS:NZ	2.40	0.54
22:LP:118:GLN:OE1	22:LP:120:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Lp:38:THR:HA	48:Lp:45:THR:HA	1.90	0.54
5:L5:1258:G:H2'	5:L5:1259:G:C8	2.42	0.54
5:L5:2520:C:H2'	5:L5:2521:G:H8	1.72	0.54
14:LG:157:ILE:HA	14:LG:201:THR:HG22	1.89	0.54
58:SR:109:LEU:HD13	67:SA:52:LYS:HB2	1.89	0.54
60:ST:62:ARG:NH2	85:S2:1543:U:OP2	2.33	0.54
80:SX:17:ARG:HH12	85:S2:659:G:H21	1.56	0.54
85:S2:543:C:H3'	85:S2:544:G:H8	1.71	0.54
85:S2:1115:U:O2'	85:S2:1117:C:OP2	2.24	0.54
3:CF:215:LYS:NZ	3:CF:216:VAL:O	2.41	0.54
5:L5:1514:U:H2'	5:L5:1515:A:C8	2.42	0.54
71:SG:13:GLN:NE2	85:S2:153:G:N3	2.56	0.54
5:L5:654:C:O3'	10:LC:268:ARG:NH1	2.39	0.54
5:L5:1509:C:H5''	33:La:2:PRO:HD3	1.90	0.54
57:SQ:42:ILE:HG23	57:SQ:44:PRO:HD2	1.89	0.54
60:ST:101:ARG:NH2	85:S2:1566:G:N7	2.54	0.54
5:L5:1305:C:OP1	7:L8:7:U:O2'	2.25	0.54
5:L5:2411:C:H2'	5:L5:2412:A:H8	1.71	0.54
5:L5:4220:6MZ:O5'	5:L5:4220:6MZ:H8	2.08	0.54
5:L5:4238:G:H2'	5:L5:4239:A:C8	2.42	0.54
8:LA:229:ALA:HB3	8:LA:234:LYS:HB3	1.89	0.54
12:LE:261:ILE:HG23	12:LE:267:LEU:HD23	1.90	0.54
67:SA:120:ARG:HD2	69:SC:266:TYR:HB3	1.89	0.54
85:S2:1208:A:H2'	85:S2:1209:A:H8	1.73	0.54
5:L5:5002:U:OP2	9:LB:385:LYS:NZ	2.38	0.53
12:LE:161:ARG:NH1	12:LE:273:SER:OG	2.40	0.53
59:SS:130:ARG:NH2	85:S2:1230:C:OP1	2.41	0.53
66:Sg:37:ASP:OD1	66:Sg:39:THR:OG1	2.23	0.53
71:SG:136:LYS:NZ	71:SG:175:LYS:O	2.30	0.53
85:S2:866:PSU:H2'	85:S2:867:OMG:C8	2.43	0.53
5:L5:518:G:H1	5:L5:643:C:H2'	1.73	0.53
5:L5:1818:G:O2'	5:L5:1820:C:OP2	2.22	0.53
5:L5:2745:A:H2'	5:L5:2746:A:C8	2.44	0.53
5:L5:4149:C:OP1	32:LZ:59:LYS:N	2.40	0.53
27:LU:28:PRO:HB2	27:LU:34:MET:HG3	1.90	0.53
50:Ls:13:TYR:O	50:Ls:17:ILE:HG12	2.08	0.53
53:SF:127:ARG:HG2	53:SF:136:ARG:HB2	1.89	0.53
60:ST:84:ARG:NH1	85:S2:1605:G:OP1	2.32	0.53
65:Sf:103:LEU:HB2	65:Sf:105:TYR:CE2	2.43	0.53
85:S2:752:G:OP2	85:S2:752:G:N2	2.34	0.53
5:L5:85:G:O2'	5:L5:97:G:O6	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:121:A:OP1	14:LG:110:LYS:NZ	2.32	0.53
5:L5:2846:G:O2'	28:LV:19:GLY:O	2.20	0.53
5:L5:4769:G:OP1	21:LO:176:ARG:NH1	2.34	0.53
5:L5:4860:G:H5'	21:LO:169:ARG:HD2	1.90	0.53
53:SF:141:VAL:HG12	63:Sc:47:LYS:HG2	1.89	0.53
70:SE:10:LYS:NZ	85:S2:95:G:OP1	2.33	0.53
72:SH:144:ILE:HG23	72:SH:154:ILE:HG13	1.90	0.53
85:S2:5:U:H2'	85:S2:6:G:H8	1.73	0.53
85:S2:1610:G:O6	85:S2:1630:A:N6	2.42	0.53
5:L5:121:A:H62	5:L5:152:U:H3	1.56	0.53
5:L5:433:A:C2	5:L5:3867:A2M:H4'	2.43	0.53
5:L5:1333:A:H2'	5:L5:1334:A:C8	2.43	0.53
5:L5:1837:A:OP2	26:LT:130:ARG:NH1	2.42	0.53
5:L5:1994:C:H2'	5:L5:1995:G:H8	1.74	0.53
5:L5:2521:G:H4'	39:Lg:26:PRO:HD2	1.89	0.53
5:L5:4940:C:H5'	5:L5:4941:G:H5''	1.89	0.53
5:L5:4967:A:H2'	5:L5:4968:A:H8	1.72	0.53
71:SG:1:MET:HE2	71:SG:106:LEU:HB2	1.91	0.53
71:SG:3:LEU:HD23	71:SG:109:LEU:HB3	1.90	0.53
4:AT:3:C:H2'	4:AT:4:U:H6	1.73	0.53
5:L5:1177:U:O2'	11:LD:286:SER:OG	2.23	0.53
5:L5:1494:U:H2'	5:L5:1495:G:H8	1.72	0.53
5:L5:1802:A:N3	26:LT:130:ARG:NH2	2.54	0.53
5:L5:4260:U:H2'	5:L5:4261:C:C6	2.44	0.53
5:L5:4617:G:OP1	9:LB:62:ARG:NH1	2.37	0.53
21:LO:168:TYR:CE2	21:LO:172:LYS:HD2	2.44	0.53
77:SO:34:PHE:HB3	77:SO:41:PHE:HB2	1.90	0.53
85:S2:629:A:O2'	85:S2:631:U:OP1	2.27	0.53
5:L5:702:U:H2'	5:L5:703:G:O4'	2.09	0.53
9:LB:14:LEU:HD22	9:LB:17:LEU:HD11	1.88	0.53
11:LD:62:CYS:HB3	11:LD:105:LEU:HD22	1.89	0.53
85:S2:107:A:H2'	85:S2:108:G:C8	2.43	0.53
85:S2:587:A:H5'	85:S2:592:C:H41	1.74	0.53
85:S2:1201:U:H2'	85:S2:1202:U:C6	2.43	0.53
85:S2:1259:A:N6	85:S2:1519:U:O5'	2.41	0.53
85:S2:1360:U:O2'	85:S2:1379:A:OP2	2.27	0.53
85:S2:1736:G:H2'	85:S2:1737:G:C8	2.43	0.53
85:S2:1754:G:OP1	85:S2:1780:G:N2	2.41	0.53
85:S2:1773:C:H2'	85:S2:1774:C:H5''	1.91	0.53
5:L5:73:A:N7	18:LL:103:ARG:NH2	2.56	0.53
5:L5:223:G:OP2	10:LC:165:LYS:NZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:1667:G:N1	5:L5:2281:U:OP2	2.31	0.53
11:LD:64:ILE:HD13	11:LD:109:LEU:HD22	1.91	0.53
32:LZ:50:PRO:HD3	32:LZ:68:ILE:HG12	1.90	0.53
34:Lb:5:LYS:HE2	34:Lb:8:THR:HB	1.89	0.53
62:SZ:80:ARG:O	85:S2:1598:G:O2'	2.18	0.53
67:SA:77:ILE:HG13	67:SA:99:ILE:HB	1.91	0.53
80:SX:48:LYS:HB3	80:SX:75:ILE:HD12	1.90	0.53
41:Li:55:ARG:O	41:Li:59:GLU:HG2	2.09	0.53
72:SH:100:ILE:HG21	72:SH:122:LEU:HD12	1.91	0.53
81:SY:21:LYS:HE2	81:SY:75:ILE:HD11	1.90	0.53
85:S2:942:G:H2'	85:S2:943:U:C6	2.44	0.53
5:L5:325:U:H2'	5:L5:326:C:C6	2.44	0.53
5:L5:351:C:OP2	10:LC:197:ARG:NH1	2.31	0.53
17:LJ:22:LEU:HD22	17:LJ:128:LEU:HD12	1.91	0.53
51:Lt:114:ARG:NH1	51:Lt:126:SER:O	2.38	0.53
57:SQ:8:GLN:HG3	57:SQ:27:ARG:HE	1.74	0.53
69:SC:191:VAL:HG11	69:SC:236:PHE:HA	1.90	0.53
73:SI:126:GLY:O	73:SI:128:LYS:NZ	2.40	0.53
76:SN:64:ARG:NH2	85:S2:919:A:OP2	2.37	0.53
85:S2:588:G:OP2	85:S2:588:G:N2	2.36	0.53
85:S2:838:G:N1	85:S2:840:C:O2'	2.41	0.53
5:L5:717:U:H2'	5:L5:718:C:C6	2.44	0.53
5:L5:2102:G:H1'	5:L5:2103:G:C8	2.44	0.53
5:L5:4260:U:H2'	5:L5:4261:C:H6	1.74	0.53
11:LD:217:ASP:N	11:LD:217:ASP:OD1	2.42	0.53
19:LM:71:LYS:O	19:LM:75:GLN:HG3	2.09	0.53
67:SA:18:PHE:HD1	67:SA:23:THR:HG21	1.74	0.53
67:SA:42:LYS:HD2	67:SA:48:ILE:HD11	1.90	0.53
72:SH:10:LYS:NZ	72:SH:16:PRO:O	2.42	0.53
37:Le:108:ARG:HD2	37:Le:128:ARG:HB2	1.91	0.52
42:Lj:27:TYR:HA	42:Lj:34:CYS:HA	1.91	0.52
72:SH:87:PHE:HB3	72:SH:90:LYS:HD2	1.89	0.52
5:L5:305:A:OP2	20:LN:15:GLN:NE2	2.29	0.52
5:L5:1178:G:H2'	11:LD:286:SER:HB3	1.90	0.52
5:L5:1646:A:O2'	42:Lj:49:TRP:O	2.22	0.52
5:L5:1718:C:O2'	13:LF:181:LYS:NZ	2.41	0.52
23:LQ:15:ARG:NH1	23:LQ:52:PHE:O	2.39	0.52
64:Sd:8:TRP:HZ3	85:S2:1512:C:H5''	1.73	0.52
79:SW:111:MET:HE1	79:SW:119:LYS:HD2	1.92	0.52
85:S2:1777:G:H2'	85:S2:1778:C:H6	1.74	0.52
5:L5:364:G:O6	42:Lj:55:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:1307:A:H2'	5:L5:1308:C:C6	2.43	0.52
5:L5:1577:G:O2'	5:L5:1612:G:H4'	2.09	0.52
5:L5:1802:A:H5''	5:L5:1803:G:H5'	1.90	0.52
5:L5:1961:G:N2	5:L5:2024:G:O2'	2.40	0.52
5:L5:2017:A:O2'	5:L5:2018:C:H6	1.92	0.52
5:L5:2848:G:O2'	5:L5:3838:U:O4	2.23	0.52
36:Ld:22:THR:HG23	36:Ld:122:VAL:HG13	1.92	0.52
43:Lk:26:LYS:HB2	43:Lk:69:LEU:HD12	1.91	0.52
3:CF:346:ILE:HD11	3:CF:394:LEU:HD13	1.91	0.52
7:L8:95:A:N3	40:Lh:63:GLN:NE2	2.57	0.52
28:LV:112:MET:SD	28:LV:135:ASN:ND2	2.73	0.52
52:SD:138:VAL:HG13	52:SD:182:LEU:HD21	1.91	0.52
85:S2:17:C:O2'	85:S2:1194:A:N1	2.36	0.52
85:S2:1098:C:H2'	85:S2:1099:G:C8	2.44	0.52
5:L5:300:A:H2'	5:L5:301:G:H8	1.74	0.52
19:LM:119:ARG:HG3	21:LO:189:ILE:HG23	1.90	0.52
47:Lo:2:VAL:N	47:Lo:90:HIS:O	2.42	0.52
5:L5:3661:G:N7	8:LA:152:SER:OG	2.39	0.52
5:L5:3707:U:H2'	5:L5:3708:C:C6	2.44	0.52
5:L5:4694:G:H4'	15:LH:71:ARG:HH12	1.74	0.52
11:LD:204:VAL:HB	11:LD:236:MET:HE1	1.91	0.52
39:Lg:44:SER:OG	39:Lg:46:CYS:SG	2.62	0.52
68:SB:144:LYS:HD3	68:SB:208:HIS:HB3	1.90	0.52
73:SI:89:GLU:OE1	73:SI:92:ARG:NH2	2.42	0.52
73:SI:98:LYS:HB3	85:S2:377:G:H5'	1.92	0.52
5:L5:180:C:H2'	5:L5:181:C:H6	1.74	0.52
5:L5:4441:A:H5''	16:LI:114:GLY:HA2	1.90	0.52
5:L5:4935:C:H2'	5:L5:4936:G:C8	2.45	0.52
65:Sf:107:LYS:NZ	65:Sf:108:VAL:O	2.42	0.52
65:Sf:133:ALA:HB3	65:Sf:140:TYR:HB3	1.92	0.52
71:SG:49:VAL:HB	71:SG:115:LYS:HG2	1.91	0.52
74:SJ:142:VAL:HG12	74:SJ:144:ILE:H	1.75	0.52
5:L5:2588:C:OP1	5:L5:2768:C:O2'	2.25	0.52
6:L7:52:C:O2'	6:L7:54:A:N7	2.40	0.52
14:LG:165:GLU:OE2	20:LN:26:ARG:NH1	2.40	0.52
54:SK:31:LYS:HZ3	54:SK:40:VAL:H	1.58	0.52
5:L5:152:U:OP2	20:LN:49:ARG:NH2	2.28	0.52
5:L5:1095:A:C2	5:L5:1200:G:N1	2.70	0.52
5:L5:1270:A:H8	5:L5:2106:G:H21	1.57	0.52
5:L5:2652:G:N1	48:Lp:58:GLY:O	2.40	0.52
5:L5:2764:A:H2'	5:L5:2765:A:H8	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LM:38:VAL:HG21	19:LM:50:MET:HB3	1.92	0.52
69:SC:259:THR:HG23	78:SV:16:LYS:HZ3	1.75	0.52
85:S2:1845:A:H2'	85:S2:1846:G:C8	2.45	0.52
5:L5:3898:G:H5'	9:LB:254:ILE:HG13	1.92	0.52
25:LS:15:ARG:HD2	25:LS:25:PRO:HG2	1.92	0.52
65:Sf:124:ASP:OD1	65:Sf:124:ASP:N	2.43	0.52
66:Sg:260:ASP:O	66:Sg:264:LYS:N	2.43	0.52
70:SE:151:ASP:OD2	71:SG:216:ARG:NH2	2.42	0.52
71:SG:92:ARG:O	85:S2:453:C:O2'	2.21	0.52
5:L5:1100:U:H3	5:L5:1194:G:H1	1.58	0.51
12:LE:222:LEU:HB2	12:LE:237:LYS:HD2	1.91	0.51
12:LE:264:ILE:HD11	12:LE:267:LEU:HD22	1.91	0.51
28:LV:42:VAL:HB	28:LV:45:ILE:HG13	1.92	0.51
51:Lt:50:THR:OG1	51:Lt:72:GLU:OE1	2.24	0.51
66:Sg:107:ASP:OD2	66:Sg:125:ARG:NH1	2.43	0.51
73:SI:143:LYS:NZ	85:S2:202:G:OP1	2.43	0.51
85:S2:1643:U:H2'	85:S2:1644:C:C6	2.44	0.51
4:AT:27:G:H22	4:AT:45:A:H2	1.59	0.51
5:L5:1914:C:H4'	21:LO:89:PRO:HD3	1.92	0.51
5:L5:2318:G:N2	5:L5:2321:G:OP2	2.39	0.51
5:L5:4456:OMC:HM21	9:LB:241:PRO:HD3	1.91	0.51
9:LB:206:PRO:HG2	9:LB:209:GLN:HG3	1.91	0.51
61:SU:40:ILE:O	61:SU:44:LYS:HG2	2.11	0.51
70:SE:29:PRO:HA	85:S2:496:C:H5'	1.91	0.51
84:Se:41:ARG:HG3	84:Se:42:PHE:HD1	1.76	0.51
85:S2:889:U:OP2	85:S2:896:U:N3	2.43	0.51
5:L5:257:C:H2'	5:L5:258:G:C8	2.46	0.51
5:L5:1317:U:H2'	5:L5:1318:C:C6	2.45	0.51
5:L5:1971:C:O2	50:Ls:41:GLN:NE2	2.43	0.51
5:L5:3697:U:H5''	5:L5:3698:G:H5'	1.91	0.51
5:L5:4685:U:H2'	5:L5:4686:G:C8	2.46	0.51
18:LL:140:SER:HA	18:LL:143:GLU:HG2	1.92	0.51
31:LY:10:ASP:HB3	31:LY:13:LYS:HB2	1.93	0.51
53:SF:171:GLU:OE2	62:SZ:106:GLN:NE2	2.42	0.51
57:SQ:37:ARG:NH2	85:S2:1543:U:OP1	2.39	0.51
57:SQ:80:GLN:O	57:SQ:84:ILE:HG13	2.11	0.51
61:SU:70:CYS:SG	85:S2:1491:G:O2'	2.54	0.51
82:Sa:12:LYS:HG3	82:Sa:15:ARG:HB2	1.92	0.51
5:L5:1328:G:O2'	5:L5:2349:A:OP1	2.28	0.51
5:L5:4875:G:H5''	25:LS:170:LYS:HE3	1.93	0.51
5:L5:4967:A:H2'	5:L5:4968:A:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LB:95:THR:OG1	9:LB:98:GLY:O	2.22	0.51
23:LQ:154:LYS:NZ	23:LQ:159:PRO:O	2.37	0.51
55:SM:110:VAL:O	55:SM:112:LYS:NZ	2.41	0.51
56:SP:31:GLU:HA	56:SP:34:MET:HE2	1.93	0.51
73:SI:141:ARG:HD3	73:SI:145:ILE:HG21	1.91	0.51
85:S2:1598:G:N2	85:S2:1599:U:O4	2.42	0.51
3:CF:272:LEU:O	3:CF:302:ALA:N	2.43	0.51
5:L5:262:G:H2'	5:L5:263:G:C8	2.44	0.51
5:L5:308:G:O6	20:LN:12:ARG:NH1	2.44	0.51
5:L5:369:G:N2	5:L5:372:A:OP2	2.37	0.51
5:L5:1767:A:H2'	5:L5:1769:G:H5''	1.92	0.51
5:L5:1857:C:H2'	5:L5:1858:A:C8	2.45	0.51
5:L5:2492:C:H2'	5:L5:2493:G:H8	1.74	0.51
5:L5:4459:U:H2'	5:L5:4460:U:C6	2.45	0.51
5:L5:4571:A2M:H2'	5:L5:4572:U:H6	1.75	0.51
6:L7:119:U:C2	11:LD:261:VAL:HG11	2.46	0.51
12:LE:141:ARG:NH1	12:LE:191:GLN:O	2.44	0.51
12:LE:161:ARG:O	12:LE:182:ASN:ND2	2.44	0.51
52:SD:32:ASP:OD2	52:SD:65:ARG:NH1	2.43	0.51
60:ST:74:SER:O	60:ST:78:ILE:HD12	2.10	0.51
69:SC:109:ILE:HD11	69:SC:151:ILE:HD11	1.92	0.51
69:SC:121:ARG:NH1	69:SC:123:ARG:HE	2.08	0.51
70:SE:38:LEU:HD23	85:S2:346:C:H5''	1.93	0.51
71:SG:4:ASN:ND2	85:S2:154:U:O2	2.34	0.51
78:SV:17:CYS:HB2	78:SV:56:CYS:HB3	1.91	0.51
82:Sa:11:ALA:HB3	82:Sa:33:ASP:HB2	1.92	0.51
5:L5:197:A:N1	5:L5:225:G:O2'	2.41	0.51
5:L5:4941:G:OP2	12:LE:188:ARG:NH2	2.36	0.51
10:LC:154:VAL:HG11	10:LC:174:LEU:HD11	1.92	0.51
15:LH:24:THR:HA	15:LH:37:ASP:HA	1.93	0.51
29:LW:123:LYS:HD2	85:S2:320:G:H5''	1.93	0.51
60:ST:40:ALA:HB3	60:ST:43:LYS:HG2	1.91	0.51
71:SG:227:GLN:HB3	71:SG:231:ARG:HH21	1.76	0.51
77:SO:45:THR:HA	77:SO:52:THR:HA	1.92	0.51
85:S2:1144:A:H2'	85:S2:1145:A:C8	2.46	0.51
5:L5:303:C:OP2	20:LN:68:ARG:NH2	2.41	0.51
5:L5:501:C:O2'	5:L5:648:G:OP1	2.29	0.51
5:L5:2468:U:O2'	5:L5:2506:G:N2	2.44	0.51
5:L5:2568:C:H2'	5:L5:2569:G:C8	2.46	0.51
5:L5:4523:A2M:H5''	5:L5:4524:G:H5'	1.93	0.51
5:L5:5016:A:C2	5:L5:5033:G:N2	2.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LB:77:THR:OG1	9:LB:335:GLY:O	2.26	0.51
12:LE:91:THR:HA	12:LE:108:LYS:HA	1.93	0.51
5:L5:711:A:H2'	5:L5:712:C:C6	2.46	0.51
5:L5:1187:G:OP2	5:L5:1187:G:N2	2.36	0.51
5:L5:1523:A:N3	5:L5:4389:C:O2'	2.42	0.51
50:Ls:110:ALA:HA	50:Ls:182:PRO:HG2	1.93	0.51
59:SS:15:VAL:HG12	59:SS:16:LEU:HG	1.93	0.51
66:Sg:251:ALA:HA	66:Sg:256:ILE:HD13	1.92	0.51
76:SN:14:SER:HB3	85:S2:1016:U:H5''	1.93	0.51
79:SW:6:VAL:HG13	79:SW:29:PRO:HB2	1.91	0.51
80:SX:105:PHE:HD1	80:SX:121:LYS:HB3	1.75	0.51
84:Se:31:ARG:NH2	85:S2:525:A:O3'	2.44	0.51
85:S2:640:A:H2'	85:S2:641:A:C8	2.46	0.51
5:L5:907:C:H2'	5:L5:908:G:H8	1.76	0.51
5:L5:1538:U:H2'	5:L5:1539:G:H8	1.76	0.51
5:L5:1617:G:H1'	5:L5:2513:A:N6	2.26	0.51
5:L5:1655:C:OP2	33:La:26:ARG:NH1	2.44	0.51
5:L5:2845:A:H61	5:L5:3843:C:N4	2.09	0.51
5:L5:3861:A:H2'	5:L5:3862:A:H8	1.74	0.51
5:L5:3917:A:H2'	5:L5:3918:G:H8	1.76	0.51
5:L5:3944:G:H1	5:L5:4069:U:H3	1.59	0.51
5:L5:4591:U:H2'	5:L5:4592:C:C6	2.46	0.51
9:LB:83:PRO:O	9:LB:167:GLN:NE2	2.43	0.51
66:Sg:133:ASN:HB3	66:Sg:139:LYS:HD2	1.92	0.51
5:L5:2020:U:H2'	5:L5:2021:G:H8	1.76	0.51
5:L5:4594:U:H2'	5:L5:4595:G:C8	2.42	0.51
17:LJ:42:GLN:HG2	17:LJ:117:ILE:HD12	1.92	0.51
77:SO:75:MET:HG3	77:SO:118:ALA:HB2	1.91	0.51
83:Sb:36:LYS:HB2	83:Sb:78:SER:HB3	1.92	0.51
85:S2:948:C:H2'	85:S2:949:G:C8	2.45	0.51
85:S2:1279:C:H2'	85:S2:1280:G:H8	1.76	0.51
5:L5:173:C:OP1	18:LL:129:ARG:NH1	2.44	0.50
5:L5:1503:A:H4'	5:L5:1504:G:H5'	1.93	0.50
5:L5:1516:G:O2'	18:LL:18:TRP:NE1	2.41	0.50
5:L5:2666:U:O2'	5:L5:2668:G:N7	2.38	0.50
5:L5:2765:A:H2'	5:L5:2766:A:C8	2.46	0.50
5:L5:3736:A:H2'	5:L5:3737:A:H8	1.76	0.50
5:L5:4492:U:O2'	5:L5:4512:U:O2	2.25	0.50
21:LO:186:GLU:OE1	21:LO:186:GLU:N	2.44	0.50
24:LR:127:VAL:HG12	24:LR:132:PHE:HD2	1.76	0.50
66:Sg:18:VAL:O	66:Sg:287:THR:OG1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SC:169:TYR:OH	69:SC:175:GLY:O	2.26	0.50
69:SC:196:ILE:HB	69:SC:223:TYR:HB2	1.92	0.50
78:SV:42:VAL:HG23	78:SV:43:THR:HG23	1.93	0.50
80:SX:90:CYS:HA	80:SX:93:PHE:HD2	1.75	0.50
5:L5:1333:A:H2'	5:L5:1334:A:H8	1.75	0.50
5:L5:2478:C:N3	5:L5:2591:A:O2'	2.44	0.50
5:L5:2638:G:H22	5:L5:2719:C:P	2.33	0.50
5:L5:4522:G:O2'	5:L5:4525:C:OP2	2.24	0.50
5:L5:4912:G:N2	9:LB:156:TYR:OH	2.44	0.50
5:L5:5030:U:H2'	5:L5:5031:G:H8	1.76	0.50
9:LB:258:HIS:HA	9:LB:260:ALA:N	2.25	0.50
9:LB:302:ASN:HB2	9:LB:313:SER:HA	1.93	0.50
51:Lt:22:VAL:HA	51:Lt:48:LYS:HG2	1.94	0.50
52:SD:51:LEU:HD12	52:SD:91:VAL:HG12	1.93	0.50
53:SF:40:ALA:HB3	53:SF:67:PRO:HA	1.92	0.50
67:SA:145:ILE:HG23	67:SA:159:ILE:HB	1.93	0.50
85:S2:57:U:OP1	85:S2:504:G:O2'	2.29	0.50
85:S2:67:C:N4	85:S2:70:G:N7	2.59	0.50
85:S2:1405:A:H2'	85:S2:1406:G:O4'	2.11	0.50
3:CF:251:GLN:N	3:CF:264:VAL:O	2.44	0.50
5:L5:68:U:OP1	20:LN:178:HIS:ND1	2.39	0.50
5:L5:153:G:H2'	5:L5:154:G:H8	1.77	0.50
5:L5:256:G:H2'	5:L5:257:C:C6	2.46	0.50
5:L5:965:G:N2	5:L5:2092:G:H1'	2.26	0.50
5:L5:1411:C:H2'	5:L5:1412:G:C8	2.46	0.50
5:L5:1683:PSU:OP1	33:La:44:ASN:ND2	2.42	0.50
5:L5:2622:G:O6	27:LU:81:ARG:NH2	2.45	0.50
5:L5:4987:C:OP2	9:LB:116:ARG:NH2	2.45	0.50
7:L8:142:U:OP1	20:LN:38:ARG:NH2	2.39	0.50
53:SF:22:LYS:HG3	53:SF:23:TRP:CD2	2.46	0.50
74:SJ:41:ARG:N	85:S2:642:U:OP1	2.45	0.50
79:SW:6:VAL:HG12	79:SW:34:ILE:HD11	1.92	0.50
85:S2:1372:U:OP1	85:S2:1385:G:N2	2.40	0.50
3:CF:42:PHE:HE1	3:CF:67:ARG:HH21	1.59	0.50
5:L5:184:U:H3	5:L5:253:G:H1	1.60	0.50
5:L5:700:G:N1	5:L5:701:G:C6	2.80	0.50
5:L5:1942:A:H2'	5:L5:1943:A:H8	1.76	0.50
5:L5:1979:A:H1'	5:L5:1988:G:N2	2.27	0.50
5:L5:1983:A:O2'	5:L5:2011:C:OP1	2.29	0.50
13:LF:41:MET:HE2	34:Lb:113:ALA:HB2	1.92	0.50
66:Sg:89:LEU:HB2	66:Sg:101:PHE:HE1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SC:70:VAL:HG21	69:SC:93:ILE:HG23	1.94	0.50
70:SE:208:VAL:HG11	70:SE:225:ILE:HG13	1.93	0.50
71:SG:224:ARG:HH21	71:SG:227:GLN:HG3	1.75	0.50
3:CF:63:LEU:HB2	3:CF:66:GLU:HB2	1.94	0.50
4:AT:18:G:N2	4:AT:59:A:OP2	2.43	0.50
5:L5:3722:G:H2'	5:L5:3723:A:H8	1.76	0.50
14:LG:175:ARG:HG2	14:LG:230:TYR:CD2	2.47	0.50
18:LL:111:GLN:O	18:LL:115:GLN:HG2	2.11	0.50
21:LO:126:VAL:HG13	21:LO:127:VAL:HG13	1.94	0.50
52:SD:211:VAL:O	58:SR:20:TYR:OH	2.26	0.50
57:SQ:53:GLU:OE1	57:SQ:85:ARG:NH2	2.44	0.50
67:SA:184:ARG:HG2	67:SA:189:ILE:HB	1.93	0.50
69:SC:167:ARG:HB3	69:SC:177:PRO:HB2	1.92	0.50
75:SL:126:VAL:HG12	75:SL:145:VAL:HG22	1.92	0.50
82:Sa:32:LYS:NZ	85:S2:989:C:O2	2.45	0.50
5:L5:371:A:N3	5:L5:1531:U:O2'	2.42	0.50
5:L5:1510:G:H2'	5:L5:1511:U:C6	2.47	0.50
9:LB:220:ILE:HB	9:LB:346:THR:HB	1.94	0.50
31:LY:2:LYS:HD2	31:LY:7:VAL:HG23	1.91	0.50
35:Lc:82:GLY:HA2	35:Lc:91:VAL:HG12	1.93	0.50
36:Ld:54:MET:HE3	36:Ld:60:PRO:HA	1.92	0.50
59:SS:27:ALA:HB2	59:SS:52:LEU:HD12	1.93	0.50
78:SV:51:LYS:NZ	78:SV:76:ASP:OD1	2.43	0.50
85:S2:60:A:N3	85:S2:316:G:O2'	2.40	0.50
85:S2:1588:A:H2'	85:S2:1589:A:C8	2.46	0.50
85:S2:1770:G:OP1	85:S2:1771:G:N2	2.36	0.50
2:Pt:29:C:H2'	2:Pt:30:G:H8	1.77	0.50
3:CF:149:ILE:HA	3:CF:188:VAL:HG23	1.92	0.50
5:L5:1332:C:H2'	5:L5:1333:A:C8	2.47	0.50
5:L5:1370:G:O6	10:LC:239:LYS:NZ	2.45	0.50
5:L5:2045:G:O6	5:L5:3870:C:O2'	2.29	0.50
5:L5:2696:A:H62	43:Lk:35:LYS:NZ	2.09	0.50
8:LA:181:LYS:HB2	8:LA:184:ARG:HG3	1.94	0.50
16:LI:152:LEU:HB3	16:LI:165:ILE:HD12	1.93	0.50
35:Lc:51:ASN:HB2	35:Lc:77:ASN:HB2	1.92	0.50
54:SK:31:LYS:NZ	54:SK:40:VAL:H	2.10	0.50
67:SA:106:GLY:N	67:SA:136:GLU:OE2	2.34	0.50
85:S2:649:PSU:H2'	85:S2:650:A:H8	1.76	0.50
85:S2:1010:G:H2'	85:S2:1011:A:H8	1.75	0.50
5:L5:293:G:N2	20:LN:178:HIS:O	2.36	0.50
5:L5:4769:G:H5''	21:LO:176:ARG:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:4965:U:H4'	5:L5:4966:A:H5'	1.94	0.50
29:LW:101:ARG:NH2	71:SG:145:PHE:O	2.39	0.50
59:SS:60:THR:OG1	59:SS:62:ASP:OD1	2.25	0.50
60:ST:73:GLY:O	60:ST:94:ARG:NH2	2.43	0.50
85:S2:528:A:H2'	85:S2:529:A:C8	2.46	0.50
85:S2:595:U:H2'	85:S2:596:U:C6	2.47	0.50
85:S2:1084:A:OP1	85:S2:1858:G:O2'	2.27	0.50
85:S2:1720:U:H5''	85:S2:1721:U:H5''	1.93	0.50
5:L5:386:A:O2'	31:LY:87:ARG:NH1	2.45	0.50
5:L5:387:G:O2'	5:L5:412:G:N1	2.38	0.50
5:L5:1326:A2M:H2'	5:L5:1327:C:H6	1.76	0.50
5:L5:1662:C:H2'	5:L5:1663:C:C6	2.47	0.50
5:L5:2347:A:C4	37:Le:31:ILE:HD11	2.47	0.50
24:LR:39:GLN:OE1	24:LR:42:ARG:NH1	2.44	0.50
53:SF:26:ASP:OD1	53:SF:26:ASP:N	2.45	0.50
55:SM:58:GLU:HB3	55:SM:61:TYR:HB2	1.94	0.50
75:SL:103:GLU:HG3	80:SX:11:ARG:HB2	1.94	0.50
79:SW:28:ARG:HH22	85:S2:1093:A:H5''	1.76	0.50
84:Se:41:ARG:HG3	84:Se:42:PHE:CD1	2.47	0.50
85:S2:964:A:H2'	85:S2:965:U:H6	1.77	0.50
85:S2:1438:A:H2'	85:S2:1439:A:C8	2.47	0.50
5:L5:66:A:O2'	5:L5:326:C:O2	2.30	0.49
5:L5:729:G:H5''	13:LF:76:ARG:HD2	1.94	0.49
5:L5:964:A:H2'	5:L5:965:G:H4'	1.93	0.49
5:L5:1307:A:H2'	5:L5:1308:C:H6	1.77	0.49
5:L5:2870:A:H2'	5:L5:2871:A:C8	2.47	0.49
5:L5:3589:G:N2	5:L5:3590:G:O6	2.45	0.49
5:L5:3796:U:HO2'	85:S2:1720:U:HO2'	1.60	0.49
5:L5:4095:G:H2'	5:L5:4096:C:C6	2.47	0.49
5:L5:4501:U:OP1	9:LB:5:LYS:NZ	2.45	0.49
5:L5:4991:U:H2'	5:L5:4992:G:C8	2.47	0.49
13:LF:37:PHE:HZ	34:Lb:113:ALA:HB1	1.77	0.49
22:LP:54:GLN:HA	22:LP:83:TRP:CD1	2.47	0.49
29:LW:7:SER:OG	29:LW:8:PHE:N	2.45	0.49
59:SS:39:ARG:NE	85:S2:1629:C:OP1	2.36	0.49
62:SZ:41:ARG:HH12	62:SZ:44:LEU:HG	1.77	0.49
64:Sd:14:PHE:HB2	85:S2:1661:A:H8	1.77	0.49
71:SG:67:VAL:HG12	71:SG:69:THR:HG22	1.93	0.49
71:SG:175:LYS:HG3	85:S2:77:A:H2	1.76	0.49
76:SN:66:VAL:HG13	76:SN:67:THR:HG23	1.93	0.49
83:Sb:11:SER:OG	83:Sb:14:GLU:OE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:S2:106:C:OP1	85:S2:431:G:O2'	2.27	0.49
5:L5:1390:G:N2	5:L5:1393:G:OP2	2.40	0.49
5:L5:2539:C:H2'	5:L5:2540:C:C6	2.47	0.49
5:L5:3788:C:N4	5:L5:3812:C:OP2	2.43	0.49
5:L5:4584:A:H2'	5:L5:4585:U:O4'	2.12	0.49
27:LU:44:GLN:HB2	27:LU:56:LEU:HD21	1.94	0.49
52:SD:40:ARG:HA	61:SU:108:PRO:HB3	1.93	0.49
55:SM:44:LYS:HE3	65:Sf:129:GLY:H	1.77	0.49
70:SE:127:ARG:HG3	70:SE:142:HIS:HA	1.93	0.49
85:S2:17:C:H2'	85:S2:18:C:C6	2.47	0.49
3:CF:15:HIS:NE2	3:CF:133:THR:OG1	2.29	0.49
5:L5:10:A:H2'	5:L5:11:G:C8	2.47	0.49
5:L5:1645:C:H2'	5:L5:1646:A:C8	2.46	0.49
5:L5:4620:OMU:OP2	5:L5:4670:C:N4	2.38	0.49
87:L5:5292:SPM:H112	21:LO:91:LYS:HD3	1.94	0.49
14:LG:81:ASN:O	14:LG:84:THR:OG1	2.25	0.49
81:SY:10:ARG:HA	85:S2:839:C:H41	1.76	0.49
2:Pt:23:C:H2'	2:Pt:24:A:H8	1.77	0.49
5:L5:97:G:OP1	18:LL:16:LYS:NZ	2.37	0.49
5:L5:1824:G:H2'	5:L5:1825:A:C8	2.47	0.49
5:L5:2407:G:O6	44:Ll:2:SER:N	2.46	0.49
8:LA:112:ILE:HG22	8:LA:135:THR:HG23	1.94	0.49
18:LL:110:LEU:O	18:LL:114:VAL:HG13	2.13	0.49
54:SK:3:MET:HE1	54:SK:11:ILE:HD12	1.92	0.49
55:SM:57:ASP:OD1	85:S2:1285:G:N1	2.34	0.49
5:L5:7:C:H2'	5:L5:8:U:C6	2.47	0.49
5:L5:691:C:H2'	5:L5:692:A:C8	2.48	0.49
5:L5:956:A:H1'	5:L5:2076:G:H5''	1.94	0.49
5:L5:2101:C:H2'	5:L5:2102:G:C8	2.48	0.49
5:L5:2724:G:O2'	5:L5:2726:G:OP2	2.30	0.49
5:L5:4251:A:H5''	17:LJ:108:GLY:HA3	1.94	0.49
12:LE:186:LEU:N	12:LE:250:GLN:OE1	2.44	0.49
12:LE:223:ARG:HB3	12:LE:224:LYS:HB2	1.93	0.49
13:LF:157:ARG:HE	13:LF:248:ASN:HB2	1.78	0.49
14:LG:162:ASP:HB3	14:LG:163:PRO:HD3	1.94	0.49
57:SQ:98:LYS:O	66:Sg:57:ARG:NH1	2.34	0.49
66:Sg:152:SER:OG	66:Sg:168:CYS:SG	2.57	0.49
67:SA:137:ALA:HB1	67:SA:142:LEU:HB3	1.93	0.49
68:SB:167:LYS:O	68:SB:171:ILE:HG12	2.11	0.49
85:S2:323:C:H2'	85:S2:327:G:H22	1.77	0.49
5:L5:2693:G:OP1	43:Lk:35:LYS:HE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:4102:C:H1'	5:L5:4108:G:H1	1.77	0.49
5:L5:4954:G:H2'	5:L5:4955:A:C8	2.48	0.49
5:L5:5024:C:H41	5:L5:5028:G:H21	1.60	0.49
40:Lh:73:TYR:HB3	40:Lh:79:LYS:HG2	1.94	0.49
58:SR:29:HIS:HA	58:SR:32:LYS:HG2	1.95	0.49
71:SG:139:SER:OG	71:SG:142:ARG:NH2	2.43	0.49
72:SH:12:ASN:ND2	72:SH:14:GLU:OE2	2.45	0.49
72:SH:118:ARG:NH1	85:S2:686:PSU:O4	2.36	0.49
79:SW:60:LYS:NZ	85:S2:921:G:O6	2.45	0.49
85:S2:1518:C:H5''	85:S2:1519:U:H5''	1.95	0.49
3:CF:7:HIS:HA	3:CF:86:TYR:O	2.12	0.49
5:L5:162:A:H2'	5:L5:163:A:C8	2.48	0.49
5:L5:169:G:O6	5:L5:170:C:N4	2.46	0.49
5:L5:2520:C:H2'	5:L5:2521:G:C8	2.48	0.49
5:L5:2543:A:H2	5:L5:2773:G:H22	1.60	0.49
16:LI:101:LYS:NZ	16:LI:102:MET:O	2.45	0.49
31:LY:31:SER:HA	31:LY:48:PRO:HA	1.94	0.49
52:SD:142:LEU:HD13	52:SD:150:MET:HE2	1.94	0.49
53:SF:123:GLU:OE1	63:Sc:63:ARG:NH2	2.46	0.49
66:Sg:254:PRO:O	66:Sg:272:GLN:NE2	2.46	0.49
85:S2:656:G:H21	85:S2:663:C:H5''	1.77	0.49
85:S2:1562:C:H2'	85:S2:1563:G:C8	2.46	0.49
5:L5:3911:C:H2'	5:L5:3912:U:H6	1.77	0.49
5:L5:4327:C:OP1	26:LT:70:HIS:NE2	2.46	0.49
5:L5:4699:U:H1'	5:L5:4700:A:H5''	1.94	0.49
6:L7:35:U:O2	6:L7:45:U:O2'	2.30	0.49
13:LF:96:ARG:HH12	13:LF:224:THR:HG22	1.78	0.49
18:LL:55:ILE:O	18:LL:97:SER:OG	2.27	0.49
61:SU:56:MET:HB2	61:SU:86:LYS:HG3	1.94	0.49
73:SI:141:ARG:NH2	85:S2:192:C:OP2	2.45	0.49
85:S2:149:A:H3'	85:S2:150:A:H8	1.78	0.49
85:S2:207:G:H3'	85:S2:208:G:H8	1.78	0.49
2:Pt:50:U:O4	2:Pt:64:G:O6	2.31	0.49
4:AT:24:C:H2'	4:AT:25:A:C8	2.48	0.49
5:L5:1308:C:H2'	5:L5:1309:C:C6	2.48	0.49
5:L5:1346:C:H2'	5:L5:1347:G:C8	2.46	0.49
5:L5:4563:U:H2'	5:L5:4564:A:H8	1.78	0.49
5:L5:4742:G:H2'	5:L5:4743:G:H8	1.78	0.49
7:L8:141:C:H2'	7:L8:142:U:C6	2.47	0.49
30:LX:127:LEU:HD11	30:LX:135:LYS:HE3	1.95	0.49
32:LZ:12:LEU:HB2	32:LZ:81:MET:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:S2:468:A2M:H2'	85:S2:469:A:O4'	2.13	0.49
85:S2:1845:A:H2'	85:S2:1846:G:H8	1.78	0.49
3:CF:101:ASN:HD21	4:AT:1:G:H4'	1.77	0.49
5:L5:1086:C:H2'	5:L5:1087:A:H8	1.78	0.49
5:L5:1700:G:H5''	5:L5:1704:C:H42	1.77	0.49
5:L5:4536:OMC:HM22	5:L5:4537:C:O4'	2.13	0.49
23:LQ:32:TYR:OH	23:LQ:123:PHE:O	2.30	0.49
28:LV:123:LYS:N	28:LV:140:ALA:OXT	2.46	0.49
31:LY:67:ILE:O	31:LY:84:ARG:NH2	2.46	0.49
55:SM:128:PHE:HD1	55:SM:131:LYS:HZ3	1.60	0.49
62:SZ:91:LEU:HG	62:SZ:96:LEU:HD21	1.95	0.49
72:SH:145:ARG:HE	79:SW:51:GLU:HB2	1.78	0.49
79:SW:30:CYS:SG	79:SW:31:SER:N	2.85	0.49
85:S2:1545:A:N3	85:S2:1671:G:O2'	2.36	0.49
85:S2:1628:C:H2'	85:S2:1629:C:C6	2.47	0.49
2:Pt:56:C:O4'	17:LJ:64:ARG:NE	2.42	0.48
5:L5:444:G:H2'	5:L5:445:U:C6	2.47	0.48
5:L5:1601:A:OP1	42:Lj:5:THR:OG1	2.23	0.48
5:L5:2061:U:O2'	25:LS:111:ARG:NH1	2.46	0.48
5:L5:2749:C:H2'	5:L5:2750:G:C8	2.48	0.48
5:L5:3726:A:H2'	5:L5:3727:A:C8	2.48	0.48
5:L5:3893:C:H2'	5:L5:3894:A:C8	2.48	0.48
10:LC:266:THR:HG22	10:LC:267:TRP:H	1.77	0.48
19:LM:100:ARG:HA	19:LM:103:LYS:HG2	1.95	0.48
56:SP:37:TYR:HB3	56:SP:41:GLN:HB2	1.94	0.48
59:SS:38:ARG:O	59:SS:42:HIS:ND1	2.34	0.48
75:SL:61:PRO:HG3	75:SL:141:ASN:HB3	1.95	0.48
85:S2:1441:U:O2	85:S2:1443:C:N4	2.35	0.48
85:S2:1755:C:H2'	85:S2:1756:C:C6	2.47	0.48
5:L5:1872:G:O2'	5:L5:4219:A:N3	2.39	0.48
5:L5:2811:G:N1	5:L5:2814:C:OP2	2.41	0.48
5:L5:4672:A:OP1	28:LV:15:ARG:NH2	2.37	0.48
5:L5:4730:C:N4	5:L5:4731:G:O6	2.46	0.48
15:LH:51:LYS:HG3	15:LH:52:LYS:H	1.77	0.48
21:LO:61:ARG:HA	21:LO:70:PRO:HD2	1.95	0.48
28:LV:88:TYR:OH	28:LV:90:ARG:NH2	2.43	0.48
30:LX:64:SER:HB2	40:Lh:69:LEU:HD13	1.95	0.48
56:SP:100:LYS:HB2	85:S2:1240:A:C6	2.48	0.48
68:SB:123:ALA:HB2	68:SB:165:ARG:HG2	1.95	0.48
71:SG:135:PRO:HA	85:S2:169:U:H5''	1.94	0.48
3:CF:215:LYS:HZ3	3:CF:222:ASN:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:AT:2:U:H2'	4:AT:3:C:C6	2.49	0.48
5:L5:2378:G:N2	5:L5:2381:A:OP2	2.46	0.48
5:L5:4736:C:H2'	5:L5:4737:G:H8	1.78	0.48
15:LH:107:GLU:N	15:LH:107:GLU:OE1	2.46	0.48
16:LI:51:HIS:CD2	16:LI:168:SER:HB3	2.48	0.48
54:SK:2:LEU:HD21	85:S2:1289:U:H4'	1.95	0.48
71:SG:52:ILE:HA	71:SG:111:LEU:HD23	1.96	0.48
81:SY:36:PRO:HG3	85:S2:570:C:H4'	1.95	0.48
85:S2:102:A:H4'	85:S2:104:A:C8	2.48	0.48
85:S2:441:C:H2'	85:S2:442:C:C6	2.48	0.48
3:CF:111:CYS:SG	3:CF:112:ALA:N	2.85	0.48
5:L5:280:G:OP2	20:LN:44:ARG:NH1	2.45	0.48
5:L5:419:A:N3	5:L5:1332:C:O2'	2.42	0.48
5:L5:438:G:OP1	37:Le:16:ARG:NH1	2.39	0.48
5:L5:2611:A:H2'	5:L5:2612:G:C8	2.49	0.48
5:L5:3664:G:H2'	5:L5:3665:G:C8	2.48	0.48
9:LB:258:HIS:HA	9:LB:260:ALA:H	1.78	0.48
15:LH:93:ARG:HG2	15:LH:182:SER:HB3	1.96	0.48
26:LT:127:GLN:NE2	26:LT:129:LYS:O	2.46	0.48
53:SF:71:ARG:NH2	53:SF:148:ASN:OD1	2.42	0.48
54:SK:14:LEU:HD22	54:SK:35:LEU:HD23	1.95	0.48
61:SU:67:LYS:HG2	61:SU:78:ASP:HB2	1.94	0.48
68:SB:120:MET:HE1	85:S2:987:A:C6	2.48	0.48
80:SX:105:PHE:CD1	80:SX:121:LYS:HB3	2.49	0.48
85:S2:90:G:OP1	85:S2:445:A:N6	2.47	0.48
85:S2:1457:U:H2'	85:S2:1458:G:H8	1.78	0.48
85:S2:1801:A:H2'	85:S2:1802:C:C6	2.47	0.48
5:L5:1327:C:H2'	5:L5:1328:G:C8	2.48	0.48
5:L5:1558:A:H2'	5:L5:1559:G:H8	1.79	0.48
5:L5:1591:U:OP2	5:L5:2856:C:O2'	2.20	0.48
5:L5:2824:OMC:H1'	5:L5:2824:OMC:HM23	1.70	0.48
5:L5:3641:U:H5	5:L5:3646:A:N7	2.11	0.48
5:L5:3856:A:H5''	22:LP:83:TRP:O	2.14	0.48
5:L5:3945:A:H2'	5:L5:3946:G:C8	2.48	0.48
6:L7:63:C:H5'	6:L7:64:G:H5''	1.95	0.48
11:LD:181:PRO:HD2	11:LD:195:HIS:CD2	2.48	0.48
29:LW:2:LYS:HE3	29:LW:15:PRO:HB3	1.95	0.48
31:LY:22:PRO:HD2	31:LY:25:ILE:HD11	1.96	0.48
32:LZ:11:VAL:HG12	32:LZ:82:PRO:HA	1.96	0.48
55:SM:128:PHE:HA	55:SM:131:LYS:HG2	1.96	0.48
71:SG:170:ARG:HA	85:S2:72:C:H42	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:SH:51:ILE:HD11	72:SH:176:VAL:HG12	1.96	0.48
85:S2:902:G:O2'	85:S2:903:A:O4'	2.32	0.48
3:CF:178:ILE:HB	3:CF:183:TYR:HB2	1.95	0.48
5:L5:679:C:H2'	5:L5:680:G:C8	2.47	0.48
5:L5:718:C:OP1	13:LF:217:ARG:NH1	2.41	0.48
5:L5:4638:U:OP1	5:L5:5044:A:O2'	2.31	0.48
7:L8:102:G:H5''	42:Lj:39:TYR:HE1	1.77	0.48
52:SD:109:LEU:HD21	52:SD:115:VAL:HA	1.96	0.48
60:ST:44:GLU:HG3	60:ST:45:LEU:HD12	1.96	0.48
70:SE:187:ALA:O	70:SE:245:ARG:NH1	2.40	0.48
85:S2:455:A:H2'	85:S2:456:C:C6	2.49	0.48
3:CF:360:VAL:HG12	3:CF:369:ALA:HB2	1.96	0.48
5:L5:318:A:H2'	5:L5:319:A:C8	2.49	0.48
5:L5:1279:A:O2'	5:L5:1281:G:N7	2.38	0.48
5:L5:1972:G:H2'	5:L5:1973:G:C8	2.49	0.48
5:L5:2018:C:H2'	5:L5:2019:C:C6	2.49	0.48
5:L5:2743:A:H2'	5:L5:2744:A:C8	2.49	0.48
5:L5:3656:A:H2'	5:L5:3657:U:H6	1.78	0.48
5:L5:3880:G:H2'	5:L5:3881:G:C8	2.48	0.48
5:L5:4069:U:H2'	5:L5:4070:U:C6	2.48	0.48
5:L5:5005:G:N2	5:L5:5041:G:O2'	2.46	0.48
7:L8:21:C:OP1	10:LC:195:LYS:NZ	2.46	0.48
21:LO:10:ASP:OD2	21:LO:37:ARG:NH2	2.47	0.48
54:SK:31:LYS:HZ3	54:SK:39:ASN:N	2.11	0.48
57:SQ:110:ASP:OD1	57:SQ:111:ILE:HD12	2.14	0.48
59:SS:36:VAL:HG21	59:SS:71:MET:HE3	1.95	0.48
66:Sg:106:LYS:HB3	66:Sg:125:ARG:HB2	1.94	0.48
70:SE:100:ARG:HB2	70:SE:114:ILE:HD13	1.94	0.48
79:SW:3:ARG:HD3	79:SW:6:VAL:HG22	1.96	0.48
85:S2:1554:C:OP2	85:S2:1555:U:O2'	2.30	0.48
85:S2:1617:G:N1	85:S2:1620:A:OP2	2.46	0.48
1:CI:78:HIS:NE2	5:L5:2706:G:N7	2.61	0.48
5:L5:93:G:H2'	5:L5:94:A:C8	2.49	0.48
5:L5:1855:G:OP1	34:Lb:4:SER:HB2	2.14	0.48
5:L5:2491:C:O2'	5:L5:2492:C:O4'	2.25	0.48
5:L5:2580:U:HO2'	32:LZ:79:HIS:CE1	2.29	0.48
5:L5:3867:A2M:H2'	5:L5:3868:G:O4'	2.14	0.48
5:L5:5064:G:N2	22:LP:75:GLN:HE22	2.11	0.48
15:LH:18:ILE:HG12	15:LH:27:VAL:HG22	1.95	0.48
33:La:102:ASP:HA	33:La:125:LYS:HB2	1.95	0.48
42:Lj:2:THR:HG22	42:Lj:4:GLY:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SD:137:VAL:HB	52:SD:185:LYS:HB2	1.94	0.48
52:SD:172:VAL:HG22	52:SD:185:LYS:HG2	1.95	0.48
55:SM:82:ASN:OD1	55:SM:83:LYS:N	2.47	0.48
58:SR:29:HIS:CD2	66:Sg:36:ARG:HH21	2.31	0.48
69:SC:257:LYS:O	78:SV:16:LYS:NZ	2.46	0.48
76:SN:55:ARG:HD3	85:S2:1017:U:H5'	1.96	0.48
77:SO:33:ILE:HB	77:SO:97:LEU:HD23	1.95	0.48
85:S2:639:C:H2'	85:S2:640:A:C8	2.48	0.48
5:L5:1552:G:O2'	5:L5:1574:G:N2	2.34	0.48
5:L5:1960:A:C8	50:Ls:63:LYS:HE2	2.48	0.48
5:L5:2298:U:OP1	10:LC:204:ARG:NE	2.46	0.48
5:L5:2696:A:OP1	43:Lk:26:LYS:NZ	2.47	0.48
5:L5:2749:C:H2'	5:L5:2750:G:H8	1.78	0.48
5:L5:2899:C:P	24:LR:108:ARG:HH22	2.36	0.48
5:L5:4239:A:H2'	5:L5:4240:G:H8	1.79	0.48
5:L5:4524:G:C2	9:LB:252:ALA:HB1	2.49	0.48
14:LG:150:LYS:NZ	14:LG:177:MET:O	2.46	0.48
21:LO:54:TYR:OH	21:LO:73:PHE:O	2.31	0.48
29:LW:97:LYS:O	29:LW:99:GLU:N	2.45	0.48
53:SF:39:ILE:HG23	53:SF:68:ILE:HD13	1.95	0.48
53:SF:51:HIS:NE2	85:S2:1674:G:OP1	2.44	0.48
67:SA:42:LYS:HD3	67:SA:46:ILE:HB	1.95	0.48
69:SC:102:LEU:HD22	69:SC:130:ILE:HD12	1.96	0.48
71:SG:2:LYS:HB3	71:SG:15:LEU:HD11	1.96	0.48
71:SG:170:ARG:HG3	85:S2:72:C:N3	2.28	0.48
85:S2:1407:U:H2'	85:S2:1408:U:C6	2.49	0.48
1:CI:75:LYS:O	27:LU:117:ILE:C	2.56	0.48
4:AT:3:C:H2'	4:AT:4:U:C6	2.49	0.48
4:AT:60:A:H2'	4:AT:61:A:O4'	2.14	0.48
5:L5:3732:A:H2'	5:L5:3733:A:C8	2.46	0.48
5:L5:3867:A2M:HM'3	5:L5:3867:A2M:H1'	1.56	0.48
5:L5:3910:C:H2'	5:L5:3911:C:H6	1.78	0.48
17:LJ:63:ARG:HH11	47:Lo:106:PHE:HB2	1.79	0.48
59:SS:88:LYS:H	59:SS:95:TYR:HD1	1.59	0.48
66:Sg:163:PRO:HB2	66:Sg:179:LEU:HD12	1.94	0.48
79:SW:44:HIS:NE2	79:SW:112:ASP:OD2	2.36	0.48
85:S2:5:U:H2'	85:S2:6:G:C8	2.49	0.48
85:S2:1550:G:O2'	85:S2:1558:C:O2	2.23	0.48
5:L5:2275:G:H2'	5:L5:2276:A:C8	2.49	0.47
5:L5:4060:U:H2'	5:L5:4061:G:C8	2.49	0.47
5:L5:4910:G:H22	21:LO:107:GLY:HA3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:5006:U:H4'	5:L5:5007:A:H5'	1.96	0.47
7:L8:75:OMG:HM23	7:L8:75:OMG:H1'	1.75	0.47
9:LB:29:VAL:HG12	9:LB:31:SER:H	1.79	0.47
22:LP:52:THR:HG23	22:LP:85:LYS:HG3	1.96	0.47
26:LT:102:ARG:O	26:LT:106:LEU:HG	2.14	0.47
53:SF:19:LEU:HD11	53:SF:50:PRO:HD3	1.96	0.47
54:SK:85:LEU:HD21	54:SK:89:ILE:HB	1.96	0.47
57:SQ:110:ASP:OD1	57:SQ:110:ASP:N	2.46	0.47
65:Sf:92:LYS:NZ	85:S2:1271:C:OP1	2.44	0.47
67:SA:172:GLY:HA3	67:SA:203:PHE:HD1	1.78	0.47
72:SH:10:LYS:HE3	72:SH:17:ASP:HB3	1.96	0.47
79:SW:57:ARG:HD2	85:S2:919:A:H4'	1.95	0.47
81:SY:105:LYS:O	81:SY:109:GLU:HG2	2.14	0.47
85:S2:325:C:N3	85:S2:326:C:O2'	2.46	0.47
85:S2:747:U:O2	85:S2:796:G:N2	2.47	0.47
85:S2:1680:G:H2'	85:S2:1681:U:C6	2.49	0.47
3:CF:79:LYS:HD2	3:CF:295:HIS:HB3	1.96	0.47
5:L5:267:G:H2'	5:L5:268:G:H8	1.78	0.47
5:L5:1340:OMC:HM23	5:L5:1340:OMC:H1'	1.72	0.47
5:L5:1899:G:O2'	37:Le:57:ASN:OD1	2.31	0.47
5:L5:2640:G:H2'	5:L5:2641:A:C8	2.49	0.47
5:L5:2861:OMC:HM23	5:L5:2861:OMC:H1'	1.68	0.47
5:L5:3595:U:H5''	5:L5:3597:G:OP2	2.14	0.47
5:L5:4088:C:H2'	5:L5:4089:G:C8	2.50	0.47
5:L5:4601:U:H2'	5:L5:4602:A:H8	1.78	0.47
8:LA:131:GLY:H	8:LA:169:VAL:HG13	1.78	0.47
11:LD:211:LEU:HB3	11:LD:219:TYR:HB2	1.96	0.47
75:SL:3:ASP:OD1	75:SL:4:ILE:N	2.47	0.47
85:S2:16:G:H2'	85:S2:17:C:C6	2.50	0.47
85:S2:66:G:H2'	85:S2:67:C:H4'	1.95	0.47
3:CF:290:LYS:HE3	85:S2:488:U:H5''	1.96	0.47
5:L5:1677:PSU:H4'	5:L5:1680:G:C2	2.49	0.47
5:L5:1696:C:H5'	5:L5:1719:A:H1'	1.97	0.47
5:L5:1867:A:H2'	5:L5:1868:A:C8	2.49	0.47
5:L5:4523:A2M:H1'	5:L5:4558:U:C4	2.50	0.47
13:LF:182:TYR:HB3	13:LF:200:ARG:HG3	1.96	0.47
20:LN:46:ASP:OD1	20:LN:47:LYS:N	2.47	0.47
56:SP:100:LYS:HG2	56:SP:101:THR:HG23	1.96	0.47
57:SQ:130:LYS:NZ	57:SQ:131:LYS:O	2.46	0.47
72:SH:113:LYS:HA	72:SH:113:LYS:HD2	1.68	0.47
74:SJ:59:GLU:O	74:SJ:62:THR:OG1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Pt:3:C:H42	2:Pt:70:A:H61	1.61	0.47
2:Pt:29:C:H2'	2:Pt:30:G:C8	2.49	0.47
4:AT:65:G:H3'	4:AT:66:G:H8	1.79	0.47
5:L5:162:A:H2'	5:L5:163:A:H8	1.78	0.47
5:L5:1175:A:H2	5:L5:1185:G:H22	1.62	0.47
5:L5:1280:C:O2'	10:LC:321:ASN:OD1	2.20	0.47
5:L5:4743:G:H2'	5:L5:4744:A:C8	2.49	0.47
8:LA:45:VAL:HG22	8:LA:61:VAL:HG22	1.96	0.47
9:LB:394:LYS:HA	9:LB:397:ILE:HG12	1.96	0.47
61:SU:80:PHE:HB3	64:Sd:52:PHE:HB3	1.95	0.47
69:SC:207:ALA:HB2	85:S2:4:C:H4'	1.96	0.47
77:SO:42:VAL:HG11	77:SO:78:ALA:HA	1.95	0.47
85:S2:945:U:H2'	85:S2:946:U:C6	2.50	0.47
5:L5:106:A:H2'	5:L5:107:G:O4'	2.14	0.47
5:L5:1371:A:N1	7:L8:28:C:O2'	2.45	0.47
5:L5:1392:A:H2'	5:L5:1393:G:C8	2.49	0.47
5:L5:2515:G:OP1	39:Lg:37:LYS:NZ	2.31	0.47
5:L5:3619:G:H22	5:L5:3624:A:H1'	1.79	0.47
32:LZ:46:ILE:HA	32:LZ:70:SER:HA	1.96	0.47
51:Lt:82:ILE:HG12	51:Lt:137:GLN:HG2	1.97	0.47
57:SQ:67:ASP:OD2	57:SQ:69:ARG:NH1	2.46	0.47
67:SA:164:ASN:OD1	67:SA:165:ASN:N	2.48	0.47
69:SC:64:THR:HG22	69:SC:66:LEU:H	1.79	0.47
77:SO:101:GLY:HA3	77:SO:134:PRO:HD2	1.97	0.47
85:S2:866:PSU:H2'	85:S2:867:OMG:H8	1.80	0.47
85:S2:1189:A:H2'	85:S2:1190:A:H8	1.80	0.47
85:S2:1533:A:H2	85:S2:1536:G:N3	2.13	0.47
5:L5:181:C:H2'	5:L5:182:G:C8	2.50	0.47
5:L5:423:G:H21	22:LP:118:GLN:NE2	2.11	0.47
5:L5:3690:U:H2'	5:L5:3691:G:O4'	2.15	0.47
5:L5:4750:G:H2'	5:L5:4751:G:C8	2.50	0.47
5:L5:4750:G:H2'	5:L5:4751:G:H8	1.79	0.47
8:LA:140:ASN:ND2	8:LA:143:THR:OG1	2.48	0.47
53:SF:145:ARG:HH12	63:Sc:47:LYS:HE2	1.79	0.47
54:SK:27:VAL:HB	54:SK:43:LEU:HD12	1.96	0.47
57:SQ:34:VAL:HG22	57:SQ:70:VAL:HB	1.96	0.47
70:SE:89:VAL:HG11	70:SE:119:ALA:HB1	1.97	0.47
85:S2:24:C:O2'	85:S2:25:A:H8	1.97	0.47
85:S2:468:A2M:HM'3	85:S2:468:A2M:H1'	1.73	0.47
85:S2:553:U:O4	85:S2:554:A:N6	2.44	0.47
3:CF:364:HIS:CD2	3:CF:365:THR:H	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:10:A:H2'	5:L5:11:G:H8	1.79	0.47
5:L5:261:G:H2'	5:L5:262:G:C8	2.50	0.47
5:L5:1175:A:H2	5:L5:1185:G:H1	1.59	0.47
5:L5:1466:G:OP2	34:Lb:44:ARG:NH2	2.48	0.47
5:L5:1504:G:H2'	5:L5:1505:C:C6	2.49	0.47
5:L5:1514:U:H2'	5:L5:1515:A:H8	1.78	0.47
5:L5:1918:U:O2'	5:L5:1920:C:OP2	2.33	0.47
5:L5:3932:U:H2'	5:L5:3933:G:H8	1.79	0.47
5:L5:4093:G:H3'	5:L5:4094:G:H8	1.80	0.47
5:L5:4188:U:H2'	5:L5:4189:U:C6	2.50	0.47
5:L5:4304:A:OP2	5:L5:4305:G:N2	2.44	0.47
5:L5:4322:G:N2	5:L5:4325:A:OP2	2.40	0.47
7:L8:67:U:H2'	7:L8:68:G:C8	2.48	0.47
8:LA:108:PRO:HB2	48:Lp:86:LEU:HD23	1.95	0.47
10:LC:289:LEU:HD21	23:LQ:31:LEU:HB2	1.97	0.47
13:LF:162:ILE:HD12	13:LF:167:ILE:HB	1.97	0.47
13:LF:241:ASN:O	13:LF:245:ARG:HG2	2.14	0.47
19:LM:96:GLU:O	19:LM:100:ARG:HG2	2.14	0.47
20:LN:200:LEU:HD22	20:LN:204:ARG:NH1	2.29	0.47
22:LP:5:SER:OG	22:LP:118:GLN:NE2	2.47	0.47
23:LQ:155:ALA:O	23:LQ:158:THR:OG1	2.31	0.47
43:Lk:25:ILE:HD13	43:Lk:57:LYS:HZ3	1.78	0.47
54:SK:65:ARG:NH1	64:Sd:20:SER:OG	2.48	0.47
66:Sg:289:LEU:HD11	66:Sg:298:LEU:HD21	1.95	0.47
69:SC:185:THR:OG1	85:S2:1155:U:OP1	2.31	0.47
70:SE:72:ILE:HD12	70:SE:77:ARG:HG3	1.97	0.47
72:SH:191:GLU:O	72:SH:193:GLN:NE2	2.33	0.47
80:SX:9:THR:HG22	85:S2:681:PSU:H4'	1.97	0.47
80:SX:28:LYS:HE2	80:SX:32:LEU:HD22	1.96	0.47
85:S2:51:U:H2'	85:S2:52:G:H8	1.80	0.47
85:S2:929:G:H2'	85:S2:930:C:O4'	2.14	0.47
5:L5:158:A:H5''	5:L5:159:C:H2'	1.97	0.47
5:L5:1503:A:H62	23:LQ:87:THR:HG21	1.79	0.47
5:L5:1811:G:H21	34:Lb:57:MET:HE2	1.80	0.47
5:L5:2279:A:O2'	37:Le:48:ARG:NH2	2.48	0.47
5:L5:3932:U:H2'	5:L5:3933:G:C8	2.49	0.47
5:L5:4742:G:H2'	5:L5:4743:G:C8	2.50	0.47
21:LO:149:TYR:O	21:LO:153:THR:OG1	2.30	0.47
31:LY:4:ASN:HB3	31:LY:7:VAL:HG22	1.96	0.47
40:Lh:89:ARG:O	40:Lh:93:ARG:HG2	2.15	0.47
48:Lp:75:SER:O	48:Lp:79:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:Ls:62:ARG:HB3	50:Ls:66:ARG:HH12	1.80	0.47
72:SH:30:LEU:O	72:SH:33:ASN:ND2	2.48	0.47
76:SN:29:THR:OG1	76:SN:31:ASP:OD1	2.23	0.47
82:Sa:79:ILE:HD11	85:S2:1864:U:H5'	1.96	0.47
85:S2:516:A:N1	85:S2:643:A:O2'	2.41	0.47
85:S2:1208:A:H2'	85:S2:1209:A:C8	2.50	0.47
85:S2:1577:G:O2'	85:S2:1579:A:N3	2.41	0.47
4:AT:18:G:O2'	4:AT:58:G:N2	2.37	0.47
5:L5:267:G:H2'	5:L5:268:G:C8	2.50	0.47
5:L5:1356:U:H2'	5:L5:1357:C:C6	2.50	0.47
5:L5:2610:G:H2'	5:L5:2611:A:C8	2.50	0.47
38:Lf:25:THR:HB	38:Lf:87:LYS:HD3	1.97	0.47
42:Lj:85:LYS:HB3	42:Lj:85:LYS:HE3	1.74	0.47
51:Lt:76:SER:OG	51:Lt:116:MET:SD	2.63	0.47
52:SD:39:VAL:HG12	52:SD:48:ILE:HG12	1.96	0.47
54:SK:85:LEU:HD12	54:SK:86:PRO:HD2	1.96	0.47
66:Sg:82:SER:OG	66:Sg:83:TRP:N	2.48	0.47
5:L5:424:U:H2'	5:L5:425:U:C6	2.50	0.47
5:L5:457:G:H2'	5:L5:458:C:H6	1.79	0.47
5:L5:1743:A:N1	5:L5:1789:C:O2'	2.45	0.47
5:L5:1869:G:C6	88:L5:5285:SPD:H32	2.50	0.47
5:L5:2083:C:P	23:LQ:14:ARG:HH22	2.37	0.47
5:L5:3951:G:H1'	5:L5:4062:A:H61	1.79	0.47
5:L5:4088:C:H2'	5:L5:4089:G:H8	1.80	0.47
5:L5:4232:U:H5''	47:Lo:3:ASN:O	2.15	0.47
5:L5:4627:U:O2'	9:LB:55:HIS:ND1	2.39	0.47
5:L5:4642:U:H2'	5:L5:4643:G:C8	2.50	0.47
9:LB:220:ILE:HG12	9:LB:278:THR:HG23	1.96	0.47
38:Lf:41:PHE:HE1	38:Lf:110:ILE:HD13	1.80	0.47
62:SZ:85:ARG:NH2	85:S2:1597:C:OP2	2.38	0.47
73:SI:57:ALA:HB2	73:SI:183:GLY:HA2	1.97	0.47
78:SV:1:MET:HB3	78:SV:10:ASP:HB2	1.96	0.47
84:Se:28:LYS:HD3	84:Se:32:ALA:HB1	1.96	0.47
85:S2:99:A2M:HM'3	85:S2:99:A2M:H1'	1.53	0.47
85:S2:1129:G:H3'	85:S2:1130:G:N2	2.30	0.47
85:S2:1844:U:H2'	85:S2:1845:A:C8	2.50	0.47
5:L5:287:U:H2'	5:L5:288:G:C8	2.50	0.46
5:L5:1468:C:H2'	5:L5:1469:C:H6	1.81	0.46
5:L5:2084:C:O2	23:LQ:16:LYS:NZ	2.47	0.46
5:L5:3841:OMC:HM23	5:L5:3841:OMC:H1'	1.72	0.46
5:L5:4728:U:OP1	9:LB:132:LYS:NZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LM:36:ALA:HB3	19:LM:55:MET:HE1	1.96	0.46
52:SD:62:LYS:O	52:SD:67:ARG:NH2	2.41	0.46
57:SQ:139:ALA:HB2	85:S2:1650:A:H5''	1.97	0.46
70:SE:204:SER:OG	70:SE:205:PHE:N	2.41	0.46
71:SG:7:PHE:CE2	71:SG:9:ALA:HB3	2.50	0.46
85:S2:352:U:H2'	85:S2:353:C:C6	2.50	0.46
85:S2:1779:G:H2'	85:S2:1780:G:C8	2.50	0.46
3:CF:145:VAL:O	3:CF:183:TYR:OH	2.25	0.46
3:CF:146:LYS:NZ	3:CF:423:ARG:HH22	2.13	0.46
5:L5:280:G:H5''	20:LN:14:LYS:HE2	1.97	0.46
5:L5:1494:U:H2'	5:L5:1495:G:C8	2.50	0.46
5:L5:1996:C:O3'	50:Ls:44:ARG:NH1	2.46	0.46
5:L5:3718:A2M:HM'3	5:L5:3718:A2M:H1'	1.70	0.46
5:L5:4345:C:H2'	5:L5:4346:U:H6	1.80	0.46
5:L5:4476:C:O2'	5:L5:4478:G:OP2	2.30	0.46
5:L5:4918:C:H2'	5:L5:4919:G:H8	1.81	0.46
5:L5:4991:U:H2'	5:L5:4992:G:H8	1.79	0.46
13:LF:171:ASP:OD1	13:LF:172:ASN:N	2.47	0.46
19:LM:46:ARG:O	19:LM:48:GLN:NE2	2.36	0.46
20:LN:155:VAL:O	20:LN:162:ARG:NH2	2.48	0.46
32:LZ:136:PHE:O	39:Lg:78:TYR:OH	2.30	0.46
39:Lg:45:ALA:HB3	39:Lg:82:MET:HE2	1.96	0.46
70:SE:134:LYS:NZ	85:S2:127:C:O2	2.48	0.46
85:S2:367:U:H4'	85:S2:371:A:C8	2.51	0.46
85:S2:656:G:H5'	85:S2:662:G:N2	2.30	0.46
85:S2:693:A:H2'	85:S2:694:G:C8	2.50	0.46
85:S2:1491:G:H2'	85:S2:1492:U:C6	2.50	0.46
5:L5:737:C:C5	5:L5:739:G:H5''	2.51	0.46
5:L5:1974:U:H4'	5:L5:1975:G:H3'	1.97	0.46
5:L5:2335:C:H2'	5:L5:2336:G:H8	1.79	0.46
5:L5:2517:A:H5'	39:Lg:62:LYS:HD3	1.97	0.46
5:L5:2671:C:H2'	5:L5:2672:C:C6	2.51	0.46
5:L5:3910:C:H2'	5:L5:3911:C:C6	2.50	0.46
5:L5:4541:G:N2	5:L5:4544:A:OP2	2.40	0.46
7:L8:19:C:H2'	7:L8:20:A:C8	2.49	0.46
57:SQ:128:GLU:HG2	57:SQ:137:ALA:HB1	1.97	0.46
65:Sf:117:LEU:HD12	65:Sf:118:ARG:HD3	1.97	0.46
66:Sg:8:ARG:HB3	66:Sg:309:VAL:HG13	1.97	0.46
67:SA:104:THR:O	67:SA:107:THR:OG1	2.33	0.46
74:SJ:114:VAL:HG23	74:SJ:126:ALA:HB1	1.97	0.46
85:S2:576:A2M:HM'3	85:S2:576:A2M:H1'	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:S2:1146:C:O2'	85:S2:1150:A:N1	2.46	0.46
5:L5:170:C:H42	5:L5:266:C:N4	2.13	0.46
5:L5:1339:U:OP1	33:La:8:THR:OG1	2.33	0.46
5:L5:1733:G:N3	5:L5:4214:A:H2'	2.30	0.46
5:L5:2835:A:O2'	9:LB:228:TYR:O	2.29	0.46
5:L5:3908:A:N7	5:L5:4449:A:N6	2.63	0.46
5:L5:4974:C:N4	5:L5:4975:G:O6	2.48	0.46
7:L8:66:A:H2'	7:L8:67:U:C6	2.50	0.46
64:Sd:2:GLY:HA3	64:Sd:6:LEU:HD21	1.97	0.46
69:SC:271:ASP:OD1	69:SC:272:HIS:N	2.48	0.46
70:SE:151:ASP:HA	71:SG:212:LEU:HD21	1.98	0.46
74:SJ:164:PRO:HB3	74:SJ:170:PRO:HA	1.97	0.46
81:SY:77:ASP:OD1	81:SY:77:ASP:N	2.48	0.46
85:S2:1142:G:N2	85:S2:1145:A:OP2	2.37	0.46
3:CF:229:LEU:HA	3:CF:232:LEU:HG	1.96	0.46
3:CF:345:ILE:N	3:CF:435:VAL:O	2.39	0.46
4:AT:44:A:H2'	4:AT:45:A:C8	2.50	0.46
4:AT:63:C:H2'	4:AT:64:G:C8	2.50	0.46
5:L5:318:A:H2'	5:L5:319:A:H8	1.81	0.46
5:L5:2306:G:H1'	5:L5:2332:A:N6	2.31	0.46
5:L5:2777:G:H5''	5:L5:2778:G:H5'	1.97	0.46
5:L5:3721:U:H2'	5:L5:3722:G:H8	1.79	0.46
5:L5:4761:G:H2'	5:L5:4762:A:C8	2.51	0.46
8:LA:206:PRO:HG3	8:LA:213:GLY:HA3	1.97	0.46
24:LR:15:LEU:HD22	24:LR:52:ARG:HB2	1.98	0.46
24:LR:176:ARG:NH2	85:S2:910:G:OP1	2.47	0.46
35:Lc:38:ILE:HD11	35:Lc:46:VAL:HG21	1.97	0.46
59:SS:38:ARG:HD2	60:ST:45:LEU:HD11	1.97	0.46
59:SS:48:ALA:O	59:SS:66:ARG:NH2	2.49	0.46
67:SA:63:ARG:HG3	67:SA:185:MET:HE1	1.97	0.46
85:S2:152:U:H2'	85:S2:153:G:C8	2.50	0.46
85:S2:563:G:O2'	85:S2:564:A:OP1	2.31	0.46
85:S2:907:G:H2'	85:S2:908:A:C8	2.50	0.46
85:S2:1808:U:H2'	85:S2:1809:A:H8	1.81	0.46
3:CF:102:MET:HE3	3:CF:136:HIS:CD2	2.51	0.46
5:L5:1438:U:H4'	13:LF:31:LYS:HE3	1.98	0.46
5:L5:2481:G:H2'	5:L5:2482:C:C6	2.50	0.46
5:L5:3720:G:H22	5:L5:3733:A:H2	1.64	0.46
5:L5:3848:U:H2'	5:L5:3849:A:C8	2.50	0.46
11:LD:146:LEU:HB2	11:LD:163:LEU:HD12	1.98	0.46
29:LW:5:LEU:HD12	29:LW:30:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Lc:34:THR:HG23	35:Lc:95:ALA:HB2	1.97	0.46
63:Sc:17:VAL:HA	63:Sc:30:VAL:HG12	1.98	0.46
68:SB:186:ASN:OD1	68:SB:187:LYS:N	2.49	0.46
78:SV:74:LYS:O	78:SV:81:LYS:NZ	2.41	0.46
80:SX:107:ARG:HG2	80:SX:112:VAL:HG22	1.97	0.46
85:S2:747:U:C2	85:S2:796:G:N1	2.84	0.46
3:CF:214:TRP:CZ2	3:CF:231:ALA:HB2	2.51	0.46
3:CF:214:TRP:HZ2	3:CF:231:ALA:HB2	1.81	0.46
5:L5:1097:C:H2'	5:L5:1098:G:C8	2.51	0.46
5:L5:1770:A:N7	5:L5:1771:U:N3	2.64	0.46
5:L5:1846:G:H2'	5:L5:1847:C:C6	2.50	0.46
5:L5:2413:U:H2'	5:L5:2414:G:H8	1.81	0.46
5:L5:2693:G:OP2	43:Lk:33:LYS:NZ	2.41	0.46
5:L5:2716:C:O3'	27:LU:107:LYS:NZ	2.48	0.46
5:L5:2765:A:H2'	5:L5:2766:A:H8	1.80	0.46
5:L5:4524:G:OP1	5:L5:4559:A:N6	2.43	0.46
15:LH:89:ARG:HD3	15:LH:91:LYS:HE3	1.98	0.46
19:LM:130:LEU:HB3	21:LO:177:LEU:HD11	1.96	0.46
29:LW:56:ARG:HE	29:LW:61:LYS:CB	2.29	0.46
30:LX:90:ILE:HG12	30:LX:96:LEU:HD23	1.98	0.46
37:Le:76:LYS:HD2	37:Le:98:GLU:CD	2.41	0.46
37:Le:99:ILE:HD13	37:Le:108:ARG:HB2	1.98	0.46
40:Lh:107:GLN:O	40:Lh:111:GLU:HG3	2.16	0.46
53:SF:142:SER:HB3	63:Sc:50:VAL:HG22	1.97	0.46
56:SP:93:MET:HE1	56:SP:106:GLU:OE1	2.16	0.46
62:SZ:106:GLN:HG3	62:SZ:108:ILE:HD11	1.96	0.46
77:SO:113:GLN:OE1	82:Sa:46:GLU:N	2.48	0.46
85:S2:17:C:H2'	85:S2:18:C:H6	1.80	0.46
85:S2:106:C:H2'	85:S2:107:A:C8	2.48	0.46
85:S2:1652:G:N2	85:S2:1672:U:O2	2.37	0.46
85:S2:1719:A:N6	85:S2:1814:G:O2'	2.49	0.46
3:CF:282:PRO:HG2	3:CF:324:ASN:HA	1.98	0.46
4:AT:26:C:H2'	4:AT:27:G:H8	1.79	0.46
5:L5:71:C:H1'	18:LL:62:PRO:O	2.16	0.46
5:L5:418:A:C2	7:L8:17:A:H1'	2.50	0.46
5:L5:1982:G:H5'	51:Lt:28:LEU:HD13	1.97	0.46
5:L5:2583:C:OP2	39:Lg:76:ARG:NH1	2.47	0.46
5:L5:3848:U:H2'	5:L5:3849:A:H8	1.81	0.46
5:L5:4457:PSU:H1'	9:LB:252:ALA:HB3	1.98	0.46
5:L5:4638:U:H2'	5:L5:4639:G:N3	2.31	0.46
5:L5:4688:C:H2'	5:L5:4689:PSU:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L7:15:C:H2'	6:L7:16:A:H8	1.81	0.46
9:LB:27:GLY:HA2	9:LB:276:HIS:CD2	2.50	0.46
38:Lf:45:LYS:NZ	38:Lf:108:SER:HA	2.31	0.46
56:SP:123:TYR:OH	59:SS:120:HIS:NE2	2.44	0.46
57:SQ:100:VAL:HG22	57:SQ:101:ASP:H	1.80	0.46
68:SB:145:LYS:HB2	68:SB:145:LYS:HE3	1.70	0.46
77:SO:40:THR:HG21	77:SO:74:ALA:HB2	1.97	0.46
85:S2:1047:C:H2'	85:S2:1048:G:O4'	2.16	0.46
3:CF:198:GLY:HA2	3:CF:201:MET:HE1	1.98	0.46
5:L5:260:C:H2'	5:L5:261:G:C8	2.51	0.46
5:L5:1084:C:H2'	5:L5:1085:C:H6	1.81	0.46
5:L5:1558:A:H2'	5:L5:1559:G:C8	2.50	0.46
5:L5:1824:G:H5''	26:LT:35:LYS:HE2	1.98	0.46
5:L5:1878:G:H2'	5:L5:1879:C:C6	2.51	0.46
5:L5:4305:G:C6	26:LT:80:VAL:HG21	2.51	0.46
7:L8:58:G:O6	42:Lj:63:ARG:NH1	2.45	0.46
16:LI:38:ARG:NH1	16:LI:45:GLU:OE1	2.44	0.46
33:La:36:GLY:HA3	33:La:40:HIS:CE1	2.50	0.46
54:SK:32:HIS:CD2	54:SK:45:VAL:HG11	2.51	0.46
57:SQ:130:LYS:HA	57:SQ:137:ALA:HA	1.98	0.46
60:ST:114:GLU:OE1	60:ST:114:GLU:N	2.48	0.46
62:SZ:86:ALA:HA	62:SZ:89:GLN:HE21	1.80	0.46
5:L5:457:G:H2'	5:L5:458:C:C6	2.51	0.46
5:L5:1457:G:O2'	23:LQ:75:ARG:NH2	2.46	0.46
7:L8:39:G:H1'	7:L8:103:A:N6	2.31	0.46
15:LH:27:VAL:HG12	15:LH:84:VAL:HG21	1.97	0.46
68:SB:23:ASP:OD1	68:SB:23:ASP:N	2.48	0.46
74:SJ:121:LYS:NZ	85:S2:528:A:H5'	2.30	0.46
85:S2:414:A:H2'	85:S2:415:A:H8	1.82	0.46
54:SK:23:ALA:HB3	54:SK:69:TRP:HZ3	1.82	0.45
55:SM:49:LEU:HD21	55:SM:123:VAL:HG11	1.97	0.45
59:SS:78:LYS:HD3	59:SS:78:LYS:HA	1.73	0.45
63:Sc:37:ASP:OD1	63:Sc:39:SER:OG	2.31	0.45
68:SB:85:LYS:HB2	68:SB:101:HIS:HB3	1.98	0.45
69:SC:110:MET:HG2	69:SC:125:LYS:HB3	1.97	0.45
72:SH:91:HIS:ND1	72:SH:169:LYS:HG2	2.30	0.45
80:SX:28:LYS:O	80:SX:32:LEU:HB2	2.16	0.45
85:S2:484:A2M:HM'3	85:S2:484:A2M:H1'	1.72	0.45
5:L5:444:G:H2'	5:L5:445:U:H6	1.81	0.45
5:L5:2412:A:H2'	5:L5:2413:U:C6	2.51	0.45
5:L5:2498:C:H2'	5:L5:2499:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:2803:U:H2'	5:L5:2804:OMC:H6	1.81	0.45
5:L5:5002:U:H2'	5:L5:5003:U:C6	2.51	0.45
18:LL:91:ALA:HB1	18:LL:96:ILE:HB	1.99	0.45
32:LZ:88:ASP:OD1	32:LZ:88:ASP:N	2.41	0.45
51:Lt:117:ARG:HG3	51:Lt:119:ARG:HG3	1.99	0.45
65:Sf:105:TYR:OH	85:S2:1310:U:OP2	2.33	0.45
69:SC:68:ARG:HG2	69:SC:277:HIS:HB2	1.97	0.45
73:SI:84:ASN:HD22	73:SI:100:CYS:HB3	1.80	0.45
83:Sb:33:MET:HE3	83:Sb:48:SER:HA	1.99	0.45
84:Se:39:ASN:HA	84:Se:43:VAL:HG12	1.99	0.45
85:S2:747:U:O2	85:S2:796:G:C2	2.69	0.45
85:S2:1390:U:H2'	85:S2:1391:OMC:C6	2.52	0.45
5:L5:1306:C:H2'	5:L5:1307:A:H8	1.81	0.45
5:L5:2361:G:O2'	5:L5:3859:G:O6	2.32	0.45
5:L5:3687:A:O2'	8:LA:236:GLY:N	2.48	0.45
5:L5:4066:U:H2'	5:L5:4067:U:H6	1.81	0.45
5:L5:4619:U:H2'	5:L5:4620:OMU:H6	1.98	0.45
5:L5:4896:G:H2'	5:L5:4897:G:C8	2.51	0.45
53:SF:59:LYS:HB3	53:SF:62:ARG:HG3	1.99	0.45
53:SF:100:ILE:HD11	53:SF:108:PRO:HB3	1.98	0.45
56:SP:22:LEU:HA	56:SP:25:LEU:HD12	1.97	0.45
57:SQ:15:ARG:HH22	85:S2:1444:U:P	2.39	0.45
72:SH:33:ASN:ND2	72:SH:36:LEU:HB3	2.31	0.45
79:SW:76:SER:OG	85:S2:1158:G:O3'	2.33	0.45
85:S2:692:G:N7	85:S2:693:A:N6	2.64	0.45
85:S2:1304:U:H2'	85:S2:1305:C:C6	2.52	0.45
85:S2:1850:MA6:H8	85:S2:1850:MA6:O5'	2.17	0.45
5:L5:270:U:H2'	5:L5:271:C:C6	2.52	0.45
5:L5:422:C:H2'	5:L5:423:G:H8	1.82	0.45
5:L5:1259:G:H2'	5:L5:1260:G:H8	1.80	0.45
5:L5:1268:G:N7	34:Lb:111:ARG:NH2	2.62	0.45
5:L5:1481:C:H5	41:Li:3:LEU:HB3	1.82	0.45
5:L5:1683:PSU:H2'	5:L5:1684:A:C8	2.52	0.45
5:L5:2021:G:OP1	50:Ls:58:ASN:N	2.42	0.45
5:L5:2607:C:O5'	24:LR:96:MET:HE1	2.16	0.45
5:L5:3785:A2M:H2	5:L5:4551:U:O2	2.16	0.45
5:L5:4882:U:OP1	19:LM:117:LYS:NZ	2.48	0.45
15:LH:4:ILE:HG12	15:LH:61:TRP:CH2	2.52	0.45
20:LN:157:LYS:O	20:LN:162:ARG:NH1	2.45	0.45
43:Lk:12:LEU:HB3	43:Lk:16:ARG:HH12	1.81	0.45
53:SF:185:SER:H	53:SF:190:ILE:HD11	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SU:38:ASP:OD1	61:SU:39:LEU:N	2.49	0.45
67:SA:184:ARG:NE	67:SA:191:ARG:HD3	2.31	0.45
72:SH:37:LYS:HD2	72:SH:40:LEU:HD23	1.99	0.45
85:S2:432:G:H2'	85:S2:433:A:C8	2.52	0.45
85:S2:1101:U:H2'	85:S2:1102:G:H8	1.80	0.45
85:S2:1495:G:H2'	85:S2:1496:U:C6	2.52	0.45
3:CF:17:ASP:H	3:CF:20:LYS:NZ	2.15	0.45
5:L5:161:G:H2'	5:L5:162:A:H8	1.82	0.45
5:L5:179:G:H2'	5:L5:180:C:C6	2.51	0.45
5:L5:400:A2M:HM'3	5:L5:400:A2M:H1'	1.60	0.45
5:L5:1942:A:N3	5:L5:4432:C:O2'	2.48	0.45
5:L5:4301:U:OP1	26:LT:78:LYS:NZ	2.40	0.45
5:L5:4589:A:N1	5:L5:4621:C:O2'	2.39	0.45
5:L5:4716:C:OP1	9:LB:276:HIS:ND1	2.49	0.45
7:L8:39:G:OP1	40:Lh:86:LYS:NZ	2.50	0.45
15:LH:61:TRP:CZ3	19:LM:33:GLN:HG3	2.51	0.45
58:SR:100:PRO:HG2	58:SR:122:PRO:HD3	1.99	0.45
58:SR:109:LEU:HG	58:SR:111:PHE:HD2	1.82	0.45
67:SA:215:GLN:O	67:SA:219:GLU:HG2	2.17	0.45
72:SH:63:PHE:HA	72:SH:95:ILE:O	2.17	0.45
73:SI:5:ARG:NE	85:S2:379:C:O2	2.49	0.45
77:SO:50:LYS:NZ	85:S2:951:C:H1'	2.32	0.45
81:SY:11:LYS:HB2	81:SY:24:VAL:HG12	1.98	0.45
85:S2:1259:A:H1'	85:S2:1264:C:N4	2.31	0.45
85:S2:1278:A:H2'	85:S2:1279:C:C6	2.52	0.45
5:L5:1534:A2M:H8	42:Lj:15:THR:OG1	2.17	0.45
5:L5:2495:U:H2'	5:L5:2496:G:H8	1.82	0.45
5:L5:2550:G:O2'	5:L5:2587:A:N1	2.49	0.45
5:L5:2809:G:O2'	5:L5:4644:G:OP1	2.30	0.45
23:LQ:110:ARG:HG3	23:LQ:120:ILE:HD12	1.98	0.45
25:LS:69:GLU:HG3	25:LS:71:SER:H	1.81	0.45
38:Lf:45:LYS:HA	38:Lf:107:PRO:HD2	1.98	0.45
72:SH:76:GLN:O	72:SH:80:VAL:HG23	2.17	0.45
72:SH:91:HIS:CE1	72:SH:169:LYS:HG2	2.52	0.45
73:SI:139:LYS:HE2	73:SI:139:LYS:HB2	1.70	0.45
80:SX:17:ARG:HH12	85:S2:659:G:N2	2.14	0.45
82:Sa:36:ILE:HD11	82:Sa:75:VAL:HG12	1.97	0.45
85:S2:671:A:H4'	85:S2:672:A:H5''	1.98	0.45
3:CF:117:ALA:HB3	3:CF:122:GLU:HG3	1.99	0.45
5:L5:264:C:H1'	40:Lh:112:ARG:HH21	1.82	0.45
5:L5:319:A:H1'	5:L5:3726:A:N3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:1396:G:HO2'	5:L5:1468:C:HO2'	1.58	0.45
5:L5:4113:U:H4'	5:L5:4115:G:C5	2.51	0.45
5:L5:4232:U:H5'	47:Lo:3:ASN:HB3	1.99	0.45
5:L5:4920:C:H2'	5:L5:4921:C:H6	1.81	0.45
7:L8:5:U:H2'	7:L8:6:C:H6	1.82	0.45
8:LA:180:LEU:HD11	48:Lp:26:VAL:HG11	1.98	0.45
82:Sa:60:ASP:OD1	82:Sa:60:ASP:N	2.43	0.45
85:S2:293:C:O2'	85:S2:294:U:H3'	2.17	0.45
85:S2:1272:OMC:H1'	85:S2:1272:OMC:HM23	1.72	0.45
85:S2:1528:G:H2'	85:S2:1529:C:C6	2.52	0.45
85:S2:1731:A:H2'	85:S2:1732:G:C8	2.52	0.45
5:L5:2249:C:H2'	5:L5:2250:C:H5	1.81	0.45
5:L5:2326:G:H5''	37:Le:127:ALA:HB1	1.98	0.45
5:L5:2579:G:N2	5:L5:2582:A:OP2	2.42	0.45
5:L5:3823:G:OP2	5:L5:3823:G:N2	2.39	0.45
6:L7:23:A:N3	6:L7:118:C:O2'	2.38	0.45
8:LA:112:ILE:HD11	48:Lp:79:VAL:HG22	1.97	0.45
11:LD:108:ARG:CZ	11:LD:253:TYR:HB2	2.47	0.45
36:Ld:33:ILE:HD11	36:Ld:45:ALA:HA	1.99	0.45
46:Ln:12:ARG:HG2	46:Ln:15:ARG:HH21	1.81	0.45
53:SF:76:MET:HE1	53:SF:158:ALA:HB3	1.99	0.45
59:SS:62:ASP:OD1	59:SS:62:ASP:N	2.49	0.45
62:SZ:42:ASP:OD1	62:SZ:42:ASP:N	2.46	0.45
66:Sg:239:LEU:HD11	66:Sg:248:LEU:HD21	1.99	0.45
68:SB:155:TYR:OH	85:S2:989:C:OP2	2.30	0.45
71:SG:56:ASN:HB2	71:SG:108:VAL:HG22	1.99	0.45
72:SH:37:LYS:HA	72:SH:40:LEU:HB3	1.99	0.45
77:SO:149:ARG:NH2	85:S2:961:G:OP1	2.50	0.45
85:S2:45:A:N1	85:S2:480:G:O2'	2.45	0.45
85:S2:674:C:H2'	85:S2:675:U:C6	2.52	0.45
85:S2:1435:C:O2'	85:S2:1436:C:O4'	2.26	0.45
85:S2:1856:C:H2'	85:S2:1857:G:H8	1.82	0.45
1:CI:79:ARG:HH22	5:L5:2708:U:H1'	1.82	0.45
3:CF:229:LEU:HD13	3:CF:232:LEU:HD11	1.98	0.45
5:L5:3606:U:H2'	5:L5:3607:U:C6	2.52	0.45
5:L5:3663:A:N6	5:L5:4168:G:O2'	2.50	0.45
5:L5:3809:G:OP2	5:L5:3809:G:N2	2.35	0.45
5:L5:5004:C:H2'	5:L5:5005:G:O4'	2.16	0.45
7:L8:96:C:H5''	40:Lh:66:LYS:HG2	1.99	0.45
9:LB:240:LEU:HB2	9:LB:248:LEU:HA	1.99	0.45
10:LC:293:LEU:O	10:LC:299:GLN:NE2	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LD:291:GLN:NE2	16:LI:213:HIS:O	2.35	0.45
18:LL:56:ARG:NH1	18:LL:74:ARG:O	2.39	0.45
25:LS:161:ARG:HD2	25:LS:164:LYS:HB2	1.99	0.45
36:Ld:53:ALA:HA	36:Ld:88:LEU:HD21	1.98	0.45
50:Ls:29:ILE:HG22	50:Ls:88:PHE:CD1	2.52	0.45
52:SD:23:GLU:OE2	52:SD:27:ARG:NE	2.49	0.45
53:SF:78:MET:HE3	85:S2:1222:G:H5''	1.99	0.45
53:SF:161:ALA:O	53:SF:165:ASN:ND2	2.44	0.45
68:SB:147:ASN:OD1	68:SB:148:ASN:N	2.49	0.45
73:SI:98:LYS:HG3	73:SI:178:ARG:HG2	1.99	0.45
85:S2:118:C:H1'	85:S2:445:A:C5	2.52	0.45
85:S2:388:U:H2'	85:S2:389:A:C8	2.52	0.45
85:S2:1289:U:H2'	85:S2:1290:G:C8	2.52	0.45
85:S2:1417:C:N3	85:S2:1422:G:N1	2.64	0.45
85:S2:1731:A:H2'	85:S2:1732:G:H8	1.82	0.45
85:S2:1856:C:H2'	85:S2:1857:G:C8	2.52	0.45
2:Pt:73:A:N3	16:LI:110:ARG:NH1	2.65	0.45
3:CF:348:ASN:HD21	3:CF:431:GLN:HG3	1.82	0.45
5:L5:423:G:H5'	22:LP:26:PHE:HZ	1.81	0.45
5:L5:1070:G:O2'	5:L5:1071:C:O5'	2.34	0.45
5:L5:1359:G:H4'	20:LN:203:TYR:HB2	1.98	0.45
5:L5:2006:U:H2'	5:L5:2007:G:O4'	2.17	0.45
5:L5:4612:C:C2	15:LH:120:GLU:HB2	2.52	0.45
6:L7:110:G:H2'	6:L7:111:C:C6	2.52	0.45
9:LB:218:ASP:OD2	9:LB:348:ARG:NH2	2.34	0.45
32:LZ:47:ASP:N	32:LZ:69:LYS:O	2.43	0.45
35:Lc:48:LEU:HD13	35:Lc:57:LYS:HG3	1.98	0.45
51:Lt:119:ARG:CZ	51:Lt:123:ARG:HH12	2.29	0.45
59:SS:132:ARG:NH1	85:S2:1623:A:N1	2.65	0.45
66:Sg:249:CYS:HB3	66:Sg:258:ILE:HD13	1.99	0.45
71:SG:133:LEU:HB2	85:S2:65:C:N3	2.32	0.45
80:SX:140:ARG:HH22	80:SX:142:ARG:HH21	1.65	0.45
85:S2:1393:G:H2'	85:S2:1394:G:C8	2.52	0.45
5:L5:1725:U:H2'	5:L5:1726:U:H6	1.82	0.44
5:L5:2664:G:H4'	5:L5:2677:G:H4'	1.98	0.44
5:L5:4364:G:H2'	5:L5:4365:C:H6	1.82	0.44
5:L5:4627:U:H5''	9:LB:373:LYS:HG2	1.98	0.44
5:L5:4723:A:H2'	5:L5:4724:A:C8	2.52	0.44
5:L5:5001:PSU:H5''	9:LB:382:MET:HE1	1.99	0.44
8:LA:22:HIS:O	8:LA:24:LYS:NZ	2.48	0.44
9:LB:36:ASP:OD1	9:LB:36:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LP:94:MET:HE1	22:LP:146:ILE:HB	2.00	0.44
50:Ls:102:LEU:HD11	50:Ls:187:LEU:HD23	1.99	0.44
58:SR:10:LYS:HG2	58:SR:53:TYR:CE2	2.52	0.44
63:Sc:29:GLN:HA	63:Sc:45:ASN:HA	2.00	0.44
68:SB:138:PHE:O	68:SB:213:ARG:N	2.50	0.44
70:SE:186:GLY:HA3	85:S2:809:A:OP1	2.17	0.44
73:SI:10:LYS:NZ	85:S2:370:G:O2'	2.50	0.44
76:SN:5:HIS:HB3	76:SN:117:LEU:HD13	1.99	0.44
82:Sa:13:LYS:HA	82:Sa:13:LYS:HD3	1.68	0.44
85:S2:750:C:H42	85:S2:793:G:H1'	1.80	0.44
85:S2:1093:A:H2'	85:S2:1094:C:H6	1.81	0.44
5:L5:212:A:H2'	5:L5:213:G:H8	1.82	0.44
5:L5:493:G:O2'	5:L5:494:U:OP1	2.35	0.44
5:L5:1326:A2M:OP2	5:L5:4445:U:O2'	2.31	0.44
5:L5:3610:A:H2'	5:L5:3611:A:C8	2.53	0.44
9:LB:86:VAL:HG12	9:LB:201:LEU:HD23	1.99	0.44
11:LD:234:ASP:OD1	11:LD:235:MET:N	2.50	0.44
25:LS:27:LEU:HB3	26:LT:148:PRO:HB3	1.99	0.44
37:Le:35:TRP:CZ2	37:Le:56:PRO:HD2	2.52	0.44
53:SF:179:ASN:HB2	53:SF:187:SER:HB3	1.98	0.44
65:Sf:110:GLU:HG2	65:Sf:113:LYS:HD3	2.00	0.44
73:SI:45:THR:HG23	73:SI:53:LYS:HG3	1.99	0.44
81:SY:23:MET:O	81:SY:73:GLY:N	2.45	0.44
85:S2:1692:U:H2'	85:S2:1693:G:C8	2.52	0.44
2:Pt:24:A:O2'	5:L5:3770:U:O5'	2.29	0.44
3:CF:242:THR:HG23	3:CF:271:VAL:HG23	1.99	0.44
5:L5:454:U:H2'	5:L5:455:C:O4'	2.18	0.44
5:L5:652:G:H2'	5:L5:653:U:C6	2.52	0.44
5:L5:1095:A:N1	5:L5:1200:G:C6	2.85	0.44
5:L5:1995:G:H2'	5:L5:1996:C:C6	2.53	0.44
5:L5:2007:G:H2'	5:L5:2008:U:C6	2.52	0.44
5:L5:2399:G:O2'	5:L5:2822:G:O2'	2.33	0.44
5:L5:2864:A:H2'	5:L5:2865:U:C6	2.53	0.44
5:L5:2867:C:OP1	85:S2:368:U:N3	2.50	0.44
5:L5:4363:A:H5''	47:Lo:36:GLN:HG2	1.99	0.44
5:L5:4507:A:HO2'	28:LV:41:SER:HG	1.65	0.44
11:LD:107:ARG:NH1	11:LD:169:GLY:O	2.44	0.44
17:LJ:56:THR:OG1	17:LJ:64:ARG:N	2.46	0.44
23:LQ:43:PHE:CD2	23:LQ:133:GLY:HA3	2.52	0.44
23:LQ:99:LYS:HZ2	23:LQ:119:LYS:HD3	1.81	0.44
44:Ll:25:GLN:OE1	44:Ll:28:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SM:68:LEU:HD11	65:Sf:106:TYR:CE2	2.51	0.44
56:SP:48:GLY:O	56:SP:50:ARG:NH1	2.51	0.44
69:SC:64:THR:HG22	69:SC:66:LEU:N	2.32	0.44
73:SI:26:LYS:HE3	85:S2:444:G:O6	2.17	0.44
79:SW:28:ARG:NH2	85:S2:1093:A:H5''	2.32	0.44
85:S2:327:G:H5''	85:S2:328:U:C2	2.53	0.44
85:S2:689:U:H2'	85:S2:690:G:C4	2.52	0.44
85:S2:1694:U:O2'	85:S2:1833:C:O2'	2.29	0.44
5:L5:268:G:H2'	5:L5:269:G:C8	2.51	0.44
5:L5:423:G:H2'	5:L5:424:U:C6	2.53	0.44
5:L5:495:C:H2'	5:L5:496:G:C8	2.52	0.44
5:L5:1084:C:H2'	5:L5:1085:C:C6	2.52	0.44
5:L5:1620:U:H5''	42:Lj:30:GLN:HE21	1.82	0.44
5:L5:2408:U:OP1	44:Ll:42:ARG:NH1	2.44	0.44
8:LA:7:GLY:HA2	8:LA:10:LYS:HG3	2.00	0.44
15:LH:41:ILE:HG22	15:LH:43:VAL:HG13	1.98	0.44
56:SP:47:ARG:NE	85:S2:1619:A:OP1	2.40	0.44
59:SS:63:GLU:O	59:SS:67:VAL:HG23	2.18	0.44
67:SA:4:ALA:HA	78:SV:80:SER:HB3	1.99	0.44
71:SG:87:ARG:HD3	71:SG:87:ARG:HA	1.71	0.44
85:S2:1417:C:O2	85:S2:1422:G:C6	2.70	0.44
5:L5:1308:C:OP1	21:LO:93:LYS:NZ	2.42	0.44
5:L5:1703:C:O2'	5:L5:1704:C:O5'	2.35	0.44
5:L5:1806:G:H2'	5:L5:1807:C:H6	1.82	0.44
5:L5:4935:C:H2'	5:L5:4936:G:H8	1.80	0.44
8:LA:130:SER:HB2	8:LA:171:GLY:HA3	2.00	0.44
11:LD:182:GLY:HA2	11:LD:194:VAL:HG23	1.99	0.44
29:LW:56:ARG:HE	29:LW:61:LYS:HB2	1.82	0.44
32:LZ:95:VAL:HG12	32:LZ:110:ALA:HA	2.00	0.44
51:Lt:79:ALA:HA	51:Lt:82:ILE:HG22	2.00	0.44
52:SD:77:PHE:HB2	52:SD:79:PHE:CE1	2.52	0.44
54:SK:64:TRP:HB3	64:Sd:23:VAL:HA	1.99	0.44
65:Sf:105:TYR:HE1	65:Sf:131:PHE:HD2	1.65	0.44
72:SH:126:HIS:CE1	72:SH:181:THR:HG23	2.52	0.44
80:SX:90:CYS:HA	80:SX:93:PHE:CD2	2.52	0.44
85:S2:1030:A:H2'	85:S2:1031:A2M:H8	1.98	0.44
2:Pt:58:A:O2'	2:Pt:60:A:OP2	2.30	0.44
5:L5:24:G:N7	42:Lj:46:LYS:NZ	2.65	0.44
5:L5:35:U:H4'	5:L5:1525:A:C2	2.52	0.44
5:L5:1697:G:H22	5:L5:2084:C:P	2.41	0.44
5:L5:1998:A:N6	50:Ls:40:MET:SD	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:2909:C:H1'	5:L5:3585:G:H1	1.81	0.44
5:L5:3893:C:H2'	5:L5:3894:A:H8	1.83	0.44
5:L5:4590:A2M:HM'3	5:L5:4590:A2M:H1'	1.84	0.44
7:L8:102:G:OP2	7:L8:104:A:O2'	2.32	0.44
9:LB:299:ILE:HB	9:LB:313:SER:HB3	1.99	0.44
12:LE:190:HIS:HB3	12:LE:193:PHE:HD2	1.82	0.44
23:LQ:178:ARG:N	33:La:51:GLY:HA2	2.32	0.44
43:Lk:24:LYS:HB2	43:Lk:35:LYS:HB2	1.99	0.44
49:Lr:47:LYS:O	49:Lr:103:ARG:HD2	2.18	0.44
53:SF:128:ILE:HD13	85:S2:1683:C:H1'	2.00	0.44
58:SR:81:ARG:O	67:SA:85:ARG:NH2	2.50	0.44
62:SZ:48:VAL:HG23	62:SZ:80:ARG:HD2	1.99	0.44
85:S2:29:G:H2'	85:S2:30:C:C6	2.53	0.44
85:S2:955:A:N1	85:S2:968:U:O2'	2.39	0.44
85:S2:996:A:H2'	85:S2:997:A:C8	2.52	0.44
2:Pt:11:U:H2'	2:Pt:12:G:C8	2.52	0.44
5:L5:1327:C:H2'	5:L5:1328:G:H8	1.83	0.44
5:L5:1444:G:H22	5:L5:2104:G:N2	2.16	0.44
5:L5:1510:G:H2'	5:L5:1511:U:H6	1.82	0.44
5:L5:1613:A:H5''	8:LA:183:GLY:CA	2.48	0.44
5:L5:1984:A:N6	5:L5:2010:A:O2'	2.50	0.44
5:L5:3599:A:H2'	5:L5:3600:G:C8	2.52	0.44
5:L5:4070:U:H2'	5:L5:4071:U:C6	2.53	0.44
5:L5:4244:A:H2'	5:L5:4245:G:O4'	2.18	0.44
5:L5:4524:G:N3	9:LB:252:ALA:HB1	2.33	0.44
5:L5:4862:G:H2'	5:L5:4863:G:C8	2.53	0.44
6:L7:57:C:H2'	6:L7:58:A:H8	1.83	0.44
10:LC:10:VAL:O	10:LC:18:SER:OG	2.29	0.44
11:LD:289:ARG:O	11:LD:292:GLU:HG3	2.18	0.44
21:LO:81:TRP:HB2	21:LO:104:VAL:HG21	2.00	0.44
21:LO:119:VAL:N	25:LS:168:THR:O	2.47	0.44
85:S2:72:C:H5'	85:S2:73:C:C5	2.53	0.44
85:S2:149:A:N7	85:S2:169:U:O2	2.51	0.44
85:S2:291:G:H2'	85:S2:292:A:C8	2.53	0.44
85:S2:1093:A:H2'	85:S2:1094:C:C6	2.52	0.44
85:S2:1337:4AC:O5'	85:S2:1337:4AC:H6	2.17	0.44
3:CF:375:LEU:HD11	3:CF:394:LEU:HD11	2.00	0.44
3:CF:393:PHE:HE2	3:CF:395:LYS:HG2	1.83	0.44
4:AT:57:C:C5	5:L5:2009:A:H1'	2.53	0.44
5:L5:308:G:OP2	5:L5:308:G:N2	2.42	0.44
5:L5:1426:G:N1	5:L5:1458:C:OP2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:1802:A:H4'	26:LT:105:PHE:CE1	2.53	0.44
5:L5:3708:C:H2'	5:L5:3709:U:C6	2.52	0.44
11:LD:110:LEU:HB3	11:LD:115:MET:O	2.18	0.44
56:SP:22:LEU:HA	56:SP:25:LEU:HB2	1.99	0.44
62:SZ:102:LYS:HA	62:SZ:102:LYS:HD3	1.85	0.44
66:Sg:100:ARG:CZ	85:S2:1399:C:H5''	2.48	0.44
69:SC:259:THR:HG21	78:SV:16:LYS:H	1.82	0.44
69:SC:271:ASP:O	69:SC:275:LYS:HG3	2.18	0.44
74:SJ:40:LYS:NZ	85:S2:641:A:OP1	2.36	0.44
74:SJ:124:HIS:CD2	84:Se:35:ARG:HD2	2.53	0.44
85:S2:943:U:C2	85:S2:944:A:C8	3.06	0.44
5:L5:684:G:H5''	12:LE:100:LYS:HE3	2.00	0.44
5:L5:972:C:H2'	5:L5:973:G:H8	1.82	0.44
5:L5:982:U:H2'	5:L5:983:C:C6	2.53	0.44
5:L5:1181:C:O2'	5:L5:1183:C:H5''	2.18	0.44
5:L5:1977:C:O2'	5:L5:1978:C:OP1	2.33	0.44
5:L5:2667:C:O4'	24:LR:96:MET:HG2	2.16	0.44
5:L5:4401:G:H2'	5:L5:4402:C:H6	1.82	0.44
5:L5:4458:C:H2'	5:L5:4459:U:C6	2.52	0.44
5:L5:4642:U:H2'	5:L5:4643:G:H8	1.82	0.44
5:L5:4745:G:H22	5:L5:4955:A:H2	1.66	0.44
5:L5:5002:U:H2'	5:L5:5003:U:H6	1.83	0.44
8:LA:114:CYS:N	8:LA:165:VAL:O	2.51	0.44
25:LS:173:ASN:ND2	25:LS:175:PHE:O	2.51	0.44
28:LV:43:LYS:HE2	28:LV:62:MET:HE3	2.00	0.44
36:Ld:57:MET:HG2	36:Ld:88:LEU:HD23	2.00	0.44
53:SF:167:LYS:HA	62:SZ:71:ALA:HB1	1.99	0.44
55:SM:20:GLU:HG2	55:SM:119:GLN:HB2	2.00	0.44
66:Sg:230:LEU:HD11	66:Sg:259:TRP:CG	2.53	0.44
85:S2:15:U:H2'	85:S2:16:G:O4'	2.18	0.44
85:S2:166:A2M:HM'3	85:S2:166:A2M:H1'	1.80	0.44
3:CF:58:TRP:CD1	3:CF:67:ARG:HG2	2.53	0.43
5:L5:178:C:N4	5:L5:179:G:O6	2.51	0.43
5:L5:189:G:H2'	5:L5:190:G:H8	1.81	0.43
5:L5:223:G:H4'	5:L5:225:G:N7	2.32	0.43
5:L5:1207:C:H2'	5:L5:1208:G:H8	1.82	0.43
5:L5:2007:G:H2'	5:L5:2008:U:H6	1.82	0.43
5:L5:2368:A:N6	5:L5:2827:G:O2'	2.50	0.43
5:L5:2491:C:H2'	5:L5:2492:C:C6	2.53	0.43
5:L5:2676:A:OP2	5:L5:2676:A:H8	2.01	0.43
5:L5:4344:U:H2'	5:L5:4345:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:4481:U:H2'	5:L5:4482:U:H6	1.82	0.43
9:LB:393:LYS:HG3	9:LB:396:ARG:HH21	1.83	0.43
14:LG:83:PHE:HA	14:LG:183:ILE:HD13	2.00	0.43
28:LV:92:ASP:O	29:LW:2:LYS:NZ	2.51	0.43
38:Lf:36:ARG:O	38:Lf:39:THR:OG1	2.31	0.43
47:Lo:11:PHE:O	47:Lo:81:ARG:NH2	2.51	0.43
55:SM:23:LYS:O	55:SM:27:ILE:HG12	2.18	0.43
65:Sf:103:LEU:HD12	65:Sf:105:TYR:CZ	2.53	0.43
72:SH:58:LYS:HA	72:SH:58:LYS:HD2	1.82	0.43
73:SI:4:SER:OG	73:SI:6:ASP:OD2	2.21	0.43
85:S2:609:U:H2'	85:S2:610:G:C8	2.51	0.43
85:S2:962:A:N1	85:S2:1055:A:O2'	2.51	0.43
85:S2:1279:C:H2'	85:S2:1280:G:C8	2.52	0.43
3:CF:428:ASP:HB3	3:CF:433:VAL:HG21	2.00	0.43
4:AT:3:C:H42	4:AT:71:A:H61	1.65	0.43
5:L5:209:U:OP1	31:LY:63:LYS:NZ	2.46	0.43
5:L5:1613:A:H5''	8:LA:183:GLY:HA2	2.00	0.43
5:L5:1890:G:OP2	5:L5:1890:G:N2	2.47	0.43
5:L5:1910:G:O2'	5:L5:1917:A:N1	2.45	0.43
5:L5:2292:C:H2'	5:L5:2293:U:C6	2.53	0.43
5:L5:2448:G:H2'	5:L5:2449:A:C8	2.53	0.43
5:L5:3825:A2M:H2'	5:L5:3826:C:O4'	2.18	0.43
5:L5:3927:U:H2'	5:L5:3928:A:C8	2.53	0.43
7:L8:90:C:H1'	31:LY:24:HIS:HB3	1.99	0.43
8:LA:145:LYS:HD3	8:LA:145:LYS:HA	1.81	0.43
10:LC:150:LEU:O	10:LC:152:LEU:N	2.51	0.43
51:Lt:12:VAL:HG11	51:Lt:65:GLN:N	2.31	0.43
53:SF:60:ARG:HD2	85:S2:1679:A:H2'	2.00	0.43
59:SS:64:VAL:O	59:SS:68:ILE:HG12	2.17	0.43
69:SC:178:HIS:HB2	69:SC:220:ASP:HB2	2.00	0.43
69:SC:202:THR:HG23	74:SJ:54:ARG:HH22	1.82	0.43
71:SG:23:LYS:HE3	71:SG:41:LEU:HA	2.00	0.43
72:SH:18:GLU:OE1	72:SH:18:GLU:N	2.51	0.43
81:SY:60:PHE:O	85:S2:571:U:O2'	2.36	0.43
85:S2:348:A:H2'	85:S2:349:A:C8	2.53	0.43
85:S2:375:U:H2'	85:S2:376:A:C8	2.54	0.43
85:S2:1705:C:H2'	85:S2:1706:G:C8	2.53	0.43
5:L5:180:C:H2'	5:L5:181:C:C6	2.53	0.43
5:L5:2409:U:H5	5:L5:2783:A:N1	2.17	0.43
5:L5:3928:A:H2'	5:L5:3929:G:O4'	2.18	0.43
5:L5:4508:C:N3	5:L5:4512:U:H5	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:5015:G:H2'	5:L5:5016:A:C2	2.53	0.43
7:L8:36:G:C5	40:Lh:89:ARG:HD3	2.54	0.43
11:LD:203:ASN:OD1	11:LD:203:ASN:N	2.51	0.43
12:LE:173:LEU:HD21	12:LE:191:GLN:HB3	2.00	0.43
23:LQ:35:LEU:O	23:LQ:39:THR:OG1	2.24	0.43
29:LW:113:LYS:O	29:LW:117:LYS:HG2	2.18	0.43
41:Li:76:ARG:HA	41:Li:76:ARG:HD3	1.79	0.43
66:Sg:65:PHE:C	66:Sg:82:SER:HG	2.26	0.43
70:SE:101:LEU:HD12	70:SE:101:LEU:HA	1.88	0.43
81:SY:113:ARG:NE	81:SY:131:PRO:HG2	2.33	0.43
85:S2:693:A:H2'	85:S2:694:G:N7	2.34	0.43
2:Pt:72:C:H3'	2:Pt:73:A:H8	1.83	0.43
5:L5:432:U:H1'	87:L5:5292:SPM:H82	2.00	0.43
5:L5:455:C:O2'	5:L5:456:C:H5'	2.17	0.43
5:L5:475:G:H2'	5:L5:476:G:H8	1.83	0.43
5:L5:654:C:H2'	5:L5:655:C:H6	1.84	0.43
5:L5:1461:C:H2'	5:L5:1462:A:C8	2.53	0.43
5:L5:3923:A:H2'	5:L5:3924:C:C6	2.53	0.43
5:L5:4911:A:OP2	9:LB:100:ARG:HD3	2.19	0.43
5:L5:5053:U:H3'	5:L5:5054:C:C6	2.53	0.43
8:LA:28:ARG:HD2	8:LA:123:ARG:HG3	2.01	0.43
29:LW:52:THR:O	29:LW:56:ARG:HG2	2.19	0.43
31:LY:23:SER:HA	31:LY:26:ARG:HB2	1.99	0.43
50:Ls:29:ILE:HD11	50:Ls:191:GLN:HG2	2.01	0.43
50:Ls:47:LEU:HD11	50:Ls:51:ALA:HB3	2.00	0.43
53:SF:185:SER:O	53:SF:185:SER:OG	2.31	0.43
61:SU:104:ILE:HB	61:SU:106:ILE:HG12	1.99	0.43
67:SA:37:TYR:CD1	67:SA:162:PRO:HG3	2.54	0.43
72:SH:30:LEU:HG	72:SH:33:ASN:HD22	1.84	0.43
72:SH:165:ASN:HA	72:SH:168:HIS:HE1	1.83	0.43
74:SJ:67:ASP:HB3	74:SJ:70:ARG:HB3	1.99	0.43
76:SN:25:TRP:CD1	83:Sb:82:LYS:HD2	2.54	0.43
85:S2:28:U:H2'	85:S2:29:G:C8	2.51	0.43
5:L5:1473:U:H2'	5:L5:1474:C:C6	2.53	0.43
5:L5:1511:U:H2'	5:L5:1512:G:H8	1.84	0.43
5:L5:2890:C:H2'	5:L5:2891:U:C6	2.54	0.43
5:L5:4277:G:H5''	26:LT:17:ARG:HG2	1.99	0.43
5:L5:4913:G:H4'	5:L5:4914:C:O5'	2.18	0.43
7:L8:47:C:H1'	7:L8:61:A:H2'	1.99	0.43
21:LO:88:LEU:HD12	21:LO:99:LEU:HD13	1.99	0.43
41:Li:33:LEU:HD21	41:Li:38:LYS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SF:103:LEU:HD11	62:SZ:67:LEU:HD22	1.99	0.43
59:SS:13:LEU:HD22	59:SS:20:ILE:HD11	1.99	0.43
59:SS:92:ASP:OD1	59:SS:92:ASP:N	2.51	0.43
83:Sb:11:SER:N	83:Sb:14:GLU:OE2	2.51	0.43
85:S2:835:C:H4'	85:S2:836:G:C8	2.54	0.43
85:S2:1017:U:H2'	85:S2:1018:U:H6	1.83	0.43
85:S2:1348:G:H2'	85:S2:1349:G:H8	1.83	0.43
85:S2:1558:C:H2'	85:S2:1559:C:C6	2.54	0.43
85:S2:1667:U:H2'	85:S2:1668:U:C6	2.54	0.43
2:Pt:22:U:H2'	2:Pt:23:C:H6	1.83	0.43
3:CF:146:LYS:HZ1	3:CF:423:ARG:HH22	1.65	0.43
5:L5:73:A:N6	18:LL:103:ARG:HH22	2.15	0.43
5:L5:716:C:OP1	10:LC:317:ASN:HB2	2.19	0.43
5:L5:1669:A:H4'	5:L5:1685:G:H22	1.82	0.43
5:L5:1996:C:N4	5:L5:2000:G:N2	2.46	0.43
5:L5:2399:G:HO2'	5:L5:2822:G:HO2'	1.63	0.43
5:L5:2844:A:O2'	5:L5:4631:G:H4'	2.19	0.43
5:L5:3871:A:H2'	5:L5:3872:A:C8	2.53	0.43
18:LL:48:PRO:HB2	40:Lh:120:ALA:HB2	2.00	0.43
42:Lj:67:LEU:HD23	42:Lj:67:LEU:HA	1.87	0.43
50:Ls:30:VAL:HA	50:Ls:189:ILE:HA	2.00	0.43
56:SP:79:HIS:HD2	85:S2:1298:G:C4	2.36	0.43
58:SR:60:ARG:HA	58:SR:63:ARG:HG2	2.00	0.43
64:Sd:54:LYS:NZ	85:S2:1482:C:OP1	2.52	0.43
71:SG:195:LYS:HD3	85:S2:126:G:H5'	2.00	0.43
75:SL:36:TYR:OH	85:S2:294:U:OP1	2.31	0.43
81:SY:7:ILE:HG12	81:SY:43:LYS:HD3	2.01	0.43
85:S2:1221:G:H2'	85:S2:1222:G:C8	2.54	0.43
85:S2:1410:C:H2'	85:S2:1411:G:H8	1.83	0.43
85:S2:1802:C:H2'	85:S2:1803:U:C6	2.54	0.43
3:CF:349:HIS:ND1	3:CF:351:GLY:O	2.52	0.43
5:L5:184:U:O2	5:L5:253:G:C2	2.72	0.43
5:L5:1302:U:H3'	5:L5:1303:A:H8	1.83	0.43
5:L5:1537:A:H2'	5:L5:1538:U:C6	2.54	0.43
5:L5:1662:C:H2'	5:L5:1663:C:H6	1.84	0.43
5:L5:2297:G:H4'	10:LC:242:PRO:HB2	2.00	0.43
5:L5:2436:U:OP2	30:LX:135:LYS:NZ	2.46	0.43
5:L5:2437:C:H1'	30:LX:125:ASN:HB3	2.00	0.43
5:L5:2695:A:OP1	43:Lk:35:LYS:NZ	2.28	0.43
5:L5:3855:C:H2'	5:L5:3856:A:H8	1.83	0.43
5:L5:4651:A:H2'	5:L5:4652:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:4680:G:H2'	5:L5:4681:A:C8	2.53	0.43
6:L7:111:C:H2'	6:L7:112:U:O4'	2.18	0.43
7:L8:70:G:H5''	31:LY:27:ARG:CZ	2.49	0.43
8:LA:173:GLY:O	48:Lp:69:TRP:NE1	2.51	0.43
11:LD:86:TYR:HE1	11:LD:247:ILE:HG13	1.83	0.43
24:LR:157:ASP:OD1	24:LR:158:GLN:N	2.52	0.43
31:LY:82:ILE:HG22	31:LY:83:GLU:H	1.84	0.43
32:LZ:41:ALA:HB2	32:LZ:77:TYR:HE1	1.83	0.43
40:Lh:70:ARG:HG2	40:Lh:83:LEU:HD22	2.01	0.43
51:Lt:85:LEU:HD13	51:Lt:109:ILE:HD12	2.01	0.43
60:ST:11:GLN:HB2	85:S2:1542:C:H4'	2.01	0.43
62:SZ:86:ALA:O	62:SZ:90:GLU:HG2	2.18	0.43
67:SA:69:GLU:HB2	69:SC:270:THR:HG21	1.99	0.43
67:SA:220:LYS:HD3	67:SA:220:LYS:HA	1.82	0.43
68:SB:97:LEU:HD23	68:SB:232:HIS:CD2	2.54	0.43
71:SG:174:PRO:O	85:S2:77:A:O2'	2.29	0.43
73:SI:3:ILE:O	73:SI:30:GLY:N	2.46	0.43
74:SJ:111:GLN:HE21	74:SJ:123:ILE:HG13	1.84	0.43
77:SO:96:LYS:HD3	77:SO:132:VAL:HG11	2.00	0.43
85:S2:634:A:H2'	85:S2:635:G:H8	1.84	0.43
85:S2:641:A:H2'	85:S2:642:U:O4'	2.18	0.43
85:S2:1831:A:O2'	85:S2:1832:6MZ:O5'	2.28	0.43
2:Pt:22:U:H2'	2:Pt:23:C:C6	2.53	0.43
3:CF:39:ILE:HD11	3:CF:56:TYR:CD1	2.54	0.43
3:CF:225:GLY:HA2	3:CF:230:GLU:CD	2.44	0.43
5:L5:381:U:H4'	5:L5:415:G:H5'	2.01	0.43
5:L5:1504:G:H2'	5:L5:1505:C:H6	1.84	0.43
5:L5:4113:U:H4'	5:L5:4115:G:C6	2.54	0.43
5:L5:4163:U:OP2	14:LG:53:ARG:NH2	2.52	0.43
5:L5:4578:G:H2'	5:L5:4579:PSU:C6	2.54	0.43
7:L8:52:A:H4'	44:Ll:19:GLN:HA	2.00	0.43
8:LA:20:VAL:HA	8:LA:23:ARG:HG3	1.99	0.43
8:LA:115:CYS:SG	8:LA:124:GLY:HA3	2.58	0.43
9:LB:57:VAL:HB	9:LB:367:PHE:HB3	2.00	0.43
12:LE:183:ARG:HA	12:LE:183:ARG:HD2	1.84	0.43
16:LI:54:SER:HB3	16:LI:135:ILE:HD11	2.01	0.43
18:LL:48:PRO:HG3	40:Lh:118:LYS:HE2	2.00	0.43
27:LU:23:LEU:HD23	27:LU:110:TYR:HB2	2.00	0.43
61:SU:87:ARG:HH22	85:S2:1447:G:P	2.42	0.43
67:SA:73:ASP:HB3	67:SA:120:ARG:HB2	2.01	0.43
69:SC:74:LYS:HA	69:SC:74:LYS:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:S2:159:A2M:HM'3	85:S2:159:A2M:H1'	1.55	0.43
85:S2:575:A:H2'	85:S2:576:A2M:O4'	2.18	0.43
85:S2:1511:U:H2'	85:S2:1512:C:C6	2.54	0.43
85:S2:1514:G:H2'	85:S2:1515:G:C8	2.54	0.43
3:CF:352:GLN:HA	3:CF:395:LYS:HD3	2.01	0.43
5:L5:662:C:H2'	5:L5:663:G:C8	2.54	0.43
5:L5:978:G:H2'	5:L5:979:C:C6	2.53	0.43
5:L5:2407:G:H2'	44:L1:13:LEU:HD22	2.01	0.43
5:L5:3927:U:H2'	5:L5:3928:A:H8	1.84	0.43
5:L5:4156:G:H5''	5:L5:4157:A:H2'	2.00	0.43
14:LG:209:SER:HA	14:LG:212:LYS:HG3	2.00	0.43
24:LR:35:ALA:HA	24:LR:40:GLN:OE1	2.19	0.43
36:Ld:114:PHE:HA	36:Ld:117:LEU:HD12	2.01	0.43
46:Ln:2:ARG:NE	85:S2:1842:4AC:OP2	2.35	0.43
66:Sg:207:CYS:HB3	66:Sg:221:LEU:HD21	2.01	0.43
68:SB:29:ASP:OD1	68:SB:29:ASP:N	2.52	0.43
69:SC:85:SER:OG	78:SV:25:GLY:O	2.30	0.43
70:SE:31:PRO:HA	70:SE:81:THR:HB	2.00	0.43
70:SE:100:ARG:NH2	70:SE:118:GLU:OE2	2.51	0.43
71:SG:138:ALA:HA	71:SG:176:ILE:HD11	2.00	0.43
80:SX:70:VAL:HG11	80:SX:94:ILE:HG21	2.01	0.43
81:SY:93:ARG:HH21	85:S2:575:A:P	2.42	0.43
85:S2:517:OMC:H2'	85:S2:518:G:O4'	2.18	0.43
85:S2:1117:C:H2'	85:S2:1118:C:C6	2.53	0.43
3:CF:266:ARG:HD3	3:CF:305:GLY:HA2	2.01	0.43
4:AT:4:U:H2'	4:AT:5:C:C6	2.53	0.43
5:L5:689:U:H2'	5:L5:690:C:C6	2.54	0.43
5:L5:1194:G:H2'	5:L5:1195:G:H8	1.84	0.43
5:L5:1309:C:H2'	5:L5:1310:C:C6	2.53	0.43
5:L5:1628:C:OP2	8:LA:9:ARG:HD2	2.19	0.43
5:L5:1687:U:H2'	5:L5:1688:G:C8	2.54	0.43
5:L5:1779:U:H2'	5:L5:1780:A:C8	2.54	0.43
5:L5:2540:C:H5''	39:Lg:65:MET:HE3	2.00	0.43
5:L5:2823:G:N7	24:LR:20:LYS:HD3	2.33	0.43
5:L5:4563:U:C2	5:L5:4564:A:C8	3.07	0.43
5:L5:4918:C:H2'	5:L5:4919:G:C8	2.54	0.43
10:LC:144:ILE:HG13	10:LC:144:ILE:O	2.19	0.43
63:Sc:21:THR:OG1	63:Sc:22:GLY:N	2.51	0.43
67:SA:6:ASP:OD1	67:SA:6:ASP:N	2.51	0.43
74:SJ:29:LEU:HD23	84:Se:41:ARG:HD2	2.00	0.43
77:SO:141:ARG:NH2	85:S2:1856:C:OP1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:S2:51:U:H2'	85:S2:52:G:C8	2.54	0.43
85:S2:753:C:C4	85:S2:791:C:H4'	2.53	0.43
85:S2:881:G:N2	85:S2:906:U:H1'	2.34	0.43
85:S2:1287:A:N6	85:S2:1288:OMU:O2	2.52	0.43
3:CF:267:VAL:HG21	3:CF:302:ALA:HB1	2.01	0.42
5:L5:2648:G:H2'	5:L5:2649:G:H8	1.83	0.42
5:L5:2815:A2M:H2'	5:L5:2816:G:C8	2.53	0.42
5:L5:3721:U:H2'	5:L5:3722:G:C8	2.53	0.42
7:L8:6:C:H2'	7:L8:7:U:H6	1.84	0.42
13:LF:46:ARG:HH21	34:Lb:102:PRO:HG3	1.84	0.42
17:LJ:35:ARG:O	17:LJ:39:VAL:HG23	2.19	0.42
24:LR:80:LYS:HA	24:LR:80:LYS:HD2	1.83	0.42
37:Le:91:CYS:HB3	37:Le:95:TYR:HD2	1.84	0.42
58:SR:128:PHE:CD2	58:SR:129:LYS:HG3	2.54	0.42
60:ST:71:GLY:O	60:ST:75:MET:HG2	2.18	0.42
60:ST:96:SER:OG	85:S2:1568:C:OP1	2.32	0.42
68:SB:136:ARG:HB3	68:SB:216:LYS:HG3	2.01	0.42
85:S2:551:U:H2'	85:S2:552:G:C8	2.53	0.42
85:S2:564:A:H2'	85:S2:565:G:O4'	2.18	0.42
85:S2:1189:A:H2'	85:S2:1190:A:C8	2.54	0.42
85:S2:1597:C:H4'	85:S2:1603:G:C6	2.53	0.42
5:L5:374:G:OP2	42:Lj:56:ARG:NH1	2.43	0.42
5:L5:974:C:H5''	13:LF:43:ARG:NH1	2.34	0.42
5:L5:1932:A:H8	21:LO:49:ARG:NH2	2.17	0.42
5:L5:2421:G:OP2	5:L5:2828:U:H1'	2.19	0.42
5:L5:4507:A:H2'	5:L5:4508:C:C6	2.53	0.42
13:LF:214:SER:OG	13:LF:215:SER:N	2.52	0.42
23:LQ:66:MET:HE1	23:LQ:86:ILE:HD13	2.01	0.42
35:Lc:31:TYR:OH	35:Lc:59:GLU:OE1	2.27	0.42
50:Ls:77:LYS:HE2	50:Ls:193:PHE:HE1	1.84	0.42
50:Ls:159:GLN:NE2	50:Ls:162:LYS:HG3	2.34	0.42
56:SP:83:MET:HB3	56:SP:116:LEU:HD12	2.00	0.42
56:SP:115:TYR:OH	85:S2:1620:A:OP1	2.29	0.42
58:SR:33:ARG:HD3	58:SR:33:ARG:HA	1.85	0.42
59:SS:102:GLY:HA2	59:SS:105:ASN:HD21	1.84	0.42
67:SA:176:TRP:NE1	67:SA:197:VAL:O	2.50	0.42
82:Sa:10:ARG:HH12	85:S2:1859:A:P	2.41	0.42
85:S2:152:U:H2'	85:S2:153:G:H8	1.84	0.42
85:S2:909:G:H2'	85:S2:910:G:C8	2.53	0.42
85:S2:1174:PSU:H2'	85:S2:1175:G:H8	1.84	0.42
85:S2:1383:A2M:H1'	85:S2:1383:A2M:HM'3	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:S2:1777:G:H2'	85:S2:1778:C:C6	2.54	0.42
5:L5:1086:C:H2'	5:L5:1087:A:C8	2.54	0.42
5:L5:1545:G:H2'	5:L5:1546:C:C6	2.54	0.42
5:L5:1563:A:H2'	5:L5:1564:A:C8	2.54	0.42
5:L5:1631:A:C2	8:LA:204:MET:HG2	2.53	0.42
5:L5:1847:C:H2'	5:L5:1848:C:C6	2.53	0.42
5:L5:2018:C:H2'	5:L5:2019:C:H6	1.83	0.42
5:L5:2296:G:O2'	10:LC:242:PRO:O	2.30	0.42
5:L5:2654:C:H2'	5:L5:2655:C:H6	1.84	0.42
5:L5:2903:G:H1'	5:L5:2904:U:C5	2.54	0.42
5:L5:4345:C:H2'	5:L5:4346:U:C6	2.53	0.42
9:LB:154:LYS:HE2	9:LB:154:LYS:HB2	1.72	0.42
17:LJ:95:ARG:H	17:LJ:98:ASN:ND2	2.17	0.42
24:LR:139:MET:HG2	24:LR:143:HIS:CE1	2.54	0.42
31:LY:50:ARG:HB3	31:LY:53:ASP:OD2	2.18	0.42
43:Lk:68:GLU:HG3	43:Lk:70:LYS:H	1.85	0.42
45:Lm:79:GLU:CD	45:Lm:81:SER:HG	2.26	0.42
60:ST:23:LYS:HD3	60:ST:51:ASN:HD22	1.83	0.42
69:SC:190:SER:HB3	85:S2:1143:A:H5'	2.02	0.42
70:SE:36:HIS:CG	70:SE:85:GLY:HA3	2.54	0.42
70:SE:247:THR:N	70:SE:250:GLU:OE2	2.45	0.42
72:SH:17:ASP:OD1	72:SH:17:ASP:N	2.52	0.42
74:SJ:174:LYS:NZ	85:S2:560:A:OP1	2.46	0.42
85:S2:601:OMG:HM23	85:S2:601:OMG:H1'	1.68	0.42
85:S2:649:PSU:H2'	85:S2:650:A:C8	2.53	0.42
85:S2:815:U:C2	85:S2:816:A:C8	3.07	0.42
85:S2:1291:A:OP2	85:S2:1302:G:O2'	2.33	0.42
5:L5:92:C:OP2	5:L5:4341:C:O2'	2.26	0.42
5:L5:150:U:OP2	14:LG:200:THR:OG1	2.27	0.42
5:L5:921:C:H2'	5:L5:922:C:C6	2.54	0.42
5:L5:1806:G:H2'	5:L5:1807:C:C6	2.54	0.42
5:L5:1981:G:N1	5:L5:1982:G:O6	2.52	0.42
5:L5:2034:G:H2'	5:L5:2035:C:C6	2.54	0.42
5:L5:2634:C:H2'	5:L5:2635:U:C6	2.54	0.42
5:L5:3633:C:H2'	5:L5:3634:G:C8	2.54	0.42
5:L5:5030:U:H2'	5:L5:5031:G:C8	2.55	0.42
32:LZ:123:LYS:O	32:LZ:124:THR:OG1	2.25	0.42
55:SM:17:ALA:O	55:SM:20:GLU:HG3	2.18	0.42
67:SA:37:TYR:HA	67:SA:53:ARG:HD3	2.00	0.42
67:SA:184:ARG:HE	67:SA:191:ARG:HD3	1.84	0.42
78:SV:74:LYS:NZ	78:SV:83:PHE:HB3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:S2:1595:U:H2'	85:S2:1596:U:C6	2.54	0.42
1:CI:79:ARG:CZ	5:L5:2708:U:O2'	2.55	0.42
3:CF:255:LYS:HB2	3:CF:317:VAL:HG11	2.02	0.42
5:L5:737:C:C4	5:L5:739:G:H5''	2.54	0.42
5:L5:1351:G:O6	23:LQ:55:ARG:NH1	2.52	0.42
5:L5:1554:A:OP1	48:Lp:5:THR:OG1	2.31	0.42
5:L5:1642:A:H61	8:LA:2:GLY:C	2.27	0.42
5:L5:1976:G:N7	5:L5:2002:A:H2'	2.35	0.42
5:L5:2464:C:HO2'	5:L5:2465:C:H6	1.68	0.42
5:L5:4195:G:OP1	5:L5:4221:C:O2'	2.35	0.42
5:L5:4318:C:H4'	47:Lo:17:LYS:HA	2.01	0.42
5:L5:4563:U:H2'	5:L5:4564:A:C8	2.54	0.42
6:L7:22:A:H2'	6:L7:23:A:C8	2.55	0.42
9:LB:288:GLY:HA3	9:LB:330:PHE:CE1	2.54	0.42
10:LC:221:PHE:O	10:LC:222:ARG:HG2	2.20	0.42
11:LD:66:TYR:HE2	11:LD:68:ARG:HE	1.68	0.42
33:La:76:ASP:HB3	33:La:115:GLY:HA3	2.01	0.42
53:SF:60:ARG:NH2	85:S2:1679:A:OP1	2.49	0.42
60:ST:60:THR:HG22	60:ST:75:MET:HE2	2.02	0.42
66:Sg:131:LEU:O	66:Sg:139:LYS:N	2.52	0.42
70:SE:75:LYS:NZ	85:S2:122:G:OP1	2.37	0.42
71:SG:56:ASN:ND2	71:SG:60:GLY:O	2.52	0.42
73:SI:132:GLU:O	73:SI:136:ILE:HG23	2.19	0.42
80:SX:17:ARG:HH22	85:S2:659:G:H21	1.67	0.42
81:SY:102:THR:OG1	81:SY:106:GLN:OE1	2.37	0.42
84:Se:58:ASN:ND2	85:S2:606:G:H1'	2.35	0.42
85:S2:382:C:H2'	85:S2:383:G:C8	2.54	0.42
85:S2:1088:U:H4'	85:S2:1089:G:OP2	2.20	0.42
85:S2:1227:G:C2	85:S2:1228:A:C8	3.07	0.42
3:CF:76:SER:N	3:CF:91:ASP:OD1	2.47	0.42
4:AT:7:G:O2'	4:AT:50:C:H5'	2.19	0.42
5:L5:664:G:H2'	5:L5:665:C:C6	2.55	0.42
5:L5:2864:A:H2'	5:L5:2865:U:H6	1.85	0.42
5:L5:4637:OMG:HM23	5:L5:4637:OMG:H1'	1.70	0.42
5:L5:4920:C:H2'	5:L5:4921:C:C6	2.54	0.42
10:LC:305:PRO:HB2	10:LC:307:LYS:HG3	2.01	0.42
13:LF:228:VAL:HA	25:LS:39:VAL:HG22	2.01	0.42
35:Lc:47:ILE:HD12	35:Lc:94:LEU:HD11	2.02	0.42
63:Sc:44:ARG:NH1	63:Sc:61:SER:O	2.52	0.42
66:Sg:270:LEU:HD13	66:Sg:310:TRP:CE3	2.55	0.42
67:SA:111:GLN:HA	67:SA:116:PHE:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SA:172:GLY:HA3	67:SA:203:PHE:CD1	2.54	0.42
68:SB:141:GLY:HA3	68:SB:207:LEU:HD23	2.01	0.42
70:SE:59:ASP:O	70:SE:63:LYS:HG3	2.20	0.42
70:SE:149:TYR:CD2	71:SG:205:GLU:HB3	2.54	0.42
76:SN:15:ALA:HB2	83:Sb:20:LYS:HD3	2.00	0.42
79:SW:106:THR:OG1	79:SW:111:MET:HE2	2.19	0.42
85:S2:70:G:N2	85:S2:79:A:H62	2.15	0.42
85:S2:1199:A:H2'	85:S2:1200:A:C8	2.54	0.42
5:L5:288:G:H2'	5:L5:289:C:C6	2.55	0.42
5:L5:677:G:H2'	5:L5:678:C:C6	2.54	0.42
5:L5:1096:C:H2'	5:L5:1097:C:C6	2.54	0.42
5:L5:1195:G:H2'	5:L5:1196:G:C8	2.55	0.42
5:L5:1875:C:H2'	5:L5:1876:U:C6	2.55	0.42
5:L5:4571:A2M:H1'	5:L5:4571:A2M:HM'3	1.81	0.42
5:L5:4739:C:H2'	5:L5:4740:G:H5'	2.02	0.42
6:L7:4:U:H2'	6:L7:5:A:H8	1.85	0.42
9:LB:59:GLU:HB2	9:LB:366:LYS:HE2	2.01	0.42
12:LE:99:ASP:OD1	12:LE:99:ASP:N	2.51	0.42
24:LR:99:MET:HE1	24:LR:127:VAL:O	2.20	0.42
59:SS:73:ASN:HB3	59:SS:76:GLN:OE1	2.19	0.42
66:Sg:230:LEU:HD21	66:Sg:259:TRP:CE2	2.55	0.42
70:SE:121:TYR:HA	70:SE:163:ASP:HA	2.01	0.42
85:S2:461:U:H2'	85:S2:462:OMC:H6	1.84	0.42
85:S2:697:G:OP2	85:S2:733:C:N4	2.35	0.42
85:S2:1324:G:HO2'	85:S2:1510:G:HO2'	1.63	0.42
3:CF:60:LEU:HD13	3:CF:78:TRP:HD1	1.84	0.42
5:L5:734:G:C2	5:L5:735:G:C8	3.07	0.42
5:L5:1419:G:H5''	23:LQ:71:LYS:NZ	2.35	0.42
5:L5:2732:G:H2'	5:L5:2733:C:C6	2.54	0.42
5:L5:4761:G:H2'	5:L5:4762:A:H8	1.85	0.42
6:L7:112:U:H2'	6:L7:113:G:H8	1.85	0.42
12:LE:223:ARG:HH22	12:LE:238:GLU:HG3	1.85	0.42
16:LI:73:ASN:HB2	16:LI:87:MET:HE1	2.01	0.42
31:LY:13:LYS:O	31:LY:17:ARG:HD3	2.20	0.42
52:SD:109:LEU:HD23	52:SD:109:LEU:HA	1.82	0.42
62:SZ:46:ASN:ND2	85:S2:1599:U:OP2	2.48	0.42
67:SA:126:ASP:OD2	67:SA:129:ALA:N	2.45	0.42
72:SH:81:ARG:O	72:SH:85:LYS:HG3	2.20	0.42
73:SI:130:THR:O	73:SI:134:GLU:HB2	2.20	0.42
74:SJ:2:PRO:HA	85:S2:509:OMG:OP1	2.19	0.42
79:SW:125:ILE:HD12	79:SW:125:ILE:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:S2:14:C:H2'	85:S2:15:U:C6	2.55	0.42
85:S2:27:A2M:HM'3	85:S2:27:A2M:H1'	1.60	0.42
85:S2:508:A:H3'	85:S2:509:OMG:C8	2.51	0.42
85:S2:1345:G:OP1	85:S2:1688:C:O2'	2.37	0.42
85:S2:1514:G:H2'	85:S2:1515:G:H8	1.85	0.42
85:S2:1716:C:H2'	85:S2:1717:C:H6	1.85	0.42
1:CI:63:ARG:HD2	1:CI:63:ARG:HA	1.85	0.42
5:L5:173:C:H5''	18:LL:129:ARG:HH12	1.83	0.42
5:L5:1403:G:N2	5:L5:1415:G:C4	2.88	0.42
5:L5:1685:G:N3	34:Lb:15:LYS:NZ	2.68	0.42
5:L5:1912:G:N2	21:LO:87:MET:HE2	2.34	0.42
5:L5:1953:U:H2'	5:L5:1954:U:C6	2.55	0.42
5:L5:2008:U:N3	5:L5:2011:C:OP2	2.32	0.42
5:L5:2413:U:H2'	5:L5:2414:G:C8	2.55	0.42
5:L5:2570:U:H2'	5:L5:2571:C:C6	2.55	0.42
5:L5:4272:G:OP2	5:L5:4272:G:N2	2.31	0.42
7:L8:8:U:H2'	7:L8:9:A:C8	2.54	0.42
35:Lc:30:GLY:O	35:Lc:34:THR:OG1	2.26	0.42
50:Ls:119:CYS:SG	50:Ls:120:GLU:N	2.93	0.42
60:ST:82:ARG:NH1	85:S2:1654:G:OP1	2.53	0.42
66:Sg:44:LYS:HG2	66:Sg:56:GLN:HB2	2.01	0.42
67:SA:184:ARG:HE	67:SA:191:ARG:HA	1.85	0.42
80:SX:46:HIS:CD2	80:SX:103:ALA:HB2	2.55	0.42
83:Sb:22:LYS:HE3	85:S2:1129:G:H5''	2.01	0.42
85:S2:737:G:H2'	85:S2:738:C:H4'	2.02	0.42
85:S2:863:PSU:O2	85:S2:864:A:N6	2.53	0.42
85:S2:1217:A:H2'	85:S2:1218:C:C6	2.54	0.42
85:S2:1568:C:H2'	85:S2:1569:A:C8	2.55	0.42
3:CF:113:VAL:HA	3:CF:149:ILE:O	2.20	0.42
5:L5:161:G:H2'	5:L5:162:A:C8	2.55	0.42
5:L5:475:G:H2'	5:L5:476:G:C8	2.55	0.42
5:L5:1413:C:H2'	5:L5:1414:C:C6	2.55	0.42
5:L5:2495:U:H2'	5:L5:2496:G:C8	2.55	0.42
5:L5:2846:G:OP1	28:LV:85:ARG:NH2	2.53	0.42
5:L5:3607:U:H2'	5:L5:3608:A:C8	2.55	0.42
5:L5:3627:OMG:HM23	5:L5:3627:OMG:H1'	1.87	0.42
5:L5:3656:A:H2'	5:L5:3657:U:C6	2.54	0.42
5:L5:4192:A:H2'	5:L5:4193:C:H6	1.84	0.42
5:L5:4306:OMU:HM23	5:L5:4306:OMU:H1'	1.87	0.42
5:L5:4979:A:OP1	9:LB:228:TYR:HB2	2.20	0.42
7:L8:89:U:H2'	7:L8:90:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LB:216:MET:HE2	9:LB:281:ASN:HB3	2.02	0.42
39:Lg:33:LEU:HD23	39:Lg:33:LEU:HA	1.89	0.42
66:Sg:24:THR:HA	66:Sg:25:PRO:HD3	1.91	0.42
76:SN:55:ARG:NH1	85:S2:1015:U:O2'	2.53	0.42
76:SN:140:LYS:HA	76:SN:140:LYS:HD3	1.90	0.42
80:SX:60:LYS:H	80:SX:114:ASP:HB2	1.84	0.42
85:S2:300:U:H2'	85:S2:301:A:H8	1.85	0.42
85:S2:613:G:N2	85:S2:626:G:OP1	2.52	0.42
85:S2:1174:PSU:H2'	85:S2:1175:G:C8	2.55	0.42
1:CI:76:VAL:O	24:LR:47:ASP:HB3	2.20	0.41
5:L5:513:U:H1'	5:L5:516:C:H41	1.85	0.41
5:L5:689:U:H2'	5:L5:690:C:H6	1.85	0.41
5:L5:1602:U:OP1	42:Lj:2:THR:OG1	2.30	0.41
5:L5:1764:G:H4'	5:L5:1769:G:C6	2.55	0.41
5:L5:1787:A:N3	5:L5:4210:U:O2'	2.48	0.41
5:L5:1895:G:OP1	13:LF:96:ARG:NH2	2.53	0.41
5:L5:2034:G:O2'	25:LS:118:ARG:NH1	2.46	0.41
5:L5:2376:A:H2'	5:L5:2377:C:C6	2.55	0.41
5:L5:2497:C:H2'	5:L5:2498:C:C6	2.55	0.41
5:L5:3718:A2M:H2'	5:L5:3719:A:O4'	2.20	0.41
9:LB:17:LEU:HD23	9:LB:17:LEU:HA	1.76	0.41
13:LF:126:ASN:H	13:LF:129:SER:HG	1.68	0.41
20:LN:149:GLN:NE2	40:Lh:99:GLU:O	2.53	0.41
21:LO:84:VAL:HG11	21:LO:102:LEU:HD22	2.02	0.41
25:LS:93:MET:HE1	25:LS:117:HIS:CE1	2.55	0.41
29:LW:99:GLU:HB3	29:LW:102:LYS:HE3	2.01	0.41
54:SK:22:VAL:HG22	54:SK:68:TYR:HD1	1.85	0.41
56:SP:59:ARG:HH21	56:SP:76:VAL:HG23	1.84	0.41
57:SQ:125:ARG:HB2	85:S2:1648:G:H5''	2.01	0.41
59:SS:55:ARG:N	59:SS:58:GLU:OE2	2.37	0.41
62:SZ:69:THR:H	62:SZ:72:VAL:HG22	1.85	0.41
67:SA:57:LYS:HD2	67:SA:57:LYS:HA	1.80	0.41
85:S2:641:A:O2'	85:S2:645:C:OP1	2.38	0.41
85:S2:1317:C:H2'	85:S2:1318:G:C8	2.55	0.41
3:CF:34:ILE:HD11	3:CF:39:ILE:HD12	2.02	0.41
5:L5:269:G:H2'	5:L5:270:U:C6	2.55	0.41
5:L5:462:G:H2'	5:L5:463:A:C8	2.54	0.41
5:L5:467:U:C4	5:L5:468:U:H1'	2.56	0.41
5:L5:1590:C:H3'	5:L5:1591:U:H4'	2.02	0.41
5:L5:2870:A:H2'	5:L5:2871:A:H8	1.84	0.41
5:L5:3661:G:H4'	5:L5:3662:A:H5'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:3822:PSU:H3'	5:L5:3823:G:N2	2.35	0.41
5:L5:3911:C:H2'	5:L5:3912:U:C6	2.53	0.41
5:L5:4543:G:H2'	5:L5:4544:A:C8	2.55	0.41
12:LE:223:ARG:HA	12:LE:224:LYS:HA	1.80	0.41
19:LM:37:LEU:HD22	25:LS:75:VAL:HG23	2.02	0.41
25:LS:99:ASP:OD1	25:LS:100:LEU:N	2.51	0.41
39:Lg:41:ALA:O	39:Lg:52:ARG:HD3	2.20	0.41
39:Lg:69:LYS:HG3	39:Lg:73:HIS:CD2	2.55	0.41
54:SK:7:ASN:HB2	54:SK:40:VAL:HG22	2.01	0.41
54:SK:37:ASP:N	54:SK:37:ASP:OD1	2.48	0.41
60:ST:39:LEU:HD23	60:ST:39:LEU:HA	1.76	0.41
67:SA:81:ASN:OD1	67:SA:82:THR:N	2.52	0.41
68:SB:40:ASN:OD1	68:SB:41:ILE:HD12	2.20	0.41
68:SB:171:ILE:HD11	68:SB:197:ILE:HA	2.02	0.41
74:SJ:2:PRO:HD2	85:S2:429:C:P	2.60	0.41
85:S2:1457:U:H2'	85:S2:1458:G:C8	2.55	0.41
3:CF:335:MET:SD	3:CF:443:LYS:HE3	2.60	0.41
5:L5:473:C:H2'	5:L5:474:C:C6	2.55	0.41
5:L5:1207:C:H2'	5:L5:1208:G:C8	2.55	0.41
5:L5:1497:A:N6	23:LQ:175:GLU:O	2.53	0.41
5:L5:1730:U:H2'	5:L5:1731:C:C6	2.55	0.41
5:L5:2385:U:H2'	5:L5:2386:U:H6	1.86	0.41
5:L5:2621:A:H2'	5:L5:2622:G:C8	2.56	0.41
5:L5:2648:G:H2'	5:L5:2649:G:C8	2.55	0.41
5:L5:4069:U:H2'	5:L5:4070:U:H6	1.85	0.41
5:L5:4578:G:H2'	5:L5:4579:PSU:H6	1.85	0.41
6:L7:40:U:O2	17:LJ:75:ARG:NE	2.39	0.41
13:LF:213:LEU:HB3	13:LF:247:MET:HG3	2.03	0.41
24:LR:4:LEU:HD11	24:LR:29:THR:HG23	2.02	0.41
37:Le:85:LEU:HD21	37:Le:115:ALA:HB2	2.02	0.41
43:Lk:25:ILE:HD13	43:Lk:57:LYS:NZ	2.35	0.41
51:Lt:109:ILE:HA	51:Lt:112:ILE:HG12	2.03	0.41
51:Lt:119:ARG:NH2	51:Lt:123:ARG:HH12	2.18	0.41
62:SZ:90:GLU:O	62:SZ:93:SER:OG	2.27	0.41
63:Sc:66:ARG:NH1	63:Sc:68:LEU:HD23	2.34	0.41
73:SI:42:ARG:HH21	73:SI:59:ARG:NH1	2.17	0.41
74:SJ:132:GLN:HB2	74:SJ:134:HIS:CD2	2.55	0.41
75:SL:153:LYS:HD3	75:SL:153:LYS:HA	1.87	0.41
78:SV:27:LYS:HD3	78:SV:27:LYS:HA	1.87	0.41
85:S2:391:C:H2'	85:S2:392:A:H8	1.85	0.41
85:S2:399:C:H5	85:S2:680:G:H5''	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:S2:433:A:H2'	85:S2:434:G:C8	2.55	0.41
85:S2:1026:C:H4'	85:S2:1161:U:H4'	2.03	0.41
85:S2:1330:G:N7	85:S2:1492:U:H3'	2.36	0.41
85:S2:1511:U:H2'	85:S2:1512:C:H6	1.85	0.41
5:L5:99:A:H2'	5:L5:100:C:O2	2.20	0.41
5:L5:212:A:H2'	5:L5:213:G:C8	2.55	0.41
5:L5:1282:G:OP2	12:LE:128:HIS:NE2	2.54	0.41
5:L5:1534:A2M:N3	42:Lj:11:ARG:HB2	2.35	0.41
5:L5:2380:G:N2	5:L5:2424:OMG:H5''	2.34	0.41
5:L5:2602:G:H2'	5:L5:2603:C:C6	2.56	0.41
5:L5:3610:A:H2'	5:L5:3611:A:H8	1.86	0.41
5:L5:4573:G:H2'	5:L5:4574:U:C6	2.55	0.41
5:L5:4704:C:H2'	5:L5:4705:A:C8	2.55	0.41
14:LG:95:LEU:HD23	14:LG:184:ILE:HD12	2.03	0.41
14:LG:123:ALA:HA	14:LG:124:GLY:HA2	1.86	0.41
15:LH:41:ILE:HG21	15:LH:73:ILE:HD11	2.01	0.41
26:LT:119:ALA:O	26:LT:123:GLY:N	2.53	0.41
27:LU:80:LYS:HG2	27:LU:110:TYR:CE2	2.54	0.41
33:La:72:THR:HG22	33:La:110:LYS:HB3	2.02	0.41
40:Lh:52:LYS:HA	40:Lh:52:LYS:HD3	1.84	0.41
44:Ll:25:GLN:NE2	44:Ll:28:ARG:HH12	2.19	0.41
70:SE:252:ARG:O	70:SE:256:LEU:HG	2.21	0.41
71:SG:133:LEU:HD23	71:SG:133:LEU:H	1.84	0.41
73:SI:114:GLU:HG3	73:SI:119:LEU:O	2.20	0.41
85:S2:155:G:C6	85:S2:164:A:C6	3.08	0.41
85:S2:880:G:H3'	85:S2:881:G:H8	1.84	0.41
85:S2:1114:U:O2'	85:S2:1115:U:H2'	2.20	0.41
85:S2:1406:G:H2'	85:S2:1407:U:C6	2.55	0.41
85:S2:1706:G:H2'	85:S2:1707:U:H6	1.86	0.41
2:Pt:47:U:O2'	2:Pt:50:U:OP1	2.30	0.41
3:CF:85:TYR:OH	3:CF:232:LEU:O	2.28	0.41
5:L5:347:A:H2'	5:L5:348:G:C8	2.54	0.41
5:L5:1194:G:H2'	5:L5:1195:G:C8	2.55	0.41
5:L5:1478:C:H2'	5:L5:1479:G:H8	1.85	0.41
5:L5:4892:A:H2'	5:L5:4893:A:O4'	2.21	0.41
12:LE:165:LEU:HD11	12:LE:176:THR:HG22	2.02	0.41
20:LN:80:THR:O	20:LN:80:THR:OG1	2.38	0.41
24:LR:176:ARG:NH1	24:LR:177:LEU:HG	2.36	0.41
26:LT:4:THR:OG1	26:LT:9:ARG:HD3	2.21	0.41
37:Le:19:LYS:HE3	37:Le:19:LYS:HB3	1.87	0.41
50:Ls:57:LYS:O	50:Ls:61:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SF:83:ASN:OD1	85:S2:1651:A:O2'	2.29	0.41
58:SR:34:VAL:O	58:SR:38:ILE:HG12	2.19	0.41
66:Sg:230:LEU:HD11	66:Sg:259:TRP:CD1	2.56	0.41
67:SA:34:MET:HE1	67:SA:162:PRO:HB3	2.03	0.41
71:SG:149:LYS:HD2	71:SG:149:LYS:HA	1.92	0.41
73:SI:149:TYR:O	73:SI:153:LYS:HG2	2.20	0.41
78:SV:18:SER:HB3	78:SV:72:LEU:HD21	2.03	0.41
80:SX:140:ARG:NH2	80:SX:142:ARG:HH21	2.18	0.41
81:SY:68:LYS:HE2	81:SY:68:LYS:HB3	1.75	0.41
85:S2:496:C:H2'	85:S2:497:C:H6	1.86	0.41
85:S2:1025:U:H2'	85:S2:1026:C:O4'	2.20	0.41
85:S2:1177:PSU:H2'	85:S2:1178:U:C6	2.56	0.41
85:S2:1264:C:H4'	85:S2:1265:A:O4'	2.20	0.41
3:CF:132:GLN:HB3	3:CF:136:HIS:CE1	2.55	0.41
3:CF:166:ARG:O	3:CF:169:GLU:HG2	2.20	0.41
5:L5:20:U:H3'	5:L5:21:G:H8	1.84	0.41
5:L5:749:G:N2	5:L5:750:U:O4	2.36	0.41
5:L5:1338:G:H4'	5:L5:1339:U:H6	1.85	0.41
5:L5:1354:A:H5'	23:LQ:108:ARG:HH21	1.84	0.41
5:L5:2079:G:H2'	5:L5:2080:U:C6	2.56	0.41
5:L5:2640:G:H2'	5:L5:2641:A:H8	1.85	0.41
5:L5:3762:U:C2	5:L5:3763:A:C8	3.09	0.41
5:L5:3925:OMU:H1'	5:L5:3925:OMU:HM23	1.80	0.41
5:L5:4473:A:H5''	45:Lm:95:ILE:HD12	2.03	0.41
5:L5:4620:OMU:HM23	5:L5:4620:OMU:H1'	1.86	0.41
7:L8:92:U:H2'	7:L8:93:C:O4'	2.20	0.41
25:LS:83:ARG:HG3	25:LS:125:GLN:HB2	2.02	0.41
51:Lt:28:LEU:H	51:Lt:28:LEU:HD23	1.86	0.41
52:SD:115:VAL:HG21	52:SD:138:VAL:HG11	2.03	0.41
67:SA:110:ASN:HB3	67:SA:113:GLN:HE22	1.84	0.41
79:SW:111:MET:HE3	79:SW:116:ALA:HA	2.02	0.41
82:Sa:98:PRO:HA	82:Sa:99:PRO:HD3	1.96	0.41
84:Se:11:LYS:O	84:Se:15:GLN:HG3	2.20	0.41
85:S2:24:C:O2'	85:S2:25:A:O5'	2.39	0.41
85:S2:96:C:H2'	85:S2:97:U:C6	2.56	0.41
85:S2:1336:C:H2'	85:S2:1337:4AC:O4'	2.20	0.41
85:S2:1401:A:H2'	85:S2:1402:A:C8	2.55	0.41
3:CF:5:LYS:HG3	3:CF:85:TYR:HA	2.03	0.41
3:CF:220:ASP:OD1	3:CF:221:GLY:N	2.54	0.41
5:L5:683:C:H2'	5:L5:684:G:O4'	2.21	0.41
5:L5:947:C:H5''	12:LE:51:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:1186:U:H2'	5:L5:1187:G:N3	2.36	0.41
5:L5:1297:U:OP1	38:Lf:56:ASN:HB2	2.19	0.41
5:L5:1567:U:H2'	5:L5:1568:C:C6	2.56	0.41
5:L5:2402:G:C2	5:L5:2403:A:C8	3.08	0.41
5:L5:2610:G:H2'	5:L5:2611:A:H8	1.85	0.41
5:L5:2634:C:H2'	5:L5:2635:U:H6	1.85	0.41
5:L5:2898:G:OP2	24:LR:135:LYS:NZ	2.38	0.41
5:L5:3777:G:O2'	5:L5:3815:G:O6	2.32	0.41
5:L5:4622:A:H4'	9:LB:13:SER:HB2	2.02	0.41
5:L5:4657:U:O2'	5:L5:4659:G:OP2	2.39	0.41
5:L5:4954:G:H2'	5:L5:4955:A:H8	1.83	0.41
7:L8:144:U:H2'	7:L8:145:C:C6	2.55	0.41
12:LE:101:ASN:O	12:LE:105:ARG:NH2	2.53	0.41
24:LR:82:LYS:HA	24:LR:82:LYS:HD2	1.86	0.41
32:LZ:22:LYS:NZ	32:LZ:132:GLN:O	2.47	0.41
37:Le:89:LEU:HD13	37:Le:118:LEU:HD22	2.02	0.41
43:Lk:61:PRO:HA	43:Lk:62:PRO:HD3	1.91	0.41
44:Ll:27:ILE:HG22	44:Ll:33:ASN:HD21	1.85	0.41
66:Sg:85:GLY:HA2	66:Sg:108:VAL:HG23	2.03	0.41
79:SW:57:ARG:HG2	85:S2:920:A:H4'	2.02	0.41
83:Sb:34:ASP:O	83:Sb:79:PHE:HA	2.21	0.41
85:S2:525:A:H2'	85:S2:526:A:C8	2.56	0.41
85:S2:1244:PSU:H2'	85:S2:1245:G:H8	1.84	0.41
85:S2:1616:U:O2'	85:S2:1661:A:N3	2.43	0.41
5:L5:108:A:N1	5:L5:333:U:O2'	2.50	0.41
5:L5:441:G:H2'	5:L5:442:G:H8	1.85	0.41
5:L5:467:U:N3	5:L5:468:U:O2'	2.51	0.41
5:L5:1100:U:H1'	5:L5:1167:C:H42	1.85	0.41
5:L5:1979:A:H61	5:L5:1984:A:P	2.43	0.41
5:L5:2364:OMG:HM23	5:L5:2364:OMG:H1'	1.82	0.41
5:L5:4173:G:H2'	5:L5:4174:U:C6	2.56	0.41
5:L5:4273:A:H2'	5:L5:4274:A:C8	2.56	0.41
5:L5:4616:A:H2'	5:L5:4617:G:O4'	2.21	0.41
5:L5:4966:A:H5''	9:LB:128:LYS:HG3	2.03	0.41
8:LA:116:LEU:HB3	8:LA:126:LEU:HB2	2.02	0.41
11:LD:41:LYS:HB2	26:LT:68:THR:O	2.21	0.41
12:LE:150:LEU:HD11	12:LE:164:PHE:HB2	2.03	0.41
14:LG:51:LEU:O	14:LG:55:VAL:HG23	2.21	0.41
15:LH:114:ILE:HB	15:LH:124:ARG:HB2	2.03	0.41
16:LI:36:LEU:HD11	16:LI:69:ARG:HD2	2.03	0.41
18:LL:7:GLY:O	33:La:49:HIS:NE2	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Lb:99:ILE:O	34:Lb:109:ARG:NH1	2.54	0.41
52:SD:114:ALA:HB3	52:SD:117:ARG:HG3	2.02	0.41
52:SD:204:LEU:HB2	52:SD:207:HIS:HB2	2.02	0.41
59:SS:89:ASP:OD1	59:SS:90:VAL:N	2.54	0.41
72:SH:118:ARG:HD3	72:SH:118:ARG:HA	1.92	0.41
73:SI:91:VAL:HG21	73:SI:205:ARG:HH12	1.85	0.41
73:SI:91:VAL:HG11	73:SI:205:ARG:HH12	1.84	0.41
77:SO:80:ASP:O	77:SO:83:GLN:HG3	2.20	0.41
79:SW:42:MET:HB3	79:SW:42:MET:HE2	1.85	0.41
85:S2:656:G:N2	85:S2:663:C:H5''	2.36	0.41
85:S2:1037:G:H4'	85:S2:1845:A:H4'	2.02	0.41
85:S2:1533:A:N7	85:S2:1604:G:H1'	2.36	0.41
85:S2:1620:A:H1'	85:S2:1624:U:OP2	2.21	0.41
85:S2:1621:U:O2'	85:S2:1622:U:H2'	2.21	0.41
3:CF:22:THR:HG23	3:CF:56:TYR:HB2	2.03	0.41
5:L5:135:G:N7	40:Lh:97:LYS:HE3	2.36	0.41
5:L5:935:A:O2'	5:L5:936:C:OP1	2.39	0.41
5:L5:959:G:C8	12:LE:123:ARG:HG2	2.56	0.41
5:L5:1600:A:H5'	22:LP:133:HIS:HA	2.03	0.41
5:L5:1739:G:H2'	5:L5:1740:C:C6	2.56	0.41
5:L5:1846:G:H2'	5:L5:1847:C:H6	1.85	0.41
5:L5:1956:A:H2'	5:L5:1957:U:C6	2.56	0.41
5:L5:2019:C:H2'	5:L5:2020:U:C6	2.56	0.41
5:L5:2045:G:O2'	5:L5:2046:G:H5''	2.21	0.41
5:L5:2303:C:H5''	37:Le:104:SER:HB3	2.03	0.41
5:L5:2415:U:H2'	5:L5:2416:G:C8	2.55	0.41
5:L5:2480:G:H2'	5:L5:2481:G:C8	2.56	0.41
5:L5:2863:G:O2'	24:LR:82:LYS:O	2.37	0.41
5:L5:3606:U:H2'	5:L5:3607:U:H6	1.86	0.41
5:L5:3870:C:H2'	5:L5:3871:A:H8	1.86	0.41
5:L5:4084:G:O6	8:LA:72:ARG:NH2	2.45	0.41
5:L5:4232:U:H1'	5:L5:4233:A:C2	2.55	0.41
5:L5:4593:C:H2'	5:L5:4594:U:H6	1.86	0.41
7:L8:7:U:H2'	7:L8:8:U:C6	2.56	0.41
17:LJ:48:PRO:HB3	17:LJ:72:CYS:HB3	2.03	0.41
18:LL:18:TRP:CD1	18:LL:18:TRP:H	2.38	0.41
23:LQ:32:TYR:HD2	23:LQ:51:LEU:HD11	1.86	0.41
24:LR:21:LYS:HE3	24:LR:55:VAL:HA	2.02	0.41
24:LR:103:ARG:HG2	24:LR:124:TYR:CE2	2.55	0.41
24:LR:175:GLU:O	24:LR:178:GLN:HG3	2.21	0.41
26:LT:50:LYS:HB3	26:LT:50:LYS:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LZ:33:THR:C	32:LZ:35:ASP:H	2.29	0.41
38:Lf:106:TYR:O	38:Lf:108:SER:N	2.54	0.41
39:Lg:82:MET:HE3	39:Lg:82:MET:HB2	1.90	0.41
41:Li:68:ARG:HA	41:Li:68:ARG:HD3	1.80	0.41
44:Ll:28:ARG:HA	44:Ll:33:ASN:ND2	2.33	0.41
51:Lt:114:ARG:NH2	51:Lt:162:CYS:SG	2.94	0.41
54:SK:32:HIS:ND1	54:SK:33:PRO:HD2	2.36	0.41
55:SM:95:ASP:HB3	55:SM:99:LYS:HB3	2.01	0.41
55:SM:112:LYS:HE2	55:SM:112:LYS:HB2	1.84	0.41
56:SP:100:LYS:HB2	85:S2:1240:A:C5	2.56	0.41
69:SC:116:THR:HA	85:S2:1203:G:H4'	2.03	0.41
69:SC:183:LYS:HA	69:SC:195:LEU:O	2.20	0.41
70:SE:242:LYS:HD3	70:SE:242:LYS:HA	1.74	0.41
71:SG:7:PHE:HD1	71:SG:113:ILE:HB	1.86	0.41
73:SI:150:ASP:HA	73:SI:153:LYS:CG	2.50	0.41
74:SJ:64:ASP:OD1	74:SJ:65:GLU:N	2.54	0.41
75:SL:128:VAL:HG12	75:SL:142:VAL:HA	2.01	0.41
83:Sb:17:ARG:HH11	85:S2:1127:C:H4'	1.86	0.41
85:S2:520:A:O2'	85:S2:825:A:N3	2.45	0.41
85:S2:1656:G:O6	85:S2:1668:U:O4	2.39	0.41
3:CF:178:ILE:HA	3:CF:181:ILE:HG22	2.03	0.41
5:L5:441:G:H2'	5:L5:442:G:C8	2.56	0.41
5:L5:499:G:H2'	5:L5:499:G:N3	2.36	0.41
5:L5:1189:G:H2'	5:L5:1190:C:C6	2.55	0.41
5:L5:1345:A:H2'	5:L5:1346:C:C6	2.56	0.41
5:L5:1672:U:H2'	5:L5:1673:U:C6	2.57	0.41
5:L5:1984:A:H5'	5:L5:1986:U:P	2.61	0.41
9:LB:217:ILE:HD12	9:LB:347:LEU:HB3	2.02	0.41
9:LB:289:GLN:NE2	9:LB:292:LEU:HD11	2.32	0.41
13:LF:48:LYS:HE3	34:Lb:96:LEU:HD21	2.03	0.41
16:LI:187:LYS:HE3	16:LI:189:CYS:SG	2.61	0.41
22:LP:15:CYS:SG	22:LP:150:LEU:HB2	2.61	0.41
23:LQ:86:ILE:HD11	23:LQ:100:VAL:HG11	2.02	0.41
25:LS:5:GLY:O	25:LS:111:ARG:NH2	2.54	0.41
36:Ld:63:ARG:HD3	36:Ld:103:TYR:CD2	2.56	0.41
51:Lt:11:LYS:HD2	51:Lt:11:LYS:HA	1.95	0.41
57:SQ:97:GLN:HB2	57:SQ:105:LYS:HG3	2.03	0.41
59:SS:24:ARG:H	59:SS:24:ARG:HG2	1.73	0.41
59:SS:62:ASP:O	59:SS:65:GLU:HG3	2.21	0.41
66:Sg:35:SER:OG	66:Sg:36:ARG:N	2.54	0.41
66:Sg:314:ILE:HD12	66:Sg:314:ILE:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SA:10:MET:SD	67:SA:15:VAL:HG22	2.61	0.41
67:SA:184:ARG:HG3	67:SA:189:ILE:HD12	2.02	0.41
67:SA:198:MET:HG2	67:SA:200:ASP:H	1.86	0.41
73:SI:141:ARG:HA	73:SI:141:ARG:CZ	2.51	0.41
79:SW:77:PRO:HG2	79:SW:79:PHE:CE2	2.56	0.41
80:SX:128:VAL:HG23	80:SX:138:LYS:HD2	2.02	0.41
85:S2:495:U:H2'	85:S2:496:C:O4'	2.20	0.41
85:S2:672:A:N6	85:S2:1027:A:OP1	2.50	0.41
85:S2:1309:C:H2'	85:S2:1310:U:O4'	2.20	0.41
85:S2:1323:U:H2'	85:S2:1324:G:C8	2.56	0.41
85:S2:1348:G:C8	85:S2:1349:G:C8	3.09	0.41
85:S2:1760:G:N1	85:S2:1774:C:OP1	2.54	0.41
85:S2:1797:U:H2'	85:S2:1798:C:C6	2.56	0.41
3:CF:274:PRO:HA	3:CF:289:VAL:HG13	2.03	0.40
3:CF:378:LYS:HE2	3:CF:391:PRO:HB3	2.02	0.40
5:L5:270:U:H2'	5:L5:271:C:H6	1.86	0.40
5:L5:705:G:H2'	5:L5:706:C:C6	2.56	0.40
5:L5:1588:U:H2'	5:L5:1589:C:C6	2.57	0.40
5:L5:2764:A:H2'	5:L5:2765:A:C8	2.54	0.40
7:L8:64:U:C2	7:L8:65:A:C8	3.09	0.40
8:LA:180:LEU:HD21	48:Lp:22:LEU:HB3	2.03	0.40
10:LC:328:LEU:HB3	13:LF:187:MET:HG3	2.03	0.40
12:LE:128:HIS:ND1	12:LE:128:HIS:O	2.54	0.40
19:LM:118:MET:HG2	21:LO:192:TYR:CZ	2.56	0.40
30:LX:77:ILE:HD13	30:LX:100:VAL:HG12	2.03	0.40
41:Li:90:LEU:HA	41:Li:93:VAL:HG22	2.03	0.40
46:Ln:17:ARG:NH1	85:S2:1173:A:OP1	2.54	0.40
51:Lt:32:ILE:HA	51:Lt:35:LEU:HD23	2.03	0.40
60:ST:72:VAL:O	60:ST:76:THR:HG23	2.21	0.40
63:Sc:10:LYS:HE2	63:Sc:34:PHE:CD2	2.56	0.40
69:SC:78:LEU:HD12	69:SC:81:ILE:HD12	2.04	0.40
71:SG:174:PRO:HB3	85:S2:65:C:C6	2.56	0.40
71:SG:191:ARG:NH2	85:S2:312:G:H2'	2.36	0.40
76:SN:64:ARG:HD3	76:SN:70:LYS:HG2	2.03	0.40
79:SW:28:ARG:HB3	79:SW:29:PRO:HD3	2.03	0.40
81:SY:111:LYS:NZ	85:S2:56:G:OP1	2.38	0.40
82:Sa:41:ILE:HD12	82:Sa:68:TYR:CD2	2.56	0.40
85:S2:432:G:H2'	85:S2:433:A:H8	1.85	0.40
5:L5:943:A:N6	13:LF:151:ASN:OD1	2.51	0.40
5:L5:1961:G:H8	50:Ls:59:THR:HG21	1.86	0.40
5:L5:2638:G:N1	5:L5:2718:U:H2'	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L5:4927:G:H5''	5:L5:4928:C:C5	2.57	0.40
12:LE:45:SER:C	12:LE:47:ASN:H	2.29	0.40
23:LQ:177:ALA:O	23:LQ:184:ARG:HB2	2.22	0.40
30:LX:88:LYS:O	30:LX:92:ASP:HB2	2.20	0.40
34:Lb:43:MET:HE2	34:Lb:47:LYS:NZ	2.36	0.40
47:Lo:4:VAL:HG23	47:Lo:93:LEU:HD23	2.03	0.40
53:SF:48:TYR:CE1	57:SQ:56:LEU:HD13	2.56	0.40
53:SF:120:GLY:HA2	53:SF:121:PRO:HD3	1.94	0.40
53:SF:167:LYS:HE3	53:SF:172:CYS:SG	2.61	0.40
66:Sg:183:LYS:HA	66:Sg:183:LYS:HD2	1.83	0.40
67:SA:5:LEU:HD11	78:SV:41:LYS:HD2	2.03	0.40
85:S2:35:C:H2'	85:S2:36:U:C6	2.56	0.40
85:S2:43:U:OP2	85:S2:485:A:N6	2.46	0.40
85:S2:1221:G:H2'	85:S2:1222:G:H8	1.86	0.40
85:S2:1349:G:H2'	85:S2:1350:U:C6	2.56	0.40
85:S2:1683:C:H2'	85:S2:1684:C:H6	1.87	0.40
3:CF:168:GLU:O	3:CF:172:LYS:HG2	2.21	0.40
3:CF:291:SER:O	3:CF:311:ASN:N	2.45	0.40
4:AT:61:A:H5''	4:AT:62:C:C5	2.56	0.40
5:L5:65:A:N6	5:L5:75:G:H1'	2.36	0.40
5:L5:1266:G:O6	34:Lb:91:ARG:HB2	2.22	0.40
5:L5:1338:G:H4'	5:L5:1339:U:C6	2.56	0.40
5:L5:1772:C:H2'	5:L5:1773:U:H6	1.86	0.40
5:L5:1952:G:OP1	25:LS:139:ARG:NE	2.55	0.40
5:L5:2022:C:H2'	5:L5:2023:C:O4'	2.21	0.40
5:L5:3685:C:H5'	8:LA:193:ARG:CZ	2.51	0.40
5:L5:3873:G:H2'	5:L5:3874:G:C8	2.57	0.40
5:L5:3945:A:H2'	5:L5:3946:G:H8	1.86	0.40
5:L5:4601:U:OP2	5:L5:4609:G:N1	2.42	0.40
9:LB:160:ILE:HG12	9:LB:193:LYS:HD3	2.02	0.40
10:LC:266:THR:HG22	10:LC:267:TRP:N	2.37	0.40
11:LD:84:PRO:HG3	11:LD:89:LYS:HA	2.03	0.40
11:LD:156:GLY:HA2	11:LD:181:PRO:HG3	2.03	0.40
12:LE:203:ILE:O	12:LE:206:VAL:HG22	2.21	0.40
21:LO:89:PRO:O	21:LO:95:GLY:HA3	2.21	0.40
42:Lj:19:CYS:SG	42:Lj:34:CYS:HB2	2.60	0.40
61:SU:99:LYS:HA	61:SU:99:LYS:HD3	1.89	0.40
63:Sc:13:ARG:CZ	63:Sc:35:MET:HE1	2.52	0.40
71:SG:174:PRO:HG3	85:S2:65:C:C2	2.56	0.40
76:SN:94:LYS:HE2	76:SN:94:LYS:HB2	1.93	0.40
77:SO:138:ASP:HB3	85:S2:984:C:O2'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:S2:1239:U:N3	85:S2:1242:U:OP2	2.42	0.40
85:S2:1513:C:H2'	85:S2:1514:G:C8	2.54	0.40
5:L5:37:U:H2'	5:L5:38:A:O4'	2.22	0.40
5:L5:460:C:H2'	5:L5:461:G:H8	1.86	0.40
5:L5:1199:G:H2'	5:L5:1200:G:C8	2.57	0.40
5:L5:1241:C:H5'	12:LE:72:LYS:HZ2	1.85	0.40
5:L5:1772:C:H2'	5:L5:1773:U:C6	2.57	0.40
5:L5:1972:G:C6	5:L5:1973:G:C6	3.10	0.40
5:L5:2539:C:H2'	5:L5:2540:C:H6	1.85	0.40
9:LB:147:GLU:CD	9:LB:198:ARG:HH22	2.26	0.40
28:LV:65:VAL:HG23	28:LV:73:ARG:HA	2.02	0.40
37:Le:35:TRP:HH2	37:Le:55:MET:HG2	1.86	0.40
52:SD:68:GLU:HB3	54:SK:70:TYR:CE1	2.57	0.40
54:SK:90:VAL:HG21	54:SK:95:ARG:HB2	2.04	0.40
55:SM:87:GLU:HG3	55:SM:103:VAL:HG11	2.04	0.40
57:SQ:49:TYR:O	57:SQ:53:GLU:HB2	2.21	0.40
59:SS:102:GLY:HA2	59:SS:105:ASN:ND2	2.36	0.40
69:SC:256:TRP:CD2	79:SW:68:ARG:HD3	2.56	0.40
76:SN:102:LEU:HD12	76:SN:102:LEU:HA	1.94	0.40
77:SO:98:ARG:HG2	77:SO:99:ALA:O	2.22	0.40
81:SY:10:ARG:HA	85:S2:839:C:N4	2.37	0.40
83:Sb:51:GLN:NE2	85:S2:927:C:O2	2.54	0.40
85:S2:12:U:H2'	85:S2:13:C:C6	2.56	0.40
85:S2:64:A:N6	85:S2:83:A:OP2	2.51	0.40
85:S2:669:A:H2'	85:S2:670:A:C8	2.57	0.40
85:S2:1749:G:H2'	85:S2:1750:C:C6	2.57	0.40
2:Pt:27:U:H2'	2:Pt:28:U:C6	2.57	0.40
3:CF:237:PRO:HA	3:CF:238:PRO:HD3	1.97	0.40
3:CF:266:ARG:HA	3:CF:307:ASN:HA	2.04	0.40
5:L5:190:G:H2'	5:L5:191:G:H8	1.87	0.40
5:L5:1647:U:OP1	88:L5:5290:SPD:H51	2.21	0.40
5:L5:2787:A2M:H1'	5:L5:2787:A2M:HM'2	1.82	0.40
5:L5:2804:OMC:C2	5:L5:2805:C:C5	3.10	0.40
5:L5:3760:A:C5	85:S2:1826:G:H4'	2.56	0.40
5:L5:3870:C:H2'	5:L5:3871:A:C8	2.56	0.40
5:L5:4320:G:H2'	5:L5:4321:U:C6	2.57	0.40
5:L5:4500:PSU:H2'	5:L5:4501:U:C6	2.57	0.40
5:L5:4633:G:N2	5:L5:4664:A:N7	2.70	0.40
5:L5:4749:C:H2'	5:L5:4750:G:O4'	2.21	0.40
5:L5:4862:G:H2'	5:L5:4863:G:H8	1.87	0.40
5:L5:4993:G:H22	5:L5:5058:A:H2	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L7:15:C:H2'	6:L7:16:A:C8	2.55	0.40
8:LA:28:ARG:HE	8:LA:28:ARG:HB2	1.76	0.40
11:LD:37:VAL:HG12	11:LD:50:ARG:HD3	2.03	0.40
16:LI:43:VAL:HG21	16:LI:197:VAL:HG13	2.03	0.40
19:LM:6:PHE:H	19:LM:11:ARG:NH2	2.20	0.40
21:LO:180:GLN:NE2	21:LO:184:ASN:OD1	2.53	0.40
51:Lt:81:ILE:HD13	51:Lt:113:ALA:HB1	2.04	0.40
54:SK:26:ASP:HB3	54:SK:29:MET:HB2	2.04	0.40
67:SA:124:VAL:HG13	67:SA:130:ASP:HB2	2.02	0.40
73:SI:114:GLU:HB3	73:SI:136:ILE:HD12	2.04	0.40
75:SL:111:VAL:HG12	75:SL:140:PHE:HB2	2.04	0.40
85:S2:194:C:H2'	85:S2:195:C:H6	1.87	0.40
85:S2:472:C:O2	85:S2:475:C:N4	2.54	0.40
85:S2:946:U:H2'	85:S2:947:G:H8	1.87	0.40
85:S2:1421:A:H3'	85:S2:1422:G:C8	2.57	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
3	CF	438/441 (99%)	420 (96%)	18 (4%)	0	100	100
8	LA	246/248 (99%)	229 (93%)	17 (7%)	0	100	100
9	LB	400/402 (100%)	383 (96%)	17 (4%)	0	100	100
10	LC	366/368 (100%)	353 (96%)	13 (4%)	0	100	100
11	LD	291/293 (99%)	280 (96%)	11 (4%)	0	100	100
12	LE	236/250 (94%)	221 (94%)	15 (6%)	0	100	100
13	LF	223/225 (99%)	215 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	LG	239/241 (99%)	223 (93%)	16 (7%)	0	100	100
15	LH	188/190 (99%)	182 (97%)	6 (3%)	0	100	100
16	LI	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
17	LJ	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
18	LL	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
19	LM	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
20	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
21	LO	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
22	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
23	LQ	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
24	LR	185/187 (99%)	179 (97%)	6 (3%)	0	100	100
25	LS	173/175 (99%)	163 (94%)	10 (6%)	0	100	100
26	LT	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
27	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
28	LV	129/131 (98%)	125 (97%)	4 (3%)	0	100	100
29	LW	112/124 (90%)	108 (96%)	4 (4%)	0	100	100
30	LX	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
31	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
32	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
33	La	145/147 (99%)	141 (97%)	4 (3%)	0	100	100
34	Lb	105/121 (87%)	100 (95%)	5 (5%)	0	100	100
35	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
36	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
37	Le	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
38	Lf	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
39	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
40	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
41	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
42	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
43	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
44	Ll	48/50 (96%)	47 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	Lm	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
46	Ln	22/24 (92%)	22 (100%)	0	0	100	100
47	Lo	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
48	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
49	Lr	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
50	Ls	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
51	Lt	128/157 (82%)	111 (87%)	17 (13%)	0	100	100
52	SD	225/227 (99%)	218 (97%)	7 (3%)	0	100	100
53	SF	187/189 (99%)	176 (94%)	11 (6%)	0	100	100
54	SK	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
55	SM	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
56	SP	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
57	SQ	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
58	SR	133/135 (98%)	125 (94%)	7 (5%)	1 (1%)	16	31
59	SS	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
60	ST	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
61	SU	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
62	SZ	73/75 (97%)	64 (88%)	9 (12%)	0	100	100
63	Sc	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
64	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
65	Sf	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
66	Sg	311/313 (99%)	293 (94%)	18 (6%)	0	100	100
67	SA	219/221 (99%)	204 (93%)	15 (7%)	0	100	100
68	SB	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
69	SC	218/220 (99%)	206 (94%)	12 (6%)	0	100	100
70	SE	260/262 (99%)	249 (96%)	11 (4%)	0	100	100
71	SG	235/237 (99%)	222 (94%)	13 (6%)	0	100	100
72	SH	182/189 (96%)	168 (92%)	14 (8%)	0	100	100
73	SI	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
74	SJ	183/185 (99%)	175 (96%)	7 (4%)	1 (0%)	24	43
75	SL	151/153 (99%)	144 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
76	SN	148/150 (99%)	144 (97%)	4 (3%)	0	100	100
77	SO	135/137 (98%)	126 (93%)	9 (7%)	0	100	100
78	SV	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
79	SW	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
80	SX	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
81	SY	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
82	Sa	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
83	Sb	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
84	Se	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
All	All	12110/12343 (98%)	11574 (96%)	534 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
58	SR	129	LYS
74	SJ	138	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CI	25/25 (100%)	25 (100%)	0	100	100
3	CF	365/366 (100%)	365 (100%)	0	100	100
8	LA	190/190 (100%)	190 (100%)	0	100	100
9	LB	348/348 (100%)	348 (100%)	0	100	100
10	LC	306/306 (100%)	306 (100%)	0	100	100
11	LD	246/247 (100%)	246 (100%)	0	100	100
12	LE	212/222 (96%)	212 (100%)	0	100	100
13	LF	194/194 (100%)	194 (100%)	0	100	100
14	LG	203/205 (99%)	203 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	LH	169/169 (100%)	169 (100%)	0	100	100
16	LI	180/180 (100%)	180 (100%)	0	100	100
17	LJ	143/148 (97%)	143 (100%)	0	100	100
18	LL	176/176 (100%)	176 (100%)	0	100	100
19	LM	118/118 (100%)	118 (100%)	0	100	100
20	LN	171/171 (100%)	171 (100%)	0	100	100
21	LO	173/173 (100%)	173 (100%)	0	100	100
22	LP	134/134 (100%)	134 (100%)	0	100	100
23	LQ	164/164 (100%)	164 (100%)	0	100	100
24	LR	166/166 (100%)	166 (100%)	0	100	100
25	LS	156/156 (100%)	156 (100%)	0	100	100
26	LT	139/139 (100%)	139 (100%)	0	100	100
27	LU	91/91 (100%)	91 (100%)	0	100	100
28	LV	101/101 (100%)	101 (100%)	0	100	100
29	LW	95/103 (92%)	95 (100%)	0	100	100
30	LX	108/108 (100%)	108 (100%)	0	100	100
31	LY	124/124 (100%)	124 (100%)	0	100	100
32	LZ	117/117 (100%)	117 (100%)	0	100	100
33	La	120/120 (100%)	120 (100%)	0	100	100
34	Lb	88/101 (87%)	88 (100%)	0	100	100
35	Lc	83/83 (100%)	83 (100%)	0	100	100
36	Ld	98/98 (100%)	98 (100%)	0	100	100
37	Le	114/114 (100%)	114 (100%)	0	100	100
38	Lf	88/88 (100%)	88 (100%)	0	100	100
39	Lg	98/98 (100%)	98 (100%)	0	100	100
40	Lh	109/109 (100%)	109 (100%)	0	100	100
41	Li	86/86 (100%)	86 (100%)	0	100	100
42	Lj	73/73 (100%)	73 (100%)	0	100	100
43	Lk	64/64 (100%)	64 (100%)	0	100	100
44	Ll	47/47 (100%)	47 (100%)	0	100	100
45	Lm	48/48 (100%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	Ln	23/23 (100%)	23 (100%)	0	100	100
47	Lo	93/93 (100%)	93 (100%)	0	100	100
48	Lp	74/74 (100%)	74 (100%)	0	100	100
49	Lr	109/109 (100%)	109 (100%)	0	100	100
50	Ls	162/164 (99%)	162 (100%)	0	100	100
51	Lt	107/130 (82%)	107 (100%)	0	100	100
52	SD	190/190 (100%)	190 (100%)	0	100	100
53	SF	159/159 (100%)	159 (100%)	0	100	100
54	SK	89/89 (100%)	89 (100%)	0	100	100
55	SM	102/104 (98%)	102 (100%)	0	100	100
56	SP	107/107 (100%)	107 (100%)	0	100	100
57	SQ	119/119 (100%)	119 (100%)	0	100	100
58	SR	122/122 (100%)	122 (100%)	0	100	100
59	SS	126/126 (100%)	126 (100%)	0	100	100
60	ST	113/113 (100%)	113 (100%)	0	100	100
61	SU	94/94 (100%)	94 (100%)	0	100	100
62	SZ	66/66 (100%)	66 (100%)	0	100	100
63	Sc	57/57 (100%)	57 (100%)	0	100	100
64	Sd	48/48 (100%)	48 (100%)	0	100	100
65	Sf	60/60 (100%)	60 (100%)	0	100	100
66	Sg	272/272 (100%)	272 (100%)	0	100	100
67	SA	183/183 (100%)	183 (100%)	0	100	100
68	SB	195/195 (100%)	195 (100%)	0	100	100
69	SC	186/186 (100%)	186 (100%)	0	100	100
70	SE	224/224 (100%)	224 (100%)	0	100	100
71	SG	207/207 (100%)	207 (100%)	0	100	100
72	SH	166/169 (98%)	166 (100%)	0	100	100
73	SI	178/178 (100%)	178 (100%)	0	100	100
74	SJ	161/161 (100%)	161 (100%)	0	100	100
75	SL	137/137 (100%)	137 (100%)	0	100	100
76	SN	130/130 (100%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	SO	107/107 (100%)	107 (100%)	0	100	100
78	SV	67/67 (100%)	67 (100%)	0	100	100
79	SW	112/112 (100%)	112 (100%)	0	100	100
80	SX	113/113 (100%)	113 (100%)	0	100	100
81	SY	113/113 (100%)	113 (100%)	0	100	100
82	Sa	89/89 (100%)	89 (100%)	0	100	100
83	Sb	75/75 (100%)	75 (100%)	0	100	100
84	Se	47/47 (100%)	47 (100%)	0	100	100
All	All	10512/10582 (99%)	10512 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
3	CF	331	ASN
3	CF	352	GLN
8	LA	97	ASN
9	LB	68	ASN
9	LB	121	ASN
9	LB	289	GLN
9	LB	301	ASN
10	LC	41	HIS
10	LC	329	ASN
11	LD	202	GLN
13	LF	235	ASN
14	LG	112	GLN
15	LH	98	HIS
15	LH	138	GLN
16	LI	59	GLN
17	LJ	110	GLN
18	LL	111	GLN
18	LL	205	GLN
19	LM	34	ASN
20	LN	199	GLN
21	LO	26	GLN
21	LO	50	ASN
22	LP	75	GLN
22	LP	97	ASN

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Mol	Chain	Res	Type
22	LP	118	GLN
22	LP	120	ASN
22	LP	133	HIS
22	LP	137	ASN
24	LR	134	ASN
27	LU	94	ASN
29	LW	50	ASN
29	LW	79	GLN
30	LX	125	ASN
31	LY	61	HIS
33	La	34	ASN
33	La	67	GLN
33	La	120	GLN
34	Lb	60	ASN
35	Lc	51	ASN
35	Lc	72	HIS
37	Le	52	GLN
38	Lf	99	HIS
44	Ll	33	ASN
48	Lp	33	GLN
50	Ls	71	ASN
50	Ls	159	GLN
50	Ls	179	ASN
53	SF	29	GLN
53	SF	101	HIS
53	SF	118	ASN
53	SF	149	GLN
54	SK	32	HIS
54	SK	50	GLN
57	SQ	77	HIS
57	SQ	80	GLN
57	SQ	97	GLN
59	SS	11	HIS
60	ST	63	HIS
60	ST	85	ASN
62	SZ	89	GLN
64	Sd	37	ASN
65	Sf	93	HIS
65	Sf	139	HIS
66	Sg	26	GLN
66	Sg	119	GLN
66	Sg	272	GLN

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Mol	Chain	Res	Type
66	Sg	285	GLN
67	SA	9	GLN
67	SA	84	GLN
67	SA	132	GLN
68	SB	76	ASN
68	SB	118	GLN
68	SB	149	GLN
68	SB	158	HIS
68	SB	202	GLN
69	SC	267	GLN
72	SH	76	GLN
72	SH	162	GLN
73	SI	52	ASN
75	SL	65	ASN
76	SN	105	ASN
78	SV	35	ASN
79	SW	5	ASN
79	SW	90	GLN
80	SX	31	HIS
81	SY	112	ASN
82	Sa	72	HIS
83	Sb	51	GLN
84	Se	58	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Pt	72/74 (97%)	15 (20%)	0
4	AT	74/76 (97%)	27 (36%)	0
5	L5	3643/3655 (99%)	731 (20%)	16 (0%)
6	L7	119/120 (99%)	11 (9%)	0
7	L8	155/156 (99%)	21 (13%)	0
85	S2	1714/1740 (98%)	378 (22%)	4 (0%)
All	All	5777/5821 (99%)	1183 (20%)	20 (0%)

All (1183) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Pt	9	A
2	Pt	13	U
2	Pt	19	G

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Mol	Chain	Res	Type
2	Pt	21	A
2	Pt	46	G
2	Pt	47	U
2	Pt	48	C
2	Pt	49	C
2	Pt	58	A
2	Pt	61	C
2	Pt	66	C
2	Pt	67	G
2	Pt	70	A
2	Pt	74	C
2	Pt	76	A
4	AT	4	U
4	AT	8	U
4	AT	9	A
4	AT	12	G
4	AT	13	U
4	AT	14	A
4	AT	16	C
4	AT	20	U
4	AT	21	U
4	AT	22	A
4	AT	26	C
4	AT	27	G
4	AT	33	C
4	AT	37	C
4	AT	47	G
4	AT	48	U
4	AT	49	C
4	AT	50	C
4	AT	53	G
4	AT	57	C
4	AT	59	A
4	AT	60	A
4	AT	62	C
4	AT	65	G
4	AT	74	A
4	AT	76	C
4	AT	77	A
5	L5	25	A
5	L5	30	C
5	L5	39	A

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Mol	Chain	Res	Type
5	L5	42	A
5	L5	48	G
5	L5	56	A
5	L5	59	A
5	L5	64	A
5	L5	65	A
5	L5	73	A
5	L5	74	G
5	L5	91	G
5	L5	104	G
5	L5	109	G
5	L5	110	C
5	L5	119	G
5	L5	120	A
5	L5	132	G
5	L5	133	C
5	L5	134	G
5	L5	135	G
5	L5	145	G
5	L5	151	G
5	L5	157	U
5	L5	159	C
5	L5	165	A
5	L5	172	C
5	L5	176	G
5	L5	182	G
5	L5	183	C
5	L5	184	U
5	L5	185	C
5	L5	186	G
5	L5	187	U
5	L5	188	G
5	L5	189	G
5	L5	200	U
5	L5	209	U
5	L5	210	C
5	L5	216	C
5	L5	218	A
5	L5	220	C
5	L5	234	G
5	L5	237	G
5	L5	255	C

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Mol	Chain	Res	Type
5	L5	256	G
5	L5	261	G
5	L5	264	C
5	L5	265	C
5	L5	266	C
5	L5	267	G
5	L5	276	C
5	L5	280	G
5	L5	297	U
5	L5	306	A
5	L5	315	G
5	L5	316	U
5	L5	340	C
5	L5	373	G
5	L5	385	A
5	L5	387	G
5	L5	388	A
5	L5	396	A
5	L5	407	A
5	L5	409	G
5	L5	410	A
5	L5	411	G
5	L5	412	G
5	L5	413	G
5	L5	415	G
5	L5	432	U
5	L5	440	U
5	L5	449	C
5	L5	452	A
5	L5	453	G
5	L5	454	U
5	L5	456	C
5	L5	457	G
5	L5	467	U
5	L5	472	C
5	L5	484	U
5	L5	485	C
5	L5	486	C
5	L5	489	C
5	L5	493	G
5	L5	494	U
5	L5	497	G

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Mol	Chain	Res	Type
5	L5	498	C
5	L5	499	G
5	L5	500	G
5	L5	502	C
5	L5	503	C
5	L5	504	G
5	L5	509	A
5	L5	510	U
5	L5	512	U
5	L5	513	U
5	L5	514	U
5	L5	518	G
5	L5	643	C
5	L5	646	G
5	L5	653	U
5	L5	654	C
5	L5	655	C
5	L5	656	C
5	L5	657	C
5	L5	659	G
5	L5	666	G
5	L5	667	A
5	L5	668	C
5	L5	669	C
5	L5	673	C
5	L5	685	C
5	L5	686	A
5	L5	687	U
5	L5	703	G
5	L5	704	C
5	L5	708	G
5	L5	730	G
5	L5	731	G
5	L5	738	C
5	L5	739	G
5	L5	742	G
5	L5	746	A
5	L5	759	G
5	L5	904	C
5	L5	905	C
5	L5	906	C
5	L5	910	G

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Mol	Chain	Res	Type
5	L5	913	U
5	L5	914	U
5	L5	915	A
5	L5	917	A
5	L5	923	C
5	L5	924	C
5	L5	926	G
5	L5	932	A
5	L5	933	G
5	L5	935	A
5	L5	936	C
5	L5	941	C
5	L5	943	A
5	L5	945	U
5	L5	956	A
5	L5	959	G
5	L5	960	A
5	L5	961	G
5	L5	962	C
5	L5	965	G
5	L5	966	A
5	L5	967	C
5	L5	969	C
5	L5	970	G
5	L5	982	U
5	L5	985	C
5	L5	1070	G
5	L5	1071	C
5	L5	1072	C
5	L5	1075	G
5	L5	1082	C
5	L5	1083	U
5	L5	1168	G
5	L5	1171	G
5	L5	1172	C
5	L5	1173	G
5	L5	1179	U
5	L5	1180	C
5	L5	1181	C
5	L5	1182	C
5	L5	1183	C
5	L5	1202	C

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Mol	Chain	Res	Type
5	L5	1203	G
5	L5	1210	C
5	L5	1211	G
5	L5	1214	C
5	L5	1215	C
5	L5	1216	C
5	L5	1218	G
5	L5	1219	G
5	L5	1222	A
5	L5	1246	G
5	L5	1253	G
5	L5	1254	A
5	L5	1257	A
5	L5	1258	G
5	L5	1266	G
5	L5	1267	C
5	L5	1269	G
5	L5	1271	G
5	L5	1272	C
5	L5	1273	G
5	L5	1275	G
5	L5	1280	C
5	L5	1284	G
5	L5	1285	U
5	L5	1287	G
5	L5	1293	G
5	L5	1294	A
5	L5	1295	C
5	L5	1296	G
5	L5	1301	C
5	L5	1302	U
5	L5	1314	C
5	L5	1326	A2M
5	L5	1354	A
5	L5	1359	G
5	L5	1365	C
5	L5	1366	G
5	L5	1367	C
5	L5	1381	U
5	L5	1387	A
5	L5	1394	G
5	L5	1397	A

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Mol	Chain	Res	Type
5	L5	1398	A
5	L5	1404	G
5	L5	1407	C
5	L5	1409	C
5	L5	1410	U
5	L5	1411	C
5	L5	1414	C
5	L5	1416	G
5	L5	1417	C
5	L5	1420	A
5	L5	1437	C
5	L5	1438	U
5	L5	1439	C
5	L5	1442	C
5	L5	1443	A
5	L5	1444	G
5	L5	1446	C
5	L5	1447	C
5	L5	1482	G
5	L5	1483	C
5	L5	1497	A
5	L5	1498	G
5	L5	1502	G
5	L5	1517	G
5	L5	1524	A2M
5	L5	1534	A2M
5	L5	1537	A
5	L5	1547	A
5	L5	1564	A
5	L5	1566	C
5	L5	1578	U
5	L5	1591	U
5	L5	1596	U
5	L5	1621	A
5	L5	1624	G
5	L5	1625	OMG
5	L5	1626	G
5	L5	1631	A
5	L5	1633	G
5	L5	1634	A
5	L5	1637	A
5	L5	1638	A

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Mol	Chain	Res	Type
5	L5	1640	C
5	L5	1641	G
5	L5	1642	A
5	L5	1654	G
5	L5	1661	C
5	L5	1676	C
5	L5	1677	PSU
5	L5	1678	C
5	L5	1697	G
5	L5	1699	A
5	L5	1700	G
5	L5	1701	A
5	L5	1702	C
5	L5	1704	C
5	L5	1705	G
5	L5	1717	C
5	L5	1718	C
5	L5	1719	A
5	L5	1731	C
5	L5	1734	G
5	L5	1742	A
5	L5	1750	G
5	L5	1755	C
5	L5	1757	U
5	L5	1758	G
5	L5	1760	G
5	L5	1761	G
5	L5	1762	C
5	L5	1763	C
5	L5	1764	G
5	L5	1765	A
5	L5	1766	A
5	L5	1767	A
5	L5	1768	C
5	L5	1769	G
5	L5	1770	A
5	L5	1775	A
5	L5	1785	C
5	L5	1787	A
5	L5	1804	A
5	L5	1806	G
5	L5	1810	G

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Mol	Chain	Res	Type
5	L5	1815	G
5	L5	1821	G
5	L5	1822	U
5	L5	1834	U
5	L5	1836	G
5	L5	1837	A
5	L5	1842	G
5	L5	1855	G
5	L5	1869	G
5	L5	1882	U
5	L5	1892	A
5	L5	1897	A
5	L5	1917	A
5	L5	1918	U
5	L5	1919	G
5	L5	1920	C
5	L5	1921	C
5	L5	1922	G
5	L5	1925	G
5	L5	1931	C
5	L5	1932	A
5	L5	1936	C
5	L5	1948	G
5	L5	1951	G
5	L5	1961	G
5	L5	1962	A
5	L5	1974	U
5	L5	1975	G
5	L5	1978	C
5	L5	1980	U
5	L5	1981	G
5	L5	1982	G
5	L5	1983	A
5	L5	1984	A
5	L5	1985	G
5	L5	1986	U
5	L5	1991	A
5	L5	1993	C
5	L5	1997	U
5	L5	1998	A
5	L5	1999	A
5	L5	2001	G

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Mol	Chain	Res	Type
5	L5	2002	A
5	L5	2003	G
5	L5	2004	U
5	L5	2011	C
5	L5	2017	A
5	L5	2018	C
5	L5	2024	G
5	L5	2026	A
5	L5	2046	G
5	L5	2048	U
5	L5	2055	G
5	L5	2056	G
5	L5	2062	C
5	L5	2069	A
5	L5	2084	C
5	L5	2092	G
5	L5	2093	A
5	L5	2095	A
5	L5	2096	G
5	L5	2097	U
5	L5	2098	G
5	L5	2101	C
5	L5	2102	G
5	L5	2107	C
5	L5	2110	C
5	L5	2111	G
5	L5	2112	G
5	L5	2250	C
5	L5	2252	G
5	L5	2256	C
5	L5	2258	C
5	L5	2289	C
5	L5	2300	A
5	L5	2301	G
5	L5	2313	A
5	L5	2331	G
5	L5	2333	G
5	L5	2348	G
5	L5	2351	OMC
5	L5	2360	A
5	L5	2395	A
5	L5	2397	G

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Mol	Chain	Res	Type
5	L5	2408	U
5	L5	2417	A
5	L5	2425	U
5	L5	2453	A
5	L5	2464	C
5	L5	2465	C
5	L5	2469	C
5	L5	2471	G
5	L5	2474	G
5	L5	2475	G
5	L5	2478	C
5	L5	2479	G
5	L5	2483	G
5	L5	2484	A
5	L5	2485	U
5	L5	2486	G
5	L5	2487	G
5	L5	2488	C
5	L5	2489	C
5	L5	2490	U
5	L5	2494	U
5	L5	2504	C
5	L5	2505	C
5	L5	2506	G
5	L5	2513	A
5	L5	2519	U
5	L5	2520	C
5	L5	2529	A
5	L5	2537	A
5	L5	2544	G
5	L5	2546	G
5	L5	2547	G
5	L5	2554	U
5	L5	2555	G
5	L5	2560	C
5	L5	2565	A
5	L5	2573	A
5	L5	2583	C
5	L5	2586	G
5	L5	2587	A
5	L5	2589	C
5	L5	2601	A

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Mol	Chain	Res	Type
5	L5	2618	G
5	L5	2627	C
5	L5	2653	C
5	L5	2662	G
5	L5	2669	C
5	L5	2675	G
5	L5	2676	A
5	L5	2687	U
5	L5	2694	G
5	L5	2695	A
5	L5	2696	A
5	L5	2706	G
5	L5	2707	U
5	L5	2708	U
5	L5	2710	C
5	L5	2711	G
5	L5	2721	G
5	L5	2724	G
5	L5	2726	G
5	L5	2739	C
5	L5	2742	G
5	L5	2743	A
5	L5	2746	A
5	L5	2761	U
5	L5	2763	U
5	L5	2769	U
5	L5	2770	C
5	L5	2788	U
5	L5	2790	U
5	L5	2806	A
5	L5	2814	C
5	L5	2825	A
5	L5	2826	U
5	L5	2827	G
5	L5	2829	U
5	L5	2838	G
5	L5	2855	G
5	L5	2877	G
5	L5	2894	A
5	L5	2900	U
5	L5	2902	G
5	L5	2903	G

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Mol	Chain	Res	Type
5	L5	2904	U
5	L5	2905	C
5	L5	2907	G
5	L5	2908	U
5	L5	3588	C
5	L5	3590	G
5	L5	3591	C
5	L5	3592	G
5	L5	3594	C
5	L5	3595	U
5	L5	3596	A
5	L5	3597	G
5	L5	3604	A
5	L5	3605	C
5	L5	3626	G
5	L5	3630	A
5	L5	3635	A
5	L5	3644	U
5	L5	3646	A
5	L5	3648	A
5	L5	3662	A
5	L5	3670	C
5	L5	3673	C
5	L5	3674	G
5	L5	3691	G
5	L5	3701	OMC
5	L5	3710	G
5	L5	3711	A
5	L5	3713	U
5	L5	3727	A
5	L5	3748	A
5	L5	3753	G
5	L5	3760	A
5	L5	3764	U
5	L5	3770	U
5	L5	3774	A
5	L5	3775	A
5	L5	3776	G
5	L5	3777	G
5	L5	3785	A2M
5	L5	3786	U
5	L5	3792	OMG

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Mol	Chain	Res	Type
5	L5	3811	G
5	L5	3814	U
5	L5	3817	A
5	L5	3819	G
5	L5	3824	A
5	L5	3838	U
5	L5	3839	G
5	L5	3840	U
5	L5	3867	A2M
5	L5	3868	G
5	L5	3877	A
5	L5	3878	C
5	L5	3879	G
5	L5	3885	G
5	L5	3892	U
5	L5	3897	G
5	L5	3901	A
5	L5	3906	A
5	L5	3907	G
5	L5	3908	A
5	L5	3915	U
5	L5	3923	A
5	L5	3938	G
5	L5	3939	G
5	L5	3942	A
5	L5	3944	G
5	L5	3947	A
5	L5	3949	A
5	L5	3950	U
5	L5	3952	A
5	L5	3953	G
5	L5	4057	C
5	L5	4058	U
5	L5	4059	C
5	L5	4060	U
5	L5	4061	G
5	L5	4062	A
5	L5	4064	C
5	L5	4065	G
5	L5	4068	U
5	L5	4076	G
5	L5	4084	G

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Mol	Chain	Res	Type
5	L5	4095	G
5	L5	4097	G
5	L5	4098	A
5	L5	4099	G
5	L5	4101	C
5	L5	4104	G
5	L5	4108	G
5	L5	4111	U
5	L5	4114	C
5	L5	4115	G
5	L5	4116	C
5	L5	4117	U
5	L5	4119	C
5	L5	4122	G
5	L5	4127	A
5	L5	4141	G
5	L5	4142	C
5	L5	4143	G
5	L5	4144	C
5	L5	4146	G
5	L5	4149	C
5	L5	4150	G
5	L5	4162	C
5	L5	4163	U
5	L5	4168	G
5	L5	4170	A
5	L5	4183	G
5	L5	4184	G
5	L5	4191	G
5	L5	4203	A
5	L5	4212	A
5	L5	4222	G
5	L5	4225	G
5	L5	4228	OMG
5	L5	4229	U
5	L5	4233	A
5	L5	4251	A
5	L5	4254	G
5	L5	4257	A
5	L5	4258	C
5	L5	4265	U
5	L5	4268	A

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Mol	Chain	Res	Type
5	L5	4273	A
5	L5	4281	A
5	L5	4291	G
5	L5	4295	U
5	L5	4304	A
5	L5	4305	G
5	L5	4314	C
5	L5	4319	C
5	L5	4329	G
5	L5	4330	G
5	L5	4332	C
5	L5	4349	C
5	L5	4350	C
5	L5	4354	U
5	L5	4364	G
5	L5	4373	G
5	L5	4376	A
5	L5	4377	G
5	L5	4378	A
5	L5	4379	A
5	L5	4387	C
5	L5	4391	G
5	L5	4394	A
5	L5	4405	G
5	L5	4420	U
5	L5	4421	C
5	L5	4422	A
5	L5	4433	G
5	L5	4438	U
5	L5	4448	G
5	L5	4449	A
5	L5	4452	U
5	L5	4464	A
5	L5	4466	C
5	L5	4475	G
5	L5	4488	A
5	L5	4500	PSU
5	L5	4512	U
5	L5	4513	A
5	L5	4519	C
5	L5	4524	G
5	L5	4525	C

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Mol	Chain	Res	Type
5	L5	4545	G
5	L5	4548	A
5	L5	4557	U
5	L5	4560	C
5	L5	4567	G
5	L5	4575	G
5	L5	4584	A
5	L5	4589	A
5	L5	4590	A2M
5	L5	4600	G
5	L5	4601	U
5	L5	4617	G
5	L5	4636	PSU
5	L5	4637	OMG
5	L5	4652	G
5	L5	4656	A
5	L5	4670	C
5	L5	4672	A
5	L5	4679	G
5	L5	4693	C
5	L5	4694	G
5	L5	4695	C
5	L5	4700	A
5	L5	4708	A
5	L5	4709	U
5	L5	4719	G
5	L5	4733	C
5	L5	4734	A
5	L5	4740	G
5	L5	4741	C
5	L5	4742	G
5	L5	4745	G
5	L5	4750	G
5	L5	4754	G
5	L5	4757	C
5	L5	4759	C
5	L5	4761	G
5	L5	4765	G
5	L5	4771	C
5	L5	4772	C
5	L5	4775	C
5	L5	4859	C

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Mol	Chain	Res	Type
5	L5	4870	G
5	L5	4871	C
5	L5	4875	G
5	L5	4881	U
5	L5	4882	U
5	L5	4883	C
5	L5	4887	C
5	L5	4889	G
5	L5	4895	C
5	L5	4896	G
5	L5	4897	G
5	L5	4899	G
5	L5	4900	C
5	L5	4901	G
5	L5	4910	G
5	L5	4912	G
5	L5	4914	C
5	L5	4922	C
5	L5	4925	U
5	L5	4926	C
5	L5	4927	G
5	L5	4928	C
5	L5	4934	A
5	L5	4937	C
5	L5	4940	C
5	L5	4941	G
5	L5	4943	A
5	L5	4944	C
5	L5	4947	U
5	L5	4951	G
5	L5	4955	A
5	L5	4960	G
5	L5	4976	U
5	L5	4985	U
5	L5	4988	U
5	L5	4989	U
5	L5	4990	C
5	L5	4991	U
5	L5	5007	A
5	L5	5013	C
5	L5	5014	A
5	L5	5017	G

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Mol	Chain	Res	Type
5	L5	5022	U
5	L5	5023	C
5	L5	5024	C
5	L5	5028	G
5	L5	5030	U
5	L5	5032	C
5	L5	5034	A
5	L5	5041	G
5	L5	5047	C
5	L5	5050	C
5	L5	5054	C
5	L5	5055	G
5	L5	5061	A
5	L5	5069	U
6	L7	7	G
6	L7	22	A
6	L7	33	U
6	L7	38	U
6	L7	53	U
6	L7	54	A
6	L7	64	G
6	L7	97	G
6	L7	100	A
6	L7	110	G
6	L7	120	U
7	L8	25	G
7	L8	34	U
7	L8	35	C
7	L8	59	A
7	L8	62	A
7	L8	63	U
7	L8	80	A
7	L8	82	A
7	L8	84	A
7	L8	85	U
7	L8	87	G
7	L8	94	G
7	L8	103	A
7	L8	105	C
7	L8	111	U
7	L8	114	G
7	L8	123	U

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Mol	Chain	Res	Type
7	L8	124	U
7	L8	125	C
7	L8	126	C
7	L8	127	U
85	S2	13	C
85	S2	14	C
85	S2	25	A
85	S2	33	G
85	S2	42	A
85	S2	44	U
85	S2	45	A
85	S2	46	A
85	S2	56	G
85	S2	58	C
85	S2	59	U
85	S2	62	G
85	S2	65	C
85	S2	67	C
85	S2	68	A
85	S2	72	C
85	S2	73	C
85	S2	74	G
85	S2	75	G
85	S2	76	U
85	S2	99	A2M
85	S2	103	A
85	S2	113	G
85	S2	115	U
85	S2	130	G
85	S2	143	U
85	S2	149	A
85	S2	158	A
85	S2	160	U
85	S2	162	C
85	S2	168	C
85	S2	170	A
85	S2	175	A
85	S2	179	C
85	S2	190	G
85	S2	191	A
85	S2	196	C
85	S2	197	U

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Mol	Chain	Res	Type
85	S2	198	U
85	S2	200	G
85	S2	203	G
85	S2	204	G
85	S2	207	G
85	S2	208	G
85	S2	214	U
85	S2	291	G
85	S2	292	A
85	S2	295	C
85	S2	302	A
85	S2	306	C
85	S2	307	G
85	S2	308	G
85	S2	309	G
85	S2	311	C
85	S2	312	G
85	S2	313	A
85	S2	318	A
85	S2	319	C
85	S2	323	C
85	S2	324	C
85	S2	325	C
85	S2	326	C
85	S2	328	U
85	S2	329	G
85	S2	332	G
85	S2	339	A
85	S2	340	C
85	S2	347	G
85	S2	351	G
85	S2	360	A
85	S2	362	C
85	S2	364	A
85	S2	368	U
85	S2	370	G
85	S2	385	G
85	S2	386	C
85	S2	398	A
85	S2	407	G
85	S2	408	A
85	S2	409	C

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Mol	Chain	Res	Type
85	S2	426	A
85	S2	436	OMG
85	S2	438	G
85	S2	448	A
85	S2	449	A
85	S2	450	C
85	S2	452	G
85	S2	464	A
85	S2	465	A
85	S2	471	G
85	S2	472	C
85	S2	473	A
85	S2	474	G
85	S2	476	A
85	S2	482	G
85	S2	487	U
85	S2	488	U
85	S2	492	C
85	S2	493	A
85	S2	502	C
85	S2	516	A
85	S2	517	OMC
85	S2	531	A
85	S2	532	C
85	S2	536	A
85	S2	537	C
85	S2	540	U
85	S2	542	U
85	S2	544	G
85	S2	546	G
85	S2	547	G
85	S2	557	U
85	S2	558	G
85	S2	563	G
85	S2	564	A
85	S2	566	U
85	S2	576	A2M
85	S2	583	A
85	S2	587	A
85	S2	589	G
85	S2	590	A
85	S2	591	U

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Mol	Chain	Res	Type
85	S2	593	C
85	S2	604	A
85	S2	611	G
85	S2	614	C
85	S2	617	G
85	S2	623	G
85	S2	627	OMU
85	S2	628	A
85	S2	631	U
85	S2	643	A
85	S2	644	OMG
85	S2	655	A
85	S2	660	C
85	S2	664	A
85	S2	668	A2M
85	S2	669	A
85	S2	671	A
85	S2	672	A
85	S2	673	G
85	S2	678	U
85	S2	684	G
85	S2	688	U
85	S2	689	U
85	S2	692	G
85	S2	695	C
85	S2	696	G
85	S2	697	G
85	S2	698	G
85	S2	731	G
85	S2	732	U
85	S2	733	C
85	S2	736	C
85	S2	737	G
85	S2	738	C
85	S2	749	U
85	S2	751	G
85	S2	752	G
85	S2	753	C
85	S2	788	G
85	S2	791	C
85	S2	792	C
85	S2	798	G

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Mol	Chain	Res	Type
85	S2	799	OMU
85	S2	801	PSU
85	S2	821	G
85	S2	822	U
85	S2	823	U
85	S2	824	C
85	S2	830	A
85	S2	834	C
85	S2	835	C
85	S2	836	G
85	S2	837	A
85	S2	838	G
85	S2	839	C
85	S2	842	C
85	S2	844	U
85	S2	847	A
85	S2	867	OMG
85	S2	870	A
85	S2	874	G
85	S2	877	C
85	S2	878	G
85	S2	880	G
85	S2	888	U
85	S2	889	U
85	S2	891	G
85	S2	893	U
85	S2	896	U
85	S2	897	U
85	S2	898	U
85	S2	899	U
85	S2	900	C
85	S2	901	G
85	S2	903	A
85	S2	904	A
85	S2	913	A
85	S2	917	U
85	S2	920	A
85	S2	922	A
85	S2	933	G
85	S2	934	G
85	S2	943	U
85	S2	963	A

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Mol	Chain	Res	Type
85	S2	970	G
85	S2	971	G
85	S2	972	A
85	S2	985	G
85	S2	990	A
85	S2	992	A
85	S2	997	A
85	S2	999	G
85	S2	1008	A
85	S2	1017	U
85	S2	1023	A
85	S2	1027	A
85	S2	1060	A
85	S2	1061	U
85	S2	1062	A
85	S2	1083	A
85	S2	1085	C
85	S2	1087	A
85	S2	1109	C
85	S2	1113	A
85	S2	1114	U
85	S2	1116	C
85	S2	1121	G
85	S2	1123	C
85	S2	1133	A
85	S2	1138	C
85	S2	1148	A
85	S2	1150	A
85	S2	1153	C
85	S2	1154	U
85	S2	1170	A
85	S2	1195	A
85	S2	1207	G
85	S2	1208	A
85	S2	1215	C
85	S2	1216	C
85	S2	1217	A
85	S2	1224	G
85	S2	1227	G
85	S2	1242	U
85	S2	1243	U
85	S2	1248	B8N

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Mol	Chain	Res	Type
85	S2	1251	A
85	S2	1253	A
85	S2	1256	G
85	S2	1257	G
85	S2	1259	A
85	S2	1271	C
85	S2	1272	OMC
85	S2	1274	G
85	S2	1275	G
85	S2	1283	C
85	S2	1286	G
85	S2	1288	OMU
85	S2	1290	G
85	S2	1294	G
85	S2	1295	A
85	S2	1301	A
85	S2	1302	G
85	S2	1303	C
85	S2	1308	U
85	S2	1342	U
85	S2	1357	A
85	S2	1358	U
85	S2	1371	U
85	S2	1372	U
85	S2	1373	C
85	S2	1376	A
85	S2	1378	A
85	S2	1402	A
85	S2	1406	G
85	S2	1413	G
85	S2	1418	C
85	S2	1419	C
85	S2	1420	G
85	S2	1421	A
85	S2	1422	G
85	S2	1423	C
85	S2	1433	C
85	S2	1435	C
85	S2	1436	C
85	S2	1437	C
85	S2	1438	A
85	S2	1439	A

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Mol	Chain	Res	Type
85	S2	1442	OMU
85	S2	1449	G
85	S2	1454	A
85	S2	1463	U
85	S2	1466	G
85	S2	1478	U
85	S2	1479	G
85	S2	1487	A
85	S2	1489	A
85	S2	1490	OMG
85	S2	1492	U
85	S2	1494	U
85	S2	1495	G
85	S2	1497	G
85	S2	1498	A
85	S2	1521	C
85	S2	1522	A
85	S2	1531	A
85	S2	1533	A
85	S2	1534	C
85	S2	1544	C
85	S2	1552	G
85	S2	1553	C
85	S2	1556	A
85	S2	1558	C
85	S2	1560	U
85	S2	1573	G
85	S2	1574	C
85	S2	1575	G
85	S2	1578	U
85	S2	1580	A
85	S2	1581	C
85	S2	1587	G
85	S2	1588	A
85	S2	1600	G
85	S2	1604	G
85	S2	1606	G
85	S2	1621	U
85	S2	1623	A
85	S2	1631	U
85	S2	1633	A
85	S2	1634	A

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Mol	Chain	Res	Type
85	S2	1637	A
85	S2	1648	G
85	S2	1654	G
85	S2	1663	A
85	S2	1665	G
85	S2	1686	G
85	S2	1695	A
85	S2	1698	C
85	S2	1699	A
85	S2	1715	A
85	S2	1721	U
85	S2	1722	G
85	S2	1744	G
85	S2	1745	A
85	S2	1752	C
85	S2	1753	C
85	S2	1754	G
85	S2	1755	C
85	S2	1757	G
85	S2	1759	G
85	S2	1761	U
85	S2	1772	C
85	S2	1773	C
85	S2	1774	C
85	S2	1777	G
85	S2	1782	G
85	S2	1783	C
85	S2	1784	G
85	S2	1786	U
85	S2	1798	C
85	S2	1809	A
85	S2	1810	U
85	S2	1821	U
85	S2	1825	A
85	S2	1826	G
85	S2	1829	G
85	S2	1831	A
85	S2	1835	A
85	S2	1838	U
85	S2	1849	G
85	S2	1851	MA6
85	S2	1861	G

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Mol	Chain	Res	Type
85	S2	1862	G
85	S2	1863	A
85	S2	1864	U
85	S2	1865	C

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L5	406	C
5	L5	493	G
5	L5	914	U
5	L5	1082	C
5	L5	1590	C
5	L5	1633	G
5	L5	1703	C
5	L5	1977	C
5	L5	2416	G
5	L5	2485	U
5	L5	2675	G
5	L5	2760	G
5	L5	3673	C
5	L5	4600	G
5	L5	4699	U
5	L5	4913	G
85	S2	291	G
85	S2	563	G
85	S2	688	U
85	S2	1477	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
5	OMC	L5	1340	5	19,22,23	0.59	0	25,31,34	0.83	0
85	A2M	S2	1031	85	22,25,26	1.15	1 (4%)	30,36,39	1.58	7 (23%)
85	PSU	S2	1177	85	18,21,22	1.06	1 (5%)	21,30,33	1.82	4 (19%)
5	PSU	L5	4579	5	18,21,22	1.04	1 (5%)	21,30,33	1.86	4 (19%)
5	PSU	L5	3920	5,86	18,21,22	1.05	1 (5%)	21,30,33	1.85	4 (19%)
5	PSU	L5	1536	5	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
5	PSU	L5	4521	5,86	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
5	OMG	L5	3627	5	23,26,27	0.49	0	32,38,41	0.60	0
5	PSU	L5	4973	5	18,21,22	1.10	1 (5%)	21,30,33	1.94	4 (19%)
85	OMU	S2	1288	85	19,22,23	3.39	7 (36%)	25,31,34	1.75	5 (20%)
5	PSU	L5	1744	5,86	18,21,22	1.08	1 (5%)	21,30,33	1.90	4 (19%)
5	OMG	L5	4499	5	23,26,27	0.49	0	32,38,41	0.47	0
85	PSU	S2	93	85	18,21,22	1.09	1 (5%)	21,30,33	1.78	4 (19%)
5	OMU	L5	4306	5	19,22,23	3.31	7 (36%)	25,31,34	1.82	4 (16%)
85	4AC	S2	1337	85	21,24,25	0.38	0	28,34,37	0.71	1 (3%)
5	OMC	L5	2824	5	19,22,23	0.55	0	25,31,34	0.63	0
85	OMG	S2	683	85	23,26,27	0.48	0	32,38,41	0.50	0
85	PSU	S2	651	85	18,21,22	1.10	1 (5%)	21,30,33	1.92	4 (19%)
85	OMG	S2	436	85	23,26,27	0.47	0	32,38,41	0.53	0
5	A2M	L5	398	5	22,25,26	1.15	1 (4%)	30,36,39	1.60	7 (23%)
5	A2M	L5	4523	5,86	22,25,26	1.21	2 (9%)	30,36,39	1.61	8 (26%)
5	PSU	L5	3695	5	18,21,22	1.07	1 (5%)	21,30,33	1.90	5 (23%)
5	PSU	L5	4500	5	18,21,22	1.11	1 (5%)	21,30,33	1.99	5 (23%)
5	PSU	L5	4972	5	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
5	PSU	L5	4471	5	18,21,22	1.05	1 (5%)	21,30,33	1.87	4 (19%)
5	OMG	L5	4228	5	23,26,27	0.49	0	32,38,41	0.62	0
5	A2M	L5	3867	5	22,25,26	1.14	1 (4%)	30,36,39	1.46	8 (26%)
5	UR3	L5	4530	5	19,22,23	2.72	7 (36%)	26,32,35	1.60	3 (11%)
85	OMU	S2	1326	85	19,22,23	3.39	7 (36%)	25,31,34	1.83	5 (20%)
5	PSU	L5	2632	5	18,21,22	1.06	1 (5%)	21,30,33	1.82	4 (19%)
85	OMC	S2	1391	85	19,22,23	0.52	0	25,31,34	0.68	0
85	OMU	S2	116	85	19,22,23	3.36	7 (36%)	25,31,34	1.77	4 (16%)
5	PSU	L5	2839	5	18,21,22	1.04	1 (5%)	21,30,33	1.82	4 (19%)
85	6MZ	S2	1832	85,86	26,26,26	2.82	5 (19%)	36,39,39	2.06	9 (25%)
5	OMC	L5	3701	5	19,22,23	0.68	0	25,31,34	1.68	4 (16%)
5	OMC	L5	3887	5	19,22,23	0.57	0	25,31,34	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PSU	L5	1782	5	18,21,22	1.07	1 (5%)	21,30,33	1.83	4 (19%)
5	UY1	L5	3818	5	19,22,23	4.90	9 (47%)	21,31,34	1.92	5 (23%)
5	PSU	L5	4552	5	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
85	PSU	S2	406	85	18,21,22	1.11	1 (5%)	21,30,33	1.98	5 (23%)
5	PSU	L5	1860	5	18,21,22	1.03	1 (5%)	21,30,33	1.85	4 (19%)
85	A2M	S2	576	85	22,25,26	1.19	1 (4%)	30,36,39	1.53	7 (23%)
5	OMC	L5	2861	5	19,22,23	0.56	0	25,31,34	0.80	1 (4%)
5	PSU	L5	4689	5	18,21,22	1.06	1 (5%)	21,30,33	1.97	4 (19%)
5	PSU	L5	1677	5	18,21,22	1.06	1 (5%)	21,30,33	1.87	3 (14%)
5	A2M	L5	1323	5	22,25,26	1.16	2 (9%)	30,36,39	1.58	9 (30%)
5	PSU	L5	1582	5	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
5	A2M	L5	3785	5,86	22,25,26	1.08	1 (4%)	30,36,39	1.61	9 (30%)
5	OMC	L5	3869	5	19,22,23	0.60	0	25,31,34	0.70	0
7	OMG	L8	75	7	23,26,27	0.48	0	32,38,41	0.51	0
5	PSU	L5	3884	5	18,21,22	1.07	1 (5%)	21,30,33	1.89	4 (19%)
5	PSU	L5	1862	5	18,21,22	1.05	1 (5%)	21,30,33	1.91	4 (19%)
5	OMC	L5	2351	5,86	19,22,23	0.62	0	25,31,34	1.18	2 (8%)
5	6MZ	L5	4220	5	22,25,26	3.98	11 (50%)	29,36,39	2.37	11 (37%)
5	OMG	L5	2424	5	23,26,27	0.51	0	32,38,41	0.45	0
5	OMC	L5	2804	5	19,22,23	0.61	0	25,31,34	0.88	1 (4%)
85	PSU	S2	109	85	18,21,22	1.06	1 (5%)	21,30,33	1.92	4 (19%)
5	A2M	L5	2815	5	22,25,26	1.16	1 (4%)	30,36,39	1.50	8 (26%)
85	PSU	S2	105	85	18,21,22	1.07	1 (5%)	21,30,33	1.84	4 (19%)
85	OMU	S2	799	85	19,22,23	3.39	7 (36%)	25,31,34	1.81	5 (20%)
85	PSU	S2	801	85	18,21,22	1.11	1 (5%)	21,30,33	1.86	4 (19%)
85	OMG	S2	867	85	23,26,27	0.50	0	32,38,41	0.46	0
85	A2M	S2	1383	85	22,25,26	1.17	1 (4%)	30,36,39	1.61	5 (16%)
5	OMG	L5	4494	5	23,26,27	0.51	0	32,38,41	0.54	0
5	A2M	L5	400	5	22,25,26	1.18	1 (4%)	30,36,39	1.59	9 (30%)
85	A2M	S2	159	85	22,25,26	1.20	1 (4%)	30,36,39	1.52	9 (30%)
85	OMG	S2	509	85	23,26,27	0.48	0	32,38,41	0.51	0
85	PSU	S2	686	85	18,21,22	1.08	1 (5%)	21,30,33	1.85	4 (19%)
5	A2M	L5	4590	5	22,25,26	1.16	1 (4%)	30,36,39	1.53	6 (20%)
85	PSU	S2	1232	85	18,21,22	1.09	1 (5%)	21,30,33	1.85	4 (19%)
85	PSU	S2	866	85	18,21,22	1.09	1 (5%)	21,30,33	1.81	5 (23%)
5	PSU	L5	5001	5	18,21,22	1.08	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
5	PSU	L5	3853	5,86	18,21,22	1.04	1 (5%)	21,30,33	1.81	4 (19%)
85	A2M	S2	166	85	22,25,26	1.28	2 (9%)	30,36,39	1.53	7 (23%)
5	PSU	L5	4353	5	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
85	OMU	S2	121	85	19,22,23	3.34	7 (36%)	25,31,34	1.85	5 (20%)
85	OMU	S2	1442	85	19,22,23	3.40	7 (36%)	25,31,34	1.82	5 (20%)
85	PSU	S2	814	85	18,21,22	1.09	1 (5%)	21,30,33	1.79	4 (19%)
5	A2M	L5	4571	5	22,25,26	1.20	1 (4%)	30,36,39	1.54	7 (23%)
85	OMG	S2	644	85	23,26,27	0.46	0	32,38,41	0.48	0
85	PSU	S2	681	85	18,21,22	1.06	1 (5%)	21,30,33	1.83	4 (19%)
5	OMG	L5	4392	5	23,26,27	0.51	0	32,38,41	0.46	0
85	OMU	S2	627	85	19,22,23	3.41	7 (36%)	25,31,34	1.82	4 (16%)
5	OMC	L5	2422	5,86	19,22,23	0.58	0	25,31,34	0.69	0
5	OMC	L5	4536	5	19,22,23	0.59	0	25,31,34	0.69	0
5	PSU	L5	4673	5,86	18,21,22	1.05	1 (5%)	21,30,33	1.82	4 (19%)
85	OMC	S2	1703	85	19,22,23	0.55	0	25,31,34	0.60	0
85	OMC	S2	517	85	19,22,23	0.53	0	25,31,34	0.64	0
5	PSU	L5	1781	5	18,21,22	1.05	1 (5%)	21,30,33	1.78	4 (19%)
5	PSU	L5	4457	5	18,21,22	1.04	1 (5%)	21,30,33	1.96	5 (23%)
85	PSU	S2	1056	85	18,21,22	1.08	1 (5%)	21,30,33	1.91	4 (19%)
5	A2M	L5	3718	5	22,25,26	1.11	1 (4%)	30,36,39	1.51	5 (16%)
5	OMG	L5	2876	5	23,26,27	0.51	0	32,38,41	0.55	0
5	A2M	L5	3830	5	22,25,26	1.13	1 (4%)	30,36,39	1.58	7 (23%)
85	PSU	S2	1004	85	18,21,22	1.13	1 (5%)	21,30,33	1.86	4 (19%)
85	PSU	S2	1367	85	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
5	A2M	L5	2401	5	22,25,26	1.16	1 (4%)	30,36,39	1.59	6 (20%)
5	PSU	L5	4442	5	18,21,22	1.08	1 (5%)	21,30,33	1.90	5 (23%)
85	OMU	S2	354	85	19,22,23	3.33	7 (36%)	25,31,34	1.88	5 (20%)
85	A2M	S2	27	85	22,25,26	1.19	1 (4%)	30,36,39	1.52	7 (23%)
85	PSU	S2	863	85	18,21,22	1.11	1 (5%)	21,30,33	1.85	4 (19%)
5	OMU	L5	2837	5	19,22,23	3.36	7 (36%)	25,31,34	1.86	4 (16%)
5	OMG	L5	1316	5	23,26,27	0.52	0	32,38,41	0.57	0
5	OMU	L5	4227	5	19,22,23	3.35	7 (36%)	25,31,34	1.82	5 (20%)
85	PSU	S2	1174	85	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
85	PSU	S2	1244	85	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
5	PSU	L5	4431	5	18,21,22	1.04	1 (5%)	21,30,33	1.87	4 (19%)
85	PSU	S2	1045	85	18,21,22	1.06	1 (5%)	21,30,33	1.87	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OMG	L5	3744	5	23,26,27	0.49	0	32,38,41	0.47	0
85	PSU	S2	1046	85	18,21,22	1.12	1 (5%)	21,30,33	1.83	4 (19%)
85	OMC	S2	174	85	19,22,23	0.53	0	25,31,34	0.65	0
85	OMU	S2	172	85	19,22,23	3.37	7 (36%)	25,31,34	1.81	5 (20%)
5	A2M	L5	2787	5	22,25,26	1.15	1 (4%)	30,36,39	1.50	8 (26%)
85	OMG	S2	1490	85	23,26,27	0.50	0	32,38,41	0.46	0
5	PSU	L5	3637	5	18,21,22	1.06	1 (5%)	21,30,33	2.02	5 (23%)
5	OMG	L5	4618	5	23,26,27	0.50	0	32,38,41	0.53	0
85	PSU	S2	649	85	18,21,22	1.08	1 (5%)	21,30,33	1.93	3 (14%)
5	PSU	L5	5010	5	18,21,22	1.08	1 (5%)	21,30,33	1.85	4 (19%)
85	OMG	S2	601	85	23,26,27	0.47	0	32,38,41	0.44	0
7	PSU	L8	69	7	18,21,22	1.08	1 (5%)	21,30,33	1.82	5 (23%)
5	OMG	L5	4623	5	23,26,27	0.52	0	32,38,41	0.58	0
85	B8N	S2	1248	85	25,29,30	3.28	6 (24%)	28,42,45	2.03	7 (25%)
5	1MA	L5	1322	5,86	21,25,26	0.55	0	30,37,40	0.78	1 (3%)
5	PSU	L5	4299	5	18,21,22	1.01	1 (5%)	21,30,33	1.81	4 (19%)
5	OMU	L5	4498	5	19,22,23	3.34	7 (36%)	25,31,34	1.86	5 (20%)
5	PSU	L5	4532	5	18,21,22	1.10	1 (5%)	21,30,33	1.85	4 (19%)
7	PSU	L8	55	7	18,21,22	1.05	1 (5%)	21,30,33	1.89	4 (19%)
5	PSU	L5	1792	5	18,21,22	1.02	1 (5%)	21,30,33	1.89	3 (14%)
5	5MC	L5	3782	5,86	19,22,23	0.60	0	26,32,35	0.71	0
5	OMG	L5	3899	5	23,26,27	0.54	0	32,38,41	0.51	0
5	PSU	L5	3822	5	18,21,22	1.06	1 (5%)	21,30,33	1.82	5 (23%)
5	A2M	L5	1871	5,86	22,25,26	1.17	1 (4%)	30,36,39	1.63	6 (20%)
5	A2M	L5	1326	5	22,25,26	1.14	1 (4%)	30,36,39	1.47	9 (30%)
5	PSU	L5	4361	5	18,21,22	1.01	1 (5%)	21,30,33	1.80	3 (14%)
85	OMG	S2	1328	85	23,26,27	0.46	0	32,38,41	0.45	0
5	A2M	L5	2363	5,86	22,25,26	1.15	2 (9%)	30,36,39	1.57	8 (26%)
5	PSU	L5	1683	5	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
85	G7M	S2	1639	85,2	23,26,27	2.66	8 (34%)	34,39,42	2.63	11 (32%)
5	OMG	L5	1522	5	23,26,27	0.52	0	32,38,41	0.57	0
3	SEP	CF	163	3	8,9,10	1.61	1 (12%)	7,12,14	1.30	1 (14%)
5	OMU	L5	4620	5	19,22,23	3.24	7 (36%)	25,31,34	1.75	5 (20%)
5	PSU	L5	4296	5	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
5	OMG	L5	4637	5	23,26,27	0.50	0	32,38,41	0.48	0
85	OMU	S2	428	85	19,22,23	3.35	7 (36%)	25,31,34	1.85	5 (20%)
85	A2M	S2	484	85	22,25,26	1.17	1 (4%)	30,36,39	1.47	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OMG	L5	1625	5	23,26,27	0.50	0	32,38,41	0.45	0
5	PSU	L5	4293	5	18,21,22	1.12	1 (5%)	21,30,33	1.96	4 (19%)
85	A2M	S2	668	85,86	22,25,26	1.29	2 (9%)	30,36,39	1.61	8 (26%)
5	PSU	L5	4312	5	18,21,22	1.06	1 (5%)	21,30,33	1.90	4 (19%)
85	OMC	S2	462	85	19,22,23	0.54	0	25,31,34	0.71	0
85	A2M	S2	99	85,86	22,25,26	1.16	1 (4%)	30,36,39	1.57	8 (26%)
5	OMU	L5	3925	5	19,22,23	3.32	7 (36%)	25,31,34	1.90	5 (20%)
5	PSU	L5	4403	5	18,21,22	1.04	1 (5%)	21,30,33	1.95	4 (19%)
85	MA6	S2	1851	85	23,26,27	1.28	2 (8%)	33,38,41	3.42	13 (39%)
85	OMC	S2	1272	85	19,22,23	0.57	0	25,31,34	1.10	2 (8%)
85	PSU	S2	966	85,86	18,21,22	1.09	1 (5%)	21,30,33	1.92	4 (19%)
85	MA6	S2	1850	85	23,26,27	1.27	2 (8%)	33,38,41	3.34	13 (39%)
5	PSU	L5	3844	5	18,21,22	1.12	1 (5%)	21,30,33	1.84	4 (19%)
5	OMC	L5	4456	5	19,22,23	0.64	0	25,31,34	0.84	1 (4%)
85	PSU	S2	1081	85	18,21,22	1.04	1 (5%)	21,30,33	1.82	5 (23%)
5	OMC	L5	3841	5	19,22,23	0.56	0	25,31,34	0.69	1 (4%)
5	5MC	L5	4447	5	19,22,23	0.76	0	26,32,35	0.65	0
5	OMC	L5	3808	5	19,22,23	0.64	0	25,31,34	0.78	1 (4%)
5	PSU	L5	3639	5	18,21,22	1.08	1 (5%)	21,30,33	1.85	4 (19%)
5	OMG	L5	4370	5	23,26,27	0.48	0	32,38,41	0.49	0
5	PSU	L5	4628	5	18,21,22	1.00	1 (5%)	21,30,33	1.82	4 (19%)
5	PSU	L5	4493	5	18,21,22	1.05	1 (5%)	21,30,33	1.86	3 (14%)
85	4AC	S2	1842	85	21,24,25	0.37	0	28,34,37	0.48	0
5	PSU	L5	3851	5	18,21,22	1.02	1 (5%)	21,30,33	1.86	3 (14%)
5	PSU	L5	4576	5	18,21,22	1.08	1 (5%)	21,30,33	1.85	5 (23%)
5	OMG	L5	4196	5,2	23,26,27	0.49	0	32,38,41	0.45	0
5	OMG	L5	2364	5	23,26,27	0.50	0	32,38,41	0.45	0
85	A2M	S2	468	85	22,25,26	1.18	1 (4%)	30,36,39	1.57	6 (20%)
5	PSU	L5	4636	5	18,21,22	1.10	1 (5%)	21,30,33	2.05	6 (28%)
5	OMG	L5	3792	5	23,26,27	0.49	0	32,38,41	0.53	0
5	A2M	L5	1534	5,86	22,25,26	1.16	2 (9%)	30,36,39	1.52	9 (30%)
5	OMC	L5	2365	5	19,22,23	0.57	0	25,31,34	0.60	0
5	A2M	L5	1524	5	22,25,26	1.22	2 (9%)	30,36,39	1.52	6 (20%)
5	A2M	L5	3825	5	22,25,26	1.13	1 (4%)	30,36,39	1.54	7 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
 '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OMC	L5	1340	5	-	1/9/27/28	0/2/2/2
85	A2M	S2	1031	85	-	0/9/27/28	0/3/3/3
85	PSU	S2	1177	85	-	0/7/25/26	0/2/2/2
5	PSU	L5	4579	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	3920	5,86	-	0/7/25/26	0/2/2/2
5	PSU	L5	1536	5	-	2/7/25/26	0/2/2/2
5	PSU	L5	4521	5,86	-	0/7/25/26	0/2/2/2
5	OMG	L5	3627	5	-	0/9/27/28	0/3/3/3
5	PSU	L5	4973	5	-	0/7/25/26	0/2/2/2
85	OMU	S2	1288	85	-	2/9/27/28	0/2/2/2
5	PSU	L5	1744	5,86	-	0/7/25/26	0/2/2/2
5	OMG	L5	4499	5	-	1/9/27/28	0/3/3/3
85	PSU	S2	93	85	-	0/7/25/26	0/2/2/2
5	OMU	L5	4306	5	-	0/9/27/28	0/2/2/2
85	4AC	S2	1337	85	-	1/11/29/30	0/2/2/2
5	OMC	L5	2824	5	-	1/9/27/28	0/2/2/2
85	OMG	S2	683	85	-	0/9/27/28	0/3/3/3
85	PSU	S2	651	85	-	0/7/25/26	0/2/2/2
85	OMG	S2	436	85	-	2/9/27/28	0/3/3/3
5	A2M	L5	398	5	-	1/9/27/28	0/3/3/3
5	A2M	L5	4523	5,86	-	0/9/27/28	0/3/3/3
5	PSU	L5	3695	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4500	5	-	3/7/25/26	0/2/2/2
5	PSU	L5	4972	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4471	5	-	1/7/25/26	0/2/2/2
5	OMG	L5	4228	5	-	2/9/27/28	0/3/3/3
5	A2M	L5	3867	5	-	3/9/27/28	0/3/3/3
5	UR3	L5	4530	5	-	0/7/25/26	0/2/2/2
85	OMU	S2	1326	85	-	0/9/27/28	0/2/2/2
5	PSU	L5	2632	5	-	0/7/25/26	0/2/2/2
85	OMC	S2	1391	85	-	0/9/27/28	0/2/2/2
85	OMU	S2	116	85	-	0/9/27/28	0/2/2/2
5	PSU	L5	2839	5	-	0/7/25/26	0/2/2/2
85	6MZ	S2	1832	85,86	-	4/12/28/28	0/3/3/3
5	OMC	L5	3701	5	-	6/9/27/28	0/2/2/2
5	OMC	L5	3887	5	-	1/9/27/28	0/2/2/2
5	PSU	L5	1782	5	-	0/7/25/26	0/2/2/2
5	UY1	L5	3818	5	-	2/9/27/28	0/2/2/2
5	PSU	L5	4552	5	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	PSU	S2	406	85	-	0/7/25/26	0/2/2/2
5	PSU	L5	1860	5	-	0/7/25/26	0/2/2/2
85	A2M	S2	576	85	-	4/9/27/28	0/3/3/3
5	OMC	L5	2861	5	-	1/9/27/28	0/2/2/2
5	PSU	L5	4689	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	1677	5	-	3/7/25/26	0/2/2/2
5	A2M	L5	1323	5	-	2/9/27/28	0/3/3/3
5	PSU	L5	1582	5	-	0/7/25/26	0/2/2/2
5	A2M	L5	3785	5,86	-	3/9/27/28	0/3/3/3
5	OMC	L5	3869	5	-	1/9/27/28	0/2/2/2
7	OMG	L8	75	7	-	1/9/27/28	0/3/3/3
5	PSU	L5	3884	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	1862	5	-	0/7/25/26	0/2/2/2
5	OMC	L5	2351	5,86	-	3/9/27/28	0/2/2/2
5	6MZ	L5	4220	5	-	0/9/27/28	0/3/3/3
5	OMG	L5	2424	5	-	0/9/27/28	0/3/3/3
5	OMC	L5	2804	5	-	0/9/27/28	0/2/2/2
85	PSU	S2	109	85	-	0/7/25/26	0/2/2/2
5	A2M	L5	2815	5	-	2/9/27/28	0/3/3/3
85	PSU	S2	105	85	-	0/7/25/26	0/2/2/2
85	OMU	S2	799	85	-	2/9/27/28	0/2/2/2
85	PSU	S2	801	85	-	2/7/25/26	0/2/2/2
85	OMG	S2	867	85	-	2/9/27/28	0/3/3/3
85	A2M	S2	1383	85	-	3/9/27/28	0/3/3/3
5	OMG	L5	4494	5	-	0/9/27/28	0/3/3/3
5	A2M	L5	400	5	-	1/9/27/28	0/3/3/3
85	A2M	S2	159	85	-	1/9/27/28	0/3/3/3
85	OMG	S2	509	85	-	0/9/27/28	0/3/3/3
85	PSU	S2	686	85	-	0/7/25/26	0/2/2/2
5	A2M	L5	4590	5	-	3/9/27/28	0/3/3/3
85	PSU	S2	1232	85	-	0/7/25/26	0/2/2/2
85	PSU	S2	866	85	-	0/7/25/26	0/2/2/2
5	PSU	L5	5001	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	3853	5,86	-	0/7/25/26	0/2/2/2
85	A2M	S2	166	85	-	0/9/27/28	0/3/3/3
5	PSU	L5	4353	5	-	0/7/25/26	0/2/2/2
85	OMU	S2	121	85	-	0/9/27/28	0/2/2/2
85	OMU	S2	1442	85	-	2/9/27/28	0/2/2/2
85	PSU	S2	814	85	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A2M	L5	4571	5	-	0/9/27/28	0/3/3/3
85	OMG	S2	644	85	-	4/9/27/28	0/3/3/3
85	PSU	S2	681	85	-	0/7/25/26	0/2/2/2
5	OMG	L5	4392	5	-	0/9/27/28	0/3/3/3
85	OMU	S2	627	85	-	4/9/27/28	0/2/2/2
5	OMC	L5	2422	5,86	-	2/9/27/28	0/2/2/2
5	OMC	L5	4536	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	4673	5,86	-	0/7/25/26	0/2/2/2
85	OMC	S2	1703	85	-	1/9/27/28	0/2/2/2
85	OMC	S2	517	85	-	2/9/27/28	0/2/2/2
5	PSU	L5	1781	5	-	1/7/25/26	0/2/2/2
5	PSU	L5	4457	5	-	0/7/25/26	0/2/2/2
85	PSU	S2	1056	85	-	0/7/25/26	0/2/2/2
5	A2M	L5	3718	5	-	1/9/27/28	0/3/3/3
5	OMG	L5	2876	5	-	1/9/27/28	0/3/3/3
5	A2M	L5	3830	5	-	0/9/27/28	0/3/3/3
85	PSU	S2	1004	85	-	0/7/25/26	0/2/2/2
85	PSU	S2	1367	85	-	0/7/25/26	0/2/2/2
5	A2M	L5	2401	5	-	2/9/27/28	0/3/3/3
5	PSU	L5	4442	5	-	0/7/25/26	0/2/2/2
85	OMU	S2	354	85	-	0/9/27/28	0/2/2/2
85	A2M	S2	27	85	-	1/9/27/28	0/3/3/3
85	PSU	S2	863	85	-	0/7/25/26	0/2/2/2
5	OMU	L5	2837	5	-	0/9/27/28	0/2/2/2
5	OMG	L5	1316	5	-	0/9/27/28	0/3/3/3
5	OMU	L5	4227	5	-	0/9/27/28	0/2/2/2
85	PSU	S2	1174	85	-	0/7/25/26	0/2/2/2
85	PSU	S2	1244	85	-	0/7/25/26	0/2/2/2
5	PSU	L5	4431	5	-	0/7/25/26	0/2/2/2
85	PSU	S2	1045	85	-	2/7/25/26	0/2/2/2
5	OMG	L5	3744	5	-	0/9/27/28	0/3/3/3
85	PSU	S2	1046	85	-	0/7/25/26	0/2/2/2
85	OMC	S2	174	85	-	1/9/27/28	0/2/2/2
85	OMU	S2	172	85	-	0/9/27/28	0/2/2/2
5	A2M	L5	2787	5	-	6/9/27/28	0/3/3/3
85	OMG	S2	1490	85	-	1/9/27/28	0/3/3/3
5	PSU	L5	3637	5	-	0/7/25/26	0/2/2/2
5	OMG	L5	4618	5	-	2/9/27/28	0/3/3/3
85	PSU	S2	649	85	-	0/7/25/26	0/2/2/2
5	PSU	L5	5010	5	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	OMG	S2	601	85	-	1/9/27/28	0/3/3/3
7	PSU	L8	69	7	-	0/7/25/26	0/2/2/2
5	OMG	L5	4623	5	-	0/9/27/28	0/3/3/3
85	B8N	S2	1248	85	-	5/16/34/35	0/2/2/2
5	1MA	L5	1322	5,86	-	2/7/25/26	0/3/3/3
5	PSU	L5	4299	5	-	0/7/25/26	0/2/2/2
5	OMU	L5	4498	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	4532	5	-	0/7/25/26	0/2/2/2
7	PSU	L8	55	7	-	0/7/25/26	0/2/2/2
5	PSU	L5	1792	5	-	0/7/25/26	0/2/2/2
5	5MC	L5	3782	5,86	-	1/7/25/26	0/2/2/2
5	OMG	L5	3899	5	-	2/9/27/28	0/3/3/3
5	PSU	L5	3822	5	-	0/7/25/26	0/2/2/2
5	A2M	L5	1871	5,86	-	0/9/27/28	0/3/3/3
5	A2M	L5	1326	5	-	3/9/27/28	0/3/3/3
5	PSU	L5	4361	5	-	0/7/25/26	0/2/2/2
85	OMG	S2	1328	85	-	1/9/27/28	0/3/3/3
5	A2M	L5	2363	5,86	-	0/9/27/28	0/3/3/3
5	PSU	L5	1683	5	-	0/7/25/26	0/2/2/2
85	G7M	S2	1639	85,2	-	0/7/25/26	0/3/3/3
5	OMG	L5	1522	5	-	0/9/27/28	0/3/3/3
3	SEP	CF	163	3	-	6/6/8/10	-
5	OMU	L5	4620	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	4296	5	-	2/7/25/26	0/2/2/2
5	OMG	L5	4637	5	-	3/9/27/28	0/3/3/3
85	OMU	S2	428	85	-	6/9/27/28	0/2/2/2
85	A2M	S2	484	85	-	0/9/27/28	0/3/3/3
5	OMG	L5	1625	5	-	2/9/27/28	0/3/3/3
5	PSU	L5	4293	5	-	0/7/25/26	0/2/2/2
85	A2M	S2	668	85,86	-	2/9/27/28	0/3/3/3
5	PSU	L5	4312	5	-	0/7/25/26	0/2/2/2
85	OMC	S2	462	85	-	0/9/27/28	0/2/2/2
85	A2M	S2	99	85,86	-	3/9/27/28	0/3/3/3
5	OMU	L5	3925	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	4403	5	-	0/7/25/26	0/2/2/2
85	MA6	S2	1851	85	-	1/11/29/30	0/3/3/3
85	OMC	S2	1272	85	-	5/9/27/28	0/2/2/2
85	PSU	S2	966	85,86	-	0/7/25/26	0/2/2/2
85	MA6	S2	1850	85	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	L5	3844	5	-	1/7/25/26	0/2/2/2
5	OMC	L5	4456	5	-	0/9/27/28	0/2/2/2
85	PSU	S2	1081	85	-	1/7/25/26	0/2/2/2
5	OMC	L5	3841	5	-	1/9/27/28	0/2/2/2
5	5MC	L5	4447	5	-	4/7/25/26	0/2/2/2
5	OMC	L5	3808	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	3639	5	-	0/7/25/26	0/2/2/2
5	OMG	L5	4370	5	-	1/9/27/28	0/3/3/3
5	PSU	L5	4628	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4493	5	-	0/7/25/26	0/2/2/2
85	4AC	S2	1842	85	-	0/11/29/30	0/2/2/2
5	PSU	L5	3851	5	-	1/7/25/26	0/2/2/2
5	PSU	L5	4576	5	-	0/7/25/26	0/2/2/2
5	OMG	L5	4196	5,2	-	1/9/27/28	0/3/3/3
5	OMG	L5	2364	5	-	1/9/27/28	0/3/3/3
85	A2M	S2	468	85	-	0/9/27/28	0/3/3/3
5	PSU	L5	4636	5	-	1/7/25/26	0/2/2/2
5	OMG	L5	3792	5	-	2/9/27/28	0/3/3/3
5	A2M	L5	1534	5,86	-	1/9/27/28	0/3/3/3
5	OMC	L5	2365	5	-	0/9/27/28	0/2/2/2
5	A2M	L5	1524	5	-	2/9/27/28	0/3/3/3
5	A2M	L5	3825	5	-	0/9/27/28	0/3/3/3

All (271) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L5	3818	UY1	C6-C5	12.73	1.49	1.35
85	S2	1832	6MZ	C6-N6	12.64	1.48	1.34
5	L5	4220	6MZ	C6-N6	12.38	1.48	1.34
5	L5	3818	UY1	C2-N1	11.79	1.52	1.36
85	S2	1442	OMU	C2-N1	8.47	1.51	1.38
85	S2	799	OMU	C2-N1	8.45	1.51	1.38
85	S2	627	OMU	C2-N1	8.41	1.51	1.38
5	L5	2837	OMU	C2-N1	8.34	1.51	1.38
85	S2	1288	OMU	C2-N1	8.33	1.51	1.38
85	S2	172	OMU	C2-N1	8.31	1.51	1.38
5	L5	4220	6MZ	C3'-C2'	-8.31	1.30	1.53
5	L5	3925	OMU	C2-N1	8.29	1.51	1.38
85	S2	116	OMU	C2-N1	8.29	1.51	1.38
85	S2	1326	OMU	C2-N1	8.29	1.51	1.38
5	L5	4227	OMU	C2-N1	8.28	1.51	1.38
5	L5	4498	OMU	C2-N1	8.25	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L5	4306	OMU	C2-N1	8.20	1.51	1.38
85	S2	428	OMU	C2-N1	8.19	1.51	1.38
85	S2	121	OMU	C2-N1	8.16	1.51	1.38
85	S2	354	OMU	C2-N1	8.09	1.51	1.38
5	L5	4620	OMU	C2-N1	7.90	1.50	1.38
85	S2	1248	B8N	C6-N1	7.84	1.55	1.36
85	S2	1248	B8N	C4-N3	-7.84	1.26	1.40
5	L5	3818	UY1	C2-N3	7.78	1.50	1.37
85	S2	1248	B8N	C4-C5	7.11	1.63	1.47
85	S2	627	OMU	C2-N3	7.00	1.50	1.38
85	S2	1326	OMU	C2-N3	7.00	1.50	1.38
85	S2	1442	OMU	C2-N3	7.00	1.50	1.38
85	S2	172	OMU	C2-N3	6.97	1.50	1.38
85	S2	428	OMU	C2-N3	6.92	1.50	1.38
85	S2	116	OMU	C2-N3	6.91	1.50	1.38
85	S2	799	OMU	C2-N3	6.90	1.50	1.38
85	S2	1288	OMU	C2-N3	6.89	1.50	1.38
85	S2	354	OMU	C2-N3	6.86	1.49	1.38
5	L5	4227	OMU	C2-N3	6.85	1.49	1.38
85	S2	121	OMU	C2-N3	6.84	1.49	1.38
5	L5	2837	OMU	C2-N3	6.81	1.49	1.38
5	L5	4498	OMU	C2-N3	6.78	1.49	1.38
5	L5	4306	OMU	C2-N3	6.75	1.49	1.38
5	L5	3925	OMU	C2-N3	6.70	1.49	1.38
85	S2	1639	G7M	C4-N3	6.68	1.49	1.34
5	L5	4620	OMU	C2-N3	6.60	1.49	1.38
5	L5	4530	UR3	C2-N1	6.40	1.47	1.38
5	L5	4530	UR3	C6-C5	6.23	1.49	1.35
85	S2	1248	B8N	C2-N1	5.97	1.56	1.39
85	S2	1288	OMU	C6-C5	5.94	1.48	1.35
85	S2	627	OMU	C6-C5	5.93	1.48	1.35
85	S2	121	OMU	C6-C5	5.92	1.48	1.35
85	S2	172	OMU	C6-C5	5.89	1.48	1.35
85	S2	428	OMU	C6-C5	5.88	1.48	1.35
5	L5	2837	OMU	C6-C5	5.87	1.48	1.35
5	L5	4498	OMU	C6-C5	5.85	1.48	1.35
85	S2	1326	OMU	C6-C5	5.84	1.48	1.35
5	L5	4227	OMU	C6-C5	5.84	1.48	1.35
85	S2	799	OMU	C6-C5	5.83	1.48	1.35
85	S2	116	OMU	C6-C5	5.81	1.48	1.35
85	S2	354	OMU	C6-C5	5.80	1.48	1.35
85	S2	1442	OMU	C6-C5	5.78	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L5	3925	OMU	C6-C5	5.76	1.48	1.35
5	L5	4306	OMU	C6-C5	5.71	1.48	1.35
5	L5	4530	UR3	C2-N3	5.71	1.50	1.39
5	L5	4620	OMU	C6-C5	5.70	1.48	1.35
5	L5	4620	OMU	O4-C4	-5.56	1.13	1.24
5	L5	4306	OMU	O4-C4	-5.53	1.13	1.24
85	S2	1639	G7M	C2-N3	5.51	1.46	1.33
85	S2	1326	OMU	O4-C4	-5.48	1.13	1.24
85	S2	121	OMU	O4-C4	-5.47	1.13	1.24
5	L5	3925	OMU	O4-C4	-5.47	1.13	1.24
5	L5	2837	OMU	O4-C4	-5.47	1.13	1.24
85	S2	1442	OMU	O4-C4	-5.45	1.13	1.24
85	S2	116	OMU	O4-C4	-5.44	1.13	1.24
5	L5	4227	OMU	O4-C4	-5.42	1.13	1.24
5	L5	4498	OMU	O4-C4	-5.42	1.13	1.24
85	S2	354	OMU	O4-C4	-5.41	1.14	1.24
85	S2	428	OMU	O4-C4	-5.41	1.14	1.24
5	L5	3818	UY1	C6-N1	5.40	1.45	1.36
85	S2	799	OMU	O4-C4	-5.39	1.14	1.24
85	S2	627	OMU	O4-C4	-5.38	1.14	1.24
85	S2	172	OMU	O4-C4	-5.38	1.14	1.24
85	S2	1248	B8N	C6-C5	5.34	1.42	1.35
85	S2	1288	OMU	O4-C4	-5.34	1.14	1.24
85	S2	1639	G7M	C2-N2	4.95	1.45	1.34
5	L5	4220	6MZ	O4'-C4'	4.88	1.55	1.45
85	S2	1639	G7M	C5-N7	-4.68	1.33	1.39
5	L5	4220	6MZ	O4'-C1'	-4.66	1.31	1.42
5	L5	3818	UY1	C4-N3	4.50	1.47	1.38
85	S2	1326	OMU	C4-N3	4.48	1.46	1.38
85	S2	627	OMU	C4-N3	4.47	1.46	1.38
85	S2	1288	OMU	C4-N3	4.45	1.46	1.38
85	S2	1442	OMU	C4-N3	4.43	1.46	1.38
85	S2	799	OMU	C4-N3	4.37	1.46	1.38
85	S2	172	OMU	C4-N3	4.35	1.46	1.38
85	S2	428	OMU	C4-N3	4.35	1.46	1.38
85	S2	116	OMU	C4-N3	4.34	1.46	1.38
5	L5	4220	6MZ	C5'-C4'	-4.27	1.38	1.51
5	L5	4227	OMU	C4-N3	4.24	1.45	1.38
85	S2	354	OMU	C4-N3	4.21	1.45	1.38
5	L5	4498	OMU	C4-N3	4.19	1.45	1.38
5	L5	2837	OMU	C4-N3	4.17	1.45	1.38
85	S2	121	OMU	C4-N3	4.17	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L5	4306	OMU	C4-N3	4.10	1.45	1.38
5	L5	3925	OMU	C4-N3	4.07	1.45	1.38
5	L5	4620	OMU	C4-N3	3.93	1.45	1.38
85	S2	1639	G7M	C5-C6	3.86	1.54	1.43
85	S2	1248	B8N	C1'-C5	3.74	1.58	1.50
85	S2	1004	PSU	C6-C5	3.73	1.39	1.35
5	L5	3844	PSU	C6-C5	3.72	1.39	1.35
85	S2	93	PSU	C6-C5	3.67	1.39	1.35
85	S2	863	PSU	C6-C5	3.64	1.39	1.35
85	S2	651	PSU	C6-C5	3.62	1.39	1.35
5	L5	3818	UY1	O4-C4	-3.62	1.16	1.23
85	S2	406	PSU	C6-C5	3.61	1.39	1.35
85	S2	1367	PSU	C6-C5	3.61	1.39	1.35
5	L5	4293	PSU	C6-C5	3.61	1.39	1.35
85	S2	866	PSU	C6-C5	3.60	1.39	1.35
85	S2	1046	PSU	C6-C5	3.60	1.39	1.35
85	S2	1174	PSU	C6-C5	3.60	1.39	1.35
85	S2	966	PSU	C6-C5	3.59	1.39	1.35
85	S2	814	PSU	C6-C5	3.57	1.39	1.35
85	S2	801	PSU	C6-C5	3.57	1.39	1.35
85	S2	1244	PSU	C6-C5	3.57	1.39	1.35
5	L5	1782	PSU	C6-C5	3.55	1.39	1.35
5	L5	4532	PSU	C6-C5	3.54	1.39	1.35
85	S2	1232	PSU	C6-C5	3.54	1.39	1.35
5	L5	1781	PSU	C6-C5	3.53	1.39	1.35
3	CF	163	SEP	P-O1P	3.51	1.61	1.50
5	L5	2632	PSU	C6-C5	3.50	1.39	1.35
5	L5	4973	PSU	C6-C5	3.50	1.39	1.35
5	L5	5010	PSU	C6-C5	3.50	1.39	1.35
85	S2	649	PSU	C6-C5	3.50	1.39	1.35
85	S2	105	PSU	C6-C5	3.49	1.39	1.35
5	L5	4972	PSU	C6-C5	3.49	1.39	1.35
85	S2	686	PSU	C6-C5	3.48	1.39	1.35
5	L5	4500	PSU	C6-C5	3.47	1.39	1.35
5	L5	1744	PSU	C6-C5	3.45	1.39	1.35
5	L5	4552	PSU	C6-C5	3.45	1.39	1.35
85	S2	576	A2M	O5'-C5'	-3.44	1.34	1.44
5	L5	1683	PSU	C6-C5	3.43	1.39	1.35
5	L5	4220	6MZ	C5-N7	-3.43	1.32	1.39
5	L5	4353	PSU	C6-C5	3.43	1.39	1.35
5	L5	2401	A2M	O5'-C5'	-3.43	1.34	1.44
85	S2	1045	PSU	C6-C5	3.43	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L5	4312	PSU	C6-C5	3.42	1.39	1.35
5	L5	4296	PSU	C6-C5	3.42	1.39	1.35
5	L5	3884	PSU	C6-C5	3.41	1.39	1.35
5	L5	400	A2M	O5'-C5'	-3.41	1.34	1.44
85	S2	1056	PSU	C6-C5	3.41	1.39	1.35
5	L5	1862	PSU	C6-C5	3.41	1.39	1.35
5	L5	4521	PSU	C6-C5	3.41	1.39	1.35
5	L5	1582	PSU	C6-C5	3.41	1.39	1.35
85	S2	1081	PSU	C6-C5	3.41	1.39	1.35
5	L5	3825	A2M	O5'-C5'	-3.40	1.34	1.44
5	L5	3818	UY1	C1'-C5	3.40	1.58	1.50
5	L5	3830	A2M	O5'-C5'	-3.40	1.34	1.44
7	L8	69	PSU	C6-C5	3.40	1.39	1.35
85	S2	1177	PSU	C6-C5	3.40	1.39	1.35
7	L8	55	PSU	C6-C5	3.40	1.39	1.35
5	L5	2787	A2M	O5'-C5'	-3.39	1.34	1.44
5	L5	4636	PSU	C6-C5	3.39	1.39	1.35
5	L5	5001	PSU	C6-C5	3.38	1.39	1.35
5	L5	4442	PSU	C6-C5	3.38	1.39	1.35
85	S2	99	A2M	O5'-C5'	-3.38	1.34	1.44
5	L5	3639	PSU	C6-C5	3.38	1.39	1.35
5	L5	4571	A2M	O5'-C5'	-3.37	1.34	1.44
5	L5	3822	PSU	C6-C5	3.37	1.39	1.35
85	S2	681	PSU	C6-C5	3.37	1.39	1.35
5	L5	1536	PSU	C6-C5	3.37	1.39	1.35
85	S2	109	PSU	C6-C5	3.37	1.39	1.35
5	L5	4576	PSU	C6-C5	3.37	1.39	1.35
5	L5	1323	A2M	O5'-C5'	-3.36	1.34	1.44
5	L5	3637	PSU	C6-C5	3.36	1.39	1.35
5	L5	3695	PSU	C6-C5	3.36	1.39	1.35
5	L5	1871	A2M	O5'-C5'	-3.36	1.34	1.44
5	L5	4523	A2M	O5'-C5'	-3.36	1.34	1.44
5	L5	4431	PSU	C6-C5	3.36	1.39	1.35
5	L5	1524	A2M	O5'-C5'	-3.35	1.34	1.44
85	S2	1383	A2M	O5'-C5'	-3.34	1.34	1.44
5	L5	3853	PSU	C6-C5	3.34	1.39	1.35
85	S2	166	A2M	O5'-C5'	-3.34	1.34	1.44
5	L5	4493	PSU	C6-C5	3.33	1.39	1.35
5	L5	1326	A2M	O5'-C5'	-3.33	1.34	1.44
5	L5	3785	A2M	O5'-C5'	-3.33	1.34	1.44
5	L5	3920	PSU	C6-C5	3.33	1.39	1.35
85	S2	668	A2M	O5'-C5'	-3.31	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L5	4471	PSU	C6-C5	3.31	1.39	1.35
5	L5	2815	A2M	O5'-C5'	-3.30	1.34	1.44
5	L5	398	A2M	O5'-C5'	-3.30	1.34	1.44
5	L5	4673	PSU	C6-C5	3.29	1.38	1.35
85	S2	1031	A2M	O5'-C5'	-3.29	1.34	1.44
5	L5	1860	PSU	C6-C5	3.29	1.38	1.35
85	S2	27	A2M	O5'-C5'	-3.28	1.34	1.44
85	S2	468	A2M	O5'-C5'	-3.26	1.34	1.44
5	L5	3867	A2M	O5'-C5'	-3.26	1.34	1.44
85	S2	484	A2M	O5'-C5'	-3.26	1.34	1.44
5	L5	2363	A2M	O5'-C5'	-3.26	1.34	1.44
5	L5	4579	PSU	C6-C5	3.26	1.38	1.35
85	S2	1851	MA6	C6-N6	3.25	1.45	1.36
5	L5	4689	PSU	C6-C5	3.25	1.38	1.35
5	L5	4361	PSU	C6-C5	3.22	1.38	1.35
5	L5	3718	A2M	O5'-C5'	-3.22	1.34	1.44
5	L5	2839	PSU	C6-C5	3.22	1.38	1.35
5	L5	3818	UY1	O2-C2	-3.22	1.16	1.23
5	L5	1792	PSU	C6-C5	3.21	1.38	1.35
5	L5	4220	6MZ	C5-C4	-3.20	1.33	1.39
85	S2	1850	MA6	C6-N6	3.18	1.45	1.36
5	L5	4457	PSU	C6-C5	3.18	1.38	1.35
5	L5	4299	PSU	C6-C5	3.17	1.38	1.35
5	L5	3851	PSU	C6-C5	3.16	1.38	1.35
5	L5	4590	A2M	O5'-C5'	-3.15	1.35	1.44
5	L5	4220	6MZ	C2'-C1'	3.13	1.63	1.53
85	S2	1832	6MZ	C5-N7	-3.12	1.33	1.39
5	L5	4628	PSU	C6-C5	3.10	1.38	1.35
5	L5	1677	PSU	C6-C5	3.09	1.38	1.35
5	L5	4403	PSU	C6-C5	3.08	1.38	1.35
85	S2	159	A2M	O5'-C5'	-3.08	1.35	1.44
5	L5	1534	A2M	O5'-C5'	-3.05	1.35	1.44
85	S2	1832	6MZ	C5-C4	-3.04	1.33	1.39
85	S2	627	OMU	C5-C4	2.99	1.50	1.43
85	S2	1288	OMU	C5-C4	2.98	1.50	1.43
85	S2	799	OMU	C5-C4	2.86	1.49	1.43
85	S2	172	OMU	C5-C4	2.84	1.49	1.43
85	S2	428	OMU	C5-C4	2.82	1.49	1.43
5	L5	4498	OMU	C5-C4	2.82	1.49	1.43
85	S2	1832	6MZ	C8-N9	-2.82	1.32	1.37
5	L5	4227	OMU	C5-C4	2.81	1.49	1.43
85	S2	1326	OMU	C5-C4	2.81	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L5	4220	6MZ	C8-N9	-2.80	1.32	1.37
85	S2	1442	OMU	C5-C4	2.80	1.49	1.43
85	S2	1639	G7M	C2-N1	2.79	1.44	1.37
85	S2	354	OMU	C5-C4	2.78	1.49	1.43
5	L5	4220	6MZ	O3'-C3'	2.77	1.49	1.43
5	L5	3925	OMU	C5-C4	2.77	1.49	1.43
85	S2	116	OMU	C5-C4	2.75	1.49	1.43
5	L5	2837	OMU	C5-C4	2.75	1.49	1.43
85	S2	121	OMU	C5-C4	2.73	1.49	1.43
85	S2	799	OMU	C6-N1	2.73	1.44	1.38
85	S2	1288	OMU	C6-N1	2.71	1.44	1.38
85	S2	354	OMU	C6-N1	2.71	1.44	1.38
5	L5	4530	UR3	O2-C2	-2.70	1.17	1.22
5	L5	4498	OMU	C6-N1	2.69	1.44	1.38
85	S2	627	OMU	C6-N1	2.68	1.44	1.38
85	S2	1326	OMU	C6-N1	2.68	1.44	1.38
85	S2	1442	OMU	C6-N1	2.67	1.44	1.38
85	S2	121	OMU	C6-N1	2.66	1.44	1.38
5	L5	4306	OMU	C6-N1	2.64	1.44	1.38
5	L5	4306	OMU	C5-C4	2.63	1.49	1.43
85	S2	668	A2M	O4'-C4'	-2.63	1.39	1.45
5	L5	4530	UR3	C6-N1	2.61	1.44	1.38
5	L5	2837	OMU	C6-N1	2.60	1.44	1.38
85	S2	172	OMU	C6-N1	2.59	1.44	1.38
85	S2	428	OMU	C6-N1	2.58	1.44	1.38
5	L5	4620	OMU	C5-C4	2.58	1.49	1.43
5	L5	4227	OMU	C6-N1	2.57	1.44	1.38
85	S2	116	OMU	C6-N1	2.57	1.44	1.38
85	S2	1639	G7M	O6-C6	-2.54	1.18	1.23
5	L5	3925	OMU	C6-N1	2.51	1.44	1.38
5	L5	4620	OMU	C6-N1	2.48	1.44	1.38
85	S2	1851	MA6	C5-C4	-2.37	1.34	1.39
85	S2	1639	G7M	C6-N1	2.36	1.43	1.38
85	S2	1832	6MZ	C6-N1	-2.36	1.31	1.35
5	L5	4530	UR3	C5-C4	2.31	1.49	1.43
5	L5	1534	A2M	O4'-C4'	-2.27	1.40	1.45
5	L5	2363	A2M	O4'-C4'	-2.25	1.40	1.45
85	S2	1850	MA6	C5-C4	-2.25	1.35	1.39
5	L5	4220	6MZ	C6-N1	-2.20	1.31	1.35
5	L5	1524	A2M	O4'-C4'	-2.16	1.40	1.45
5	L5	4530	UR3	C3U-N3	2.15	1.50	1.47
5	L5	3818	UY1	C4-C5	2.12	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L5	1323	A2M	O4'-C4'	-2.06	1.40	1.45
85	S2	166	A2M	C5-C4	2.01	1.42	1.39
5	L5	4523	A2M	O4'-C4'	-2.01	1.40	1.45

All (672) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	S2	1851	MA6	N1-C6-N6	-12.17	102.03	116.86
85	S2	1850	MA6	N1-C6-N6	-11.70	102.60	116.86
85	S2	1851	MA6	C5-C6-N6	8.11	138.17	125.33
85	S2	1850	MA6	C5-C6-N6	7.86	137.77	125.33
85	S2	1639	G7M	C1'-N9-C4	7.66	149.10	126.49
85	S2	1639	G7M	C1'-N9-C8	-7.49	101.45	126.74
5	L5	3925	OMU	C4-N3-C2	-5.91	119.28	126.61
85	S2	428	OMU	C4-N3-C2	-5.75	119.48	126.61
5	L5	4498	OMU	C4-N3-C2	-5.70	119.54	126.61
85	S2	627	OMU	C4-N3-C2	-5.69	119.55	126.61
85	S2	354	OMU	C4-N3-C2	-5.66	119.58	126.61
5	L5	4530	UR3	C4-N3-C2	-5.63	120.05	124.58
5	L5	4227	OMU	C4-N3-C2	-5.62	119.63	126.61
5	L5	2837	OMU	C4-N3-C2	-5.59	119.67	126.61
85	S2	1326	OMU	C4-N3-C2	-5.58	119.68	126.61
85	S2	172	OMU	C4-N3-C2	-5.57	119.69	126.61
5	L5	4220	6MZ	N1-C2-N3	-5.56	120.16	128.58
85	S2	1851	MA6	N1-C2-N3	-5.56	120.16	128.58
85	S2	1851	MA6	N9-C8-N7	-5.56	106.05	113.94
85	S2	121	OMU	C4-N3-C2	-5.55	119.72	126.61
85	S2	1442	OMU	C4-N3-C2	-5.52	119.76	126.61
5	L5	4306	OMU	C4-N3-C2	-5.51	119.77	126.61
85	S2	1832	6MZ	N1-C2-N3	-5.49	120.26	128.58
85	S2	799	OMU	C4-N3-C2	-5.48	119.81	126.61
85	S2	1288	OMU	C4-N3-C2	-5.43	119.87	126.61
85	S2	1248	B8N	C5-C4-N3	5.38	125.92	116.15
85	S2	1850	MA6	N1-C2-N3	-5.36	120.46	128.58
85	S2	116	OMU	C4-N3-C2	-5.35	119.97	126.61
5	L5	3637	PSU	N1-C2-N3	5.32	120.78	115.17
85	S2	1850	MA6	N9-C8-N7	-5.28	106.44	113.94
5	L5	4636	PSU	C4-N3-C2	-5.27	119.11	126.37
5	L5	3701	OMC	C1'-N1-C2	5.18	129.89	118.44
5	L5	1677	PSU	C4-N3-C2	-5.18	119.23	126.37
5	L5	3637	PSU	C4-N3-C2	-5.12	119.31	126.37
5	L5	4457	PSU	C4-N3-C2	-5.09	119.36	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L5	4403	PSU	C4-N3-C2	-5.08	119.37	126.37
5	L5	4620	OMU	C4-N3-C2	-5.07	120.31	126.61
5	L5	4521	PSU	C4-N3-C2	-5.06	119.41	126.37
85	S2	649	PSU	C4-N3-C2	-5.06	119.41	126.37
5	L5	1792	PSU	C4-N3-C2	-5.04	119.42	126.37
5	L5	4500	PSU	C4-N3-C2	-5.03	119.45	126.37
5	L5	4973	PSU	C4-N3-C2	-5.01	119.47	126.37
5	L5	4636	PSU	N1-C2-N3	5.00	120.45	115.17
5	L5	4689	PSU	N1-C2-N3	5.00	120.44	115.17
5	L5	4689	PSU	C4-N3-C2	-4.99	119.50	126.37
85	S2	109	PSU	C4-N3-C2	-4.99	119.50	126.37
5	L5	4293	PSU	N1-C2-N3	4.98	120.42	115.17
5	L5	4500	PSU	N1-C2-N3	4.97	120.41	115.17
85	S2	406	PSU	C4-N3-C2	-4.97	119.53	126.37
5	L5	4471	PSU	C4-N3-C2	-4.96	119.54	126.37
85	S2	1174	PSU	C4-N3-C2	-4.95	119.55	126.37
85	S2	1056	PSU	C4-N3-C2	-4.95	119.55	126.37
5	L5	4312	PSU	C4-N3-C2	-4.93	119.58	126.37
85	S2	406	PSU	N1-C2-N3	4.93	120.36	115.17
5	L5	1744	PSU	C4-N3-C2	-4.92	119.59	126.37
5	L5	4552	PSU	C4-N3-C2	-4.92	119.60	126.37
5	L5	1862	PSU	C4-N3-C2	-4.92	119.60	126.37
5	L5	4293	PSU	C4-N3-C2	-4.91	119.60	126.37
85	S2	966	PSU	C4-N3-C2	-4.91	119.61	126.37
5	L5	4521	PSU	N1-C2-N3	4.91	120.34	115.17
5	L5	4493	PSU	C4-N3-C2	-4.90	119.62	126.37
85	S2	1045	PSU	C4-N3-C2	-4.90	119.63	126.37
5	L5	4442	PSU	C4-N3-C2	-4.89	119.63	126.37
5	L5	1582	PSU	C4-N3-C2	-4.89	119.63	126.37
85	S2	651	PSU	C4-N3-C2	-4.88	119.64	126.37
5	L5	1860	PSU	C4-N3-C2	-4.88	119.65	126.37
5	L5	3695	PSU	C4-N3-C2	-4.87	119.66	126.37
5	L5	4296	PSU	C4-N3-C2	-4.87	119.66	126.37
5	L5	4973	PSU	N1-C2-N3	4.86	120.29	115.17
5	L5	1683	PSU	C4-N3-C2	-4.86	119.68	126.37
5	L5	3884	PSU	C4-N3-C2	-4.86	119.68	126.37
5	L5	4353	PSU	C4-N3-C2	-4.85	119.69	126.37
5	L5	3851	PSU	C4-N3-C2	-4.85	119.69	126.37
85	S2	1832	6MZ	C5-C4-N3	-4.84	120.05	126.72
85	S2	651	PSU	N1-C2-N3	4.84	120.27	115.17
5	L5	4431	PSU	C4-N3-C2	-4.83	119.71	126.37
5	L5	4457	PSU	N1-C2-N3	4.83	120.26	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	S2	1244	PSU	C4-N3-C2	-4.83	119.72	126.37
85	S2	1232	PSU	C4-N3-C2	-4.83	119.72	126.37
85	S2	1367	PSU	C4-N3-C2	-4.83	119.72	126.37
5	L5	1862	PSU	N1-C2-N3	4.82	120.25	115.17
5	L5	1536	PSU	C4-N3-C2	-4.82	119.73	126.37
7	L8	55	PSU	C4-N3-C2	-4.82	119.74	126.37
85	S2	1046	PSU	C4-N3-C2	-4.81	119.75	126.37
5	L5	5010	PSU	C4-N3-C2	-4.81	119.75	126.37
5	L5	3818	UY1	C4-N3-C2	-4.81	119.75	126.37
85	S2	801	PSU	C4-N3-C2	-4.80	119.75	126.37
5	L5	1782	PSU	C4-N3-C2	-4.80	119.75	126.37
5	L5	4532	PSU	C4-N3-C2	-4.80	119.76	126.37
5	L5	4299	PSU	C4-N3-C2	-4.79	119.77	126.37
5	L5	3639	PSU	C4-N3-C2	-4.79	119.77	126.37
85	S2	1367	PSU	N1-C2-N3	4.79	120.22	115.17
85	S2	1177	PSU	C4-N3-C2	-4.78	119.79	126.37
85	S2	1832	6MZ	N9-C8-N7	-4.78	107.16	113.94
85	S2	966	PSU	N1-C2-N3	4.78	120.21	115.17
5	L5	4972	PSU	C4-N3-C2	-4.78	119.79	126.37
85	S2	686	PSU	C4-N3-C2	-4.77	119.80	126.37
85	S2	863	PSU	C4-N3-C2	-4.77	119.80	126.37
5	L5	4673	PSU	C4-N3-C2	-4.77	119.80	126.37
5	L5	4312	PSU	N1-C2-N3	4.77	120.20	115.17
5	L5	5001	PSU	C4-N3-C2	-4.77	119.80	126.37
5	L5	3920	PSU	C4-N3-C2	-4.77	119.81	126.37
7	L8	55	PSU	N1-C2-N3	4.77	120.19	115.17
85	S2	1004	PSU	C4-N3-C2	-4.76	119.81	126.37
5	L5	4361	PSU	C4-N3-C2	-4.75	119.83	126.37
5	L5	4552	PSU	N1-C2-N3	4.75	120.18	115.17
5	L5	4576	PSU	C4-N3-C2	-4.74	119.83	126.37
5	L5	1536	PSU	N1-C2-N3	4.74	120.16	115.17
85	S2	1081	PSU	C4-N3-C2	-4.74	119.85	126.37
5	L5	1744	PSU	N1-C2-N3	4.73	120.15	115.17
5	L5	4972	PSU	N1-C2-N3	4.72	120.15	115.17
5	L5	3884	PSU	N1-C2-N3	4.72	120.15	115.17
85	S2	814	PSU	C4-N3-C2	-4.72	119.87	126.37
85	S2	649	PSU	N1-C2-N3	4.71	120.13	115.17
85	S2	1850	MA6	C5-C4-N3	-4.71	120.24	126.72
5	L5	2839	PSU	C4-N3-C2	-4.70	119.89	126.37
5	L5	1792	PSU	N1-C2-N3	4.70	120.13	115.17
5	L5	4628	PSU	C4-N3-C2	-4.70	119.90	126.37
5	L5	2632	PSU	C4-N3-C2	-4.69	119.91	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L5	4442	PSU	N1-C2-N3	4.69	120.12	115.17
5	L5	4353	PSU	N1-C2-N3	4.69	120.12	115.17
5	L5	3822	PSU	C4-N3-C2	-4.69	119.91	126.37
5	L5	3695	PSU	N1-C2-N3	4.69	120.11	115.17
5	L5	4431	PSU	N1-C2-N3	4.69	120.11	115.17
5	L5	3844	PSU	C4-N3-C2	-4.69	119.92	126.37
85	S2	1248	B8N	C4-N3-C2	-4.68	119.85	125.62
5	L5	4403	PSU	N1-C2-N3	4.68	120.11	115.17
85	S2	1244	PSU	N1-C2-N3	4.68	120.11	115.17
5	L5	4532	PSU	N1-C2-N3	4.68	120.11	115.17
85	S2	109	PSU	N1-C2-N3	4.68	120.10	115.17
85	S2	863	PSU	N1-C2-N3	4.68	120.10	115.17
5	L5	3920	PSU	N1-C2-N3	4.67	120.10	115.17
5	L5	3853	PSU	C4-N3-C2	-4.67	119.94	126.37
85	S2	105	PSU	N1-C2-N3	4.67	120.09	115.17
5	L5	4579	PSU	C4-N3-C2	-4.67	119.94	126.37
85	S2	1174	PSU	N1-C2-N3	4.67	120.09	115.17
5	L5	4471	PSU	N1-C2-N3	4.66	120.08	115.17
5	L5	1683	PSU	N1-C2-N3	4.65	120.08	115.17
5	L5	3844	PSU	N1-C2-N3	4.64	120.07	115.17
85	S2	105	PSU	C4-N3-C2	-4.64	119.98	126.37
7	L8	69	PSU	C4-N3-C2	-4.64	119.98	126.37
5	L5	4296	PSU	N1-C2-N3	4.64	120.06	115.17
5	L5	2632	PSU	N1-C2-N3	4.63	120.06	115.17
85	S2	1056	PSU	N1-C2-N3	4.63	120.05	115.17
5	L5	5010	PSU	N1-C2-N3	4.63	120.05	115.17
5	L5	4628	PSU	N1-C2-N3	4.62	120.04	115.17
5	L5	1781	PSU	C4-N3-C2	-4.62	120.01	126.37
5	L5	4493	PSU	N1-C2-N3	4.62	120.04	115.17
85	S2	1046	PSU	N1-C2-N3	4.61	120.03	115.17
5	L5	1582	PSU	N1-C2-N3	4.61	120.03	115.17
5	L5	4579	PSU	N1-C2-N3	4.61	120.03	115.17
5	L5	3853	PSU	N1-C2-N3	4.60	120.02	115.17
85	S2	681	PSU	C4-N3-C2	-4.60	120.04	126.37
85	S2	866	PSU	C4-N3-C2	-4.59	120.05	126.37
5	L5	1860	PSU	N1-C2-N3	4.59	120.01	115.17
85	S2	1045	PSU	N1-C2-N3	4.59	120.01	115.17
85	S2	686	PSU	N1-C2-N3	4.59	120.00	115.17
85	S2	1004	PSU	N1-C2-N3	4.58	120.00	115.17
85	S2	1232	PSU	N1-C2-N3	4.58	120.00	115.17
5	L5	4220	6MZ	C5-C4-N3	-4.58	120.41	126.72
85	S2	801	PSU	N1-C2-N3	4.57	119.99	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	S2	93	PSU	C4-N3-C2	-4.57	120.08	126.37
85	S2	681	PSU	N1-C2-N3	4.56	119.98	115.17
5	L5	5001	PSU	N1-C2-N3	4.56	119.98	115.17
85	S2	1639	G7M	C2-N3-C4	4.55	120.14	112.30
5	L5	1782	PSU	N1-C2-N3	4.55	119.97	115.17
5	L5	4576	PSU	N1-C2-N3	4.55	119.97	115.17
5	L5	3639	PSU	N1-C2-N3	4.55	119.97	115.17
85	S2	93	PSU	N1-C2-N3	4.55	119.97	115.17
85	S2	1851	MA6	C5-C4-N3	-4.55	120.46	126.72
85	S2	1177	PSU	N1-C2-N3	4.54	119.96	115.17
85	S2	1081	PSU	N1-C2-N3	4.54	119.95	115.17
5	L5	4299	PSU	N1-C2-N3	4.53	119.95	115.17
5	L5	1677	PSU	N1-C2-N3	4.53	119.94	115.17
5	L5	3851	PSU	N1-C2-N3	4.51	119.92	115.17
85	S2	866	PSU	N1-C2-N3	4.50	119.92	115.17
5	L5	4673	PSU	N1-C2-N3	4.50	119.91	115.17
5	L5	1781	PSU	N1-C2-N3	4.50	119.91	115.17
5	L5	2839	PSU	N1-C2-N3	4.49	119.90	115.17
7	L8	69	PSU	N1-C2-N3	4.49	119.90	115.17
5	L5	3822	PSU	N1-C2-N3	4.46	119.87	115.17
5	L5	4361	PSU	N1-C2-N3	4.46	119.87	115.17
5	L5	4220	6MZ	N9-C8-N7	-4.44	107.64	113.94
85	S2	121	OMU	N3-C2-N1	4.41	120.64	114.89
85	S2	814	PSU	N1-C2-N3	4.41	119.82	115.17
5	L5	4220	6MZ	C9-N6-C6	-4.41	118.76	122.85
5	L5	4498	OMU	N3-C2-N1	4.34	120.54	114.89
5	L5	3830	A2M	C3'-C2'-C1'	-4.28	94.60	102.81
5	L5	3925	OMU	N3-C2-N1	4.27	120.45	114.89
5	L5	2837	OMU	N3-C2-N1	4.23	120.40	114.89
85	S2	1851	MA6	C4-N9-C8	4.19	110.14	105.74
85	S2	1639	G7M	C5-C4-N3	-4.18	120.24	128.15
5	L5	1871	A2M	C3'-C2'-C1'	-4.17	94.82	102.81
85	S2	354	OMU	N3-C2-N1	4.16	120.31	114.89
5	L5	3818	UY1	N1-C2-N3	4.16	119.55	115.17
85	S2	1383	A2M	C3'-C2'-C1'	-4.14	94.89	102.81
85	S2	1248	B8N	C1'-C5-C4	4.09	123.82	117.61
85	S2	1639	G7M	C5-C6-N1	4.07	120.26	111.84
5	L5	4523	A2M	C3'-C2'-C1'	-4.06	95.03	102.81
5	L5	4227	OMU	N3-C2-N1	4.04	120.16	114.89
85	S2	1850	MA6	C4-N9-C8	4.03	109.97	105.74
5	L5	3701	OMC	C1'-N1-C6	-4.01	112.21	120.78
5	L5	4306	OMU	N3-C2-N1	3.98	120.07	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L5	4620	OMU	N3-C2-N1	3.92	119.99	114.89
85	S2	428	OMU	N3-C2-N1	3.92	119.99	114.89
85	S2	1850	MA6	C4-C5-C6	3.90	119.94	115.91
5	L5	398	A2M	C3'-C2'-C1'	-3.84	95.45	102.81
85	S2	627	OMU	N3-C2-N1	3.82	119.87	114.89
85	S2	116	OMU	N3-C2-N1	3.78	119.81	114.89
85	S2	172	OMU	N3-C2-N1	3.78	119.81	114.89
85	S2	1288	OMU	N3-C2-N1	3.78	119.81	114.89
85	S2	1442	OMU	N3-C2-N1	3.77	119.80	114.89
85	S2	1326	OMU	N3-C2-N1	3.76	119.78	114.89
85	S2	799	OMU	N3-C2-N1	3.74	119.76	114.89
85	S2	468	A2M	C3'-C2'-C1'	-3.74	95.65	102.81
5	L5	398	A2M	O3'-C3'-C2'	3.73	121.63	111.19
5	L5	2351	OMC	C1'-N1-C2	3.72	126.67	118.44
85	S2	799	OMU	C5-C4-N3	3.68	119.95	114.80
85	S2	1031	A2M	C3'-C2'-C1'	-3.61	95.89	102.81
85	S2	627	OMU	C5-C4-N3	3.60	119.84	114.80
85	S2	428	OMU	C5-C4-N3	3.60	119.84	114.80
5	L5	3925	OMU	C5-C4-N3	3.58	119.81	114.80
85	S2	576	A2M	O3'-C3'-C2'	3.56	121.15	111.19
85	S2	1326	OMU	C5-C4-N3	3.55	119.78	114.80
5	L5	2401	A2M	O3'-C3'-C2'	3.55	121.11	111.19
85	S2	576	A2M	C3'-C2'-C1'	-3.54	96.03	102.81
5	L5	1534	A2M	C3'-C2'-C1'	-3.54	96.04	102.81
85	S2	1442	OMU	C5-C4-N3	3.52	119.74	114.80
85	S2	1851	MA6	C4-C5-C6	3.52	119.55	115.91
85	S2	172	OMU	C5-C4-N3	3.52	119.73	114.80
5	L5	4306	OMU	C5-C4-N3	3.51	119.71	114.80
5	L5	4530	UR3	C5-C4-N3	3.50	119.65	115.04
85	S2	354	OMU	C5-C4-N3	3.49	119.69	114.80
85	S2	1851	MA6	C2-N1-C6	3.49	120.34	111.83
5	L5	2787	A2M	O3'-C3'-C2'	3.48	120.92	111.19
85	S2	1288	OMU	C5-C4-N3	3.47	119.67	114.80
85	S2	116	OMU	C5-C4-N3	3.47	119.66	114.80
5	L5	2401	A2M	C3'-C2'-C1'	-3.47	96.17	102.81
5	L5	4227	OMU	C5-C4-N3	3.46	119.65	114.80
5	L5	3825	A2M	C3'-C2'-C1'	-3.46	96.18	102.81
85	S2	1639	G7M	O6-C6-C5	-3.44	120.33	128.01
85	S2	1850	MA6	C2-N1-C6	3.44	120.22	111.83
5	L5	4498	OMU	C5-C4-N3	3.42	119.60	114.80
85	S2	1851	MA6	C5-N7-C8	3.42	108.83	103.45
85	S2	1850	MA6	N3-C4-N9	3.40	132.95	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	S2	99	A2M	O3'-C3'-C2'	3.40	120.71	111.19
85	S2	1639	G7M	N9-C4-N3	3.39	132.74	125.95
85	S2	1383	A2M	O3'-C3'-C2'	3.39	120.68	111.19
5	L5	400	A2M	O3'-C3'-C2'	3.38	120.64	111.19
85	S2	468	A2M	O3'-C3'-C2'	3.36	120.60	111.19
85	S2	99	A2M	C3'-C2'-C1'	-3.36	96.38	102.81
85	S2	1832	6MZ	C4-C5-C6	3.35	119.57	116.78
85	S2	1832	6MZ	C2-N3-C4	3.34	120.00	111.83
5	L5	2837	OMU	C5-C4-N3	3.34	119.48	114.80
85	S2	1639	G7M	CN7-N7-C5	3.34	130.96	126.80
85	S2	1272	OMC	C1'-N1-C2	3.34	125.81	118.44
5	L5	1871	A2M	O3'-C3'-C2'	3.33	120.50	111.19
85	S2	166	A2M	O3'-C3'-C2'	3.32	120.47	111.19
5	L5	4571	A2M	O3'-C3'-C2'	3.31	120.45	111.19
5	L5	1524	A2M	O3'-C3'-C2'	3.31	120.45	111.19
85	S2	121	OMU	C5-C4-N3	3.29	119.41	114.80
85	S2	1248	B8N	N3-C2-N1	3.29	120.73	116.72
5	L5	3830	A2M	O3'-C3'-C2'	3.28	120.35	111.19
85	S2	1031	A2M	O3'-C3'-C2'	3.27	120.34	111.19
5	L5	4220	6MZ	C2-N3-C4	3.26	119.79	111.83
85	S2	1832	6MZ	C5-N7-C8	3.25	108.56	103.45
85	S2	1850	MA6	C5-N7-C8	3.24	108.55	103.45
5	L5	4620	OMU	C5-C4-N3	3.22	119.31	114.80
85	S2	1851	MA6	C2-N3-C4	3.22	119.69	111.83
5	L5	3718	A2M	O3'-C3'-C2'	3.22	120.19	111.19
85	S2	1851	MA6	N3-C4-N9	3.22	132.64	127.17
5	L5	4590	A2M	C3'-C2'-C1'	-3.21	96.66	102.81
5	L5	1323	A2M	C2'-C1'-N9	3.21	119.03	113.75
5	L5	4220	6MZ	C4-C5-C6	3.21	119.45	116.78
85	S2	668	A2M	C4-N9-C1'	-3.19	119.17	126.63
5	L5	3825	A2M	O3'-C3'-C2'	3.16	120.03	111.19
85	S2	159	A2M	O3'-C3'-C2'	3.14	119.98	111.19
5	L5	4571	A2M	C3'-C2'-C1'	-3.14	96.79	102.81
85	S2	1850	MA6	C2-N3-C4	3.14	119.50	111.83
85	S2	1832	6MZ	N3-C4-N9	3.11	132.46	127.17
5	L5	4523	A2M	O3'-C3'-C2'	3.11	119.88	111.19
5	L5	3718	A2M	C3'-C2'-C1'	-3.09	96.88	102.81
85	S2	1442	OMU	O4-C4-C5	-3.09	119.83	125.16
5	L5	2363	A2M	C3'-C2'-C1'	-3.08	96.91	102.81
5	L5	2363	A2M	O3'-C3'-C2'	3.08	119.80	111.19
85	S2	1326	OMU	O4-C4-C5	-3.07	119.87	125.16
5	L5	3851	PSU	O2-C2-N1	-3.06	119.63	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	S2	1639	G7M	C2-N1-C6	-3.06	119.55	125.11
5	L5	1323	A2M	O3'-C3'-C2'	3.05	119.73	111.19
5	L5	400	A2M	C3'-C2'-C1'	-3.04	96.98	102.81
85	S2	428	OMU	O4-C4-C5	-3.04	119.91	125.16
85	S2	484	A2M	O3'-C3'-C2'	3.04	119.70	111.19
85	S2	406	PSU	O2-C2-N1	-3.04	119.66	122.79
85	S2	668	A2M	C1'-N9-C8	3.03	133.83	127.09
5	L5	2815	A2M	C2'-C1'-N9	3.02	118.73	113.75
5	L5	1871	A2M	C4-N9-C1'	-3.01	119.58	126.63
5	L5	4689	PSU	O2-C2-N1	-3.00	119.70	122.79
85	S2	1248	B8N	O4-C4-N3	-3.00	115.12	119.99
85	S2	1832	6MZ	C4-N9-C8	3.00	108.88	105.74
5	L5	4220	6MZ	N3-C4-N9	2.99	132.25	127.17
5	L5	3785	A2M	O3'-C3'-C2'	2.98	119.51	111.19
85	S2	627	OMU	O4-C4-C5	-2.97	120.05	125.16
5	L5	3701	OMC	O2-C2-N3	-2.97	117.66	122.33
5	L5	2815	A2M	O3'-C3'-C2'	2.96	119.47	111.19
5	L5	4579	PSU	O2-C2-N1	-2.96	119.74	122.79
5	L5	1326	A2M	O3'-C3'-C2'	2.95	119.45	111.19
5	L5	4457	PSU	O2-C2-N1	-2.95	119.74	122.79
5	L5	4353	PSU	O2-C2-N1	-2.93	119.76	122.79
5	L5	2363	A2M	C2'-C1'-N9	2.93	118.58	113.75
85	S2	109	PSU	O2-C2-N1	-2.93	119.77	122.79
85	S2	172	OMU	O4-C4-C5	-2.92	120.12	125.16
85	S2	799	OMU	O4-C4-C5	-2.92	120.12	125.16
5	L5	1871	A2M	C1'-N9-C8	2.92	133.57	127.09
85	S2	27	A2M	O3'-C3'-C2'	2.91	119.34	111.19
85	S2	668	A2M	C2'-C1'-N9	2.91	118.53	113.75
5	L5	2401	A2M	C4-N9-C1'	-2.90	119.85	126.63
5	L5	4523	A2M	C4-N9-C1'	-2.88	119.89	126.63
5	L5	3925	OMU	O4-C4-C5	-2.88	120.19	125.16
85	S2	651	PSU	O2-C2-N1	-2.88	119.82	122.79
5	L5	4293	PSU	O2-C2-N1	-2.88	119.82	122.79
85	S2	966	PSU	O2-C2-N1	-2.87	119.83	122.79
85	S2	99	A2M	C4-N9-C1'	-2.87	119.93	126.63
85	S2	116	OMU	O4-C4-C5	-2.86	120.23	125.16
5	L5	4500	PSU	O2-C2-N1	-2.86	119.84	122.79
5	L5	3818	UY1	C6-N1-C2	-2.86	120.04	122.69
5	L5	4590	A2M	C4-N9-C1'	-2.84	119.99	126.63
85	S2	1367	PSU	O2-C2-N1	-2.84	119.86	122.79
85	S2	1031	A2M	C4-N9-C1'	-2.84	119.99	126.63
5	L5	1536	PSU	O2-C2-N1	-2.84	119.86	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L5	4220	6MZ	C5-N7-C8	2.84	107.91	103.45
5	L5	3818	UY1	C6-C5-C4	2.83	120.09	118.17
85	S2	1383	A2M	C4-N9-C1'	-2.83	120.02	126.63
85	S2	1045	PSU	O2-C2-N1	-2.83	119.87	122.79
5	L5	2401	A2M	C1'-N9-C8	2.83	133.37	127.09
85	S2	468	A2M	C4-N9-C1'	-2.83	120.03	126.63
85	S2	681	PSU	O2-C2-N1	-2.82	119.88	122.79
5	L5	4306	OMU	O4-C4-C5	-2.81	120.31	125.16
85	S2	354	OMU	O4-C4-C5	-2.81	120.31	125.16
5	L5	3844	PSU	O2-C2-N1	-2.80	119.90	122.79
5	L5	4227	OMU	O4-C4-C5	-2.80	120.33	125.16
5	L5	4590	A2M	O3'-C3'-C2'	2.80	119.02	111.19
5	L5	1860	PSU	O2-C2-N1	-2.80	119.90	122.79
5	L5	3718	A2M	C1'-N9-C8	2.79	133.30	127.09
5	L5	4523	A2M	C1'-N9-C8	2.79	133.29	127.09
85	S2	27	A2M	C3'-C2'-C1'	-2.79	97.46	102.81
85	S2	1288	OMU	O4-C4-C5	-2.78	120.36	125.16
5	L5	4521	PSU	O2-C2-N1	-2.78	119.92	122.79
5	L5	4403	PSU	O2-C2-N1	-2.78	119.92	122.79
85	S2	1031	A2M	C1'-N9-C8	2.77	133.25	127.09
85	S2	99	A2M	C1'-N9-C8	2.77	133.24	127.09
85	S2	1244	PSU	O2-C2-N1	-2.76	119.94	122.79
5	L5	3867	A2M	C2'-C1'-N9	2.76	118.30	113.75
7	L8	69	PSU	O2-C2-N1	-2.76	119.94	122.79
5	L5	4972	PSU	O2-C2-N1	-2.76	119.94	122.79
5	L5	4498	OMU	O4-C4-C5	-2.76	120.40	125.16
5	L5	4312	PSU	O2-C2-N1	-2.76	119.94	122.79
5	L5	3884	PSU	O2-C2-N1	-2.76	119.94	122.79
5	L5	4590	A2M	C1'-N9-C8	2.75	133.20	127.09
85	S2	1639	G7M	CN7-N7-C8	-2.75	120.63	124.79
5	L5	4493	PSU	O2-C2-N1	-2.75	119.95	122.79
85	S2	801	PSU	O2-C2-N1	-2.75	119.96	122.79
85	S2	1174	PSU	O2-C2-N1	-2.75	119.96	122.79
5	L5	4552	PSU	O2-C2-N1	-2.74	119.96	122.79
5	L5	4296	PSU	O2-C2-N1	-2.74	119.96	122.79
5	L5	2351	OMC	C1'-N1-C6	-2.74	114.93	120.78
5	L5	1781	PSU	O2-C2-N1	-2.73	119.97	122.79
5	L5	3785	A2M	C4-N9-C1'	-2.73	120.26	126.63
85	S2	1004	PSU	O2-C2-N1	-2.72	119.98	122.79
5	L5	4689	PSU	C6-N1-C2	-2.72	120.17	122.69
5	L5	2837	OMU	O4-C4-C5	-2.72	120.47	125.16
85	S2	668	A2M	O3'-C3'-C2'	2.72	118.79	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L5	2839	PSU	O2-C2-N1	-2.72	119.99	122.79
85	S2	468	A2M	C1'-N9-C8	2.71	133.12	127.09
5	L5	3695	PSU	O2-C2-N1	-2.71	120.00	122.79
5	L5	4220	6MZ	C4-N9-C8	2.71	108.58	105.74
5	L5	4973	PSU	O2-C2-N1	-2.71	120.00	122.79
5	L5	3818	UY1	O2-C2-N1	-2.70	120.00	122.79
85	S2	166	A2M	C3'-C2'-C1'	-2.70	97.63	102.81
85	S2	159	A2M	C1'-N9-C8	2.70	133.09	127.09
85	S2	93	PSU	O2-C2-N1	-2.70	120.00	122.79
85	S2	1056	PSU	O2-C2-N1	-2.70	120.00	122.79
5	L5	3825	A2M	C4-N9-C1'	-2.70	120.32	126.63
85	S2	159	A2M	C4-N9-C1'	-2.69	120.33	126.63
5	L5	1524	A2M	C4'-O4'-C1'	-2.69	103.52	109.47
5	L5	398	A2M	C4-N9-C1'	-2.68	120.36	126.63
7	L8	55	PSU	O2-C2-N1	-2.68	120.03	122.79
5	L5	3830	A2M	C4-N9-C1'	-2.68	120.37	126.63
5	L5	400	A2M	C1'-N9-C8	2.68	133.04	127.09
5	L5	4620	OMU	O4-C4-C5	-2.68	120.54	125.16
85	S2	105	PSU	O2-C2-N1	-2.68	120.03	122.79
85	S2	1383	A2M	C1'-N9-C8	2.67	133.03	127.09
5	L5	3822	PSU	O2-C2-N1	-2.67	120.03	122.79
5	L5	2787	A2M	O4'-C1'-C2'	2.67	111.19	106.59
3	CF	163	SEP	OG-CB-CA	2.67	110.74	108.14
85	S2	27	A2M	C4-N9-C1'	-2.67	120.40	126.63
5	L5	1683	PSU	O2-C2-N1	-2.66	120.04	122.79
5	L5	3830	A2M	C1'-N9-C8	2.66	133.00	127.09
5	L5	1792	PSU	O2-C2-N1	-2.66	120.05	122.79
5	L5	400	A2M	C4-N9-C1'	-2.66	120.42	126.63
5	L5	4442	PSU	O2-C2-N1	-2.65	120.05	122.79
85	S2	27	A2M	C1'-N9-C8	2.65	132.98	127.09
85	S2	484	A2M	C1'-N9-C8	2.65	132.97	127.09
5	L5	4532	PSU	O2-C2-N1	-2.65	120.06	122.79
85	S2	484	A2M	C4-N9-C1'	-2.64	120.46	126.63
5	L5	3825	A2M	C1'-N9-C8	2.64	132.95	127.09
5	L5	1862	PSU	O2-C2-N1	-2.63	120.07	122.79
85	S2	1081	PSU	O2-C2-N1	-2.63	120.08	122.79
5	L5	398	A2M	C1'-N9-C8	2.63	132.93	127.09
5	L5	4576	PSU	O2-C2-N1	-2.62	120.08	122.79
5	L5	3853	PSU	O2-C2-N1	-2.62	120.08	122.79
5	L5	4530	UR3	C6-N1-C2	-2.62	119.66	121.80
5	L5	2632	PSU	O2-C2-N1	-2.62	120.09	122.79
85	S2	1232	PSU	O2-C2-N1	-2.62	120.09	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L5	3701	OMC	O2-C2-N1	2.61	124.01	118.90
5	L5	2804	OMC	C1'-N1-C2	2.61	124.19	118.44
5	L5	4636	PSU	O2-C2-N1	-2.60	120.10	122.79
85	S2	121	OMU	O4-C4-C5	-2.60	120.68	125.16
5	L5	4471	PSU	O2-C2-N1	-2.60	120.11	122.79
5	L5	3920	PSU	O2-C2-N1	-2.59	120.11	122.79
5	L5	5010	PSU	O2-C2-N1	-2.59	120.12	122.79
5	L5	4628	PSU	O2-C2-N1	-2.58	120.13	122.79
85	S2	649	PSU	O2-C2-N1	-2.58	120.13	122.79
5	L5	3785	A2M	C1'-N9-C8	2.57	132.80	127.09
5	L5	3639	PSU	O2-C2-N1	-2.56	120.14	122.79
85	S2	686	PSU	O2-C2-N1	-2.56	120.14	122.79
85	S2	1046	PSU	O2-C2-N1	-2.56	120.14	122.79
5	L5	2861	OMC	C1'-N1-C2	2.56	124.09	118.44
5	L5	3785	A2M	C4'-O4'-C1'	-2.55	103.83	109.47
85	S2	166	A2M	C4-N9-C1'	-2.55	120.66	126.63
5	L5	4431	PSU	O2-C2-N1	-2.55	120.16	122.79
5	L5	1323	A2M	O4'-C1'-C2'	2.55	110.98	106.59
85	S2	799	OMU	C1'-N1-C2	2.55	122.17	117.59
5	L5	1782	PSU	O2-C2-N1	-2.54	120.16	122.79
85	S2	1272	OMC	C1'-N1-C6	-2.54	115.36	120.78
85	S2	681	PSU	C6-N1-C2	-2.53	120.34	122.69
85	S2	668	A2M	O4'-C1'-C2'	2.53	110.95	106.59
5	L5	3718	A2M	C4-N9-C1'	-2.53	120.72	126.63
5	L5	1744	PSU	O2-C2-N1	-2.53	120.18	122.79
5	L5	1524	A2M	O4'-C1'-C2'	2.52	110.93	106.59
85	S2	866	PSU	O2-C2-N1	-2.52	120.19	122.79
5	L5	4293	PSU	C6-N1-C2	-2.52	120.35	122.69
5	L5	1677	PSU	O2-C2-N1	-2.52	120.19	122.79
5	L5	1323	A2M	C3'-C2'-C1'	-2.51	98.00	102.81
5	L5	3808	OMC	C1'-N1-C2	2.51	123.98	118.44
5	L5	5001	PSU	O2-C2-N1	-2.51	120.20	122.79
85	S2	814	PSU	O2-C2-N1	-2.50	120.21	122.79
5	L5	3867	A2M	O3'-C3'-C2'	2.49	118.17	111.19
5	L5	3867	A2M	C1'-N9-C8	2.49	132.63	127.09
5	L5	4571	A2M	C1'-N9-C8	2.48	132.61	127.09
5	L5	4636	PSU	C6-C5-C4	2.48	119.85	118.17
5	L5	4571	A2M	C4-N9-C1'	-2.48	120.83	126.63
85	S2	863	PSU	O2-C2-N1	-2.48	120.23	122.79
85	S2	1337	4AC	N4-C4-N3	2.47	117.88	113.87
5	L5	1582	PSU	O2-C2-N1	-2.47	120.24	122.79
5	L5	3785	A2M	C3'-C2'-C1'	-2.47	98.08	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L5	1323	A2M	C1'-N9-C8	2.46	132.56	127.09
5	L5	2363	A2M	C1'-N9-C8	2.45	132.53	127.09
5	L5	4361	PSU	O2-C2-N1	-2.45	120.26	122.79
5	L5	4299	PSU	O2-C2-N1	-2.44	120.27	122.79
5	L5	2363	A2M	O4'-C1'-C2'	2.43	110.78	106.59
5	L5	4673	PSU	O2-C2-N1	-2.43	120.28	122.79
5	L5	1326	A2M	C1'-N9-C8	2.43	132.49	127.09
85	S2	354	OMU	O2-C2-N1	-2.43	119.64	122.80
85	S2	166	A2M	C1'-N9-C8	2.43	132.48	127.09
5	L5	4579	PSU	C6-N1-C2	-2.42	120.44	122.69
5	L5	4500	PSU	C6-N1-C2	-2.42	120.45	122.69
5	L5	1534	A2M	C2'-C1'-N9	2.41	117.72	113.75
85	S2	159	A2M	C3'-C2'-C1'	-2.41	98.19	102.81
5	L5	2363	A2M	C4-N9-C1'	-2.40	121.02	126.63
5	L5	1326	A2M	C2'-C1'-N9	2.40	117.70	113.75
5	L5	3785	A2M	C2-N1-C6	-2.40	114.79	118.73
5	L5	3867	A2M	C4-N9-C1'	-2.40	121.03	126.63
85	S2	1177	PSU	O2-C2-N1	-2.39	120.32	122.79
85	S2	105	PSU	C6-N1-C2	-2.39	120.47	122.69
5	L5	2787	A2M	C4-N9-C1'	-2.39	121.05	126.63
5	L5	1323	A2M	C4-N9-C1'	-2.38	121.07	126.63
5	L5	2815	A2M	C1'-N9-C8	2.37	132.36	127.09
85	S2	428	OMU	O2-C2-N1	-2.37	119.71	122.80
5	L5	1534	A2M	C1'-N9-C8	2.37	132.35	127.09
85	S2	406	PSU	C6-N1-C2	-2.37	120.50	122.69
5	L5	1534	A2M	O3'-C3'-C4'	-2.36	104.29	111.08
5	L5	3695	PSU	C6-N1-C2	-2.36	120.50	122.69
5	L5	4403	PSU	O4'-C1'-C2'	2.36	108.41	105.15
85	S2	1367	PSU	C6-N1-C2	-2.36	120.50	122.69
5	L5	2787	A2M	C1'-N9-C8	2.36	132.32	127.09
85	S2	576	A2M	C4-N9-C1'	-2.35	121.13	126.63
5	L5	4628	PSU	C6-N1-C2	-2.35	120.51	122.69
85	S2	1832	6MZ	C4-C5-N7	-2.35	107.89	110.58
85	S2	1248	B8N	O4'-C1'-C2'	2.35	108.40	105.15
85	S2	651	PSU	C6-N1-C2	-2.34	120.52	122.69
85	S2	93	PSU	C6-N1-C2	-2.33	120.53	122.69
5	L5	4590	A2M	C6-C5-C4	-2.33	114.00	117.18
5	L5	1326	A2M	C3'-C2'-C1'	-2.33	98.35	102.81
5	L5	4456	OMC	C1'-N1-C2	2.32	123.57	118.44
5	L5	1322	1MA	N1-C6-N6	2.32	125.54	119.71
85	S2	1850	MA6	C1'-N9-C8	-2.32	121.95	127.09
5	L5	3637	PSU	C6-N1-C2	-2.31	120.54	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L5	1871	A2M	C6-C5-C4	-2.31	114.02	117.18
85	S2	121	OMU	O2-C2-N1	-2.31	119.79	122.80
5	L5	4973	PSU	C6-N1-C2	-2.31	120.55	122.69
5	L5	1326	A2M	C4-N9-C1'	-2.31	121.24	126.63
85	S2	484	A2M	O4'-C1'-C2'	2.30	110.56	106.59
7	L8	55	PSU	C6-N1-C2	-2.30	120.55	122.69
5	L5	1534	A2M	C4-N9-C1'	-2.30	121.25	126.63
5	L5	3884	PSU	C6-N1-C2	-2.30	120.56	122.69
85	S2	576	A2M	C1'-N9-C8	2.30	132.19	127.09
5	L5	4552	PSU	C6-N1-C2	-2.29	120.57	122.69
5	L5	4220	6MZ	C3'-C2'-C1'	2.29	105.79	101.46
5	L5	1524	A2M	C1'-N9-C8	2.28	132.17	127.09
85	S2	863	PSU	C6-N1-C2	-2.28	120.57	122.69
5	L5	3844	PSU	C6-N1-C2	-2.28	120.57	122.69
85	S2	668	A2M	C6-C5-C4	-2.28	114.06	117.18
7	L8	69	PSU	C6-N1-C2	-2.28	120.57	122.69
5	L5	2839	PSU	C6-N1-C2	-2.28	120.58	122.69
5	L5	3637	PSU	C6-C5-C4	2.27	119.71	118.17
85	S2	1442	OMU	C1'-N1-C2	2.27	121.68	117.59
5	L5	2815	A2M	C4-N9-C1'	-2.27	121.32	126.63
5	L5	4353	PSU	C6-N1-C2	-2.27	120.58	122.69
5	L5	4972	PSU	C6-N1-C2	-2.27	120.58	122.69
5	L5	3637	PSU	O2-C2-N1	-2.27	120.45	122.79
5	L5	3785	A2M	O4'-C4'-C3'	2.26	109.65	105.15
85	S2	1244	PSU	C6-N1-C2	-2.26	120.59	122.69
5	L5	4442	PSU	O4'-C1'-C2'	2.26	108.28	105.15
5	L5	1536	PSU	C6-N1-C2	-2.25	120.60	122.69
85	S2	1004	PSU	C6-N1-C2	-2.25	120.61	122.69
5	L5	2632	PSU	C6-N1-C2	-2.24	120.61	122.69
5	L5	5010	PSU	C6-N1-C2	-2.24	120.61	122.69
5	L5	2787	A2M	O4'-C4'-C3'	2.24	109.60	105.15
85	S2	1383	A2M	C6-C5-C4	-2.24	114.12	117.18
5	L5	2401	A2M	C6-C5-C4	-2.23	114.13	117.18
85	S2	686	PSU	C6-N1-C2	-2.23	120.62	122.69
85	S2	801	PSU	C6-N1-C2	-2.23	120.62	122.69
7	L8	69	PSU	O4'-C1'-C2'	2.23	108.23	105.15
5	L5	3785	A2M	C5-C6-N1	2.22	123.16	117.51
5	L5	4312	PSU	C6-N1-C2	-2.22	120.63	122.69
5	L5	3867	A2M	C2-N1-C6	-2.22	115.09	118.73
5	L5	4296	PSU	C6-N1-C2	-2.21	120.64	122.69
5	L5	1534	A2M	O3'-C3'-C2'	2.21	117.37	111.19
5	L5	400	A2M	C2'-C1'-N9	2.21	117.39	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L5	3920	PSU	C6-N1-C2	-2.21	120.64	122.69
5	L5	4498	OMU	O2-C2-N1	-2.20	119.93	122.80
85	S2	27	A2M	O4'-C1'-C2'	2.20	110.38	106.59
5	L5	4442	PSU	C6-N1-C2	-2.20	120.65	122.69
5	L5	3853	PSU	C6-N1-C2	-2.20	120.65	122.69
85	S2	1046	PSU	C6-N1-C2	-2.20	120.65	122.69
5	L5	2815	A2M	C3'-C2'-C1'	-2.20	98.60	102.81
85	S2	866	PSU	C6-N1-C2	-2.20	120.65	122.69
5	L5	4576	PSU	C6-N1-C2	-2.19	120.66	122.69
85	S2	1639	G7M	N9-C8-N7	-2.19	107.16	112.48
85	S2	1851	MA6	C4-C5-N7	-2.19	108.08	110.58
85	S2	1031	A2M	C6-C5-C4	-2.19	114.19	117.18
85	S2	866	PSU	O4'-C1'-C2'	2.18	108.17	105.15
5	L5	1683	PSU	C6-N1-C2	-2.18	120.67	122.69
5	L5	4532	PSU	C6-N1-C2	-2.18	120.67	122.69
5	L5	3822	PSU	O4'-C1'-C2'	2.18	108.17	105.15
5	L5	400	A2M	O4'-C1'-C2'	2.18	110.34	106.59
5	L5	1524	A2M	C4-N9-C1'	-2.18	121.55	126.63
5	L5	4431	PSU	C6-N1-C2	-2.17	120.67	122.69
5	L5	1862	PSU	C6-N1-C2	-2.17	120.68	122.69
5	L5	1326	A2M	C5-C6-N1	2.17	123.02	117.51
85	S2	27	A2M	C6-C5-C4	-2.17	114.22	117.18
5	L5	4457	PSU	C6-N1-C2	-2.16	120.68	122.69
85	S2	966	PSU	C6-N1-C2	-2.16	120.68	122.69
5	L5	1534	A2M	C2-N1-C6	-2.16	115.18	118.73
85	S2	166	A2M	O4'-C1'-C2'	2.16	110.31	106.59
5	L5	5001	PSU	C6-N1-C2	-2.16	120.69	122.69
85	S2	1177	PSU	C6-N1-C2	-2.16	120.69	122.69
5	L5	4523	A2M	C6-C5-C4	-2.15	114.24	117.18
85	S2	99	A2M	C6-C5-C4	-2.15	114.24	117.18
5	L5	2815	A2M	O4'-C1'-C2'	2.15	110.29	106.59
85	S2	1232	PSU	C6-N1-C2	-2.15	120.70	122.69
5	L5	400	A2M	C6-C5-C4	-2.15	114.25	117.18
85	S2	468	A2M	C6-C5-C4	-2.15	114.25	117.18
5	L5	3785	A2M	C6-C5-C4	-2.14	114.25	117.18
5	L5	1744	PSU	C6-N1-C2	-2.14	120.70	122.69
5	L5	1326	A2M	C2-N1-C6	-2.14	115.21	118.73
5	L5	4521	PSU	C6-N1-C2	-2.14	120.71	122.69
5	L5	3825	A2M	C6-C5-C4	-2.13	114.26	117.18
85	S2	1851	MA6	C1'-N9-C8	-2.13	122.36	127.09
5	L5	3639	PSU	C6-N1-C2	-2.13	120.72	122.69
5	L5	1323	A2M	C2-N1-C6	-2.13	115.24	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L5	4636	PSU	O4'-C1'-C2'	2.12	108.09	105.15
5	L5	4457	PSU	O4'-C1'-C2'	2.12	108.09	105.15
85	S2	814	PSU	C6-N1-C2	-2.12	120.72	122.69
85	S2	159	A2M	O4'-C1'-C2'	2.12	110.24	106.59
5	L5	3822	PSU	C6-N1-C2	-2.12	120.72	122.69
5	L5	3925	OMU	O2-C2-N1	-2.12	120.04	122.80
5	L5	4620	OMU	O2-C2-N1	-2.12	120.04	122.80
5	L5	3830	A2M	C6-C5-C4	-2.12	114.28	117.18
5	L5	3718	A2M	C2-N1-C6	-2.12	115.25	118.73
5	L5	4220	6MZ	C5-C6-N1	2.11	120.42	118.15
85	S2	1326	OMU	O2-C2-N1	-2.11	120.05	122.80
5	L5	4571	A2M	C6-C5-C4	-2.11	114.30	117.18
5	L5	4521	PSU	C6-C5-C4	2.10	119.59	118.17
5	L5	1524	A2M	C2-N1-C6	-2.10	115.27	118.73
5	L5	4523	A2M	C4'-O4'-C1'	-2.10	104.83	109.47
5	L5	1781	PSU	C6-N1-C2	-2.10	120.75	122.69
85	S2	1248	B8N	O4-C4-C5	-2.09	118.96	122.58
5	L5	3867	A2M	O4'-C4'-C3'	2.09	109.31	105.15
5	L5	1534	A2M	C5-C6-N1	2.09	122.83	117.51
5	L5	1871	A2M	C4'-O4'-C1'	-2.09	104.85	109.47
5	L5	3867	A2M	C6-C5-C4	-2.09	114.32	117.18
85	S2	1174	PSU	C6-N1-C2	-2.09	120.75	122.69
5	L5	1323	A2M	C5-C6-N1	2.09	122.81	117.51
85	S2	1081	PSU	C6-N1-C2	-2.08	120.76	122.69
85	S2	406	PSU	C6-C5-C4	2.08	119.58	118.17
5	L5	398	A2M	C5-C6-N1	2.08	122.80	117.51
5	L5	398	A2M	C6-C5-C4	-2.08	114.34	117.18
5	L5	4523	A2M	C2-N1-C6	-2.08	115.32	118.73
5	L5	3830	A2M	C5-C6-N1	2.08	122.79	117.51
85	S2	484	A2M	C6-C5-C4	-2.08	114.34	117.18
5	L5	4227	OMU	O2-C2-N1	-2.08	120.09	122.80
85	S2	159	A2M	C6-C5-C4	-2.08	114.34	117.18
85	S2	1031	A2M	O4'-C1'-C2'	2.07	110.16	106.59
5	L5	4673	PSU	C6-N1-C2	-2.07	120.77	122.69
5	L5	2363	A2M	C2-N1-C6	-2.07	115.33	118.73
5	L5	2787	A2M	C2-N1-C6	-2.07	115.33	118.73
85	S2	99	A2M	O4'-C1'-C2'	2.07	110.15	106.59
5	L5	2815	A2M	C6-C5-C4	-2.07	114.35	117.18
5	L5	398	A2M	C2-N1-C6	-2.06	115.34	118.73
5	L5	1582	PSU	C6-N1-C2	-2.06	120.78	122.69
5	L5	1323	A2M	C6-C5-C4	-2.06	114.37	117.18
5	L5	4590	A2M	O4'-C1'-C2'	2.06	110.13	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	S2	1850	MA6	C4-C5-N7	-2.06	108.23	110.58
5	L5	4571	A2M	C2-N1-C6	-2.05	115.36	118.73
5	L5	3825	A2M	C2-N1-C6	-2.05	115.36	118.73
85	S2	27	A2M	C5-C6-N1	2.05	122.72	117.51
5	L5	2363	A2M	C5-C6-N1	2.05	122.72	117.51
5	L5	1326	A2M	O4'-C1'-C2'	2.05	110.12	106.59
85	S2	172	OMU	O2-C2-N1	-2.05	120.13	122.80
85	S2	159	A2M	C5-C6-N1	2.05	122.71	117.51
5	L5	4500	PSU	C6-C5-C4	2.05	119.55	118.17
5	L5	3695	PSU	O4'-C1'-C2'	2.04	107.98	105.15
5	L5	1782	PSU	C6-N1-C2	-2.04	120.80	122.69
5	L5	2787	A2M	C5-C6-N1	2.04	122.69	117.51
5	L5	4523	A2M	C5-C6-N1	2.04	122.69	117.51
85	S2	576	A2M	C5-C6-N1	2.04	122.69	117.51
85	S2	1031	A2M	C5-C6-N1	2.04	122.69	117.51
85	S2	576	A2M	C6-C5-C4	-2.04	114.39	117.18
5	L5	1534	A2M	C6-C5-C4	-2.04	114.40	117.18
85	S2	1056	PSU	C6-N1-C2	-2.03	120.80	122.69
85	S2	99	A2M	C2-N1-C6	-2.03	115.39	118.73
85	S2	166	A2M	C5-C6-N1	2.03	122.68	117.51
85	S2	109	PSU	C6-N1-C2	-2.03	120.80	122.69
5	L5	400	A2M	C5-C6-N1	2.03	122.67	117.51
5	L5	1860	PSU	C6-N1-C2	-2.03	120.81	122.69
5	L5	2815	A2M	C5-C6-N1	2.03	122.67	117.51
5	L5	400	A2M	C2-N1-C6	-2.03	115.39	118.73
85	S2	1081	PSU	O4'-C1'-C2'	2.03	107.96	105.15
5	L5	3830	A2M	C2-N1-C6	-2.03	115.40	118.73
85	S2	668	A2M	C2-N1-C6	-2.03	115.40	118.73
85	S2	1288	OMU	O2-C2-N1	-2.03	120.16	122.80
5	L5	2401	A2M	C5-C6-N1	2.03	122.66	117.51
5	L5	4576	PSU	O4'-C1'-C2'	2.03	107.96	105.15
85	S2	468	A2M	C5-C6-N1	2.03	122.66	117.51
5	L5	1326	A2M	C6-C5-C4	-2.03	114.41	117.18
5	L5	3825	A2M	C5-C6-N1	2.02	122.65	117.51
5	L5	4471	PSU	C6-N1-C2	-2.02	120.82	122.69
5	L5	3867	A2M	C5-C6-N1	2.02	122.64	117.51
85	S2	99	A2M	C5-C6-N1	2.02	122.64	117.51
5	L5	3841	OMC	C1'-N1-C2	2.02	122.90	118.44
85	S2	668	A2M	C4'-O4'-C1'	-2.02	105.01	109.47
5	L5	2787	A2M	C6-C5-C4	-2.02	114.42	117.18
5	L5	4571	A2M	C5-C6-N1	2.02	122.63	117.51
85	S2	159	A2M	C2-N1-C6	-2.02	115.42	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L5	4636	PSU	C6-N1-C2	-2.01	120.82	122.69
85	S2	166	A2M	C6-C5-C4	-2.01	114.44	117.18
85	S2	484	A2M	C5-C6-N1	2.01	122.61	117.51
5	L5	4299	PSU	C6-N1-C2	-2.00	120.83	122.69
85	S2	159	A2M	C2'-C1'-N9	2.00	117.05	113.75
85	S2	1045	PSU	C6-N1-C2	-2.00	120.83	122.69
85	S2	576	A2M	C2-N1-C6	-2.00	115.44	118.73

There are no chirality outliers.

All (162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	CF	163	SEP	N-CA-CB-OG
3	CF	163	SEP	C-CA-CB-OG
3	CF	163	SEP	CA-CB-OG-P
3	CF	163	SEP	CB-OG-P-O2P
3	CF	163	SEP	CB-OG-P-O3P
7	L8	75	OMG	C1'-C2'-O2'-CM2
5	L5	400	A2M	C1'-C2'-O2'-CM'
5	L5	1326	A2M	O4'-C4'-C5'-O5'
5	L5	1340	OMC	C1'-C2'-O2'-CM2
5	L5	1625	OMG	O4'-C4'-C5'-O5'
5	L5	2351	OMC	C1'-C2'-O2'-CM2
5	L5	2787	A2M	C1'-C2'-O2'-CM'
5	L5	2824	OMC	C1'-C2'-O2'-CM2
5	L5	2861	OMC	C1'-C2'-O2'-CM2
5	L5	3701	OMC	O4'-C4'-C5'-O5'
5	L5	3792	OMG	O4'-C4'-C5'-O5'
5	L5	3841	OMC	C1'-C2'-O2'-CM2
5	L5	3867	A2M	C3'-C4'-C5'-O5'
5	L5	3867	A2M	C1'-C2'-O2'-CM'
5	L5	4196	OMG	C1'-C2'-O2'-CM2
5	L5	4500	PSU	O4'-C4'-C5'-O5'
5	L5	4590	A2M	O4'-C4'-C5'-O5'
5	L5	4637	OMG	O4'-C4'-C5'-O5'
5	L5	4637	OMG	C1'-C2'-O2'-CM2
85	S2	27	A2M	C1'-C2'-O2'-CM'
85	S2	99	A2M	C1'-C2'-O2'-CM'
85	S2	159	A2M	C1'-C2'-O2'-CM'
85	S2	576	A2M	C1'-C2'-O2'-CM'
85	S2	601	OMG	C1'-C2'-O2'-CM2
85	S2	644	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
85	S2	644	OMG	C1'-C2'-O2'-CM2
85	S2	1248	B8N	O4'-C4'-C5'-O5'
85	S2	1272	OMC	C1'-C2'-O2'-CM2
85	S2	1272	OMC	O4'-C4'-C5'-O5'
85	S2	1288	OMU	O4'-C4'-C5'-O5'
85	S2	1328	OMG	C1'-C2'-O2'-CM2
85	S2	1337	4AC	N3-C4-N4-C7
85	S2	1383	A2M	C1'-C2'-O2'-CM'
85	S2	1442	OMU	O4'-C4'-C5'-O5'
85	S2	1832	6MZ	C5-C6-N6-C9
85	S2	1832	6MZ	N1-C6-N6-C9
5	L5	1326	A2M	C3'-C4'-C5'-O5'
5	L5	3701	OMC	C3'-C4'-C5'-O5'
5	L5	4500	PSU	C3'-C4'-C5'-O5'
5	L5	4590	A2M	C3'-C4'-C5'-O5'
85	S2	436	OMG	O4'-C4'-C5'-O5'
85	S2	576	A2M	O4'-C4'-C5'-O5'
85	S2	576	A2M	C3'-C4'-C5'-O5'
85	S2	801	PSU	C3'-C4'-C5'-O5'
85	S2	867	OMG	C3'-C4'-C5'-O5'
85	S2	1272	OMC	C3'-C4'-C5'-O5'
5	L5	3701	OMC	C2'-C1'-N1-C2
5	L5	1323	A2M	O4'-C4'-C5'-O5'
5	L5	1536	PSU	C3'-C4'-C5'-O5'
5	L5	1536	PSU	O4'-C4'-C5'-O5'
5	L5	2401	A2M	C3'-C4'-C5'-O5'
5	L5	2815	A2M	O4'-C4'-C5'-O5'
5	L5	3867	A2M	O4'-C4'-C5'-O5'
5	L5	3899	OMG	O4'-C4'-C5'-O5'
5	L5	3899	OMG	C3'-C4'-C5'-O5'
85	S2	99	A2M	O4'-C4'-C5'-O5'
85	S2	517	OMC	C3'-C4'-C5'-O5'
85	S2	517	OMC	O4'-C4'-C5'-O5'
85	S2	799	OMU	C3'-C4'-C5'-O5'
85	S2	867	OMG	O4'-C4'-C5'-O5'
85	S2	1442	OMU	C3'-C4'-C5'-O5'
5	L5	1625	OMG	C3'-C4'-C5'-O5'
5	L5	3792	OMG	C3'-C4'-C5'-O5'
5	L5	4637	OMG	C3'-C4'-C5'-O5'
85	S2	644	OMG	C3'-C4'-C5'-O5'
85	S2	668	A2M	O4'-C4'-C5'-O5'
85	S2	799	OMU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
85	S2	1248	B8N	C3'-C4'-C5'-O5'
85	S2	1288	OMU	C3'-C4'-C5'-O5'
5	L5	3701	OMC	C2'-C1'-N1-C6
5	L5	4447	5MC	C2'-C1'-N1-C6
5	L5	2787	A2M	C3'-C4'-C5'-O5'
85	S2	668	A2M	C3'-C4'-C5'-O5'
5	L5	1524	A2M	O4'-C4'-C5'-O5'
5	L5	1677	PSU	O4'-C4'-C5'-O5'
5	L5	4228	OMG	O4'-C4'-C5'-O5'
5	L5	4618	OMG	C3'-C4'-C5'-O5'
85	S2	436	OMG	C3'-C4'-C5'-O5'
85	S2	627	OMU	O4'-C4'-C5'-O5'
85	S2	801	PSU	O4'-C4'-C5'-O5'
5	L5	1524	A2M	C3'-C4'-C5'-O5'
5	L5	1677	PSU	C3'-C4'-C5'-O5'
5	L5	2401	A2M	O4'-C4'-C5'-O5'
5	L5	2815	A2M	C3'-C4'-C5'-O5'
5	L5	3785	A2M	O4'-C4'-C5'-O5'
5	L5	4228	OMG	C3'-C4'-C5'-O5'
85	S2	1248	B8N	N34-C33-C34-O36
3	CF	163	SEP	CB-OG-P-O1P
5	L5	2787	A2M	C2'-C1'-N9-C8
5	L5	3818	UY1	C4'-C5'-O5'-P
5	L5	4590	A2M	C4'-C5'-O5'-P
5	L5	1323	A2M	C3'-C4'-C5'-O5'
5	L5	4296	PSU	O4'-C4'-C5'-O5'
85	S2	99	A2M	C3'-C4'-C5'-O5'
85	S2	428	OMU	O4'-C4'-C5'-O5'
5	L5	2422	OMC	O4'-C4'-C5'-O5'
5	L5	4296	PSU	C3'-C4'-C5'-O5'
5	L5	2422	OMC	C3'-C4'-C5'-O5'
5	L5	3851	PSU	C3'-C4'-C5'-O5'
85	S2	1045	PSU	O4'-C4'-C5'-O5'
85	S2	1832	6MZ	C5'-O5'-P-OP2
85	S2	1248	B8N	C31-C32-C33-C34
5	L5	3782	5MC	O4'-C4'-C5'-O5'
5	L5	4618	OMG	O4'-C4'-C5'-O5'
85	S2	428	OMU	C3'-C4'-C5'-O5'
85	S2	1045	PSU	C3'-C4'-C5'-O5'
85	S2	428	OMU	C2'-C1'-N1-C6
5	L5	4447	5MC	C2'-C1'-N1-C2
5	L5	4447	5MC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
5	L5	3701	OMC	O4'-C1'-N1-C6
5	L5	398	A2M	O4'-C4'-C5'-O5'
85	S2	627	OMU	C2'-C1'-N1-C6
5	L5	4447	5MC	O4'-C1'-N1-C2
5	L5	4499	OMG	C3'-C2'-O2'-CM2
5	L5	1534	A2M	C4'-C5'-O5'-P
85	S2	644	OMG	C4'-C5'-O5'-P
5	L5	3818	UY1	O4'-C1'-C5-C4
85	S2	1248	B8N	O4'-C1'-C5-C4
5	L5	2787	A2M	C2'-C1'-N9-C4
5	L5	4500	PSU	C4'-C5'-O5'-P
5	L5	1781	PSU	C3'-C4'-C5'-O5'
5	L5	2876	OMG	C3'-C4'-C5'-O5'
85	S2	576	A2M	C4'-C5'-O5'-P
85	S2	1851	MA6	C4'-C5'-O5'-P
85	S2	1383	A2M	O4'-C4'-C5'-O5'
5	L5	3701	OMC	O4'-C1'-N1-C2
85	S2	428	OMU	O4'-C1'-N1-C6
5	L5	3785	A2M	C3'-C2'-O2'-CM'
5	L5	3869	OMC	C3'-C2'-O2'-CM2
5	L5	4370	OMG	C3'-C2'-O2'-CM2
85	S2	174	OMC	C3'-C2'-O2'-CM2
5	L5	2364	OMG	O4'-C4'-C5'-O5'
5	L5	3785	A2M	C3'-C4'-C5'-O5'
85	S2	1832	6MZ	O4'-C4'-C5'-O5'
85	S2	627	OMU	O4'-C1'-N1-C6
5	L5	3844	PSU	C4'-C5'-O5'-P
85	S2	1490	OMG	C4'-C5'-O5'-P
85	S2	1703	OMC	O4'-C4'-C5'-O5'
5	L5	1322	1MA	C2'-C1'-N9-C8
5	L5	3718	A2M	C1'-C2'-O2'-CM'
5	L5	3887	OMC	C4'-C5'-O5'-P
85	S2	1383	A2M	C3'-C4'-C5'-O5'
5	L5	1677	PSU	O4'-C1'-C5-C6
5	L5	4636	PSU	O4'-C1'-C5-C6
5	L5	2351	OMC	C2'-C1'-N1-C6
5	L5	1326	A2M	C4'-C5'-O5'-P
5	L5	4471	PSU	C3'-C4'-C5'-O5'
5	L5	1322	1MA	C2'-C1'-N9-C4
5	L5	2351	OMC	O4'-C4'-C5'-O5'
5	L5	2787	A2M	O4'-C4'-C5'-O5'
85	S2	428	OMU	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
85	S2	627	OMU	O4'-C1'-N1-C2
85	S2	1272	OMC	C2'-C1'-N1-C6
5	L5	2787	A2M	O4'-C1'-N9-C8
85	S2	1081	PSU	C4'-C5'-O5'-P
85	S2	428	OMU	C2'-C1'-N1-C2
85	S2	1272	OMC	C2'-C1'-N1-C2

There are no ring outliers.

75 monomers are involved in 106 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L5	1340	OMC	2	0
85	S2	1031	A2M	1	0
85	S2	1177	PSU	1	0
5	L5	4579	PSU	2	0
5	L5	3627	OMG	1	0
85	S2	1288	OMU	1	0
5	L5	4306	OMU	1	0
85	S2	1337	4AC	4	0
5	L5	2824	OMC	1	0
85	S2	436	OMG	1	0
5	L5	4523	A2M	2	0
5	L5	4500	PSU	1	0
5	L5	3867	A2M	3	0
85	S2	1391	OMC	1	0
85	S2	1832	6MZ	1	0
5	L5	3701	OMC	1	0
85	S2	576	A2M	2	0
5	L5	2861	OMC	1	0
5	L5	4689	PSU	1	0
5	L5	1677	PSU	1	0
5	L5	3785	A2M	1	0
7	L8	75	OMG	2	0
5	L5	3884	PSU	1	0
5	L5	2351	OMC	1	0
5	L5	4220	6MZ	1	0
5	L5	2424	OMG	1	0
5	L5	2804	OMC	2	0
5	L5	2815	A2M	1	0
85	S2	867	OMG	2	0
85	S2	1383	A2M	1	0
5	L5	400	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	S2	159	A2M	2	0
85	S2	509	OMG	3	0
85	S2	686	PSU	1	0
5	L5	4590	A2M	1	0
85	S2	866	PSU	2	0
5	L5	5001	PSU	1	0
85	S2	166	A2M	2	0
85	S2	121	OMU	1	0
5	L5	4571	A2M	2	0
85	S2	681	PSU	1	0
5	L5	4536	OMC	1	0
85	S2	517	OMC	1	0
5	L5	4457	PSU	1	0
5	L5	3718	A2M	4	0
5	L5	2876	OMG	1	0
85	S2	27	A2M	1	0
85	S2	863	PSU	1	0
85	S2	1174	PSU	2	0
85	S2	1244	PSU	1	0
5	L5	4431	PSU	1	0
5	L5	2787	A2M	1	0
5	L5	4618	OMG	1	0
85	S2	649	PSU	2	0
85	S2	601	OMG	1	0
5	L5	3822	PSU	2	0
5	L5	1326	A2M	4	0
5	L5	2363	A2M	1	0
5	L5	1683	PSU	2	0
3	CF	163	SEP	1	0
5	L5	4620	OMU	3	0
5	L5	4637	OMG	1	0
85	S2	484	A2M	1	0
85	S2	462	OMC	1	0
85	S2	99	A2M	1	0
5	L5	3925	OMU	1	0
85	S2	1272	OMC	1	0
85	S2	1850	MA6	2	0
5	L5	4456	OMC	1	0
5	L5	3841	OMC	1	0
85	S2	1842	4AC	1	0
5	L5	2364	OMG	1	0
85	S2	468	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L5	1534	A2M	2	0
5	L5	3825	A2M	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	$\# Z > 2$
87	SPM	L5	5264	-	13,13,13	0.34	0	12,12,12	0.92	0
88	SPD	L5	5289	-	9,9,9	0.33	0	8,8,8	0.86	0
88	SPD	L5	5290	-	9,9,9	0.33	0	8,8,8	0.68	0
88	SPD	L5	5286	-	9,9,9	0.33	0	8,8,8	0.88	0
88	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.81	0
88	SPD	LN	301	-	9,9,9	0.32	0	8,8,8	0.84	0
87	SPM	L5	5291	-	13,13,13	0.36	0	12,12,12	0.88	0
87	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.91	0
88	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.84	0
87	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	1.00	0
87	SPM	L5	5267	-	13,13,13	0.35	0	12,12,12	0.99	0
88	SPD	L5	5282	-	9,9,9	0.34	0	8,8,8	0.84	0
88	SPD	L5	5261	-	9,9,9	0.32	0	8,8,8	0.95	0
88	SPD	L5	5283	-	9,9,9	0.32	0	8,8,8	0.88	0
87	SPM	L5	5288	-	13,13,13	0.36	0	12,12,12	0.98	0
88	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.87	0
87	SPM	L5	5258	-	13,13,13	0.35	0	12,12,12	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPM	L5	5264	-	-	2/11/11/11	-
88	SPD	L5	5289	-	-	2/7/7/7	-
88	SPD	L5	5290	-	-	2/7/7/7	-
88	SPD	L5	5286	-	-	3/7/7/7	-
88	SPD	L5	5285	-	-	1/7/7/7	-
88	SPD	LN	301	-	-	1/7/7/7	-
87	SPM	L5	5291	-	-	3/11/11/11	-
87	SPM	L5	5292	-	-	5/11/11/11	-
88	SPD	L5	5287	-	-	1/7/7/7	-
87	SPM	L5	5263	-	-	6/11/11/11	-
87	SPM	L5	5267	-	-	4/11/11/11	-
88	SPD	L5	5282	-	-	1/7/7/7	-
88	SPD	L5	5261	-	-	0/7/7/7	-
88	SPD	L5	5283	-	-	4/7/7/7	-
87	SPM	L5	5288	-	-	5/11/11/11	-
88	SPD	L5	5284	-	-	4/7/7/7	-
87	SPM	L5	5258	-	-	2/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	L5	5264	SPM	N5-C6-C7-C8
87	L5	5291	SPM	C7-C8-C9-N10
88	L5	5286	SPD	C3-C4-C5-N6
87	L5	5291	SPM	N5-C6-C7-C8
87	L5	5292	SPM	N10-C11-C12-C13
88	L5	5284	SPD	N6-C7-C8-C9
87	L5	5292	SPM	C8-C9-N10-C11
88	L5	5290	SPD	C8-C7-N6-C5
87	L5	5263	SPM	C7-C8-C9-N10
87	L5	5258	SPM	C3-C4-N5-C6
87	L5	5263	SPM	C3-C4-N5-C6
88	L5	5290	SPD	C4-C5-N6-C7
88	L5	5284	SPD	C3-C4-C5-N6

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Mol	Chain	Res	Type	Atoms
88	L5	5284	SPD	C4-C5-N6-C7
87	L5	5263	SPM	C8-C9-N10-C11
87	L5	5288	SPM	C7-C6-N5-C4
88	L5	5283	SPD	C8-C7-N6-C5
87	L5	5267	SPM	C2-C3-C4-N5
88	L5	5284	SPD	C2-C3-C4-C5
88	L5	5282	SPD	C2-C3-C4-C5
88	L5	5289	SPD	C2-C3-C4-C5
87	L5	5288	SPM	N1-C2-C3-C4
88	L5	5283	SPD	C7-C8-C9-N10
88	LN	301	SPD	C4-C5-N6-C7
87	L5	5288	SPM	C7-C8-C9-N10
87	L5	5292	SPM	C7-C6-N5-C4
88	L5	5283	SPD	N1-C2-C3-C4
87	L5	5288	SPM	C12-C11-N10-C9
88	L5	5286	SPD	C8-C7-N6-C5
87	L5	5292	SPM	C6-C7-C8-C9
87	L5	5263	SPM	N10-C11-C12-C13
87	L5	5263	SPM	C11-C12-C13-N14
87	L5	5288	SPM	C8-C9-N10-C11
87	L5	5292	SPM	C11-C12-C13-N14
88	L5	5283	SPD	C3-C4-C5-N6
87	L5	5264	SPM	C12-C11-N10-C9
87	L5	5267	SPM	C7-C6-N5-C4
87	L5	5263	SPM	C2-C3-C4-N5
87	L5	5267	SPM	N10-C11-C12-C13
88	L5	5286	SPD	N6-C7-C8-C9
88	L5	5285	SPD	C3-C4-C5-N6
87	L5	5258	SPM	C6-C7-C8-C9
87	L5	5267	SPM	C6-C7-C8-C9
87	L5	5291	SPM	C7-C6-N5-C4
88	L5	5287	SPD	C8-C7-N6-C5
88	L5	5289	SPD	C7-C8-C9-N10

There are no ring outliers.

5 monomers are involved in 7 short contacts:

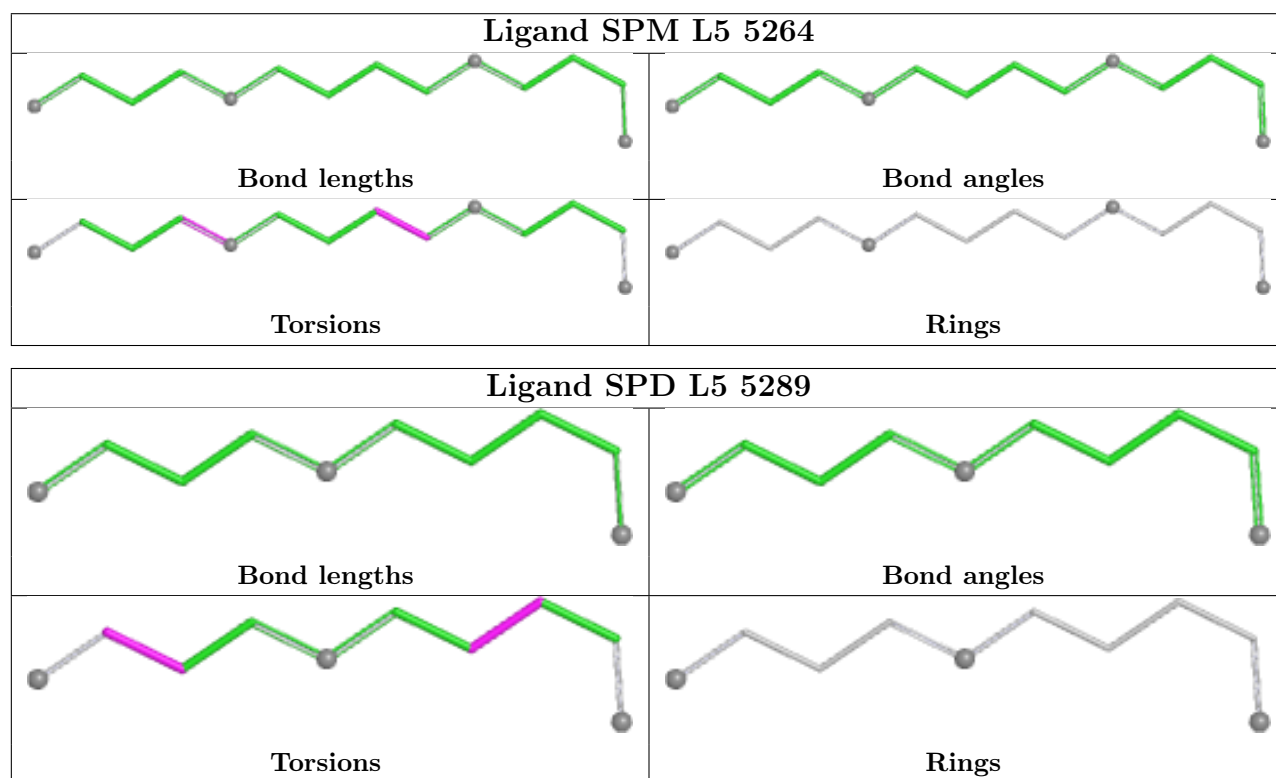
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5290	SPD	1	0
88	L5	5285	SPD	1	0
87	L5	5291	SPM	2	0
87	L5	5292	SPM	2	0

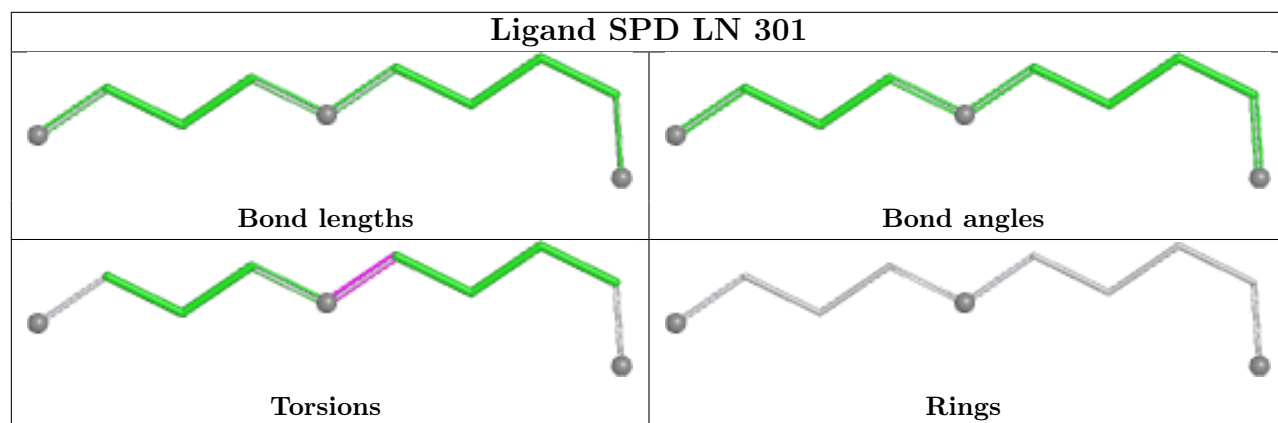
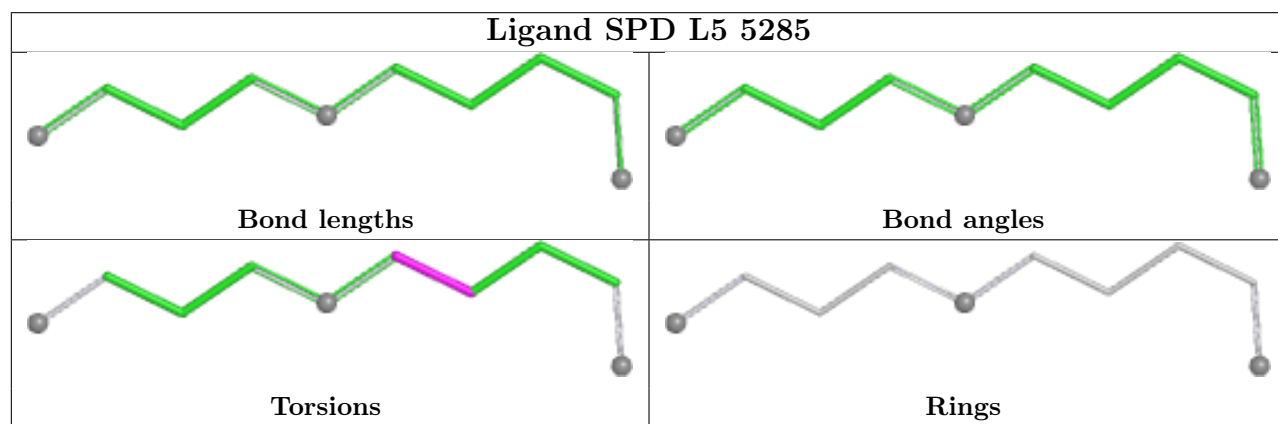
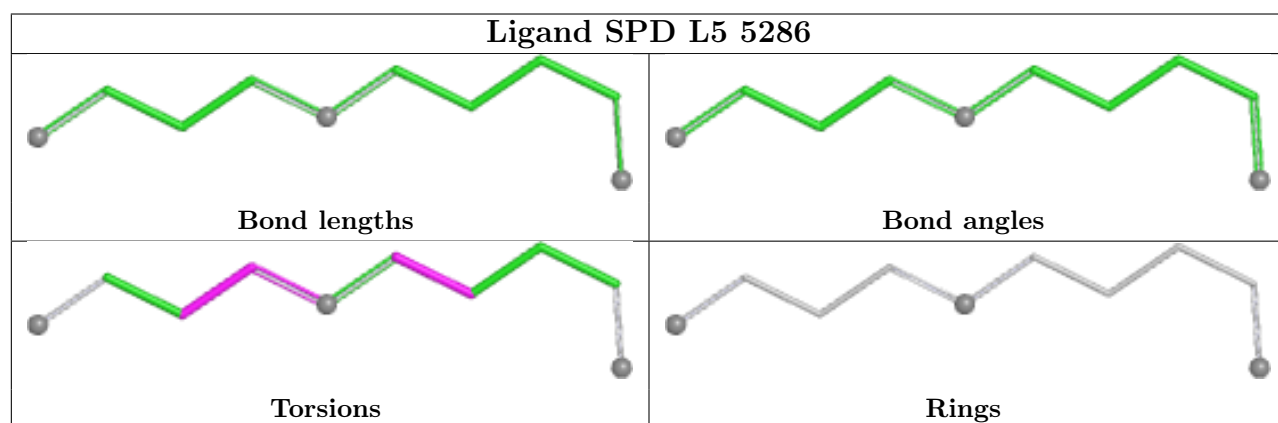
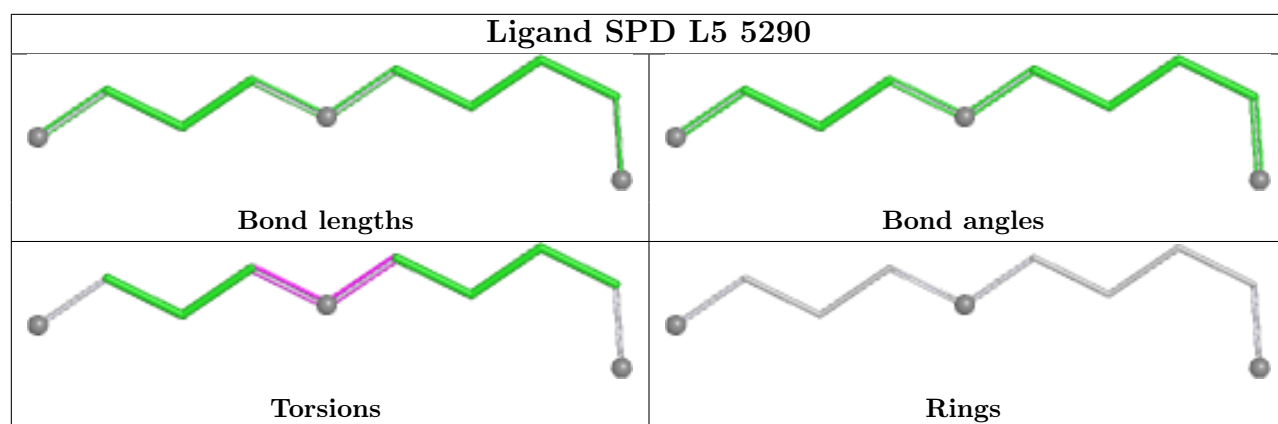
Continued on next page...

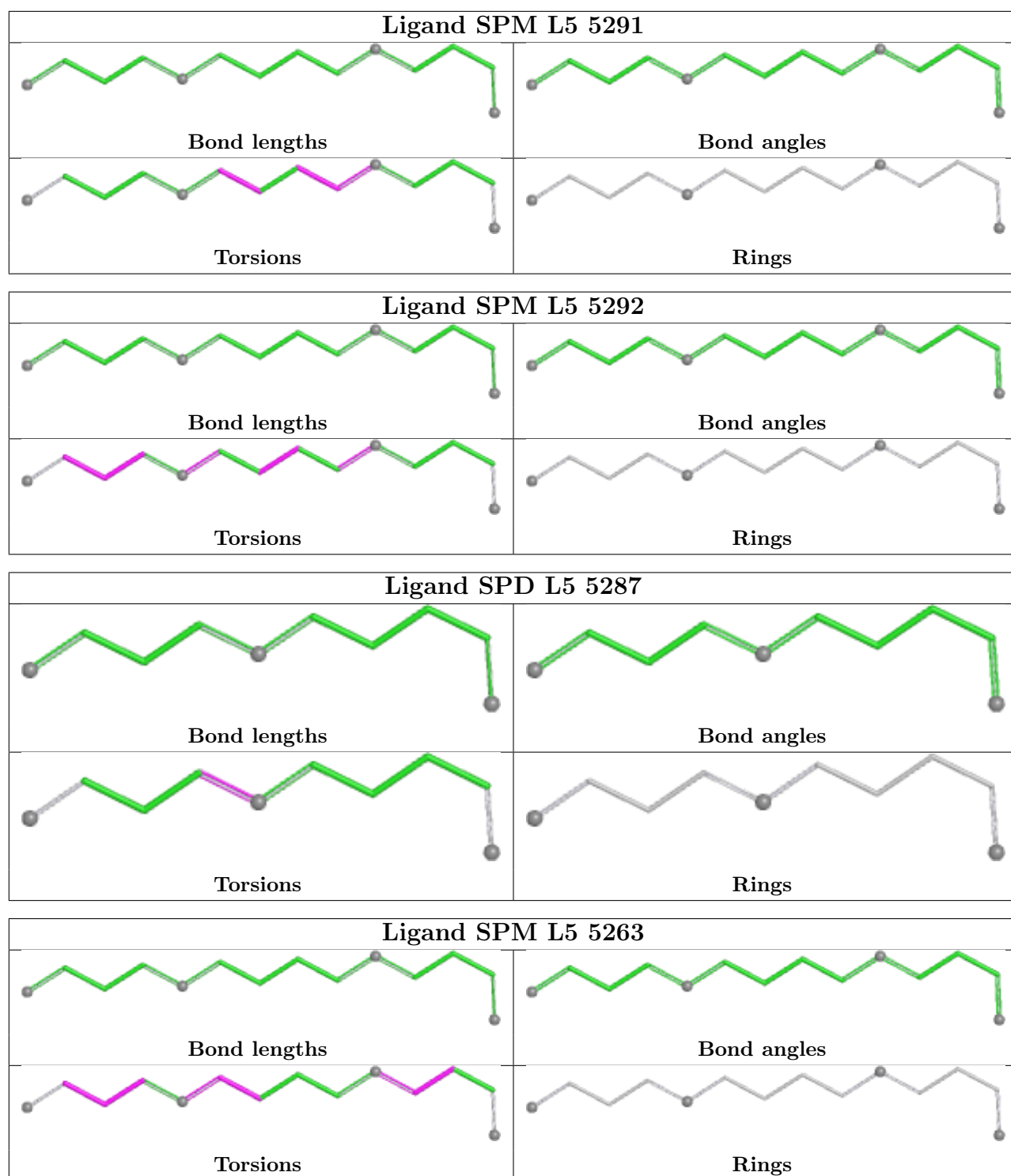
Continued from previous page...

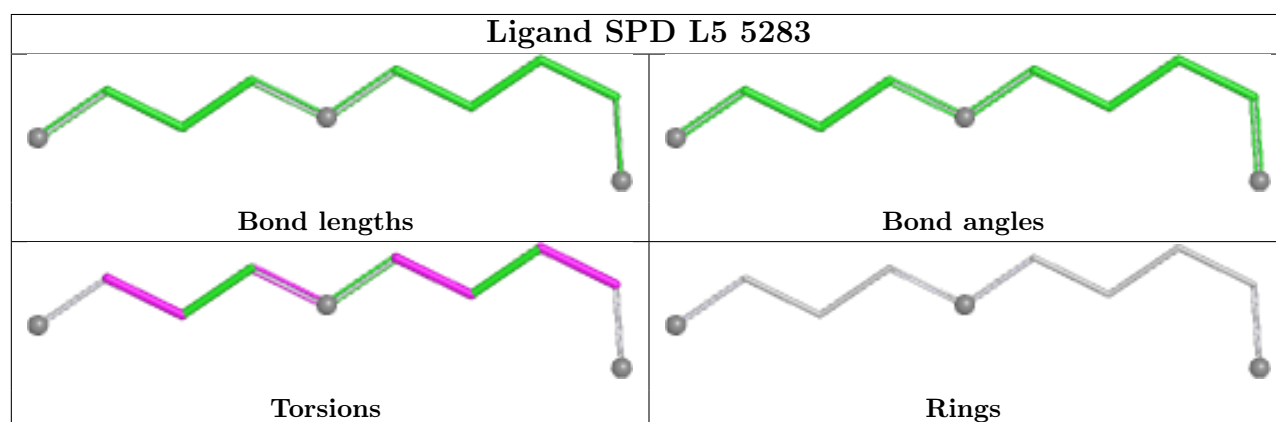
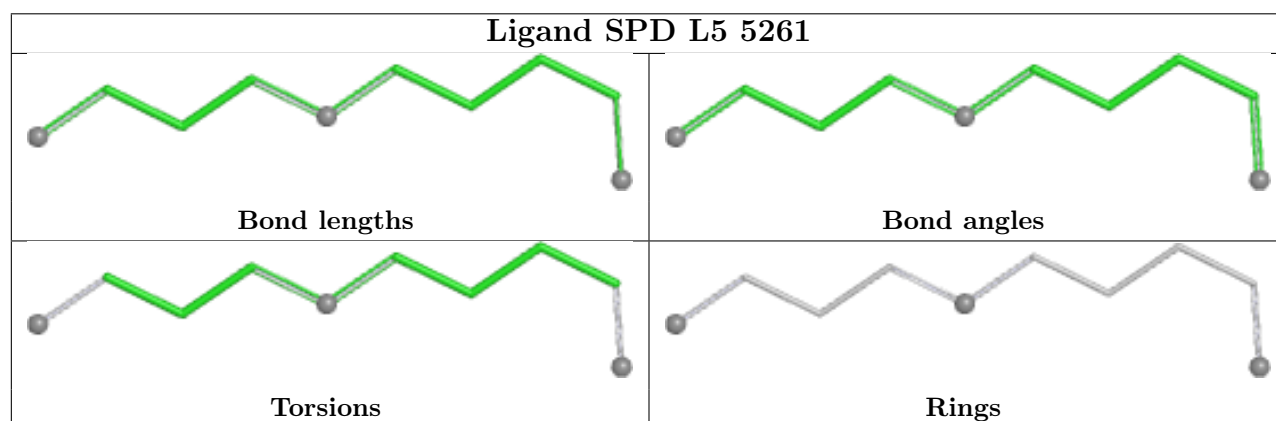
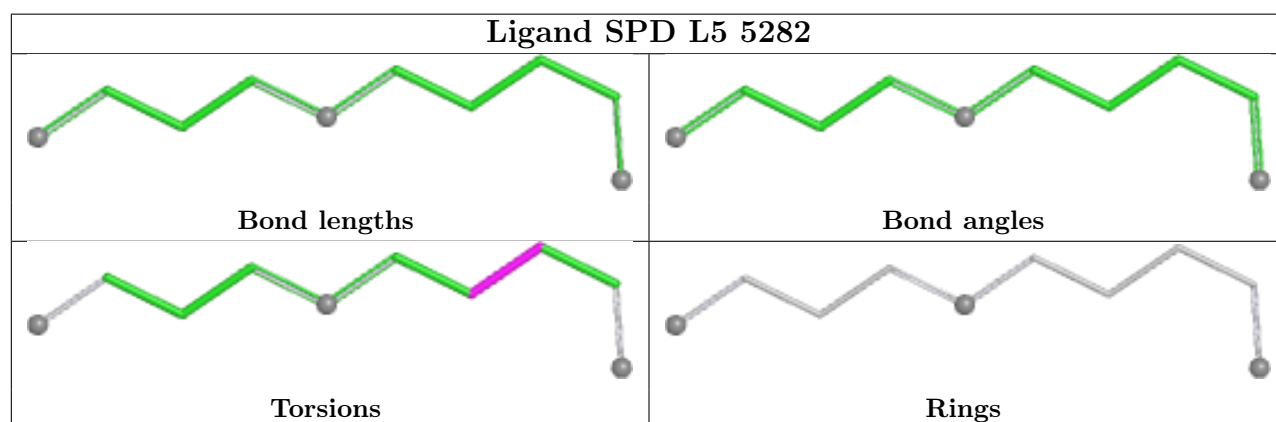
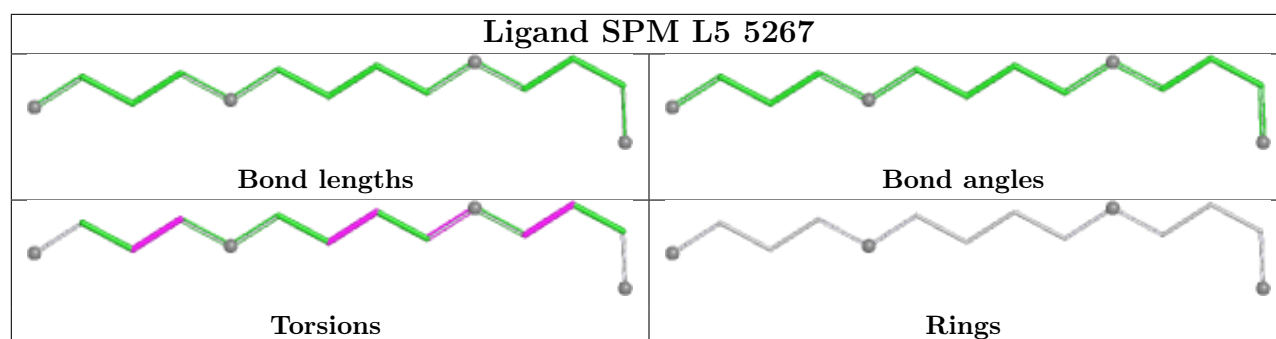
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5261	SPD	1	0

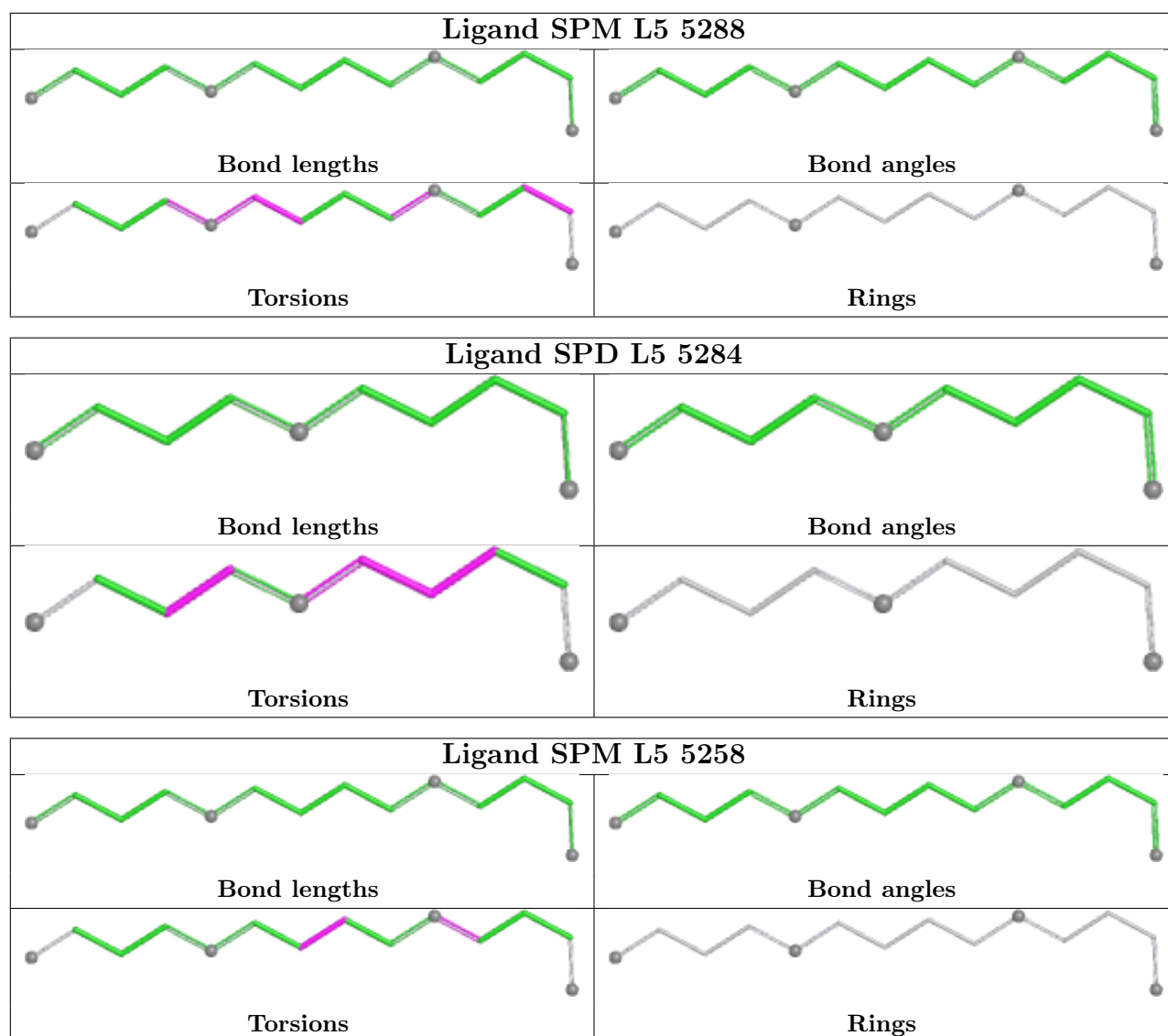
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	L5	10
85	S2	5
2	Pt	1
4	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	28.79
1	L5	1706:A	O3'	1716:G	P	21.22
1	L5	2910:G	O3'	3584:C	P	21.08
1	L5	760:G	O3'	903:C	P	16.76
1	L5	519:C	O3'	642:G	P	15.26
1	S2	698:G	O3'	730:C	P	15.19
1	L5	4776:G	O3'	4858:C	P	15.09
1	L5	2112:G	O3'	2249:C	P	14.73
1	L5	3954:A	O3'	4056:A	P	14.36
1	S2	739:C	O3'	746:C	P	12.45
1	L5	990:C	O3'	1064:G	P	12.31
1	L5	1222:A	O3'	1234:G	P	10.58
1	Pt	15:G	O3'	18:G	P	9.82
1	S2	225:G	O3'	287:U	P	7.34
1	L5	1100:U	O3'	1167:C	P	6.76
1	S2	1831:A	O3'	1832:6MZ	P	4.39
1	AT	16:C	O3'	18:G	P	4.04

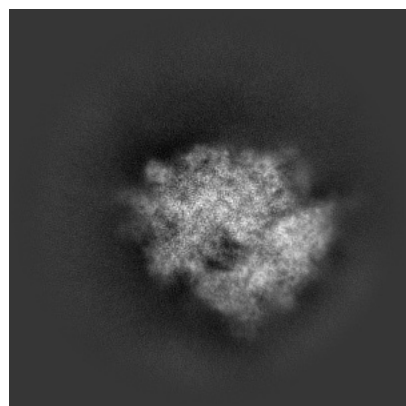
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71333. These allow visual inspection of the internal detail of the map and identification of artifacts.

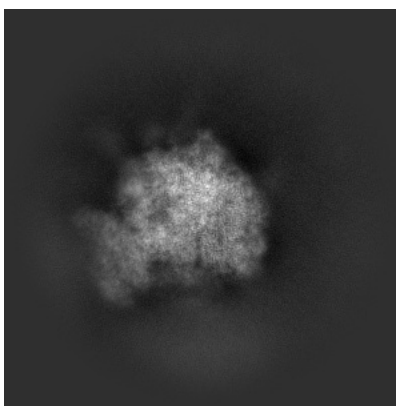
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

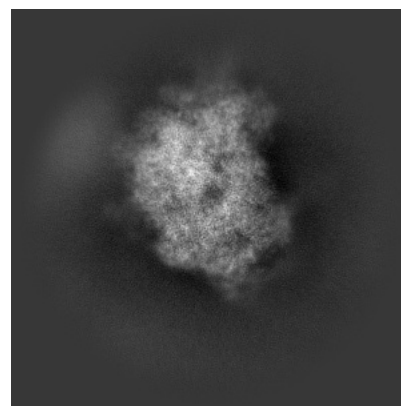
6.1.1 Primary map



X

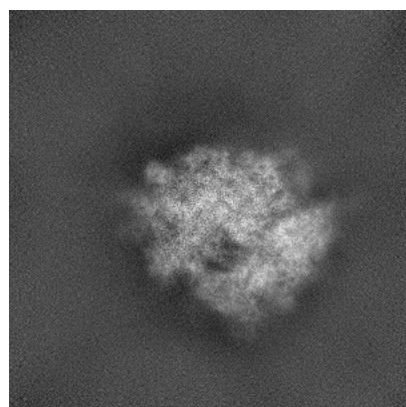


Y

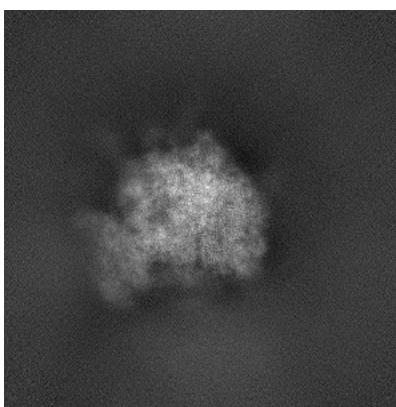


Z

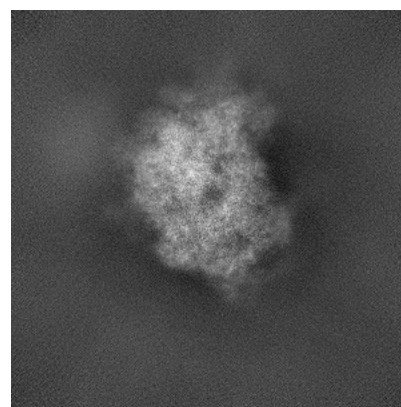
6.1.2 Raw map



X



Y

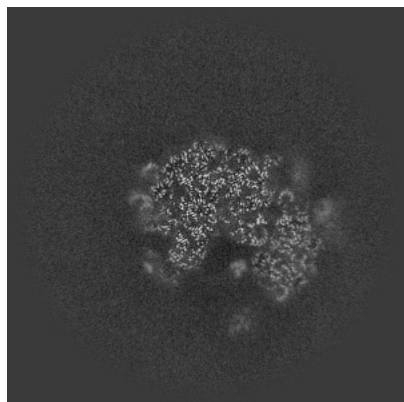


Z

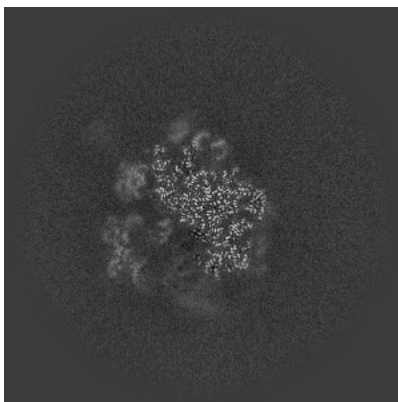
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

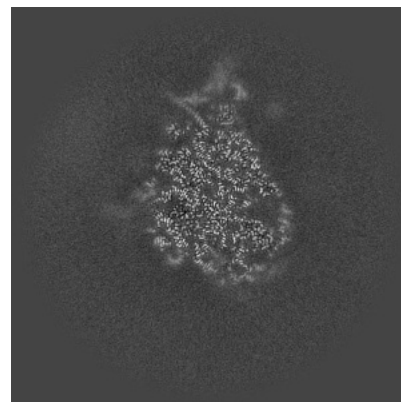
6.2.1 Primary map



X Index: 256

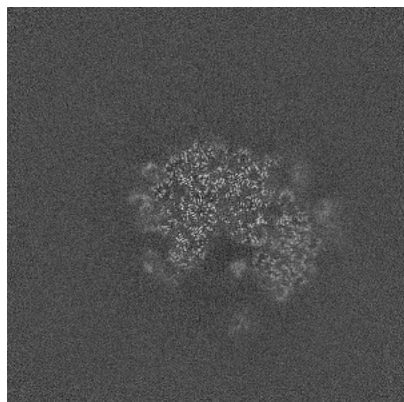


Y Index: 256

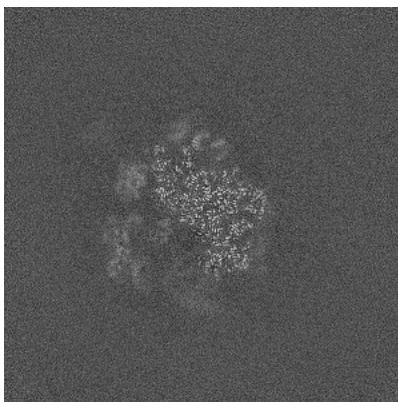


Z Index: 256

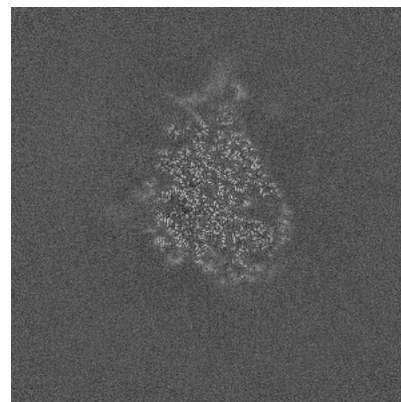
6.2.2 Raw map



X Index: 256



Y Index: 256

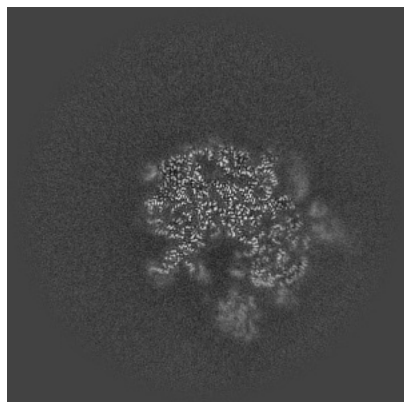


Z Index: 256

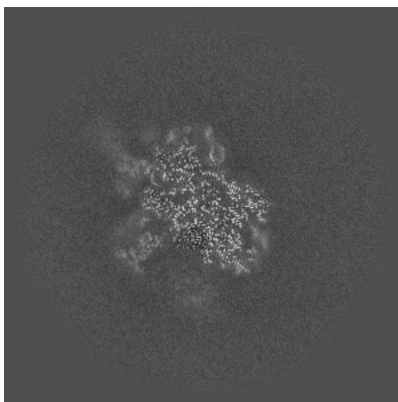
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

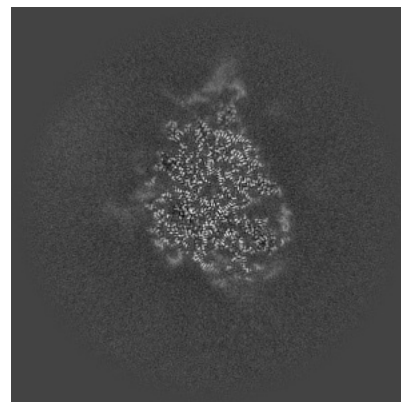
6.3.1 Primary map



X Index: 244

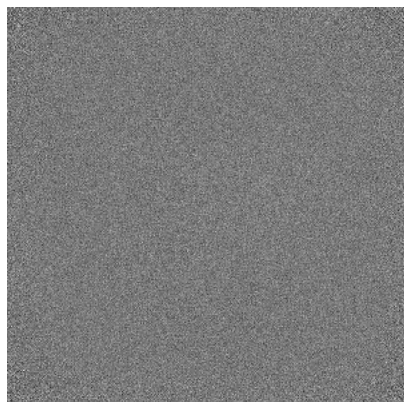


Y Index: 243

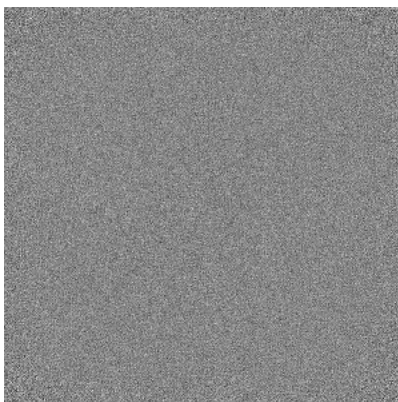


Z Index: 258

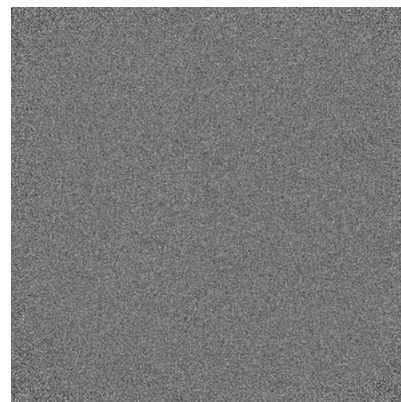
6.3.2 Raw map



X Index: 0



Y Index: 0

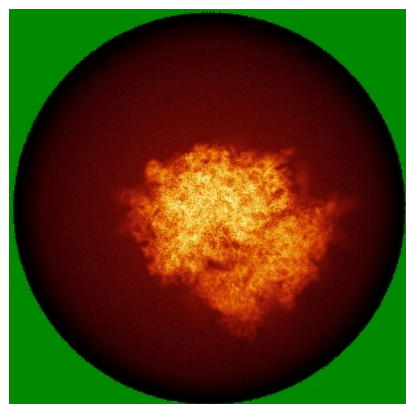


Z Index: 0

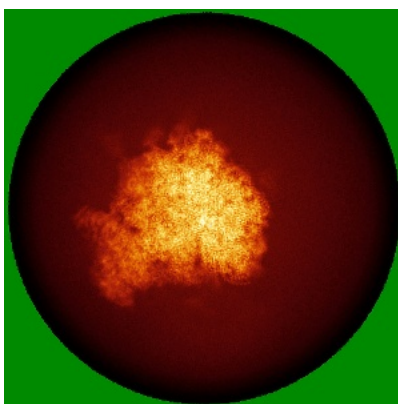
The images above show the largest variance slices of the map in three orthogonal directions.

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

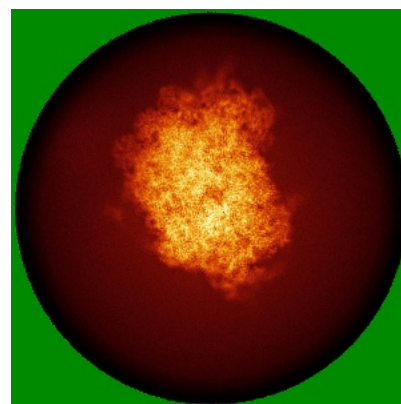
6.4.1 Primary map



X

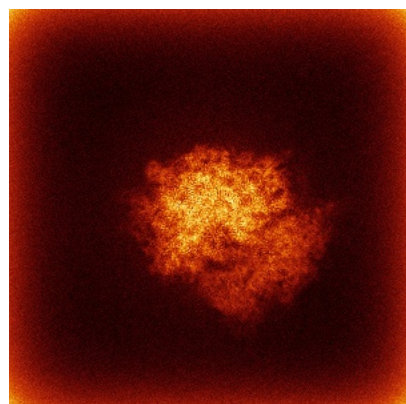


Y

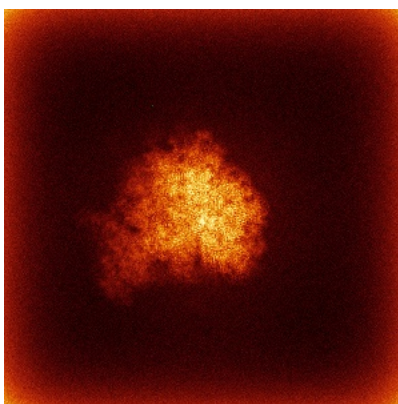


Z

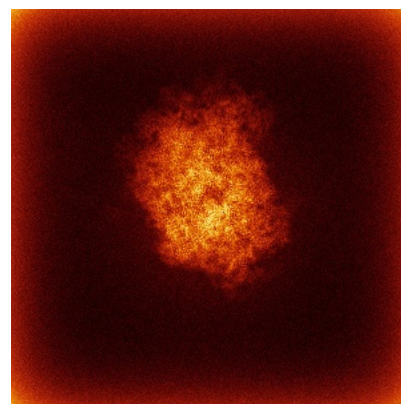
6.4.2 Raw map



X



Y

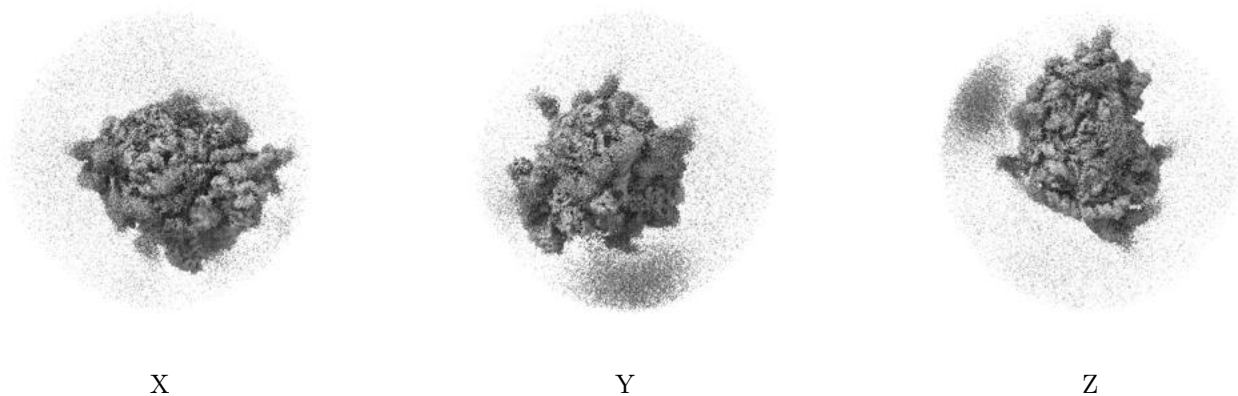


Z

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

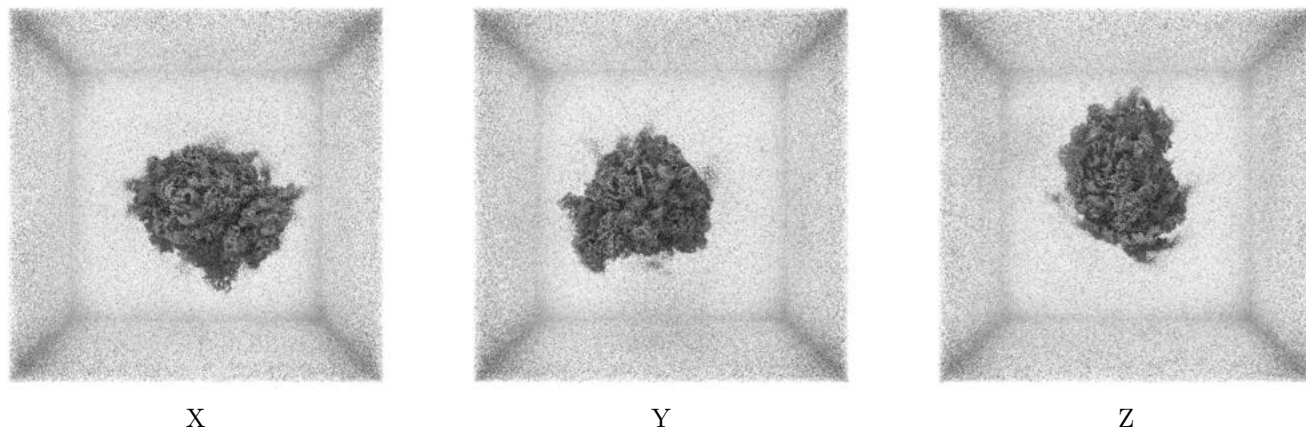
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. 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.

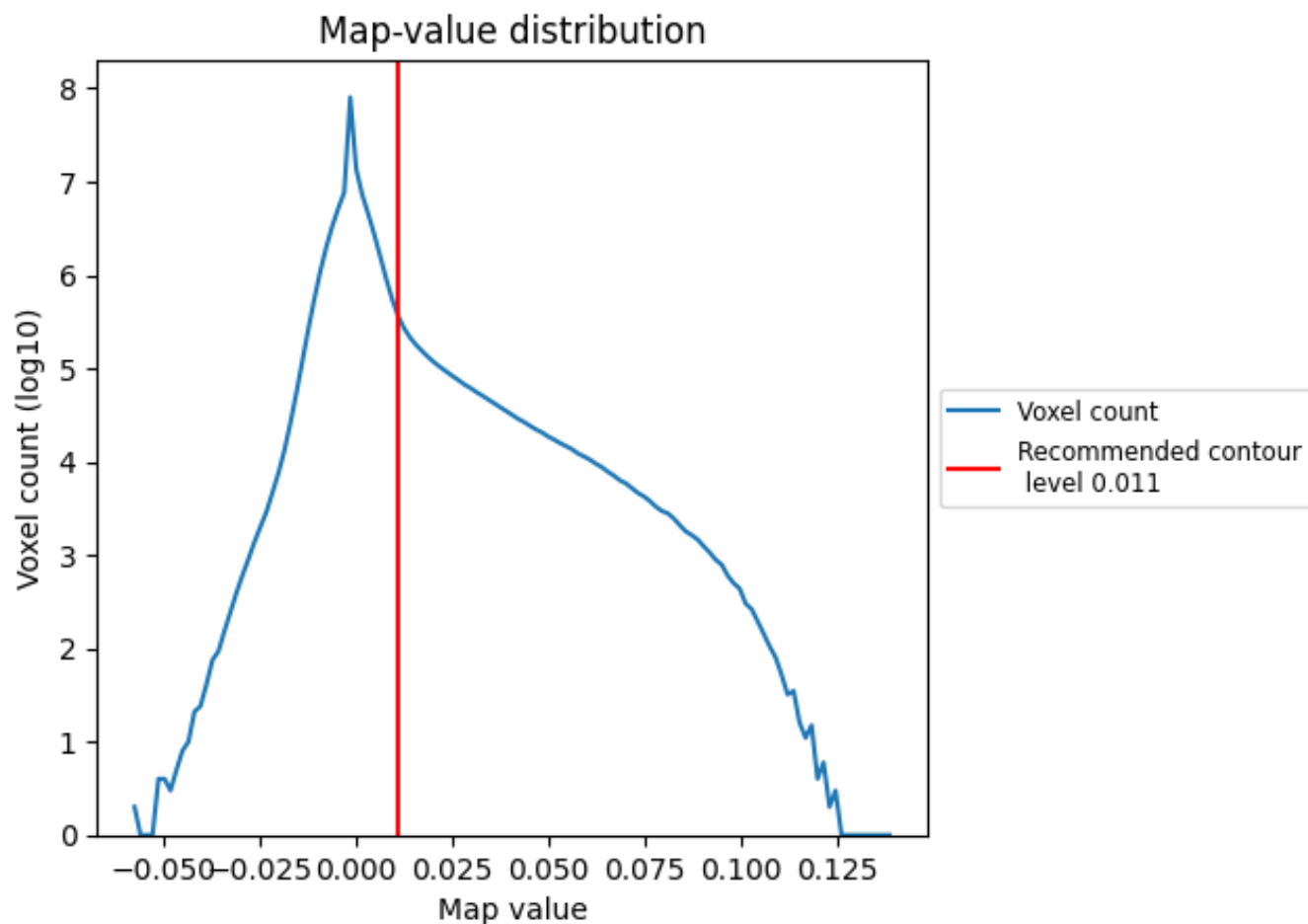
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

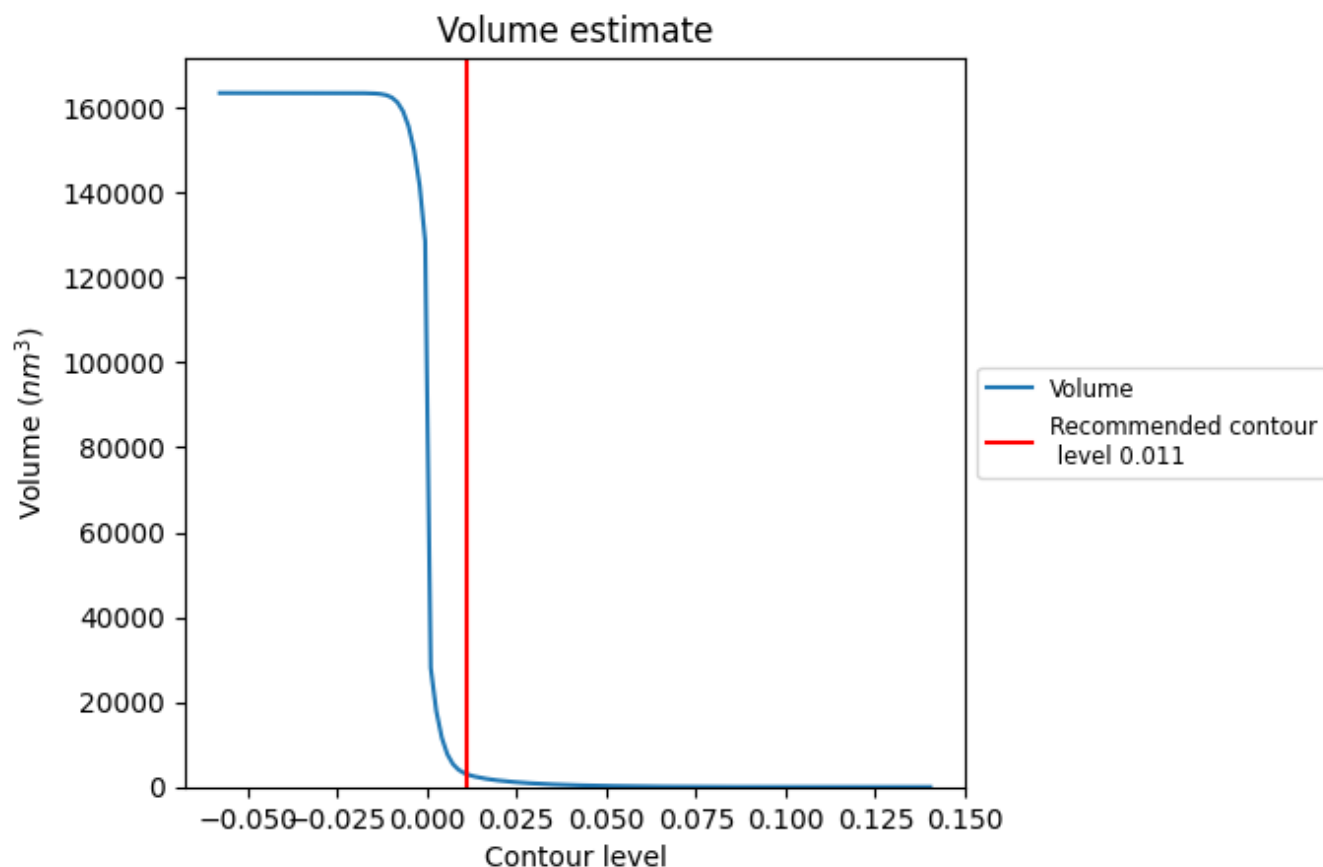
This section contains the results of statistical analysis of the map.

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.

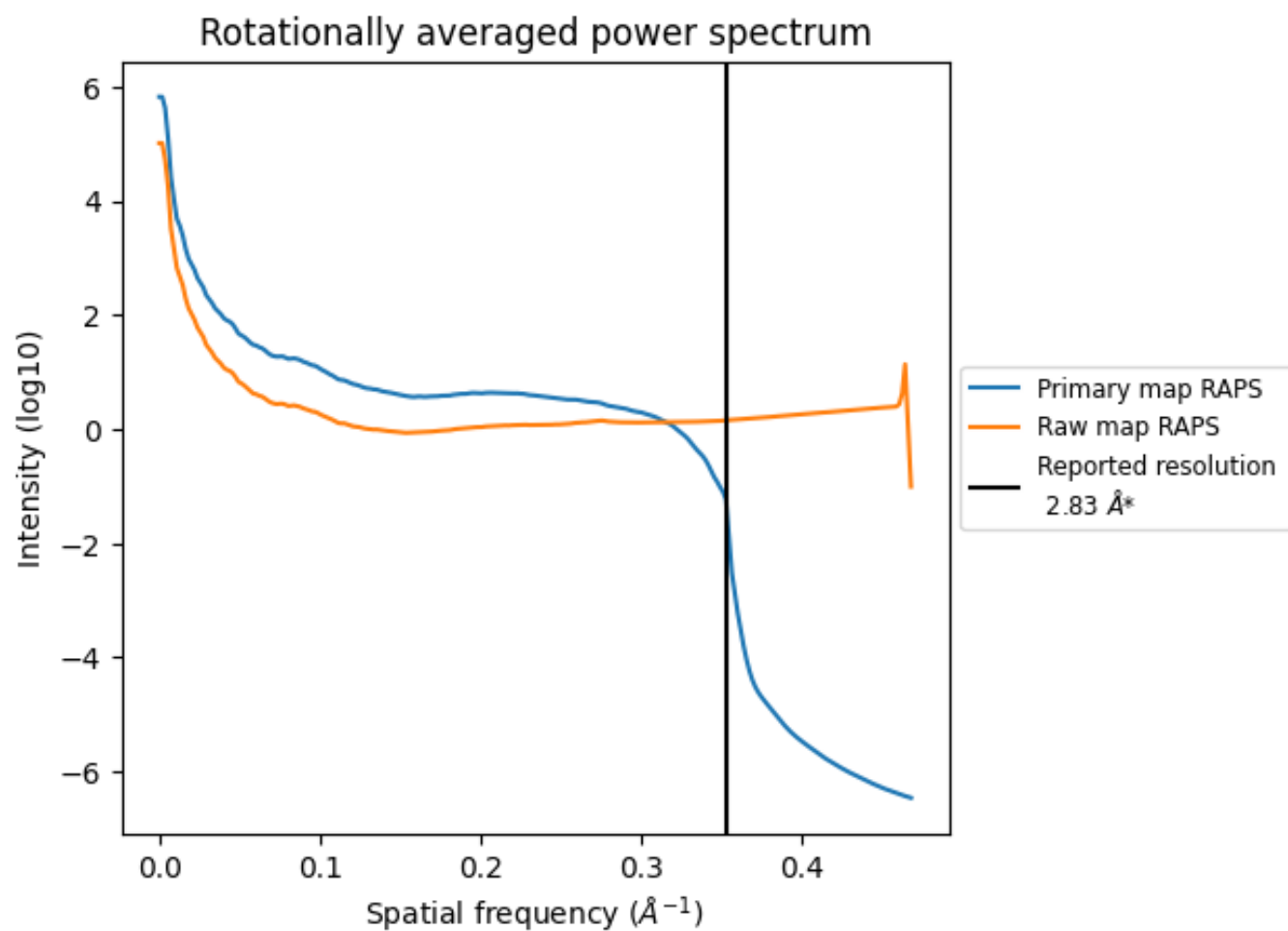
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3087 nm^3 ; this corresponds to an approximate mass of 2789 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 ⓘ

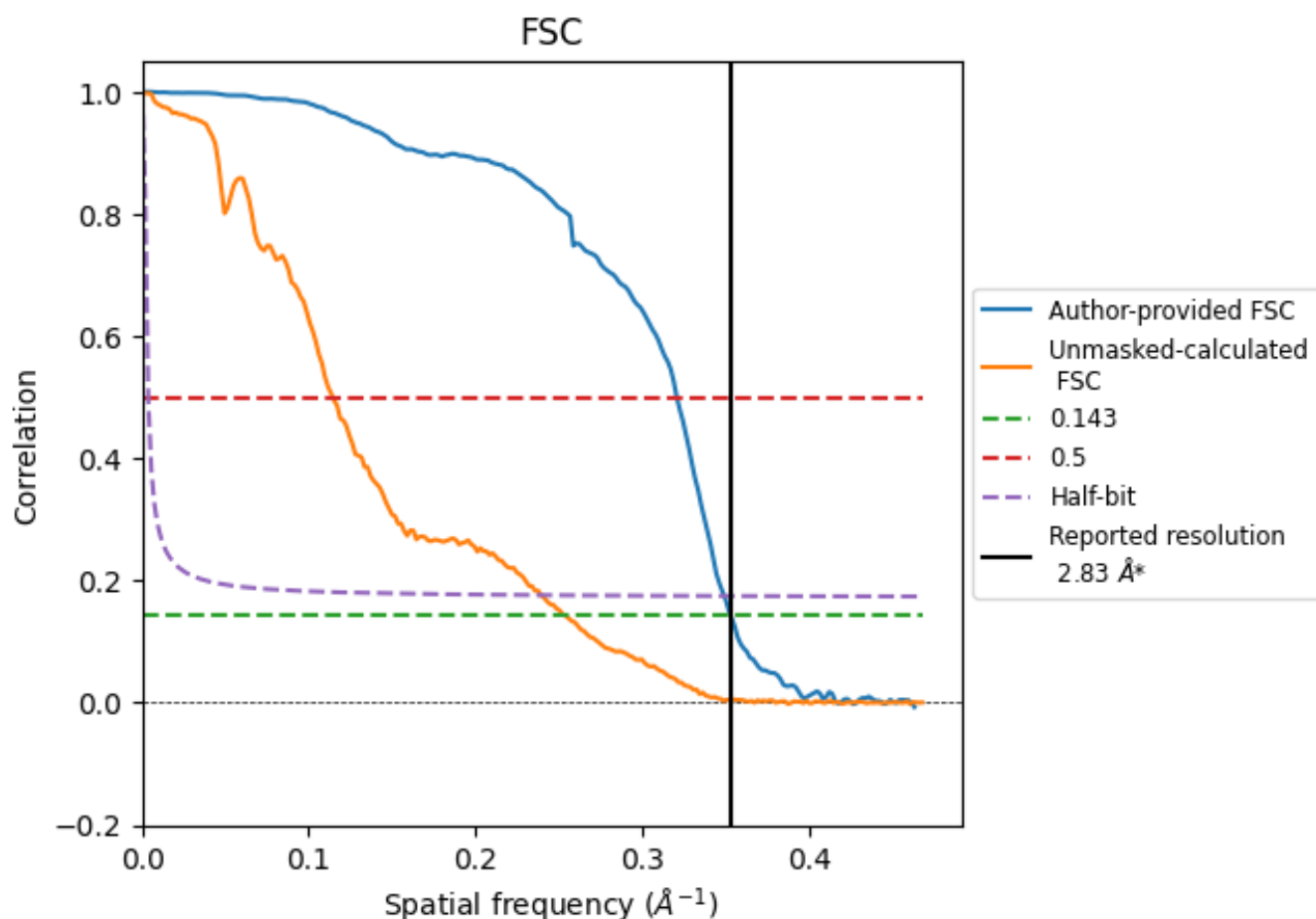


*Reported resolution corresponds to spatial frequency of 0.353 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.353 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

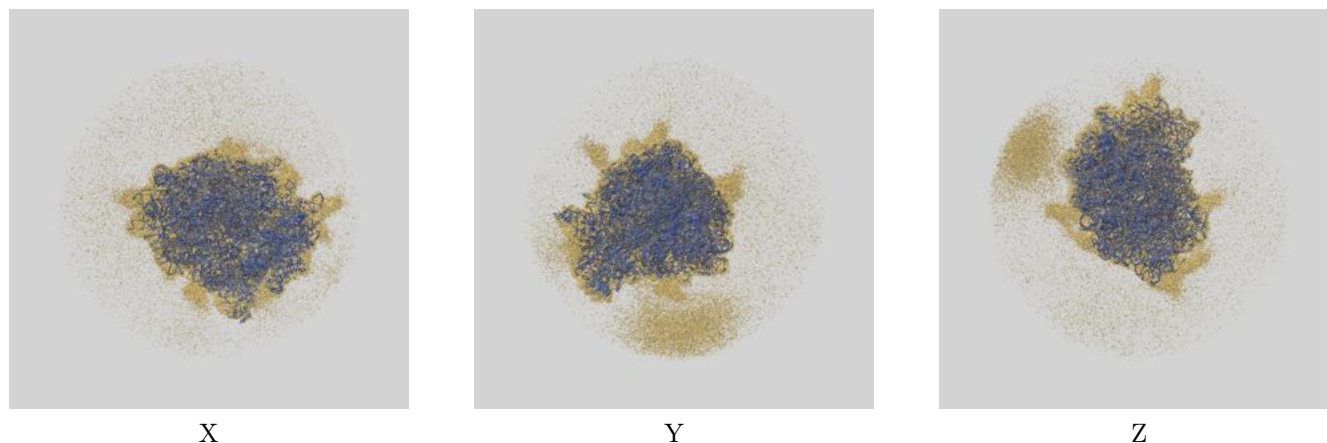
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.12	2.86
Unmasked-calculated*	3.94	8.74	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

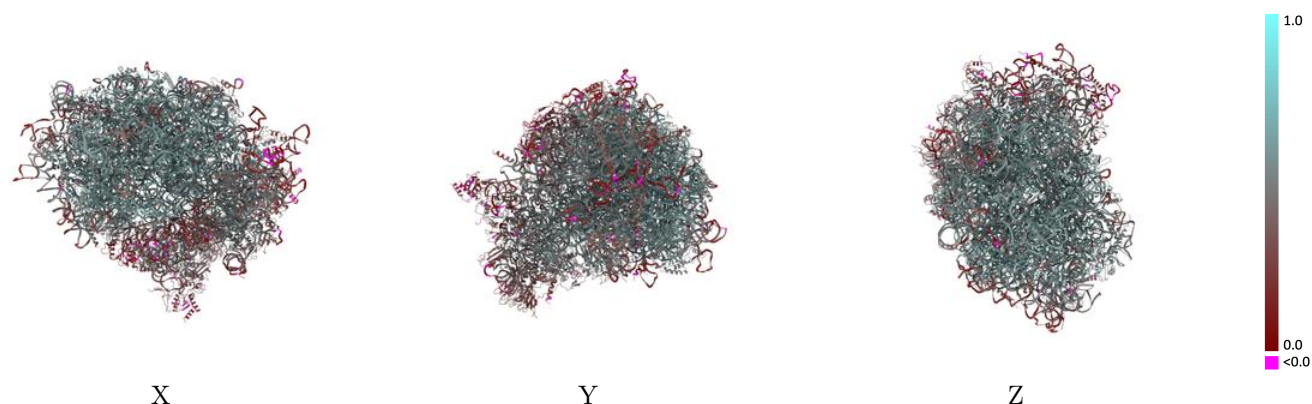
This section contains information regarding the fit between EMDB map EMD-71333 and PDB model 9P76. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



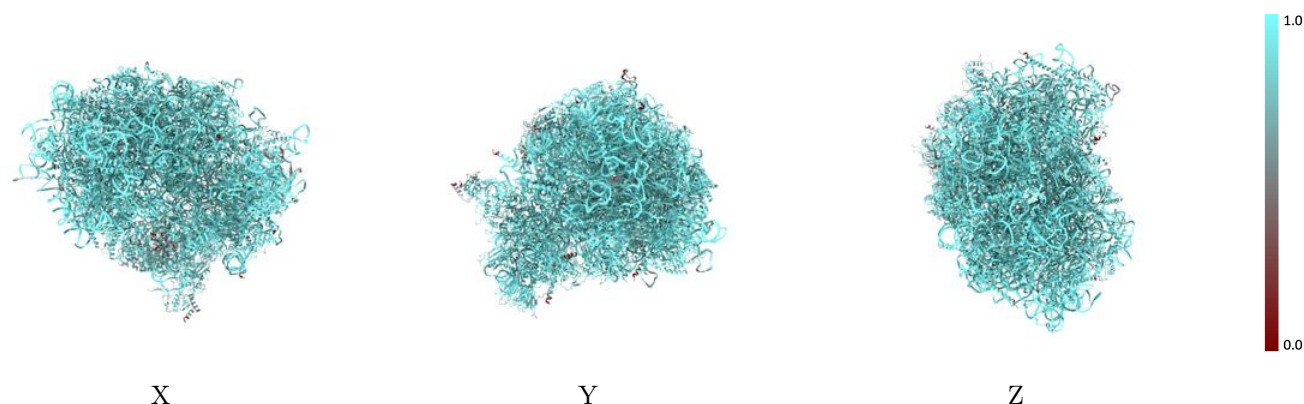
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



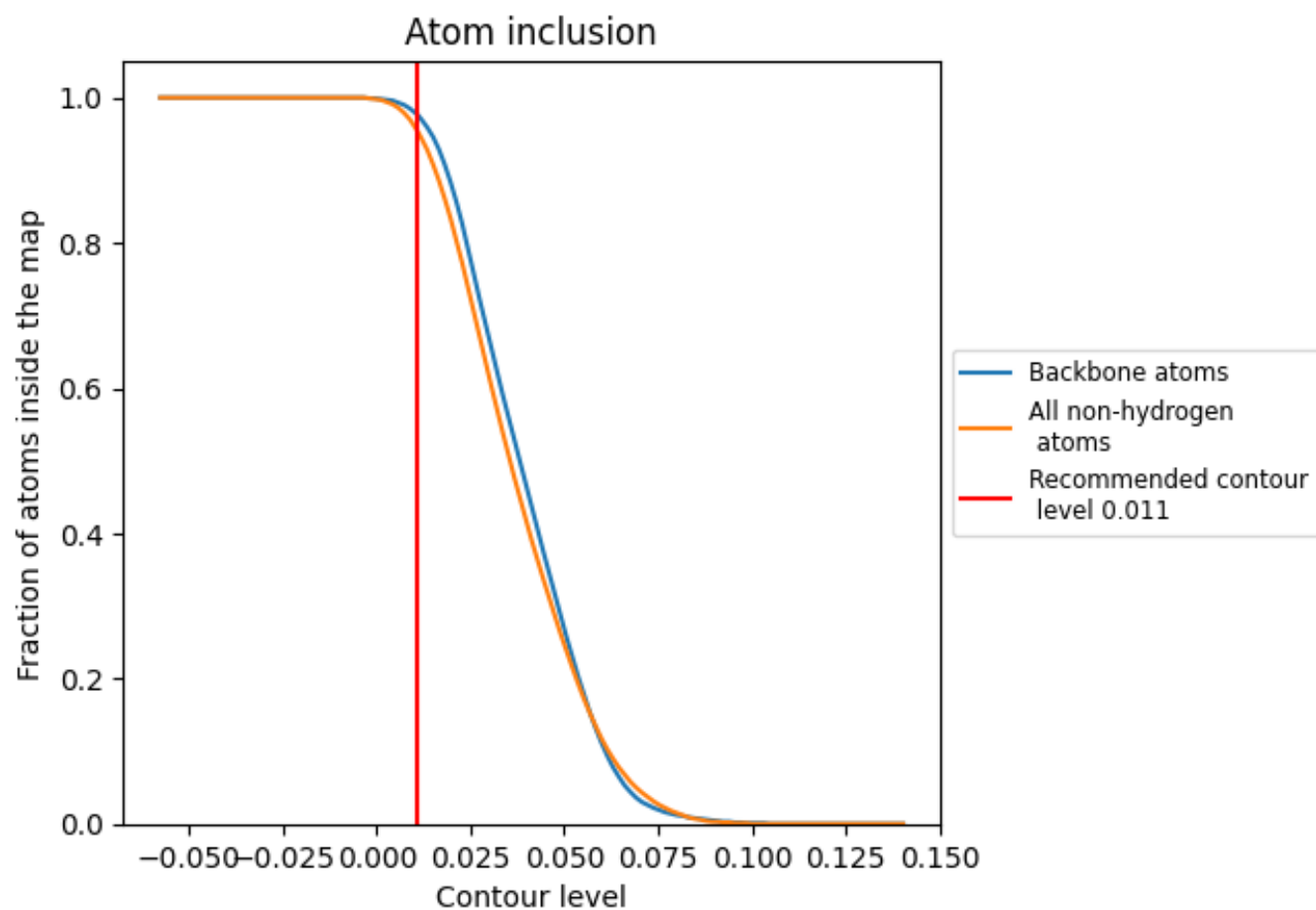
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.4970
AT	 0.9730	 0.2490
CF	 0.9150	 0.2820
CI	 0.7280	 0.4080
L5	 0.9810	 0.5300
L7	 0.9970	 0.5750
L8	 0.9880	 0.5580
LA	 0.9800	 0.5910
LB	 0.9500	 0.5700
LC	 0.9570	 0.5720
LD	 0.9520	 0.5310
LE	 0.9030	 0.5020
LF	 0.9730	 0.5730
LG	 0.9080	 0.5060
LH	 0.9560	 0.5580
LI	 0.9480	 0.5660
LJ	 0.9310	 0.5030
LL	 0.9210	 0.5420
LM	 0.9650	 0.5600
LN	 0.9910	 0.6100
LO	 0.9630	 0.5730
LP	 0.9650	 0.5840
LQ	 0.9660	 0.5950
LR	 0.9110	 0.5140
LS	 0.9710	 0.5920
LT	 0.9450	 0.5530
LU	 0.9390	 0.4820
LV	 0.9550	 0.5770
LW	 0.8720	 0.3930
LX	 0.9380	 0.5510
LY	 0.9580	 0.5570
LZ	 0.9730	 0.5440
La	 0.9740	 0.5940
Lb	 0.9050	 0.4940
Lc	 0.9480	 0.5320



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Chain	Atom inclusion	Q-score
Ld	 0.9350	 0.5520
Le	 0.9750	 0.5900
Lf	 0.9830	 0.6020
Lg	 0.9620	 0.5680
Lh	 0.9400	 0.5480
Li	 0.9520	 0.5410
Lj	 0.9790	 0.5970
Lk	 0.8900	 0.4930
Ll	 0.9690	 0.5790
Lm	 0.9380	 0.5730
Ln	 0.9570	 0.5540
Lo	 0.8180	 0.5720
Lp	 0.9420	 0.5640
Lr	 0.9640	 0.5750
Ls	 0.6340	 0.2010
Lt	 0.6340	 0.1710
Pt	 0.9190	 0.4450
S2	 0.9840	 0.4680
SA	 0.9180	 0.4560
SB	 0.9170	 0.4900
SC	 0.9540	 0.4920
SD	 0.9020	 0.3800
SE	 0.9450	 0.4600
SF	 0.7670	 0.4200
SG	 0.8820	 0.3620
SH	 0.8830	 0.3780
SI	 0.9140	 0.4770
SJ	 0.9270	 0.4520
SK	 0.9120	 0.3390
SL	 0.9020	 0.5050
SM	 0.6910	 0.1680
SN	 0.9430	 0.5200
SO	 0.8930	 0.5140
SP	 0.8520	 0.3570
SQ	 0.9190	 0.4040
SR	 0.8860	 0.3890
SS	 0.8840	 0.3950
ST	 0.9310	 0.3990
SU	 0.9040	 0.3540
SV	 0.9500	 0.4620
SW	 0.9630	 0.5230
SX	 0.9260	 0.5080

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Chain	Atom inclusion	Q-score
SY	 0.8980	 0.3880
SZ	 0.6450	 0.3720
Sa	 0.9480	 0.5120
Sb	 0.9220	 0.4580
Sc	 0.8020	 0.3950
Sd	 0.9550	 0.4510
Se	 0.8290	 0.3980
Sf	 0.7860	 0.2150
Sg	 0.8850	 0.3180