



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 02:16 AM EDT

PDB ID : 9P9H / pdb_00009p9h
EMDB ID : EMD-71411
Title : In situ human unrotated hibernating with CCDC124 state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-24
Resolution : 2.84 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

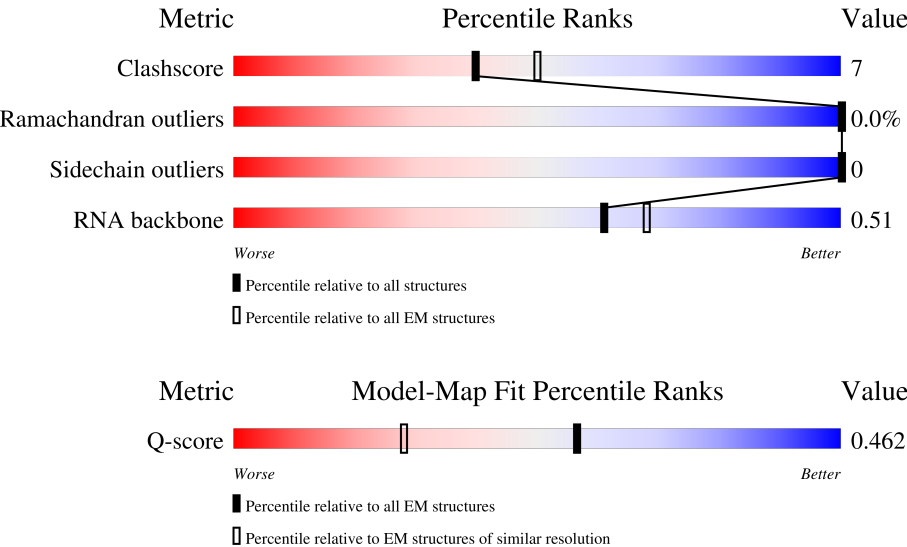
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.84 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.



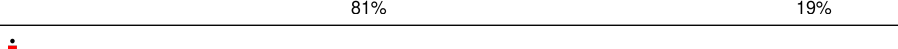
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11884 (2.34 - 3.34)

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	L5	3675	
3	L7	120	

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Mol	Chain	Length	Quality of chain
4	L8	156	
5	LA	248	
6	LB	402	
7	LC	368	
8	LD	293	
9	LE	250	
10	LF	225	
11	LG	241	
12	LH	190	
13	LI	213	
14	LJ	176	
15	LL	210	
16	LM	139	
17	LN	203	
18	LO	201	
19	LP	153	
20	LQ	187	
21	LR	187	
22	LS	175	
23	LT	159	
24	LU	101	
25	LV	131	
26	LW	124	
27	LX	120	
28	LY	134	

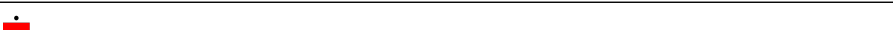
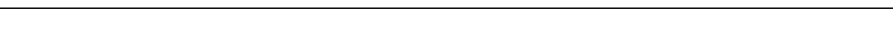
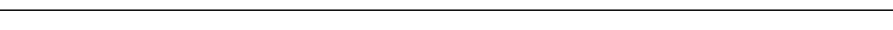
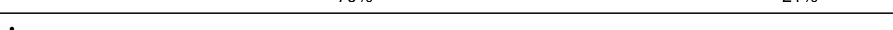
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Mol	Chain	Length	Quality of chain
29	LZ	135	
30	La	147	
31	Lb	121	
32	Lc	98	
33	Ld	107	
34	Le	128	
35	Lf	109	
36	Lg	114	
37	Lh	122	
38	Li	102	
39	Lj	86	
40	Lk	69	
41	Ll	50	
42	Lm	52	
43	Ln	24	
44	Lo	105	
45	Lp	91	
46	Lr	125	
47	Ls	196	
48	Lt	157	
49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

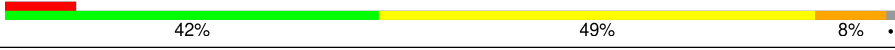
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Mol	Chain	Length	Quality of chain
54	SQ	144	
55	SR	135	
56	SS	145	
57	ST	143	
58	SU	104	
59	SZ	75	
60	Sc	64	
61	Sd	55	
62	Sf	67	
63	Sg	313	
64	SA	221	
65	SB	214	
66	SC	222	
67	SE	262	
68	SG	237	
69	SH	189	
70	SI	206	
71	SJ	185	
72	SL	153	
73	SN	150	
74	SO	140	
75	SV	83	
76	SW	129	
77	SX	141	
78	SY	131	

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Mol	Chain	Length	Quality of chain
79	Sa	102	
80	Sb	83	
81	Se	58	
82	S2	1740	
83	CB	856	
84	Et	76	
85	CE	73	

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 225614 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 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L5	3655	Total	C	N	O	P	1	0
			78445	34968	14346	25476	3655		

- Molecule 3 is a RNA chain called 5S rRNA.

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

- Molecule 4 is a RNA chain called 5.8S rRNA.

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

- Molecule 5 is a protein called 60S ribosomal protein L8.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 7 is a protein called 60S ribosomal protein L4.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 9 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 10 is a protein called 60S ribosomal protein L7.

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

- Molecule 11 is a protein called 60S ribosomal protein L7a.

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

- Molecule 12 is a protein called 60S ribosomal protein L9.

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

- Molecule 13 is a protein called Ribosomal protein uL16-like.

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

- Molecule 14 is a protein called 60S ribosomal protein L11.

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

- Molecule 15 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 16 is a protein called 60S ribosomal protein L14.

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

- Molecule 17 is a protein called 60S ribosomal protein L15.

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

- Molecule 18 is a protein called 60S ribosomal protein L13a.

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

- Molecule 19 is a protein called 60S ribosomal protein L17.

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

- Molecule 20 is a protein called 60S ribosomal protein L18.

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

- Molecule 21 is a protein called 60S ribosomal protein L19.

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

- Molecule 22 is a protein called 60S ribosomal protein L18a.

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

- Molecule 23 is a protein called 60S ribosomal protein L21.

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

- Molecule 24 is a protein called Heparin-binding protein HBp15.

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

- Molecule 25 is a protein called 60S ribosomal protein L23.

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

- Molecule 26 is a protein called Ribosomal protein L24.

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

- Molecule 27 is a protein called 60S ribosomal protein L23a.

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

- Molecule 28 is a protein called 60S ribosomal protein L26.

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

- Molecule 29 is a protein called 60S ribosomal protein L27.

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

- Molecule 30 is a protein called 60S ribosomal protein L27a.

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

- Molecule 31 is a protein called Large ribosomal subunit protein eL29.

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

- Molecule 32 is a protein called 60S ribosomal protein L30.

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

- Molecule 33 is a protein called 60S ribosomal protein L31.

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

- Molecule 34 is a protein called 60S ribosomal protein L32.

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

- Molecule 35 is a protein called 60S ribosomal protein L35a.

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

- Molecule 36 is a protein called 60S ribosomal protein L34.

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

- Molecule 37 is a protein called 60S ribosomal protein L35.

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

- Molecule 38 is a protein called 60S ribosomal protein L36.

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

- Molecule 39 is a protein called 60S ribosomal protein L37.

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

- Molecule 40 is a protein called 60S ribosomal protein L38.

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

- Molecule 41 is a protein called 60S ribosomal protein L39.

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

- Molecule 42 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 43 is a protein called 60S ribosomal protein L41.

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

- Molecule 44 is a protein called 60S ribosomal protein L36a.

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

- Molecule 45 is a protein called 60S ribosomal protein L37a.

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

- Molecule 46 is a protein called 60S ribosomal protein L28.

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

- Molecule 47 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 49 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 50 is a protein called 40S ribosomal protein S5.

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

- Molecule 51 is a protein called 40S ribosomal protein S10.

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

- Molecule 52 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 53 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 54 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 55 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 56 is a protein called 40S ribosomal protein S18.

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

- Molecule 57 is a protein called 40S ribosomal protein S19.

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

- Molecule 58 is a protein called 40S ribosomal protein S20.

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

- Molecule 59 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 60 is a protein called 40S ribosomal protein S28.

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

- Molecule 61 is a protein called 40S ribosomal protein S29.

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

- Molecule 62 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 63 is a protein called Receptor of activated protein C kinase 1.

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

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

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

- Molecule 65 is a protein called 40S ribosomal protein S3a.

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

- Molecule 66 is a protein called 40S ribosomal protein S2.

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

- Molecule 67 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 68 is a protein called 40S ribosomal protein S6.

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

- Molecule 69 is a protein called Small ribosomal subunit protein eS7.

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

- Molecule 70 is a protein called 40S ribosomal protein S8.

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

- Molecule 71 is a protein called 40S ribosomal protein S9.

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

- Molecule 72 is a protein called 40S ribosomal protein S11.

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

- Molecule 73 is a protein called 40S ribosomal protein S13.

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

- Molecule 74 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 75 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 76 is a protein called 40S ribosomal protein S15a.

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

- Molecule 77 is a protein called 40S ribosomal protein S23.

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

- Molecule 78 is a protein called 40S ribosomal protein S24.

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

- Molecule 79 is a protein called 40S ribosomal protein S26.

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

- Molecule 80 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 81 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 82 is a RNA chain called 18S rRNA.

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

- Molecule 83 is a protein called Elongation factor 2.

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

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

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

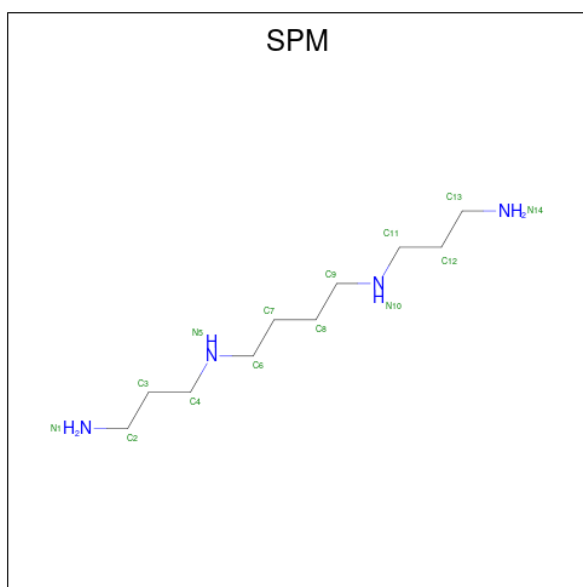
- Molecule 85 is a protein called Coiled-coil domain-containing protein 124.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	CE	73	Total	C	N	O	S	0	0
			613	369	122	121	1		

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

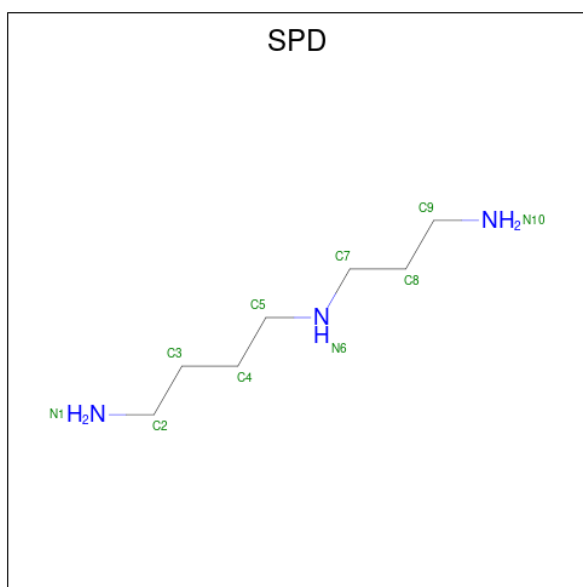
Mol	Chain	Residues	Atoms		AltConf
86	L5	177	Total	Mg	0
			177	177	
86	L7	3	Total	Mg	0
			3	3	
86	L8	5	Total	Mg	0
			5	5	
86	LA	1	Total	Mg	0
			1	1	
86	LB	1	Total	Mg	0
			1	1	
86	LP	1	Total	Mg	0
			1	1	
86	LV	1	Total	Mg	0
			1	1	
86	Le	1	Total	Mg	0
			1	1	
86	Lj	1	Total	Mg	0
			1	1	
86	SS	1	Total	Mg	0
			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: C₁₀H₂₆N₄) (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	

- 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	L8	1	Total	C	N	0
			10	7	3	
88	LN	1	Total	C	N	0
			10	7	3	

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

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

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

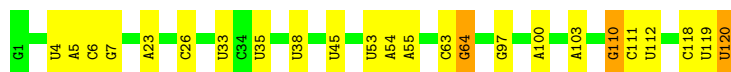
C2702	C2589	U2495	A2404	A2276	A2030	G1948	U1834	G1750	C1662	U1536	U1410	U1320	U
G2590	G2590	G2496	G2404	C2277	A2033	G1951	G1835	A1751	C1663	A1537	C1411	G1321	C
A2591	A2591	C2497	G2407	A2278	G2046	G1961	A1837	G1752	A1669	G1539	C1412	A1322	U
G2601	G2601	C2498	U2408	G2284	G2047	A1962	G1842	U1755	C1676	A1547	C1414	A1324	C
A2602	A2602	G2502	U2409	G2289	U2048	G1969	G1846	U1756	U1677	G1548	G1415	A1325	G
C2607	C2607	C2503	C2410	C2289	G2049	G1972	C1847	G1757	C1678	G1548	G1416	A1326	
A2611	A2611	C2504	C2411	C2295	G2055	G1973	C1848	G1758	C1679	A1559	C1417	G1327	
C2505	C2505	G2506	A2412	G2298	G2056	G1974	G1855	G1759	C1680	G1559	C1418	A1328	
A2507	A2507	G2507	U2413	G2299	G2060	G1975	G1856	G1760	U1684	G1563	A1420	C1332	
A2513	A2513	A2513	U2415	A2300	G2069	U1976	U1860	G1761	U1684	A1563	G1425	A1334	
G2618	G2618	G2516	A2417	A2301	A2069	C1977	U1861	G1762	C1685	C1566		A1334	
G2622	G2622	A2517	G2421	C2302	G2072	C1978	U1862	C1763	C1694	C1566	C1437	G1263	
A2623	A2623	G2518	C2422	C2303	C2073	A1979	U1863	G1764	U1695	G1577	U1438	A1254	
G2624	G2624	U2519	A2423	G2306	G2076	G1980	U1866	A1765	C1696	U1578	C1439	U1339	
C2627	C2627	C2520	G2424	G2306	G2077	G1981	A1867	A1767	C1697	U1582	C1442	C1340	
A2725	A2725	G2521	U2425	A2313	G2083	G1982	A1868	G1768	C1698		C1443	C1344	
G2726	G2726	A2529	G2448	G2318	U2080	A1983	A1869	G1769	A1699	U1589	A1444	A1345	
U2730	U2730	A2537	A2449	G2318	G2089	A1984	C1870	A1770	G1700	C1589	U1445	C1346	
C2731	C2731	G2538	G2450	G2321	C2083	G1985	A1871	U1773	A1701	C1590	U1446	G1347	
C2739	C2739	U2537	A2453	G2326	G2084	U1986	G1877	A1776	C1702	U1591	C1447	G1262	
G2742	G2742	G2538	G2453	G2326	G2085	G1988	U1882	C1777	C1704	U1596	C1461	G1266	
A2743	A2743	C2539	C2458	U2329	G2092	A1991	A1891	U1781	G1705	A1601	A1462	C1267	
A2744	A2744	A2543	U2459	G2329	A2093	U1992	A1891	U1782	A1706		G1466	G1268	
A2745	A2745	G2544	A2460	G2332	G2094	C1994	G1895	U1783	C	G1612	C1467	G1269	
A2746	A2746	U2545	C2461	C2333	A2095	G1995	A1896	A1787	C	A1613	C1468	G1270	
		G2546	C2462	C2334	G2096	C1996	A1897	A1788	A	G1617		G1359	
		G2547	G2463	C2335	U2097	U1997	A1898	C1789	C		C1480	C1365	
		U2554	C2464	G2336	G2098	A1998	G1899	C1790	C		C1481	G1366	
		G2555	G2465	G2336	G2098	A1999	G1899	U1792	C	A1621	C1483	C1367	
		G2556	G2466	A2347	C2101	G2000	G1912	A1793	C	G1624	C1369	G1278	
		G2557	U2467	G2348	G2102	G2001	C1913	A1794	G1716	G1625	U1494	A1279	
		C2558	U2468	A2349	G2103	A2002	C1914	A1802	C1717		G1495	C1280	
		G2559	C2469	G2350	G2104	G2003	A1917	G1803	C1718		G1496	G1281	
		G2560	G2471	C2351	A2105	U2004	U1918	A1804	A1719		G1497	G1282	
		A2565	G2474	A2360	G2106	G2007	G1919	A1805	C1720	A1631	G1498	G1283	
		G2566	G2475	G2361	C2107	U2008	G1920	G1806	G1721	A1632	C1499	G1284	
		G2567	C2478	U2362	C2110	A2009	C1921	C1807	U1725	G1633	A1500	U1285	
		G2568	C2479	A2363	G2111	A2010	G1922	G1810	U1726	A1634	C1501	C1286	
		G2569	G2478	G2364	G2112	C2011	G1925	G1811	U1727		G1502	G1287	
		U2570	G2479	C2364	C2249	A2012	G1925	G1815	C1731		A1503	G1293	
		C2572	A2483	A2368	G2250	A2017	U1930	G1818	C1732	U1639	G1504	A1294	
		A2573	U2484	A2382	G2251	C2018	C1931	G1819	G1733	G1640	C1295	C1295	
		G2577	U2485	C2383	G2252	C2019	A1932	C1820	U1735	G1641	U1395	G1296	
		U2580	C2486	A2395	C2256	U2020	G1933	G1821	U1736	A1645	G1396	U1297	
		G2583	C2487	A2396	G2261	G2021	A1934	U1822	G1739	G1646	A1398	C1298	
		C2588	C2489	A2397	G2262	G2024	G1940	G1823	C1740	U1647	G1403	G1300	
		A2587	U2490	U2398	A2263	A2025	A1941	G1824	G1741		A1524	C1301	
		G2588	C2491	G2399	G2265	A2026	A1942	A1825	A1742		A1534	A1307	
		A2587	G2492	G2400	G2265	A2029	A1943	G1826	U1744		C1407	C1308	
		G2588	U2494	A2401							C1409	C1309	

C4942	A4943	U4946	C4972	G4769	G4652	U4557	U4460	C4341	A4251	C4140	A3949	A3865	C3753	G3654	C2903
A4943	U4946	C4972	G4769	U4770	A4656	U4558	A4464	C4345	A4251	G4141	U3950	A3866	C3753	G3654	U2904
U4946	C4972	A4656	U4770	A4559	C4656	C4560	A4464	U4346	A4254	C4142	U3950	A3867	A3760	C3659	C2905
C4951	G4954	C4773	C4774	C4775	C4670	C4567	C4466	U4466	A4257	C4143	A3952	C3660	U3770	C3661	C2907
G4954	A4955	C4774	C4775	C4672	C4671	A4571	U4471	C4349	A4258	C4144	A3954	C3663	A3774	A3662	U2908
A4955	G4960	C4775	C4673	A4672	A4673	U4572	C4472	C4350	C4259	C4145	A4056	C3663	A3775	C3664	C2910
C4859	G4860	A4679	U4673	G4679	U4673	U4572	G4475	U4353	U4260	G4146	U4058	A3877	A3776	C3665	C2914
G4860	A4861	C4679	U4673	U4679	U4673	U4576	C4476	U4354	C4261	C4149	U4060	C3879	C3782	C3670	A2815
C4870	A4871	U4576	G4477	C4477	A4477	U4577	A4477	U4361	U4265	C4153	G4061	C3880	C3673	C3673	G3590
C4871	U4577	A4681	G4478	C4478	A4478	C4578	G4478	U4362	A4268	G4154	A4062	C3881	C3674	C3674	C3591
U4685	C4686	U4578	A4488	A4363	A4362	U4579	A4488	A4363	A4273	C4155	C4064	G3884	A3785	C3674	C3592
G4686	C4687	U4579	U4493	A4373	A4363	U4579	A4488	A4373	A4274	C4156	C4065	U3884	U3786	C3674	C3593
C4687	U4688	A4584	U4493	G4373	A4373	U4579	U4493	G4373	C4275	A4157	U4066	C3885	G3684	C3685	C3594
C4688	U4689	A4585	U4498	A4376	A4376	C4587	U4498	A4376	C4275	C4162	U4067	U3892	G3684	C3685	C3595
U4689	C4694	C4586	U4498	A4377	A4377	U4588	G4499	A4377	A4260	U4163	U4068	U3893	U3688	U3689	U2826
C4694	C4695	C4587	U4500	A4378	A4378	U4588	G4499	A4378	A4260	G4169	U4069	U3894	U3689	C3689	U2827
C4695	U4699	U4589	U4500	A4379	A4379	U4589	U4500	A4379	A4261	A4170	U4070	U3895	U3690	C3690	C3596
U4699	A4700	C4590	C4504	C4387	C4387	A4590	C4504	C4387	A4282	C4171	U4071	C3899	C3691	C3691	C3597
C4708	A4709	C4591	C4505	C4388	C4388	A4591	C4505	C4388	A4282	C4171	G4076	C3900	C3692	C3692	A2832
C4709	C4592	C4592	C4506	C4389	C4389	A4592	C4506	C4389	G4291	G4183	C4088	C3901	A3693	C3693	A2835
C4895	U4594	C4593	C4508	A4390	A4390	C4593	C4508	A4390	U4293	G4184	C4089	C3902	A3694	C3694	A2836
C4896	C4595	C4594	C4509	G4391	A4391	C4595	C4509	G4391	C4294	G4187	C4090	C3903	U3695	C3695	U2837
C4897	U4710	C4596	U4512	G4392	A4392	C4596	U4512	G4392	U4295	U4188	C4091	C3904	U3696	C3696	U2838
C4898	C4711	U4601	G4514	A4393	A4393	C4597	G4514	A4393	U4296	U4189	C4092	C3905	U3697	C3697	U2839
C4900	A4717	A4602	G4515	A4394	A4394	C4598	G4515	A4394	U4299	U4190	C4093	C3906	U3698	C3698	A2844
C4901	C4718	C4616	G4515	A4401	A4401	A4602	G4515	A4401	U4300	G4191	C4094	C3907	U3699	C3699	A2845
C4906	G4719	A4607	C4519	C4402	C4402	C4606	C4519	C4402	U4301	G4195	C4095	C3908	U3707	C3708	C2846
C4907	C4725	C4617	G4520	U4403	U4403	A4607	G4520	U4403	U4302	G4196	C4096	C3909	U3709	C3709	C2847
G4910	C4733	A4611	C4522	C4413	C4413	A4612	C4522	C4413	C4303	C4197	C4097	C3910	U3710	C3617	C2848
C4911	A4734	C4612	C4523	C4414	C4414	C4613	C4523	C4414	C4304	A4203	C4098	C3911	A3711	C3618	C2849
C4912	C4739	A4616	C4524	A4415	A4415	C4614	G4524	A4415	U4306	A4214	C4099	C3912	A3712	C3619	C2850
C4913	U4740	C4617	C4525	U4419	U4419	C4618	C4525	U4419	U4312	A4220	C4101	C3913	U3713	C3620	C2851
C4914	C4741	U4619	C4530	U4420	U4420	C4619	C4530	U4420	C4313	A4221	C4102	C3914	A3714	C3621	A2864
C4920	G4742	C4621	U4532	A4422	A4422	U4620	U4532	A4422	C4314	G4222	C4103	C3915	A3715	C3622	U2865
C4921	C4743	A4622	C4535	U4431	U4431	C4623	C4535	U4431	U4315	A4223	C4104	C3916	A3716	C3623	C2866
C4922	A4744	A4623	C4536	U4438	U4438	C4624	C4536	U4438	C4318	G4224	C4105	C3917	A3717	C3624	U2867
U4925	C4745	C4625	C4538	U4442	U4442	U4627	C4538	U4442	C4319	A4225	C4106	C3918	A3718	C3625	C2868
C4926	C4749	A4626	C4539	U4449	U4449	A4628	C4539	U4449	C4322	U4227	C4107	C3919	A3719	C3626	C2869
C4927	G4750	U4627	C4540	A4441	A4441	U4628	C4540	A4441	C4325	U4228	C4108	C3920	A3720	C3627	C2870
C4928	G4754	U4628	C4541	U4442	U4442	U4629	C4541	U4442	G4326	G4229	C4109	C3921	U3721	C3628	A2871
U4932	C4757	C4631	C4544	U4447	U4447	C4632	C4544	U4447	C4327	U4230	C4110	C3922	U3722	C3629	C2872
C4933	U4758	U4632	C4545	C4447	C4447	C4633	C4545	C4447	C4328	A4231	C4111	C3923	G3722	C3630	C2873
A4934	C4759	U4633	C4546	C4448	C4448	C4634	C4546	C4448	C4329	G4232	C4112	C3924	A3723	C3631	C2874
C4935	U4760	C4634	C4547	C4449	C4449	U4635	C4547	C4449	C4330	U4233	C4113	C3925	A3724	C3632	C2875
C5028	G4761	C4635	C4548	C4450	C4450	U4636	C4548	C4450	C4331	G4234	C4114	C3926	A3725	C3633	C2876
C5029	C4762	U4637	C4549	C4451	C4451	U4637	C4549	C4451	C4332	U4235	C4115	C3927	A3726	C3634	C2877
C5030	G4763	C4636	C4550	C4452	C4452	U4638	C4550	C4452	C4333	U4236	C4116	C3928	A3727	C3635	C2878
C4940	C4765	C4644	C4551	U4453	U4453	C4639	C4551	U4453	C4334	G4237	C4117	C3929	A3728	C3636	C2879
C4941	C4765	C4644	C4552	U4454	U4454	C4640	C4552	U4454	U4340	U4238	C4118	C3930	A3729	C3637	C2880
C5033	C4765	C4644	C4552	U4454	U4454	C4641	C4552	U4454	U4340	U4238	C4118	C3931	A3730	C3638	C2881
C5034	C4765	C4644	C4552	U4454	U4454	C4642	C4552	U4454	U4340	U4238	C4118	C3932	A3731	C3639	C2882
C5035	C4765	C4644	C4552	U4454	U4454	C4643	C4552	U4454	U4340	U4238	C4118	C3933	A3732	C3640	C2883
C5036	C4765	C4644	C4552	U4454	U4454	C4644	C4552	U4454	U4340	U4238	C4118	C3934	A3733	C3641	C2884
C5037	C4765	C4644	C4552	U4454	U4454	C4645	C4552	U4454	U4340	U4238	C4118	C3935	A3734	C3642	C2885
C5038	C4765	C4644	C4552	U4454	U4454	C4646	C4552	U4454	U4340	U4238	C4118	C3936	A3735	C3643	C2886
C5039	C4765	C4644	C4552	U4454	U4454	C4647	C4552	U4454	U4340	U4238	C4118	C3937	A3736	C3644	C2887
C5040	C4765	C4644	C4552	U4454	U4454	C4648	C4552	U4454	U4340	U4238	C4118	C3938	A3737	C3645	C2888
C5041	C4765	C4644	C4552	U4454	U4454	C4649	C4552	U4454	U4340	U4238	C4118	C3939	A3738	C3646	C2889
C5042	C4765	C4644	C4552	U4454	U4454	C4650	C4552	U4454	U4340	U4238	C4118	C3940	A3739	C3647	C2890
C5043	C4765	C4644	C4552	U4454	U4454	C4651	C4552	U4454	U4340	U4238	C4118	C3941	A3740	C3648	C2891
C5044	C4765	C4644	C4552	U4454	U4454	C4652	C4552	U4454	U4340	U4238	C4118	C3942	A3741	C3649	C2892
C5045	C4765	C4644	C4552	U4454	U4454	C4653	C4552	U4454	U4340	U4238	C4118	C3943	A3742	C3650	C2893
C5046	C4765	C4644	C4552	U4454	U4454	C4654	C4552	U4454	U4340	U4238	C4118	C3944	A3743	C3651	C2894
C5047	C4765	C4644	C4552	U4454	U4454	C4655	C4552	U4454	U4340	U4238	C4118	C3945	A3744	C3652	C2895
C5048	C4765	C4644	C4552	U4454	U4454	C4656	C4552	U4454	U4340	U4238	C4118	C3946	A3745	C3653	C2896
C5049	C4765	C4644	C4552	U4454	U4454	C4657	C4552	U4454	U4340	U4238	C4118	C3947	A3746	C3654	C2897
C5050	C4765	C4644	C4552	U4454	U4454	C4658	C4552	U4454	U4340	U4238	C4118	C3948	A3747	C3655	C2898
C5051	C4765	C4644	C4552	U4454	U4454	C4659	C4552	U4454	U4340	U4238	C4118	C3949	A3748	C3656	C2899
C5052	C4765	C4644	C4552	U4454	U4454	C4660	C4552	U4454	U4340	U4238	C4118	C3950	A3749	C3657	C2900
C5053	C4765	C4644	C4552	U4454	U4454	C4661	C4552	U4454	U4340	U4238	C4118	C3951	A3750	C3658	C2901
C5054	C4765	C4644	C4552	U4454	U4454	C4662	C4552	U4454	U4340	U4238	C4118	C3952	A3751	C3659	C2902



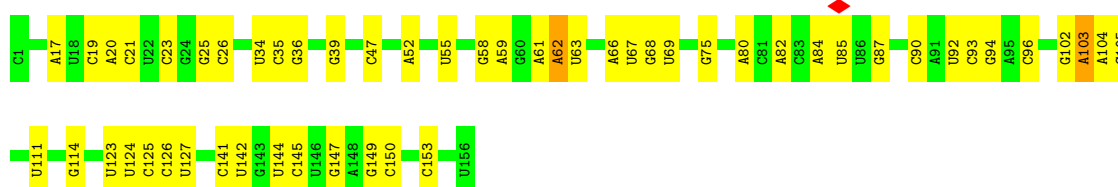
- Molecule 3: 5S rRNA

Chain L7: 80% 18%



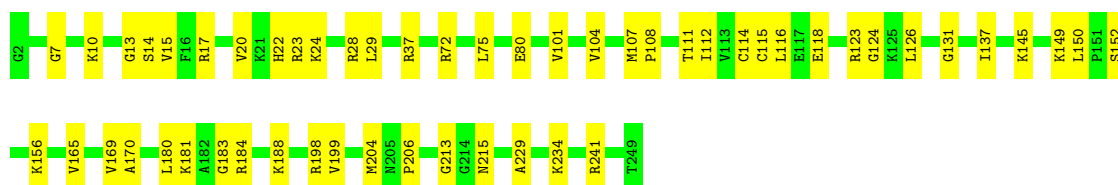
- Molecule 4: 5.8S rRNA

Chain L8: 66% 33%



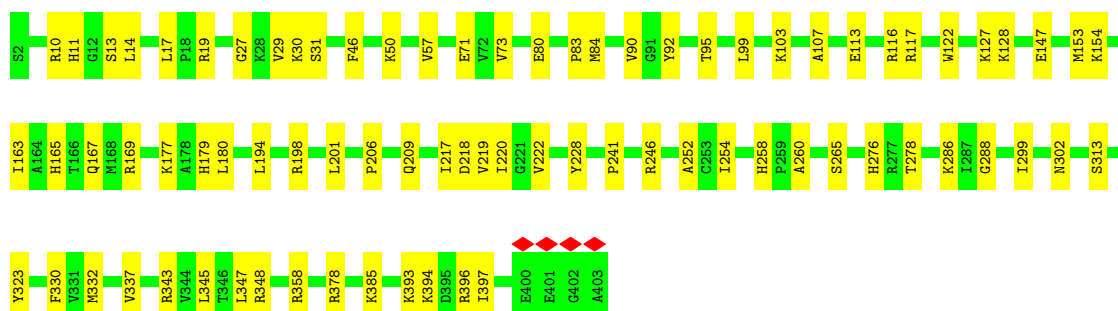
- Molecule 5: 60S ribosomal protein L8

Chain LA: 79% 21%



- Molecule 6: Large ribosomal subunit protein uL3

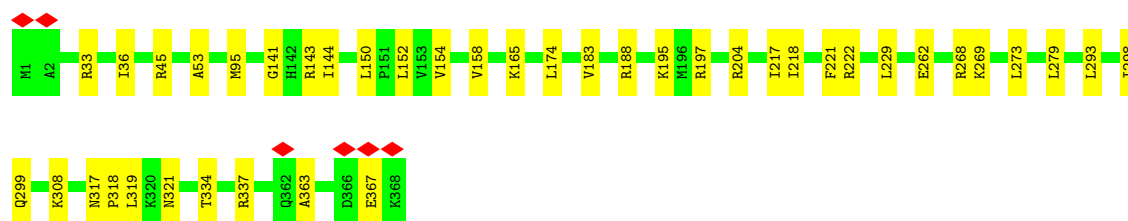
Chain LB: 80% 20%



- Molecule 7: 60S ribosomal protein L4

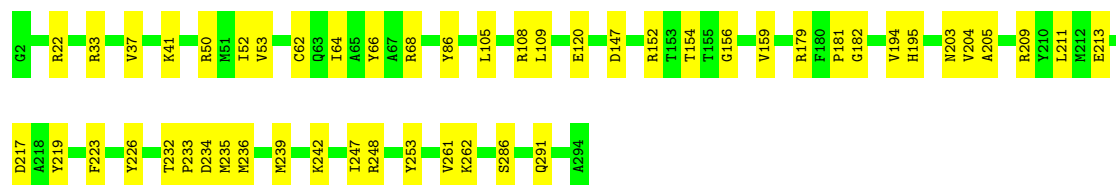
Chain LC: 89% 11%





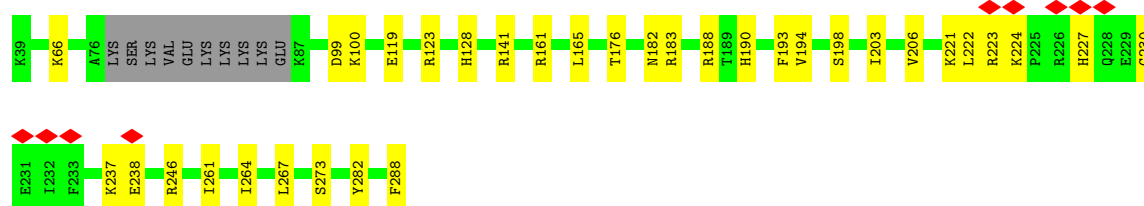
- Molecule 8: Large ribosomal subunit protein uL18

Chain LD: 83% 17%



- Molecule 9: Large ribosomal subunit protein eL6

Chain LE: 82% 14%



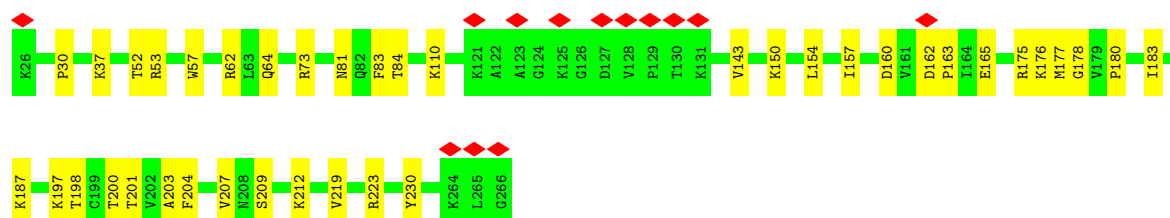
- Molecule 10: 60S ribosomal protein L7

Chain LF: 81% 19%

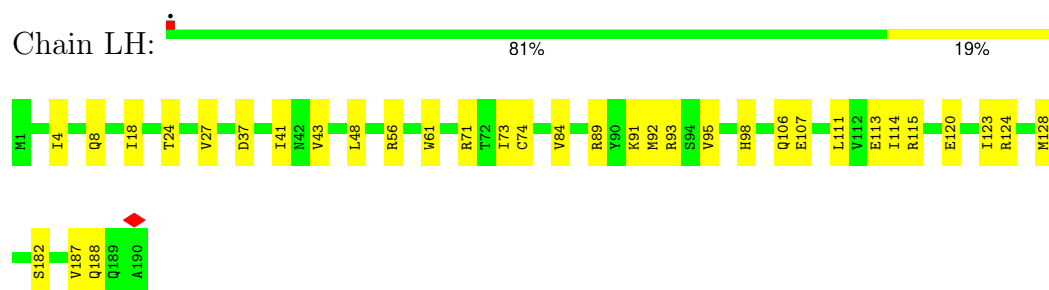


- Molecule 11: 60S ribosomal protein L7a

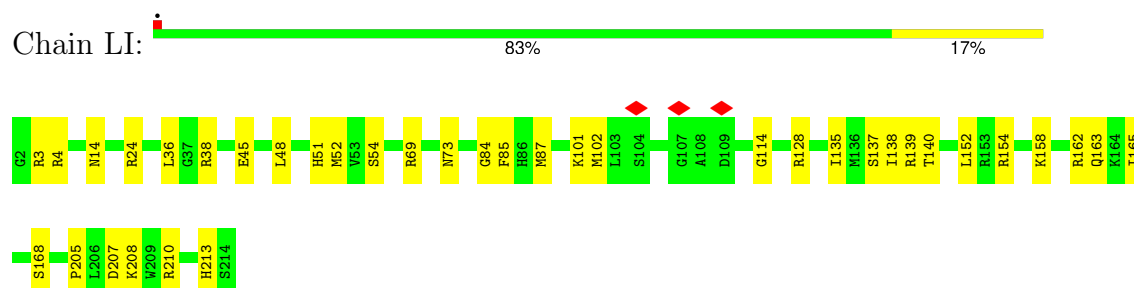
Chain LG: 84% 16%



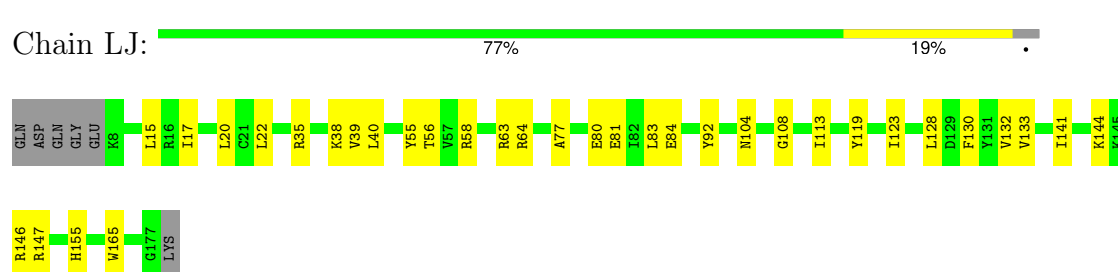
- Molecule 12: 60S ribosomal protein L9



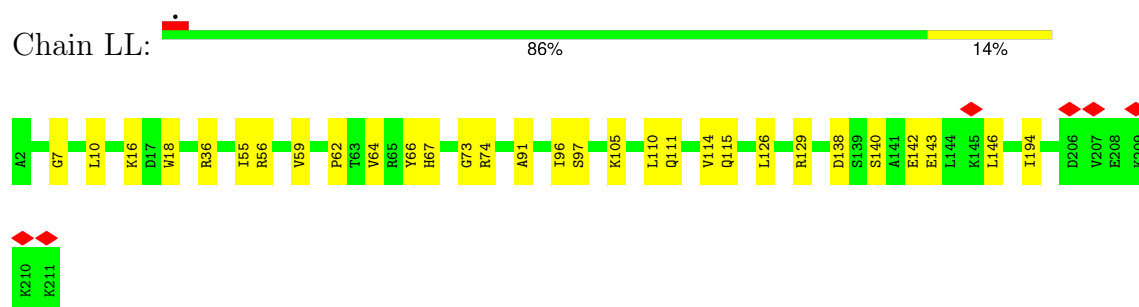
- Molecule 13: Ribosomal protein uL16-like



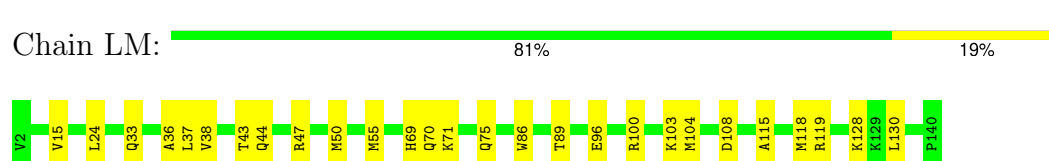
- Molecule 14: 60S ribosomal protein L11



- Molecule 15: Large ribosomal subunit protein eL13



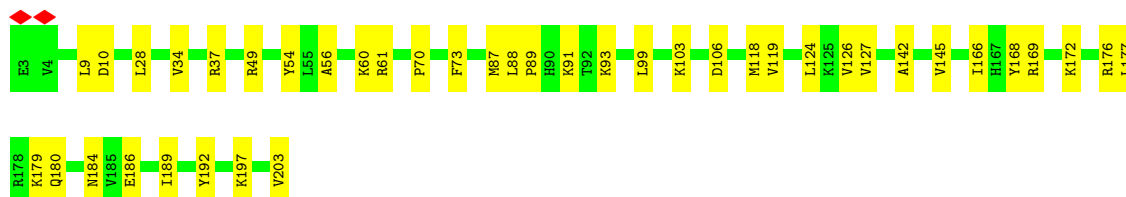
- Molecule 16: 60S ribosomal protein L14



● Molecule 17: 60S ribosomal protein L15

Chain LN:  86% 14%

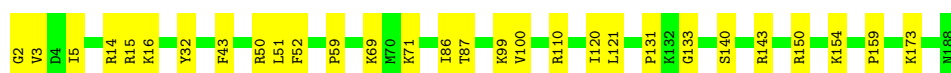
● Molecule 18: 60S ribosomal protein L13a

Chain LO:  80% 20%

● Molecule 19: 60S ribosomal protein L17

Chain LP:  82% 18%

● Molecule 20: 60S ribosomal protein L18

Chain LQ:  84% 16%

● Molecule 21: 60S ribosomal protein L19

Chain LR:  86% 14%

● Molecule 22: 60S ribosomal protein L18a

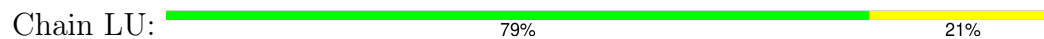
Chain LS:  88% 12%

● Molecule 23: 60S ribosomal protein L21

Chain LT:  87% 13%



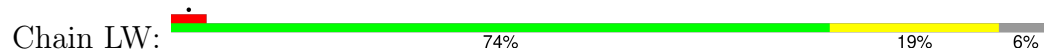
- Molecule 24: Heparin-binding protein HBp15



- Molecule 25: 60S ribosomal protein L23



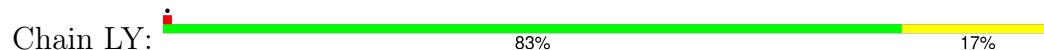
- Molecule 26: Ribosomal protein L24



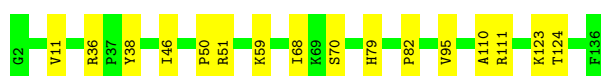
- Molecule 27: 60S ribosomal protein L23a



- Molecule 28: 60S ribosomal protein L26



- Molecule 29: 60S ribosomal protein L27

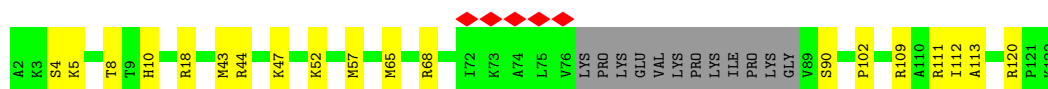
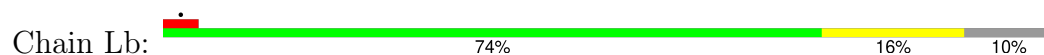


- Molecule 30: 60S ribosomal protein L27a

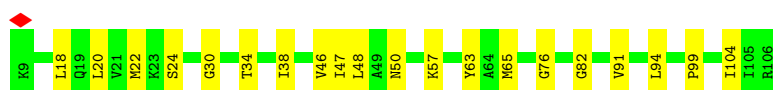
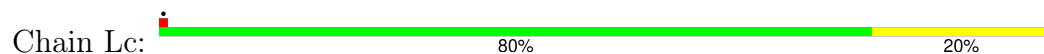




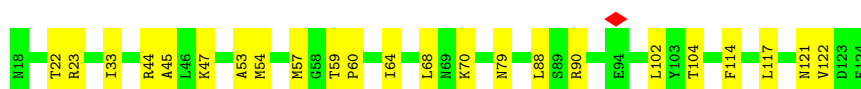
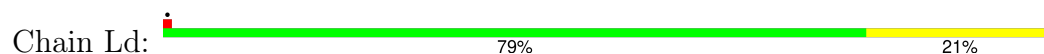
- Molecule 31: Large ribosomal subunit protein eL29



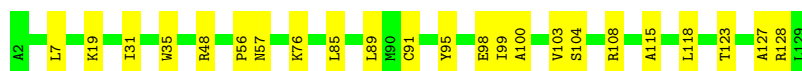
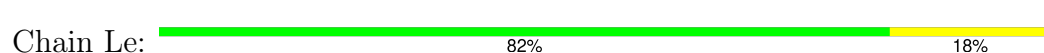
- Molecule 32: 60S ribosomal protein L30



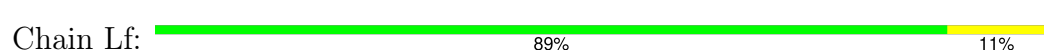
- Molecule 33: 60S ribosomal protein L31



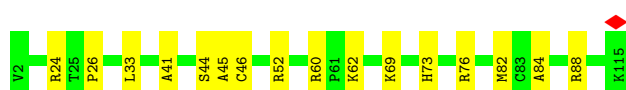
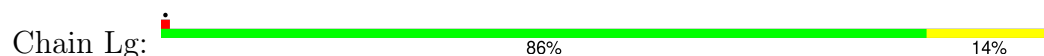
- Molecule 34: 60S ribosomal protein L32



- Molecule 35: 60S ribosomal protein L35a



- Molecule 36: 60S ribosomal protein L34



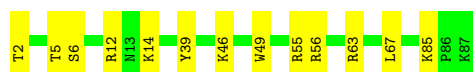
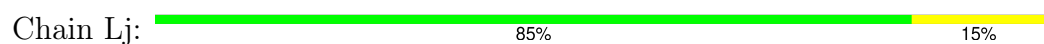
- Molecule 37: 60S ribosomal protein L35



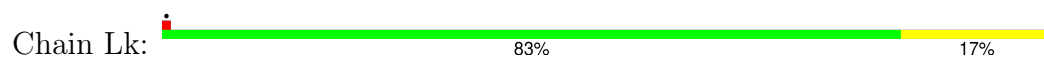
- Molecule 38: 60S ribosomal protein L36



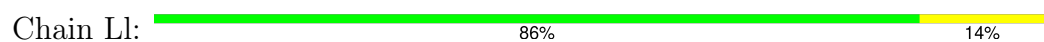
- Molecule 39: 60S ribosomal protein L37



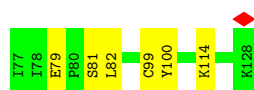
- Molecule 40: 60S ribosomal protein L38



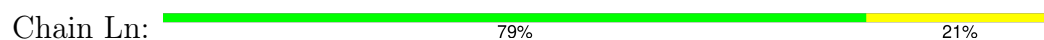
- Molecule 41: 60S ribosomal protein L39



- Molecule 42: Large ribosomal subunit protein eL40



- Molecule 43: 60S ribosomal protein L41

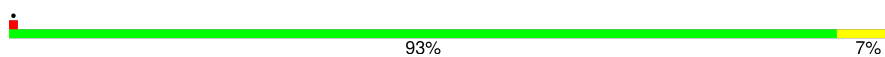


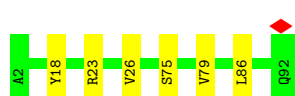
- Molecule 44: 60S ribosomal protein L36a

Chain Lo:  86% 14%



- Molecule 45: 60S ribosomal protein L37a

Chain Lp:  93% 7%



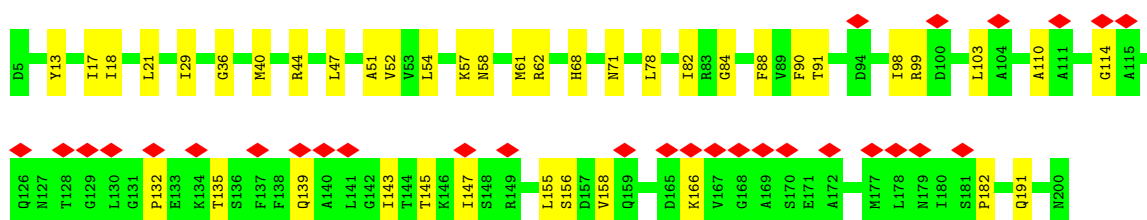
- Molecule 46: 60S ribosomal protein L28

Chain Lr:  92% 8%



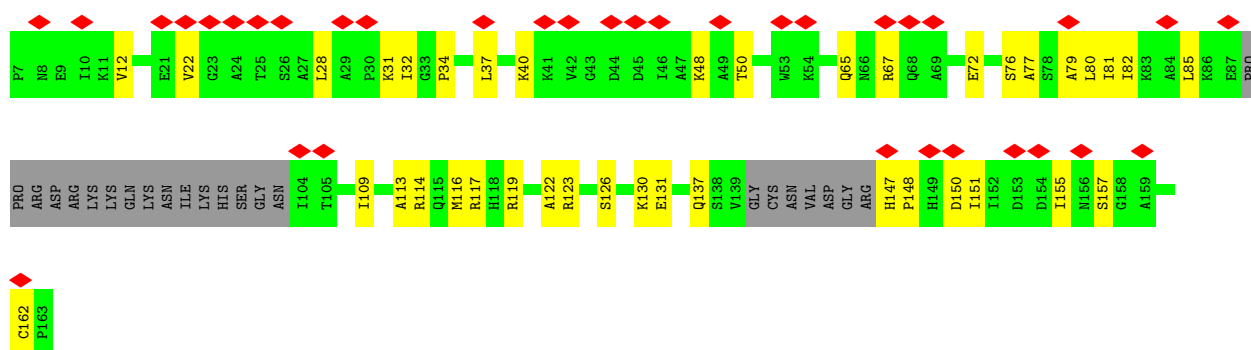
- Molecule 47: 60S acidic ribosomal protein P0

Chain Ls:  15% 79% 21%



- Molecule 48: Large ribosomal subunit protein uL11

Chain Lt:  22% 61% 25% 15%

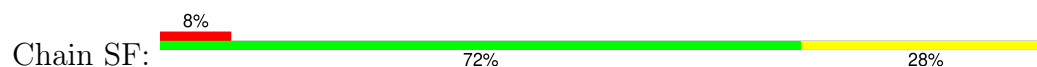


- Molecule 49: Small ribosomal subunit protein uS3

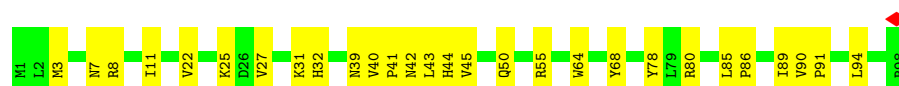
Chain SD:  88% 12%



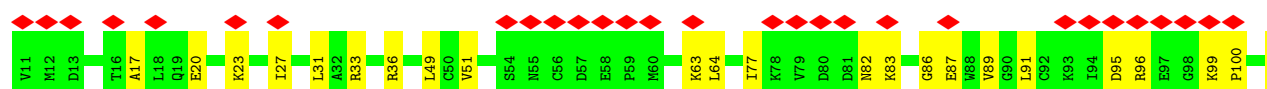
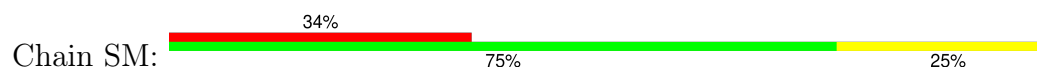
- Molecule 50: 40S ribosomal protein S5



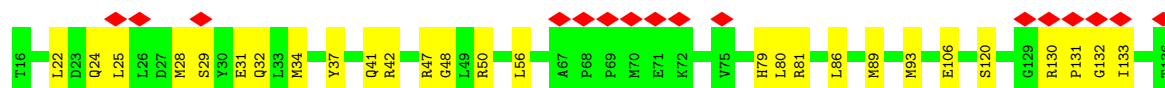
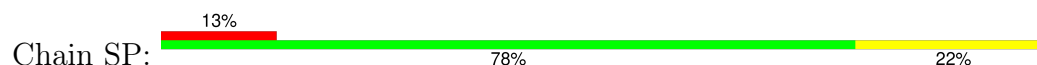
- Molecule 51: 40S ribosomal protein S10



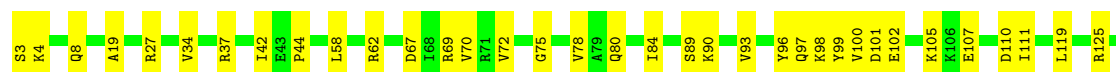
- Molecule 52: Small ribosomal subunit protein eS12

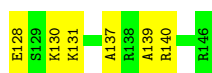


- Molecule 53: Small ribosomal subunit protein uS19

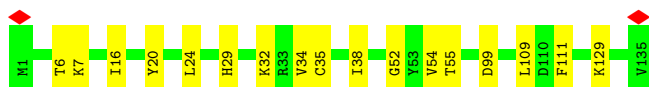
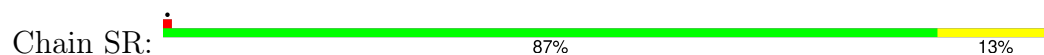


- Molecule 54: Small ribosomal subunit protein uS9

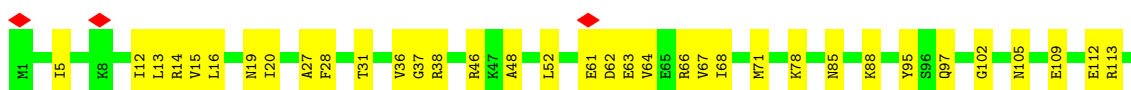




- Molecule 55: Small ribosomal subunit protein eS17



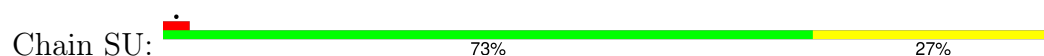
- Molecule 56: 40S ribosomal protein S18



- Molecule 57: 40S ribosomal protein S19



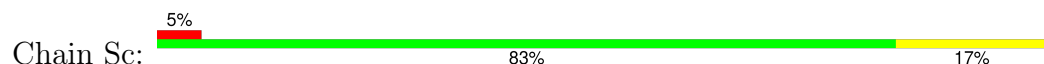
- Molecule 58: 40S ribosomal protein S20



- Molecule 59: Small ribosomal subunit protein eS25



- Molecule 60: 40S ribosomal protein S28





- Molecule 61: 40S ribosomal protein S29

Chain Sd: 67% 33%



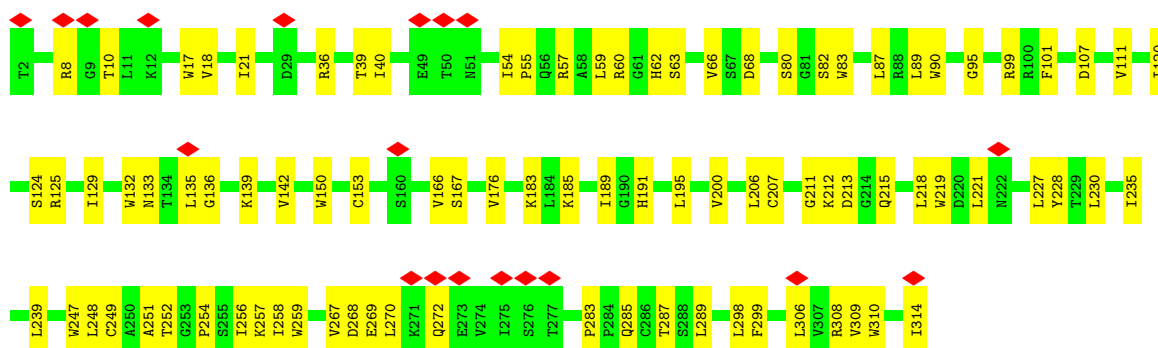
- Molecule 62: Ubiquitin-40S ribosomal protein S27a

Chain Sf: 13% 64% 36%



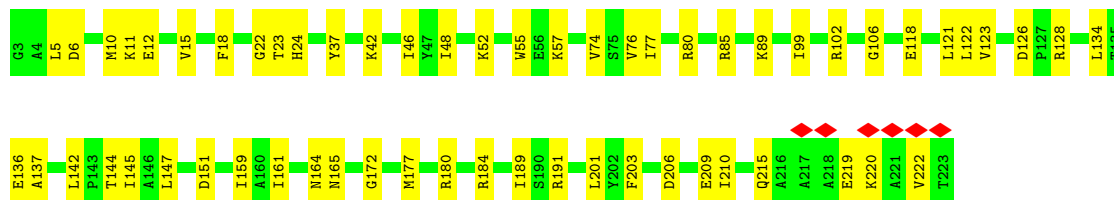
- Molecule 63: Receptor of activated protein C kinase 1

Chain Sg: 6% 72% 28%



- Molecule 64: 40S ribosomal protein SA

Chain SA: 73% 27%



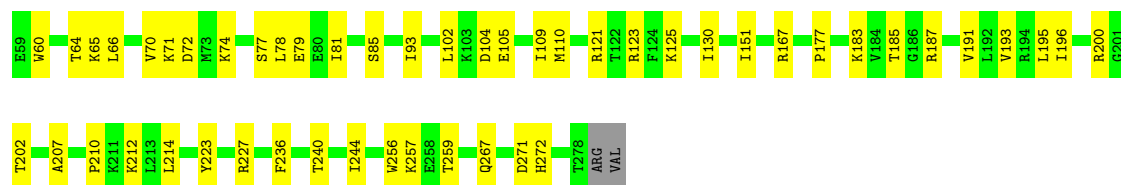
- Molecule 65: 40S ribosomal protein S3a

Chain SB: 79% 21%



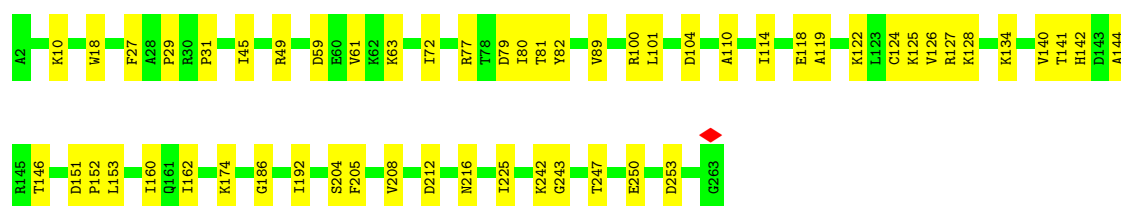
- Molecule 66: 40S ribosomal protein S2

Chain SC: 77% 23%



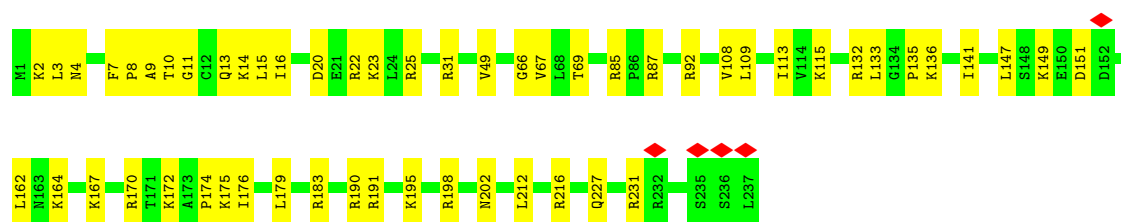
- Molecule 67: Small ribosomal subunit protein eS4, X isoform

Chain SE: 79% 21%



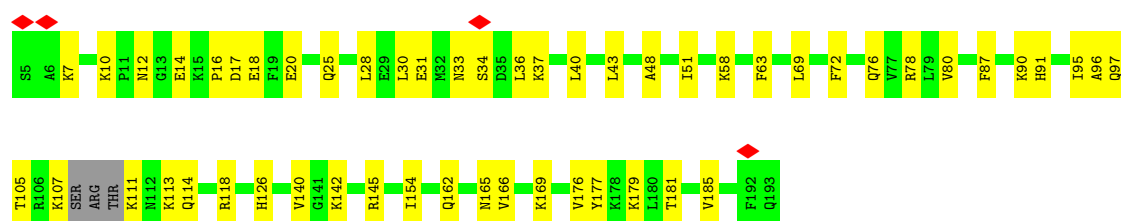
- Molecule 68: 40S ribosomal protein S6

Chain SG: 77% 23%

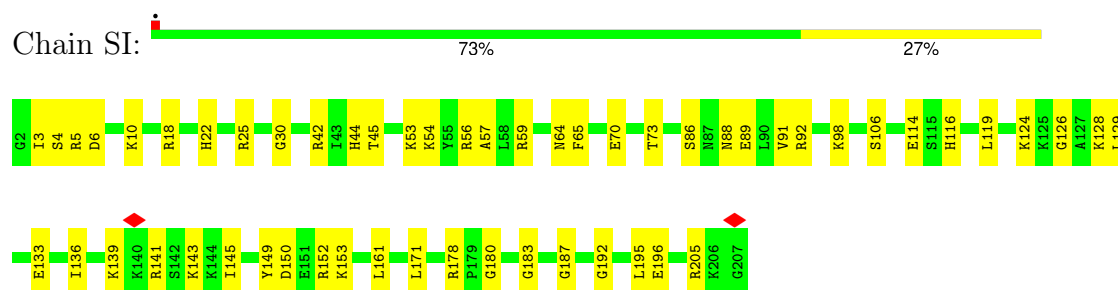


- Molecule 69: Small ribosomal subunit protein eS7

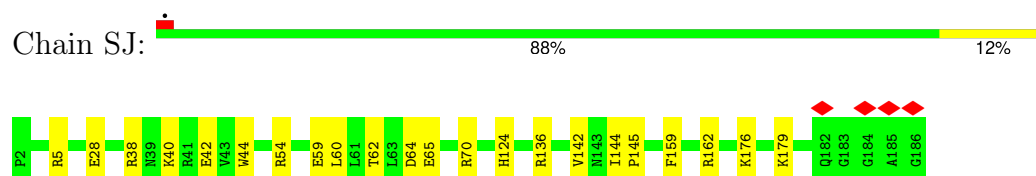
Chain SH: 70% 28%



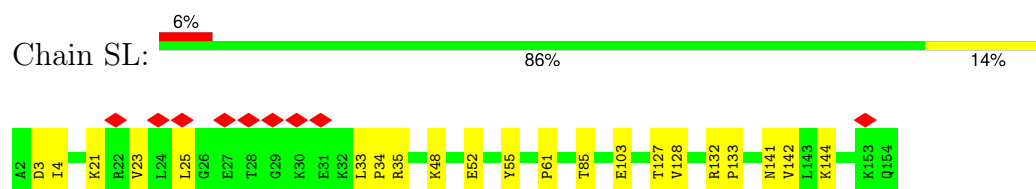
- Molecule 70: 40S ribosomal protein S8



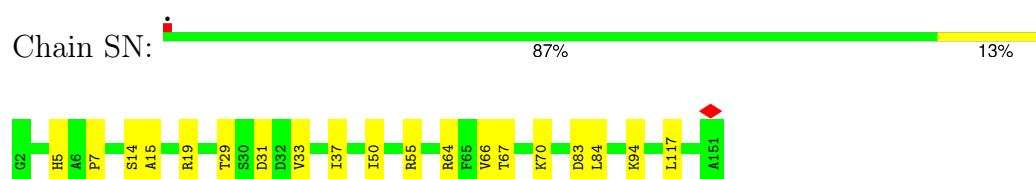
- Molecule 71: 40S ribosomal protein S9



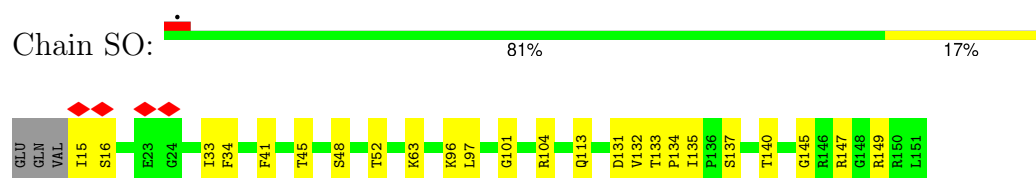
- Molecule 72: 40S ribosomal protein S11



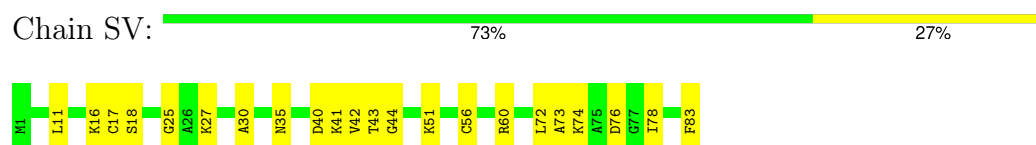
- Molecule 73: 40S ribosomal protein S13



- Molecule 74: Small ribosomal subunit protein uS11



- Molecule 75: Small ribosomal subunit protein eS21



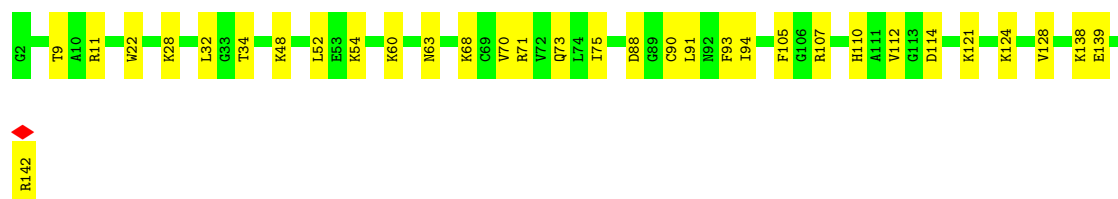
- Molecule 76: 40S ribosomal protein S15a

Chain SW:  81% 19%



- Molecule 77: 40S ribosomal protein S23

Chain SX:  77% 23%



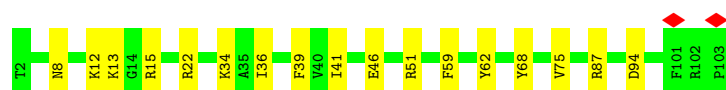
- Molecule 78: 40S ribosomal protein S24

Chain SY:  78% 22%



- Molecule 79: 40S ribosomal protein S26

Chain Sa:  83% 17%



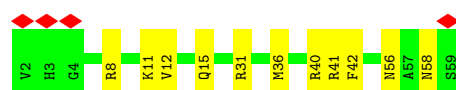
- Molecule 80: Small ribosomal subunit protein eS27

Chain Sb:  76% 24%



- Molecule 81: Small ribosomal subunit protein eS30

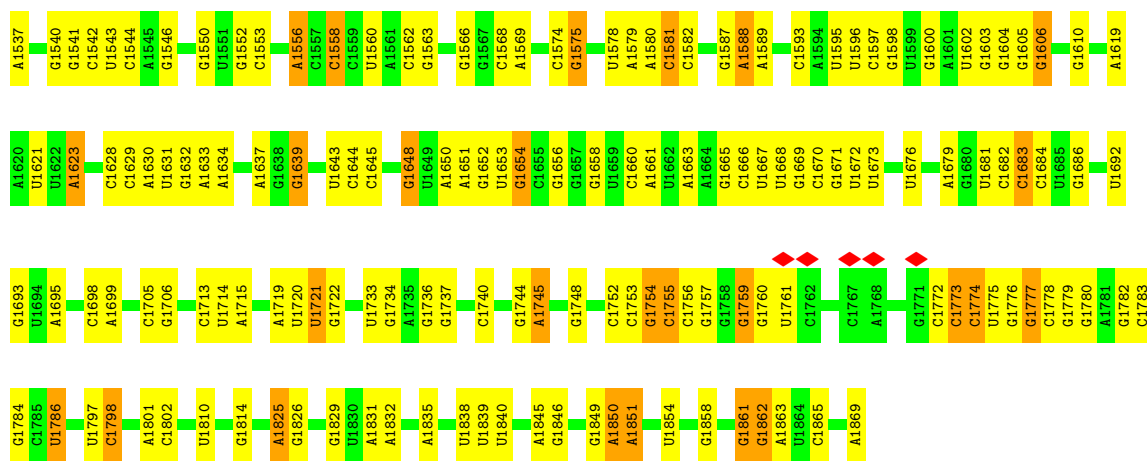
Chain Se:  7% 81% 19%



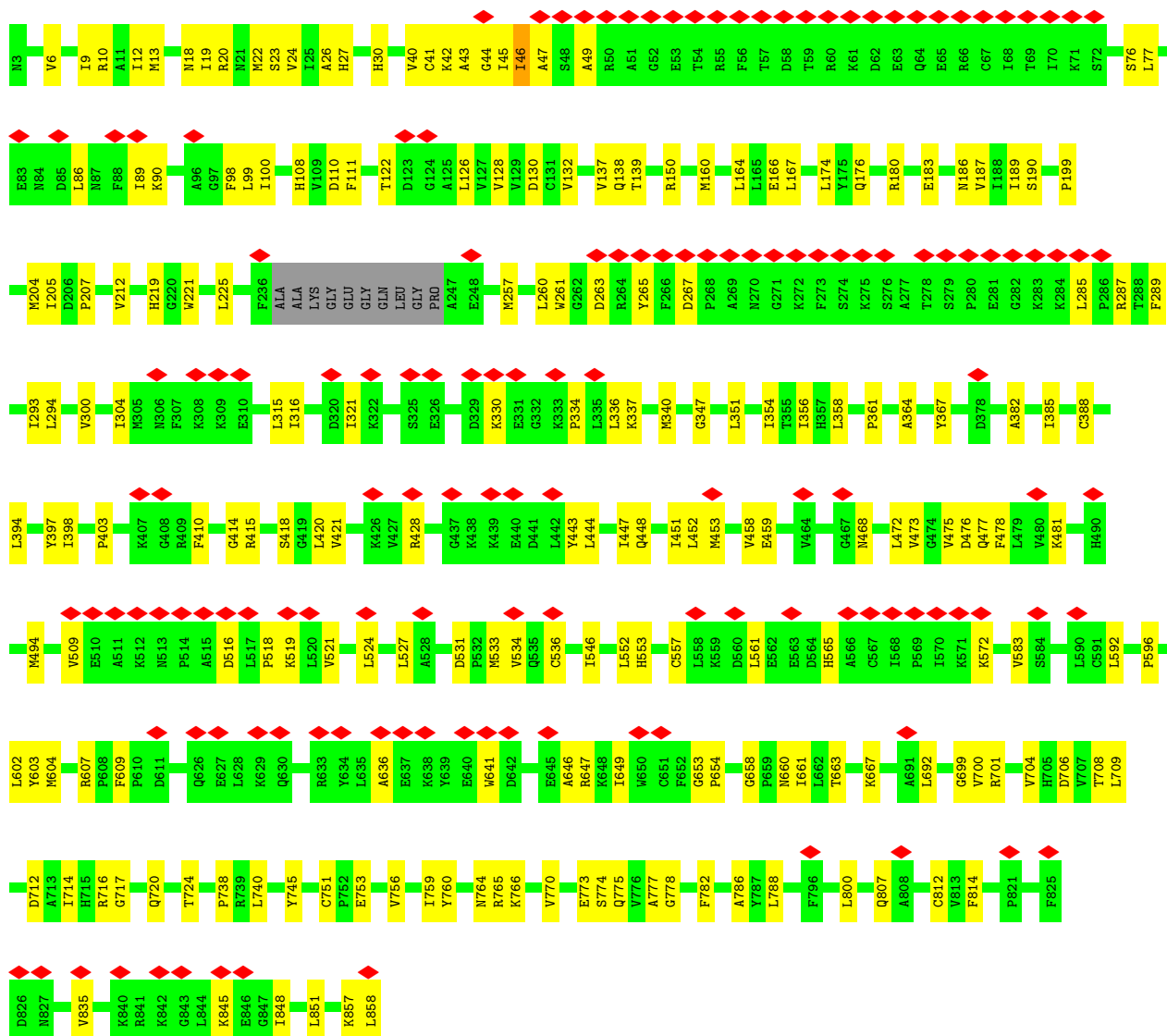
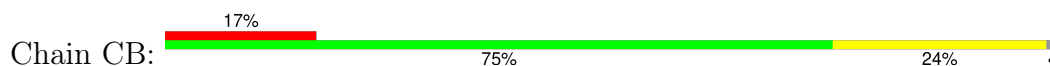
- Molecule 82: 18S rRNA

Chain S2:  56% 36% 8%

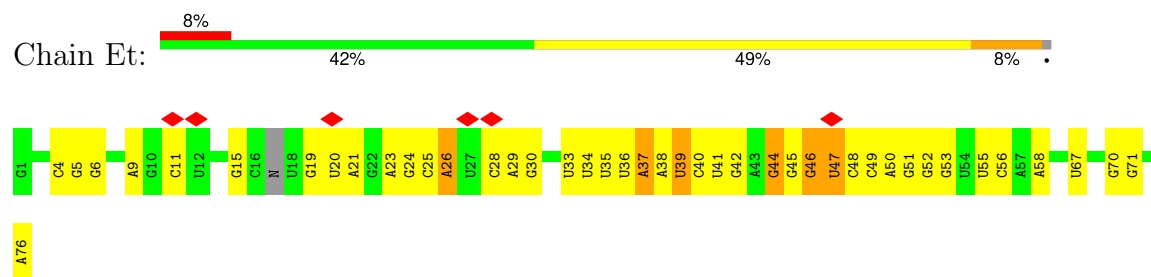
U1	G95	C179	U928	G436	A519	G601	U689	G836	G925	A1020	A1133	U1239	U1326	C1433
C4	A95	C186	G329	G437	A520	G604	G692	A837	G928	A1023	A1138	A1240	G1327	C1434
G6	A102	C187	G330	G438	A522	A604	A693	G838	G929	A1024	C1138	U1242	G1328	C1435
C13	A103	G187	G331	C441	A525	G606	G695	G840	G930	U1025	C1139	U1243	N1337	C1436
C14	A104	C190	G332	C442	A526	G607	G696	G841	G931	U1026	G1140	U1244	G1338	C1437
G16	A105	A191	G333	A445	G527	G608	G697	G842	G932	A1027	A1143	B81248	U1342	A1438
C17	A106	C192	G334	A448	A528	C614	G698	G843	G933	A1028	A1144		U1347	A1439
C18	A107	C193	C334	A449	A529	G615	G699	G844	G934	A1031	A1145		U1348	
C19	A108	C194	C335	A450	A530	G616	G700	G845	G935	G1032	A1146		U1349	
C20	A109	C195	C336	A451	A531	A616	G701	G846	G936	G1033	A1147		U1350	
G25	G113	U197	G337	A452	A532	G617	G702	A847	G937	A1034	A1148		G1351	
U26	G114	U198	A347	A453	A533	G623	G703	C851	G938	G1035	A1149		U1352	
A27	U115	U199	A348	A454	A534	G624	G704	G852	G939	U1045	A1150		U1353	
U28	U116	C200	A349	A455	A535	G625	G705	G853	G940	U1046	A1151		U1354	
G29	C117	G201	A350	A456	A536	G626	G706	G854	G941	C1047	A1152		U1355	
C30	C118	G202	A351	A457	A537	G627	G707	G855	G942	G1048	A1153		U1356	
G33	U121	G203	A352	A458	A538	G628	G708	G856	G943	U1055	U1173		U1357	
A38	G122	G204	A353	A459	A539	G629	G709	G857	G944	U1056	U1174		U1371	
G41	C125	G207	A354	A460	A540	G630	G710	G858	G945	U1057	U1175		U1372	
A42	G126	G208	A355	A461	A541	G631	G711	G859	G946	C1057	U1176		U1373	
U43	G130	U214	A356	A462	A542	G632	G712	G860	G947	U1058	U1177		U1374	
U44	G136	C223	A357	A463	A543	G633	G713	G861	G948	G1059	U1178		U1375	
A45	U137	A224	A358	A464	A544	G634	G714	G862	G949	U1060	U1179		U1376	
A46	G142	G291	A359	A465	A545	G635	G715	G863	G950	U1061	U1180		U1377	
C49	U143	C292	A360	A466	A546	G636	G716	G864	G951	U1062	U1181		U1378	
A50	U144	C293	A361	A467	A547	G637	G717	G865	G952	U1063	U1182		U1379	
U51	U145	U294	A362	A468	A548	G638	G718	G866	G953	U1064	U1183		A1383	
G52	G146	C295	A363	A469	A549	G639	G719	G867	G954	U1065	U1184		U1388	
G56	G149	G298	A364	A470	A550	G640	G720	G868	G955	C1085	U1207		U1494	
U57	A149	A302	A365	A471	A551	G641	G721	G869	G956	U1080	A1208		U1495	
C58	C151	C306	A366	A472	A552	G642	G722	G870	G957	U1081	A1209		U1496	
U59	U152	C382	A367	A473	A553	G643	G723	G871	G958	U1082	C1215		U1497	
A64	U153	G307	A368	A474	A554	G644	G724	G872	G959	U1083	C1216		U1498	
G65	U154	U154	A369	A475	A555	G645	G725	G873	G960	U1084	A1217		G1398	
C66	A158	G309	A370	A476	A556	G646	G726	G874	G961	C1085	C1218		U1499	
G67	A159	C311	A371	A477	A557	G647	G727	G875	G962	U1085	U1201		A1401	
A69	U160	A313	A372	A478	A558	G648	G728	G876	G963	U1086	U1202		A1402	
G71	C162	G316	A373	A479	A559	G649	G729	G877	G964	U1087	U1203		A1405	
C72	G165	A318	A374	A480	A560	G650	G730	G878	G965	U1088	U1204		G1406	
C73	A166	C319	A375	A481	A561	G651	G731	G879	G966	U1089	U1205		U1407	
G74	G167	G320	A376	A482	A562	G652	G732	G880	G967	U1090	U1206		U1408	
U76	C168	G321	A377	A483	A563	G653	G733	G881	G968	U1091	U1207		G1413	
A83	U169	G322	A378	A484	A564	G654	G734	G882	G969	C1109	G1221		C1417	
A84	A171	C323	A379	A485	A565	G655	G735	G883	G970	U1112	A1222		C1418	
A85	U172	C324	A380	A486	A566	G656	G736	G884	G971	U1113	G1223		C1419	
U93	A175	C325	A381	A487	A567	G657	G737	G885	G972	U1114	U1224		G1420	
G94	G327	A433	A382	A488	A568	G658	G738	G886	G973	U1115	U1225		A1421	
		A434	A383	A489	A569	G659	G739	G887	G974	U1116	U1226		G1500	
		A435	A384	A490	A570	G660	G740	G888	G975	U1117	G1227		C1512	
			A385	A491	A571	G661	G741	G889	G976	U1118	U1228		C1513	
			A386	A492	A572	G662	G742	G890	G977	U1119	A1229		G1514	
			A387	A493	A573	G663	G743	G891	G978	U1120	U1230		C1518	
			A388	A494	A574	G664	G744	G892	G979	U1121	U1231		U1519	
			A389	A495	A575	G665	G745	G893	G980	U1122	U1232		G1520	
			A390	A496	A576	G666	G746	G894	G981	U1123	U1233		C1521	
			A391	A497	A577	G667	G747	G895	G982	U1124	U1234		G1528	
			A392	A498	A578	G668	G748	G896	G983	U1125	U1235		A1531	
			A393	A499	A579	G669	G749	G897	G984	U1126	U1236		G1532	
			A394	A500	A580	G670	G750	G898	G985	U1127	U1237		A1533	
			A395	A501	A581	G671	G751	G899	G986	U1128	U1238		G1536	
			A396	A502	A582	G672	G752	G900	G987	U1129	U1239			
			A397	A503	A583	G673	G753	G901	G988	U1130	U1240			
			A398	A504	A584	G674	G754	G902	G989		U1241			
			A399	A505	A585	G675	G755	G903	G990		U1242			
			A400	A506	A586	G676	G756	G904	G991		U1243			
			A401	A507	A587	G677	G757	G905	G992		U1244			
			A402	A508	A588	G678	G758	G906	G993		U1245			
			A403	A509	A589	G679	G759	G907	G994		U1246			
			A404	A510	A590	G680	G760	G908	G995		U1247			
			A405	A511	A591	G681	G761	G909	G996		U1248			
			A406	A512	A592	G682	G762	G910	G997		U1249			
			A407	A513	A593	G683	G763	G911	G998		U1250			
			A408	A514	A594	G684	G764	G912	G999		U1251			
			A409	A515	A595	G685	G765	G913	G1000		U1252			
			A410	A516	A596	G686	G766	G914	A1001		U1253			
			A411	A517	A597	G687	G767	G915	U1002		U1254			
			A412	A518	A598	G688	G768	G916	U1003		U1255			
			A413	A519	A599	G689	G769	G917	U1004		U1256			
			A414	A520	A600	G690	G770	G918	U1005		U1257			
			A415	A521	A601	G691	G771	G919	U1006		U1258			
			A416	A522	A602	G692	G772	G920	U1007		U1259			
			A417	A523	A603	G693	G773	G921	U1008		U1260			
			A418	A524	A604	G694	G774	G922	U1009		U1261			
			A419	A525	A605	G695	G775	G923	U1010		U1262			
			A420	A526	A606	G696	G776	G924	U1011		U1263			
			A421	A527	A607	G697	G777	G925	U1012		U1264			
			A422	A528	A608	G698	G778	G926	U1013		U1265			
			A423	A529	A609	G699	G779	G927	U1014		U1266			
			A424	A530	A610	G700	G780	G928	U1015		U1267			
			A425	A531	A611	G701	G781	G929	U1016		U1268			
			A426	A532	A612	G702	G782	G930	U1017		U1269			
			A427	A533	A613	G703	G783	G931	U1018		U1270			
			A428	A534	A614	G704	G784	G932	U1019		U1271			
			A429	A535	A615	G705	G785	G933	U1020		U1272			
			A430	A536	A616	G706	G786	G934	U1021		U1273			
			A431	A537	A617	G707	G787	G935	U1022		U1274			
			A432	A538	A618	G708	G788	G936	U1023		U1275			
			A433	A539	A619	G709	G789	G937	U1024		U1276			
			A434	A540	A620	G710	G790	G938	U1025		U1277			
			A435	A541	A621	G711	G791	G939	U1026		U1278			
			A436	A542	A622	G712	G792	G940	U1027		U1279			
			A437	A543	A623	G713	G793	G941	U1028		U1280			
			A438	A544	A624	G714	G794	G942	U1029		U1281			
			A439	A545	A625	G715	G795	G943	U1030		U1282			
			A440	A546	A626	G716	G796	G944	U1031		U1283			
			A441	A547	A627	G717	G797	G945	U1032		U1284			
			A442	A548	A628	G718	G798	G946	U1033		U1285			
			A443	A549	A629	G719	G799	G947	U1034		U1286			
			A444	A550	A630	G720	G800	G948	U1035		U1287			
			A445	A551	A631	G721	G801	G949	U1036		U1288			
			A446	A552	A632	G722	G802	G950	U1037		U1289			



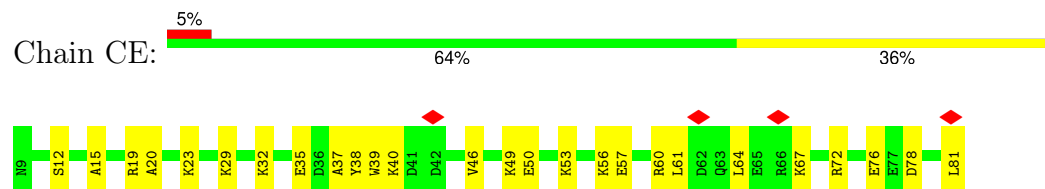
• Molecule 83: Elongation factor 2



● Molecule 84: E site tRNA



● Molecule 85: Coiled-coil domain-containing protein 124



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	86934	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	0.165	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0136	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: MG, B8N, G7M, SPD, MA6, ZN, UY1, 5MC, UR3, OMC, OMG, A2M, 6MZ, PSU, OMU, 4AC, SPM, 1MA

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	L5	0.29	0/85098	0.30	0/132762
3	L7	0.27	0/2861	0.25	0/4459
4	L8	0.28	0/3631	0.28	0/5657
5	LA	0.29	0/1936	0.42	0/2596
6	LB	0.26	0/3306	0.40	0/4424
7	LC	0.27	0/2981	0.37	0/4002
8	LD	0.22	0/2428	0.33	0/3252
9	LE	0.22	0/1973	0.40	0/2645
10	LF	0.26	0/1905	0.33	0/2539
11	LG	0.23	0/1960	0.38	0/2637
12	LH	0.23	0/1537	0.36	0/2066
13	LI	0.24	0/1751	0.35	0/2340
14	LJ	0.20	0/1385	0.40	0/1852
15	LL	0.23	0/1732	0.31	0/2315
16	LM	0.26	0/1161	0.40	0/1554
17	LN	0.28	0/1746	0.34	0/2338
18	LO	0.27	0/1682	0.37	0/2250
19	LP	0.28	0/1268	0.41	0/1701
20	LQ	0.28	0/1537	0.37	0/2052
21	LR	0.24	0/1582	0.37	0/2091
22	LS	0.27	0/1493	0.36	0/2003
23	LT	0.24	0/1326	0.33	0/1770
24	LU	0.25	0/839	0.52	0/1126
25	LV	0.25	0/993	0.37	0/1332
26	LW	0.22	0/959	0.37	0/1270
27	LX	0.23	0/1002	0.36	0/1345
28	LY	0.24	0/1132	0.36	0/1504
29	LZ	0.23	0/1130	0.37	0/1507
30	La	0.26	0/1191	0.32	0/1591
31	Lb	0.21	0/889	0.38	0/1175

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lc	0.25	0/774	0.38	0/1038
33	Ld	0.25	0/903	0.38	0/1216
34	Le	0.27	0/1071	0.33	0/1429
35	Lf	0.28	0/895	0.37	0/1198
36	Lg	0.25	0/916	0.33	0/1220
37	Lh	0.22	0/1023	0.33	0/1351
38	Li	0.21	0/843	0.30	0/1115
39	Lj	0.28	0/720	0.40	0/952
40	Lk	0.21	0/575	0.42	0/761
41	Ll	0.26	0/454	0.30	0/599
42	Lm	0.23	0/435	0.35	0/575
43	Ln	0.26	0/231	0.35	0/294
44	Lo	0.26	0/876	0.35	0/1156
45	Lp	0.25	0/718	0.34	0/953
46	Lr	0.25	0/1017	0.33	0/1364
47	Ls	0.13	0/1519	0.34	0/2052
48	Lt	0.16	0/1009	0.48	0/1363
49	SD	0.15	0/1793	0.30	0/2414
50	SF	0.18	0/1516	0.37	0/2037
51	SK	0.18	0/851	0.46	0/1147
52	SM	0.14	0/950	0.39	0/1275
53	SP	0.17	0/1003	0.39	0/1342
54	SQ	0.18	0/1160	0.40	0/1553
55	SR	0.19	0/1105	0.47	0/1484
56	SS	0.18	0/1216	0.38	0/1628
57	ST	0.17	0/1131	0.38	0/1515
58	SU	0.19	0/831	0.49	0/1115
59	SZ	0.19	0/604	0.46	0/810
60	Sc	0.19	0/508	0.39	0/680
61	Sd	0.18	0/470	0.32	0/623
62	Sf	0.15	0/560	0.46	0/745
63	Sg	0.15	0/2493	0.39	0/3394
64	SA	0.19	0/1778	0.37	0/2416
65	SB	0.19	0/1765	0.38	0/2362
66	SC	0.21	0/1744	0.36	0/2357
67	SE	0.18	0/2118	0.36	0/2849
68	SG	0.16	0/1946	0.36	0/2590
69	SH	0.18	0/1519	0.42	0/2033
70	SI	0.21	0/1715	0.37	0/2287
71	SJ	0.17	0/1550	0.32	0/2069
72	SL	0.21	0/1268	0.31	0/1696
73	SN	0.19	0/1232	0.27	0/1656
74	SO	0.23	0/1037	0.41	0/1391

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SV	0.20	0/643	0.38	0/860
76	SW	0.23	0/1051	0.35	0/1406
77	SX	0.20	0/1116	0.37	0/1490
78	SY	0.18	0/1083	0.42	0/1438
79	Sa	0.22	0/836	0.35	0/1121
80	Sb	0.20	0/665	0.37	0/891
81	Se	0.16	0/465	0.38	0/612
82	S2	0.24	0/39756	0.28	0/61939
83	CB	0.15	0/6734	0.37	1/9094 (0.0%)
84	Et	0.27	0/1778	0.44	0/2767
85	CE	0.21	0/616	0.47	0/812
All	All	0.25	0/237246	0.33	1/347012 (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
54	SQ	0	1
74	SO	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	CB	46	ILE	N-CA-C	-6.57	106.89	113.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
74	SO	137	SER	Peptide
54	SQ	107	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CI	247	0	283	12	0
2	L5	78445	0	39719	780	0
3	L7	2561	0	1295	15	0
4	L8	3315	0	1685	26	0
5	LA	1898	0	1993	40	0
6	LB	3238	0	3376	58	0
7	LC	2927	0	3104	32	0
8	LD	2382	0	2410	34	0
9	LE	1935	0	2096	27	0
10	LF	1870	0	1996	33	0
11	LG	1927	0	2074	28	0
12	LH	1518	0	1601	24	0
13	LI	1711	0	1749	25	0
14	LJ	1362	0	1396	31	0
15	LL	1701	0	1818	25	0
16	LM	1138	0	1204	20	0
17	LN	1701	0	1749	23	0
18	LO	1650	0	1794	32	0
19	LP	1242	0	1269	19	0
20	LQ	1513	0	1628	20	0
21	LR	1566	0	1729	21	0
22	LS	1453	0	1490	15	0
23	LT	1298	0	1366	18	0
24	LU	825	0	850	15	0
25	LV	979	0	1039	10	0
26	LW	945	0	1003	23	0
27	LX	985	0	1066	9	0
28	LY	1115	0	1205	16	0
29	LZ	1107	0	1182	12	0
30	La	1162	0	1213	10	0
31	Lb	876	0	948	19	0
32	Lc	764	0	804	12	0
33	Ld	888	0	930	14	0
34	Le	1053	0	1147	16	0
35	Lf	876	0	912	10	0
36	Lg	906	0	998	14	0
37	Lh	1015	0	1148	14	0
38	Li	832	0	917	7	0
39	Lj	705	0	737	13	0
40	Lk	569	0	637	8	0
41	Ll	444	0	483	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	Lm	429	0	465	5	0
43	Ln	230	0	276	4	0
44	Lo	862	0	929	35	0
45	Lp	708	0	756	5	0
46	Lr	1002	0	1068	6	0
47	Ls	1496	0	1540	79	0
48	Lt	998	0	1032	54	0
49	SD	1765	0	1865	18	0
50	SF	1495	0	1549	64	0
51	SK	827	0	854	21	0
52	SM	940	0	965	18	0
53	SP	985	0	1031	38	0
54	SQ	1142	0	1213	28	0
55	SR	1090	0	1149	14	0
56	SS	1198	0	1261	28	0
57	ST	1112	0	1146	29	0
58	SU	821	0	883	21	0
59	SZ	598	0	656	17	0
60	Sc	506	0	536	11	0
61	Sd	459	0	452	16	0
62	Sf	548	0	551	19	0
63	Sg	2436	0	2393	57	0
64	SA	1741	0	1746	42	0
65	SB	1738	0	1809	31	0
66	SC	1707	0	1791	35	0
67	SE	2076	0	2177	37	0
68	SG	1923	0	2089	49	0
69	SH	1497	0	1590	39	0
70	SI	1686	0	1772	40	0
71	SJ	1525	0	1640	15	0
72	SL	1247	0	1323	14	0
73	SN	1208	0	1294	14	0
74	SO	1024	0	1050	17	0
75	SV	636	0	637	16	0
76	SW	1034	0	1080	19	0
77	SX	1098	0	1165	28	0
78	SY	1065	0	1142	21	0
79	Sa	821	0	870	13	0
80	Sb	651	0	672	15	0
81	Se	459	0	503	12	0
82	S2	36953	0	18679	457	0
83	CB	6605	0	6678	273	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	Et	1593	0	810	50	0
85	CE	613	0	625	63	0
86	L5	177	0	0	0	0
86	L7	3	0	0	0	0
86	L8	5	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	80	0	152	4	0
88	L8	10	0	19	0	0
88	LN	10	0	19	1	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	225614	0	170127	2733	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 (2733) 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)
44:Lo:106:PHE:CZ	85:CE:39:TRP:CG	1.93	1.53
53:SP:130:ARG:NH1	83:CB:858:LEU:HD23	1.24	1.43
82:S2:1825:A:N6	83:CB:717:GLY:HA3	1.12	1.39
53:SP:133:ILE:HG21	83:CB:709:LEU:N	1.36	1.37
82:S2:1825:A:N6	83:CB:717:GLY:CA	1.87	1.37
82:S2:1825:A:C2	83:CB:714:ILE:HG13	1.59	1.37
48:Lt:34:PRO:CG	83:CB:775:GLN:O	1.79	1.31
82:S2:1825:A:H2	83:CB:714:ILE:CG1	1.42	1.30
47:Ls:147:ILE:CG1	83:CB:204:MET:SD	2.20	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Lo:106:PHE:CZ	85:CE:39:TRP:CD2	2.20	1.28
53:SP:130:ARG:NH1	83:CB:858:LEU:CD2	1.95	1.28
47:Ls:155:LEU:CD1	83:CB:263:ASP:OD2	1.82	1.27
1:CI:79:ARG:NH1	2:L5:2708:U:O2'	1.68	1.26
47:Ls:155:LEU:HD12	83:CB:263:ASP:OD2	1.23	1.25
50:SF:133:THR:HA	84:Et:40:C:O5'	1.35	1.24
50:SF:131:ALA:O	84:Et:39:U:H4'	1.35	1.24
48:Lt:34:PRO:HB3	83:CB:777:ALA:N	1.52	1.22
82:S2:1825:A:C2	83:CB:714:ILE:CG1	2.19	1.22
47:Ls:139:GLN:HB3	83:CB:180:ARG:CD	1.70	1.20
53:SP:133:ILE:HG23	83:CB:708:THR:CB	1.71	1.19
53:SP:130:ARG:HH11	83:CB:858:LEU:CD2	1.54	1.19
47:Ls:139:GLN:OE1	83:CB:180:ARG:HD3	1.03	1.18
50:SF:133:THR:C	84:Et:39:U:HO2'	1.51	1.17
2:L5:4419:U:O2	83:CB:765:ARG:NE	1.80	1.15
47:Ls:147:ILE:CG2	83:CB:204:MET:SD	2.35	1.14
50:SF:131:ALA:O	84:Et:39:U:C4'	1.96	1.14
44:Lo:106:PHE:CE2	85:CE:39:TRP:CE2	2.36	1.13
44:Lo:106:PHE:HZ	85:CE:39:TRP:CD2	1.59	1.13
2:L5:1776:A:H5''	85:CE:64:LEU:CD1	1.78	1.13
44:Lo:106:PHE:HE2	85:CE:39:TRP:CE2	1.66	1.13
47:Ls:147:ILE:HG13	83:CB:204:MET:SD	1.86	1.12
2:L5:1776:A:C5'	85:CE:64:LEU:HD13	1.78	1.12
47:Ls:139:GLN:OE1	83:CB:180:ARG:CD	1.97	1.12
50:SF:134:VAL:CG2	84:Et:40:C:O2'	1.99	1.11
47:Ls:139:GLN:CD	83:CB:180:ARG:HD3	1.76	1.11
48:Lt:34:PRO:HG2	83:CB:775:GLN:O	0.94	1.10
50:SF:130:ARG:NH1	84:Et:37:A:H8	1.48	1.10
2:L5:4419:U:O2	83:CB:765:ARG:CD	2.00	1.10
53:SP:133:ILE:HG23	83:CB:708:THR:HB	1.17	1.09
53:SP:133:ILE:HG23	83:CB:708:THR:CA	1.81	1.08
50:SF:130:ARG:NH1	84:Et:37:A:C8	2.17	1.08
48:Lt:37:LEU:HD11	83:CB:777:ALA:HB1	1.20	1.08
50:SF:133:THR:CA	84:Et:39:U:O2'	2.01	1.08
53:SP:133:ILE:CG2	83:CB:709:LEU:N	2.17	1.07
50:SF:133:THR:C	84:Et:39:U:O2'	1.96	1.06
53:SP:133:ILE:CG2	83:CB:708:THR:HB	1.85	1.06
82:S2:1825:A:H62	83:CB:717:GLY:CA	1.56	1.05
48:Lt:34:PRO:HA	83:CB:777:ALA:HA	1.39	1.04
44:Lo:106:PHE:CZ	85:CE:39:TRP:CD1	2.44	1.04
44:Lo:106:PHE:HZ	85:CE:39:TRP:CG	1.49	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SF:134:VAL:HG23	84:Et:40:C:O2'	1.55	1.04
53:SP:133:ILE:HG21	83:CB:709:LEU:H	0.89	1.03
47:Ls:147:ILE:HG12	83:CB:204:MET:SD	1.94	1.03
14:LJ:55:TYR:OH	85:CE:49:LYS:HE2	1.59	1.03
48:Lt:34:PRO:HG2	83:CB:775:GLN:C	1.84	1.02
2:L5:1996:C:H42	2:L5:2000:G:N2	1.55	1.02
44:Lo:106:PHE:CE1	85:CE:39:TRP:HA	1.95	1.02
47:Ls:147:ILE:HG23	83:CB:204:MET:SD	1.99	1.02
44:Lo:106:PHE:CE2	85:CE:39:TRP:CD2	2.48	0.99
50:SF:133:THR:CA	84:Et:40:C:O5'	2.11	0.99
2:L5:2009:A:H1'	83:CB:760:TYR:CE2	1.96	0.98
47:Ls:139:GLN:NE2	83:CB:180:ARG:HA	1.78	0.97
47:Ls:132:PRO:O	83:CB:187:VAL:HB	1.64	0.97
48:Lt:34:PRO:CG	83:CB:777:ALA:H	1.78	0.96
48:Lt:37:LEU:HD11	83:CB:777:ALA:CB	1.95	0.96
48:Lt:34:PRO:HB3	83:CB:777:ALA:CA	1.95	0.95
48:Lt:34:PRO:CB	83:CB:777:ALA:N	2.29	0.95
47:Ls:139:GLN:HB3	83:CB:180:ARG:HD2	1.44	0.95
44:Lo:106:PHE:CZ	85:CE:39:TRP:CB	2.48	0.95
53:SP:130:ARG:HH12	83:CB:858:LEU:HD23	1.14	0.95
44:Lo:106:PHE:CE2	85:CE:39:TRP:CD1	2.54	0.94
2:L5:1996:C:N4	2:L5:2000:G:H22	1.66	0.93
47:Ls:155:LEU:CD1	83:CB:263:ASP:CG	2.42	0.93
82:S2:1748:G:H1	82:S2:1786:U:H3	1.00	0.93
82:S2:1825:A:H61	83:CB:717:GLY:CA	1.77	0.92
2:L5:3946:G:H1	2:L5:4067:U:H3	1.13	0.92
53:SP:130:ARG:HH11	83:CB:858:LEU:HD21	1.31	0.92
82:S2:1825:A:H2	83:CB:714:ILE:HG12	1.34	0.92
2:L5:1996:C:H42	2:L5:2000:G:H22	0.96	0.91
12:LH:98:HIS:HE1	83:CB:166:GLU:OE2	1.52	0.91
1:CI:74:LYS:HA	24:LU:116:GLN:O	1.70	0.90
2:L5:4419:U:C1'	83:CB:765:ARG:HG3	2.00	0.90
2:L5:1776:A:H5''	85:CE:64:LEU:HD13	0.93	0.90
48:Lt:34:PRO:HG3	83:CB:777:ALA:H	1.34	0.90
50:SF:130:ARG:HH12	84:Et:37:A:H8	0.91	0.90
47:Ls:139:GLN:CD	83:CB:180:ARG:CD	2.42	0.89
47:Ls:147:ILE:HG21	83:CB:204:MET:CG	2.03	0.89
53:SP:133:ILE:CG2	83:CB:708:THR:C	2.45	0.89
50:SF:133:THR:HA	84:Et:39:U:O2'	1.72	0.88
47:Ls:139:GLN:HE22	83:CB:180:ARG:HA	1.39	0.88
44:Lo:106:PHE:CE2	85:CE:39:TRP:CG	2.62	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:Lo:106:PHE:CE2	85:CE:39:TRP:NE1	2.41	0.88
82:S2:1825:A:N3	83:CB:714:ILE:HG13	1.87	0.88
48:Lt:34:PRO:CB	83:CB:777:ALA:H	1.87	0.88
47:Ls:139:GLN:HB3	83:CB:180:ARG:NE	1.87	0.88
53:SP:133:ILE:CG2	83:CB:708:THR:CA	2.52	0.88
2:L5:2007:G:H21	2:L5:2012:A:H62	1.20	0.87
65:SB:103:MET:HG3	65:SB:215:VAL:HG12	1.56	0.87
2:L5:4419:U:H1'	83:CB:765:ARG:HG3	1.55	0.86
82:S2:1825:A:N6	83:CB:717:GLY:N	2.25	0.85
62:Sf:126:CYS:SG	62:Sf:144:CYS:N	2.49	0.84
15:LL:64:VAL:HA	15:LL:67:HIS:HD2	1.39	0.84
47:Ls:139:GLN:CB	83:CB:180:ARG:NE	2.41	0.84
47:Ls:139:GLN:CB	83:CB:180:ARG:CD	2.55	0.84
47:Ls:156:SER:HB3	83:CB:263:ASP:OD2	1.76	0.84
48:Lt:34:PRO:CA	83:CB:777:ALA:HA	2.08	0.84
47:Ls:139:GLN:NE2	83:CB:183:GLU:HB2	1.94	0.83
53:SP:133:ILE:CG2	83:CB:709:LEU:H	1.83	0.83
2:L5:1100:U:H3	2:L5:1194:G:H1	1.27	0.83
48:Lt:31:LYS:HA	83:CB:774:SER:HB2	1.60	0.83
47:Ls:139:GLN:CG	83:CB:180:ARG:NE	2.43	0.82
47:Ls:147:ILE:HG21	83:CB:204:MET:HB3	1.60	0.82
2:L5:4419:U:O2	83:CB:765:ARG:CG	2.27	0.82
44:Lo:106:PHE:CE1	85:CE:39:TRP:CA	2.63	0.81
47:Ls:147:ILE:CG1	83:CB:204:MET:CE	2.59	0.80
2:L5:2009:A:H1'	83:CB:760:TYR:HE2	1.41	0.80
47:Ls:147:ILE:HG21	83:CB:204:MET:CB	2.10	0.80
47:Ls:147:ILE:HG21	83:CB:204:MET:SD	2.22	0.80
82:S2:925:G:H1	82:S2:1017:U:H3	1.30	0.80
82:S2:1825:A:H61	83:CB:717:GLY:N	1.78	0.80
2:L5:1777:C:OP2	85:CE:64:LEU:HD21	1.81	0.79
47:Ls:139:GLN:CD	83:CB:180:ARG:NE	2.40	0.79
66:SC:210:PRO:HB3	66:SC:240:THR:HG21	1.63	0.79
14:LJ:55:TYR:OH	85:CE:49:LYS:CE	2.31	0.79
82:S2:1776:G:N2	82:S2:1777:G:N7	2.31	0.79
82:S2:1239:U:C5	83:CB:667:LYS:HD2	2.18	0.79
26:LW:100:VAL:HG12	26:LW:104:GLN:HE22	1.47	0.79
53:SP:133:ILE:HG23	83:CB:708:THR:HA	1.63	0.78
47:Ls:147:ILE:HG12	83:CB:204:MET:CE	2.13	0.78
2:L5:1095:A:H2	2:L5:1200:G:H1	1.24	0.77
2:L5:1776:A:O5'	85:CE:64:LEU:HD22	1.85	0.77
47:Ls:139:GLN:CD	83:CB:180:ARG:HE	1.92	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4419:U:O2	83:CB:765:ARG:HG3	1.84	0.77
65:SB:122:GLU:HG2	65:SB:140:VAL:HG12	1.67	0.77
2:L5:4910:G:H4'	6:LB:95:THR:HG22	1.67	0.76
48:Lt:31:LYS:HA	83:CB:774:SER:CB	2.15	0.76
82:S2:1239:U:C4	83:CB:667:LYS:HD3	2.20	0.76
82:S2:1239:U:O4	83:CB:667:LYS:HG3	1.85	0.76
47:Ls:147:ILE:CB	83:CB:204:MET:SD	2.72	0.76
53:SP:133:ILE:HG21	83:CB:708:THR:C	2.11	0.76
82:S2:1239:U:O4	83:CB:667:LYS:CG	2.34	0.76
83:CB:110:ASP:HB3	83:CB:553:HIS:HB2	1.67	0.75
2:L5:5024:C:H41	2:L5:5028:G:H21	1.31	0.75
54:SQ:72:VAL:HG11	54:SQ:80:GLN:HG3	1.68	0.75
66:SC:193:VAL:HG11	66:SC:240:THR:HG22	1.69	0.75
48:Lt:34:PRO:O	83:CB:777:ALA:O	2.04	0.75
48:Lt:34:PRO:CB	83:CB:777:ALA:CA	2.65	0.74
47:Ls:139:GLN:CD	83:CB:180:ARG:HA	2.11	0.74
2:L5:3701:OMC:H5	2:L5:3748:A:H62	1.35	0.74
50:SF:134:VAL:HG12	50:SF:135:ARG:HG2	1.68	0.74
14:LJ:55:TYR:CE1	85:CE:46:VAL:HG12	2.22	0.74
82:S2:1239:U:C4	83:CB:667:LYS:CD	2.69	0.74
50:SF:133:THR:O	84:Et:39:U:O2'	1.93	0.73
19:LP:109:VAL:HA	19:LP:112:LEU:HD13	1.70	0.73
47:Ls:147:ILE:CG2	83:CB:204:MET:HB3	2.18	0.73
2:L5:2611:A:H5'	2:L5:2688:G:H4'	1.71	0.73
82:S2:94:G:HO2'	82:S2:508:A:HO2'	1.36	0.72
2:L5:1702:C:H4'	7:LC:308:LYS:HD2	1.72	0.72
33:Ld:90:ARG:HD3	33:Ld:102:LEU:HD13	1.72	0.72
69:SH:154:ILE:HB	69:SH:185:VAL:HG22	1.71	0.72
47:Ls:139:GLN:CG	83:CB:180:ARG:HE	1.99	0.72
63:Sg:247:TRP:HB3	63:Sg:258:ILE:HD11	1.70	0.72
2:L5:497:G:H1	2:L5:657:C:H42	1.38	0.71
2:L5:1982:G:H5'	48:Lt:28:LEU:HD13	1.71	0.71
68:SG:2:LYS:HB2	68:SG:108:VAL:HG12	1.71	0.71
84:Et:44:G:H2'	84:Et:45:G:C8	2.24	0.71
16:LM:15:VAL:HG22	16:LM:50:MET:HE1	1.72	0.71
82:S2:1239:U:O4	83:CB:667:LYS:CD	2.38	0.71
2:L5:3594:C:O2	2:L5:3597:G:N2	2.24	0.71
50:SF:133:THR:CB	84:Et:40:C:O5'	2.39	0.71
57:ST:12:GLN:NE2	82:S2:1593:C:O2	2.23	0.71
2:L5:4546:A:N7	5:LA:215:ASN:ND2	2.39	0.70
69:SH:105:THR:HG23	69:SH:107:LYS:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:664:G:N2	2:L5:666:G:O6	2.25	0.70
2:L5:387:G:HO2'	2:L5:412:G:H1	1.39	0.70
5:LA:104:VAL:HA	5:LA:107:MET:HE3	1.73	0.70
67:SE:208:VAL:HG11	67:SE:225:ILE:HG13	1.73	0.70
84:Et:15:G:N2	84:Et:48:C:O2	2.25	0.70
47:Ls:155:LEU:HD13	83:CB:263:ASP:CG	2.15	0.70
76:SW:2:VAL:N	82:S2:1091:C:HO2'	1.90	0.70
47:Ls:147:ILE:CG2	83:CB:204:MET:CB	2.70	0.69
83:CB:42:LYS:HG2	83:CB:347:GLY:HA3	1.73	0.69
44:Lo:106:PHE:CE1	85:CE:39:TRP:CB	2.75	0.69
2:L5:2484:A:H62	2:L5:2494:U:H3	1.41	0.69
83:CB:225:LEU:HD12	83:CB:260:LEU:HB3	1.74	0.69
2:L5:2009:A:C8	83:CB:756:VAL:CG1	2.75	0.69
2:L5:2092:G:O2'	2:L5:2262:G:N2	2.26	0.69
2:L5:2351:OMC:HM22	7:LC:95:MET:HG3	1.74	0.69
2:L5:3954:A:H1'	2:L5:4058:U:H5'	1.75	0.69
82:S2:1658:G:OP2	82:S2:1660:C:N4	2.25	0.69
82:S2:1684:C:HO2'	84:Et:34:U:H6	1.38	0.69
2:L5:184:U:O2	2:L5:253:G:N2	2.23	0.69
2:L5:2702:C:OP1	24:LU:101:ARG:NH2	2.24	0.69
2:L5:4946:U:HO2'	35:Lf:2:SER:N	1.90	0.69
47:Ls:147:ILE:HG13	83:CB:204:MET:CE	2.22	0.69
48:Lt:65:GLN:HG3	48:Lt:67:ARG:H	1.57	0.69
52:SM:51:VAL:HG12	52:SM:77:ILE:HB	1.74	0.69
2:L5:3937:C:H1'	17:LN:125:SER:HB3	1.74	0.69
2:L5:4242:U:H3	2:L5:4281:A:H2	1.38	0.68
62:Sf:99:LYS:NZ	82:S2:1287:A:OP1	2.25	0.68
26:LW:80:ARG:NH2	68:SG:8:PRO:O	2.26	0.68
2:L5:748:G:O6	22:LS:98:ARG:NH2	2.26	0.68
49:SD:106:ARG:HG3	49:SD:175:VAL:HG22	1.75	0.68
83:CB:561:LEU:HA	83:CB:565:HIS:HB2	1.74	0.68
2:L5:1995:G:O2'	48:Lt:122:ALA:O	2.11	0.68
13:LI:205:PRO:HD2	13:LI:208:LYS:HE2	1.76	0.68
2:L5:2007:G:N2	2:L5:2012:A:H62	1.91	0.68
68:SG:183:ARG:NH2	82:S2:316:G:OP2	2.26	0.68
80:Sb:14:GLU:HA	80:Sb:17:ARG:HG2	1.76	0.68
5:LA:107:MET:HB3	5:LA:111:THR:HG21	1.73	0.68
66:SC:187:ARG:NH2	82:S2:1143:A:OP2	2.27	0.67
87:L5:5290:SPM:H112	18:LO:91:LYS:HD3	1.75	0.67
57:ST:124:THR:HG23	57:ST:127:GLY:H	1.60	0.67
2:L5:1669:A:OP1	31:Lb:18:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4607:A:H4'	83:CB:552:LEU:HD13	1.77	0.67
17:LN:157:LYS:O	17:LN:162:ARG:NH1	2.27	0.67
18:LO:34:VAL:HG22	18:LO:103:LYS:HB2	1.77	0.67
2:L5:665:C:H4'	2:L5:666:G:H5'	1.75	0.67
82:S2:940:U:H3	82:S2:1002:U:H3	1.40	0.67
26:LW:56:ARG:HE	26:LW:61:LYS:HB2	1.59	0.67
84:Et:28:C:H2'	84:Et:29:A:H8	1.60	0.67
82:S2:1058:A:H5'	85:CE:12:SER:CB	2.24	0.67
50:SF:124:ASP:OD1	50:SF:125:SER:N	2.25	0.67
76:SW:71:LYS:NZ	82:S2:1156:U:OP1	2.28	0.67
63:Sg:87:LEU:HB2	63:Sg:101:PHE:HB2	1.77	0.67
2:L5:2458:C:H5''	17:LN:67:ARG:HD2	1.77	0.67
5:LA:29:LEU:O	5:LA:123:ARG:NH1	2.28	0.67
2:L5:1414:C:H2'	2:L5:1415:G:H8	1.60	0.66
6:LB:90:VAL:HG23	6:LB:163:ILE:HD11	1.77	0.66
74:SO:104:ARG:NH2	82:S2:959:G:OP1	2.27	0.66
82:S2:1239:U:O4	83:CB:667:LYS:HD3	1.95	0.66
2:L5:2554:U:O2	2:L5:2764:A:N7	2.28	0.66
21:LR:172:ARG:NH1	82:S2:909:G:OP1	2.28	0.66
76:SW:107:SER:HB2	82:S2:860:G:H21	1.59	0.66
12:LH:106:GLN:HB2	12:LH:111:LEU:HB3	1.78	0.66
82:S2:747:U:N3	82:S2:796:G:N1	2.44	0.66
12:LH:98:HIS:CE1	83:CB:166:GLU:OE2	2.42	0.66
51:SK:50:GLN:HE22	82:S2:1276:A:H1'	1.60	0.66
68:SG:132:ARG:NH2	82:S2:152:U:O4'	2.28	0.66
6:LB:222:VAL:O	6:LB:343:ARG:NH1	2.29	0.66
14:LJ:55:TYR:CD1	85:CE:46:VAL:CG1	2.79	0.66
81:Se:41:ARG:NH2	82:S2:639:C:OP1	2.29	0.66
80:Sb:34:ASP:O	80:Sb:79:PHE:HA	1.95	0.66
1:CI:79:ARG:NH1	2:L5:2708:U:HO2'	1.93	0.66
25:LV:35:LYS:HB2	25:LV:67:LYS:HG3	1.76	0.66
56:SS:85:ASN:OD1	56:SS:97:GLN:NE2	2.28	0.66
2:L5:2520:C:O2	2:L5:2640:G:N2	2.28	0.66
40:Lk:8:ILE:HD11	40:Lk:56:LEU:HD13	1.77	0.66
85:CE:46:VAL:HA	85:CE:49:LYS:HD2	1.78	0.66
83:CB:604:MET:HG2	83:CB:704:VAL:HA	1.78	0.65
82:S2:533:A:H61	82:S2:550:C:H42	1.44	0.65
4:L8:75:OMG:OP2	28:LY:74:TYR:OH	2.15	0.65
30:La:84:GLU:OE1	30:La:87:ARG:NH2	2.30	0.65
48:Lt:151:ILE:O	48:Lt:155:ILE:HB	1.97	0.65
2:L5:1095:A:N1	2:L5:1200:G:O6	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:SG:7:PHE:HD2	68:SG:10:THR:HG22	1.62	0.65
2:L5:4525:C:OP1	6:LB:246:ARG:NH2	2.28	0.65
2:L5:4910:G:N2	18:LO:106:ASP:O	2.30	0.65
47:Ls:58:ASN:ND2	47:Ls:84:GLY:O	2.24	0.65
50:SF:168:THR:OG1	50:SF:171:GLU:OE1	2.15	0.65
68:SG:135:PRO:HG2	68:SG:141:ILE:HG22	1.78	0.65
82:S2:1536:G:H2'	82:S2:1537:A:H8	1.62	0.65
83:CB:509:VAL:HG12	83:CB:572:LYS:HG3	1.79	0.65
22:LS:76:LYS:NZ	22:LS:100:LEU:O	2.31	0.64
6:LB:10:ARG:NH1	6:LB:11:HIS:O	2.30	0.64
48:Lt:130:LYS:NZ	48:Lt:157:SER:O	2.30	0.64
82:S2:751:G:H1'	82:S2:793:G:H21	1.61	0.64
1:CI:78:HIS:NE2	2:L5:2706:G:N7	2.44	0.64
82:S2:628:A:N6	82:S2:1500:G:O2'	2.30	0.64
2:L5:68:U:OP1	17:LN:178:HIS:ND1	2.31	0.64
40:Lk:54:GLU:OE2	40:Lk:58:GLN:NE2	2.27	0.64
2:L5:4281:A:H2'	2:L5:4282:A:H2'	1.79	0.64
19:LP:39:MET:HG2	19:LP:43:LYS:HD3	1.79	0.64
69:SH:114:GLN:HE22	82:S2:874:G:H21	1.45	0.64
23:LT:43:LYS:O	23:LT:58:HIS:ND1	2.31	0.64
64:SA:89:LYS:HD2	64:SA:201:LEU:HG	1.79	0.64
2:L5:2601:A:N6	2:L5:2744:A:OP2	2.28	0.64
82:S2:928:G:H2'	82:S2:929:G:C8	2.32	0.64
2:L5:1994:C:H2'	2:L5:1995:G:C8	2.33	0.64
2:L5:3641:U:OP2	2:L5:3646:A:N6	2.31	0.64
46:Lr:26:SER:OG	46:Lr:28:GLU:OE1	2.15	0.64
49:SD:142:LEU:HD13	49:SD:150:MET:HE2	1.80	0.64
70:SI:98:LYS:HB3	82:S2:377:G:H5'	1.80	0.64
2:L5:1704:C:O3'	10:LF:46:ARG:NH1	2.31	0.63
53:SP:133:ILE:CG2	83:CB:708:THR:CB	2.52	0.63
24:LU:65:ARG:HG2	24:LU:67:LYS:H	1.63	0.63
58:SU:51:LYS:HB3	58:SU:90:ASP:HB2	1.80	0.63
83:CB:692:LEU:HD11	83:CB:738:PRO:HB2	1.80	0.63
54:SQ:19:ALA:HB2	54:SQ:75:GLY:HA3	1.81	0.63
71:SJ:162:ARG:NH1	82:S2:582:U:OP1	2.30	0.63
83:CB:385:ILE:HG22	83:CB:418:SER:HB2	1.81	0.63
68:SG:22:ARG:HG3	68:SG:25:ARG:HH12	1.64	0.63
82:S2:1829:G:H1'	82:S2:1850:MA6:H2	1.79	0.63
2:L5:1982:G:N2	2:L5:2009:A:O2'	2.32	0.63
2:L5:2495:U:H2'	2:L5:2496:G:H8	1.64	0.63
48:Lt:117:ARG:HE	48:Lt:119:ARG:H	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SE:45:ILE:HG13	67:SE:61:VAL:HG11	1.79	0.63
67:SE:153:LEU:O	67:SE:174:LYS:NZ	2.31	0.63
12:LH:106:GLN:NE2	12:LH:113:GLU:OE2	2.31	0.63
2:L5:3946:G:N2	2:L5:4067:U:O2	2.32	0.63
2:L5:170:C:H42	2:L5:266:C:H42	1.47	0.63
2:L5:4431:PSU:OP2	13:LI:3:ARG:NH2	2.28	0.62
31:Lb:109:ARG:HA	31:Lb:112:ILE:HG12	1.81	0.62
67:SE:79:ASP:HB3	67:SE:82:TYR:HB2	1.81	0.62
2:L5:4092:G:N7	2:L5:4114:C:N4	2.45	0.62
5:LA:137:ILE:HD11	5:LA:149:LYS:HB2	1.82	0.62
63:Sg:252:THR:HG21	63:Sg:257:LYS:HD2	1.81	0.62
14:LJ:55:TYR:CD1	85:CE:46:VAL:HG12	2.35	0.62
2:L5:1100:U:O3'	2:L5:1167:C:N4	2.32	0.62
2:L5:2009:A:C1'	83:CB:760:TYR:CE2	2.78	0.62
14:LJ:146:ARG:HG2	14:LJ:147:ARG:HG3	1.81	0.62
2:L5:327:U:O2'	38:Li:30:ARG:NH1	2.32	0.62
2:L5:4987:C:OP2	6:LB:116:ARG:NH2	2.32	0.62
84:Et:6:G:H1	84:Et:67:U:H3	1.47	0.62
40:Lk:26:LYS:HB2	40:Lk:69:LEU:HD12	1.81	0.62
49:SD:40:ARG:NH2	58:SU:106:ILE:O	2.32	0.62
58:SU:80:PHE:HB3	61:Sd:52:PHE:HB3	1.81	0.62
82:S2:587:A:H5'	82:S2:592:C:H41	1.64	0.62
2:L5:67:C:OP2	2:L5:312:G:N2	2.30	0.62
33:Ld:64:ILE:HG23	33:Ld:68:LEU:HD23	1.82	0.62
44:Lo:106:PHE:HZ	85:CE:39:TRP:CB	1.98	0.62
47:Ls:145:THR:O	83:CB:183:GLU:CG	2.47	0.62
51:SK:85:LEU:HD21	51:SK:89:ILE:HB	1.80	0.62
67:SE:144:ALA:HB3	82:S2:121:OMU:HM23	1.80	0.62
2:L5:1499:C:OP1	20:LQ:150:ARG:NH2	2.33	0.62
11:LG:209:SER:HA	11:LG:212:LYS:HG3	1.82	0.62
77:SX:105:PHE:HD1	77:SX:121:LYS:HB3	1.65	0.62
82:S2:106:C:H2'	82:S2:107:A:H8	1.65	0.62
82:S2:1417:C:O2	82:S2:1422:G:O6	2.18	0.62
2:L5:2758:G:O2'	2:L5:2765:A:N3	2.30	0.62
2:L5:4419:U:O4'	83:CB:765:ARG:HG3	2.00	0.61
82:S2:1639:G7M:H5''	84:Et:30:G:OP1	2.00	0.61
2:L5:4992:G:H2'	2:L5:4993:G:C8	2.36	0.61
50:SF:127:ARG:HG2	50:SF:136:ARG:HE	1.64	0.61
64:SA:118:GLU:HG3	66:SC:65:LYS:HE2	1.82	0.61
14:LJ:141:ILE:HA	14:LJ:144:LYS:HD2	1.82	0.61
18:LO:180:GLN:NE2	18:LO:184:ASN:OD1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SF:34:SER:HA	60:Sc:55:VAL:HG23	1.81	0.61
54:SQ:58:LEU:HB3	54:SQ:62:ARG:HD2	1.82	0.61
70:SI:70:GLU:OE2	72:SL:21:LYS:NZ	2.32	0.61
82:S2:1536:G:H2'	82:S2:1537:A:C8	2.35	0.61
2:L5:3811:G:O2'	2:L5:3814:U:OP2	2.18	0.61
62:Sf:108:VAL:HG12	62:Sf:114:ILE:HA	1.81	0.61
13:LI:87:MET:HG2	13:LI:138:ILE:HG12	1.81	0.61
47:Ls:139:GLN:HE21	83:CB:183:GLU:CD	2.08	0.61
50:SF:84:GLY:O	82:S2:1673:U:O2'	2.16	0.61
59:SZ:99:LEU:HD21	59:SZ:102:LYS:HB2	1.82	0.61
2:L5:2899:C:OP1	21:LR:108:ARG:NH2	2.31	0.61
47:Ls:17:ILE:HD12	47:Ls:54:LEU:HD21	1.82	0.61
48:Lt:37:LEU:CD1	83:CB:777:ALA:HB1	2.13	0.61
82:S2:1422:G:H4'	82:S2:1423:C:H3'	1.82	0.61
62:Sf:144:CYS:HB2	62:Sf:146:LEU:HD23	1.82	0.61
72:SL:85:THR:HG21	82:S2:373:G:H4'	1.83	0.61
2:L5:2695:A:OP1	40:Lk:35:LYS:NZ	2.27	0.61
58:SU:70:CYS:SG	82:S2:1491:G:O2'	2.57	0.61
63:Sg:213:ASP:OD2	63:Sg:215:GLN:NE2	2.34	0.61
83:CB:636:ALA:HA	83:CB:641:TRP:H	1.66	0.61
26:LW:80:ARG:HH22	82:S2:167:G:H4'	1.66	0.61
67:SE:29:PRO:HA	82:S2:496:C:H5'	1.83	0.61
2:L5:1802:A:N3	23:LT:130:ARG:NH2	2.48	0.61
2:L5:3688:U:OP2	5:LA:198:ARG:NH2	2.34	0.61
49:SD:99:ILE:HG23	49:SD:173:ARG:HH21	1.63	0.61
55:SR:109:LEU:HD13	64:SA:52:LYS:HB2	1.83	0.61
2:L5:2557:G:H1	2:L5:2570:U:H3	1.48	0.60
2:L5:4088:C:OP1	5:LA:37:ARG:NH1	2.34	0.60
49:SD:8:LYS:HG2	58:SU:61:LEU:HD11	1.82	0.60
56:SS:27:ALA:HB2	56:SS:52:LEU:HD12	1.82	0.60
58:SU:26:SER:HB3	58:SU:110:VAL:HA	1.83	0.60
66:SC:200:ARG:O	71:SJ:54:ARG:NH2	2.30	0.60
2:L5:4472:G:O2'	42:Lm:100:TYR:O	2.20	0.60
5:LA:114:CYS:HB3	5:LA:165:VAL:HB	1.84	0.60
17:LN:155:VAL:O	17:LN:162:ARG:NH2	2.33	0.60
82:S2:1228:A:H2'	82:S2:1229:G:C8	2.36	0.60
83:CB:745:TYR:HB2	83:CB:814:PHE:HA	1.83	0.60
50:SF:131:ALA:O	84:Et:39:U:C5'	2.49	0.60
72:SL:35:ARG:NH2	72:SL:55:TYR:O	2.35	0.60
72:SL:133:PRO:HG2	82:S2:383:G:H21	1.66	0.60
83:CB:137:VAL:HG22	83:CB:807:GLN:HE21	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:500:G:N2	2:L5:504:G:O2'	2.28	0.60
2:L5:2658:G:N2	2:L5:2676:A:OP2	2.33	0.60
6:LB:107:ALA:HB2	6:LB:201:LEU:HD22	1.82	0.60
52:SM:91:LEU:HD12	52:SM:106:CYS:HB2	1.82	0.60
53:SP:48:GLY:O	53:SP:50:ARG:NH1	2.35	0.60
61:Sd:54:LYS:NZ	82:S2:1482:C:OP1	2.35	0.60
67:SE:49:ARG:NH2	82:S2:496:C:OP1	2.32	0.60
69:SH:177:TYR:O	69:SH:181:THR:HB	2.02	0.60
82:S2:1239:U:C5	83:CB:667:LYS:CD	2.84	0.60
2:L5:4618:OMG:H5'	25:LV:15:ARG:HB2	1.83	0.60
71:SJ:40:LYS:NZ	82:S2:641:A:OP1	2.32	0.60
82:S2:1058:A:H5'	85:CE:12:SER:HB3	1.83	0.60
83:CB:524:LEU:HD22	83:CB:561:LEU:HD11	1.84	0.60
50:SF:185:SER:H	50:SF:190:ILE:HD11	1.67	0.60
51:SK:25:LYS:NZ	82:S2:1497:G:N7	2.44	0.60
57:ST:22:LEU:HG	57:ST:28:LEU:HD21	1.82	0.60
78:SY:11:LYS:HB2	78:SY:24:VAL:HG12	1.84	0.60
78:SY:21:LYS:HE2	78:SY:75:ILE:HD11	1.83	0.60
82:S2:1550:G:H3'	82:S2:1579:A:H61	1.66	0.60
2:L5:4153:C:H5''	27:LX:38:LYS:HD2	1.83	0.60
21:LR:39:GLN:OE1	21:LR:42:ARG:NH1	2.34	0.60
2:L5:1175:A:H2	2:L5:1185:G:H22	1.49	0.60
2:L5:1366:G:H5''	15:LL:36:ARG:HH12	1.67	0.60
2:L5:2362:U:H2'	2:L5:2363:A2M:H8	1.83	0.60
44:Lo:106:PHE:CZ	85:CE:39:TRP:HB3	2.37	0.60
70:SI:88:ASN:OD1	70:SI:205:ARG:NH2	2.34	0.60
77:SX:107:ARG:HG3	77:SX:110:HIS:HB3	1.83	0.60
82:S2:1277:C:H2'	82:S2:1278:A:H8	1.66	0.60
83:CB:43:ALA:HB2	83:CB:351:LEU:HD21	1.84	0.60
2:L5:1776:A:C4'	85:CE:64:LEU:HD13	2.32	0.60
43:Ln:1:MET:HG3	82:S2:1706:G:H5'	1.83	0.60
56:SS:130:ARG:NH2	82:S2:1230:C:OP1	2.35	0.60
59:SZ:58:LEU:HD12	59:SZ:62:VAL:HG21	1.84	0.60
66:SC:183:LYS:HA	66:SC:195:LEU:O	2.02	0.60
82:S2:1639:G7M:C5'	84:Et:30:G:OP1	2.50	0.60
2:L5:4419:U:O2	83:CB:765:ARG:HD3	1.99	0.60
8:LD:223:PHE:HB3	8:LD:226:TYR:HB2	1.84	0.60
53:SP:130:ARG:HD3	53:SP:131:PRO:HD2	1.84	0.60
2:L5:500:G:OP1	2:L5:504:G:N2	2.35	0.59
2:L5:1503:A:H62	20:LQ:87:THR:HG21	1.66	0.59
47:Ls:147:ILE:HG12	83:CB:204:MET:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:CB:641:TRP:HZ3	83:CB:649:ILE:HD11	1.67	0.59
50:SF:131:ALA:C	84:Et:39:U:H4'	2.23	0.59
68:SG:66:GLY:HA2	82:S2:1745:A:H1'	1.84	0.59
53:SP:130:ARG:HH12	83:CB:858:LEU:CD2	1.87	0.59
82:S2:838:G:H1	82:S2:840:C:HO2'	1.48	0.59
49:SD:172:VAL:HG22	49:SD:185:LYS:HG2	1.85	0.59
82:S2:554:A:HO2'	82:S2:555:A:H8	1.48	0.59
82:S2:874:G:H2'	82:S2:875:A:H8	1.67	0.59
2:L5:4594:U:H2'	2:L5:4595:G:H8	1.67	0.59
64:SA:77:ILE:HG13	64:SA:99:ILE:HB	1.84	0.59
2:L5:659:G:H2'	2:L5:660:A:H8	1.67	0.59
2:L5:4107:G:N2	2:L5:4108:G:O6	2.33	0.59
47:Ls:139:GLN:HE22	83:CB:183:GLU:HB2	1.67	0.59
2:L5:4097:G:O6	2:L5:4098:A:N6	2.36	0.59
16:LM:100:ARG:HA	16:LM:103:LYS:HG2	1.85	0.59
54:SQ:78:VAL:HG12	82:S2:1673:U:H5''	1.85	0.59
63:Sg:206:LEU:HD12	63:Sg:218:LEU:HD12	1.84	0.59
70:SI:150:ASP:HA	70:SI:153:LYS:HG2	1.84	0.59
78:SY:34:THR:O	82:S2:570:C:O2'	2.20	0.59
2:L5:1703:C:O2'	2:L5:1704:C:O4'	2.21	0.59
2:L5:3868:G:H22	2:L5:3900:G:H1'	1.66	0.59
2:L5:513:U:N3	2:L5:516:C:OP2	2.33	0.58
42:Lm:99:CYS:HB2	42:Lm:114:LYS:HE3	1.85	0.58
50:SF:134:VAL:HG22	84:Et:40:C:O2'	1.99	0.58
83:CB:759:ILE:HG12	83:CB:800:LEU:HD11	1.85	0.58
84:Et:5:G:H2'	84:Et:6:G:H8	1.67	0.58
2:L5:1339:U:H2'	2:L5:1340:OMC:C6	2.38	0.58
2:L5:1996:C:O3'	47:Ls:44:ARG:NH1	2.35	0.58
2:L5:3717:A:H2'	2:L5:3718:A2M:H8	1.84	0.58
44:Lo:2:VAL:N	44:Lo:90:HIS:O	2.36	0.58
49:SD:32:ASP:OD1	49:SD:57:ASN:ND2	2.35	0.58
65:SB:99:ASN:OD1	65:SB:100:PHE:N	2.37	0.58
75:SV:51:LYS:NZ	75:SV:76:ASP:OD1	2.23	0.58
82:S2:640:A:H2'	82:S2:641:A:C8	2.39	0.58
84:Et:28:C:H2'	84:Et:29:A:C8	2.39	0.58
8:LD:64:ILE:HD13	8:LD:109:LEU:HD22	1.85	0.58
59:SZ:80:ARG:O	82:S2:1598:G:O2'	2.18	0.58
82:S2:1825:A:N6	83:CB:717:GLY:H	2.00	0.58
2:L5:1739:G:N3	2:L5:1742:A:N6	2.51	0.58
2:L5:2017:A:O2'	2:L5:2018:C:H6	1.86	0.58
2:L5:2460:A:OP2	88:LN:301:SPD:N10	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LD:62:CYS:HB3	8:LD:105:LEU:HD22	1.84	0.58
26:LW:80:ARG:NH1	82:S2:167:G:O2'	2.36	0.58
40:Lk:27:LYS:O	40:Lk:70:LYS:NZ	2.35	0.58
72:SL:33:LEU:HD12	72:SL:34:PRO:HD2	1.85	0.58
2:L5:919:C:OP1	16:LM:69:HIS:ND1	2.22	0.58
2:L5:3736:A:H2'	2:L5:3737:A:C8	2.38	0.58
2:L5:4887:C:H42	2:L5:4932:U:H3	1.50	0.58
24:LU:44:GLN:HB2	24:LU:56:LEU:HD21	1.84	0.58
54:SQ:125:ARG:HB2	82:S2:1648:G:H5''	1.86	0.58
63:Sg:68:ASP:HB3	63:Sg:111:VAL:HG22	1.84	0.58
2:L5:2007:G:H21	2:L5:2012:A:N6	1.97	0.58
13:LI:85:PHE:HE2	13:LI:87:MET:HE2	1.67	0.58
28:LY:67:ILE:O	28:LY:84:ARG:NH2	2.36	0.58
52:SM:63:LYS:HD3	52:SM:64:LEU:HD22	1.85	0.58
66:SC:267:GLN:OE1	75:SV:35:ASN:ND2	2.36	0.58
69:SH:7:LYS:HD3	69:SH:10:LYS:HB3	1.84	0.58
2:L5:24:G:N7	39:Lj:46:LYS:NZ	2.50	0.58
2:L5:184:U:O2'	2:L5:189:G:O4'	2.22	0.58
2:L5:1396:G:N7	30:La:110:LYS:NZ	2.49	0.58
2:L5:2020:U:H2'	2:L5:2021:G:H8	1.68	0.58
42:Lm:79:GLU:OE2	42:Lm:81:SER:OG	2.19	0.58
51:SK:31:LYS:HZ3	51:SK:40:VAL:H	1.52	0.58
62:Sf:92:LYS:NZ	82:S2:1271:C:OP1	2.33	0.58
68:SG:176:ILE:HG12	68:SG:179:LEU:HD11	1.86	0.58
83:CB:257:MET:HA	83:CB:260:LEU:HB2	1.86	0.58
83:CB:596:PRO:HD3	83:CB:724:THR:HB	1.86	0.58
2:L5:1776:A:H5''	85:CE:64:LEU:CG	2.32	0.58
52:SM:36:ARG:NH1	82:S2:1310:U:OP1	2.36	0.58
54:SQ:100:VAL:HG22	54:SQ:101:ASP:H	1.68	0.58
74:SO:15:ILE:HG23	74:SO:16:SER:H	1.68	0.58
82:S2:165:G:OP2	82:S2:165:G:N2	2.29	0.58
83:CB:189:ILE:HD11	83:CB:204:MET:HA	1.86	0.58
2:L5:2093:A:N3	2:L5:2094:G:N1	2.51	0.58
2:L5:2468:U:O2'	2:L5:2506:G:N2	2.37	0.58
6:LB:165:HIS:HB3	6:LB:180:LEU:HD23	1.86	0.58
39:Lj:14:LYS:NZ	41:Ll:51:LEU:OXT	2.37	0.58
2:L5:4076:G:OP1	11:LG:73:ARG:NE	2.36	0.58
8:LD:120:GLU:O	8:LD:248:ARG:NH1	2.36	0.58
69:SH:165:ASN:O	69:SH:169:LYS:NZ	2.31	0.58
70:SI:22:HIS:HB3	82:S2:433:A:H5''	1.84	0.58
84:Et:46:G:H5'	84:Et:47:U:H5''	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:935:A:O2'	16:LM:44:GLN:O	2.22	0.57
9:LE:161:ARG:NH1	9:LE:273:SER:OG	2.37	0.57
47:Ls:135:THR:HG21	83:CB:187:VAL:HG11	1.85	0.57
50:SF:133:THR:HA	84:Et:40:C:P	2.43	0.57
51:SK:8:ARG:NH2	82:S2:1314:U:O2'	2.37	0.57
68:SG:133:LEU:HD12	82:S2:65:C:C4	2.39	0.57
83:CB:44:GLY:HA3	83:CB:47:ALA:HB3	1.86	0.57
2:L5:1961:G:N2	2:L5:2024:G:O2'	2.37	0.57
4:L8:52:A:H5'	41:Ll:21:ARG:HD3	1.86	0.57
7:LC:298:ILE:HD13	20:LQ:131:PRO:HB3	1.85	0.57
83:CB:304:ILE:HG21	83:CB:336:LEU:HD13	1.86	0.57
83:CB:447:ILE:HG12	83:CB:472:LEU:HD13	1.85	0.57
2:L5:1094:G:O6	2:L5:1201:U:O2	2.22	0.57
2:L5:2017:A:O2'	2:L5:2018:C:O5'	2.19	0.57
6:LB:10:ARG:NH2	6:LB:265:SER:O	2.36	0.57
83:CB:524:LEU:HD12	83:CB:536:CYS:HB3	1.86	0.57
2:L5:4098:A:H2'	2:L5:4099:G:H4'	1.86	0.57
68:SG:11:GLY:HA2	82:S2:166:A2M:HM'1	1.86	0.57
2:L5:1992:U:H4'	2:L5:1993:C:H5''	1.86	0.57
2:L5:4873:G:N7	18:LO:179:LYS:NZ	2.49	0.57
63:Sg:107:ASP:HB2	63:Sg:125:ARG:HG3	1.87	0.57
69:SH:63:PHE:HA	69:SH:95:ILE:O	2.05	0.57
57:ST:126:GLN:HB2	57:ST:129:ARG:HH21	1.69	0.57
70:SI:106:SER:HB3	70:SI:171:LEU:HG	1.87	0.57
2:L5:2295:C:O2'	7:LC:45:ARG:NH2	2.38	0.57
6:LB:80:GLU:OE1	6:LB:323:TYR:OH	2.23	0.57
8:LD:41:LYS:NZ	23:LT:32:ARG:O	2.35	0.57
46:Lr:28:GLU:OE2	46:Lr:31:ASN:ND2	2.32	0.57
67:SE:100:ARG:HB2	67:SE:114:ILE:HD13	1.86	0.57
68:SG:92:ARG:O	82:S2:453:C:O2'	2.21	0.57
83:CB:607:ARG:HD3	83:CB:701:ARG:HD3	1.87	0.57
2:L5:62:A:N3	2:L5:77:U:O2'	2.33	0.57
2:L5:2516:G:O2'	36:Lg:62:LYS:NZ	2.38	0.57
4:L8:62:A:OP1	37:Lh:52:LYS:NZ	2.34	0.57
24:LU:28:PRO:HB2	24:LU:34:MET:HG3	1.87	0.57
50:SF:133:THR:OG1	84:Et:40:C:O5'	2.22	0.57
63:Sg:63:SER:HB2	82:S2:1398:G:H1'	1.86	0.57
63:Sg:254:PRO:O	63:Sg:272:GLN:NE2	2.38	0.57
77:SX:68:LYS:HB3	77:SX:91:LEU:HD13	1.85	0.57
2:L5:4725:C:OP1	6:LB:103:LYS:NZ	2.37	0.57
17:LN:164:LEU:O	17:LN:169:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:Ls:68:HIS:O	47:Ls:71:ASN:ND2	2.38	0.57
54:SQ:67:ASP:OD2	54:SQ:69:ARG:NH1	2.38	0.57
54:SQ:80:GLN:O	54:SQ:84:ILE:HG13	2.05	0.57
82:S2:695:C:N4	82:S2:736:C:O2'	2.38	0.57
47:Ls:145:THR:O	83:CB:183:GLU:HG2	2.05	0.57
58:SU:85:HIS:ND1	82:S2:1447:G:OP1	2.37	0.57
82:S2:508:A:H3'	82:S2:509:OMG:H8	1.69	0.57
2:L5:966:A:OP2	2:L5:2092:G:N2	2.38	0.56
11:LG:180:PRO:HG3	11:LG:219:VAL:HG13	1.86	0.56
16:LM:71:LYS:O	16:LM:75:GLN:HG3	2.05	0.56
44:Lo:106:PHE:CE1	85:CE:39:TRP:CG	2.82	0.56
56:SS:5:ILE:N	59:SZ:50:PHE:O	2.36	0.56
69:SH:12:ASN:ND2	69:SH:14:GLU:OE2	2.38	0.56
83:CB:27:HIS:ND1	83:CB:138:GLN:HB2	2.20	0.56
2:L5:267:G:OP1	37:Lh:109:ARG:NH2	2.37	0.56
2:L5:1281:G:N1	9:LE:128:HIS:HB2	2.20	0.56
2:L5:5002:U:OP2	6:LB:385:LYS:NZ	2.39	0.56
48:Lt:77:ALA:HB3	48:Lt:80:LEU:HB2	1.87	0.56
74:SO:135:ILE:O	82:S2:943:U:O2'	2.22	0.56
83:CB:76:SER:HB3	83:CB:99:LEU:HD11	1.87	0.56
2:L5:1914:C:H4'	18:LO:89:PRO:HD3	1.86	0.56
2:L5:1942:A:H2'	2:L5:1943:A:C8	2.39	0.56
2:L5:2613:C:OP1	36:Lg:24:ARG:NH2	2.38	0.56
3:L7:6:C:O2'	8:LD:50:ARG:NH2	2.38	0.56
6:LB:17:LEU:O	6:LB:19:ARG:N	2.37	0.56
9:LE:165:LEU:HD11	9:LE:176:THR:HG22	1.87	0.56
21:LR:176:ARG:NH2	82:S2:910:G:OP1	2.38	0.56
48:Lt:37:LEU:HD21	83:CB:777:ALA:C	2.30	0.56
51:SK:31:LYS:NZ	51:SK:40:VAL:H	2.04	0.56
62:Sf:97:LYS:NZ	82:S2:1289:U:OP2	2.36	0.56
74:SO:134:PRO:HB3	82:S2:944:A:H5''	1.87	0.56
82:S2:1228:A:H2'	82:S2:1229:G:H8	1.70	0.56
2:L5:1993:C:H2'	2:L5:1994:C:C6	2.41	0.56
2:L5:4094:G:N2	2:L5:4115:G:OP2	2.39	0.56
16:LM:36:ALA:HB3	16:LM:55:MET:HE1	1.87	0.56
44:Lo:106:PHE:O	85:CE:38:TYR:CZ	2.58	0.56
68:SG:198:ARG:NH1	82:S2:126:G:OP2	2.37	0.56
74:SO:34:PHE:HB3	74:SO:41:PHE:HB2	1.88	0.56
82:S2:1354:G:N2	82:S2:1357:A:OP2	2.34	0.56
2:L5:966:A:H5''	2:L5:2092:G:H22	1.69	0.56
6:LB:83:PRO:O	6:LB:167:GLN:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LP:17:SER:HB2	19:LP:98:ALA:HB2	1.88	0.56
50:SF:36:GLN:NE2	50:SF:37:ASP:OD1	2.39	0.56
53:SP:31:GLU:HA	53:SP:34:MET:HE2	1.86	0.56
73:SN:55:ARG:HD3	82:S2:1017:U:H5'	1.88	0.56
82:S2:1226:G:N1	82:S2:1639:G7M:OP2	2.30	0.56
2:L5:1079:C:O2	2:L5:1221:G:N2	2.29	0.56
41:Ll:28:ARG:HA	41:Ll:33:ASN:HD22	1.71	0.56
48:Lt:34:PRO:CA	83:CB:777:ALA:CA	2.83	0.56
69:SH:111:LYS:HE3	82:S2:796:G:H21	1.71	0.56
78:SY:80:ASP:OD1	78:SY:81:TYR:N	2.39	0.56
2:L5:2478:C:N3	2:L5:2591:A:O2'	2.39	0.56
2:L5:4220:6MZ:H2'	2:L5:4222:G:H5''	1.88	0.56
2:L5:4340:U:O2	88:L5:5260:SPD:N10	2.39	0.56
19:LP:116:HIS:HB3	19:LP:149:ILE:HB	1.86	0.56
44:Lo:33:LEU:HA	44:Lo:38:LYS:HG2	1.88	0.56
61:Sd:19:ARG:NH2	82:S2:1661:A:OP1	2.38	0.56
82:S2:543:C:H3'	82:S2:544:G:H8	1.71	0.56
2:L5:1969:G:H4'	47:Ls:36:GLY:HA2	1.88	0.56
2:L5:2832:A:OP1	33:Ld:47:LYS:NZ	2.29	0.56
2:L5:3611:A:H2	2:L5:5016:A:H8	1.52	0.56
2:L5:4279:A:H5'	2:L5:4281:A:H1'	1.87	0.56
83:CB:745:TYR:HE2	83:CB:812:CYS:HB2	1.71	0.56
28:LY:4:ASN:HB3	28:LY:7:VAL:HG22	1.86	0.56
2:L5:2407:G:O6	41:Ll:2:SER:N	2.39	0.56
11:LG:165:GLU:OE2	17:LN:26:ARG:NH1	2.36	0.56
18:LO:9:LEU:HD23	18:LO:118:MET:HB2	1.88	0.56
52:SM:96:ARG:NH2	52:SM:100:PRO:O	2.39	0.56
2:L5:184:U:H3	2:L5:253:G:H1	1.54	0.55
36:Lg:45:ALA:HB3	36:Lg:82:MET:HE2	1.88	0.55
64:SA:22:GLY:O	64:SA:24:HIS:ND1	2.38	0.55
83:CB:835:VAL:HG11	83:CB:848:ILE:HD11	1.88	0.55
2:L5:2083:C:OP2	20:LQ:14:ARG:NH2	2.33	0.55
2:L5:4163:U:OP2	11:LG:53:ARG:NH2	2.40	0.55
5:LA:118:GLU:OE2	5:LA:156:LYS:NZ	2.39	0.55
6:LB:219:VAL:HG11	6:LB:337:VAL:HG13	1.88	0.55
66:SC:259:THR:HG23	75:SV:16:LYS:HZ3	1.70	0.55
68:SG:136:LYS:NZ	68:SG:175:LYS:O	2.34	0.55
69:SH:34:SER:OG	69:SH:78:ARG:NH2	2.38	0.55
2:L5:158:A:N1	2:L5:276:C:O2'	2.37	0.55
2:L5:4098:A:N1	2:L5:4112:C:N4	2.53	0.55
13:LI:152:LEU:HB3	13:LI:165:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Lc:38:ILE:HD11	32:Lc:46:VAL:HG21	1.89	0.55
48:Lt:50:THR:OG1	48:Lt:72:GLU:OE1	2.23	0.55
58:SU:48:LEU:HG	58:SU:93:SER:HB3	1.88	0.55
2:L5:2009:A:C1'	83:CB:760:TYR:HE2	2.14	0.55
2:L5:5023:C:OP2	70:SI:124:LYS:NZ	2.40	0.55
72:SL:103:GLU:HG3	77:SX:11:ARG:HB2	1.87	0.55
82:S2:795:A:H2'	82:S2:796:G:C8	2.42	0.55
83:CB:388:CYS:HB2	83:CB:418:SER:HA	1.88	0.55
2:L5:1759:G:H1	2:L5:1773:U:H3	1.54	0.55
2:L5:4537:C:H2'	2:L5:4538:G:H8	1.70	0.55
22:LS:173:ASN:ND2	22:LS:175:PHE:O	2.40	0.55
67:SE:146:THR:HG21	82:S2:122:G:H21	1.70	0.55
69:SH:31:GLU:HA	69:SH:37:LYS:HG3	1.89	0.55
1:CI:50:MET:HG3	24:LU:114:TYR:CD2	2.42	0.55
2:L5:109:G:OP2	15:LL:74:ARG:NH2	2.35	0.55
5:LA:229:ALA:HB3	5:LA:234:LYS:HB3	1.87	0.55
8:LD:204:VAL:HB	8:LD:236:MET:HE1	1.88	0.55
8:LD:232:THR:OG1	8:LD:234:ASP:OD1	2.20	0.55
10:LF:243:LEU:O	10:LF:247:MET:HB2	2.06	0.55
13:LI:38:ARG:NH1	13:LI:45:GLU:OE1	2.37	0.55
26:LW:100:VAL:O	26:LW:104:GLN:NE2	2.40	0.55
50:SF:39:ILE:HG23	50:SF:68:ILE:HD13	1.88	0.55
60:Sc:37:ASP:OD1	60:Sc:39:SER:OG	2.25	0.55
64:SA:126:ASP:OD1	64:SA:165:ASN:ND2	2.39	0.55
83:CB:453:MET:HA	83:CB:458:VAL:HG12	1.89	0.55
83:CB:583:VAL:HG22	83:CB:700:VAL:HG22	1.87	0.55
2:L5:1332:C:H2'	2:L5:1333:A:H8	1.72	0.55
54:SQ:4:LYS:HE3	82:S2:1423:C:H41	1.72	0.55
66:SC:109:ILE:HD11	66:SC:151:ILE:HD11	1.88	0.55
2:L5:702:U:H2'	2:L5:703:G:O4'	2.07	0.55
2:L5:1726:U:H5'	10:LF:135:ILE:HD11	1.89	0.55
2:L5:2318:G:N2	2:L5:2321:G:OP2	2.34	0.55
7:LC:262:GLU:HB3	7:LC:273:LEU:HD13	1.89	0.55
11:LG:57:TRP:O	11:LG:62:ARG:NH1	2.40	0.55
50:SF:40:ALA:HB3	50:SF:67:PRO:HA	1.88	0.55
57:ST:2:PRO:HD2	82:S2:1419:C:H42	1.71	0.55
63:Sg:89:LEU:HB3	63:Sg:99:ARG:HB3	1.88	0.55
67:SE:151:ASP:HA	68:SG:212:LEU:HD21	1.89	0.55
2:L5:121:A:OP1	11:LG:110:LYS:NZ	2.32	0.55
2:L5:261:G:H2'	2:L5:262:G:C8	2.42	0.55
2:L5:4413:C:O2	13:LI:158:LYS:NZ	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LW:105:ARG:NH2	68:SG:149:LYS:O	2.40	0.55
33:Ld:22:THR:HG23	33:Ld:122:VAL:HG13	1.88	0.55
47:Ls:110:ALA:HA	47:Ls:182:PRO:HG2	1.89	0.55
66:SC:102:LEU:HD22	66:SC:130:ILE:HD12	1.87	0.55
68:SG:7:PHE:HD1	68:SG:113:ILE:HB	1.72	0.55
70:SI:91:VAL:HG11	70:SI:205:ARG:HH12	1.72	0.55
82:S2:888:U:H4'	82:S2:889:U:H5'	1.89	0.55
2:L5:1100:U:O4	2:L5:1194:G:O6	2.25	0.55
29:LZ:46:ILE:HA	29:LZ:70:SER:HA	1.88	0.55
57:ST:74:SER:O	57:ST:78:ILE:HD12	2.07	0.55
65:SB:144:LYS:HD3	65:SB:208:HIS:HB3	1.88	0.55
83:CB:18:ASN:HD22	83:CB:98:PHE:HE1	1.53	0.55
50:SF:171:GLU:OE2	59:SZ:106:GLN:NE2	2.37	0.54
56:SS:36:VAL:HG21	56:SS:71:MET:HE3	1.89	0.54
62:Sf:110:GLU:HG2	62:Sf:113:LYS:HD3	1.89	0.54
74:SO:145:GLY:O	79:Sa:22:ARG:NH2	2.40	0.54
75:SV:42:VAL:HG23	75:SV:43:THR:HG23	1.88	0.54
82:S2:942:G:H2'	82:S2:943:U:C6	2.42	0.54
82:S2:1255:G:OP1	82:S2:1256:G:O2'	2.23	0.54
85:CE:72:ARG:HH11	85:CE:76:GLU:HG2	1.71	0.54
2:L5:502:C:H3'	2:L5:503:C:H3'	1.89	0.54
2:L5:2486:G:O6	2:L5:2493:G:O6	2.26	0.54
15:LL:64:VAL:HA	15:LL:67:HIS:CD2	2.31	0.54
22:LS:161:ARG:HD2	22:LS:164:LYS:HB2	1.88	0.54
24:LU:23:LEU:HD23	24:LU:110:TYR:HB2	1.89	0.54
36:Lg:44:SER:OG	36:Lg:46:CYS:SG	2.65	0.54
63:Sg:258:ILE:HG23	63:Sg:267:VAL:HG23	1.89	0.54
2:L5:1328:G:O2'	2:L5:2349:A:OP1	2.25	0.54
5:LA:101:VAL:HG22	5:LA:165:VAL:HG22	1.88	0.54
56:SS:88:LYS:H	56:SS:95:TYR:HD1	1.55	0.54
83:CB:26:ALA:HB2	83:CB:128:VAL:HB	1.90	0.54
83:CB:354:ILE:HG23	83:CB:358:LEU:HD12	1.90	0.54
2:L5:2495:U:H2'	2:L5:2496:G:C8	2.42	0.54
40:Lk:24:LYS:HD3	40:Lk:69:LEU:HD21	1.89	0.54
70:SI:143:LYS:NZ	82:S2:202:G:OP1	2.41	0.54
82:S2:981:A:H2'	82:S2:982:G:C8	2.42	0.54
82:S2:1513:C:H2'	82:S2:1514:G:H8	1.72	0.54
2:L5:305:A:OP2	17:LN:15:GLN:NE2	2.36	0.54
2:L5:729:G:H5''	10:LF:76:ARG:HD2	1.90	0.54
2:L5:2845:A:H61	2:L5:3843:C:H42	1.54	0.54
2:L5:4363:A:H5''	44:Lo:36:GLN:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LL:91:ALA:HB1	15:LL:96:ILE:HB	1.90	0.54
50:SF:30:ILE:HG23	50:SF:117:ILE:HD11	1.89	0.54
55:SR:16:ILE:HD11	55:SR:54:VAL:HG21	1.89	0.54
61:Sd:17:GLY:O	61:Sd:27:ARG:NH1	2.41	0.54
82:S2:1606:G:N2	82:S2:1632:G:H1'	2.22	0.54
83:CB:12:ILE:HD12	83:CB:99:LEU:HB2	1.88	0.54
2:L5:223:G:OP2	7:LC:165:LYS:NZ	2.40	0.54
2:L5:1333:A:H2'	2:L5:1334:A:C8	2.43	0.54
2:L5:4620:OMU:OP2	2:L5:4670:C:N4	2.33	0.54
2:L5:4774:C:O2'	2:L5:4775:C:O2	2.25	0.54
18:LO:54:TYR:OH	18:LO:73:PHE:O	2.25	0.54
57:ST:62:ARG:NH2	82:S2:1543:U:OP2	2.36	0.54
63:Sg:8:ARG:HB3	63:Sg:309:VAL:HG13	1.89	0.54
69:SH:10:LYS:NZ	69:SH:16:PRO:O	2.41	0.54
2:L5:4617:G:OP2	6:LB:358:ARG:NH2	2.40	0.54
2:L5:4941:G:OP2	9:LE:188:ARG:NH2	2.32	0.54
8:LD:156:GLY:HA2	8:LD:181:PRO:HG3	1.89	0.54
18:LO:186:GLU:OE1	18:LO:186:GLU:N	2.40	0.54
57:ST:65:TYR:HE1	57:ST:128:GLN:HG3	1.72	0.54
63:Sg:249:CYS:HB3	63:Sg:258:ILE:HD13	1.90	0.54
2:L5:4967:A:H2'	2:L5:4968:A:C8	2.42	0.54
8:LD:291:GLN:NE2	13:LI:213:HIS:O	2.32	0.54
30:La:87:ARG:HG3	30:La:120:GLN:HE22	1.73	0.54
50:SF:133:THR:N	84:Et:39:U:O2'	2.41	0.54
54:SQ:3:SER:OG	54:SQ:4:LYS:N	2.40	0.54
57:ST:121:ARG:HH21	82:S2:1563:G:H5''	1.71	0.54
1:CI:79:ARG:HH22	2:L5:2708:U:H1'	1.72	0.54
2:L5:1591:U:OP2	2:L5:2856:C:O2'	2.20	0.54
2:L5:1933:G:H2'	2:L5:1934:A:C8	2.43	0.54
2:L5:2745:A:H2'	2:L5:2746:A:C8	2.43	0.54
2:L5:3717:A:H2'	2:L5:3718:A2M:C8	2.38	0.54
5:LA:108:PRO:HB2	45:Lp:86:LEU:HD23	1.90	0.54
48:Lt:82:ILE:HG12	48:Lt:137:GLN:HG2	1.90	0.54
48:Lt:114:ARG:NH2	48:Lt:126:SER:OG	2.41	0.54
51:SK:27:VAL:HB	51:SK:43:LEU:HD12	1.90	0.54
56:SS:109:GLU:HA	56:SS:112:GLU:HG2	1.90	0.54
66:SC:72:ASP:OD2	66:SC:272:HIS:NE2	2.40	0.54
1:CI:50:MET:HG3	24:LU:114:TYR:CE2	2.42	0.54
2:L5:88:A:N7	20:LQ:173:LYS:NZ	2.56	0.54
2:L5:364:G:O6	39:Lj:55:ARG:NH2	2.41	0.54
16:LM:119:ARG:HG3	18:LO:189:ILE:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LQ:99:LYS:HZ2	20:LQ:121:LEU:HD11	1.73	0.54
35:Lf:43:LEU:O	35:Lf:109:ARG:NH2	2.41	0.54
63:Sg:18:VAL:O	63:Sg:287:THR:OG1	2.26	0.54
63:Sg:129:ILE:HB	63:Sg:142:VAL:HB	1.89	0.54
82:S2:557:U:H2'	82:S2:558:G:C8	2.43	0.54
82:S2:889:U:OP2	82:S2:896:U:N3	2.41	0.54
82:S2:1203:G:H2'	82:S2:1204:A:C8	2.42	0.54
83:CB:40:VAL:HG13	83:CB:47:ALA:HB1	1.88	0.54
2:L5:4220:6MZ:O5'	2:L5:4220:6MZ:H8	2.09	0.53
4:L8:58:G:N7	39:Lj:63:ARG:NH2	2.44	0.53
10:LF:96:ARG:HH12	10:LF:224:THR:HG22	1.72	0.53
14:LJ:84:GLU:OE2	14:LJ:92:TYR:OH	2.25	0.53
50:SF:134:VAL:HG23	84:Et:40:C:HO2'	1.70	0.53
54:SQ:130:LYS:NZ	54:SQ:131:LYS:O	2.41	0.53
64:SA:37:TYR:OH	64:SA:57:LYS:NZ	2.38	0.53
82:S2:118:C:H1'	82:S2:445:A:C5	2.43	0.53
2:L5:1214:C:N3	31:Lb:90:SER:OG	2.41	0.53
2:L5:1734:G:N2	2:L5:1735:U:O4	2.34	0.53
2:L5:1837:A:OP2	23:LT:130:ARG:NH1	2.38	0.53
2:L5:4537:C:H2'	2:L5:4538:G:C8	2.42	0.53
32:Lc:99:PRO:HG3	32:Lc:104:ILE:HB	1.90	0.53
48:Lt:34:PRO:HB3	83:CB:777:ALA:C	2.32	0.53
58:SU:68:THR:O	61:Sd:40:ARG:NH1	2.40	0.53
64:SA:18:PHE:HD1	64:SA:23:THR:HG21	1.71	0.53
70:SI:10:LYS:O	70:SI:18:ARG:NH1	2.41	0.53
2:L5:4694:G:H4'	12:LH:71:ARG:HH12	1.73	0.53
51:SK:55:ARG:NH1	51:SK:78:TYR:OH	2.41	0.53
66:SC:77:SER:OG	66:SC:79:GLU:OE1	2.26	0.53
74:SO:33:ILE:HB	74:SO:97:LEU:HD23	1.91	0.53
83:CB:150:ARG:HH22	83:CB:199:PRO:HD2	1.73	0.53
72:SL:128:VAL:HG12	72:SL:142:VAL:HA	1.90	0.53
76:SW:111:MET:HE1	76:SW:119:LYS:HD2	1.89	0.53
80:Sb:20:LYS:NZ	82:S2:1016:U:OP2	2.41	0.53
82:S2:851:C:H5''	82:S2:852:G:H5'	1.89	0.53
83:CB:27:HIS:HB2	83:CB:139:THR:HG23	1.90	0.53
49:SD:138:VAL:HG13	49:SD:182:LEU:HD21	1.91	0.53
72:SL:133:PRO:O	82:S2:383:G:O2'	2.25	0.53
77:SX:70:VAL:HG11	77:SX:94:ILE:HG21	1.89	0.53
82:S2:1013:U:OP1	82:S2:1129:G:O2'	2.26	0.53
2:L5:1994:C:H2'	2:L5:1995:G:H8	1.73	0.53
2:L5:3911:C:H2'	2:L5:3912:U:H6	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4260:U:H2'	2:L5:4261:C:C6	2.44	0.53
7:LC:218:ILE:HA	7:LC:229:LEU:HD22	1.89	0.53
28:LY:2:LYS:HD2	28:LY:7:VAL:HG23	1.89	0.53
47:Ls:139:GLN:HG2	83:CB:180:ARG:HE	1.74	0.53
73:SN:70:LYS:NZ	82:S2:1020:A:N7	2.55	0.53
80:Sb:62:VAL:HG23	80:Sb:74:THR:HG21	1.91	0.53
82:S2:1581:C:H5'	82:S2:1582:C:H5	1.74	0.53
82:S2:1825:A:C2	83:CB:714:ILE:HG12	2.19	0.53
2:L5:691:C:H2'	2:L5:692:A:C8	2.43	0.53
2:L5:735:G:H5''	16:LM:70:GLN:HG3	1.91	0.53
9:LE:223:ARG:HH22	9:LE:238:GLU:HG3	1.74	0.53
18:LO:168:TYR:CE2	18:LO:172:LYS:HD2	2.44	0.53
59:SZ:106:GLN:HG3	59:SZ:108:ILE:HD11	1.89	0.53
66:SC:257:LYS:O	75:SV:16:LYS:NZ	2.40	0.53
73:SN:66:VAL:HG13	73:SN:67:THR:HG23	1.90	0.53
82:S2:902:G:O2'	82:S2:903:A:O4'	2.27	0.53
2:L5:71:C:H1'	15:LL:62:PRO:O	2.09	0.53
19:LP:118:GLN:OE1	19:LP:120:ASN:ND2	2.41	0.53
28:LY:76:LYS:HE2	41:Ll:31:THR:HB	1.89	0.53
47:Ls:29:ILE:HG22	47:Ls:88:PHE:HD1	1.72	0.53
50:SF:78:MET:HE3	82:S2:1222:G:H5''	1.90	0.53
80:Sb:11:SER:N	80:Sb:14:GLU:OE2	2.42	0.53
25:LV:92:ASP:O	26:LW:2:LYS:NZ	2.42	0.53
46:Lr:38:PHE:O	46:Lr:45:HIS:NE2	2.31	0.53
82:S2:455:A:H2'	82:S2:456:C:H6	1.74	0.53
2:L5:267:G:H2'	2:L5:268:G:H8	1.74	0.53
2:L5:1756:U:O2'	2:L5:1758:G:OP2	2.24	0.53
26:LW:123:LYS:HD2	82:S2:320:G:H5''	1.90	0.53
47:Ls:135:THR:CG2	83:CB:187:VAL:HG11	2.39	0.53
51:SK:3:MET:HE1	51:SK:11:ILE:HD12	1.90	0.53
64:SA:85:ARG:NH1	64:SA:203:PHE:O	2.40	0.53
2:L5:1241:C:O2'	31:Lb:120:ARG:O	2.27	0.52
2:L5:1258:G:H2'	2:L5:1259:G:C8	2.44	0.52
2:L5:1548:G:O2'	2:L5:2812:A:N3	2.38	0.52
2:L5:2084:C:O2	20:LQ:16:LYS:NZ	2.42	0.52
7:LC:293:LEU:O	7:LC:299:GLN:NE2	2.39	0.52
31:Lb:102:PRO:O	31:Lb:109:ARG:NH2	2.41	0.52
54:SQ:131:LYS:HB2	54:SQ:140:ARG:HH22	1.74	0.52
56:SS:48:ALA:O	56:SS:66:ARG:NH2	2.42	0.52
60:Sc:66:ARG:HH12	60:Sc:68:LEU:HD23	1.74	0.52
81:Se:58:ASN:ND2	82:S2:608:C:O4'	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:S2:553:U:O4	82:S2:554:A:N6	2.40	0.52
82:S2:1684:C:O2'	84:Et:34:U:H6	1.92	0.52
82:S2:1773:C:H2'	82:S2:1774:C:H5''	1.91	0.52
35:Lf:78:HIS:HB3	35:Lf:83:MET:HB3	1.91	0.52
39:Lj:2:THR:HB	39:Lj:6:SER:HB2	1.90	0.52
79:Sa:41:ILE:HD12	79:Sa:68:TYR:HD2	1.74	0.52
83:CB:410:PHE:HB2	83:CB:476:ASP:CG	2.34	0.52
2:L5:2624:G:OP2	24:LU:97:ARG:NH2	2.42	0.52
2:L5:5016:A:C2	2:L5:5033:G:N2	2.74	0.52
20:LQ:15:ARG:NH1	20:LQ:52:PHE:O	2.41	0.52
72:SL:3:ASP:OD1	72:SL:4:ILE:N	2.42	0.52
2:L5:93:G:H2'	2:L5:94:A:C8	2.45	0.52
2:L5:2568:C:H2'	2:L5:2569:G:H8	1.73	0.52
2:L5:4612:C:C2	12:LH:120:GLU:HB2	2.44	0.52
2:L5:4717:A:OP2	6:LB:30:LYS:NZ	2.32	0.52
18:LO:54:TYR:CD1	18:LO:145:VAL:HG21	2.44	0.52
52:SM:82:ASN:OD1	52:SM:83:LYS:N	2.42	0.52
53:SP:79:HIS:HD2	82:S2:1298:G:C4	2.28	0.52
66:SC:60:TRP:O	66:SC:71:LYS:NZ	2.37	0.52
68:SG:13:GLN:NE2	82:S2:153:G:N3	2.57	0.52
83:CB:394:LEU:HD11	83:CB:421:VAL:HG23	1.92	0.52
84:Et:26:A:H62	84:Et:44:G:H21	1.58	0.52
2:L5:2696:A:OP1	40:Lk:26:LYS:NZ	2.42	0.52
47:Ls:99:ARG:HG3	47:Ls:103:LEU:HD13	1.92	0.52
66:SC:207:ALA:HB2	82:S2:4:C:H4'	1.92	0.52
69:SH:51:ILE:HG21	69:SH:179:LYS:HG2	1.91	0.52
82:S2:1777:G:H2'	82:S2:1778:C:H6	1.73	0.52
83:CB:30:HIS:CE1	83:CB:130:ASP:H	2.28	0.52
10:LF:41:MET:HE2	31:Lb:113:ALA:HB2	1.90	0.52
18:LO:197:LYS:NZ	18:LO:203:VAL:O	2.42	0.52
50:SF:60:ARG:HD2	82:S2:1679:A:H2'	1.92	0.52
54:SQ:42:ILE:HG23	54:SQ:44:PRO:HD2	1.91	0.52
56:SS:15:VAL:HG12	56:SS:16:LEU:HG	1.91	0.52
67:SE:125:LYS:O	67:SE:142:HIS:N	2.42	0.52
2:L5:1270:A:H8	2:L5:2106:G:H21	1.57	0.52
2:L5:2745:A:H2'	2:L5:2746:A:H8	1.75	0.52
2:L5:2756:G:O6	29:LZ:51:ARG:NH2	2.30	0.52
37:Lh:80:PRO:HD2	37:Lh:83:LEU:HD12	1.91	0.52
54:SQ:89:SER:OG	54:SQ:119:LEU:O	2.25	0.52
58:SU:40:ILE:O	58:SU:44:LYS:HG2	2.09	0.52
64:SA:10:MET:HE3	64:SA:55:TRP:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:SN:64:ARG:NH2	82:S2:919:A:OP2	2.41	0.52
48:Lt:119:ARG:NH1	48:Lt:123:ARG:HH12	2.08	0.52
49:SD:161:GLY:HA3	82:S2:1388:A:H61	1.75	0.52
61:Sd:2:GLY:N	82:S2:1271:C:O2	2.42	0.52
82:S2:367:U:H4'	82:S2:371:A:C8	2.45	0.52
82:S2:1010:G:H2'	82:S2:1011:A:C8	2.45	0.52
82:S2:1405:A:H2'	82:S2:1406:G:O4'	2.10	0.52
2:L5:2517:A:H5'	36:Lg:62:LYS:HD3	1.91	0.52
2:L5:4601:U:H2'	2:L5:4602:A:H8	1.75	0.52
9:LE:264:ILE:HD11	9:LE:267:LEU:HD22	1.92	0.52
48:Lt:85:LEU:HD13	48:Lt:109:ILE:HD12	1.90	0.52
57:ST:11:GLN:HB2	82:S2:1542:C:H4'	1.92	0.52
72:SL:61:PRO:HG3	72:SL:141:ASN:HB3	1.92	0.52
83:CB:646:ALA:HA	83:CB:649:ILE:HG12	1.92	0.52
2:L5:4478:G:O2'	2:L5:4602:A:N1	2.42	0.52
4:L8:39:G:OP1	37:Lh:86:LYS:NZ	2.43	0.52
65:SB:32:ASP:OD1	65:SB:46:LYS:NZ	2.38	0.52
68:SG:20:ASP:HB3	68:SG:23:LYS:HB2	1.91	0.52
2:L5:1961:G:O2'	2:L5:2025:A:N6	2.44	0.51
2:L5:3823:G:OP2	2:L5:3823:G:N2	2.35	0.51
33:Ld:23:ARG:HG2	33:Ld:121:ASN:HA	1.92	0.51
44:Lo:106:PHE:HZ	85:CE:39:TRP:CE3	2.19	0.51
54:SQ:140:ARG:HB2	82:S2:1644:C:H4'	1.92	0.51
78:SY:119:GLY:HA2	82:S2:85:A:H5'	1.91	0.51
83:CB:518:PRO:HA	83:CB:521:VAL:HG22	1.91	0.51
2:L5:268:G:H2'	2:L5:269:G:H8	1.75	0.51
2:L5:1070:G:O2'	2:L5:1071:C:O5'	2.26	0.51
2:L5:1509:C:H5''	30:La:2:PRO:HD3	1.92	0.51
7:LC:363:ALA:O	7:LC:367:GLU:HB3	2.10	0.51
51:SK:85:LEU:HD12	51:SK:86:PRO:HD2	1.91	0.51
62:Sf:102:VAL:HG22	62:Sf:104:LYS:HG2	1.92	0.51
76:SW:6:VAL:HG12	76:SW:34:ILE:HD11	1.93	0.51
76:SW:6:VAL:HG13	76:SW:29:PRO:HB2	1.91	0.51
83:CB:527:LEU:HD21	83:CB:557:CYS:HB3	1.93	0.51
48:Lt:34:PRO:HB3	83:CB:777:ALA:O	2.10	0.51
64:SA:76:VAL:HG12	64:SA:123:VAL:HB	1.91	0.51
65:SB:167:LYS:O	65:SB:171:ILE:HG12	2.10	0.51
68:SG:3:LEU:HD23	68:SG:109:LEU:HB3	1.91	0.51
68:SG:191:ARG:HH12	82:S2:312:G:H2'	1.75	0.51
69:SH:162:GLN:HE22	69:SH:166:VAL:HB	1.75	0.51
76:SW:111:MET:HE3	76:SW:116:ALA:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:S2:672:A:N6	82:S2:1027:A:OP1	2.41	0.51
82:S2:1130:G:OP2	82:S2:1130:G:N2	2.34	0.51
82:S2:1748:G:O6	82:S2:1786:U:O4	2.28	0.51
82:S2:1801:A:H2'	82:S2:1802:C:C6	2.46	0.51
2:L5:1718:C:O2'	10:LF:181:LYS:NZ	2.43	0.51
2:L5:3898:G:H5'	6:LB:254:ILE:HG13	1.92	0.51
6:LB:50:LYS:HB2	6:LB:345:LEU:HD11	1.92	0.51
17:LN:146:PRO:HB2	37:Lh:104:THR:HG23	1.93	0.51
53:SP:37:TYR:O	56:SS:88:LYS:NZ	2.43	0.51
77:SX:124:LYS:NZ	82:S2:29:G:OP1	2.40	0.51
82:S2:1610:G:O6	82:S2:1630:A:N6	2.43	0.51
2:L5:1268:G:N7	31:Lb:111:ARG:NH2	2.53	0.51
2:L5:1411:C:H2'	2:L5:1412:G:C8	2.45	0.51
2:L5:4274:A:H2'	2:L5:4275:G:C8	2.45	0.51
2:L5:4967:A:H2'	2:L5:4968:A:H8	1.75	0.51
59:SZ:41:ARG:HH12	59:SZ:44:LEU:HG	1.75	0.51
62:Sf:103:LEU:HB2	62:Sf:105:TYR:CE2	2.45	0.51
65:SB:26:SER:O	65:SB:51:ARG:NH2	2.43	0.51
77:SX:48:LYS:HB3	77:SX:75:ILE:HD12	1.91	0.51
2:L5:1683:PSU:OP1	30:La:44:ASN:ND2	2.42	0.51
9:LE:141:ARG:NH2	35:Lf:110:ILE:O	2.44	0.51
11:LG:157:ILE:HA	11:LG:201:THR:HG22	1.93	0.51
17:LN:46:ASP:OD1	17:LN:47:LYS:N	2.43	0.51
56:SS:28:PHE:O	56:SS:31:THR:OG1	2.25	0.51
66:SC:121:ARG:NH1	66:SC:123:ARG:HE	2.09	0.51
82:S2:525:A:H2'	82:S2:526:A:H8	1.75	0.51
2:L5:308:G:OP2	2:L5:308:G:N2	2.35	0.51
2:L5:1867:A:H2'	2:L5:1868:A:C8	2.46	0.51
6:LB:288:GLY:HA3	6:LB:330:PHE:CE1	2.46	0.51
10:LF:171:ASP:OD1	10:LF:172:ASN:N	2.43	0.51
14:LJ:104:ASN:HD22	14:LJ:133:VAL:HG13	1.75	0.51
47:Ls:29:ILE:HG22	47:Ls:88:PHE:CD1	2.46	0.51
52:SM:23:LYS:O	52:SM:27:ILE:HG12	2.10	0.51
58:SU:96:GLU:OE1	58:SU:99:LYS:N	2.36	0.51
63:Sg:239:LEU:HD11	63:Sg:248:LEU:HD21	1.93	0.51
67:SE:204:SER:OG	67:SE:205:PHE:N	2.39	0.51
67:SE:247:THR:N	67:SE:250:GLU:OE2	2.39	0.51
70:SI:3:ILE:O	70:SI:30:GLY:N	2.42	0.51
82:S2:145:G:H2'	82:S2:146:G:C8	2.45	0.51
6:LB:57:VAL:HG22	6:LB:73:VAL:HG22	1.93	0.51
47:Ls:139:GLN:NE2	83:CB:183:GLU:CB	2.70	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SI:45:THR:HG23	70:SI:53:LYS:HG3	1.93	0.51
80:Sb:67:THR:OG1	80:Sb:70:LYS:O	2.21	0.51
85:CE:60:ARG:NH1	85:CE:61:LEU:HG	2.26	0.51
2:L5:2009:A:C8	83:CB:756:VAL:HG13	2.46	0.51
47:Ls:13:TYR:O	47:Ls:17:ILE:HG12	2.11	0.51
67:SE:31:PRO:HA	67:SE:81:THR:HB	1.93	0.51
67:SE:126:VAL:HA	67:SE:141:THR:HA	1.93	0.51
82:S2:57:U:OP1	82:S2:504:G:O2'	2.29	0.51
82:S2:964:A:H2'	82:S2:965:U:H6	1.76	0.51
82:S2:1421:A:H5''	82:S2:1422:G:H2'	1.92	0.51
82:S2:1588:A:H2'	82:S2:1589:A:C8	2.46	0.51
12:LH:92:MET:HE2	12:LH:179:ILE:HG22	1.93	0.51
14:LJ:58:ARG:CZ	85:CE:39:TRP:CD2	2.87	0.51
33:Ld:59:THR:OG1	33:Ld:104:THR:OG1	2.25	0.51
38:Li:55:ARG:O	38:Li:59:GLU:HG2	2.11	0.51
56:SS:14:ARG:HH11	56:SS:19:ASN:HB3	1.76	0.51
61:Sd:12:ARG:NH1	82:S2:1513:C:OP1	2.31	0.51
66:SC:191:VAL:HG11	66:SC:236:PHE:HA	1.93	0.51
69:SH:10:LYS:HE3	69:SH:17:ASP:HB3	1.93	0.51
85:CE:29:LYS:HA	85:CE:32:LYS:HZ2	1.75	0.51
2:L5:351:C:OP2	7:LC:197:ARG:NH1	2.34	0.50
2:L5:2102:G:H1'	2:L5:2103:G:C8	2.46	0.50
2:L5:4636:PSU:N1	33:Ld:79:ASN:OD1	2.43	0.50
2:L5:4896:G:H2'	2:L5:4897:G:C8	2.47	0.50
12:LH:107:GLU:N	12:LH:107:GLU:OE1	2.44	0.50
18:LO:126:VAL:HG13	18:LO:127:VAL:HG13	1.92	0.50
47:Ls:147:ILE:CG2	83:CB:186:ASN:HB3	2.41	0.50
78:SY:108:LYS:NZ	82:S2:506:G:OP1	2.38	0.50
82:S2:1058:A:H5'	85:CE:12:SER:HB2	1.93	0.50
2:L5:387:G:O2'	2:L5:412:G:N1	2.36	0.50
2:L5:717:U:H2'	2:L5:718:C:C6	2.46	0.50
2:L5:1438:U:H4'	10:LF:31:LYS:HE3	1.93	0.50
2:L5:4927:G:H5''	2:L5:4928:C:H5	1.76	0.50
18:LO:10:ASP:OD2	18:LO:37:ARG:NH2	2.44	0.50
53:SP:56:LEU:HD22	53:SP:80:LEU:HD11	1.92	0.50
57:ST:44:GLU:HG3	57:ST:45:LEU:HD12	1.93	0.50
65:SB:40:ASN:HD21	65:SB:76:ASN:HB2	1.77	0.50
71:SJ:136:ARG:NH1	71:SJ:159:PHE:O	2.40	0.50
77:SX:142:ARG:C	83:CB:477:GLN:O	2.54	0.50
82:S2:28:U:H2'	82:S2:29:G:H8	1.76	0.50
82:S2:107:A:H2'	82:S2:108:G:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:2577:C:OP1	29:LZ:111:ARG:NH2	2.44	0.50
4:L8:21:C:OP1	7:LC:195:LYS:NZ	2.42	0.50
15:LL:7:GLY:O	30:La:49:HIS:NE2	2.40	0.50
63:Sg:40:ILE:HB	63:Sg:59:LEU:HB2	1.93	0.50
79:Sa:41:ILE:HD12	79:Sa:68:TYR:CD2	2.45	0.50
82:S2:1033:G:N1	82:S2:1080:A:O2'	2.39	0.50
82:S2:1845:A:H2'	82:S2:1846:G:C8	2.46	0.50
1:CI:78:HIS:NE2	2:L5:2706:G:C8	2.75	0.50
2:L5:2018:C:H2'	2:L5:2019:C:C6	2.46	0.50
2:L5:4589:A:N1	2:L5:4621:C:O2'	2.41	0.50
13:LI:207:ASP:OD1	13:LI:210:ARG:NH1	2.44	0.50
26:LW:7:SER:OG	26:LW:8:PHE:N	2.45	0.50
50:SF:22:LYS:HG3	50:SF:23:TRP:CD2	2.46	0.50
64:SA:128:ARG:NH2	64:SA:151:ASP:O	2.44	0.50
2:L5:418:A:C2	4:L8:17:A:H1'	2.47	0.50
2:L5:1802:A:H5''	2:L5:1803:G:H5'	1.93	0.50
2:L5:3732:A:H2'	2:L5:3733:A:H8	1.76	0.50
7:LC:144:ILE:HG13	7:LC:144:ILE:O	2.11	0.50
24:LU:36:ALA:HB1	24:LU:70:ILE:HD11	1.93	0.50
47:Ls:139:GLN:CG	83:CB:180:ARG:CD	2.88	0.50
64:SA:137:ALA:HB1	64:SA:142:LEU:HB3	1.94	0.50
69:SH:140:VAL:HG12	73:SN:19:ARG:HD3	1.94	0.50
71:SJ:38:ARG:N	71:SJ:42:GLU:OE2	2.30	0.50
82:S2:436:OMG:OP2	82:S2:471:G:O2'	2.23	0.50
83:CB:27:HIS:HB3	83:CB:30:HIS:CD2	2.47	0.50
2:L5:1697:G:H22	2:L5:2084:C:P	2.35	0.50
2:L5:3707:U:H2'	2:L5:3708:C:C6	2.46	0.50
2:L5:5064:G:N2	19:LP:75:GLN:HE22	2.10	0.50
6:LB:378:ARG:HE	26:LW:32:LEU:HD21	1.75	0.50
21:LR:92:LYS:HG2	21:LR:96:MET:HE3	1.94	0.50
63:Sg:57:ARG:HE	63:Sg:95:GLY:HA3	1.76	0.50
66:SC:78:LEU:HD12	66:SC:81:ILE:HD12	1.93	0.50
66:SC:196:ILE:HB	66:SC:223:TYR:HB2	1.92	0.50
82:S2:455:A:H2'	82:S2:456:C:C6	2.46	0.50
2:L5:654:C:H2'	2:L5:655:C:C6	2.47	0.50
2:L5:2300:A:N7	7:LC:143:ARG:NH1	2.60	0.50
2:L5:3910:C:H2'	2:L5:3911:C:C6	2.47	0.50
19:LP:107:LEU:HD13	19:LP:152:GLU:HG3	1.93	0.50
63:Sg:176:VAL:HG23	63:Sg:185:LYS:HB2	1.94	0.50
70:SI:133:GLU:HA	70:SI:136:ILE:HG12	1.92	0.50
82:S2:159:A2M:O5'	82:S2:159:A2M:H8	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:137:G:H2'	2:L5:138:G:H8	1.77	0.50
2:L5:1617:G:H1'	2:L5:2513:A:N6	2.26	0.50
14:LJ:38:LYS:HD2	14:LJ:123:ILE:HD11	1.94	0.50
58:SU:79:ARG:NH2	82:S2:1669:G:OP1	2.42	0.50
68:SG:135:PRO:HA	82:S2:169:U:H5''	1.93	0.50
68:SG:190:ARG:NH2	82:S2:334:C:OP2	2.40	0.50
82:S2:482:G:N1	82:S2:485:A:OP2	2.39	0.50
2:L5:1655:C:OP2	30:La:26:ARG:NH1	2.45	0.50
2:L5:3697:U:H5''	2:L5:3698:G:H5'	1.93	0.50
2:L5:4239:A:H2'	2:L5:4240:G:C8	2.47	0.50
2:L5:4591:U:H2'	2:L5:4592:C:C6	2.47	0.50
4:L8:141:C:H2'	4:L8:142:U:C6	2.47	0.50
6:LB:147:GLU:OE2	6:LB:198:ARG:NH2	2.32	0.50
8:LD:182:GLY:HA2	8:LD:194:VAL:HG23	1.93	0.50
12:LH:48:LEU:HD21	12:LH:56:ARG:HB2	1.93	0.50
45:Lp:75:SER:O	45:Lp:79:VAL:HG23	2.12	0.50
51:SK:22:VAL:HG22	51:SK:68:TYR:HD1	1.76	0.50
51:SK:64:TRP:HB3	61:Sd:23:VAL:HA	1.94	0.50
63:Sg:195:LEU:HA	63:Sg:211:GLY:HA3	1.93	0.50
66:SC:85:SER:OG	75:SV:25:GLY:O	2.29	0.50
69:SH:20:GLU:HG2	69:SH:48:ALA:HB3	1.93	0.50
70:SI:141:ARG:HD3	70:SI:145:ILE:HG21	1.93	0.50
74:SO:45:THR:HA	74:SO:52:THR:HA	1.94	0.50
78:SY:51:THR:OG1	78:SY:53:ASP:OD1	2.23	0.50
78:SY:119:GLY:O	82:S2:84:A:O2'	2.27	0.50
82:S2:149:A:H3'	82:S2:150:A:H8	1.76	0.50
83:CB:609:PHE:CZ	83:CB:661:ILE:HG12	2.46	0.50
85:CE:72:ARG:NH1	85:CE:76:GLU:HG2	2.27	0.50
2:L5:1628:C:OP1	5:LA:14:SER:OG	2.29	0.49
2:L5:2809:G:O2'	2:L5:4644:G:OP1	2.28	0.49
5:LA:181:LYS:HB2	5:LA:184:ARG:HG3	1.94	0.49
6:LB:218:ASP:OD2	6:LB:348:ARG:NH2	2.32	0.49
15:LL:111:GLN:O	15:LL:115:GLN:HG2	2.12	0.49
57:ST:60:THR:HG22	57:ST:75:MET:HE2	1.94	0.49
65:SB:97:LEU:HB3	65:SB:232:HIS:NE2	2.27	0.49
82:S2:960:U:O2'	82:S2:962:A:N7	2.37	0.49
2:L5:1662:C:H2'	2:L5:1663:C:C6	2.47	0.49
2:L5:3641:U:H5	2:L5:3646:A:N7	2.09	0.49
10:LF:157:ARG:HE	10:LF:248:ASN:HB2	1.77	0.49
50:SF:60:ARG:NH2	82:S2:1679:A:OP1	2.43	0.49
50:SF:141:VAL:HG12	60:Sc:47:LYS:HG2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SA:184:ARG:HE	64:SA:191:ARG:HA	1.77	0.49
68:SG:170:ARG:HG3	82:S2:72:C:N3	2.27	0.49
82:S2:1562:C:H2'	82:S2:1563:G:H8	1.76	0.49
2:L5:433:A:C2	2:L5:3867:A2M:H4'	2.46	0.49
6:LB:394:LYS:HA	6:LB:397:ILE:HG12	1.94	0.49
8:LD:217:ASP:N	8:LD:217:ASP:OD1	2.41	0.49
9:LE:190:HIS:HB3	9:LE:193:PHE:HD2	1.77	0.49
12:LH:18:ILE:HG12	12:LH:27:VAL:HG22	1.94	0.49
14:LJ:58:ARG:HG2	85:CE:39:TRP:HE3	1.76	0.49
26:LW:2:LYS:HE3	26:LW:15:PRO:HB3	1.94	0.49
47:Ls:139:GLN:OE1	83:CB:180:ARG:HA	2.12	0.49
47:Ls:143:ILE:HD12	47:Ls:158:VAL:HG11	1.95	0.49
52:SM:49:LEU:HD21	52:SM:123:VAL:HG11	1.94	0.49
77:SX:28:LYS:HE2	77:SX:32:LEU:HD22	1.93	0.49
78:SY:105:LYS:NZ	82:S2:507:G:O6	2.36	0.49
82:S2:1337:4AC:O5'	82:S2:1337:4AC:H6	2.12	0.49
2:L5:173:C:OP1	15:LL:129:ARG:NH1	2.46	0.49
2:L5:325:U:H2'	2:L5:326:C:C6	2.47	0.49
2:L5:512:U:H3	2:L5:647:G:H1	1.60	0.49
2:L5:1283:G:N1	2:L5:2076:G:OP1	2.33	0.49
2:L5:3659:G:OP1	5:LA:241:ARG:NH1	2.45	0.49
6:LB:258:HIS:HA	6:LB:260:ALA:N	2.26	0.49
8:LD:66:TYR:HE2	8:LD:68:ARG:HE	1.60	0.49
22:LS:27:LEU:HB3	23:LT:148:PRO:HB3	1.94	0.49
48:Lt:76:SER:OG	48:Lt:116:MET:SD	2.69	0.49
61:Sd:46:TYR:O	61:Sd:50:ILE:HD12	2.12	0.49
73:SN:14:SER:HB3	82:S2:1016:U:H5''	1.95	0.49
76:SW:3:ARG:HH22	76:SW:28:ARG:HH21	1.60	0.49
76:SW:44:HIS:NE2	76:SW:112:ASP:OD2	2.42	0.49
79:Sa:8:ASN:ND2	82:S2:1861:G:OP1	2.42	0.49
82:S2:928:G:H1	82:S2:1013:U:H3	1.59	0.49
2:L5:10:A:H2'	2:L5:11:G:C8	2.48	0.49
2:L5:1480:C:O2'	2:L5:1482:G:OP2	2.31	0.49
2:L5:1516:G:O2'	15:LL:18:TRP:NE1	2.45	0.49
2:L5:3880:G:H2'	2:L5:3881:G:C8	2.47	0.49
2:L5:4188:U:H2'	2:L5:4189:U:C6	2.48	0.49
50:SF:81:ARG:O	50:SF:85:LYS:NZ	2.34	0.49
56:SS:46:ARG:NH1	57:ST:50:GLU:OE2	2.45	0.49
82:S2:1288:OMU:HN3	82:S2:1311:C:H42	1.60	0.49
82:S2:1720:U:H5''	82:S2:1721:U:H5''	1.94	0.49
2:L5:2279:A:O2'	34:Le:48:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:2491:C:H2'	2:L5:2492:C:C6	2.47	0.49
2:L5:2739:C:O2	5:LA:188:LYS:NZ	2.43	0.49
2:L5:3615:G:H1'	26:LW:44:ARG:HD3	1.95	0.49
2:L5:3720:G:H22	2:L5:3733:A:H2	1.58	0.49
75:SV:73:ALA:HB1	75:SV:78:ILE:HB	1.95	0.49
82:S2:49:C:H2'	82:S2:472:C:H41	1.76	0.49
2:L5:2101:C:H2'	2:L5:2102:G:C8	2.47	0.49
2:L5:2539:C:H2'	2:L5:2540:C:C6	2.48	0.49
2:L5:2568:C:H2'	2:L5:2569:G:C8	2.48	0.49
2:L5:4459:U:H2'	2:L5:4460:U:C6	2.47	0.49
6:LB:299:ILE:HB	6:LB:313:SER:HB3	1.94	0.49
29:LZ:50:PRO:HD3	29:LZ:68:ILE:HG12	1.95	0.49
56:SS:132:ARG:NH1	82:S2:1623:A:N1	2.60	0.49
67:SE:104:ASP:HB3	67:SE:110:ALA:HB2	1.93	0.49
69:SH:87:PHE:HB3	69:SH:90:LYS:HD2	1.95	0.49
70:SI:116:HIS:O	70:SI:152:ARG:NH2	2.38	0.49
71:SJ:60:LEU:HD22	71:SJ:70:ARG:HA	1.95	0.49
82:S2:1098:C:H2'	82:S2:1099:G:C8	2.47	0.49
82:S2:1407:U:H2'	82:S2:1408:U:C6	2.47	0.49
83:CB:403:PRO:HA	83:CB:410:PHE:HA	1.94	0.49
1:CI:78:HIS:CD2	2:L5:2706:G:N7	2.81	0.49
2:L5:1646:A:O2'	39:Lj:49:TRP:O	2.25	0.49
2:L5:1985:G:N2	2:L5:2003:G:O2'	2.46	0.49
2:L5:4699:U:H1'	2:L5:4700:A:H5''	1.94	0.49
18:LO:119:VAL:N	22:LS:168:THR:O	2.44	0.49
25:LV:87:SER:OG	26:LW:19:ARG:NH1	2.46	0.49
55:SR:32:LYS:NZ	82:S2:1452:A:OP2	2.45	0.49
64:SA:106:GLY:N	64:SA:136:GLU:OE2	2.34	0.49
82:S2:207:G:H3'	82:S2:208:G:H8	1.78	0.49
82:S2:1277:C:H2'	82:S2:1278:A:C8	2.47	0.49
82:S2:1528:G:O2'	82:S2:1666:C:OP1	2.30	0.49
82:S2:1684:C:H1'	84:Et:34:U:OP1	2.13	0.49
2:L5:148:C:OP2	11:LG:197:LYS:NZ	2.42	0.49
2:L5:280:G:H5''	17:LN:14:LYS:HE2	1.93	0.49
2:L5:308:G:O6	17:LN:12:ARG:NH1	2.46	0.49
2:L5:2764:A:H2'	2:L5:2765:A:H8	1.78	0.49
2:L5:2835:A:O2'	6:LB:228:TYR:O	2.27	0.49
2:L5:4966:A:H5''	6:LB:128:LYS:HG3	1.93	0.49
6:LB:217:ILE:HD12	6:LB:347:LEU:HB3	1.95	0.49
53:SP:132:GLY:HA2	83:CB:708:THR:HG21	1.95	0.49
77:SX:128:VAL:HG23	77:SX:138:LYS:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:SY:7:ILE:HG12	78:SY:43:LYS:HD3	1.94	0.49
78:SY:41:ARG:NH2	78:SY:52:PRO:O	2.45	0.49
2:L5:1097:C:H2'	2:L5:1098:G:C8	2.48	0.49
2:L5:1332:C:H2'	2:L5:1333:A:C8	2.47	0.49
2:L5:1500:A:H5''	2:L5:1501:C:H5''	1.95	0.49
2:L5:1743:A:N1	2:L5:1789:C:O2'	2.44	0.49
2:L5:1998:A:O2'	2:L5:1999:A:O4'	2.29	0.49
2:L5:2744:A:H2'	2:L5:2745:A:C8	2.47	0.49
2:L5:4225:G:OP1	13:LI:24:ARG:NH2	2.39	0.49
2:L5:4457:PSU:H1'	6:LB:252:ALA:HB3	1.95	0.49
2:L5:4935:C:H2'	2:L5:4936:G:C8	2.47	0.49
14:LJ:22:LEU:HD22	14:LJ:128:LEU:HD12	1.94	0.49
15:LL:56:ARG:NH1	15:LL:74:ARG:O	2.40	0.49
26:LW:56:ARG:HE	26:LW:61:LYS:CB	2.26	0.49
43:Ln:12:ARG:HG2	43:Ln:15:ARG:HH21	1.78	0.49
50:SF:49:LEU:HD12	50:SF:50:PRO:HD2	1.94	0.49
50:SF:161:ALA:O	50:SF:165:ASN:ND2	2.40	0.49
51:SK:41:PRO:HG2	51:SK:44:HIS:CG	2.48	0.49
68:SG:172:LYS:NZ	82:S2:67:C:OP2	2.34	0.49
73:SN:29:THR:OG1	73:SN:31:ASP:OD1	2.27	0.49
85:CE:78:ASP:HA	85:CE:81:LEU:HB3	1.95	0.49
2:L5:158:A:H5''	2:L5:159:C:H2'	1.96	0.48
2:L5:2716:C:O3'	24:LU:107:LYS:NZ	2.46	0.48
2:L5:3664:G:H2'	2:L5:3665:G:H8	1.78	0.48
22:LS:99:ASP:OD1	22:LS:100:LEU:N	2.43	0.48
34:Le:108:ARG:HD2	34:Le:128:ARG:HB2	1.93	0.48
54:SQ:96:TYR:HA	54:SQ:100:VAL:HG12	1.95	0.48
65:SB:171:ILE:HG22	65:SB:174:ARG:HE	1.78	0.48
81:Se:11:LYS:O	81:Se:15:GLN:HG3	2.13	0.48
82:S2:84:A:N3	82:S2:150:A:O2'	2.46	0.48
2:L5:1326:A2M:H2'	2:L5:1327:C:C6	2.48	0.48
2:L5:1503:A:H4'	2:L5:1504:G:H5'	1.95	0.48
7:LC:154:VAL:HG11	7:LC:174:LEU:HD11	1.95	0.48
9:LE:119:GLU:HG3	34:Le:7:LEU:HD22	1.94	0.48
31:Lb:5:LYS:HE2	31:Lb:8:THR:HB	1.94	0.48
69:SH:69:LEU:HD13	69:SH:96:ALA:HB2	1.96	0.48
75:SV:30:ALA:O	75:SV:60:ARG:HD3	2.13	0.48
80:Sb:49:HIS:ND1	80:Sb:69:GLY:O	2.46	0.48
82:S2:1533:A:H62	82:S2:1602:U:H3	1.61	0.48
82:S2:1568:C:H2'	82:S2:1569:A:C8	2.48	0.48
82:S2:1595:U:H2'	82:S2:1596:U:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:121:A:H62	2:L5:152:U:H3	1.62	0.48
2:L5:369:G:N2	2:L5:372:A:OP2	2.42	0.48
2:L5:497:G:N2	2:L5:498:C:H41	2.11	0.48
2:L5:1344:C:H1'	15:LL:10:LEU:HD11	1.95	0.48
2:L5:1866:U:OP1	13:LI:4:ARG:NH1	2.36	0.48
2:L5:2903:G:H1'	2:L5:2904:U:H5	1.78	0.48
2:L5:3619:G:H22	2:L5:3624:A:H1'	1.77	0.48
2:L5:4940:C:O2'	9:LE:246:ARG:NH2	2.45	0.48
5:LA:180:LEU:HD22	45:Lp:18:TYR:HB3	1.96	0.48
34:Le:91:CYS:HB3	34:Le:95:TYR:HD2	1.77	0.48
60:Sc:39:SER:HB2	79:Sa:51:ARG:HH12	1.77	0.48
62:Sf:95:ARG:HH12	82:S2:1291:A:H62	1.60	0.48
63:Sg:207:CYS:HB3	63:Sg:221:LEU:HD21	1.95	0.48
64:SA:134:LEU:HD21	64:SA:144:THR:HG21	1.96	0.48
70:SI:54:LYS:NZ	82:S2:381:C:OP2	2.45	0.48
2:L5:467:U:C4	2:L5:468:U:H1'	2.48	0.48
2:L5:1320:U:O2'	2:L5:1891:A:N1	2.45	0.48
2:L5:1461:C:H2'	2:L5:1462:A:C8	2.48	0.48
2:L5:4584:A:H2'	2:L5:4585:U:O4'	2.13	0.48
12:LH:41:ILE:HG22	12:LH:43:VAL:HG13	1.95	0.48
12:LH:61:TRP:CZ3	16:LM:33:GLN:HG3	2.49	0.48
13:LI:54:SER:HB3	13:LI:135:ILE:HD11	1.95	0.48
19:LP:54:GLN:HA	19:LP:83:TRP:CD1	2.47	0.48
27:LX:122:ALA:N	27:LX:139:ARG:O	2.43	0.48
63:Sg:82:SER:OG	63:Sg:83:TRP:N	2.45	0.48
65:SB:85:LYS:HB2	65:SB:101:HIS:HB3	1.94	0.48
70:SI:89:GLU:OE1	70:SI:92:ARG:NH2	2.46	0.48
82:S2:5:U:H2'	82:S2:6:G:H8	1.78	0.48
82:S2:106:C:H2'	82:S2:107:A:C8	2.46	0.48
82:S2:1144:A:H2'	82:S2:1145:A:C8	2.48	0.48
82:S2:1652:G:H1	82:S2:1672:U:H3	1.60	0.48
83:CB:205:ILE:HD12	83:CB:212:VAL:HG22	1.96	0.48
2:L5:1095:A:N1	2:L5:1200:G:C6	2.81	0.48
2:L5:1324:A:O2'	2:L5:1326:A2M:OP1	2.24	0.48
2:L5:1777:C:P	85:CE:64:LEU:HD11	2.54	0.48
2:L5:2049:G:HO2'	2:L5:3884:PSU:HO2'	1.54	0.48
2:L5:2588:C:OP1	2:L5:2768:C:O2'	2.27	0.48
2:L5:4769:G:H5''	18:LO:176:ARG:HD3	1.96	0.48
7:LC:268:ARG:NH1	7:LC:269:LYS:HE2	2.29	0.48
11:LG:150:LYS:NZ	11:LG:177:MET:O	2.46	0.48
78:SY:29:HIS:O	78:SY:67:GLY:HA2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:S2:1115:U:O2'	82:S2:1117:C:OP2	2.30	0.48
2:L5:1326:A2M:HM'3	2:L5:1326:A2M:H1'	1.63	0.48
2:L5:4347:G:H2'	2:L5:4348:A:C8	2.48	0.48
70:SI:25:ARG:HA	82:S2:448:A:H5''	1.95	0.48
82:S2:1438:A:H2'	82:S2:1439:A:C8	2.49	0.48
2:L5:172:C:H4'	2:L5:173:C:H5'	1.96	0.48
2:L5:423:G:H21	19:LP:118:GLN:NE2	2.10	0.48
2:L5:500:G:H1'	2:L5:504:G:H3'	1.95	0.48
2:L5:4345:C:H2'	2:L5:4346:U:C6	2.48	0.48
6:LB:153:MET:HB3	6:LB:194:LEU:HD11	1.95	0.48
14:LJ:63:ARG:HH11	44:Lo:106:PHE:HB2	1.79	0.48
44:Lo:106:PHE:HE1	85:CE:39:TRP:CA	2.22	0.48
50:SF:142:SER:HB3	60:Sc:50:VAL:HG22	1.94	0.48
51:SK:32:HIS:CD2	51:SK:45:VAL:HG11	2.48	0.48
52:SM:128:PHE:HA	52:SM:131:LYS:HG2	1.96	0.48
54:SQ:110:ASP:OD1	54:SQ:111:ILE:HD12	2.13	0.48
59:SZ:42:ASP:OD1	59:SZ:42:ASP:N	2.44	0.48
62:Sf:139:HIS:O	62:Sf:147:THR:HA	2.13	0.48
63:Sg:166:VAL:HG12	63:Sg:176:VAL:HG12	1.95	0.48
68:SG:202:ASN:ND2	82:S2:125:C:OP1	2.39	0.48
69:SH:51:ILE:HD11	69:SH:176:VAL:HG12	1.96	0.48
70:SI:57:ALA:HB2	70:SI:183:GLY:HA2	1.95	0.48
82:S2:17:C:O2'	82:S2:1194:A:N1	2.38	0.48
82:S2:1337:4AC:H2'	82:S2:1338:G:H8	1.78	0.48
82:S2:1435:C:O2'	82:S2:1436:C:O4'	2.30	0.48
83:CB:221:TRP:CG	83:CB:340:MET:HB3	2.49	0.48
2:L5:1367:C:O2'	2:L5:1369:C:OP2	2.26	0.48
2:L5:2009:A:N6	83:CB:782:PHE:CZ	2.82	0.48
2:L5:2583:C:OP2	36:Lg:76:ARG:NH1	2.46	0.48
2:L5:4113:U:H4'	2:L5:4115:G:C6	2.48	0.48
2:L5:4897:G:OP1	16:LM:128:LYS:NZ	2.45	0.48
7:LC:141:GLY:O	7:LC:204:ARG:NH1	2.35	0.48
12:LH:114:ILE:HB	12:LH:124:ARG:HB2	1.95	0.48
15:LL:142:GLU:HA	15:LL:146:LEU:HD12	1.95	0.48
21:LR:127:VAL:HG12	21:LR:132:PHE:HD2	1.78	0.48
24:LU:63:ILE:HD13	24:LU:72:VAL:HG22	1.96	0.48
44:Lo:106:PHE:HZ	85:CE:39:TRP:HB3	1.75	0.48
56:SS:64:VAL:O	56:SS:68:ILE:HG12	2.13	0.48
82:S2:329:G:H2'	82:S2:330:G:C8	2.49	0.48
82:S2:907:G:H2'	82:S2:908:A:C8	2.48	0.48
83:CB:361:PRO:HB3	83:CB:415:ARG:NH2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:2411:C:H2'	2:L5:2412:A:C8	2.49	0.48
2:L5:4305:G:N7	23:LT:87:LYS:NZ	2.53	0.48
2:L5:4769:G:OP1	18:LO:176:ARG:NH1	2.43	0.48
4:L8:19:C:H2'	4:L8:20:A:C8	2.48	0.48
8:LD:234:ASP:OD1	8:LD:235:MET:N	2.47	0.48
10:LF:127:LYS:HB2	23:LT:133:ALA:HB3	1.96	0.48
10:LF:237:GLU:HG2	22:LS:38:VAL:HG22	1.96	0.48
58:SU:56:MET:HB2	58:SU:86:LYS:HG3	1.95	0.48
65:SB:168:MET:HB2	65:SB:197:ILE:HD13	1.96	0.48
69:SH:30:LEU:O	69:SH:33:ASN:ND2	2.47	0.48
83:CB:41:CYS:HA	83:CB:49:ALA:HA	1.96	0.48
2:L5:138:G:H2'	2:L5:139:G:H8	1.79	0.48
2:L5:737:C:C5	2:L5:739:G:H5'	2.49	0.48
2:L5:1095:A:C2	2:L5:1200:G:N1	2.65	0.48
2:L5:2018:C:H2'	2:L5:2019:C:H6	1.79	0.48
2:L5:2846:G:OP1	25:LV:85:ARG:NH2	2.47	0.48
2:L5:3732:A:H2'	2:L5:3733:A:C8	2.49	0.48
3:L7:23:A:N3	3:L7:118:C:O2'	2.36	0.48
8:LD:86:TYR:HE1	8:LD:247:ILE:HG13	1.78	0.48
19:LP:114:ILE:HA	19:LP:150:LEU:HD23	1.96	0.48
55:SR:29:HIS:CD2	63:Sg:36:ARG:HH21	2.32	0.48
57:ST:40:ALA:HB3	57:ST:43:LYS:HG2	1.96	0.48
59:SZ:85:ARG:NH2	82:S2:1597:C:OP2	2.39	0.48
67:SE:192:ILE:HG12	67:SE:243:GLY:HA3	1.96	0.48
73:SN:15:ALA:HB2	80:Sb:20:LYS:HD3	1.95	0.48
77:SX:105:PHE:CD1	77:SX:121:LYS:HB3	2.45	0.48
2:L5:374:G:OP2	39:Lj:56:ARG:NH1	2.38	0.47
2:L5:490:C:H2'	2:L5:491:G:C8	2.48	0.47
2:L5:1942:A:H2'	2:L5:1943:A:H8	1.78	0.47
6:LB:27:GLY:HA2	6:LB:276:HIS:CD2	2.49	0.47
24:LU:39:PHE:HD1	24:LU:90:TYR:CD2	2.32	0.47
50:SF:26:ASP:N	50:SF:26:ASP:OD1	2.46	0.47
50:SF:83:ASN:OD1	82:S2:1651:A:O2'	2.28	0.47
65:SB:171:ILE:HD11	65:SB:197:ILE:HA	1.95	0.47
80:Sb:11:SER:OG	80:Sb:14:GLU:OE1	2.30	0.47
83:CB:19:ILE:HD12	83:CB:99:LEU:HD23	1.95	0.47
2:L5:178:C:N4	2:L5:179:G:O6	2.47	0.47
2:L5:1176:C:H42	2:L5:1184:A:H61	1.61	0.47
2:L5:1776:A:P	85:CE:64:LEU:HD22	2.54	0.47
2:L5:4622:A:H4'	6:LB:13:SER:HB2	1.95	0.47
6:LB:14:LEU:HD22	6:LB:17:LEU:HD11	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LJ:58:ARG:CZ	85:CE:39:TRP:CE3	2.96	0.47
15:LL:110:LEU:O	15:LL:114:VAL:HG13	2.15	0.47
25:LV:43:LYS:HE2	25:LV:62:MET:HE3	1.95	0.47
63:Sg:212:LYS:HA	63:Sg:235:ILE:HG13	1.95	0.47
78:SY:105:LYS:O	78:SY:109:GLU:HG2	2.14	0.47
79:Sa:13:LYS:HD3	79:Sa:13:LYS:HA	1.71	0.47
82:S2:325:C:N3	82:S2:326:C:O2'	2.45	0.47
82:S2:1383:A2M:HM'3	82:S2:1383:A2M:H1'	1.64	0.47
2:L5:256:G:H2'	2:L5:257:C:C6	2.49	0.47
2:L5:519:C:H1'	2:L5:643:C:C2	2.49	0.47
2:L5:667:A:H5''	2:L5:668:C:H5''	1.96	0.47
2:L5:2029:A:H2'	2:L5:2030:A:C8	2.48	0.47
2:L5:4095:G:H2'	2:L5:4096:C:C6	2.50	0.47
2:L5:4149:C:OP1	29:LZ:59:LYS:N	2.47	0.47
4:L8:150:C:N4	11:LG:52:THR:O	2.47	0.47
10:LF:213:LEU:HB3	10:LF:247:MET:HG3	1.97	0.47
10:LF:241:ASN:O	10:LF:245:ARG:HG2	2.14	0.47
12:LH:89:ARG:HD3	12:LH:91:LYS:HE3	1.96	0.47
13:LI:36:LEU:HD11	13:LI:69:ARG:HD2	1.97	0.47
21:LR:157:ASP:OD1	21:LR:158:GLN:N	2.47	0.47
37:Lh:89:ARG:O	37:Lh:93:ARG:HG2	2.15	0.47
50:SF:19:LEU:HD11	50:SF:50:PRO:HD3	1.95	0.47
51:SK:42:ASN:HA	51:SK:45:VAL:HG12	1.96	0.47
63:Sg:133:ASN:HB3	63:Sg:139:LYS:HD2	1.97	0.47
68:SG:162:LEU:HG	68:SG:167:LYS:HE3	1.95	0.47
82:S2:1550:G:O2'	82:S2:1558:C:O2	2.25	0.47
2:L5:1461:C:H2'	2:L5:1462:A:H8	1.78	0.47
2:L5:1727:U:OP1	10:LF:131:ASN:ND2	2.46	0.47
2:L5:2811:G:N1	2:L5:2814:C:OP2	2.42	0.47
2:L5:4301:U:OP2	2:L5:4303:C:N4	2.47	0.47
14:LJ:55:TYR:CE1	85:CE:46:VAL:CG1	2.94	0.47
47:Ls:114:GLY:HA2	47:Ls:166:LYS:HD2	1.96	0.47
52:SM:110:VAL:O	52:SM:112:LYS:NZ	2.45	0.47
63:Sg:124:SER:OG	63:Sg:125:ARG:N	2.46	0.47
82:S2:223:C:H2'	82:S2:224:A:C8	2.50	0.47
82:S2:329:G:H2'	82:S2:330:G:H8	1.79	0.47
2:L5:97:G:OP1	15:LL:16:LYS:NZ	2.37	0.47
2:L5:170:C:H42	2:L5:266:C:N4	2.12	0.47
2:L5:2284:G:OP1	30:La:7:LYS:NZ	2.43	0.47
2:L5:2411:C:H2'	2:L5:2412:A:H8	1.78	0.47
2:L5:2580:U:OP1	29:LZ:36:ARG:NH1	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:2640:G:H2'	2:L5:2641:A:C8	2.50	0.47
2:L5:3917:A:H2'	2:L5:3918:G:H8	1.79	0.47
4:L8:75:OMG:HM23	4:L8:75:OMG:H1'	1.70	0.47
17:LN:140:LYS:HD3	17:LN:140:LYS:HA	1.66	0.47
47:Ls:139:GLN:HA	83:CB:180:ARG:CZ	2.44	0.47
54:SQ:102:GLU:HA	54:SQ:105:LYS:HB3	1.97	0.47
63:Sg:39:THR:HG22	63:Sg:60:ARG:HG2	1.96	0.47
67:SE:247:THR:OG1	67:SE:250:GLU:OE1	2.33	0.47
68:SG:191:ARG:HH22	82:S2:312:G:H2'	1.80	0.47
82:S2:17:C:H2'	82:S2:18:C:C6	2.49	0.47
82:S2:604:A:N3	82:S2:639:C:O2'	2.42	0.47
82:S2:996:A:H2'	82:S2:997:A:C8	2.49	0.47
83:CB:6:VAL:HA	83:CB:9:ILE:HB	1.96	0.47
83:CB:190:SER:HB2	83:CB:204:MET:HE2	1.96	0.47
2:L5:169:G:O6	2:L5:170:C:N4	2.48	0.47
2:L5:1194:G:H2'	2:L5:1195:G:C8	2.50	0.47
2:L5:3661:G:N7	5:LA:152:SER:OG	2.44	0.47
6:LB:29:VAL:HG12	6:LB:31:SER:H	1.80	0.47
23:LT:102:ARG:O	23:LT:106:LEU:HG	2.14	0.47
57:ST:83:GLN:OE1	57:ST:93:SER:OG	2.30	0.47
82:S2:747:U:C2	82:S2:796:G:N1	2.83	0.47
82:S2:1491:G:H2'	82:S2:1492:U:C6	2.49	0.47
2:L5:99:A:H5''	17:LN:184:ILE:HD12	1.96	0.47
2:L5:257:C:H2'	2:L5:258:G:C8	2.50	0.47
2:L5:1846:G:H2'	2:L5:1847:C:C6	2.49	0.47
2:L5:1855:G:OP1	31:Lb:4:SER:HB2	2.14	0.47
2:L5:1899:G:O2'	34:Le:57:ASN:OD1	2.31	0.47
2:L5:2910:G:N2	2:L5:3585:G:O2'	2.47	0.47
2:L5:3796:U:HO2'	82:S2:1720:U:HO2'	1.56	0.47
2:L5:4251:A:H5''	14:LJ:108:GLY:HA3	1.96	0.47
10:LF:57:TYR:OH	10:LF:189:ASP:OD1	2.30	0.47
12:LH:115:ARG:HD3	12:LH:123:ILE:HD12	1.96	0.47
20:LQ:154:LYS:NZ	20:LQ:159:PRO:O	2.46	0.47
46:Lr:119:ARG:HA	46:Lr:122:LYS:HE3	1.95	0.47
49:SD:32:ASP:OD2	49:SD:65:ARG:NH1	2.48	0.47
49:SD:77:PHE:HB2	49:SD:79:PHE:CE1	2.49	0.47
51:SK:32:HIS:HD2	51:SK:45:VAL:HG11	1.80	0.47
57:ST:84:ARG:NH1	82:S2:1605:G:OP1	2.41	0.47
62:Sf:105:TYR:HE1	62:Sf:131:PHE:HD2	1.62	0.47
66:SC:110:MET:HG2	66:SC:125:LYS:HB3	1.97	0.47
66:SC:227:ARG:NH2	82:S2:663:C:O2'	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SE:127:ARG:HG3	67:SE:142:HIS:HA	1.96	0.47
75:SV:74:LYS:HZ1	75:SV:83:PHE:HB3	1.80	0.47
82:S2:16:G:H2'	82:S2:17:C:C6	2.50	0.47
82:S2:349:A:H2'	82:S2:350:C:C6	2.49	0.47
82:S2:520:A:O2'	82:S2:825:A:N3	2.40	0.47
2:L5:1194:G:H2'	2:L5:1195:G:H8	1.80	0.47
2:L5:1877:G:O6	31:Lb:10:HIS:NE2	2.46	0.47
2:L5:1932:A:OP1	18:LO:49:ARG:NH2	2.27	0.47
9:LE:223:ARG:HB3	9:LE:224:LYS:HB2	1.96	0.47
10:LF:182:TYR:HB3	10:LF:200:ARG:HG3	1.96	0.47
12:LH:4:ILE:HG12	12:LH:61:TRP:CH2	2.50	0.47
16:LM:130:LEU:HB3	18:LO:177:LEU:HD11	1.96	0.47
20:LQ:50:ARG:HH21	20:LQ:140:SER:HB2	1.80	0.47
63:Sg:120:ILE:HB	63:Sg:132:TRP:HB2	1.97	0.47
65:SB:23:ASP:N	65:SB:23:ASP:OD1	2.48	0.47
70:SI:4:SER:OG	70:SI:6:ASP:OD2	2.26	0.47
82:S2:66:G:H2'	82:S2:67:C:H4'	1.97	0.47
82:S2:159:A2M:HM'3	82:S2:159:A2M:H1'	1.58	0.47
83:CB:653:GLY:HA2	83:CB:660:ASN:HB2	1.97	0.47
85:CE:56:LYS:O	85:CE:60:ARG:HD3	2.14	0.47
2:L5:715:G:OP1	7:LC:321:ASN:ND2	2.44	0.47
2:L5:2382:A:N1	2:L5:2829:U:O2'	2.45	0.47
2:L5:3923:A:H2'	2:L5:3924:C:C6	2.50	0.47
2:L5:4441:A:H5''	13:LI:114:GLY:HA2	1.97	0.47
2:L5:4606:G:P	83:CB:27:HIS:HE2	2.37	0.47
11:LG:154:LEU:HB3	11:LG:204:PHE:HB2	1.97	0.47
47:Ls:91:THR:HG21	47:Ls:98:ILE:HG13	1.97	0.47
71:SJ:64:ASP:OD1	71:SJ:65:GLU:N	2.48	0.47
79:Sa:87:ARG:NH1	79:Sa:94:ASP:OD1	2.48	0.47
81:Se:41:ARG:HG3	81:Se:42:PHE:HD1	1.80	0.47
81:Se:41:ARG:HG3	81:Se:42:PHE:CD1	2.50	0.47
82:S2:1144:A:H5'	82:S2:1355:C:H41	1.80	0.47
82:S2:1736:G:H2'	82:S2:1737:G:C8	2.49	0.47
2:L5:1298:C:H2'	2:L5:1299:G:C8	2.50	0.47
2:L5:2021:G:OP1	47:Ls:58:ASN:N	2.44	0.47
2:L5:3799:A:N3	2:L5:4506:C:O2'	2.42	0.47
2:L5:3841:OMC:HM23	2:L5:3841:OMC:H1'	1.76	0.47
2:L5:4742:G:H2'	2:L5:4743:G:H8	1.80	0.47
11:LG:162:ASP:HB3	11:LG:163:PRO:HD3	1.96	0.47
14:LJ:56:THR:OG1	14:LJ:64:ARG:N	2.44	0.47
50:SF:187:SER:OG	50:SF:190:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:SA:206:ASP:HB3	64:SA:209:GLU:OE1	2.15	0.47
82:S2:793:G:H2'	82:S2:794:A:H8	1.80	0.47
84:Et:51:G:H2'	84:Et:52:G:H8	1.81	0.47
2:L5:106:A:H2'	2:L5:107:G:O4'	2.15	0.46
2:L5:444:G:H2'	2:L5:445:U:C6	2.50	0.46
2:L5:1188:C:H2'	2:L5:1189:G:H8	1.80	0.46
2:L5:1333:A:H2'	2:L5:1334:A:H8	1.78	0.46
2:L5:1601:A:OP1	39:Lj:5:THR:OG1	2.22	0.46
2:L5:1995:G:H2'	2:L5:1996:C:C6	2.50	0.46
2:L5:2299:G:O6	7:LC:188:ARG:NH2	2.48	0.46
2:L5:3908:A:N7	2:L5:4449:A:N6	2.63	0.46
2:L5:4954:G:H2'	2:L5:4955:A:C8	2.49	0.46
5:LA:206:PRO:HG3	5:LA:213:GLY:HA3	1.96	0.46
8:LD:205:ALA:HB1	8:LD:233:PRO:HB3	1.97	0.46
17:LN:75:VAL:HG21	17:LN:80:THR:HG22	1.97	0.46
49:SD:115:VAL:HG21	49:SD:138:VAL:HG11	1.97	0.46
54:SQ:8:GLN:HG3	54:SQ:27:ARG:HE	1.80	0.46
63:Sg:289:LEU:HD11	63:Sg:298:LEU:HD21	1.97	0.46
78:SY:77:ASP:OD1	78:SY:77:ASP:N	2.47	0.46
82:S2:51:U:H2'	82:S2:52:G:C8	2.50	0.46
82:S2:454:U:H2'	82:S2:455:A:H8	1.80	0.46
82:S2:656:G:N2	82:S2:663:C:H5''	2.30	0.46
82:S2:656:G:H5'	82:S2:662:G:N2	2.30	0.46
82:S2:1692:U:H2'	82:S2:1693:G:C8	2.50	0.46
83:CB:207:PRO:HG2	83:CB:261:TRP:CE2	2.50	0.46
2:L5:497:G:H21	2:L5:498:C:H41	1.63	0.46
2:L5:2298:U:OP1	7:LC:204:ARG:NE	2.47	0.46
2:L5:2637:U:HO2'	2:L5:2718:U:HO2'	1.62	0.46
2:L5:3950:U:H3	2:L5:4063:U:H3	1.62	0.46
2:L5:4504:C:H2'	2:L5:4505:C:C6	2.50	0.46
20:LQ:3:VAL:HG13	20:LQ:5:ILE:HG12	1.97	0.46
32:Lc:47:ILE:HD12	32:Lc:94:LEU:HD11	1.96	0.46
49:SD:223:ILE:HD11	63:Sg:189:ILE:HD12	1.97	0.46
51:SK:7:ASN:HB2	51:SK:40:VAL:HG22	1.98	0.46
64:SA:102:ARG:NH1	82:S2:1378:A:OP2	2.46	0.46
66:SC:70:VAL:HG21	66:SC:93:ILE:HG23	1.97	0.46
68:SG:85:ARG:O	68:SG:87:ARG:NH1	2.49	0.46
82:S2:528:A:H2'	82:S2:529:A:C8	2.50	0.46
82:S2:1286:G:N2	82:S2:1312:G:O2'	2.49	0.46
82:S2:1337:4AC:H2'	82:S2:1338:G:C8	2.50	0.46
2:L5:907:C:H2'	2:L5:908:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:908:G:H2'	2:L5:909:A:H8	1.79	0.46
2:L5:1308:C:OP1	18:LO:93:LYS:NZ	2.46	0.46
2:L5:1408:G:O2'	2:L5:1411:C:N4	2.48	0.46
2:L5:1696:C:H5'	2:L5:1719:A:H1'	1.97	0.46
2:L5:2009:A:C8	83:CB:756:VAL:HG11	2.49	0.46
2:L5:2725:A:N6	21:LR:88:ARG:O	2.48	0.46
2:L5:4115:G:O2'	2:L5:4116:C:O5'	2.32	0.46
11:LG:83:PHE:HA	11:LG:183:ILE:HD13	1.97	0.46
18:LO:166:ILE:HG12	18:LO:169:ARG:HH21	1.80	0.46
19:LP:122:ALA:HB3	19:LP:143:PRO:HG2	1.97	0.46
34:Le:76:LYS:HD2	34:Le:98:GLU:CD	2.41	0.46
54:SQ:139:ALA:HB2	82:S2:1650:A:H5''	1.96	0.46
57:ST:42:HIS:NE2	57:ST:43:LYS:HE3	2.30	0.46
57:ST:114:GLU:OE1	57:ST:114:GLU:N	2.47	0.46
77:SX:90:CYS:HA	77:SX:93:PHE:HD2	1.79	0.46
82:S2:51:U:H2'	82:S2:52:G:H8	1.81	0.46
82:S2:468:A2M:HM'3	82:S2:468:A2M:H1'	1.68	0.46
82:S2:693:A:H2'	82:S2:694:G:C8	2.51	0.46
82:S2:962:A:N1	82:S2:1055:A:O2'	2.47	0.46
82:S2:1755:C:H2'	82:S2:1756:C:C6	2.51	0.46
83:CB:132:VAL:HG13	83:CB:167:LEU:HD11	1.97	0.46
2:L5:965:G:N2	2:L5:2092:G:H1'	2.30	0.46
14:LJ:83:LEU:HD22	14:LJ:132:VAL:HG11	1.97	0.46
16:LM:96:GLU:O	16:LM:100:ARG:HG2	2.15	0.46
25:LV:42:VAL:HB	25:LV:45:ILE:HG13	1.98	0.46
61:Sd:14:PHE:HB2	82:S2:1661:A:H8	1.81	0.46
65:SB:186:ASN:HA	65:SB:189:ILE:HD12	1.98	0.46
67:SE:100:ARG:NH2	67:SE:118:GLU:OE2	2.48	0.46
69:SH:145:ARG:HE	76:SW:51:GLU:HB2	1.81	0.46
82:S2:598:G:O2'	82:S2:605:A:N1	2.46	0.46
82:S2:1189:A:H2'	82:S2:1190:A:H8	1.81	0.46
82:S2:1656:G:H1	82:S2:1668:U:H3	1.63	0.46
83:CB:219:HIS:HB2	83:CB:221:TRP:CD1	2.50	0.46
2:L5:2111:G:N2	2:L5:2251:G:O2'	2.48	0.46
2:L5:2112:G:H5''	2:L5:2251:G:H1	1.79	0.46
2:L5:3796:U:O2'	82:S2:1720:U:O2'	2.26	0.46
33:Ld:53:ALA:HA	33:Ld:88:LEU:HD21	1.97	0.46
50:SF:103:LEU:HD11	59:SZ:67:LEU:HD22	1.97	0.46
55:SR:52:GLY:O	55:SR:55:THR:OG1	2.33	0.46
62:Sf:124:ASP:OD1	62:Sf:124:ASP:N	2.45	0.46
68:SG:2:LYS:HB3	68:SG:15:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:SJ:145:PRO:HD2	82:S2:522:A:H5''	1.98	0.46
73:SN:5:HIS:HB3	73:SN:117:LEU:HD13	1.98	0.46
82:S2:1643:U:H2'	82:S2:1644:C:C6	2.50	0.46
2:L5:300:A:H2'	2:L5:301:G:H8	1.81	0.46
2:L5:1414:C:H2'	2:L5:1415:G:C8	2.47	0.46
2:L5:1695:U:O2'	2:L5:1719:A:N3	2.39	0.46
2:L5:4476:C:O2'	2:L5:4478:G:OP2	2.26	0.46
2:L5:4543:G:H2'	2:L5:4544:A:C8	2.50	0.46
4:L8:96:C:H5''	37:Lh:66:LYS:HG2	1.98	0.46
9:LE:161:ARG:O	9:LE:182:ASN:ND2	2.49	0.46
10:LF:46:ARG:HH21	31:Lb:102:PRO:HG3	1.81	0.46
32:Lc:48:LEU:HD13	32:Lc:57:LYS:HG3	1.98	0.46
47:Ls:139:GLN:HE22	83:CB:180:ARG:CA	2.19	0.46
60:Sc:10:LYS:HE2	60:Sc:34:PHE:HD2	1.81	0.46
70:SI:141:ARG:NH2	82:S2:192:C:OP2	2.49	0.46
70:SI:149:TYR:O	70:SI:153:LYS:HG2	2.16	0.46
76:SW:27:ILE:HG13	76:SW:61:ILE:HB	1.97	0.46
80:Sb:68:GLY:O	82:S2:928:G:N2	2.44	0.46
83:CB:164:LEU:HD21	83:CB:174:LEU:HD22	1.98	0.46
2:L5:455:C:O2'	2:L5:456:C:H5'	2.15	0.46
2:L5:1390:G:N2	2:L5:1393:G:OP2	2.40	0.46
2:L5:3867:A2M:HM'3	2:L5:3867:A2M:H1'	1.65	0.46
6:LB:302:ASN:HB2	6:LB:313:SER:HA	1.98	0.46
50:SF:127:ARG:HG2	50:SF:136:ARG:HB2	1.98	0.46
56:SS:137:LYS:NZ	82:S2:1236:G:O6	2.49	0.46
63:Sg:10:THR:HG22	63:Sg:308:ARG:HG2	1.97	0.46
64:SA:184:ARG:HG2	64:SA:189:ILE:HB	1.97	0.46
65:SB:136:ARG:HB3	65:SB:216:LYS:HG3	1.96	0.46
65:SB:214:LYS:NZ	82:S2:943:U:OP1	2.39	0.46
69:SH:126:HIS:CE1	69:SH:181:THR:HG23	2.51	0.46
77:SX:52:LEU:HD11	77:SX:73:GLN:HB2	1.97	0.46
82:S2:5:U:H2'	82:S2:6:G:C8	2.51	0.46
82:S2:327:G:H5''	82:S2:328:U:C2	2.50	0.46
82:S2:1775:U:H2'	82:S2:1776:G:C2	2.51	0.46
2:L5:4088:C:H2'	2:L5:4089:G:C8	2.51	0.46
7:LC:183:VAL:HA	7:LC:204:ARG:HB3	1.97	0.46
26:LW:7:SER:HB2	26:LW:13:ILE:HD11	1.97	0.46
28:LY:10:ASP:HB3	28:LY:13:LYS:HB2	1.98	0.46
30:La:72:THR:HG22	30:La:110:LYS:HB3	1.98	0.46
48:Lt:31:LYS:CB	83:CB:773:GLU:O	2.64	0.46
66:SC:121:ARG:HH12	66:SC:123:ARG:HE	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:SC:271:ASP:OD1	66:SC:272:HIS:N	2.49	0.46
67:SE:134:LYS:N	82:S2:298:G:OP1	2.45	0.46
69:SH:30:LEU:HG	69:SH:33:ASN:HD22	1.81	0.46
70:SI:126:GLY:O	70:SI:128:LYS:NZ	2.48	0.46
82:S2:102:A:H4'	82:S2:104:A:C8	2.51	0.46
82:S2:1189:A:H2'	82:S2:1190:A:C8	2.51	0.46
83:CB:89:ILE:HG12	83:CB:356:ILE:HA	1.97	0.46
2:L5:162:A:H2'	2:L5:163:A:C8	2.51	0.46
2:L5:1647:U:OP1	88:L5:5288:SPD:H51	2.16	0.46
2:L5:2474:G:H2'	2:L5:2502:G:N2	2.30	0.46
5:LA:116:LEU:HB3	5:LA:126:LEU:HB2	1.96	0.46
9:LE:261:ILE:HG23	9:LE:267:LEU:HD23	1.97	0.46
48:Lt:28:LEU:HD23	48:Lt:28:LEU:H	1.81	0.46
50:SF:132:GLY:C	84:Et:39:U:O2'	2.59	0.46
54:SQ:37:ARG:NH2	82:S2:1543:U:OP1	2.39	0.46
56:SS:37:GLY:N	82:S2:1630:A:H5'	2.31	0.46
68:SG:4:ASN:ND2	82:S2:154:U:O2	2.47	0.46
70:SI:98:LYS:HG3	70:SI:178:ARG:HG2	1.98	0.46
76:SW:62:VAL:HG11	80:Sb:8:LEU:HG	1.97	0.46
78:SY:76:TYR:OH	78:SY:86:GLU:OE1	2.19	0.46
82:S2:420:G:O2'	82:S2:660:C:N3	2.45	0.46
2:L5:197:A:N1	2:L5:225:G:O2'	2.47	0.46
2:L5:233:U:HO2'	2:L5:234:G:H8	1.63	0.46
2:L5:417:G:OP1	2:L5:2329:U:O2'	2.28	0.46
2:L5:1398:A:N1	2:L5:1419:G:O2'	2.48	0.46
2:L5:1725:U:H2'	2:L5:1726:U:H6	1.81	0.46
2:L5:2033:A:OP1	13:LI:162:ARG:NH2	2.46	0.46
87:L5:5290:SPM:H31	87:L5:5290:SPM:H62	1.79	0.46
3:L7:120:U:H5''	8:LD:262:LYS:HG2	1.96	0.46
8:LD:181:PRO:HD2	8:LD:195:HIS:CD2	2.51	0.46
10:LF:162:ILE:HD12	10:LF:167:ILE:HB	1.98	0.46
19:LP:52:THR:HG23	19:LP:85:LYS:HG3	1.98	0.46
35:Lf:45:LYS:NZ	35:Lf:108:SER:HA	2.31	0.46
36:Lg:82:MET:HE3	36:Lg:82:MET:HB2	1.88	0.46
46:Lr:47:LYS:O	46:Lr:103:ARG:HD2	2.16	0.46
52:SM:87:GLU:HG3	52:SM:103:VAL:HG11	1.98	0.46
67:SE:59:ASP:O	67:SE:63:LYS:HG3	2.16	0.46
69:SH:33:ASN:ND2	69:SH:36:LEU:HB3	2.30	0.46
70:SI:44:HIS:ND1	82:S2:1740:C:OP1	2.38	0.46
82:S2:1420:G:O2'	82:S2:1421:A:N3	2.49	0.46
82:S2:1667:U:H2'	82:S2:1668:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:659:G:H2'	2:L5:660:A:C8	2.50	0.45
2:L5:1340:OMC:HM23	2:L5:1340:OMC:H1'	1.75	0.45
2:L5:2580:U:O2'	29:LZ:79:HIS:ND1	2.44	0.45
2:L5:2724:G:O2'	2:L5:2726:G:OP2	2.31	0.45
8:LD:179:ARG:HD3	8:LD:179:ARG:HA	1.72	0.45
11:LG:187:LYS:HB2	11:LG:198:THR:HG23	1.97	0.45
64:SA:74:VAL:HG23	64:SA:121:LEU:HB3	1.97	0.45
72:SL:132:ARG:HD3	82:S2:114:G:H5'	1.97	0.45
77:SX:60:LYS:H	77:SX:114:ASP:HB2	1.81	0.45
2:L5:4389:C:H2'	2:L5:4390:A:C8	2.51	0.45
2:L5:4775:C:H41	2:L5:4859:C:N4	2.14	0.45
2:L5:5004:C:H2'	2:L5:5005:G:O4'	2.15	0.45
5:LA:114:CYS:N	5:LA:165:VAL:O	2.49	0.45
12:LH:93:ARG:HG2	12:LH:182:SER:HB3	1.97	0.45
21:LR:175:GLU:O	21:LR:178:GLN:HG3	2.17	0.45
53:SP:22:LEU:HA	53:SP:25:LEU:HB2	1.99	0.45
57:ST:6:VAL:HG12	57:ST:135:ALA:HB2	1.99	0.45
81:Se:31:ARG:NH2	82:S2:525:A:O3'	2.49	0.45
82:S2:115:U:H2'	82:S2:116:OMU:C6	2.46	0.45
82:S2:1010:G:H2'	82:S2:1011:A:H8	1.81	0.45
83:CB:531:ASP:HB3	83:CB:534:VAL:HG12	1.98	0.45
2:L5:150:U:OP2	11:LG:200:THR:OG1	2.27	0.45
2:L5:498:C:C2	2:L5:499:G:H1'	2.51	0.45
2:L5:2009:A:N6	83:CB:782:PHE:HZ	2.14	0.45
2:L5:3856:A:H5''	19:LP:83:TRP:O	2.16	0.45
2:L5:4401:G:H2'	2:L5:4402:C:H6	1.80	0.45
14:LJ:15:LEU:HD12	14:LJ:165:TRP:HB2	1.98	0.45
26:LW:19:ARG:NH2	26:LW:37:GLU:OE2	2.50	0.45
29:LZ:123:LYS:O	29:LZ:124:THR:OG1	2.24	0.45
47:Ls:18:ILE:HD12	47:Ls:21:LEU:HD11	1.98	0.45
53:SP:81:ARG:NH1	53:SP:120:SER:OG	2.49	0.45
63:Sg:21:ILE:HG21	63:Sg:299:PHE:HB2	1.98	0.45
69:SH:18:GLU:OE1	69:SH:18:GLU:N	2.49	0.45
70:SI:56:ARG:HA	70:SI:180:GLY:HA2	1.98	0.45
82:S2:932:G:O2'	82:S2:934:G:OP2	2.28	0.45
82:S2:1240:A:N3	82:S2:1267:C:O2'	2.41	0.45
83:CB:18:ASN:HB3	83:CB:98:PHE:HD1	1.81	0.45
2:L5:318:A:H2'	2:L5:319:A:C8	2.52	0.45
2:L5:1494:U:H2'	2:L5:1495:G:H8	1.81	0.45
2:L5:3595:U:H5''	2:L5:3597:G:OP2	2.16	0.45
6:LB:258:HIS:HA	6:LB:260:ALA:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LE:222:LEU:HB2	9:LE:237:LYS:HD2	1.97	0.45
11:LG:73:ARG:HD3	11:LG:73:ARG:HA	1.81	0.45
18:LO:61:ARG:HA	18:LO:70:PRO:HD2	1.98	0.45
57:ST:72:VAL:O	57:ST:76:THR:HG23	2.16	0.45
68:SG:170:ARG:NH1	82:S2:72:C:O2	2.50	0.45
83:CB:428:ARG:HG2	83:CB:444:LEU:HD13	1.99	0.45
2:L5:252:C:H2'	2:L5:253:G:H8	1.82	0.45
2:L5:1269:G:O2'	2:L5:1270:A:O4'	2.30	0.45
2:L5:1733:G:N3	2:L5:4214:A:H2'	2.31	0.45
2:L5:2072:C:OP1	20:LQ:2:GLY:N	2.50	0.45
2:L5:4508:C:N3	2:L5:4512:U:H5	2.14	0.45
2:L5:4536:OMC:HM22	2:L5:4537:C:O4'	2.17	0.45
4:L8:66:A:H2'	4:L8:67:U:C6	2.51	0.45
4:L8:67:U:H2'	4:L8:68:G:H8	1.81	0.45
8:LD:108:ARG:CZ	8:LD:253:TYR:HB2	2.47	0.45
33:Ld:114:PHE:HA	33:Ld:117:LEU:HD12	1.99	0.45
47:Ls:29:ILE:HD11	47:Ls:191:GLN:HG2	1.97	0.45
54:SQ:98:LYS:O	63:Sg:57:ARG:NH1	2.38	0.45
56:SS:63:GLU:O	56:SS:67:VAL:HG23	2.17	0.45
61:Sd:8:TRP:HZ3	82:S2:1512:C:H5''	1.82	0.45
63:Sg:17:TRP:HB2	63:Sg:36:ARG:HD3	1.98	0.45
66:SC:104:ASP:OD1	66:SC:105:GLU:N	2.49	0.45
68:SG:49:VAL:HB	68:SG:115:LYS:HG2	1.97	0.45
78:SY:68:LYS:HE2	78:SY:68:LYS:HB3	1.78	0.45
80:Sb:42:LYS:HE3	80:Sb:57:VAL:HG22	1.98	0.45
82:S2:1221:G:O2'	82:S2:1676:U:O2	2.33	0.45
2:L5:303:C:OP2	17:LN:68:ARG:NH2	2.44	0.45
2:L5:327:U:HO2'	38:Li:30:ARG:HH11	1.60	0.45
2:L5:1577:G:O2'	2:L5:1612:G:H4'	2.16	0.45
2:L5:1912:G:N2	18:LO:87:MET:HE2	2.32	0.45
2:L5:2306:G:H1'	2:L5:2332:A:N6	2.32	0.45
2:L5:2611:A:H2'	2:L5:2612:G:C8	2.51	0.45
2:L5:3861:A:H2'	2:L5:3862:A:C8	2.52	0.45
2:L5:3932:U:H2'	2:L5:3933:G:C8	2.52	0.45
2:L5:4345:C:H2'	2:L5:4346:U:H6	1.81	0.45
2:L5:4775:C:H41	2:L5:4859:C:H42	1.65	0.45
5:LA:28:ARG:HD2	5:LA:123:ARG:HG3	1.99	0.45
37:Lh:95:LEU:HD22	37:Lh:99:GLU:HG3	1.97	0.45
48:Lt:34:PRO:HG3	83:CB:775:GLN:O	1.98	0.45
50:SF:132:GLY:C	84:Et:39:U:H4'	2.41	0.45
54:SQ:97:GLN:HB2	54:SQ:105:LYS:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:SR:99:ASP:OD2	64:SA:42:LYS:NZ	2.31	0.45
64:SA:42:LYS:HD3	64:SA:46:ILE:HB	1.98	0.45
68:SG:7:PHE:CE2	68:SG:9:ALA:HB3	2.51	0.45
77:SX:142:ARG:CG	83:CB:443:TYR:OH	2.65	0.45
81:Se:12:VAL:HG23	82:S2:616:A:H1'	1.97	0.45
82:S2:525:A:H2'	82:S2:526:A:C8	2.51	0.45
82:S2:563:G:O2'	82:S2:564:A:OP1	2.33	0.45
82:S2:929:G:H2'	82:S2:930:C:O4'	2.17	0.45
83:CB:23:SER:HB3	83:CB:122:THR:HG21	1.98	0.45
2:L5:162:A:H2'	2:L5:163:A:H8	1.81	0.45
2:L5:381:U:H4'	2:L5:415:G:H5'	1.98	0.45
2:L5:1811:G:H21	31:Lb:57:MET:HE2	1.82	0.45
2:L5:2846:G:O2'	25:LV:19:GLY:O	2.28	0.45
2:L5:3664:G:H2'	2:L5:3665:G:C8	2.52	0.45
2:L5:3726:A:H2'	2:L5:3727:A:C8	2.51	0.45
2:L5:4587:G:OP1	18:LO:61:ARG:NH1	2.46	0.45
6:LB:50:LYS:NZ	6:LB:337:VAL:O	2.47	0.45
8:LD:152:ARG:HG3	8:LD:154:THR:HG23	1.99	0.45
10:LF:37:PHE:HZ	31:Lb:113:ALA:HB1	1.82	0.45
10:LF:182:TYR:CZ	10:LF:203:GLU:HG2	2.52	0.45
38:Li:35:LYS:HE3	38:Li:35:LYS:HB3	1.81	0.45
49:SD:55:THR:HA	49:SD:58:VAL:HG12	1.98	0.45
81:Se:8:ARG:HG2	81:Se:11:LYS:HD3	1.99	0.45
82:S2:29:G:H2'	82:S2:30:C:C6	2.52	0.45
82:S2:629:A:O2'	82:S2:631:U:OP1	2.34	0.45
82:S2:1201:U:H2'	82:S2:1202:U:C6	2.52	0.45
82:S2:1231:C:O2'	82:S2:1253:A:N6	2.50	0.45
82:S2:1232:PSU:H2'	82:S2:1233:G:C8	2.52	0.45
82:S2:1736:G:H2'	82:S2:1737:G:H8	1.82	0.45
82:S2:1825:A:H62	83:CB:717:GLY:HA3	0.60	0.45
83:CB:316:ILE:HA	83:CB:321:ILE:HD12	1.98	0.45
85:CE:35:GLU:HA	85:CE:38:TYR:HB3	1.98	0.45
2:L5:1613:A:H5''	5:LA:183:GLY:CA	2.47	0.45
2:L5:2521:G:H4'	36:Lg:26:PRO:HD2	1.98	0.45
2:L5:4315:A:OP1	23:LT:69:GLN:NE2	2.47	0.45
2:L5:4524:G:C2	6:LB:252:ALA:HB1	2.52	0.45
16:LM:24:LEU:HB2	16:LM:43:THR:HG21	1.99	0.45
21:LR:19:LYS:HB2	21:LR:19:LYS:HE2	1.82	0.45
53:SP:24:GLN:O	53:SP:28:MET:HB2	2.16	0.45
55:SR:29:HIS:HA	55:SR:32:LYS:HG2	1.99	0.45
56:SS:62:ASP:OD1	56:SS:62:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SS:121:ARG:HG3	56:SS:131:VAL:HB	1.99	0.45
57:ST:39:LEU:HA	57:ST:39:LEU:HD23	1.74	0.45
59:SZ:91:LEU:HG	59:SZ:96:LEU:HD21	1.99	0.45
64:SA:145:ILE:HG12	64:SA:159:ILE:HB	1.98	0.45
69:SH:142:LYS:HB3	76:SW:54:ASP:HB3	1.98	0.45
80:Sb:42:LYS:HZ1	80:Sb:58:GLY:H	1.65	0.45
83:CB:160:MET:HE3	83:CB:174:LEU:HD21	1.99	0.45
83:CB:516:ASP:HA	83:CB:519:LYS:HE2	1.97	0.45
83:CB:603:TYR:HE2	83:CB:708:THR:HG23	1.81	0.45
2:L5:2676:A:OP2	2:L5:2676:A:H8	2.00	0.45
2:L5:4093:G:H3'	2:L5:4094:G:H8	1.82	0.45
20:LQ:32:TYR:HD2	20:LQ:51:LEU:HD11	1.80	0.45
32:Lc:65:MET:HE3	32:Lc:65:MET:HB3	1.90	0.45
48:Lt:81:ILE:HD13	48:Lt:113:ALA:HB1	1.99	0.45
53:SP:130:ARG:NH1	83:CB:858:LEU:HD21	2.00	0.45
68:SG:67:VAL:HG12	68:SG:69:THR:HG22	1.99	0.45
73:SN:83:ASP:OD1	73:SN:84:LEU:N	2.49	0.45
77:SX:105:PHE:CE2	77:SX:112:VAL:HB	2.51	0.45
85:CE:50:GLU:HA	85:CE:53:LYS:HE3	1.98	0.45
2:L5:424:U:H2'	2:L5:425:U:C6	2.52	0.45
2:L5:3611:A:C2	2:L5:5016:A:H8	2.34	0.45
6:LB:113:GLU:OE2	6:LB:169:ARG:NH1	2.50	0.45
12:LH:8:GLN:HG2	12:LH:74:CYS:SG	2.57	0.45
13:LI:52:MET:HE3	13:LI:163:GLN:HG2	1.99	0.45
37:Lh:107:GLN:O	37:Lh:111:GLU:HG3	2.17	0.45
64:SA:6:ASP:OD1	64:SA:6:ASP:N	2.49	0.45
67:SE:10:LYS:NZ	82:S2:95:G:OP1	2.33	0.45
82:S2:563:G:HO2'	82:S2:564:A:P	2.39	0.45
82:S2:1259:A:N6	82:S2:1519:U:O5'	2.50	0.45
2:L5:965:G:H21	2:L5:2092:G:H1'	1.82	0.44
2:L5:1895:G:OP1	10:LF:96:ARG:NH2	2.47	0.44
2:L5:4742:G:OP1	2:L5:4900:C:N4	2.35	0.44
15:LL:126:LEU:N	15:LL:138:ASP:OD2	2.27	0.44
19:LP:5:SER:OG	19:LP:118:GLN:NE2	2.50	0.44
27:LX:121:VAL:HA	27:LX:140:LEU:HA	1.99	0.44
54:SQ:98:LYS:HE3	54:SQ:99:TYR:CZ	2.53	0.44
63:Sg:62:HIS:NE2	63:Sg:80:SER:OG	2.35	0.44
68:SG:87:ARG:HD3	68:SG:87:ARG:HA	1.70	0.44
82:S2:674:C:H2'	82:S2:675:U:C6	2.52	0.44
82:S2:1139:C:H5	82:S2:1149:A:H62	1.66	0.44
82:S2:1217:A:H2'	82:S2:1218:C:C6	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:S2:1681:U:H2'	82:S2:1682:C:C6	2.51	0.44
2:L5:197:A:N3	2:L5:222:C:O2'	2.49	0.44
2:L5:4302:U:H4'	23:LT:5:LYS:HD3	2.00	0.44
7:LC:150:LEU:O	7:LC:152:LEU:N	2.50	0.44
15:LL:55:ILE:O	15:LL:97:SER:OG	2.32	0.44
33:Ld:54:MET:HE3	33:Ld:60:PRO:HA	1.98	0.44
47:Ls:52:VAL:HG12	47:Ls:90:PHE:HB2	1.99	0.44
63:Sg:191:HIS:ND1	63:Sg:195:LEU:HD21	2.32	0.44
65:SB:29:ASP:OD1	65:SB:29:ASP:N	2.51	0.44
65:SB:145:LYS:HB2	65:SB:145:LYS:HE3	1.73	0.44
74:SO:149:ARG:NH2	82:S2:961:G:OP1	2.50	0.44
77:SX:28:LYS:NZ	82:S2:1189:A:OP1	2.40	0.44
82:S2:99:A2M:H8	82:S2:99:A2M:O5'	2.18	0.44
82:S2:576:A2M:HM'3	82:S2:576:A2M:H1'	1.82	0.44
82:S2:1084:A:OP1	82:S2:1858:G:O2'	2.28	0.44
83:CB:654:PRO:HD2	83:CB:658:GLY:HA3	1.98	0.44
2:L5:423:G:H5'	19:LP:26:PHE:HZ	1.83	0.44
2:L5:684:G:H5''	9:LE:100:LYS:HE3	1.99	0.44
2:L5:2079:G:H2'	2:L5:2080:U:C6	2.53	0.44
2:L5:4274:A:H2'	2:L5:4275:G:H8	1.82	0.44
2:L5:4291:G:H5'	2:L5:4293:PSU:C6	2.52	0.44
2:L5:4524:G:N3	6:LB:252:ALA:HB1	2.32	0.44
5:LA:131:GLY:H	5:LA:169:VAL:HG13	1.82	0.44
20:LQ:86:ILE:HD11	20:LQ:100:VAL:HG11	1.98	0.44
21:LR:176:ARG:NH1	21:LR:177:LEU:HG	2.33	0.44
33:Ld:57:MET:HG2	33:Ld:88:LEU:HD23	2.00	0.44
51:SK:31:LYS:HZ3	51:SK:39:ASN:N	2.15	0.44
56:SS:38:ARG:HD2	57:ST:45:LEU:HD11	1.99	0.44
57:ST:39:LEU:HD21	57:ST:52:TRP:CZ3	2.53	0.44
58:SU:19:ARG:HB3	58:SU:92:HIS:CD2	2.53	0.44
59:SZ:86:ALA:HA	59:SZ:89:GLN:HE21	1.81	0.44
63:Sg:268:ASP:OD1	63:Sg:269:GLU:N	2.50	0.44
67:SE:101:LEU:HD12	67:SE:101:LEU:HA	1.85	0.44
82:S2:1850:MA6:H8	82:S2:1850:MA6:O5'	2.18	0.44
83:CB:219:HIS:CE1	83:CB:337:LYS:HE2	2.51	0.44
2:L5:4456:OMC:HM21	6:LB:241:PRO:HD3	1.99	0.44
2:L5:4594:U:H2'	2:L5:4595:G:C8	2.48	0.44
9:LE:183:ARG:HA	9:LE:183:ARG:HD2	1.80	0.44
13:LI:101:LYS:NZ	13:LI:102:MET:O	2.48	0.44
15:LL:140:SER:HA	15:LL:143:GLU:HG2	1.99	0.44
25:LV:107:ASN:ND2	25:LV:111:GLU:OE2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Lm:79:GLU:CD	42:Lm:81:SER:HG	2.21	0.44
53:SP:37:TYR:HB3	53:SP:41:GLN:HB2	1.98	0.44
55:SR:35:CYS:HA	55:SR:38:ILE:HG12	1.99	0.44
64:SA:18:PHE:CD1	64:SA:23:THR:HG21	2.51	0.44
68:SG:136:LYS:HB2	82:S2:65:C:H41	1.83	0.44
82:S2:27:A2M:HM'3	82:S2:27:A2M:H1'	1.63	0.44
82:S2:830:A:OP2	82:S2:846:G:N2	2.50	0.44
83:CB:225:LEU:HB2	83:CB:257:MET:HE3	1.99	0.44
2:L5:72:C:H5	15:LL:67:HIS:HD1	1.64	0.44
2:L5:138:G:H2'	2:L5:139:G:C8	2.52	0.44
2:L5:662:C:H2'	2:L5:663:G:H8	1.83	0.44
2:L5:979:C:OP2	9:LE:66:LYS:HD3	2.17	0.44
2:L5:1282:G:OP2	9:LE:128:HIS:NE2	2.51	0.44
2:L5:1537:A:H2'	2:L5:1538:U:C6	2.53	0.44
2:L5:1751:A:H2'	2:L5:1752:G:C8	2.53	0.44
2:L5:2347:A:C4	34:Le:31:ILE:HD11	2.53	0.44
2:L5:2570:U:H2'	2:L5:2571:C:C6	2.53	0.44
11:LG:143:VAL:HG22	11:LG:203:ALA:HB2	1.99	0.44
49:SD:27:ARG:NH1	82:S2:1498:A:OP2	2.42	0.44
50:SF:131:ALA:O	84:Et:39:U:O4'	2.33	0.44
72:SL:127:THR:HB	72:SL:144:LYS:HB3	1.99	0.44
82:S2:136:C:H5''	82:S2:137:U:H5''	2.00	0.44
82:S2:194:C:H2'	82:S2:195:C:H6	1.83	0.44
82:S2:835:C:H4'	82:S2:836:G:C8	2.53	0.44
82:S2:1215:C:O2'	82:S2:1645:C:OP2	2.34	0.44
82:S2:1628:C:H2'	82:S2:1629:C:C6	2.51	0.44
82:S2:1801:A:H2'	82:S2:1802:C:H6	1.82	0.44
83:CB:10:ARG:HH22	83:CB:420:LEU:HD11	1.83	0.44
2:L5:1327:C:H2'	2:L5:1328:G:C8	2.53	0.44
2:L5:1818:G:O2'	2:L5:1820:C:OP2	2.27	0.44
2:L5:2864:A:H2'	2:L5:2865:U:C6	2.52	0.44
2:L5:4126:C:OP1	11:LG:37:LYS:NZ	2.51	0.44
7:LC:334:THR:HG22	7:LC:337:ARG:HH21	1.82	0.44
9:LE:198:SER:OG	9:LE:288:PHE:O	2.25	0.44
12:LH:187:VAL:HG12	12:LH:188:GLN:HG3	2.00	0.44
13:LI:48:LEU:O	13:LI:139:ARG:HA	2.17	0.44
47:Ls:139:GLN:O	83:CB:180:ARG:NH1	2.50	0.44
49:SD:163:PRO:O	49:SD:167:TYR:HB2	2.18	0.44
62:Sf:85:TYR:CA	83:CB:647:ARG:HH22	2.30	0.44
82:S2:1037:G:H4'	82:S2:1845:A:H4'	1.98	0.44
82:S2:1653:U:H2'	82:S2:1654:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:CB:176:GLN:O	83:CB:180:ARG:HG2	2.18	0.44
84:Et:51:G:H2'	84:Et:52:G:C8	2.52	0.44
2:L5:132:G:H2'	2:L5:133:C:H4'	1.99	0.44
2:L5:268:G:H2'	2:L5:269:G:C8	2.52	0.44
2:L5:1359:G:H4'	17:LN:203:TYR:HB2	2.00	0.44
2:L5:1662:C:H2'	2:L5:1663:C:H6	1.83	0.44
2:L5:2848:G:O2'	2:L5:3838:U:O4	2.25	0.44
2:L5:3813:A:N3	2:L5:4538:G:O2'	2.45	0.44
2:L5:3932:U:H2'	2:L5:3933:G:H8	1.83	0.44
6:LB:165:HIS:HA	6:LB:179:HIS:O	2.17	0.44
9:LE:99:ASP:OD1	9:LE:99:ASP:N	2.50	0.44
36:Lg:69:LYS:HG3	36:Lg:73:HIS:CD2	2.53	0.44
44:Lo:74:GLU:HB3	44:Lo:77:CYS:HB3	2.00	0.44
47:Ls:139:GLN:HE21	83:CB:183:GLU:HB2	1.76	0.44
53:SP:34:MET:HB3	53:SP:42:ARG:HG3	1.98	0.44
58:SU:87:ARG:HH22	82:S2:1447:G:P	2.41	0.44
64:SA:220:LYS:HA	64:SA:220:LYS:HD3	1.84	0.44
68:SG:147:LEU:HD12	68:SG:151:ASP:HB2	2.00	0.44
69:SH:37:LYS:HA	69:SH:40:LEU:HB3	1.99	0.44
74:SO:101:GLY:HA3	74:SO:134:PRO:HD2	1.99	0.44
77:SX:63:ASN:OD1	82:S2:624:C:N4	2.42	0.44
82:S2:494:C:N4	82:S2:509:OMG:HN22	2.16	0.44
82:S2:1221:G:H2'	82:S2:1222:G:C8	2.53	0.44
82:S2:1589:A:N3	82:S2:1653:U:O2'	2.44	0.44
2:L5:1084:C:H2'	2:L5:1085:C:H6	1.83	0.44
2:L5:2326:G:H5''	34:Le:127:ALA:HB1	1.99	0.44
2:L5:3911:C:H2'	2:L5:3912:U:C6	2.51	0.44
3:L7:119:U:C2	8:LD:261:VAL:HG11	2.53	0.44
6:LB:46:PHE:CZ	6:LB:84:MET:HG2	2.52	0.44
8:LD:33:ARG:O	8:LD:37:VAL:HG22	2.18	0.44
11:LG:81:ASN:O	11:LG:84:THR:OG1	2.32	0.44
11:LG:175:ARG:HG2	11:LG:230:TYR:CD2	2.53	0.44
16:LM:115:ALA:HB1	18:LO:192:TYR:HB3	2.00	0.44
17:LN:200:LEU:HD22	17:LN:204:ARG:NH1	2.32	0.44
47:Ls:78:LEU:O	47:Ls:82:ILE:HG12	2.17	0.44
49:SD:215:ASP:OD1	49:SD:216:GLU:N	2.45	0.44
62:Sf:107:LYS:NZ	62:Sf:108:VAL:O	2.51	0.44
70:SI:45:THR:OG1	82:S2:308:G:OP1	2.28	0.44
70:SI:86:SER:OG	82:S2:376:A:N3	2.44	0.44
82:S2:116:OMU:HN3	82:S2:347:G:H1	1.65	0.44
82:S2:659:G:O2'	82:S2:662:G:O2'	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:1677:PSU:H4'	2:L5:1680:G:C2	2.53	0.44
2:L5:1741:G:O6	3:L7:103:A:O2'	2.27	0.44
2:L5:3599:A:H2'	2:L5:3600:G:C8	2.52	0.44
10:LF:46:ARG:NH2	31:Lb:102:PRO:HG3	2.33	0.44
26:LW:5:LEU:HD12	26:LW:30:GLN:NE2	2.33	0.44
33:Ld:44:ARG:HA	33:Ld:47:LYS:HE3	1.99	0.44
57:ST:104:LEU:HD22	57:ST:121:ARG:HD2	2.00	0.44
69:SH:18:GLU:C	69:SH:20:GLU:H	2.26	0.44
78:SY:9:THR:HG22	82:S2:837:A:N6	2.32	0.44
82:S2:573:U:O2	82:S2:576:A2M:H8	2.17	0.44
82:S2:1777:G:H2'	82:S2:1778:C:C6	2.53	0.44
2:L5:66:A:O2'	2:L5:326:C:O2	2.36	0.43
2:L5:454:U:H2'	2:L5:455:C:O4'	2.18	0.43
2:L5:2399:G:O2'	2:L5:2822:G:O2'	2.34	0.43
2:L5:2730:U:H2'	2:L5:2731:C:C6	2.53	0.43
2:L5:3873:G:H2'	2:L5:3874:G:C8	2.53	0.43
2:L5:4156:G:H5''	2:L5:4157:A:H2'	2.00	0.43
2:L5:4419:U:OP1	2:L5:4475:G:N2	2.49	0.43
2:L5:4611:A:H2'	2:L5:4612:C:H6	1.83	0.43
2:L5:4743:G:H2'	2:L5:4744:A:C8	2.53	0.43
2:L5:4897:G:H2'	2:L5:4898:G:H8	1.81	0.43
14:LJ:17:ILE:HD12	14:LJ:80:GLU:HG2	2.00	0.43
16:LM:104:MET:HG3	16:LM:108:ASP:HB2	2.00	0.43
16:LM:118:MET:HG2	18:LO:192:TYR:CZ	2.53	0.43
23:LT:28:ALA:O	23:LT:32:ARG:HG2	2.18	0.43
29:LZ:11:VAL:HG12	29:LZ:82:PRO:HA	2.00	0.43
41:Ll:12:PHE:CE2	41:Ll:51:LEU:HD22	2.53	0.43
66:SC:64:THR:HG22	66:SC:66:LEU:H	1.83	0.43
67:SE:72:ILE:HD12	67:SE:77:ARG:HB2	2.00	0.43
79:Sa:12:LYS:HG3	79:Sa:15:ARG:HB2	2.00	0.43
82:S2:495:U:H2'	82:S2:496:C:O4'	2.18	0.43
2:L5:696:C:H42	9:LE:221:LYS:HG3	1.82	0.43
2:L5:711:A:H2'	2:L5:712:C:C6	2.53	0.43
2:L5:3928:A:H2'	2:L5:3929:G:O4'	2.17	0.43
2:L5:4111:U:H2'	2:L5:4112:C:H5	1.83	0.43
2:L5:4419:U:O2'	83:CB:764:ASN:HB3	2.18	0.43
4:L8:26:C:O2'	7:LC:53:ALA:O	2.35	0.43
18:LO:88:LEU:HD12	18:LO:99:LEU:HD13	2.01	0.43
52:SM:91:LEU:HD23	52:SM:91:LEU:HA	1.80	0.43
56:SS:102:GLY:HA2	56:SS:105:ASN:HD21	1.83	0.43
60:Sc:10:LYS:HE2	60:Sc:34:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SE:18:TRP:HH2	67:SE:31:PRO:HD3	1.82	0.43
67:SE:80:ILE:HG23	67:SE:81:THR:HG23	2.00	0.43
67:SE:152:PRO:HG2	68:SG:216:ARG:HG3	2.00	0.43
82:S2:186:C:H2'	82:S2:187:G:H8	1.83	0.43
2:L5:473:C:H2'	2:L5:474:C:C6	2.53	0.43
2:L5:1081:C:C2'	2:L5:1082:C:H5'	2.49	0.43
2:L5:4913:G:H4'	2:L5:4914:C:O5'	2.17	0.43
4:L8:102:G:OP2	4:L8:104:A:O2'	2.30	0.43
6:LB:206:PRO:HG2	6:LB:209:GLN:HG3	1.99	0.43
27:LX:127:LEU:HD11	27:LX:135:LYS:HE3	2.01	0.43
55:SR:111:PHE:HE1	64:SA:12:GLU:HG3	1.84	0.43
57:ST:101:ARG:NH2	82:S2:1566:G:N7	2.65	0.43
59:SZ:86:ALA:O	59:SZ:90:GLU:HG2	2.18	0.43
63:Sg:10:THR:HB	63:Sg:306:LEU:HD21	2.00	0.43
64:SA:177:MET:SD	64:SA:180:ARG:NH2	2.92	0.43
66:SC:185:THR:OG1	82:S2:1155:U:OP1	2.27	0.43
68:SG:174:PRO:HB3	82:S2:65:C:C6	2.54	0.43
70:SI:65:PHE:HA	70:SI:187:GLY:O	2.18	0.43
77:SX:54:LYS:NZ	77:SX:94:ILE:O	2.49	0.43
77:SX:107:ARG:HG2	77:SX:112:VAL:HG22	2.00	0.43
82:S2:441:C:H2'	82:S2:442:C:C6	2.53	0.43
82:S2:1047:C:H2'	82:S2:1048:G:O4'	2.18	0.43
83:CB:24:VAL:HG12	83:CB:126:LEU:HD23	2.00	0.43
83:CB:108:HIS:HB2	83:CB:111:PHE:CD2	2.52	0.43
2:L5:907:C:H2'	2:L5:908:G:C8	2.53	0.43
2:L5:2864:A:H2'	2:L5:2865:U:H6	1.83	0.43
2:L5:2870:A:H2'	2:L5:2871:A:C8	2.53	0.43
2:L5:3684:G:H2'	2:L5:3685:C:C6	2.54	0.43
2:L5:4238:G:H2'	2:L5:4239:A:C8	2.53	0.43
88:L5:5282:SPD:H82	88:L5:5282:SPD:H51	1.78	0.43
9:LE:194:VAL:O	35:Lf:108:SER:OG	2.29	0.43
13:LI:73:ASN:HB2	13:LI:87:MET:HE1	2.00	0.43
50:SF:130:ARG:CZ	84:Et:37:A:C8	2.97	0.43
55:SR:24:LEU:HD23	55:SR:34:VAL:HG21	2.00	0.43
57:ST:96:SER:HB3	57:ST:99:VAL:HB	1.99	0.43
67:SE:186:GLY:HA3	82:S2:809:A:OP1	2.19	0.43
70:SI:150:ASP:HA	70:SI:153:LYS:CG	2.48	0.43
72:SL:23:VAL:HG23	72:SL:25:LEU:HG	2.00	0.43
75:SV:74:LYS:NZ	75:SV:83:PHE:HB3	2.33	0.43
83:CB:603:TYR:CD2	83:CB:706:ASP:HB3	2.54	0.43
83:CB:770:VAL:HA	83:CB:786:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:173:C:H2'	2:L5:174:C:C6	2.53	0.43
2:L5:264:C:H2'	2:L5:265:C:C4	2.53	0.43
2:L5:494:U:H2'	2:L5:495:C:C6	2.54	0.43
2:L5:1981:G:N1	2:L5:1982:G:O6	2.51	0.43
2:L5:4076:G:H5'	11:LG:73:ARG:HG3	2.00	0.43
5:LA:80:GLU:HB2	5:LA:170:ALA:HA	1.99	0.43
10:LF:236:ARG:HD3	10:LF:239:GLN:HB2	2.01	0.43
12:LH:128:MET:SD	12:LH:157:SER:HB3	2.58	0.43
62:Sf:85:TYR:C	83:CB:647:ARG:HH22	2.27	0.43
63:Sg:54:ILE:HD12	63:Sg:55:PRO:HD2	2.00	0.43
70:SI:141:ARG:NE	82:S2:191:A:OP1	2.52	0.43
82:S2:291:G:HO2'	82:S2:292:A:P	2.41	0.43
82:S2:348:A:H2'	82:S2:349:A:C8	2.53	0.43
84:Et:5:G:H2'	84:Et:6:G:C8	2.51	0.43
85:CE:37:ALA:HA	85:CE:40:LYS:HB2	2.01	0.43
1:CI:66:GLY:HA3	33:Ld:70:LYS:NZ	2.34	0.43
2:L5:491:G:H2'	2:L5:492:U:C6	2.54	0.43
2:L5:716:C:OP1	7:LC:317:ASN:HB2	2.19	0.43
2:L5:1466:G:OP2	31:Lb:44:ARG:NH2	2.51	0.43
2:L5:2465:C:H2'	2:L5:2466:G:O4'	2.19	0.43
2:L5:4088:C:H2'	2:L5:4089:G:H8	1.83	0.43
2:L5:4392:OMG:H2'	2:L5:4447:5MC:HM51	2.01	0.43
2:L5:5057:C:H2'	2:L5:5058:A:C8	2.54	0.43
4:L8:58:G:O6	39:Lj:63:ARG:NH1	2.52	0.43
8:LD:203:ASN:OD1	8:LD:203:ASN:N	2.51	0.43
14:LJ:104:ASN:HB2	14:LJ:133:VAL:HA	1.99	0.43
17:LN:90:ASN:O	44:Lo:48:TYR:OH	2.33	0.43
28:LY:22:PRO:HD2	28:LY:25:ILE:HD11	2.00	0.43
65:SB:124:HIS:HA	65:SB:137:LEU:O	2.19	0.43
70:SI:64:ASN:OD1	70:SI:73:THR:HG22	2.18	0.43
70:SI:139:LYS:HE2	70:SI:139:LYS:HB2	1.70	0.43
71:SJ:28:GLU:OE2	71:SJ:44:TRP:NE1	2.41	0.43
82:S2:194:C:H2'	82:S2:195:C:C6	2.53	0.43
82:S2:1278:A:H2'	82:S2:1279:C:C6	2.54	0.43
2:L5:2404:A:H1'	39:Lj:12:ARG:HH21	1.82	0.43
2:L5:2667:C:O4'	21:LR:96:MET:HG2	2.18	0.43
2:L5:3690:U:H2'	2:L5:3691:G:O4'	2.19	0.43
2:L5:4322:G:N2	2:L5:4325:A:OP2	2.43	0.43
3:L7:110:G:H2'	3:L7:111:C:C6	2.54	0.43
5:LA:13:GLY:O	5:LA:17:ARG:HG3	2.18	0.43
5:LA:22:HIS:O	5:LA:24:LYS:NZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LB:393:LYS:HG3	6:LB:396:ARG:HH21	1.83	0.43
9:LE:203:ILE:O	9:LE:206:VAL:HG22	2.19	0.43
10:LF:105:VAL:HG13	10:LF:136:VAL:HG12	2.01	0.43
19:LP:76:TRP:CD1	19:LP:76:TRP:H	2.36	0.43
26:LW:52:THR:O	26:LW:56:ARG:HG2	2.18	0.43
50:SF:79:HIS:O	50:SF:81:ARG:N	2.47	0.43
58:SU:38:ASP:OD1	58:SU:39:LEU:N	2.51	0.43
63:Sg:183:LYS:HA	63:Sg:183:LYS:HD2	1.85	0.43
75:SV:17:CYS:HB2	75:SV:56:CYS:HB3	2.01	0.43
78:SY:36:PRO:O	78:SY:40:ILE:HD12	2.18	0.43
82:S2:152:U:H2'	82:S2:153:G:C8	2.54	0.43
82:S2:1243:U:OP2	82:S2:1518:C:O2'	2.25	0.43
83:CB:382:ALA:HA	83:CB:385:ILE:HG12	2.00	0.43
84:Et:23:A:H2'	84:Et:24:G:C8	2.54	0.43
2:L5:262:G:H2'	2:L5:263:G:C8	2.53	0.43
2:L5:1195:G:H2'	2:L5:1196:G:C8	2.54	0.43
2:L5:3827:G:O2'	2:L5:3829:G:OP2	2.36	0.43
2:L5:4238:G:H2'	2:L5:4239:A:H8	1.84	0.43
3:L7:63:C:H5'	3:L7:64:G:H5''	2.01	0.43
4:L8:36:G:C5	37:Lh:89:ARG:HD3	2.54	0.43
4:L8:144:U:H2'	4:L8:145:C:C6	2.53	0.43
7:LC:279:LEU:HD23	7:LC:279:LEU:HA	1.87	0.43
12:LH:24:THR:HA	12:LH:37:ASP:HA	2.01	0.43
18:LO:124:LEU:HD23	18:LO:124:LEU:HA	1.87	0.43
54:SQ:90:LYS:HA	54:SQ:93:VAL:HG22	2.00	0.43
64:SA:184:ARG:NE	64:SA:191:ARG:HD3	2.33	0.43
65:SB:83:LYS:HD3	65:SB:106:THR:HG22	2.01	0.43
68:SG:14:LYS:HE2	68:SG:16:ILE:HD11	2.01	0.43
71:SJ:5:ARG:HB3	82:S2:38:A:H5''	2.01	0.43
75:SV:18:SER:HB3	75:SV:72:LEU:HD21	2.01	0.43
76:SW:28:ARG:HB3	76:SW:29:PRO:HD3	2.00	0.43
78:SY:9:THR:HG22	82:S2:837:A:H61	1.84	0.43
79:Sa:59:PHE:HB2	79:Sa:62:TYR:HB2	2.01	0.43
82:S2:293:C:O2'	82:S2:294:U:H3'	2.19	0.43
82:S2:517:OMC:H2'	82:S2:518:G:O4'	2.18	0.43
83:CB:851:LEU:HD23	83:CB:857:LYS:HZ1	1.84	0.43
2:L5:922:C:H2'	2:L5:923:C:O4'	2.19	0.43
2:L5:1175:A:H2	2:L5:1185:G:H1	1.66	0.43
2:L5:2421:G:OP2	2:L5:2828:U:H1'	2.19	0.43
2:L5:4887:C:N4	2:L5:4932:U:H3	2.15	0.43
7:LC:318:PRO:O	7:LC:319:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LF:147:LEU:O	10:LF:151:ASN:ND2	2.43	0.43
10:LF:214:SER:OG	10:LF:215:SER:N	2.51	0.43
34:Le:35:TRP:CZ2	34:Le:56:PRO:HD2	2.54	0.43
37:Lh:52:LYS:HA	37:Lh:52:LYS:HD3	1.81	0.43
44:Lo:106:PHE:CZ	85:CE:39:TRP:CE3	2.97	0.43
47:Ls:156:SER:CB	83:CB:263:ASP:OD2	2.58	0.43
48:Lt:37:LEU:HD21	83:CB:778:GLY:N	2.34	0.43
63:Sg:59:LEU:HD23	63:Sg:90:TRP:CD2	2.54	0.43
69:SH:58:LYS:HA	69:SH:58:LYS:HD2	1.82	0.43
82:S2:639:C:H2'	82:S2:640:A:C8	2.54	0.43
82:S2:1560:U:O2	82:S2:1575:G:O6	2.37	0.43
82:S2:1683:C:H2'	82:S2:1684:C:H6	1.84	0.43
83:CB:20:ARG:HB3	83:CB:100:ILE:HG23	2.01	0.43
2:L5:1563:A:N6	82:S2:1028:A:N1	2.66	0.43
2:L5:1683:PSU:H2'	2:L5:1684:A:C8	2.54	0.43
2:L5:1826:G:H4'	31:Lb:43:MET:HE3	2.01	0.43
2:L5:1998:A:N6	47:Ls:40:MET:SD	2.92	0.43
2:L5:2664:G:H4'	2:L5:2677:G:H4'	2.00	0.43
2:L5:2671:C:H2'	2:L5:2672:C:C6	2.54	0.43
3:L7:55:A:H4'	14:LJ:155:HIS:HB2	2.00	0.43
6:LB:154:LYS:HE2	6:LB:154:LYS:HB2	1.70	0.43
14:LJ:77:ALA:O	14:LJ:81:GLU:HG2	2.18	0.43
14:LJ:113:ILE:HD11	56:SS:14:ARG:HD3	2.00	0.43
15:LL:111:GLN:HA	15:LL:114:VAL:HG22	2.01	0.43
28:LY:72:GLN:HE21	28:LY:74:TYR:HD1	1.67	0.43
32:Lc:38:ILE:HG21	32:Lc:63:TYR:HB3	1.99	0.43
51:SK:91:PRO:HB2	51:SK:94:LEU:HD23	2.01	0.43
56:SS:13:LEU:HD22	56:SS:20:ILE:HD11	2.00	0.43
63:Sg:270:LEU:HD13	63:Sg:310:TRP:CE3	2.54	0.43
64:SA:11:LYS:O	64:SA:15:VAL:HG23	2.18	0.43
67:SE:122:LYS:HE2	67:SE:124:CYS:SG	2.58	0.43
82:S2:166:A2M:HM'3	82:S2:166:A2M:H1'	1.68	0.43
82:S2:693:A:H2'	82:S2:694:G:N7	2.33	0.43
82:S2:834:C:H42	82:S2:839:C:H42	1.66	0.43
82:S2:1101:U:H2'	82:S2:1102:G:C8	2.54	0.43
82:S2:1217:A:H2'	82:S2:1218:C:H6	1.83	0.43
83:CB:452:LEU:HD23	83:CB:459:GLU:O	2.19	0.43
2:L5:1278:C:H2'	2:L5:1279:A:O4'	2.18	0.42
2:L5:1404:G:N7	2:L5:1408:G:N1	2.67	0.42
2:L5:1613:A:H5''	5:LA:183:GLY:HA2	2.01	0.42
2:L5:1631:A:C2	5:LA:204:MET:HG2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:1847:C:H2'	2:L5:1848:C:C6	2.54	0.42
2:L5:2017:A:HO2'	2:L5:2018:C:C5'	2.31	0.42
2:L5:2809:G:H5''	21:LR:63:CYS:SG	2.59	0.42
2:L5:3654:G:O2'	2:L5:3693:U:OP1	2.28	0.42
2:L5:3782:5MC:OP1	43:Ln:23:ARG:NH2	2.52	0.42
2:L5:4084:G:O6	5:LA:72:ARG:NH2	2.51	0.42
2:L5:4590:A2M:HM'3	2:L5:4590:A2M:H1'	1.79	0.42
2:L5:4859:C:H2'	2:L5:4860:G:H8	1.84	0.42
2:L5:4927:G:H5''	2:L5:4928:C:C5	2.54	0.42
7:LC:33:ARG:HG2	7:LC:36:ILE:HD12	2.01	0.42
12:LH:95:VAL:HG12	42:Lm:82:LEU:HD13	2.01	0.42
26:LW:47:ARG:HE	26:LW:54:LEU:HD22	1.84	0.42
28:LY:23:SER:HA	28:LY:26:ARG:HB2	2.00	0.42
35:Lf:45:LYS:HA	35:Lf:107:PRO:HD2	2.01	0.42
60:Sc:44:ARG:NH2	60:Sc:63:ARG:HH11	2.17	0.42
66:SC:167:ARG:HB3	66:SC:177:PRO:HB2	2.00	0.42
82:S2:1259:A:H1'	82:S2:1264:C:N4	2.34	0.42
2:L5:490:C:H2'	2:L5:491:G:H8	1.83	0.42
2:L5:1669:A:H4'	2:L5:1685:G:N2	2.34	0.42
2:L5:3861:A:H2'	2:L5:3862:A:H8	1.84	0.42
2:L5:4327:C:OP1	23:LT:70:HIS:NE2	2.51	0.42
2:L5:5006:U:H4'	2:L5:5007:A:H5'	2.01	0.42
6:LB:92:TYR:HB3	6:LB:99:LEU:HD22	2.00	0.42
7:LC:221:PHE:O	7:LC:222:ARG:HG2	2.20	0.42
23:LT:44:GLY:HA2	23:LT:95:HIS:HB3	2.01	0.42
32:Lc:47:ILE:HB	32:Lc:94:LEU:HG	2.02	0.42
38:Li:76:ARG:HD3	38:Li:76:ARG:HA	1.79	0.42
48:Lt:114:ARG:NH2	48:Lt:162:CYS:SG	2.92	0.42
56:SS:61:GLU:HA	56:SS:64:VAL:HG12	2.01	0.42
57:ST:62:ARG:CZ	82:S2:1542:C:H5''	2.49	0.42
63:Sg:135:LEU:HD23	63:Sg:135:LEU:HA	1.89	0.42
63:Sg:200:VAL:HA	63:Sg:206:LEU:O	2.19	0.42
64:SA:42:LYS:HD2	64:SA:48:ILE:HD11	2.01	0.42
65:SB:147:ASN:OD1	65:SB:148:ASN:N	2.52	0.42
73:SN:29:THR:O	73:SN:33:VAL:HG23	2.19	0.42
82:S2:454:U:H2'	82:S2:455:A:C8	2.54	0.42
82:S2:1139:C:H2'	82:S2:1140:G:O4'	2.18	0.42
82:S2:1705:C:H2'	82:S2:1706:G:C8	2.54	0.42
83:CB:90:LYS:HE3	83:CB:90:LYS:HB2	1.74	0.42
85:CE:20:ALA:O	85:CE:23:LYS:HG3	2.18	0.42
2:L5:92:C:OP2	2:L5:4341:C:O2'	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:457:G:H2'	2:L5:458:C:C6	2.54	0.42
2:L5:1346:C:H2'	2:L5:1347:G:H8	1.84	0.42
2:L5:1979:A:H1'	2:L5:1988:G:N2	2.34	0.42
2:L5:4187:G:OP1	87:L5:5266:SPM:H111	2.19	0.42
2:L5:4742:G:H2'	2:L5:4743:G:C8	2.54	0.42
3:L7:111:C:H2'	3:L7:112:U:O4'	2.19	0.42
6:LB:17:LEU:HD23	6:LB:17:LEU:HA	1.78	0.42
10:LF:92:VAL:O	10:LF:120:GLY:HA2	2.19	0.42
13:LI:14:ASN:O	13:LI:128:ARG:NH2	2.24	0.42
18:LO:56:ALA:O	18:LO:60:LYS:HG2	2.18	0.42
31:Lb:43:MET:HE2	31:Lb:47:LYS:NZ	2.34	0.42
32:Lc:18:LEU:O	32:Lc:22:MET:HG2	2.19	0.42
43:Ln:17:ARG:NH1	82:S2:1173:A:OP1	2.53	0.42
48:Lt:34:PRO:CG	83:CB:777:ALA:N	2.58	0.42
54:SQ:110:ASP:OD1	54:SQ:110:ASP:N	2.49	0.42
65:SB:167:LYS:HE2	65:SB:167:LYS:HB2	1.82	0.42
70:SI:161:LEU:HD23	70:SI:195:LEU:HG	2.00	0.42
74:SO:63:LYS:HD3	74:SO:63:LYS:HA	1.87	0.42
74:SO:147:ARG:HH22	82:S2:1854:U:P	2.43	0.42
76:SW:5:ASN:HB3	76:SW:8:ALA:HB3	2.00	0.42
82:S2:1347:U:H2'	82:S2:1348:G:N3	2.34	0.42
82:S2:1540:G:H2'	82:S2:1541:G:H8	1.85	0.42
82:S2:1779:G:H2'	82:S2:1780:G:C8	2.53	0.42
83:CB:86:LEU:HD12	83:CB:89:ILE:HD12	2.00	0.42
2:L5:89:C:OP1	30:La:59:LYS:NZ	2.41	0.42
2:L5:1084:C:H2'	2:L5:1085:C:C6	2.54	0.42
2:L5:1625:OMG:HM23	17:LN:81:TYR:HE2	1.84	0.42
2:L5:2073:C:OP1	10:LF:212:LYS:HE3	2.19	0.42
2:L5:2765:A:H2'	2:L5:2766:A:C8	2.54	0.42
2:L5:2808:G:O3'	21:LR:60:ARG:NH1	2.51	0.42
4:L8:102:G:H5''	39:Lj:39:TYR:HE1	1.83	0.42
6:LB:220:ILE:HG12	6:LB:278:THR:HG23	2.00	0.42
11:LG:176:LYS:HD3	38:Li:43:MET:HE1	2.02	0.42
19:LP:85:LYS:O	19:LP:89:GLU:HG3	2.20	0.42
27:LX:82:THR:HG21	37:Lh:37:THR:HG22	2.01	0.42
44:Lo:78:ARG:O	44:Lo:80:LYS:NZ	2.52	0.42
47:Ls:47:LEU:HD11	47:Ls:51:ALA:HB3	2.02	0.42
65:SB:214:LYS:HE2	65:SB:216:LYS:HE3	2.02	0.42
82:S2:1733:U:H2'	82:S2:1734:G:O4'	2.20	0.42
82:S2:1797:U:H2'	82:S2:1798:C:C6	2.54	0.42
2:L5:120:A:H2'	2:L5:149:A:H61	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:252:C:H2'	2:L5:253:G:C8	2.54	0.42
2:L5:408:A:O2'	2:L5:411:G:OP2	2.26	0.42
2:L5:1703:C:O2'	2:L5:1704:C:O5'	2.37	0.42
2:L5:2368:A:N6	2:L5:2827:G:O2'	2.51	0.42
2:L5:2424:OMG:H1'	2:L5:2424:OMG:HM23	1.80	0.42
2:L5:2492:C:H2'	2:L5:2493:G:C8	2.54	0.42
2:L5:2558:C:H2'	2:L5:2559:G:H8	1.84	0.42
2:L5:2638:G:H22	2:L5:2719:C:P	2.42	0.42
2:L5:3718:A2M:H2'	2:L5:3719:A:O4'	2.19	0.42
2:L5:3937:C:O2'	17:LN:124:ASP:OD1	2.38	0.42
2:L5:4685:U:H2'	2:L5:4686:G:C8	2.54	0.42
5:LA:20:VAL:HA	5:LA:23:ARG:HG3	1.99	0.42
10:LF:228:VAL:HG12	22:LS:38:VAL:HG12	2.02	0.42
16:LM:86:TRP:O	16:LM:89:THR:OG1	2.33	0.42
26:LW:97:LYS:O	26:LW:99:GLU:N	2.51	0.42
64:SA:180:ARG:HH11	64:SA:184:ARG:HH11	1.68	0.42
64:SA:206:ASP:O	64:SA:210:ILE:HD12	2.18	0.42
67:SE:253:ASP:N	67:SE:253:ASP:OD1	2.51	0.42
75:SV:40:ASP:OD1	75:SV:44:GLY:N	2.52	0.42
82:S2:804:U:H2'	82:S2:805:U:C6	2.54	0.42
83:CB:265:TYR:HA	83:CB:287:ARG:HA	2.01	0.42
83:CB:448:GLN:HB3	83:CB:473:VAL:HG23	2.01	0.42
2:L5:37:U:H2'	2:L5:38:A:O4'	2.19	0.42
2:L5:400:A2M:H1'	2:L5:400:A2M:HM'3	1.63	0.42
2:L5:959:G:C8	9:LE:123:ARG:HG2	2.55	0.42
2:L5:2303:C:H5''	34:Le:104:SER:HB3	2.02	0.42
2:L5:2492:C:H2'	2:L5:2493:G:H8	1.85	0.42
2:L5:2517:A:N3	2:L5:2539:C:O2'	2.50	0.42
2:L5:2607:C:O5'	21:LR:96:MET:HE1	2.20	0.42
2:L5:3725:G:N7	38:Li:67:LYS:NZ	2.50	0.42
2:L5:4419:U:C2	83:CB:765:ARG:HG3	2.54	0.42
4:L8:90:C:H1'	28:LY:24:HIS:HB3	2.01	0.42
23:LT:4:THR:OG1	23:LT:9:ARG:HD3	2.19	0.42
28:LY:74:TYR:HE2	28:LY:77:LYS:HG3	1.85	0.42
44:Lo:4:VAL:HG23	44:Lo:93:LEU:HD23	2.02	0.42
63:Sg:227:LEU:HD23	63:Sg:228:TYR:HB2	2.01	0.42
66:SC:202:THR:HG23	71:SJ:54:ARG:HH22	1.85	0.42
67:SE:128:LYS:HG2	67:SE:140:VAL:HB	2.01	0.42
67:SE:242:LYS:HD3	67:SE:242:LYS:HA	1.75	0.42
68:SG:31:ARG:NH1	82:S2:1745:A:O3'	2.52	0.42
68:SG:164:LYS:HE2	68:SG:164:LYS:HB2	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:SG:227:GLN:HB3	68:SG:231:ARG:HH21	1.84	0.42
77:SX:28:LYS:O	77:SX:32:LEU:HB2	2.19	0.42
77:SX:34:THR:HG21	82:S2:1189:A:H4'	2.01	0.42
83:CB:174:LEU:HD23	83:CB:294:LEU:HD13	2.02	0.42
83:CB:289:PHE:HA	83:CB:293:ILE:HD12	2.00	0.42
83:CB:592:LEU:HA	83:CB:602:LEU:O	2.20	0.42
83:CB:609:PHE:CD2	83:CB:699:GLY:HA2	2.55	0.42
84:Et:52:G:H2'	84:Et:53:G:C8	2.54	0.42
2:L5:398:A2M:HM'3	2:L5:398:A2M:H1'	1.79	0.42
2:L5:1396:G:HO2'	2:L5:1468:C:HO2'	1.57	0.42
2:L5:1410:U:H3	31:Lb:52:LYS:NZ	2.17	0.42
2:L5:4535:A:H2'	2:L5:4536:OMC:H6	1.84	0.42
2:L5:4940:C:H5'	2:L5:4941:G:H5''	2.01	0.42
5:LA:7:GLY:HA2	5:LA:10:LYS:HG3	2.02	0.42
8:LD:211:LEU:HB3	8:LD:219:TYR:HB2	2.02	0.42
16:LM:37:LEU:HD12	16:LM:37:LEU:HA	1.82	0.42
20:LQ:110:ARG:HG3	20:LQ:120:ILE:HD12	2.01	0.42
22:LS:69:GLU:HG3	22:LS:71:SER:H	1.84	0.42
32:Lc:30:GLY:O	32:Lc:34:THR:OG1	2.26	0.42
33:Ld:33:ILE:HD11	33:Ld:45:ALA:HA	2.00	0.42
39:Lj:67:LEU:HD23	39:Lj:67:LEU:HA	1.87	0.42
41:Ll:28:ARG:HA	41:Ll:33:ASN:ND2	2.33	0.42
44:Lo:106:PHE:HE2	85:CE:39:TRP:CZ2	2.27	0.42
59:SZ:48:VAL:HG23	59:SZ:80:ARG:HD2	2.01	0.42
63:Sg:101:PHE:CD2	63:Sg:136:GLY:HA2	2.54	0.42
63:Sg:207:CYS:SG	63:Sg:219:TRP:HB2	2.60	0.42
66:SC:214:LEU:HD22	66:SC:244:ILE:HD11	2.02	0.42
72:SL:48:LYS:HD3	72:SL:52:GLU:OE2	2.20	0.42
77:SX:88:ASP:HA	82:S2:617:G:H4'	2.01	0.42
82:S2:1393:G:H2'	82:S2:1394:G:C8	2.55	0.42
82:S2:1401:A:H2'	82:S2:1402:A:C8	2.54	0.42
2:L5:85:G:O2'	2:L5:97:G:O6	2.31	0.42
2:L5:137:G:H2'	2:L5:138:G:C8	2.53	0.42
2:L5:1281:G:C6	9:LE:128:HIS:HB2	2.55	0.42
2:L5:1444:G:H22	2:L5:2104:G:N2	2.18	0.42
2:L5:1824:G:H5''	23:LT:35:LYS:HE2	2.01	0.42
2:L5:3867:A2M:H2'	2:L5:3868:G:O4'	2.19	0.42
2:L5:4458:C:H2'	2:L5:4459:U:C6	2.55	0.42
2:L5:4859:C:H2'	2:L5:4860:G:C8	2.55	0.42
15:LL:59:VAL:HG21	15:LL:73:GLY:HA3	2.01	0.42
15:LL:194:ILE:HD12	15:LL:194:ILE:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LQ:43:PHE:CD2	20:LQ:133:GLY:HA3	2.55	0.42
23:LT:39:ILE:HG13	23:LT:102:ARG:HE	1.85	0.42
28:LY:47:MET:HE3	28:LY:48:PRO:HD2	2.01	0.42
28:LY:50:ARG:NH1	28:LY:51:LYS:HB3	2.35	0.42
34:Le:98:GLU:HG2	34:Le:123:THR:OG1	2.20	0.42
39:Lj:85:LYS:HB3	39:Lj:85:LYS:HE3	1.71	0.42
50:SF:167:LYS:HA	59:SZ:71:ALA:HB1	2.02	0.42
64:SA:5:LEU:HD11	75:SV:41:LYS:HD2	2.01	0.42
64:SA:215:GLN:O	64:SA:219:GLU:HG2	2.19	0.42
67:SE:212:ASP:OD1	67:SE:216:ASN:N	2.52	0.42
69:SH:63:PHE:HB3	69:SH:97:GLN:HG3	2.01	0.42
81:Se:56:ASN:ND2	82:S2:606:G:O4'	2.48	0.42
82:S2:601:OMG:HM23	82:S2:601:OMG:H1'	1.71	0.42
82:S2:888:U:O2'	82:S2:898:U:N3	2.49	0.42
1:CI:63:ARG:HD2	1:CI:63:ARG:HA	1.85	0.42
2:L5:108:A:N1	2:L5:333:U:O2'	2.50	0.42
2:L5:1178:G:H2'	8:LD:286:SER:HB3	2.01	0.42
2:L5:1392:A:H2'	2:L5:1393:G:C8	2.55	0.42
2:L5:2521:G:H5'	2:L5:2640:G:H1'	2.02	0.42
2:L5:3610:A:H2'	2:L5:3611:A:C8	2.55	0.42
2:L5:4113:U:H4'	2:L5:4115:G:C5	2.55	0.42
2:L5:4195:G:OP1	2:L5:4221:C:O2'	2.36	0.42
6:LB:117:ARG:HA	6:LB:177:LYS:HD2	2.01	0.42
13:LI:51:HIS:CD2	13:LI:168:SER:HB3	2.54	0.42
16:LM:38:VAL:O	16:LM:47:ARG:HA	2.18	0.42
28:LY:50:ARG:HB3	28:LY:53:ASP:OD2	2.20	0.42
48:Lt:34:PRO:CB	83:CB:777:ALA:O	2.68	0.42
48:Lt:147:HIS:HA	48:Lt:148:PRO:HD3	1.83	0.42
52:SM:20:GLU:HG2	52:SM:119:GLN:HB2	2.00	0.42
52:SM:31:LEU:HG	52:SM:33:ARG:HG3	2.01	0.42
53:SP:93:MET:HE1	53:SP:106:GLU:OE1	2.19	0.42
56:SS:78:LYS:HD3	56:SS:78:LYS:HA	1.76	0.42
66:SC:74:LYS:HA	66:SC:74:LYS:HD3	1.89	0.42
69:SH:76:GLN:O	69:SH:80:VAL:HG23	2.20	0.42
74:SO:113:GLN:OE1	79:Sa:46:GLU:N	2.53	0.42
79:Sa:34:LYS:NZ	82:S2:1862:G:N7	2.61	0.42
83:CB:9:ILE:O	83:CB:13:MET:HB2	2.20	0.42
83:CB:398:ILE:HD13	83:CB:414:GLY:HA3	2.02	0.42
1:CI:72:ARG:NH2	21:LR:25:ASP:OD2	2.48	0.42
2:L5:462:G:H2'	2:L5:463:A:C8	2.54	0.42
2:L5:499:G:H2'	2:L5:499:G:N3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:691:C:H2'	2:L5:692:A:H8	1.85	0.42
2:L5:730:G:OP2	10:LF:76:ARG:NE	2.48	0.42
2:L5:982:U:H2'	2:L5:983:C:C6	2.55	0.42
2:L5:1345:A:H2'	2:L5:1346:C:C6	2.55	0.42
2:L5:1538:U:H2'	2:L5:1539:G:H8	1.85	0.42
2:L5:2335:C:H2'	2:L5:2336:G:H8	1.85	0.42
2:L5:2415:U:H2'	2:L5:2416:G:C8	2.55	0.42
2:L5:2845:A:H61	2:L5:3843:C:N4	2.18	0.42
2:L5:4638:U:H2'	2:L5:4639:G:N3	2.35	0.42
2:L5:4987:C:P	6:LB:116:ARG:HH22	2.42	0.42
4:L8:67:U:H2'	4:L8:68:G:C8	2.55	0.42
4:L8:92:U:H2'	4:L8:93:C:O4'	2.20	0.42
9:LE:227:HIS:HE1	9:LE:230:GLY:HA2	1.83	0.42
14:LJ:35:ARG:O	14:LJ:39:VAL:HG23	2.20	0.42
19:LP:32:THR:HG23	19:LP:58:VAL:HG11	2.00	0.42
21:LR:105:LEU:HD23	21:LR:138:LEU:HD23	2.01	0.42
32:Lc:82:GLY:HA2	32:Lc:91:VAL:HG12	2.02	0.42
36:Lg:41:ALA:O	36:Lg:52:ARG:HD3	2.20	0.42
50:SF:112:LEU:HD13	50:SF:177:LEU:HD21	2.02	0.42
52:SM:17:ALA:O	52:SM:20:GLU:HG3	2.18	0.42
58:SU:104:ILE:HB	58:SU:106:ILE:HG12	2.01	0.42
60:Sc:44:ARG:HH22	60:Sc:63:ARG:HH11	1.68	0.42
65:SB:71:LEU:HD22	65:SB:82:ARG:HD2	2.02	0.42
74:SO:96:LYS:HD3	74:SO:132:VAL:HG11	2.02	0.42
78:SY:93:ARG:HH21	82:S2:575:A:P	2.42	0.42
82:S2:562:U:H2'	82:S2:563:G:C8	2.55	0.42
82:S2:867:OMG:H1'	82:S2:867:OMG:HM23	1.75	0.42
82:S2:1232:PSU:H2'	82:S2:1233:G:H8	1.85	0.42
82:S2:1759:G:N2	82:S2:1760:G:O6	2.51	0.42
83:CB:300:VAL:HG12	83:CB:315:LEU:HD13	2.01	0.42
83:CB:475:VAL:HA	83:CB:478:PHE:CD2	2.55	0.42
85:CE:67:LYS:H	85:CE:67:LYS:HG2	1.56	0.42
2:L5:223:G:H4'	2:L5:225:G:C8	2.54	0.41
2:L5:1870:C:H2'	2:L5:1871:A2M:H8	2.02	0.41
2:L5:2622:G:O6	24:LU:81:ARG:NH2	2.53	0.41
2:L5:2823:G:N7	21:LR:20:LYS:HD3	2.35	0.41
2:L5:3760:A:N6	83:CB:720:GLN:OE1	2.53	0.41
2:L5:3893:C:O2'	2:L5:4979:A:N1	2.50	0.41
2:L5:4524:G:OP1	2:L5:4559:A:N6	2.47	0.41
5:LA:115:CYS:SG	5:LA:124:GLY:HA3	2.60	0.41
21:LR:99:MET:HE2	21:LR:99:MET:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LS:15:ARG:HD2	22:LS:25:PRO:HG2	2.01	0.41
25:LV:111:GLU:H	25:LV:111:GLU:CD	2.28	0.41
31:Lb:65:MET:HG3	31:Lb:68:ARG:HH12	1.85	0.41
48:Lt:79:ALA:HA	48:Lt:82:ILE:HG22	2.01	0.41
57:ST:71:GLY:O	57:ST:75:MET:HG2	2.20	0.41
58:SU:19:ARG:HH11	58:SU:92:HIS:HB3	1.85	0.41
58:SU:32:LEU:CD1	58:SU:85:HIS:HB2	2.50	0.41
82:S2:186:C:H2'	82:S2:187:G:C8	2.55	0.41
82:S2:838:G:N1	82:S2:840:C:O2'	2.50	0.41
82:S2:1597:C:H4'	82:S2:1603:G:O6	2.19	0.41
82:S2:1713:C:H2'	82:S2:1714:U:C6	2.55	0.41
83:CB:740:LEU:HD11	83:CB:835:VAL:HG23	2.01	0.41
2:L5:513:U:H3'	2:L5:514:U:H4'	2.01	0.41
2:L5:1172:C:O2'	2:L5:1173:G:H8	2.03	0.41
2:L5:1382:G:OP1	15:LL:66:TYR:OH	2.34	0.41
2:L5:2264:C:H2'	2:L5:2265:G:O4'	2.20	0.41
2:L5:3822:PSU:OP1	87:L5:5289:SPM:N5	2.32	0.41
2:L5:4389:C:H2'	2:L5:4390:A:H8	1.85	0.41
3:L7:35:U:O2	3:L7:45:U:O2'	2.35	0.41
6:LB:29:VAL:HA	6:LB:220:ILE:HD13	2.01	0.41
11:LG:178:GLY:O	11:LG:223:ARG:NH2	2.53	0.41
21:LR:35:ALA:HA	21:LR:40:GLN:OE1	2.20	0.41
46:Lr:47:LYS:HB2	46:Lr:102:TYR:CZ	2.55	0.41
49:SD:213:PRO:HB3	55:SR:20:TYR:CE1	2.55	0.41
53:SP:29:SER:HB3	53:SP:32:GLN:NE2	2.34	0.41
69:SH:25:GLN:O	69:SH:28:LEU:HG	2.20	0.41
74:SO:131:ASP:OD1	74:SO:133:THR:OG1	2.33	0.41
82:S2:1348:G:OP2	82:S2:1348:G:N2	2.50	0.41
82:S2:1417:C:O2	82:S2:1422:G:C6	2.74	0.41
83:CB:364:ALA:HA	83:CB:367:TYR:CZ	2.56	0.41
83:CB:533:MET:HE3	83:CB:533:MET:HB3	1.75	0.41
85:CE:57:GLU:HA	85:CE:60:ARG:NH1	2.35	0.41
2:L5:956:A:H1'	2:L5:2076:G:H5''	2.01	0.41
2:L5:3722:G:H2'	2:L5:3723:A:H8	1.84	0.41
2:L5:4227:OMU:HM23	2:L5:4227:OMU:H1'	1.85	0.41
5:LA:112:ILE:HD11	45:Lp:79:VAL:HG22	2.03	0.41
14:LJ:119:TYR:CG	56:SS:12:ILE:HG12	2.56	0.41
27:LX:64:SER:HB2	37:Lh:69:LEU:HD13	2.01	0.41
50:SF:123:GLU:OE1	60:Sc:63:ARG:NH2	2.53	0.41
50:SF:131:ALA:HB3	84:Et:39:U:H1'	2.02	0.41
58:SU:61:LEU:HB2	58:SU:82:MET:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:Sd:56:ASP:OXT	82:S2:1480:A:O2'	2.32	0.41
63:Sg:283:PRO:O	63:Sg:285:GLN:NE2	2.53	0.41
68:SG:174:PRO:HG3	82:S2:65:C:C2	2.55	0.41
69:SH:118:ARG:HA	69:SH:118:ARG:HD3	1.91	0.41
78:SY:42:GLU:O	78:SY:46:LYS:HG3	2.20	0.41
82:S2:1839:U:H2'	82:S2:1840:U:C6	2.55	0.41
83:CB:753:GLU:HA	83:CB:756:VAL:HB	2.01	0.41
2:L5:302:C:H2'	2:L5:303:C:C6	2.55	0.41
2:L5:1777:C:OP2	85:CE:64:LEU:CD2	2.63	0.41
2:L5:1869:G:C6	88:L5:5284:SPD:H32	2.55	0.41
2:L5:2409:U:H5	2:L5:2783:A:N1	2.18	0.41
2:L5:3865:A:H61	2:L5:3881:G:H1	1.67	0.41
2:L5:4619:U:H2'	2:L5:4620:OMU:H6	2.01	0.41
7:LC:334:THR:HG21	10:LF:51:TYR:OH	2.20	0.41
20:LQ:69:LYS:HA	20:LQ:69:LYS:HD3	1.90	0.41
50:SF:130:ARG:NH2	84:Et:37:A:N7	2.69	0.41
56:SS:113:ARG:O	56:SS:117:ILE:HG12	2.19	0.41
61:Sd:13:LYS:HG3	82:S2:1556:A:C8	2.55	0.41
62:Sf:108:VAL:HB	62:Sf:113:LYS:H	1.86	0.41
63:Sg:153:CYS:O	63:Sg:167:SER:HA	2.20	0.41
65:SB:141:GLY:HA3	65:SB:207:LEU:HD23	2.03	0.41
71:SJ:176:LYS:HA	71:SJ:179:LYS:HG2	2.01	0.41
79:Sa:39:PHE:CE2	79:Sa:41:ILE:HD11	2.54	0.41
81:Se:8:ARG:NH1	82:S2:615:C:O3'	2.53	0.41
83:CB:766:LYS:HB3	83:CB:788:LEU:HD11	2.02	0.41
2:L5:2861:OMC:H1'	2:L5:2861:OMC:HM23	1.86	0.41
2:L5:4522:G:O2'	2:L5:4525:C:OP2	2.31	0.41
2:L5:4607:A:H5'	83:CB:552:LEU:HD22	2.02	0.41
2:L5:4637:OMG:HM23	2:L5:4637:OMG:H1'	1.78	0.41
6:LB:337:VAL:HG11	6:LB:345:LEU:HD13	2.03	0.41
9:LE:282:TYR:HE1	35:Lf:31:GLU:HG2	1.85	0.41
13:LI:84:GLY:O	13:LI:140:THR:OG1	2.29	0.41
19:LP:95:LEU:HD23	19:LP:95:LEU:HA	1.95	0.41
22:LS:93:MET:HE1	22:LS:117:HIS:CE1	2.55	0.41
32:Lc:50:ASN:ND2	32:Lc:76:GLY:O	2.54	0.41
50:SF:59:LYS:HB3	50:SF:62:ARG:HG3	2.03	0.41
50:SF:60:ARG:HE	82:S2:1679:A:P	2.43	0.41
63:Sg:101:PHE:CE2	63:Sg:136:GLY:HA2	2.55	0.41
63:Sg:125:ARG:HD3	63:Sg:150:TRP:CE2	2.56	0.41
69:SH:43:LEU:HB3	69:SH:72:PHE:CE1	2.56	0.41
82:S2:71:G:H2'	82:S2:72:C:H4'	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:S2:1328:OMG:H1'	82:S2:1328:OMG:HM23	1.81	0.41
82:S2:1670:C:H2'	82:S2:1671:G:C8	2.55	0.41
82:S2:1845:A:H2'	82:S2:1846:G:H8	1.84	0.41
83:CB:44:GLY:HA2	83:CB:77:LEU:HA	2.02	0.41
83:CB:451:ILE:HG13	83:CB:459:GLU:O	2.20	0.41
84:Et:25:C:H2'	84:Et:26:A:H5''	2.02	0.41
2:L5:279:A:OP2	17:LN:8:GLN:NE2	2.42	0.41
2:L5:654:C:O3'	7:LC:268:ARG:NH1	2.52	0.41
2:L5:1973:G:O2'	48:Lt:117:ARG:NH2	2.48	0.41
2:L5:2743:A:H2'	2:L5:2744:A:C8	2.56	0.41
2:L5:4318:C:H4'	44:Lo:17:LYS:HA	2.02	0.41
2:L5:4739:C:H2'	2:L5:4740:G:H5'	2.03	0.41
8:LD:52:ILE:HA	8:LD:147:ASP:HB3	2.02	0.41
8:LD:86:TYR:CE1	8:LD:247:ILE:HG13	2.55	0.41
11:LG:30:PRO:HG2	29:LZ:124:THR:HA	2.02	0.41
17:LN:159:ARG:HB3	17:LN:164:LEU:HB2	2.01	0.41
34:Le:19:LYS:HE3	34:Le:19:LYS:HB3	1.90	0.41
34:Le:89:LEU:HD13	34:Le:118:LEU:HD22	2.03	0.41
34:Le:99:ILE:HD13	34:Le:108:ARG:HB2	2.03	0.41
47:Ls:57:LYS:O	47:Ls:61:MET:HG2	2.20	0.41
51:SK:64:TRP:CD2	61:Sd:23:VAL:HG22	2.55	0.41
53:SP:86:LEU:H	53:SP:89:MET:CE	2.33	0.41
66:SC:212:LYS:HE2	66:SC:212:LYS:HB3	1.86	0.41
68:SG:191:ARG:NH1	82:S2:312:G:H2'	2.35	0.41
73:SN:7:PRO:HG3	82:S2:996:A:H5''	2.01	0.41
82:S2:352:U:H2'	82:S2:353:C:C6	2.56	0.41
82:S2:382:C:H2'	82:S2:383:G:C8	2.56	0.41
82:S2:1754:G:N7	82:S2:1779:G:N2	2.67	0.41
83:CB:27:HIS:HB3	83:CB:30:HIS:NE2	2.36	0.41
2:L5:270:U:H2'	2:L5:271:C:C6	2.56	0.41
2:L5:492:U:H2'	2:L5:493:G:O4'	2.20	0.41
2:L5:1174:G:H1	2:L5:1186:U:H3	1.68	0.41
2:L5:1972:G:H2'	2:L5:1973:G:C8	2.56	0.41
2:L5:2060:G:N2	22:LS:115:ALA:HB2	2.36	0.41
2:L5:2422:OMC:HM23	2:L5:2422:OMC:H1'	1.90	0.41
2:L5:2656:U:H5''	29:LZ:38:TYR:HB3	2.02	0.41
2:L5:2844:A:O2'	2:L5:4631:G:H4'	2.21	0.41
2:L5:3689:G:O2'	2:L5:3818:UY1:OP2	2.34	0.41
2:L5:3785:A2M:H2	2:L5:4551:U:O2	2.20	0.41
2:L5:4102:C:H1'	2:L5:4108:G:H1	1.86	0.41
2:L5:4260:U:H2'	2:L5:4261:C:H6	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L8:39:G:H1'	4:L8:103:A:N6	2.36	0.41
4:L8:47:C:H1'	4:L8:61:A:H2'	2.01	0.41
6:LB:286:LYS:HB3	6:LB:332:MET:HB3	2.03	0.41
8:LD:209:ARG:O	8:LD:213:GLU:HG2	2.21	0.41
18:LO:28:LEU:HD23	18:LO:28:LEU:HA	1.95	0.41
22:LS:83:ARG:HG3	22:LS:125:GLN:HB2	2.02	0.41
27:LX:81:LEU:HG	27:LX:83:THR:HG23	2.03	0.41
55:SR:7:LYS:HG3	82:S2:1373:C:OP1	2.20	0.41
55:SR:109:LEU:HG	55:SR:111:PHE:HD2	1.85	0.41
62:Sf:117:LEU:HD12	62:Sf:118:ARG:HD3	2.01	0.41
64:SA:147:LEU:HD13	64:SA:161:ILE:HB	2.03	0.41
67:SE:27:PHE:O	82:S2:495:U:O2'	2.38	0.41
70:SI:114:GLU:HG3	70:SI:119:LEU:O	2.21	0.41
71:SJ:142:VAL:HG12	71:SJ:144:ILE:H	1.85	0.41
76:SW:106:THR:OG1	76:SW:111:MET:HE2	2.21	0.41
82:S2:1374:C:H2'	82:S2:1375:G:O4'	2.21	0.41
83:CB:397:TYR:HB2	83:CB:494:MET:SD	2.61	0.41
83:CB:712:ASP:O	83:CB:716:ARG:HG2	2.20	0.41
83:CB:751:CYS:O	83:CB:782:PHE:HB2	2.21	0.41
85:CE:15:ALA:O	85:CE:19:ARG:HB2	2.21	0.41
2:L5:135:G:N3	2:L5:135:G:H2'	2.36	0.41
2:L5:1308:C:H2'	2:L5:1309:C:C6	2.56	0.41
2:L5:3607:U:H2'	2:L5:3608:A:C8	2.56	0.41
2:L5:4291:G:H4'	2:L5:4292:A:H5''	2.03	0.41
2:L5:4306:OMU:HM23	2:L5:4306:OMU:H1'	1.93	0.41
2:L5:4419:U:O4'	83:CB:765:ARG:CG	2.66	0.41
2:L5:4578:G:H2'	2:L5:4579:PSU:C6	2.56	0.41
2:L5:4770:U:H2'	2:L5:4771:C:C6	2.56	0.41
8:LD:37:VAL:HG12	8:LD:50:ARG:HD3	2.02	0.41
11:LG:160:ASP:OD1	11:LG:160:ASP:N	2.54	0.41
15:LL:18:TRP:CD1	15:LL:18:TRP:H	2.38	0.41
29:LZ:95:VAL:HG12	29:LZ:110:ALA:HA	2.03	0.41
32:Lc:20:LEU:O	32:Lc:24:SER:HB3	2.21	0.41
34:Le:85:LEU:HD21	34:Le:115:ALA:HB2	2.02	0.41
35:Lf:29:LYS:HB2	35:Lf:83:MET:HE1	2.02	0.41
53:SP:133:ILE:HG22	83:CB:708:THR:HB	1.91	0.41
59:SZ:102:LYS:HA	59:SZ:102:LYS:HD3	1.81	0.41
64:SA:80:ARG:HH21	64:SA:126:ASP:HB2	1.86	0.41
65:SB:120:MET:HE1	82:S2:987:A:C6	2.56	0.41
66:SC:64:THR:HG22	66:SC:66:LEU:N	2.35	0.41
68:SG:195:LYS:HD3	82:S2:126:G:H5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SH:58:LYS:HB2	69:SH:90:LYS:HG2	2.03	0.41
75:SV:27:LYS:HD3	75:SV:27:LYS:HA	1.86	0.41
77:SX:9:THR:HG22	82:S2:681:PSU:H4'	2.03	0.41
83:CB:330:LYS:HD3	83:CB:334:PRO:HB2	2.03	0.41
2:L5:260:C:H2'	2:L5:261:G:C8	2.55	0.41
2:L5:262:G:H2'	2:L5:263:G:H8	1.85	0.41
2:L5:1352:C:O2'	2:L5:1356:U:OP1	2.34	0.41
2:L5:1403:G:N2	2:L5:1415:G:C4	2.89	0.41
2:L5:1751:A:H2'	2:L5:1752:G:H8	1.86	0.41
2:L5:1776:A:C5'	85:CE:64:LEU:HD22	2.51	0.41
2:L5:2276:A:H2'	2:L5:2277:C:O4'	2.21	0.41
2:L5:2448:G:H2'	2:L5:2449:A:C8	2.56	0.41
2:L5:2461:G:H2'	2:L5:2462:C:C6	2.55	0.41
2:L5:2543:A:H2	2:L5:2773:G:H22	1.68	0.41
2:L5:2876:OMG:HM22	2:L5:2877:G:H5'	2.02	0.41
2:L5:2878:G:OP2	2:L5:2879:A:O2'	2.28	0.41
2:L5:4236:G:H4'	2:L5:4328:G:O2'	2.21	0.41
2:L5:4680:G:H2'	2:L5:4681:A:C8	2.55	0.41
2:L5:4710:C:H2'	2:L5:4711:C:C6	2.56	0.41
2:L5:4749:C:H2'	2:L5:4750:G:O4'	2.21	0.41
2:L5:4920:C:H2'	2:L5:4921:C:H6	1.86	0.41
2:L5:5002:U:H2'	2:L5:5003:U:C6	2.56	0.41
3:L7:7:G:H5''	8:LD:22:ARG:HD3	2.03	0.41
4:L8:149:G:H21	11:LG:64:GLN:HE22	1.69	0.41
6:LB:71:GLU:HB2	26:LW:2:LYS:HD3	2.02	0.41
6:LB:122:TRP:CE2	6:LB:127:LYS:HE3	2.56	0.41
13:LI:207:ASP:HA	13:LI:210:ARG:HG2	2.03	0.41
14:LJ:20:LEU:HD21	14:LJ:130:PHE:CD2	2.56	0.41
14:LJ:55:TYR:CD1	85:CE:46:VAL:HG11	2.54	0.41
16:LM:37:LEU:HD22	22:LS:75:VAL:HG23	2.02	0.41
18:LO:142:ALA:HA	18:LO:145:VAL:HG12	2.02	0.41
28:LY:74:TYR:CE2	28:LY:77:LYS:HG3	2.56	0.41
34:Le:100:ALA:HB3	34:Le:103:VAL:HG23	2.03	0.41
35:Lf:92:LEU:HD23	35:Lf:92:LEU:HA	1.90	0.41
36:Lg:33:LEU:HD23	36:Lg:33:LEU:HA	1.91	0.41
47:Ls:139:GLN:OE1	83:CB:180:ARG:CB	2.69	0.41
47:Ls:145:THR:O	83:CB:183:GLU:CD	2.63	0.41
48:Lt:12:VAL:HG11	48:Lt:65:GLN:N	2.36	0.41
48:Lt:114:ARG:NH1	48:Lt:126:SER:O	2.44	0.41
52:SM:95:ASP:HB3	52:SM:99:LYS:HB3	2.03	0.41
53:SP:133:ILE:CG2	83:CB:708:THR:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:SQ:128:GLU:HG2	54:SQ:137:ALA:HB1	2.02	0.41
57:ST:113:VAL:HG22	57:ST:123:LEU:HD23	2.02	0.41
59:SZ:68:ILE:HB	59:SZ:109:TYR:HB2	2.03	0.41
64:SA:122:LEU:HD22	64:SA:137:ALA:HB2	2.01	0.41
64:SA:172:GLY:HA3	64:SA:203:PHE:HD1	1.85	0.41
64:SA:219:GLU:HA	64:SA:222:VAL:HG12	2.03	0.41
67:SE:160:ILE:HD12	67:SE:162:ILE:HD11	2.02	0.41
69:SH:91:HIS:ND1	69:SH:169:LYS:HG2	2.35	0.41
70:SI:42:ARG:HH21	70:SI:59:ARG:NH1	2.19	0.41
70:SI:141:ARG:HA	70:SI:141:ARG:CZ	2.51	0.41
73:SN:37:ILE:HG23	73:SN:50:ILE:HG21	2.03	0.41
75:SV:11:LEU:HD23	75:SV:11:LEU:H	1.85	0.41
76:SW:57:ARG:NH2	80:Sb:26:GLN:HB2	2.36	0.41
76:SW:125:ILE:HA	76:SW:125:ILE:HD12	1.84	0.41
77:SX:139:GLU:HG2	83:CB:443:TYR:CE1	2.56	0.41
82:S2:43:U:OP2	82:S2:485:A:N6	2.47	0.41
82:S2:484:A2M:H8	82:S2:484:A2M:O5'	2.20	0.41
82:S2:693:A:H2	82:S2:739:C:H4'	1.84	0.41
82:S2:747:U:O2	82:S2:796:G:C2	2.74	0.41
82:S2:1223:A:H2'	82:S2:1224:G:O4'	2.21	0.41
82:S2:1446:A:O2'	82:S2:1447:G:H5''	2.20	0.41
83:CB:22:MET:HE2	83:CB:22:MET:HB2	1.95	0.41
83:CB:45:ILE:HG13	83:CB:46:ILE:N	2.36	0.41
83:CB:845:LYS:HA	83:CB:845:LYS:HD2	1.92	0.41
2:L5:126:C:H2'	2:L5:127:G:H8	1.85	0.41
2:L5:267:G:H2'	2:L5:268:G:C8	2.54	0.41
2:L5:1247:U:H2'	2:L5:1248:C:C6	2.56	0.41
2:L5:2412:A:H2'	2:L5:2413:U:C6	2.56	0.41
2:L5:2749:C:H2'	2:L5:2750:G:C8	2.56	0.41
3:L7:4:U:H2'	3:L7:5:A:C8	2.56	0.41
3:L7:26:C:O2'	14:LJ:147:ARG:NH1	2.52	0.41
20:LQ:59:PRO:HG3	20:LQ:143:ARG:HA	2.02	0.41
24:LU:80:LYS:HG2	24:LU:110:TYR:CE2	2.54	0.41
37:Lh:104:THR:O	37:Lh:108:GLN:HG2	2.21	0.41
48:Lt:131:GLU:OE2	48:Lt:155:ILE:HG21	2.21	0.41
50:SF:182:LYS:HE3	50:SF:182:LYS:HB2	1.89	0.41
51:SK:80:ARG:HH22	51:SK:90:VAL:HG12	1.86	0.41
52:SM:86:GLY:HA2	52:SM:89:VAL:HG12	2.02	0.41
53:SP:47:ARG:NE	82:S2:1619:A:OP1	2.40	0.41
55:SR:6:THR:HA	82:S2:1373:C:H5'	2.03	0.41
61:Sd:3:HIS:CE1	61:Sd:5:GLN:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:Sd:41:GLN:OE1	61:Sd:41:GLN:N	2.54	0.41
62:Sf:125:GLU:HG2	62:Sf:126:CYS:N	2.36	0.41
64:SA:164:ASN:OD1	64:SA:165:ASN:N	2.54	0.41
65:SB:136:ARG:O	65:SB:215:VAL:HA	2.21	0.41
68:SG:133:LEU:HB2	82:S2:65:C:C2	2.56	0.41
68:SG:136:LYS:O	68:SG:176:ILE:HG13	2.20	0.41
71:SJ:59:GLU:O	71:SJ:62:THR:OG1	2.32	0.41
79:Sa:36:ILE:HD11	79:Sa:75:VAL:HG12	2.02	0.41
82:S2:433:A:H2'	82:S2:434:G:C8	2.57	0.41
82:S2:462:OMC:HM23	82:S2:462:OMC:H1'	1.85	0.41
82:S2:692:G:N7	82:S2:693:A:N6	2.68	0.41
82:S2:815:U:C2	82:S2:816:A:C8	3.09	0.41
82:S2:1025:U:H2'	82:S2:1026:C:O4'	2.21	0.41
82:S2:1540:G:H2'	82:S2:1541:G:C8	2.56	0.41
83:CB:267:ASP:HB2	83:CB:285:LEU:HD23	2.02	0.41
2:L5:73:A:H5''	15:LL:105:LYS:HD3	2.02	0.40
2:L5:652:G:H2'	2:L5:653:U:C6	2.56	0.40
2:L5:1086:C:H2'	2:L5:1087:A:H8	1.85	0.40
2:L5:1631:A:C8	5:LA:199:VAL:HG21	2.56	0.40
2:L5:1962:A:H2	2:L5:2024:G:H21	1.67	0.40
2:L5:2497:C:H2'	2:L5:2498:C:H6	1.86	0.40
2:L5:4070:U:H2'	2:L5:4071:U:C6	2.56	0.40
5:LA:145:LYS:HA	5:LA:145:LYS:HD3	1.86	0.40
7:LC:158:VAL:HG12	7:LC:217:ILE:HD12	2.02	0.40
8:LD:239:MET:HA	8:LD:242:LYS:NZ	2.35	0.40
10:LF:148:LYS:O	10:LF:152:GLU:HG2	2.21	0.40
11:LG:207:VAL:O	11:LG:212:LYS:NZ	2.55	0.40
13:LI:51:HIS:ND1	13:LI:137:SER:OG	2.49	0.40
21:LR:82:LYS:HA	21:LR:82:LYS:HD2	1.89	0.40
23:LT:50:LYS:HB3	23:LT:50:LYS:HE2	1.80	0.40
28:LY:126:ARG:HG2	28:LY:130:LYS:HE2	2.03	0.40
36:Lg:60:ARG:HD2	36:Lg:60:ARG:HA	1.84	0.40
48:Lt:22:VAL:HA	48:Lt:48:LYS:HG2	2.02	0.40
48:Lt:28:LEU:O	48:Lt:32:ILE:HD12	2.20	0.40
58:SU:52:GLY:HA3	82:S2:1401:A:H4'	2.03	0.40
66:SC:256:TRP:CE2	76:SW:68:ARG:HD3	2.56	0.40
69:SH:17:ASP:OD1	69:SH:17:ASP:N	2.51	0.40
70:SI:192:GLY:O	70:SI:196:GLU:HG3	2.22	0.40
82:S2:368:U:H3'	82:S2:369:C:H2'	2.03	0.40
82:S2:496:C:H2'	82:S2:497:C:H6	1.86	0.40
82:S2:880:G:H3'	82:S2:881:G:H8	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:CB:13:MET:HE2	83:CB:468:ASN:HB3	2.03	0.40
83:CB:649:ILE:HD13	83:CB:663:THR:HB	2.03	0.40
84:Et:40:C:H2'	84:Et:41:U:H6	1.86	0.40
2:L5:302:C:H2'	2:L5:303:C:H6	1.87	0.40
2:L5:423:G:H2'	2:L5:424:U:C6	2.57	0.40
2:L5:1974:U:H4'	2:L5:1975:G:H3'	2.03	0.40
2:L5:2683:C:H2'	2:L5:2684:C:C6	2.57	0.40
2:L5:4196:OMG:HM23	2:L5:4196:OMG:H1'	1.70	0.40
2:L5:4232:U:H5'	44:Lo:3:ASN:HB3	2.03	0.40
2:L5:4616:A:H2'	2:L5:4617:G:O4'	2.21	0.40
2:L5:4906:C:H2'	2:L5:4907:G:H8	1.86	0.40
2:L5:5015:G:H2'	2:L5:5016:A:C2	2.57	0.40
12:LH:27:VAL:HG12	12:LH:84:VAL:HG21	2.03	0.40
12:LH:43:VAL:HG21	12:LH:73:ILE:HD13	2.03	0.40
27:LX:80:PRO:HA	27:LX:98:PHE:HA	2.01	0.40
48:Lt:114:ARG:O	48:Lt:117:ARG:HG2	2.22	0.40
48:Lt:150:ASP:OD1	48:Lt:151:ILE:N	2.53	0.40
63:Sg:191:HIS:CD2	63:Sg:195:LEU:HD11	2.56	0.40
65:SB:114:VAL:O	82:S2:1869:A:N6	2.53	0.40
70:SI:5:ARG:NE	82:S2:379:C:O2	2.54	0.40
82:S2:64:A:N6	82:S2:83:A:OP2	2.54	0.40
82:S2:835:C:H4'	82:S2:836:G:H8	1.86	0.40
82:S2:1112:U:O2	82:S2:1121:G:O6	2.40	0.40
82:S2:1719:A:N6	82:S2:1814:G:O2'	2.54	0.40
2:L5:31:U:H2'	2:L5:32:G:O4'	2.21	0.40
2:L5:1186:U:H2'	2:L5:1187:G:N3	2.36	0.40
2:L5:1558:A:H2'	2:L5:1559:G:C8	2.56	0.40
2:L5:1794:A:H5''	2:L5:4214:A:H61	1.86	0.40
2:L5:2632:PSU:H2'	2:L5:2633:U:C6	2.56	0.40
2:L5:3951:G:H1'	2:L5:4062:A:H61	1.86	0.40
2:L5:4169:G:H4'	2:L5:4171:C:C2	2.56	0.40
2:L5:4232:U:H5''	44:Lo:3:ASN:O	2.21	0.40
5:LA:75:LEU:HD12	5:LA:75:LEU:HA	1.91	0.40
5:LA:150:LEU:HD11	5:LA:156:LYS:HD2	2.03	0.40
26:LW:102:LYS:HA	26:LW:105:ARG:HG2	2.03	0.40
36:Lg:84:ALA:O	36:Lg:88:ARG:HG3	2.20	0.40
40:Lk:25:ILE:HD13	40:Lk:57:LYS:HZ3	1.84	0.40
45:Lp:23:ARG:HA	45:Lp:26:VAL:HG12	2.04	0.40
47:Ls:58:ASN:O	47:Ls:62:ARG:NE	2.42	0.40
48:Lt:37:LEU:HA	48:Lt:40:LYS:HE3	2.03	0.40
50:SF:100:ILE:HD11	50:SF:108:PRO:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:SM:112:LYS:HE2	52:SM:112:LYS:HB2	1.83	0.40
54:SQ:34:VAL:HG22	54:SQ:70:VAL:HB	2.03	0.40
63:Sg:230:LEU:HD11	63:Sg:259:TRP:CG	2.56	0.40
63:Sg:251:ALA:HA	63:Sg:256:ILE:HD13	2.04	0.40
65:SB:67:PHE:CE2	74:SO:48:SER:HB3	2.56	0.40
74:SO:140:THR:HB	82:S2:1046:PSU:H1'	2.03	0.40
77:SX:22:TRP:HE3	77:SX:28:LYS:HD2	1.85	0.40
81:Se:36:MET:SD	81:Se:40:ARG:NE	2.87	0.40
82:S2:323:C:H5'	82:S2:324:C:OP1	2.21	0.40
82:S2:737:G:H2'	82:S2:738:C:H4'	2.03	0.40
82:S2:1406:G:H2'	82:S2:1407:U:C6	2.57	0.40
83:CB:447:ILE:HG21	83:CB:472:LEU:HD22	2.03	0.40
2:L5:223:G:N7	7:LC:165:LYS:HE3	2.37	0.40
2:L5:1307:A:H2'	2:L5:1308:C:C6	2.57	0.40
2:L5:1494:U:H2'	2:L5:1495:G:C8	2.57	0.40
2:L5:1806:G:H2'	2:L5:1807:C:H6	1.86	0.40
2:L5:3652:A:H2'	2:L5:3653:A:C5	2.56	0.40
2:L5:4153:C:H2'	2:L5:4154:G:H8	1.87	0.40
2:L5:4571:A2M:H2'	2:L5:4572:U:H6	1.86	0.40
3:L7:4:U:H2'	3:L7:5:A:H8	1.86	0.40
3:L7:7:G:OP1	8:LD:33:ARG:NH1	2.52	0.40
5:LA:131:GLY:N	5:LA:169:VAL:HG13	2.36	0.40
8:LD:53:VAL:HG11	8:LD:159:VAL:HA	2.03	0.40
20:LQ:32:TYR:HD1	20:LQ:32:TYR:HA	1.72	0.40
36:Lg:41:ALA:O	36:Lg:52:ARG:NH1	2.49	0.40
67:SE:89:VAL:HG11	67:SE:119:ALA:HB1	2.02	0.40
70:SI:129:LEU:HD12	70:SI:129:LEU:HA	1.91	0.40
77:SX:68:LYS:HG2	77:SX:91:LEU:HD22	2.04	0.40
82:S2:874:G:H2'	82:S2:875:A:C8	2.52	0.40
83:CB:521:VAL:HA	83:CB:524:LEU:HB2	2.03	0.40
83:CB:524:LEU:HD11	83:CB:546:ILE:HD11	2.04	0.40
84:Et:39:U:H2'	84:Et:40:C:H6	1.87	0.40
2:L5:683:C:H2'	2:L5:684:G:O4'	2.21	0.40
2:L5:1081:C:O2'	2:L5:1082:C:H5'	2.21	0.40
2:L5:1419:G:H5''	20:LQ:71:LYS:NZ	2.37	0.40
2:L5:1588:U:H2'	2:L5:1589:C:C6	2.57	0.40
2:L5:1645:C:H2'	2:L5:1646:A:C8	2.56	0.40
2:L5:4069:U:H2'	2:L5:4070:U:C6	2.57	0.40
2:L5:4305:G:C6	23:LT:80:VAL:HG21	2.56	0.40
2:L5:4415:A:OP1	13:LI:154:ARG:NH2	2.54	0.40
2:L5:4625:C:O2'	2:L5:4626:A:H5'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L5:4991:U:H2'	2:L5:4992:G:C8	2.56	0.40
5:LA:14:SER:OG	5:LA:15:VAL:N	2.54	0.40
14:LJ:40:LEU:HD23	14:LJ:40:LEU:HA	1.92	0.40
27:LX:88:LYS:HE3	27:LX:88:LYS:HB2	1.95	0.40
50:SF:97:PHE:HA	50:SF:100:ILE:HG12	2.03	0.40
63:Sg:66:VAL:HA	63:Sg:82:SER:HB2	2.03	0.40
63:Sg:314:ILE:HD12	63:Sg:314:ILE:HA	1.92	0.40
64:SA:57:LYS:HA	64:SA:57:LYS:HD2	1.79	0.40
65:SB:89:GLU:OE2	65:SB:99:ASN:HB3	2.21	0.40
69:SH:113:LYS:HA	69:SH:113:LYS:HD2	1.64	0.40
71:SJ:124:HIS:HD2	81:Se:31:ARG:HE	1.69	0.40
73:SN:94:LYS:HE2	73:SN:94:LYS:HB2	1.93	0.40
77:SX:52:LEU:N	77:SX:71:ARG:O	2.53	0.40
80:Sb:33:MET:HE3	80:Sb:48:SER:HA	2.04	0.40
82:S2:1351:G:O2'	82:S2:1378:A:N1	2.55	0.40
82:S2:1360:U:O2'	82:S2:1379:A:OP2	2.33	0.40
84:Et:25:C:H3'	84:Et:26:A:H5''	2.03	0.40
85:CE:57:GLU:O	85:CE:61:LEU:HB2	2.21	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
5	LA	246/248 (99%)	228 (93%)	18 (7%)	0	100	100
6	LB	400/402 (100%)	383 (96%)	17 (4%)	0	100	100
7	LC	366/368 (100%)	351 (96%)	15 (4%)	0	100	100
8	LD	291/293 (99%)	283 (97%)	8 (3%)	0	100	100
9	LE	236/250 (94%)	224 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
11	LG	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
12	LH	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
13	LI	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
14	LJ	168/176 (96%)	162 (96%)	6 (4%)	0	100	100
15	LL	208/210 (99%)	201 (97%)	7 (3%)	0	100	100
16	LM	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
17	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
18	LO	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
19	LP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
20	LQ	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
21	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
22	LS	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
23	LT	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
24	LU	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
25	LV	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
26	LW	112/124 (90%)	107 (96%)	5 (4%)	0	100	100
27	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
28	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
29	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100
30	La	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
31	Lb	105/121 (87%)	99 (94%)	6 (6%)	0	100	100
32	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
33	Ld	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
34	Le	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
35	Lf	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
36	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
37	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
38	Li	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
39	Lj	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
40	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	Ll	48/50 (96%)	48 (100%)	0	0	100	100
42	Lm	50/52 (96%)	50 (100%)	0	0	100	100
43	Ln	22/24 (92%)	22 (100%)	0	0	100	100
44	Lo	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
45	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
46	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
47	Ls	194/196 (99%)	180 (93%)	14 (7%)	0	100	100
48	Lt	128/157 (82%)	111 (87%)	17 (13%)	0	100	100
49	SD	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
50	SF	187/189 (99%)	175 (94%)	12 (6%)	0	100	100
51	SK	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
52	SM	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
53	SP	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
54	SQ	142/144 (99%)	130 (92%)	12 (8%)	0	100	100
55	SR	133/135 (98%)	126 (95%)	6 (4%)	1 (1%)	16	31
56	SS	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
57	ST	141/143 (99%)	138 (98%)	3 (2%)	0	100	100
58	SU	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
59	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
60	Sc	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
61	Sd	53/55 (96%)	53 (100%)	0	0	100	100
62	Sf	65/67 (97%)	56 (86%)	9 (14%)	0	100	100
63	Sg	311/313 (99%)	291 (94%)	20 (6%)	0	100	100
64	SA	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
65	SB	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
66	SC	218/222 (98%)	203 (93%)	15 (7%)	0	100	100
67	SE	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
68	SG	235/237 (99%)	222 (94%)	13 (6%)	0	100	100
69	SH	182/189 (96%)	169 (93%)	13 (7%)	0	100	100
70	SI	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
71	SJ	183/185 (99%)	176 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	SL	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
73	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
74	SO	135/140 (96%)	127 (94%)	8 (6%)	0	100	100
75	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
76	SW	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
77	SX	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
78	SY	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
79	Sa	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
80	Sb	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
81	Se	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
83	CB	842/856 (98%)	811 (96%)	30 (4%)	1 (0%)	48	69
85	CE	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
All	All	12585/12836 (98%)	12046 (96%)	537 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
83	CB	481	LYS
55	SR	129	LYS

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
5	LA	190/190 (100%)	190 (100%)	0	100	100
6	LB	348/348 (100%)	348 (100%)	0	100	100
7	LC	306/306 (100%)	306 (100%)	0	100	100
8	LD	246/247 (100%)	246 (100%)	0	100	100
9	LE	212/222 (96%)	212 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	LF	194/194 (100%)	194 (100%)	0	100	100
11	LG	203/205 (99%)	203 (100%)	0	100	100
12	LH	169/169 (100%)	169 (100%)	0	100	100
13	LI	180/180 (100%)	180 (100%)	0	100	100
14	LJ	143/148 (97%)	143 (100%)	0	100	100
15	LL	176/176 (100%)	176 (100%)	0	100	100
16	LM	118/118 (100%)	118 (100%)	0	100	100
17	LN	171/171 (100%)	171 (100%)	0	100	100
18	LO	173/173 (100%)	173 (100%)	0	100	100
19	LP	134/134 (100%)	134 (100%)	0	100	100
20	LQ	164/164 (100%)	164 (100%)	0	100	100
21	LR	166/166 (100%)	166 (100%)	0	100	100
22	LS	156/156 (100%)	156 (100%)	0	100	100
23	LT	139/139 (100%)	139 (100%)	0	100	100
24	LU	91/91 (100%)	91 (100%)	0	100	100
25	LV	101/101 (100%)	101 (100%)	0	100	100
26	LW	95/103 (92%)	95 (100%)	0	100	100
27	LX	108/108 (100%)	108 (100%)	0	100	100
28	LY	124/124 (100%)	124 (100%)	0	100	100
29	LZ	117/117 (100%)	117 (100%)	0	100	100
30	La	120/120 (100%)	120 (100%)	0	100	100
31	Lb	88/101 (87%)	88 (100%)	0	100	100
32	Lc	83/83 (100%)	83 (100%)	0	100	100
33	Ld	98/98 (100%)	98 (100%)	0	100	100
34	Le	114/114 (100%)	114 (100%)	0	100	100
35	Lf	88/88 (100%)	88 (100%)	0	100	100
36	Lg	98/98 (100%)	98 (100%)	0	100	100
37	Lh	109/109 (100%)	109 (100%)	0	100	100
38	Li	86/86 (100%)	86 (100%)	0	100	100
39	Lj	73/73 (100%)	73 (100%)	0	100	100
40	Lk	64/64 (100%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	Ll	47/47 (100%)	47 (100%)	0	100	100
42	Lm	48/48 (100%)	48 (100%)	0	100	100
43	Ln	23/23 (100%)	23 (100%)	0	100	100
44	Lo	93/93 (100%)	93 (100%)	0	100	100
45	Lp	74/74 (100%)	74 (100%)	0	100	100
46	Lr	109/109 (100%)	109 (100%)	0	100	100
47	Ls	162/164 (99%)	162 (100%)	0	100	100
48	Lt	107/130 (82%)	107 (100%)	0	100	100
49	SD	190/190 (100%)	190 (100%)	0	100	100
50	SF	159/159 (100%)	159 (100%)	0	100	100
51	SK	89/89 (100%)	89 (100%)	0	100	100
52	SM	102/104 (98%)	102 (100%)	0	100	100
53	SP	107/107 (100%)	107 (100%)	0	100	100
54	SQ	119/119 (100%)	119 (100%)	0	100	100
55	SR	122/122 (100%)	122 (100%)	0	100	100
56	SS	126/126 (100%)	126 (100%)	0	100	100
57	ST	113/113 (100%)	113 (100%)	0	100	100
58	SU	94/94 (100%)	94 (100%)	0	100	100
59	SZ	66/66 (100%)	66 (100%)	0	100	100
60	Sc	57/57 (100%)	57 (100%)	0	100	100
61	Sd	48/48 (100%)	48 (100%)	0	100	100
62	Sf	60/60 (100%)	60 (100%)	0	100	100
63	Sg	272/272 (100%)	272 (100%)	0	100	100
64	SA	183/183 (100%)	183 (100%)	0	100	100
65	SB	195/195 (100%)	195 (100%)	0	100	100
66	SC	186/188 (99%)	186 (100%)	0	100	100
67	SE	224/224 (100%)	224 (100%)	0	100	100
68	SG	207/207 (100%)	207 (100%)	0	100	100
69	SH	166/169 (98%)	166 (100%)	0	100	100
70	SI	178/178 (100%)	178 (100%)	0	100	100
71	SJ	161/161 (100%)	161 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
72	SL	137/137 (100%)	137 (100%)	0	100	100
73	SN	130/130 (100%)	130 (100%)	0	100	100
74	SO	107/110 (97%)	107 (100%)	0	100	100
75	SV	67/67 (100%)	67 (100%)	0	100	100
76	SW	112/112 (100%)	112 (100%)	0	100	100
77	SX	113/113 (100%)	113 (100%)	0	100	100
78	SY	113/113 (100%)	113 (100%)	0	100	100
79	Sa	89/89 (100%)	89 (100%)	0	100	100
80	Sb	75/75 (100%)	75 (100%)	0	100	100
81	Se	47/47 (100%)	47 (100%)	0	100	100
83	CB	722/728 (99%)	722 (100%)	0	100	100
85	CE	62/62 (100%)	62 (100%)	0	100	100
All	All	10931/11011 (99%)	10931 (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 (81) such sidechains are listed below:

Mol	Chain	Res	Type
5	LA	97	ASN
6	LB	68	ASN
6	LB	145	GLN
6	LB	184	GLN
6	LB	203	GLN
6	LB	301	ASN
7	LC	329	ASN
7	LC	347	HIS
10	LF	239	GLN
11	LG	64	GLN
11	LG	112	GLN
12	LH	98	HIS
12	LH	138	GLN
13	LI	59	GLN
14	LJ	112	HIS
15	LL	19	GLN
15	LL	149	GLN
16	LM	34	ASN
17	LN	117	ASN

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Mol	Chain	Res	Type
18	LO	50	ASN
18	LO	199	HIS
19	LP	97	ASN
19	LP	118	GLN
19	LP	137	ASN
22	LS	23	HIS
22	LS	37	HIS
22	LS	108	GLN
23	LT	144	ASN
24	LU	94	ASN
25	LV	77	HIS
26	LW	79	GLN
26	LW	104	GLN
28	LY	61	HIS
30	La	34	ASN
30	La	67	GLN
30	La	120	GLN
31	Lb	60	ASN
34	Le	52	GLN
38	Li	15	HIS
39	Lj	66	HIS
41	Ll	33	ASN
42	Lm	117	HIS
45	Lp	33	GLN
46	Lr	4	HIS
46	Lr	21	ASN
47	Ls	71	ASN
48	Lt	65	GLN
48	Lt	149	HIS
50	SF	29	GLN
51	SK	28	HIS
51	SK	32	HIS
52	SM	19	GLN
54	SQ	48	GLN
58	SU	81	GLN
58	SU	92	HIS
59	SZ	89	GLN
61	Sd	5	GLN
62	Sf	93	HIS
63	Sg	285	GLN
64	SA	9	GLN
64	SA	84	GLN

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Mol	Chain	Res	Type
64	SA	132	GLN
65	SB	76	ASN
65	SB	95	ASN
65	SB	158	HIS
66	SC	267	GLN
68	SG	227	GLN
69	SH	76	GLN
69	SH	114	GLN
69	SH	162	GLN
70	SI	35	ASN
70	SI	52	ASN
72	SL	19	ASN
72	SL	65	ASN
73	SN	105	ASN
75	SV	35	ASN
77	SX	16	HIS
79	Sa	72	HIS
83	CB	168	GLN
83	CB	803	ASN
83	CB	807	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L5	3643/3675 (99%)	711 (19%)	15 (0%)
3	L7	119/120 (99%)	9 (7%)	0
4	L8	155/156 (99%)	24 (15%)	0
82	S2	1714/1740 (98%)	360 (21%)	4 (0%)
84	Et	73/76 (96%)	25 (34%)	0
All	All	5704/5767 (98%)	1129 (19%)	19 (0%)

All (1129) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L5	2	G
2	L5	25	A
2	L5	30	C
2	L5	39	A
2	L5	42	A
2	L5	48	G
2	L5	56	A

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Mol	Chain	Res	Type
2	L5	59	A
2	L5	64	A
2	L5	65	A
2	L5	73	A
2	L5	91	G
2	L5	104	G
2	L5	108	A
2	L5	109	G
2	L5	110	C
2	L5	119	G
2	L5	120	A
2	L5	127	G
2	L5	132	G
2	L5	133	C
2	L5	134	G
2	L5	135	G
2	L5	136	C
2	L5	159	C
2	L5	165	A
2	L5	172	C
2	L5	173	C
2	L5	181	C
2	L5	182	G
2	L5	183	C
2	L5	184	U
2	L5	185	C
2	L5	187	U
2	L5	188	G
2	L5	189	G
2	L5	200	U
2	L5	209	U
2	L5	210	C
2	L5	216	C
2	L5	218	A
2	L5	220	C
2	L5	234	G
2	L5	237	G
2	L5	255	C
2	L5	256	G
2	L5	261	G
2	L5	263	G
2	L5	264	C

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Mol	Chain	Res	Type
2	L5	265	C
2	L5	266	C
2	L5	267	G
2	L5	280	G
2	L5	297	U
2	L5	306	A
2	L5	315	G
2	L5	316	U
2	L5	340	C
2	L5	373	G
2	L5	385	A
2	L5	387	G
2	L5	388	A
2	L5	396	A
2	L5	407	A
2	L5	409	G
2	L5	410	A
2	L5	411	G
2	L5	412	G
2	L5	432	U
2	L5	449	C
2	L5	452	A
2	L5	453	G
2	L5	454	U
2	L5	456	C
2	L5	457	G
2	L5	467	U
2	L5	484	U
2	L5	485	C
2	L5	486	C
2	L5	489	C
2	L5	494	U
2	L5	497	G
2	L5	498	C
2	L5	499	G
2	L5	500	G
2	L5	502	C
2	L5	503	C
2	L5	504	G
2	L5	509	A
2	L5	510	U
2	L5	512	U

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Mol	Chain	Res	Type
2	L5	513	U
2	L5	514	U
2	L5	518	G
2	L5	643	C
2	L5	646	G
2	L5	653	U
2	L5	654	C
2	L5	655	C
2	L5	656	C
2	L5	657	C
2	L5	659	G
2	L5	666	G
2	L5	667	A
2	L5	668	C
2	L5	669	C
2	L5	672	C
2	L5	673	C
2	L5	685	C
2	L5	686	A
2	L5	687	U
2	L5	696	C
2	L5	704	C
2	L5	708	G
2	L5	730	G
2	L5	731	G
2	L5	738	C
2	L5	739	G
2	L5	742	G
2	L5	746	A
2	L5	759	G
2	L5	904	C
2	L5	905	C
2	L5	910	G
2	L5	913	U
2	L5	914	U
2	L5	915	A
2	L5	917	A
2	L5	923	C
2	L5	924	C
2	L5	932	A
2	L5	933	G
2	L5	936	C

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Mol	Chain	Res	Type
2	L5	943	A
2	L5	944	A
2	L5	945	U
2	L5	946	C
2	L5	956	A
2	L5	959	G
2	L5	960	A
2	L5	961	G
2	L5	962	C
2	L5	965	G
2	L5	966	A
2	L5	967	C
2	L5	969	C
2	L5	970	G
2	L5	977	C
2	L5	982	U
2	L5	985	C
2	L5	1070	G
2	L5	1071	C
2	L5	1072	C
2	L5	1075	G
2	L5	1082	C
2	L5	1083	U
2	L5	1168	G
2	L5	1171	G
2	L5	1172	C
2	L5	1173	G
2	L5	1179	U
2	L5	1180	C
2	L5	1181	C
2	L5	1182	C
2	L5	1183	C
2	L5	1187	G
2	L5	1202	C
2	L5	1203	G
2	L5	1210	C
2	L5	1211	G
2	L5	1214	C
2	L5	1215	C
2	L5	1219	G
2	L5	1222	A
2	L5	1246	G

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Mol	Chain	Res	Type
2	L5	1253	G
2	L5	1254	A
2	L5	1257	A
2	L5	1258	G
2	L5	1262	G
2	L5	1266	G
2	L5	1267	C
2	L5	1269	G
2	L5	1271	G
2	L5	1272	C
2	L5	1273	G
2	L5	1275	G
2	L5	1280	C
2	L5	1284	G
2	L5	1285	U
2	L5	1287	G
2	L5	1293	G
2	L5	1294	A
2	L5	1295	C
2	L5	1296	G
2	L5	1301	C
2	L5	1326	A2M
2	L5	1337	A
2	L5	1354	A
2	L5	1359	G
2	L5	1365	C
2	L5	1366	G
2	L5	1367	C
2	L5	1379	C
2	L5	1387	A
2	L5	1394	G
2	L5	1397	A
2	L5	1398	A
2	L5	1403	G
2	L5	1404	G
2	L5	1407	C
2	L5	1409	C
2	L5	1410	U
2	L5	1411	C
2	L5	1414	C
2	L5	1417	C
2	L5	1420	A

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Mol	Chain	Res	Type
2	L5	1425	G
2	L5	1437	C
2	L5	1439	C
2	L5	1442	C
2	L5	1443	A
2	L5	1444	G
2	L5	1446	C
2	L5	1447	C
2	L5	1482	G
2	L5	1483	C
2	L5	1497	A
2	L5	1498	G
2	L5	1502	G
2	L5	1517	G
2	L5	1524	A2M
2	L5	1534	A2M
2	L5	1537	A
2	L5	1547	A
2	L5	1566	C
2	L5	1578	U
2	L5	1591	U
2	L5	1596	U
2	L5	1621	A
2	L5	1624	G
2	L5	1625	OMG
2	L5	1631	A
2	L5	1633	G
2	L5	1634	A
2	L5	1638	A
2	L5	1640	C
2	L5	1641	G
2	L5	1642	A
2	L5	1654	G
2	L5	1661	C
2	L5	1676	C
2	L5	1677	PSU
2	L5	1678	C
2	L5	1694	C
2	L5	1697	G
2	L5	1699	A
2	L5	1700	G
2	L5	1701	A

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Mol	Chain	Res	Type
2	L5	1702	C
2	L5	1704	C
2	L5	1705	G
2	L5	1717	C
2	L5	1718	C
2	L5	1719	A
2	L5	1721	G
2	L5	1726	U
2	L5	1731	C
2	L5	1734	G
2	L5	1742	A
2	L5	1750	G
2	L5	1755	C
2	L5	1757	U
2	L5	1758	G
2	L5	1760	G
2	L5	1761	G
2	L5	1762	C
2	L5	1763	C
2	L5	1764	G
2	L5	1765	A
2	L5	1766	A
2	L5	1767	A
2	L5	1768	C
2	L5	1770	A
2	L5	1787	A
2	L5	1804	A
2	L5	1806	G
2	L5	1810	G
2	L5	1815	G
2	L5	1821	G
2	L5	1822	U
2	L5	1834	U
2	L5	1836	G
2	L5	1837	A
2	L5	1842	G
2	L5	1855	G
2	L5	1869	G
2	L5	1882	U
2	L5	1897	A
2	L5	1917	A
2	L5	1918	U

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Mol	Chain	Res	Type
2	L5	1919	G
2	L5	1920	C
2	L5	1921	C
2	L5	1922	G
2	L5	1925	G
2	L5	1930	U
2	L5	1931	C
2	L5	1932	A
2	L5	1940	G
2	L5	1948	G
2	L5	1951	G
2	L5	1961	G
2	L5	1962	A
2	L5	1974	U
2	L5	1975	G
2	L5	1978	C
2	L5	1980	U
2	L5	1981	G
2	L5	1982	G
2	L5	1983	A
2	L5	1984	A
2	L5	1985	G
2	L5	1986	U
2	L5	1991	A
2	L5	1993	C
2	L5	1997	U
2	L5	1998	A
2	L5	1999	A
2	L5	2001	G
2	L5	2002	A
2	L5	2003	G
2	L5	2004	U
2	L5	2011	C
2	L5	2017	A
2	L5	2018	C
2	L5	2024	G
2	L5	2026	A
2	L5	2046	G
2	L5	2048	U
2	L5	2055	G
2	L5	2056	G
2	L5	2069	A

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Mol	Chain	Res	Type
2	L5	2084	C
2	L5	2085	G
2	L5	2092	G
2	L5	2093	A
2	L5	2095	A
2	L5	2097	U
2	L5	2098	G
2	L5	2101	C
2	L5	2102	G
2	L5	2107	C
2	L5	2110	C
2	L5	2111	G
2	L5	2112	G
2	L5	2250	C
2	L5	2252	G
2	L5	2256	C
2	L5	2261	G
2	L5	2289	C
2	L5	2300	A
2	L5	2301	G
2	L5	2313	A
2	L5	2333	G
2	L5	2348	G
2	L5	2351	OMC
2	L5	2360	A
2	L5	2364	OMG
2	L5	2383	C
2	L5	2395	A
2	L5	2397	G
2	L5	2417	A
2	L5	2425	U
2	L5	2450	G
2	L5	2453	A
2	L5	2464	C
2	L5	2465	C
2	L5	2469	C
2	L5	2471	G
2	L5	2474	G
2	L5	2475	G
2	L5	2478	C
2	L5	2479	G
2	L5	2483	G

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Mol	Chain	Res	Type
2	L5	2484	A
2	L5	2485	U
2	L5	2487	G
2	L5	2488	C
2	L5	2489	C
2	L5	2490	U
2	L5	2494	U
2	L5	2504	C
2	L5	2505	C
2	L5	2506	G
2	L5	2507	A
2	L5	2513	A
2	L5	2519	U
2	L5	2529	A
2	L5	2537	A
2	L5	2544	G
2	L5	2546	G
2	L5	2547	G
2	L5	2554	U
2	L5	2555	G
2	L5	2556	G
2	L5	2560	C
2	L5	2565	A
2	L5	2567	G
2	L5	2573	A
2	L5	2583	C
2	L5	2587	A
2	L5	2589	C
2	L5	2602	G
2	L5	2618	G
2	L5	2627	C
2	L5	2653	C
2	L5	2662	G
2	L5	2669	C
2	L5	2675	G
2	L5	2676	A
2	L5	2687	U
2	L5	2694	G
2	L5	2695	A
2	L5	2696	A
2	L5	2706	G
2	L5	2707	U

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Mol	Chain	Res	Type
2	L5	2708	U
2	L5	2710	C
2	L5	2711	G
2	L5	2712	G
2	L5	2721	G
2	L5	2724	G
2	L5	2726	G
2	L5	2739	C
2	L5	2742	G
2	L5	2743	A
2	L5	2746	A
2	L5	2761	U
2	L5	2763	U
2	L5	2769	U
2	L5	2770	C
2	L5	2788	U
2	L5	2790	U
2	L5	2806	A
2	L5	2814	C
2	L5	2826	U
2	L5	2827	G
2	L5	2829	U
2	L5	2838	G
2	L5	2855	G
2	L5	2867	C
2	L5	2877	G
2	L5	2892	C
2	L5	2894	A
2	L5	2899	C
2	L5	2900	U
2	L5	2902	G
2	L5	2903	G
2	L5	2904	U
2	L5	2905	C
2	L5	2907	G
2	L5	2908	U
2	L5	3590	G
2	L5	3591	C
2	L5	3592	G
2	L5	3594	C
2	L5	3595	U
2	L5	3596	A

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Mol	Chain	Res	Type
2	L5	3597	G
2	L5	3604	A
2	L5	3605	C
2	L5	3616	U
2	L5	3617	G
2	L5	3626	G
2	L5	3630	A
2	L5	3635	A
2	L5	3644	U
2	L5	3646	A
2	L5	3648	A
2	L5	3662	A
2	L5	3664	G
2	L5	3670	C
2	L5	3673	C
2	L5	3674	G
2	L5	3691	G
2	L5	3701	OMC
2	L5	3710	G
2	L5	3711	A
2	L5	3713	U
2	L5	3726	A
2	L5	3727	A
2	L5	3748	A
2	L5	3753	G
2	L5	3760	A
2	L5	3770	U
2	L5	3774	A
2	L5	3775	A
2	L5	3776	G
2	L5	3777	G
2	L5	3785	A2M
2	L5	3786	U
2	L5	3792	OMG
2	L5	3811	G
2	L5	3812	C
2	L5	3814	U
2	L5	3817	A
2	L5	3819	G
2	L5	3824	A
2	L5	3838	U
2	L5	3839	G

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Mol	Chain	Res	Type
2	L5	3840	U
2	L5	3867	A2M
2	L5	3877	A
2	L5	3878	C
2	L5	3879	G
2	L5	3885	G
2	L5	3892	U
2	L5	3897	G
2	L5	3901	A
2	L5	3906	A
2	L5	3907	G
2	L5	3908	A
2	L5	3915	U
2	L5	3923	A
2	L5	3938	G
2	L5	3939	G
2	L5	3942	A
2	L5	3947	A
2	L5	3949	A
2	L5	3950	U
2	L5	3953	G
2	L5	4057	C
2	L5	4058	U
2	L5	4059	C
2	L5	4061	G
2	L5	4062	A
2	L5	4064	C
2	L5	4065	G
2	L5	4068	U
2	L5	4076	G
2	L5	4084	G
2	L5	4095	G
2	L5	4097	G
2	L5	4098	A
2	L5	4099	G
2	L5	4101	C
2	L5	4104	G
2	L5	4108	G
2	L5	4111	U
2	L5	4112	C
2	L5	4114	C
2	L5	4115	G

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Mol	Chain	Res	Type
2	L5	4116	C
2	L5	4122	G
2	L5	4127	A
2	L5	4133	C
2	L5	4140	C
2	L5	4141	G
2	L5	4142	C
2	L5	4143	G
2	L5	4144	C
2	L5	4146	G
2	L5	4149	C
2	L5	4162	C
2	L5	4163	U
2	L5	4170	A
2	L5	4183	G
2	L5	4184	G
2	L5	4191	G
2	L5	4203	A
2	L5	4222	G
2	L5	4225	G
2	L5	4229	U
2	L5	4233	A
2	L5	4251	A
2	L5	4254	G
2	L5	4257	A
2	L5	4258	C
2	L5	4265	U
2	L5	4268	A
2	L5	4273	A
2	L5	4281	A
2	L5	4291	G
2	L5	4295	U
2	L5	4304	A
2	L5	4305	G
2	L5	4306	OMU
2	L5	4314	C
2	L5	4319	C
2	L5	4329	G
2	L5	4330	G
2	L5	4332	C
2	L5	4349	C
2	L5	4350	C

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Mol	Chain	Res	Type
2	L5	4354	U
2	L5	4373	G
2	L5	4376	A
2	L5	4377	G
2	L5	4378	A
2	L5	4379	A
2	L5	4387	C
2	L5	4391	G
2	L5	4394	A
2	L5	4420	U
2	L5	4421	C
2	L5	4422	A
2	L5	4438	U
2	L5	4448	G
2	L5	4449	A
2	L5	4464	A
2	L5	4466	C
2	L5	4475	G
2	L5	4488	A
2	L5	4500	PSU
2	L5	4512	U
2	L5	4513	A
2	L5	4515	G
2	L5	4519	C
2	L5	4524	G
2	L5	4525	C
2	L5	4545	G
2	L5	4548	A
2	L5	4557	U
2	L5	4560	C
2	L5	4567	G
2	L5	4575	G
2	L5	4584	A
2	L5	4589	A
2	L5	4590	A2M
2	L5	4600	G
2	L5	4601	U
2	L5	4617	G
2	L5	4636	PSU
2	L5	4637	OMG
2	L5	4652	G
2	L5	4656	A

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Mol	Chain	Res	Type
2	L5	4670	C
2	L5	4672	A
2	L5	4679	G
2	L5	4687	A
2	L5	4694	G
2	L5	4695	C
2	L5	4700	A
2	L5	4708	A
2	L5	4709	U
2	L5	4719	G
2	L5	4733	C
2	L5	4734	A
2	L5	4740	G
2	L5	4741	C
2	L5	4742	G
2	L5	4745	G
2	L5	4754	G
2	L5	4757	C
2	L5	4759	C
2	L5	4761	G
2	L5	4765	G
2	L5	4771	C
2	L5	4772	C
2	L5	4775	C
2	L5	4859	C
2	L5	4870	G
2	L5	4871	C
2	L5	4875	G
2	L5	4882	U
2	L5	4883	C
2	L5	4889	G
2	L5	4895	C
2	L5	4896	G
2	L5	4897	G
2	L5	4899	G
2	L5	4900	C
2	L5	4901	G
2	L5	4910	G
2	L5	4912	G
2	L5	4914	C
2	L5	4922	C
2	L5	4925	U

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Mol	Chain	Res	Type
2	L5	4926	C
2	L5	4927	G
2	L5	4928	C
2	L5	4934	A
2	L5	4940	C
2	L5	4941	G
2	L5	4943	A
2	L5	4951	G
2	L5	4955	A
2	L5	4960	G
2	L5	4976	U
2	L5	4985	U
2	L5	4988	U
2	L5	4989	U
2	L5	4991	U
2	L5	4995	U
2	L5	5007	A
2	L5	5013	C
2	L5	5014	A
2	L5	5017	G
2	L5	5022	U
2	L5	5023	C
2	L5	5024	C
2	L5	5028	G
2	L5	5030	U
2	L5	5034	A
2	L5	5041	G
2	L5	5050	C
2	L5	5054	C
2	L5	5055	G
2	L5	5061	A
2	L5	5069	U
3	L7	33	U
3	L7	38	U
3	L7	53	U
3	L7	54	A
3	L7	64	G
3	L7	97	G
3	L7	100	A
3	L7	110	G
3	L7	120	U
4	L8	23	C

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Mol	Chain	Res	Type
4	L8	25	G
4	L8	34	U
4	L8	35	C
4	L8	59	A
4	L8	62	A
4	L8	63	U
4	L8	80	A
4	L8	82	A
4	L8	84	A
4	L8	85	U
4	L8	87	G
4	L8	94	G
4	L8	103	A
4	L8	105	C
4	L8	111	U
4	L8	114	G
4	L8	123	U
4	L8	124	U
4	L8	125	C
4	L8	126	C
4	L8	127	U
4	L8	147	G
4	L8	153	C
82	S2	13	C
82	S2	14	C
82	S2	17	C
82	S2	25	A
82	S2	33	G
82	S2	41	G
82	S2	44	U
82	S2	45	A
82	S2	46	A
82	S2	56	G
82	S2	58	C
82	S2	59	U
82	S2	65	C
82	S2	67	C
82	S2	68	A
82	S2	72	C
82	S2	73	C
82	S2	74	G
82	S2	76	U

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Mol	Chain	Res	Type
82	S2	99	A2M
82	S2	103	A
82	S2	113	G
82	S2	114	G
82	S2	115	U
82	S2	126	G
82	S2	130	G
82	S2	142	C
82	S2	143	U
82	S2	149	A
82	S2	158	A
82	S2	160	U
82	S2	162	C
82	S2	170	A
82	S2	175	A
82	S2	179	C
82	S2	190	G
82	S2	191	A
82	S2	196	C
82	S2	197	U
82	S2	198	U
82	S2	200	G
82	S2	203	G
82	S2	204	G
82	S2	207	G
82	S2	208	G
82	S2	214	U
82	S2	291	G
82	S2	292	A
82	S2	295	C
82	S2	302	A
82	S2	306	C
82	S2	307	G
82	S2	308	G
82	S2	309	G
82	S2	311	C
82	S2	312	G
82	S2	313	A
82	S2	318	A
82	S2	319	C
82	S2	323	C
82	S2	324	C

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Mol	Chain	Res	Type
82	S2	325	C
82	S2	326	C
82	S2	328	U
82	S2	329	G
82	S2	332	G
82	S2	339	A
82	S2	340	C
82	S2	347	G
82	S2	360	A
82	S2	362	C
82	S2	364	A
82	S2	368	U
82	S2	370	G
82	S2	385	G
82	S2	386	C
82	S2	398	A
82	S2	407	G
82	S2	408	A
82	S2	409	C
82	S2	436	OMG
82	S2	438	G
82	S2	448	A
82	S2	449	A
82	S2	450	C
82	S2	452	G
82	S2	464	A
82	S2	465	A
82	S2	471	G
82	S2	472	C
82	S2	473	A
82	S2	474	G
82	S2	476	A
82	S2	482	G
82	S2	487	U
82	S2	488	U
82	S2	492	C
82	S2	493	A
82	S2	502	C
82	S2	516	A
82	S2	517	OMC
82	S2	531	A
82	S2	532	C

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Mol	Chain	Res	Type
82	S2	536	A
82	S2	537	C
82	S2	540	U
82	S2	542	U
82	S2	544	G
82	S2	546	G
82	S2	547	G
82	S2	557	U
82	S2	558	G
82	S2	559	G
82	S2	563	G
82	S2	564	A
82	S2	576	A2M
82	S2	583	A
82	S2	587	A
82	S2	589	G
82	S2	590	A
82	S2	591	U
82	S2	593	C
82	S2	604	A
82	S2	614	C
82	S2	617	G
82	S2	623	G
82	S2	628	A
82	S2	631	U
82	S2	643	A
82	S2	644	OMG
82	S2	655	A
82	S2	660	C
82	S2	664	A
82	S2	668	A2M
82	S2	669	A
82	S2	671	A
82	S2	672	A
82	S2	673	G
82	S2	683	OMG
82	S2	688	U
82	S2	689	U
82	S2	692	G
82	S2	696	G
82	S2	697	G
82	S2	698	G

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Mol	Chain	Res	Type
82	S2	731	G
82	S2	732	U
82	S2	733	C
82	S2	736	C
82	S2	737	G
82	S2	738	C
82	S2	749	U
82	S2	751	G
82	S2	752	G
82	S2	753	C
82	S2	788	G
82	S2	791	C
82	S2	792	C
82	S2	798	G
82	S2	799	OMU
82	S2	801	PSU
82	S2	821	G
82	S2	822	U
82	S2	823	U
82	S2	824	C
82	S2	830	A
82	S2	834	C
82	S2	835	C
82	S2	836	G
82	S2	837	A
82	S2	838	G
82	S2	839	C
82	S2	842	C
82	S2	844	U
82	S2	847	A
82	S2	867	OMG
82	S2	870	A
82	S2	874	G
82	S2	877	C
82	S2	878	G
82	S2	880	G
82	S2	888	U
82	S2	889	U
82	S2	891	G
82	S2	893	U
82	S2	894	G
82	S2	896	U

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Mol	Chain	Res	Type
82	S2	897	U
82	S2	898	U
82	S2	899	U
82	S2	900	C
82	S2	901	G
82	S2	903	A
82	S2	913	A
82	S2	920	A
82	S2	930	C
82	S2	933	G
82	S2	934	G
82	S2	943	U
82	S2	963	A
82	S2	970	G
82	S2	971	G
82	S2	972	A
82	S2	985	G
82	S2	990	A
82	S2	992	A
82	S2	999	G
82	S2	1001	A
82	S2	1008	A
82	S2	1017	U
82	S2	1023	A
82	S2	1027	A
82	S2	1060	A
82	S2	1061	U
82	S2	1062	A
82	S2	1080	A
82	S2	1083	A
82	S2	1085	C
82	S2	1109	C
82	S2	1113	A
82	S2	1114	U
82	S2	1116	C
82	S2	1121	G
82	S2	1123	C
82	S2	1133	A
82	S2	1138	C
82	S2	1148	A
82	S2	1150	A
82	S2	1153	C

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Mol	Chain	Res	Type
82	S2	1154	U
82	S2	1195	A
82	S2	1207	G
82	S2	1208	A
82	S2	1215	C
82	S2	1216	C
82	S2	1217	A
82	S2	1224	G
82	S2	1227	G
82	S2	1242	U
82	S2	1243	U
82	S2	1248	B8N
82	S2	1251	A
82	S2	1253	A
82	S2	1256	G
82	S2	1257	G
82	S2	1259	A
82	S2	1271	C
82	S2	1272	OMC
82	S2	1274	G
82	S2	1275	G
82	S2	1283	C
82	S2	1286	G
82	S2	1288	OMU
82	S2	1294	G
82	S2	1295	A
82	S2	1301	A
82	S2	1302	G
82	S2	1303	C
82	S2	1304	U
82	S2	1308	U
82	S2	1342	U
82	S2	1357	A
82	S2	1358	U
82	S2	1371	U
82	S2	1372	U
82	S2	1376	A
82	S2	1378	A
82	S2	1402	A
82	S2	1413	G
82	S2	1418	C
82	S2	1419	C

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Mol	Chain	Res	Type
82	S2	1420	G
82	S2	1421	A
82	S2	1422	G
82	S2	1423	C
82	S2	1433	C
82	S2	1435	C
82	S2	1437	C
82	S2	1438	A
82	S2	1439	A
82	S2	1442	OMU
82	S2	1449	G
82	S2	1454	A
82	S2	1463	U
82	S2	1478	U
82	S2	1487	A
82	S2	1489	A
82	S2	1490	OMG
82	S2	1492	U
82	S2	1494	U
82	S2	1495	G
82	S2	1497	G
82	S2	1498	A
82	S2	1521	C
82	S2	1531	A
82	S2	1533	A
82	S2	1544	C
82	S2	1546	G
82	S2	1552	G
82	S2	1553	C
82	S2	1556	A
82	S2	1558	C
82	S2	1574	C
82	S2	1575	G
82	S2	1578	U
82	S2	1580	A
82	S2	1581	C
82	S2	1587	G
82	S2	1588	A
82	S2	1600	G
82	S2	1604	G
82	S2	1606	G
82	S2	1621	U

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Mol	Chain	Res	Type
82	S2	1623	A
82	S2	1631	U
82	S2	1633	A
82	S2	1634	A
82	S2	1637	A
82	S2	1648	G
82	S2	1654	G
82	S2	1663	A
82	S2	1665	G
82	S2	1683	C
82	S2	1686	G
82	S2	1695	A
82	S2	1698	C
82	S2	1699	A
82	S2	1715	A
82	S2	1721	U
82	S2	1722	G
82	S2	1744	G
82	S2	1745	A
82	S2	1752	C
82	S2	1753	C
82	S2	1754	G
82	S2	1755	C
82	S2	1757	G
82	S2	1759	G
82	S2	1761	U
82	S2	1772	C
82	S2	1773	C
82	S2	1774	C
82	S2	1777	G
82	S2	1782	G
82	S2	1783	C
82	S2	1784	G
82	S2	1786	U
82	S2	1798	C
82	S2	1810	U
82	S2	1825	A
82	S2	1826	G
82	S2	1831	A
82	S2	1835	A
82	S2	1838	U
82	S2	1849	G

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Mol	Chain	Res	Type
82	S2	1851	MA6
82	S2	1861	G
82	S2	1862	G
82	S2	1863	A
82	S2	1865	C
84	Et	4	C
84	Et	9	A
84	Et	11	C
84	Et	19	G
84	Et	20	U
84	Et	21	A
84	Et	26	A
84	Et	33	U
84	Et	35	U
84	Et	36	U
84	Et	37	A
84	Et	38	A
84	Et	39	U
84	Et	42	G
84	Et	44	G
84	Et	46	G
84	Et	47	U
84	Et	49	C
84	Et	50	A
84	Et	55	U
84	Et	56	C
84	Et	58	A
84	Et	70	G
84	Et	71	G
84	Et	76	A

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	L5	406	C
2	L5	493	G
2	L5	914	U
2	L5	1082	C
2	L5	1590	C
2	L5	1633	G
2	L5	1703	C
2	L5	1977	C

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Mol	Chain	Res	Type
2	L5	2416	G
2	L5	2675	G
2	L5	2760	G
2	L5	3673	C
2	L5	4600	G
2	L5	4699	U
2	L5	4913	G
82	S2	291	G
82	S2	563	G
82	S2	688	U
82	S2	1477	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
82	OMG	S2	436	82	23,26,27	0.51	0	32,38,41	0.54	0
2	PSU	L5	3920	86,2	18,21,22	1.05	2 (11%)	21,30,33	1.97	5 (23%)
2	OMG	L5	4623	2	23,26,27	0.59	0	32,38,41	0.58	0
82	PSU	S2	681	82	18,21,22	1.06	1 (5%)	21,30,33	1.87	4 (19%)
2	PSU	L5	4576	2	18,21,22	1.09	1 (5%)	21,30,33	1.94	4 (19%)
82	OMU	S2	121	82	19,22,23	3.29	7 (36%)	25,31,34	1.82	5 (20%)
82	A2M	S2	159	82	22,25,26	1.15	1 (4%)	30,36,39	1.51	7 (23%)
82	OMG	S2	644	82	23,26,27	0.49	0	32,38,41	0.49	0
2	PSU	L5	3884	2	18,21,22	1.08	2 (11%)	21,30,33	1.96	4 (19%)
2	PSU	L5	1683	2	18,21,22	1.09	2 (11%)	21,30,33	2.11	5 (23%)
2	OMU	L5	4620	2	19,22,23	3.17	7 (36%)	25,31,34	1.71	4 (16%)
2	OMG	L5	4370	2	23,26,27	0.57	0	32,38,41	0.52	0
2	PSU	L5	1860	2	18,21,22	1.10	1 (5%)	21,30,33	1.97	4 (19%)
2	OMU	L5	4227	2	19,22,23	3.27	7 (36%)	25,31,34	1.87	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	4442	2	18,21,22	1.09	1 (5%)	21,30,33	2.03	6 (28%)
82	OMG	S2	601	82	23,26,27	0.52	0	32,38,41	0.43	0
2	OMC	L5	2351	86,2	19,22,23	0.67	0	25,31,34	0.90	1 (4%)
2	1MA	L5	1322	86,2	21,25,26	0.63	0	30,37,40	0.80	2 (6%)
2	PSU	L5	4552	2	18,21,22	1.11	2 (11%)	21,30,33	2.01	5 (23%)
2	OMG	L5	1625	2	23,26,27	0.55	0	32,38,41	0.50	0
82	PSU	S2	1177	82	18,21,22	1.08	2 (11%)	21,30,33	1.98	4 (19%)
2	PSU	L5	4353	2	18,21,22	1.10	2 (11%)	21,30,33	2.05	6 (28%)
82	PSU	S2	1232	82	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
82	OMU	S2	1288	82	19,22,23	3.40	7 (36%)	25,31,34	1.75	5 (20%)
2	OMG	L5	4618	2	23,26,27	0.56	0	32,38,41	0.53	0
82	OMC	S2	1391	82	19,22,23	0.56	0	25,31,34	0.68	0
2	OMG	L5	1316	2	23,26,27	0.64	0	32,38,41	0.55	0
2	OMC	L5	2824	2	19,22,23	0.61	0	25,31,34	0.63	0
2	PSU	L5	4521	86,2	18,21,22	1.11	3 (16%)	21,30,33	2.05	6 (28%)
2	PSU	L5	1677	2	18,21,22	1.05	1 (5%)	21,30,33	1.91	3 (14%)
82	OMU	S2	1442	82	19,22,23	3.33	7 (36%)	25,31,34	1.78	5 (20%)
2	OMC	L5	2804	2	19,22,23	0.63	0	25,31,34	0.67	0
2	PSU	L5	4689	2	18,21,22	1.07	2 (11%)	21,30,33	2.07	4 (19%)
2	A2M	L5	1524	2	22,25,26	1.27	2 (9%)	30,36,39	1.52	6 (20%)
82	MA6	S2	1850	82	23,26,27	1.28	2 (8%)	33,38,41	3.36	12 (36%)
82	PSU	S2	109	82	18,21,22	1.08	2 (11%)	21,30,33	1.93	4 (19%)
82	PSU	S2	649	82	18,21,22	1.06	1 (5%)	21,30,33	2.01	5 (23%)
2	PSU	L5	1744	86,2	18,21,22	1.08	1 (5%)	21,30,33	1.98	5 (23%)
82	A2M	S2	1031	82	22,25,26	1.16	2 (9%)	30,36,39	1.59	6 (20%)
82	A2M	S2	668	82,86	22,25,26	1.32	2 (9%)	30,36,39	1.63	7 (23%)
82	PSU	S2	1056	82	18,21,22	1.07	2 (11%)	21,30,33	1.97	5 (23%)
2	A2M	L5	3825	2	22,25,26	1.17	2 (9%)	30,36,39	1.58	8 (26%)
2	PSU	L5	2632	2	18,21,22	1.10	1 (5%)	21,30,33	1.97	5 (23%)
82	PSU	S2	105	82	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
2	A2M	L5	398	2	22,25,26	1.20	1 (4%)	30,36,39	1.63	7 (23%)
82	G7M	S2	1639	82	23,26,27	2.63	9 (39%)	34,39,42	2.53	11 (32%)
2	PSU	L5	5001	2	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
2	OMG	L5	2876	2	23,26,27	0.56	0	32,38,41	0.56	0
2	OMG	L5	3899	2	23,26,27	0.63	0	32,38,41	0.54	0
2	OMG	L5	4494	2	23,26,27	0.58	0	32,38,41	0.50	0
2	A2M	L5	4571	2	22,25,26	1.28	3 (13%)	30,36,39	1.59	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	L5	4499	2	23,26,27	0.54	0	32,38,41	0.45	0
82	OMC	S2	174	82	19,22,23	0.53	0	25,31,34	0.65	0
2	OMC	L5	2422	86,2	19,22,23	0.63	0	25,31,34	0.69	0
82	A2M	S2	576	82	22,25,26	1.18	1 (4%)	30,36,39	1.54	6 (20%)
82	PSU	S2	1004	82	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
2	OMG	L5	3627	2	23,26,27	0.55	0	32,38,41	0.61	0
82	OMG	S2	509	82	23,26,27	0.51	0	32,38,41	0.50	0
2	UY1	L5	3818	2	19,22,23	4.82	10 (52%)	21,31,34	2.00	5 (23%)
82	OMG	S2	1328	82	23,26,27	0.48	0	32,38,41	0.44	0
82	PSU	S2	1367	82	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
2	OMG	L5	3744	2	23,26,27	0.56	0	32,38,41	0.46	0
2	OMC	L5	3887	2	19,22,23	0.60	0	25,31,34	0.67	0
2	OMU	L5	4498	2	19,22,23	3.22	7 (36%)	25,31,34	1.85	5 (20%)
2	A2M	L5	1534	86,2	22,25,26	1.22	3 (13%)	30,36,39	1.44	7 (23%)
82	6MZ	S2	1832	82,86	26,26,26	2.83	5 (19%)	36,39,39	2.03	10 (27%)
2	OMU	L5	2837	2	19,22,23	3.24	7 (36%)	25,31,34	1.88	5 (20%)
2	PSU	L5	3853	86,2	18,21,22	1.09	1 (5%)	21,30,33	1.95	4 (19%)
2	5MC	L5	4447	2	19,22,23	0.87	0	26,32,35	0.65	0
82	A2M	S2	166	82	22,25,26	1.23	1 (4%)	30,36,39	1.59	7 (23%)
2	A2M	L5	1871	86,2	22,25,26	1.26	3 (13%)	30,36,39	1.62	6 (20%)
82	4AC	S2	1337	82	21,24,25	0.40	0	28,34,37	0.81	2 (7%)
82	OMG	S2	867	82	23,26,27	0.51	0	32,38,41	0.45	0
82	MA6	S2	1851	82	23,26,27	1.28	2 (8%)	33,38,41	3.42	12 (36%)
82	A2M	S2	1383	82	22,25,26	1.18	1 (4%)	30,36,39	1.62	7 (23%)
82	OMU	S2	354	82	19,22,23	3.25	7 (36%)	25,31,34	1.88	5 (20%)
2	A2M	L5	3785	86,2	22,25,26	1.15	1 (4%)	30,36,39	1.63	10 (33%)
2	OMG	L5	2424	2	23,26,27	0.57	0	32,38,41	0.44	0
2	PSU	L5	2839	2	18,21,22	1.08	2 (11%)	21,30,33	2.01	5 (23%)
2	OMC	L5	3869	2	19,22,23	0.62	0	25,31,34	0.71	0
82	A2M	S2	99	82,86	22,25,26	1.19	1 (4%)	30,36,39	1.57	7 (23%)
2	A2M	L5	1323	2	22,25,26	1.20	2 (9%)	30,36,39	1.60	9 (30%)
82	PSU	S2	93	82	18,21,22	1.08	1 (5%)	21,30,33	1.82	4 (19%)
82	A2M	S2	484	82	22,25,26	1.17	1 (4%)	30,36,39	1.47	7 (23%)
2	A2M	L5	2401	2	22,25,26	1.21	1 (4%)	30,36,39	1.64	7 (23%)
2	OMC	L5	4456	2	19,22,23	0.71	1 (5%)	25,31,34	0.77	1 (4%)
2	PSU	L5	3844	2	18,21,22	1.12	1 (5%)	21,30,33	1.92	4 (19%)
82	OMG	S2	1490	82	23,26,27	0.57	0	32,38,41	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	4673	86,2	18,21,22	1.07	1 (5%)	21,30,33	1.93	4 (19%)
2	PSU	L5	3822	2	18,21,22	1.09	1 (5%)	21,30,33	1.96	5 (23%)
2	OMG	L5	3792	2	23,26,27	0.56	0	32,38,41	0.47	0
2	PSU	L5	4457	2	18,21,22	1.05	2 (11%)	21,30,33	2.09	6 (28%)
2	OMC	L5	1340	2	19,22,23	0.67	0	25,31,34	0.80	0
2	PSU	L5	4296	2	18,21,22	1.05	1 (5%)	21,30,33	1.95	4 (19%)
82	PSU	S2	1045	82	18,21,22	1.06	1 (5%)	21,30,33	1.96	4 (19%)
2	OMC	L5	2365	86,2	19,22,23	0.63	0	25,31,34	0.59	0
2	PSU	L5	3695	2	18,21,22	1.05	2 (11%)	21,30,33	2.00	5 (23%)
2	PSU	L5	4972	2	18,21,22	1.02	1 (5%)	21,30,33	1.92	5 (23%)
2	PSU	L5	4293	2	18,21,22	1.08	2 (11%)	21,30,33	1.99	4 (19%)
82	OMU	S2	627	82	19,22,23	3.38	7 (36%)	25,31,34	1.80	5 (20%)
2	PSU	L5	4579	2	18,21,22	1.07	1 (5%)	21,30,33	1.99	4 (19%)
2	A2M	L5	4590	2	22,25,26	1.17	1 (4%)	30,36,39	1.53	6 (20%)
2	PSU	L5	1781	2	18,21,22	1.05	1 (5%)	21,30,33	1.83	4 (19%)
2	PSU	L5	4500	2	18,21,22	1.14	2 (11%)	21,30,33	2.05	5 (23%)
82	PSU	S2	801	82	18,21,22	1.11	1 (5%)	21,30,33	1.82	4 (19%)
2	PSU	L5	3637	2	18,21,22	1.08	1 (5%)	21,30,33	2.02	5 (23%)
4	PSU	L8	69	4	18,21,22	1.08	1 (5%)	21,30,33	2.04	6 (28%)
2	OMC	L5	4536	2	19,22,23	0.65	0	25,31,34	0.75	0
2	PSU	L5	1782	2	18,21,22	1.07	1 (5%)	21,30,33	1.89	4 (19%)
82	PSU	S2	863	82	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
2	A2M	L5	1326	2	22,25,26	1.21	2 (9%)	30,36,39	1.51	9 (30%)
2	6MZ	L5	4220	2	26,26,26	2.73	6 (23%)	36,39,39	2.90	16 (44%)
2	PSU	L5	4403	2	18,21,22	1.03	1 (5%)	21,30,33	1.98	6 (28%)
2	5MC	L5	3782	86,2	19,22,23	0.69	0	26,32,35	0.80	1 (3%)
2	PSU	L5	4532	2	18,21,22	1.07	1 (5%)	21,30,33	1.90	4 (19%)
2	A2M	L5	3718	2	22,25,26	1.13	1 (4%)	30,36,39	1.55	6 (20%)
82	PSU	S2	814	82	18,21,22	1.06	1 (5%)	21,30,33	1.83	4 (19%)
82	A2M	S2	468	82	22,25,26	1.24	1 (4%)	30,36,39	1.57	7 (23%)
2	PSU	L5	4312	2	18,21,22	1.09	2 (11%)	21,30,33	1.97	4 (19%)
2	PSU	L5	4299	2	18,21,22	1.05	1 (5%)	21,30,33	1.88	4 (19%)
2	OMC	L5	3701	2	19,22,23	0.71	0	25,31,34	1.74	4 (16%)
82	PSU	S2	966	82,86	18,21,22	1.07	1 (5%)	21,30,33	1.88	4 (19%)
2	A2M	L5	3830	2	22,25,26	1.17	1 (4%)	30,36,39	1.57	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	4471	2	18,21,22	1.05	1 (5%)	21,30,33	1.91	4 (19%)
2	PSU	L5	4493	2	18,21,22	1.06	1 (5%)	21,30,33	1.88	4 (19%)
2	OMG	L5	2364	86,2	23,26,27	0.59	0	32,38,41	0.45	0
2	PSU	L5	4361	2	18,21,22	1.05	1 (5%)	21,30,33	1.86	4 (19%)
2	PSU	L5	5010	2	18,21,22	1.10	1 (5%)	21,30,33	1.94	4 (19%)
2	PSU	L5	3851	2	18,21,22	1.04	1 (5%)	21,30,33	1.95	4 (19%)
82	OMU	S2	1326	82	19,22,23	3.32	7 (36%)	25,31,34	1.84	5 (20%)
82	PSU	S2	406	82	18,21,22	1.06	1 (5%)	21,30,33	1.98	5 (23%)
2	OMG	L5	4196	2	23,26,27	0.56	0	32,38,41	0.45	0
2	PSU	L5	4431	2	18,21,22	1.04	1 (5%)	21,30,33	1.90	4 (19%)
2	OMG	L5	4392	2	23,26,27	0.59	0	32,38,41	0.48	0
2	PSU	L5	1862	2	18,21,22	1.04	1 (5%)	21,30,33	2.01	4 (19%)
2	A2M	L5	3867	2	22,25,26	1.27	2 (9%)	30,36,39	1.50	9 (30%)
2	A2M	L5	400	2	22,25,26	1.24	3 (13%)	30,36,39	1.60	9 (30%)
82	OMU	S2	428	82	19,22,23	3.32	7 (36%)	25,31,34	1.87	5 (20%)
2	A2M	L5	4523	86,2	22,25,26	1.27	3 (13%)	30,36,39	1.58	8 (26%)
82	PSU	S2	686	82	18,21,22	1.05	1 (5%)	21,30,33	1.93	4 (19%)
82	PSU	S2	1081	82	18,21,22	1.03	1 (5%)	21,30,33	1.96	5 (23%)
2	PSU	L5	4973	2	18,21,22	1.05	1 (5%)	21,30,33	1.98	5 (23%)
82	OMU	S2	799	82	19,22,23	3.36	7 (36%)	25,31,34	1.80	5 (20%)
82	PSU	S2	651	82	18,21,22	1.08	1 (5%)	21,30,33	1.96	4 (19%)
82	PSU	S2	1244	82	18,21,22	1.08	1 (5%)	21,30,33	1.93	5 (23%)
2	OMG	L5	4637	2	23,26,27	0.57	0	32,38,41	0.49	0
82	OMC	S2	462	82	19,22,23	0.54	0	25,31,34	0.69	0
2	OMU	L5	4306	2	19,22,23	3.22	7 (36%)	25,31,34	1.88	5 (20%)
82	4AC	S2	1842	82	21,24,25	0.39	0	28,34,37	0.48	0
82	OMC	S2	1703	82	19,22,23	0.61	0	25,31,34	0.59	0
2	OMC	L5	3841	2	19,22,23	0.63	0	25,31,34	0.72	0
2	PSU	L5	4636	2	18,21,22	1.10	1 (5%)	21,30,33	2.04	6 (28%)
82	OMU	S2	172	82	19,22,23	3.31	7 (36%)	25,31,34	1.85	5 (20%)
2	A2M	L5	2815	2	22,25,26	1.18	2 (9%)	30,36,39	1.54	8 (26%)
2	A2M	L5	2787	2	22,25,26	1.15	1 (4%)	30,36,39	1.50	7 (23%)
2	PSU	L5	3639	2	18,21,22	1.08	2 (11%)	21,30,33	2.06	5 (23%)
82	PSU	S2	1174	82	18,21,22	1.06	1 (5%)	21,30,33	1.95	4 (19%)
2	OMG	L5	1522	2	23,26,27	0.58	0	32,38,41	0.64	1 (3%)
82	OMG	S2	683	82	23,26,27	0.54	0	32,38,41	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	L5	1582	2	18,21,22	1.05	1 (5%)	21,30,33	1.81	4 (19%)
2	OMC	L5	3808	86,2	19,22,23	0.69	0	25,31,34	0.81	1 (4%)
82	OMC	S2	1272	82	19,22,23	0.55	0	25,31,34	0.85	1 (4%)
2	A2M	L5	2363	86,2	22,25,26	1.19	2 (9%)	30,36,39	1.53	9 (30%)
2	OMC	L5	2861	2	19,22,23	0.63	0	25,31,34	0.77	1 (4%)
4	OMG	L8	75	4	23,26,27	0.53	0	32,38,41	0.48	0
2	OMU	L5	3925	2	19,22,23	3.21	7 (36%)	25,31,34	1.94	5 (20%)
4	PSU	L8	55	4	18,21,22	1.04	1 (5%)	21,30,33	1.98	4 (19%)
82	B8N	S2	1248	82	25,29,30	3.25	6 (24%)	28,42,45	1.98	7 (25%)
82	PSU	S2	1046	82	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
2	OMG	L5	4228	2	23,26,27	0.55	0	32,38,41	0.65	0
2	PSU	L5	1792	2	18,21,22	1.01	1 (5%)	21,30,33	1.90	4 (19%)
2	PSU	L5	1536	2	18,21,22	1.05	1 (5%)	21,30,33	1.90	4 (19%)
2	PSU	L5	4628	2	18,21,22	1.01	1 (5%)	21,30,33	1.86	5 (23%)
82	OMC	S2	517	82	19,22,23	0.56	0	25,31,34	0.64	0
82	PSU	S2	866	82	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
82	A2M	S2	27	82	22,25,26	1.19	1 (4%)	30,36,39	1.55	7 (23%)
2	UR3	L5	4530	2	19,22,23	2.63	7 (36%)	26,32,35	1.58	2 (7%)
82	OMU	S2	116	82	19,22,23	3.30	7 (36%)	25,31,34	1.76	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	OMG	S2	436	82	-	2/9/27/28	0/3/3/3
2	PSU	L5	3920	86,2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4623	2	-	0/9/27/28	0/3/3/3
82	PSU	S2	681	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	4576	2	-	0/7/25/26	0/2/2/2
82	OMU	S2	121	82	-	0/9/27/28	0/2/2/2
82	A2M	S2	159	82	-	1/9/27/28	0/3/3/3
82	OMG	S2	644	82	-	3/9/27/28	0/3/3/3
2	PSU	L5	3884	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	1683	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4620	2	-	0/9/27/28	0/2/2/2
2	OMG	L5	4370	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L5	1860	2	-	0/7/25/26	0/2/2/2
2	OMU	L5	4227	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4442	2	-	0/7/25/26	0/2/2/2
82	OMG	S2	601	82	-	1/9/27/28	0/3/3/3
2	OMC	L5	2351	86,2	-	2/9/27/28	0/2/2/2
2	1MA	L5	1322	86,2	-	2/7/25/26	0/3/3/3
2	PSU	L5	4552	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	1625	2	-	2/9/27/28	0/3/3/3
82	PSU	S2	1177	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	4353	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	1232	82	-	0/7/25/26	0/2/2/2
82	OMU	S2	1288	82	-	2/9/27/28	0/2/2/2
2	OMG	L5	4618	2	-	2/9/27/28	0/3/3/3
82	OMC	S2	1391	82	-	0/9/27/28	0/2/2/2
2	OMG	L5	1316	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	2824	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4521	86,2	-	0/7/25/26	0/2/2/2
2	PSU	L5	1677	2	-	3/7/25/26	0/2/2/2
82	OMU	S2	1442	82	-	2/9/27/28	0/2/2/2
2	OMC	L5	2804	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	4689	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	1524	2	-	2/9/27/28	0/3/3/3
82	MA6	S2	1850	82	-	0/11/29/30	0/3/3/3
82	PSU	S2	109	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	649	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	1744	86,2	-	0/7/25/26	0/2/2/2
82	A2M	S2	1031	82	-	0/9/27/28	0/3/3/3
82	A2M	S2	668	82,86	-	2/9/27/28	0/3/3/3
82	PSU	S2	1056	82	-	0/7/25/26	0/2/2/2
2	A2M	L5	3825	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	2632	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	105	82	-	0/7/25/26	0/2/2/2
2	A2M	L5	398	2	-	1/9/27/28	0/3/3/3
82	G7M	S2	1639	82	-	2/7/25/26	0/3/3/3
2	PSU	L5	5001	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	2876	2	-	2/9/27/28	0/3/3/3
2	OMG	L5	3899	2	-	2/9/27/28	0/3/3/3
2	OMG	L5	4494	2	-	0/9/27/28	0/3/3/3
2	A2M	L5	4571	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	L5	4499	2	-	0/9/27/28	0/3/3/3
82	OMC	S2	174	82	-	0/9/27/28	0/2/2/2
2	OMC	L5	2422	86,2	-	2/9/27/28	0/2/2/2
82	A2M	S2	576	82	-	3/9/27/28	0/3/3/3
82	PSU	S2	1004	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	3627	2	-	0/9/27/28	0/3/3/3
82	OMG	S2	509	82	-	0/9/27/28	0/3/3/3
2	UY1	L5	3818	2	-	2/9/27/28	0/2/2/2
82	OMG	S2	1328	82	-	0/9/27/28	0/3/3/3
82	PSU	S2	1367	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	3744	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	3887	2	-	1/9/27/28	0/2/2/2
2	OMU	L5	4498	2	-	0/9/27/28	0/2/2/2
2	A2M	L5	1534	86,2	-	1/9/27/28	0/3/3/3
82	6MZ	S2	1832	82,86	-	3/12/28/28	0/3/3/3
2	OMU	L5	2837	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	3853	86,2	-	0/7/25/26	0/2/2/2
2	5MC	L5	4447	2	-	4/7/25/26	0/2/2/2
82	A2M	S2	166	82	-	1/9/27/28	0/3/3/3
2	A2M	L5	1871	86,2	-	0/9/27/28	0/3/3/3
82	4AC	S2	1337	82	-	1/11/29/30	0/2/2/2
82	OMG	S2	867	82	-	3/9/27/28	0/3/3/3
82	MA6	S2	1851	82	-	1/11/29/30	0/3/3/3
82	A2M	S2	1383	82	-	3/9/27/28	0/3/3/3
82	OMU	S2	354	82	-	0/9/27/28	0/2/2/2
2	A2M	L5	3785	86,2	-	1/9/27/28	0/3/3/3
2	OMG	L5	2424	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	2839	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3869	2	-	1/9/27/28	0/2/2/2
82	A2M	S2	99	82,86	-	2/9/27/28	0/3/3/3
2	A2M	L5	1323	2	-	2/9/27/28	0/3/3/3
82	PSU	S2	93	82	-	0/7/25/26	0/2/2/2
82	A2M	S2	484	82	-	0/9/27/28	0/3/3/3
2	A2M	L5	2401	2	-	0/9/27/28	0/3/3/3
2	OMC	L5	4456	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	3844	2	-	1/7/25/26	0/2/2/2
82	OMG	S2	1490	82	-	1/9/27/28	0/3/3/3
2	PSU	L5	4673	86,2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3822	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	3792	2	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L5	4457	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	1340	2	-	1/9/27/28	0/2/2/2
2	PSU	L5	4296	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	1045	82	-	2/7/25/26	0/2/2/2
2	OMC	L5	2365	86,2	-	0/9/27/28	0/2/2/2
2	PSU	L5	3695	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4972	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4293	2	-	0/7/25/26	0/2/2/2
82	OMU	S2	627	82	-	1/9/27/28	0/2/2/2
2	PSU	L5	4579	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	4590	2	-	3/9/27/28	0/3/3/3
2	PSU	L5	1781	2	-	1/7/25/26	0/2/2/2
2	PSU	L5	4500	2	-	3/7/25/26	0/2/2/2
82	PSU	S2	801	82	-	2/7/25/26	0/2/2/2
2	PSU	L5	3637	2	-	0/7/25/26	0/2/2/2
4	PSU	L8	69	4	-	0/7/25/26	0/2/2/2
2	OMC	L5	4536	2	-	0/9/27/28	0/2/2/2
2	PSU	L5	1782	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	863	82	-	0/7/25/26	0/2/2/2
2	A2M	L5	1326	2	-	4/9/27/28	0/3/3/3
2	6MZ	L5	4220	2	-	2/12/28/28	0/3/3/3
2	PSU	L5	4403	2	-	0/7/25/26	0/2/2/2
2	5MC	L5	3782	86,2	-	1/7/25/26	0/2/2/2
2	PSU	L5	4532	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	3718	2	-	0/9/27/28	0/3/3/3
82	PSU	S2	814	82	-	0/7/25/26	0/2/2/2
82	A2M	S2	468	82	-	0/9/27/28	0/3/3/3
2	PSU	L5	4312	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4299	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3701	2	-	6/9/27/28	0/2/2/2
82	PSU	S2	966	82,86	-	0/7/25/26	0/2/2/2
2	A2M	L5	3830	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	4471	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	4493	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	2364	86,2	-	2/9/27/28	0/3/3/3
2	PSU	L5	4361	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	5010	2	-	0/7/25/26	0/2/2/2
2	PSU	L5	3851	2	-	1/7/25/26	0/2/2/2
82	OMU	S2	1326	82	-	0/9/27/28	0/2/2/2
82	PSU	S2	406	82	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	L5	4196	2	-	1/9/27/28	0/3/3/3
2	PSU	L5	4431	2	-	0/7/25/26	0/2/2/2
2	OMG	L5	4392	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	1862	2	-	0/7/25/26	0/2/2/2
2	A2M	L5	3867	2	-	2/9/27/28	0/3/3/3
2	A2M	L5	400	2	-	1/9/27/28	0/3/3/3
82	OMU	S2	428	82	-	6/9/27/28	0/2/2/2
2	A2M	L5	4523	86,2	-	0/9/27/28	0/3/3/3
82	PSU	S2	686	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	1081	82	-	0/7/25/26	0/2/2/2
2	PSU	L5	4973	2	-	0/7/25/26	0/2/2/2
82	OMU	S2	799	82	-	2/9/27/28	0/2/2/2
82	PSU	S2	651	82	-	0/7/25/26	0/2/2/2
82	PSU	S2	1244	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	4637	2	-	2/9/27/28	0/3/3/3
82	OMC	S2	462	82	-	0/9/27/28	0/2/2/2
2	OMU	L5	4306	2	-	0/9/27/28	0/2/2/2
82	4AC	S2	1842	82	-	0/11/29/30	0/2/2/2
82	OMC	S2	1703	82	-	1/9/27/28	0/2/2/2
2	OMC	L5	3841	2	-	1/9/27/28	0/2/2/2
2	PSU	L5	4636	2	-	0/7/25/26	0/2/2/2
82	OMU	S2	172	82	-	0/9/27/28	0/2/2/2
2	A2M	L5	2815	2	-	2/9/27/28	0/3/3/3
2	A2M	L5	2787	2	-	5/9/27/28	0/3/3/3
2	PSU	L5	3639	2	-	0/7/25/26	0/2/2/2
82	PSU	S2	1174	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	1522	2	-	0/9/27/28	0/3/3/3
82	OMG	S2	683	82	-	2/9/27/28	0/3/3/3
2	PSU	L5	1582	2	-	0/7/25/26	0/2/2/2
2	OMC	L5	3808	86,2	-	0/9/27/28	0/2/2/2
82	OMC	S2	1272	82	-	2/9/27/28	0/2/2/2
2	A2M	L5	2363	86,2	-	0/9/27/28	0/3/3/3
2	OMC	L5	2861	2	-	0/9/27/28	0/2/2/2
4	OMG	L8	75	4	-	1/9/27/28	0/3/3/3
2	OMU	L5	3925	2	-	0/9/27/28	0/2/2/2
4	PSU	L8	55	4	-	0/7/25/26	0/2/2/2
82	B8N	S2	1248	82	-	4/16/34/35	0/2/2/2
82	PSU	S2	1046	82	-	0/7/25/26	0/2/2/2
2	OMG	L5	4228	2	-	0/9/27/28	0/3/3/3
2	PSU	L5	1792	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	L5	1536	2	-	2/7/25/26	0/2/2/2
2	PSU	L5	4628	2	-	0/7/25/26	0/2/2/2
82	OMC	S2	517	82	-	2/9/27/28	0/2/2/2
82	PSU	S2	866	82	-	0/7/25/26	0/2/2/2
82	A2M	S2	27	82	-	1/9/27/28	0/3/3/3
2	UR3	L5	4530	2	-	0/7/25/26	0/2/2/2
82	OMU	S2	116	82	-	0/9/27/28	0/2/2/2

All (298) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	S2	1832	6MZ	C6-N6	12.72	1.48	1.34
2	L5	3818	UY1	C6-C5	12.47	1.49	1.35
2	L5	4220	6MZ	C6-N6	11.82	1.47	1.34
2	L5	3818	UY1	C2-N1	11.60	1.51	1.36
82	S2	1288	OMU	C2-N1	8.58	1.51	1.38
82	S2	799	OMU	C2-N1	8.31	1.51	1.38
82	S2	627	OMU	C2-N1	8.18	1.51	1.38
82	S2	1442	OMU	C2-N1	8.10	1.51	1.38
82	S2	172	OMU	C2-N1	8.09	1.51	1.38
82	S2	428	OMU	C2-N1	8.08	1.51	1.38
82	S2	116	OMU	C2-N1	8.08	1.51	1.38
82	S2	1248	B8N	C4-N3	-8.04	1.26	1.40
82	S2	1326	OMU	C2-N1	8.02	1.51	1.38
82	S2	121	OMU	C2-N1	8.00	1.51	1.38
2	L5	4227	OMU	C2-N1	7.97	1.50	1.38
2	L5	2837	OMU	C2-N1	7.86	1.50	1.38
2	L5	4306	OMU	C2-N1	7.85	1.50	1.38
82	S2	354	OMU	C2-N1	7.84	1.50	1.38
2	L5	3925	OMU	C2-N1	7.82	1.50	1.38
82	S2	1248	B8N	C6-N1	7.78	1.55	1.36
2	L5	4498	OMU	C2-N1	7.64	1.50	1.38
2	L5	4620	OMU	C2-N1	7.60	1.50	1.38
2	L5	3818	UY1	C2-N3	7.57	1.49	1.37
82	S2	627	OMU	C2-N3	6.96	1.50	1.38
82	S2	1248	B8N	C4-C5	6.91	1.63	1.47
82	S2	1442	OMU	C2-N3	6.87	1.49	1.38
82	S2	799	OMU	C2-N3	6.86	1.49	1.38
82	S2	116	OMU	C2-N3	6.84	1.49	1.38
82	S2	1288	OMU	C2-N3	6.83	1.49	1.38
82	S2	1326	OMU	C2-N3	6.81	1.49	1.38
82	S2	428	OMU	C2-N3	6.79	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	S2	172	OMU	C2-N3	6.77	1.49	1.38
82	S2	121	OMU	C2-N3	6.72	1.49	1.38
2	L5	4227	OMU	C2-N3	6.68	1.49	1.38
82	S2	354	OMU	C2-N3	6.58	1.49	1.38
2	L5	2837	OMU	C2-N3	6.57	1.49	1.38
2	L5	4306	OMU	C2-N3	6.53	1.49	1.38
2	L5	4498	OMU	C2-N3	6.51	1.49	1.38
2	L5	3925	OMU	C2-N3	6.45	1.49	1.38
2	L5	4620	OMU	C2-N3	6.40	1.49	1.38
82	S2	1639	G7M	C4-N3	6.40	1.48	1.34
2	L5	4530	UR3	C6-C5	6.20	1.49	1.35
2	L5	4530	UR3	C2-N1	5.98	1.46	1.38
82	S2	627	OMU	C6-C5	5.89	1.48	1.35
82	S2	1288	OMU	C6-C5	5.88	1.48	1.35
82	S2	1248	B8N	C2-N1	5.86	1.56	1.39
82	S2	799	OMU	C6-C5	5.83	1.48	1.35
82	S2	172	OMU	C6-C5	5.80	1.48	1.35
82	S2	428	OMU	C6-C5	5.79	1.48	1.35
82	S2	1442	OMU	C6-C5	5.79	1.48	1.35
82	S2	1326	OMU	C6-C5	5.78	1.48	1.35
2	L5	4620	OMU	O4-C4	-5.72	1.13	1.24
82	S2	121	OMU	C6-C5	5.71	1.48	1.35
82	S2	354	OMU	C6-C5	5.71	1.48	1.35
2	L5	3925	OMU	O4-C4	-5.71	1.13	1.24
2	L5	4498	OMU	C6-C5	5.68	1.48	1.35
2	L5	4227	OMU	C6-C5	5.67	1.48	1.35
2	L5	4306	OMU	O4-C4	-5.66	1.13	1.24
82	S2	116	OMU	C6-C5	5.65	1.48	1.35
2	L5	2837	OMU	C6-C5	5.63	1.48	1.35
2	L5	4498	OMU	O4-C4	-5.62	1.13	1.24
2	L5	4227	OMU	O4-C4	-5.59	1.13	1.24
2	L5	2837	OMU	O4-C4	-5.58	1.13	1.24
82	S2	116	OMU	O4-C4	-5.57	1.13	1.24
82	S2	354	OMU	O4-C4	-5.56	1.13	1.24
2	L5	4306	OMU	C6-C5	5.56	1.48	1.35
2	L5	4620	OMU	C6-C5	5.56	1.48	1.35
82	S2	1326	OMU	O4-C4	-5.55	1.13	1.24
2	L5	3925	OMU	C6-C5	5.54	1.47	1.35
2	L5	4530	UR3	C2-N3	5.49	1.49	1.39
82	S2	121	OMU	O4-C4	-5.48	1.13	1.24
82	S2	428	OMU	O4-C4	-5.48	1.13	1.24
82	S2	799	OMU	O4-C4	-5.47	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	S2	627	OMU	O4-C4	-5.46	1.13	1.24
82	S2	1442	OMU	O4-C4	-5.46	1.13	1.24
82	S2	1288	OMU	O4-C4	-5.44	1.13	1.24
82	S2	172	OMU	O4-C4	-5.43	1.13	1.24
82	S2	1639	G7M	C2-N3	5.28	1.46	1.33
2	L5	3818	UY1	C6-N1	5.26	1.44	1.36
82	S2	1248	B8N	C6-C5	5.17	1.42	1.35
82	S2	1639	G7M	C5-N7	-5.05	1.33	1.39
82	S2	1639	G7M	C2-N2	4.83	1.45	1.34
82	S2	627	OMU	C4-N3	4.47	1.46	1.38
2	L5	3818	UY1	C4-N3	4.37	1.47	1.38
82	S2	1442	OMU	C4-N3	4.35	1.46	1.38
82	S2	172	OMU	C4-N3	4.32	1.46	1.38
82	S2	1288	OMU	C4-N3	4.32	1.46	1.38
82	S2	1326	OMU	C4-N3	4.31	1.46	1.38
82	S2	428	OMU	C4-N3	4.28	1.45	1.38
82	S2	116	OMU	C4-N3	4.25	1.45	1.38
82	S2	121	OMU	C4-N3	4.20	1.45	1.38
82	S2	799	OMU	C4-N3	4.20	1.45	1.38
82	S2	354	OMU	C4-N3	4.15	1.45	1.38
2	L5	4498	OMU	C4-N3	4.06	1.45	1.38
2	L5	2837	OMU	C4-N3	4.05	1.45	1.38
2	L5	4227	OMU	C4-N3	4.05	1.45	1.38
2	L5	4306	OMU	C4-N3	4.00	1.45	1.38
2	L5	3925	OMU	C4-N3	3.84	1.45	1.38
2	L5	4620	OMU	C4-N3	3.81	1.45	1.38
2	L5	3818	UY1	O4-C4	-3.76	1.16	1.23
82	S2	1639	G7M	C5-C6	3.72	1.53	1.43
2	L5	2401	A2M	O5'-C5'	-3.70	1.33	1.44
82	S2	801	PSU	C6-C5	3.60	1.39	1.35
2	L5	3825	A2M	O5'-C5'	-3.55	1.33	1.44
2	L5	2787	A2M	O5'-C5'	-3.53	1.33	1.44
82	S2	668	A2M	O5'-C5'	-3.53	1.33	1.44
82	S2	1248	B8N	C1'-C5	3.52	1.58	1.50
2	L5	3785	A2M	O5'-C5'	-3.49	1.34	1.44
82	S2	93	PSU	C6-C5	3.48	1.39	1.35
82	S2	99	A2M	O5'-C5'	-3.48	1.34	1.44
2	L5	3830	A2M	O5'-C5'	-3.48	1.34	1.44
2	L5	3844	PSU	C6-C5	3.47	1.39	1.35
2	L5	1326	A2M	O5'-C5'	-3.47	1.34	1.44
2	L5	5010	PSU	C6-C5	3.46	1.39	1.35
2	L5	4500	PSU	C6-C5	3.46	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	1871	A2M	O5'-C5'	-3.46	1.34	1.44
82	S2	1367	PSU	C6-C5	3.46	1.39	1.35
82	S2	1031	A2M	O5'-C5'	-3.46	1.34	1.44
2	L5	400	A2M	O5'-C5'	-3.46	1.34	1.44
82	S2	1232	PSU	C6-C5	3.46	1.39	1.35
2	L5	1323	A2M	O5'-C5'	-3.45	1.34	1.44
82	S2	468	A2M	O5'-C5'	-3.44	1.34	1.44
2	L5	4220	6MZ	C5-C4	-3.44	1.33	1.39
82	S2	1244	PSU	C6-C5	3.44	1.39	1.35
2	L5	1524	A2M	O5'-C5'	-3.43	1.34	1.44
82	S2	866	PSU	C6-C5	3.42	1.39	1.35
2	L5	2363	A2M	O5'-C5'	-3.42	1.34	1.44
82	S2	966	PSU	C6-C5	3.41	1.39	1.35
82	S2	1383	A2M	O5'-C5'	-3.40	1.34	1.44
2	L5	4220	6MZ	C5-N7	-3.40	1.32	1.39
82	S2	1004	PSU	C6-C5	3.40	1.39	1.35
82	S2	27	A2M	O5'-C5'	-3.40	1.34	1.44
2	L5	2815	A2M	O5'-C5'	-3.40	1.34	1.44
82	S2	651	PSU	C6-C5	3.39	1.39	1.35
2	L5	1860	PSU	C6-C5	3.39	1.39	1.35
2	L5	4571	A2M	O5'-C5'	-3.39	1.34	1.44
82	S2	105	PSU	C6-C5	3.38	1.39	1.35
2	L5	2632	PSU	C6-C5	3.38	1.39	1.35
82	S2	576	A2M	O5'-C5'	-3.38	1.34	1.44
2	L5	4552	PSU	C6-C5	3.37	1.39	1.35
2	L5	4312	PSU	C6-C5	3.37	1.39	1.35
82	S2	863	PSU	C6-C5	3.37	1.39	1.35
2	L5	1782	PSU	C6-C5	3.36	1.39	1.35
2	L5	5001	PSU	C6-C5	3.36	1.39	1.35
82	S2	1177	PSU	C6-C5	3.35	1.39	1.35
2	L5	3867	A2M	O5'-C5'	-3.35	1.34	1.44
82	S2	814	PSU	C6-C5	3.32	1.39	1.35
2	L5	398	A2M	O5'-C5'	-3.32	1.34	1.44
82	S2	166	A2M	O5'-C5'	-3.32	1.34	1.44
2	L5	4590	A2M	O5'-C5'	-3.32	1.34	1.44
82	S2	109	PSU	C6-C5	3.31	1.39	1.35
2	L5	3718	A2M	O5'-C5'	-3.31	1.34	1.44
82	S2	484	A2M	O5'-C5'	-3.31	1.34	1.44
2	L5	4523	A2M	O5'-C5'	-3.30	1.34	1.44
2	L5	3818	UY1	O2-C2	-3.30	1.16	1.23
2	L5	4576	PSU	C6-C5	3.30	1.38	1.35
2	L5	1781	PSU	C6-C5	3.29	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	4493	PSU	C6-C5	3.28	1.38	1.35
2	L5	3818	UY1	C1'-C5	3.27	1.57	1.50
82	S2	1174	PSU	C6-C5	3.27	1.38	1.35
82	S2	1045	PSU	C6-C5	3.26	1.38	1.35
82	S2	1046	PSU	C6-C5	3.26	1.38	1.35
82	S2	686	PSU	C6-C5	3.26	1.38	1.35
2	L5	1744	PSU	C6-C5	3.25	1.38	1.35
2	L5	4532	PSU	C6-C5	3.25	1.38	1.35
2	L5	4636	PSU	C6-C5	3.24	1.38	1.35
82	S2	649	PSU	C6-C5	3.23	1.38	1.35
2	L5	3853	PSU	C6-C5	3.23	1.38	1.35
82	S2	406	PSU	C6-C5	3.23	1.38	1.35
2	L5	1862	PSU	C6-C5	3.23	1.38	1.35
4	L8	69	PSU	C6-C5	3.21	1.38	1.35
2	L5	4353	PSU	C6-C5	3.21	1.38	1.35
2	L5	3822	PSU	C6-C5	3.20	1.38	1.35
2	L5	4579	PSU	C6-C5	3.20	1.38	1.35
2	L5	4673	PSU	C6-C5	3.20	1.38	1.35
2	L5	4521	PSU	C6-C5	3.19	1.38	1.35
2	L5	1683	PSU	C6-C5	3.19	1.38	1.35
2	L5	4442	PSU	C6-C5	3.19	1.38	1.35
82	S2	1832	6MZ	C5-N7	-3.18	1.33	1.39
2	L5	3637	PSU	C6-C5	3.18	1.38	1.35
2	L5	4296	PSU	C6-C5	3.18	1.38	1.35
2	L5	4293	PSU	C6-C5	3.18	1.38	1.35
82	S2	681	PSU	C6-C5	3.18	1.38	1.35
82	S2	159	A2M	O5'-C5'	-3.16	1.35	1.44
2	L5	4973	PSU	C6-C5	3.15	1.38	1.35
2	L5	4299	PSU	C6-C5	3.15	1.38	1.35
2	L5	4431	PSU	C6-C5	3.14	1.38	1.35
82	S2	1056	PSU	C6-C5	3.14	1.38	1.35
4	L8	55	PSU	C6-C5	3.13	1.38	1.35
2	L5	4361	PSU	C6-C5	3.13	1.38	1.35
2	L5	4471	PSU	C6-C5	3.12	1.38	1.35
2	L5	1582	PSU	C6-C5	3.12	1.38	1.35
2	L5	2839	PSU	C6-C5	3.11	1.38	1.35
2	L5	3884	PSU	C6-C5	3.10	1.38	1.35
82	S2	1832	6MZ	C5-C4	-3.10	1.33	1.39
2	L5	4689	PSU	C6-C5	3.09	1.38	1.35
2	L5	1534	A2M	O5'-C5'	-3.09	1.35	1.44
2	L5	4972	PSU	C6-C5	3.08	1.38	1.35
82	S2	1851	MA6	C6-N6	3.07	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	S2	1850	MA6	C6-N6	3.06	1.45	1.36
2	L5	3695	PSU	C6-C5	3.06	1.38	1.35
82	S2	1081	PSU	C6-C5	3.05	1.38	1.35
82	S2	668	A2M	O4'-C4'	-3.04	1.38	1.45
2	L5	3851	PSU	C6-C5	3.04	1.38	1.35
2	L5	1792	PSU	C6-C5	3.03	1.38	1.35
2	L5	4220	6MZ	C8-N9	-3.00	1.32	1.37
2	L5	4628	PSU	C6-C5	2.99	1.38	1.35
2	L5	3639	PSU	C6-C5	2.93	1.38	1.35
82	S2	1832	6MZ	C8-N9	-2.93	1.32	1.37
2	L5	3920	PSU	C6-C5	2.93	1.38	1.35
2	L5	1536	PSU	C6-C5	2.92	1.38	1.35
2	L5	4403	PSU	C6-C5	2.88	1.38	1.35
82	S2	627	OMU	C5-C4	2.87	1.49	1.43
2	L5	4457	PSU	C6-C5	2.84	1.38	1.35
82	S2	1288	OMU	C5-C4	2.80	1.49	1.43
2	L5	1677	PSU	C6-C5	2.79	1.38	1.35
82	S2	799	OMU	C5-C4	2.79	1.49	1.43
82	S2	1326	OMU	C5-C4	2.78	1.49	1.43
82	S2	172	OMU	C5-C4	2.77	1.49	1.43
2	L5	4530	UR3	O2-C2	-2.76	1.17	1.22
82	S2	1639	G7M	C2-N1	2.75	1.44	1.37
82	S2	428	OMU	C5-C4	2.71	1.49	1.43
82	S2	1442	OMU	C5-C4	2.70	1.49	1.43
2	L5	4498	OMU	C5-C4	2.68	1.49	1.43
82	S2	1288	OMU	C6-N1	2.68	1.44	1.38
82	S2	627	OMU	C6-N1	2.65	1.44	1.38
2	L5	4227	OMU	C5-C4	2.65	1.49	1.43
82	S2	121	OMU	C5-C4	2.64	1.49	1.43
82	S2	354	OMU	C5-C4	2.63	1.49	1.43
2	L5	2837	OMU	C5-C4	2.62	1.49	1.43
82	S2	1639	G7M	O6-C6	-2.62	1.18	1.23
82	S2	1442	OMU	C6-N1	2.62	1.44	1.38
82	S2	799	OMU	C6-N1	2.62	1.44	1.38
2	L5	3925	OMU	C5-C4	2.61	1.49	1.43
2	L5	1524	A2M	O4'-C4'	-2.61	1.39	1.45
2	L5	4571	A2M	O4'-C4'	-2.60	1.39	1.45
82	S2	1851	MA6	C5-C4	-2.59	1.34	1.39
82	S2	116	OMU	C5-C4	2.57	1.49	1.43
82	S2	121	OMU	C6-N1	2.56	1.44	1.38
2	L5	4498	OMU	C6-N1	2.56	1.44	1.38
82	S2	354	OMU	C6-N1	2.55	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	S2	428	OMU	C6-N1	2.54	1.44	1.38
2	L5	2363	A2M	O4'-C4'	-2.53	1.39	1.45
2	L5	1534	A2M	O4'-C4'	-2.53	1.39	1.45
82	S2	1850	MA6	C5-C4	-2.52	1.34	1.39
82	S2	1326	OMU	C6-N1	2.52	1.44	1.38
2	L5	4220	6MZ	C6-N1	-2.48	1.31	1.35
2	L5	4306	OMU	C5-C4	2.47	1.49	1.43
2	L5	4620	OMU	C6-N1	2.47	1.44	1.38
82	S2	172	OMU	C6-N1	2.45	1.43	1.38
2	L5	4530	UR3	C6-N1	2.43	1.43	1.38
2	L5	2837	OMU	C6-N1	2.43	1.43	1.38
82	S2	116	OMU	C6-N1	2.43	1.43	1.38
2	L5	4306	OMU	C6-N1	2.42	1.43	1.38
2	L5	4620	OMU	C5-C4	2.40	1.48	1.43
2	L5	3867	A2M	O4'-C4'	-2.40	1.39	1.45
2	L5	4227	OMU	C6-N1	2.39	1.43	1.38
82	S2	1639	G7M	C6-N1	2.38	1.43	1.38
2	L5	3925	OMU	C6-N1	2.37	1.43	1.38
2	L5	1323	A2M	O4'-C4'	-2.36	1.39	1.45
2	L5	1326	A2M	O4'-C4'	-2.31	1.39	1.45
2	L5	1871	A2M	O4'-C4'	-2.29	1.39	1.45
2	L5	2815	A2M	O4'-C4'	-2.29	1.39	1.45
2	L5	4523	A2M	O3'-C3'	-2.26	1.37	1.43
82	S2	1832	6MZ	C6-N1	-2.25	1.31	1.35
2	L5	3818	UY1	O4'-C1'	-2.22	1.40	1.43
82	S2	1639	G7M	C4-N9	-2.19	1.32	1.38
2	L5	4530	UR3	C5-C4	2.19	1.49	1.43
2	L5	4523	A2M	O4'-C4'	-2.19	1.40	1.45
2	L5	400	A2M	O3'-C3'	-2.17	1.37	1.43
2	L5	4353	PSU	C4-C5	-2.14	1.38	1.44
2	L5	4689	PSU	C4-C5	-2.11	1.38	1.44
2	L5	4521	PSU	C4-C5	-2.11	1.38	1.44
2	L5	3884	PSU	C4-C5	-2.10	1.38	1.44
2	L5	4293	PSU	C4-C5	-2.07	1.38	1.44
2	L5	3639	PSU	C4-C5	-2.07	1.38	1.44
2	L5	3825	A2M	O4'-C4'	-2.06	1.40	1.45
2	L5	2839	PSU	C4-C5	-2.05	1.38	1.44
2	L5	1871	A2M	O3'-C3'	-2.05	1.37	1.43
2	L5	3695	PSU	C4-C5	-2.04	1.38	1.44
2	L5	4500	PSU	C4-C5	-2.04	1.38	1.44
2	L5	400	A2M	O4'-C4'	-2.04	1.40	1.45
82	S2	1031	A2M	O4'-C4'	-2.03	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L5	4521	PSU	O4'-C1'	-2.03	1.41	1.43
2	L5	4456	OMC	C4-N3	-2.03	1.30	1.34
82	S2	1177	PSU	C4-C5	-2.03	1.38	1.44
2	L5	1683	PSU	C4-C5	-2.03	1.38	1.44
2	L5	4530	UR3	C3U-N3	2.02	1.50	1.47
2	L5	4552	PSU	C4-C5	-2.02	1.38	1.44
2	L5	4220	6MZ	C4-N9	-2.02	1.33	1.37
82	S2	1056	PSU	C4-C5	-2.02	1.38	1.44
2	L5	3818	UY1	C4-C5	2.01	1.49	1.44
2	L5	4312	PSU	C4-C5	-2.01	1.38	1.44
2	L5	1534	A2M	O3'-C3'	-2.01	1.38	1.43
2	L5	3920	PSU	C4-C5	-2.01	1.38	1.44
2	L5	4571	A2M	O3'-C3'	-2.01	1.38	1.43
82	S2	109	PSU	C4-C5	-2.01	1.38	1.44
2	L5	4457	PSU	C4-C5	-2.00	1.38	1.44

All (704) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	S2	1851	MA6	N1-C6-N6	-12.27	101.91	116.86
82	S2	1850	MA6	N1-C6-N6	-12.02	102.21	116.86
82	S2	1851	MA6	C5-C6-N6	8.20	138.32	125.33
82	S2	1850	MA6	C5-C6-N6	8.04	138.06	125.33
82	S2	1639	G7M	C1'-N9-C4	7.28	147.99	126.49
82	S2	1639	G7M	C1'-N9-C8	-7.19	102.46	126.74
2	L5	3925	OMU	C4-N3-C2	-6.11	119.03	126.61
2	L5	4220	6MZ	OP3-P-OP1	-5.96	87.63	110.83
2	L5	4227	OMU	C4-N3-C2	-5.85	119.35	126.61
82	S2	1851	MA6	N1-C2-N3	-5.81	119.78	128.58
82	S2	428	OMU	C4-N3-C2	-5.79	119.42	126.61
82	S2	1832	6MZ	N1-C2-N3	-5.78	119.84	128.58
2	L5	4220	6MZ	N1-C2-N3	-5.77	119.85	128.58
2	L5	4498	OMU	C4-N3-C2	-5.76	119.45	126.61
82	S2	1326	OMU	C4-N3-C2	-5.76	119.46	126.61
2	L5	4306	OMU	C4-N3-C2	-5.76	119.46	126.61
82	S2	354	OMU	C4-N3-C2	-5.75	119.47	126.61
82	S2	172	OMU	C4-N3-C2	-5.73	119.50	126.61
2	L5	2837	OMU	C4-N3-C2	-5.69	119.55	126.61
82	S2	627	OMU	C4-N3-C2	-5.60	119.66	126.61
2	L5	4530	UR3	C4-N3-C2	-5.60	120.08	124.58
82	S2	121	OMU	C4-N3-C2	-5.56	119.71	126.61
82	S2	799	OMU	C4-N3-C2	-5.53	119.74	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	4220	6MZ	OP3-P-O5'	-5.52	92.28	106.67
82	S2	1850	MA6	N1-C2-N3	-5.51	120.23	128.58
82	S2	1442	OMU	C4-N3-C2	-5.51	119.77	126.61
2	L5	4220	6MZ	C9-N6-C6	-5.46	117.78	122.85
2	L5	1683	PSU	N1-C2-N3	5.45	120.92	115.17
82	S2	1851	MA6	N9-C8-N7	-5.44	106.22	113.94
2	L5	3701	OMC	C1'-N1-C2	5.39	130.35	118.44
2	L5	4689	PSU	N1-C2-N3	5.38	120.84	115.17
2	L5	4457	PSU	C4-N3-C2	-5.37	118.98	126.37
2	L5	3637	PSU	N1-C2-N3	5.31	120.77	115.17
82	S2	1850	MA6	N9-C8-N7	-5.30	106.42	113.94
2	L5	4220	6MZ	OP3-P-OP2	-5.27	88.03	107.80
82	S2	116	OMU	C4-N3-C2	-5.26	120.08	126.61
2	L5	4636	PSU	C4-N3-C2	-5.26	119.13	126.37
82	S2	1288	OMU	C4-N3-C2	-5.25	120.09	126.61
2	L5	4457	PSU	N1-C2-N3	5.25	120.70	115.17
2	L5	1677	PSU	C4-N3-C2	-5.20	119.21	126.37
82	S2	1248	B8N	C5-C4-N3	5.18	125.56	116.15
2	L5	4353	PSU	N1-C2-N3	5.17	120.62	115.17
2	L5	1683	PSU	C4-N3-C2	-5.16	119.27	126.37
2	L5	3637	PSU	C4-N3-C2	-5.15	119.27	126.37
2	L5	3639	PSU	N1-C2-N3	5.14	120.59	115.17
2	L5	4521	PSU	N1-C2-N3	5.13	120.58	115.17
2	L5	4220	6MZ	OP2-P-OP1	5.13	130.82	110.83
2	L5	4552	PSU	N1-C2-N3	5.13	120.57	115.17
2	L5	4403	PSU	C4-N3-C2	-5.11	119.33	126.37
2	L5	1862	PSU	C4-N3-C2	-5.11	119.33	126.37
2	L5	4500	PSU	N1-C2-N3	5.09	120.54	115.17
4	L8	69	PSU	N1-C2-N3	5.09	120.53	115.17
2	L5	1862	PSU	N1-C2-N3	5.08	120.52	115.17
2	L5	4442	PSU	N1-C2-N3	5.06	120.51	115.17
82	S2	1081	PSU	C4-N3-C2	-5.06	119.40	126.37
2	L5	2839	PSU	N1-C2-N3	5.06	120.51	115.17
2	L5	4521	PSU	C4-N3-C2	-5.06	119.40	126.37
2	L5	3695	PSU	C4-N3-C2	-5.05	119.41	126.37
2	L5	4312	PSU	N1-C2-N3	5.05	120.49	115.17
2	L5	4293	PSU	C4-N3-C2	-5.05	119.42	126.37
2	L5	4293	PSU	N1-C2-N3	5.04	120.49	115.17
2	L5	3695	PSU	N1-C2-N3	5.03	120.48	115.17
2	L5	4579	PSU	N1-C2-N3	5.03	120.47	115.17
82	S2	649	PSU	N1-C2-N3	5.03	120.47	115.17
82	S2	1056	PSU	C4-N3-C2	-5.02	119.45	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	3639	PSU	C4-N3-C2	-5.02	119.45	126.37
4	L8	55	PSU	N1-C2-N3	5.01	120.46	115.17
2	L5	3884	PSU	C4-N3-C2	-5.00	119.48	126.37
82	S2	649	PSU	C4-N3-C2	-5.00	119.48	126.37
2	L5	2632	PSU	N1-C2-N3	4.99	120.43	115.17
2	L5	3920	PSU	N1-C2-N3	4.99	120.43	115.17
82	S2	1045	PSU	C4-N3-C2	-4.99	119.50	126.37
2	L5	3853	PSU	N1-C2-N3	4.98	120.42	115.17
4	L8	55	PSU	C4-N3-C2	-4.98	119.51	126.37
2	L5	4636	PSU	N1-C2-N3	4.98	120.42	115.17
2	L5	4973	PSU	C4-N3-C2	-4.98	119.52	126.37
82	S2	1177	PSU	N1-C2-N3	4.98	120.42	115.17
2	L5	4973	PSU	N1-C2-N3	4.98	120.42	115.17
82	S2	1177	PSU	C4-N3-C2	-4.98	119.52	126.37
2	L5	4471	PSU	N1-C2-N3	4.97	120.42	115.17
2	L5	3818	UY1	C4-N3-C2	-4.97	119.52	126.37
4	L8	69	PSU	C4-N3-C2	-4.97	119.53	126.37
2	L5	1744	PSU	N1-C2-N3	4.97	120.41	115.17
82	S2	406	PSU	C4-N3-C2	-4.97	119.53	126.37
82	S2	651	PSU	N1-C2-N3	4.96	120.40	115.17
2	L5	3851	PSU	N1-C2-N3	4.96	120.40	115.17
2	L5	4442	PSU	C4-N3-C2	-4.96	119.54	126.37
2	L5	4689	PSU	C4-N3-C2	-4.96	119.54	126.37
82	S2	406	PSU	N1-C2-N3	4.96	120.40	115.17
2	L5	1860	PSU	N1-C2-N3	4.96	120.40	115.17
82	S2	1045	PSU	N1-C2-N3	4.96	120.40	115.17
2	L5	3844	PSU	N1-C2-N3	4.96	120.40	115.17
2	L5	4620	OMU	C4-N3-C2	-4.95	120.47	126.61
2	L5	4579	PSU	C4-N3-C2	-4.94	119.57	126.37
82	S2	866	PSU	C4-N3-C2	-4.94	119.57	126.37
2	L5	1860	PSU	C4-N3-C2	-4.93	119.58	126.37
2	L5	4353	PSU	C4-N3-C2	-4.93	119.58	126.37
2	L5	4500	PSU	C4-N3-C2	-4.93	119.58	126.37
2	L5	4552	PSU	C4-N3-C2	-4.93	119.58	126.37
2	L5	3822	PSU	N1-C2-N3	4.93	120.36	115.17
2	L5	4296	PSU	C4-N3-C2	-4.92	119.59	126.37
82	S2	1004	PSU	C4-N3-C2	-4.92	119.59	126.37
82	S2	1081	PSU	N1-C2-N3	4.92	120.36	115.17
2	L5	5010	PSU	N1-C2-N3	4.92	120.35	115.17
82	S2	1004	PSU	N1-C2-N3	4.91	120.35	115.17
2	L5	4673	PSU	N1-C2-N3	4.91	120.35	115.17
2	L5	2839	PSU	C4-N3-C2	-4.91	119.60	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	1792	PSU	C4-N3-C2	-4.91	119.61	126.37
82	S2	866	PSU	N1-C2-N3	4.90	120.34	115.17
2	L5	3884	PSU	N1-C2-N3	4.90	120.34	115.17
82	S2	686	PSU	C4-N3-C2	-4.90	119.62	126.37
82	S2	1174	PSU	C4-N3-C2	-4.90	119.63	126.37
2	L5	3853	PSU	C4-N3-C2	-4.89	119.63	126.37
82	S2	1056	PSU	N1-C2-N3	4.89	120.33	115.17
82	S2	105	PSU	N1-C2-N3	4.89	120.32	115.17
82	S2	1046	PSU	C4-N3-C2	-4.88	119.65	126.37
82	S2	863	PSU	C4-N3-C2	-4.87	119.66	126.37
82	S2	651	PSU	C4-N3-C2	-4.87	119.67	126.37
82	S2	1174	PSU	N1-C2-N3	4.86	120.30	115.17
82	S2	1232	PSU	N1-C2-N3	4.86	120.30	115.17
2	L5	4673	PSU	C4-N3-C2	-4.86	119.67	126.37
82	S2	109	PSU	C4-N3-C2	-4.86	119.68	126.37
2	L5	4296	PSU	N1-C2-N3	4.85	120.29	115.17
2	L5	2632	PSU	C4-N3-C2	-4.85	119.69	126.37
2	L5	1782	PSU	N1-C2-N3	4.85	120.28	115.17
2	L5	4493	PSU	C4-N3-C2	-4.85	119.69	126.37
2	L5	4576	PSU	N1-C2-N3	4.85	120.28	115.17
2	L5	4972	PSU	N1-C2-N3	4.84	120.28	115.17
2	L5	3851	PSU	C4-N3-C2	-4.84	119.70	126.37
2	L5	4403	PSU	N1-C2-N3	4.84	120.27	115.17
2	L5	1744	PSU	C4-N3-C2	-4.84	119.71	126.37
2	L5	5010	PSU	C4-N3-C2	-4.83	119.72	126.37
82	S2	1244	PSU	N1-C2-N3	4.83	120.26	115.17
2	L5	4299	PSU	C4-N3-C2	-4.83	119.72	126.37
82	S2	1046	PSU	N1-C2-N3	4.83	120.26	115.17
82	S2	1244	PSU	C4-N3-C2	-4.82	119.73	126.37
2	L5	1792	PSU	N1-C2-N3	4.82	120.25	115.17
2	L5	5001	PSU	N1-C2-N3	4.82	120.25	115.17
2	L5	4532	PSU	C4-N3-C2	-4.82	119.73	126.37
82	S2	1232	PSU	C4-N3-C2	-4.82	119.73	126.37
2	L5	3920	PSU	C4-N3-C2	-4.82	119.73	126.37
2	L5	4312	PSU	C4-N3-C2	-4.82	119.73	126.37
82	S2	966	PSU	N1-C2-N3	4.82	120.25	115.17
2	L5	4431	PSU	C4-N3-C2	-4.82	119.74	126.37
2	L5	4972	PSU	C4-N3-C2	-4.81	119.74	126.37
82	S2	686	PSU	N1-C2-N3	4.81	120.24	115.17
2	L5	1536	PSU	C4-N3-C2	-4.81	119.75	126.37
82	S2	109	PSU	N1-C2-N3	4.81	120.24	115.17
2	L5	4576	PSU	C4-N3-C2	-4.80	119.76	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	S2	1367	PSU	N1-C2-N3	4.80	120.23	115.17
82	S2	863	PSU	N1-C2-N3	4.79	120.22	115.17
2	L5	4628	PSU	N1-C2-N3	4.79	120.22	115.17
82	S2	105	PSU	C4-N3-C2	-4.78	119.78	126.37
2	L5	5001	PSU	C4-N3-C2	-4.78	119.78	126.37
2	L5	4431	PSU	N1-C2-N3	4.78	120.21	115.17
2	L5	3822	PSU	C4-N3-C2	-4.78	119.79	126.37
82	S2	814	PSU	C4-N3-C2	-4.78	119.79	126.37
2	L5	1536	PSU	N1-C2-N3	4.77	120.20	115.17
82	S2	1367	PSU	C4-N3-C2	-4.77	119.81	126.37
2	L5	4299	PSU	N1-C2-N3	4.76	120.19	115.17
82	S2	681	PSU	N1-C2-N3	4.76	120.18	115.17
2	L5	4361	PSU	C4-N3-C2	-4.75	119.83	126.37
2	L5	4532	PSU	N1-C2-N3	4.74	120.16	115.17
2	L5	4493	PSU	N1-C2-N3	4.73	120.16	115.17
2	L5	1677	PSU	N1-C2-N3	4.73	120.15	115.17
2	L5	4471	PSU	C4-N3-C2	-4.72	119.86	126.37
82	S2	1832	6MZ	N9-C8-N7	-4.72	107.24	113.94
2	L5	1582	PSU	N1-C2-N3	4.70	120.12	115.17
2	L5	1782	PSU	C4-N3-C2	-4.69	119.91	126.37
2	L5	1781	PSU	C4-N3-C2	-4.67	119.93	126.37
2	L5	4220	6MZ	N9-C8-N7	-4.67	107.31	113.94
2	L5	1781	PSU	N1-C2-N3	4.67	120.09	115.17
2	L5	3844	PSU	C4-N3-C2	-4.67	119.94	126.37
82	S2	801	PSU	N1-C2-N3	4.67	120.09	115.17
2	L5	4361	PSU	N1-C2-N3	4.66	120.09	115.17
82	S2	93	PSU	N1-C2-N3	4.65	120.07	115.17
82	S2	1248	B8N	C4-N3-C2	-4.64	119.90	125.62
82	S2	681	PSU	C4-N3-C2	-4.64	119.97	126.37
2	L5	4628	PSU	C4-N3-C2	-4.64	119.97	126.37
82	S2	93	PSU	C4-N3-C2	-4.63	119.99	126.37
82	S2	966	PSU	C4-N3-C2	-4.61	120.02	126.37
2	L5	1582	PSU	C4-N3-C2	-4.59	120.04	126.37
82	S2	1832	6MZ	C5-C4-N3	-4.55	120.46	126.72
82	S2	801	PSU	C4-N3-C2	-4.55	120.11	126.37
82	S2	814	PSU	N1-C2-N3	4.52	119.94	115.17
82	S2	1639	G7M	C2-N3-C4	4.48	120.01	112.30
2	L5	4220	6MZ	C5-C4-N3	-4.46	120.58	126.72
2	L5	3818	UY1	N1-C2-N3	4.39	119.80	115.17
82	S2	1850	MA6	C5-C4-N3	-4.38	120.69	126.72
2	L5	1871	A2M	C3'-C2'-C1'	-4.32	94.53	102.81
82	S2	1851	MA6	C5-C4-N3	-4.26	120.85	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	S2	1851	MA6	C4-N9-C8	4.25	110.20	105.74
82	S2	1383	A2M	C3'-C2'-C1'	-4.21	94.74	102.81
2	L5	3701	OMC	C1'-N1-C6	-4.20	111.81	120.78
2	L5	4523	A2M	C3'-C2'-C1'	-4.15	94.86	102.81
2	L5	3925	OMU	N3-C2-N1	4.15	120.30	114.89
2	L5	3830	A2M	C3'-C2'-C1'	-4.13	94.90	102.81
82	S2	1850	MA6	C4-N9-C8	4.13	110.07	105.74
82	S2	354	OMU	N3-C2-N1	4.08	120.21	114.89
2	L5	4306	OMU	N3-C2-N1	4.02	120.12	114.89
2	L5	2837	OMU	N3-C2-N1	4.01	120.11	114.89
2	L5	4498	OMU	N3-C2-N1	3.99	120.09	114.89
82	S2	121	OMU	N3-C2-N1	3.98	120.08	114.89
82	S2	1639	G7M	C5-C6-N1	3.97	120.06	111.84
82	S2	1639	G7M	C5-C4-N3	-3.94	120.70	128.15
82	S2	172	OMU	N3-C2-N1	3.91	119.98	114.89
2	L5	4227	OMU	N3-C2-N1	3.91	119.97	114.89
2	L5	398	A2M	C3'-C2'-C1'	-3.90	95.33	102.81
2	L5	3925	OMU	C5-C4-N3	3.89	120.25	114.80
82	S2	799	OMU	N3-C2-N1	3.87	119.92	114.89
82	S2	428	OMU	N3-C2-N1	3.86	119.92	114.89
82	S2	1326	OMU	N3-C2-N1	3.82	119.86	114.89
2	L5	4498	OMU	C5-C4-N3	3.80	120.12	114.80
2	L5	4227	OMU	C5-C4-N3	3.80	120.12	114.80
82	S2	428	OMU	C5-C4-N3	3.75	120.05	114.80
2	L5	4306	OMU	C5-C4-N3	3.73	120.03	114.80
2	L5	4620	OMU	N3-C2-N1	3.72	119.74	114.89
82	S2	1442	OMU	N3-C2-N1	3.72	119.73	114.89
2	L5	4530	UR3	C5-C4-N3	3.70	119.91	115.04
82	S2	1326	OMU	C5-C4-N3	3.69	119.97	114.80
82	S2	1031	A2M	C3'-C2'-C1'	-3.69	95.74	102.81
82	S2	627	OMU	C5-C4-N3	3.67	119.94	114.80
2	L5	398	A2M	O3'-C3'-C2'	3.65	121.40	111.19
82	S2	1851	MA6	C2-N1-C6	3.64	120.73	111.83
2	L5	2401	A2M	O3'-C3'-C2'	3.64	121.37	111.19
82	S2	116	OMU	N3-C2-N1	3.64	119.63	114.89
82	S2	627	OMU	N3-C2-N1	3.64	119.63	114.89
82	S2	1288	OMU	N3-C2-N1	3.64	119.63	114.89
82	S2	354	OMU	C5-C4-N3	3.63	119.89	114.80
82	S2	1442	OMU	C5-C4-N3	3.63	119.89	114.80
82	S2	799	OMU	C5-C4-N3	3.61	119.86	114.80
82	S2	1248	B8N	C1'-C5-C4	3.61	123.09	117.61
82	S2	99	A2M	C3'-C2'-C1'	-3.60	95.91	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	3718	A2M	C3'-C2'-C1'	-3.58	95.95	102.81
82	S2	121	OMU	C5-C4-N3	3.58	119.81	114.80
2	L5	2837	OMU	C5-C4-N3	3.55	119.78	114.80
82	S2	1248	B8N	N3-C2-N1	3.54	121.04	116.72
82	S2	116	OMU	C5-C4-N3	3.52	119.72	114.80
82	S2	172	OMU	C5-C4-N3	3.51	119.72	114.80
82	S2	1850	MA6	C2-N1-C6	3.50	120.39	111.83
82	S2	1850	MA6	C4-C5-C6	3.49	119.52	115.91
2	L5	1323	A2M	C2'-C1'-N9	3.48	119.49	113.75
82	S2	1288	OMU	C5-C4-N3	3.48	119.68	114.80
2	L5	4590	A2M	C3'-C2'-C1'	-3.45	96.21	102.81
2	L5	2787	A2M	O3'-C3'-C2'	3.42	120.77	111.19
2	L5	3825	A2M	C3'-C2'-C1'	-3.41	96.27	102.81
82	S2	468	A2M	C3'-C2'-C1'	-3.41	96.27	102.81
82	S2	1832	6MZ	C2-N3-C4	3.41	120.16	111.83
2	L5	4220	6MZ	O5'-P-OP1	3.39	115.61	106.44
82	S2	576	A2M	O3'-C3'-C2'	3.39	120.68	111.19
2	L5	4620	OMU	C5-C4-N3	3.39	119.54	114.80
2	L5	4220	6MZ	C2-N3-C4	3.35	120.01	111.83
82	S2	1639	G7M	O6-C6-C5	-3.35	120.54	128.01
82	S2	27	A2M	C3'-C2'-C1'	-3.34	96.41	102.81
82	S2	1383	A2M	O3'-C3'-C2'	3.34	120.52	111.19
82	S2	166	A2M	O3'-C3'-C2'	3.31	120.44	111.19
2	L5	2401	A2M	C3'-C2'-C1'	-3.29	96.51	102.81
82	S2	576	A2M	C3'-C2'-C1'	-3.29	96.51	102.81
82	S2	1832	6MZ	C5-N7-C8	3.27	108.60	103.45
2	L5	1683	PSU	O2-C2-N1	-3.25	119.44	122.79
2	L5	1534	A2M	C3'-C2'-C1'	-3.24	96.60	102.81
2	L5	4689	PSU	C6-N1-C2	-3.24	119.69	122.69
4	L8	69	PSU	O2-C2-N1	-3.22	119.47	122.79
2	L5	1323	A2M	O3'-C3'-C2'	3.22	120.20	111.19
82	S2	1174	PSU	O2-C2-N1	-3.21	119.47	122.79
82	S2	1851	MA6	C2-N3-C4	3.21	119.68	111.83
82	S2	1850	MA6	N3-C4-N9	3.21	132.63	127.17
82	S2	166	A2M	C3'-C2'-C1'	-3.20	96.68	102.81
2	L5	1524	A2M	O3'-C3'-C2'	3.20	120.14	111.19
2	L5	4579	PSU	O2-C2-N1	-3.20	119.49	122.79
2	L5	3718	A2M	O3'-C3'-C2'	3.19	120.11	111.19
82	S2	668	A2M	C4-N9-C1'	-3.19	119.18	126.63
82	S2	1851	MA6	C5-N7-C8	3.18	108.45	103.45
2	L5	400	A2M	C3'-C2'-C1'	-3.18	96.71	102.81
2	L5	2401	A2M	C4-N9-C1'	-3.18	119.19	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	3830	A2M	O3'-C3'-C2'	3.18	120.08	111.19
82	S2	1851	MA6	C4-C5-C6	3.18	119.20	115.91
2	L5	1871	A2M	O3'-C3'-C2'	3.16	120.02	111.19
82	S2	99	A2M	O3'-C3'-C2'	3.15	120.01	111.19
82	S2	159	A2M	O3'-C3'-C2'	3.15	120.00	111.19
82	S2	1031	A2M	O3'-C3'-C2'	3.14	119.98	111.19
2	L5	2815	A2M	C2'-C1'-N9	3.14	118.92	113.75
82	S2	1850	MA6	C5-N7-C8	3.14	108.38	103.45
2	L5	400	A2M	O3'-C3'-C2'	3.13	119.96	111.19
2	L5	3825	A2M	O3'-C3'-C2'	3.13	119.95	111.19
2	L5	4689	PSU	O2-C2-N1	-3.12	119.57	122.79
82	S2	428	OMU	O4-C4-C5	-3.12	119.78	125.16
82	S2	1850	MA6	C2-N3-C4	3.12	119.44	111.83
2	L5	4500	PSU	O2-C2-N1	-3.11	119.58	122.79
82	S2	1851	MA6	N3-C4-N9	3.10	132.44	127.17
2	L5	3639	PSU	O2-C2-N1	-3.10	119.59	122.79
2	L5	1536	PSU	O2-C2-N1	-3.10	119.59	122.79
82	S2	116	OMU	O4-C4-C5	-3.08	119.85	125.16
82	S2	1639	G7M	N9-C4-N3	3.08	132.11	125.95
2	L5	4306	OMU	O4-C4-C5	-3.07	119.87	125.16
82	S2	468	A2M	O3'-C3'-C2'	3.07	119.77	111.19
2	L5	4576	PSU	O2-C2-N1	-3.07	119.63	122.79
2	L5	3785	A2M	C4'-O4'-C1'	-3.06	102.70	109.47
2	L5	3844	PSU	O2-C2-N1	-3.04	119.65	122.79
2	L5	3818	UY1	C6-C5-C4	3.03	120.22	118.17
82	S2	1442	OMU	O4-C4-C5	-3.03	119.93	125.16
2	L5	4220	6MZ	C4-N9-C8	3.03	108.92	105.74
2	L5	3851	PSU	O2-C2-N1	-3.03	119.67	122.79
82	S2	1639	G7M	C2-N1-C6	-3.03	119.62	125.11
2	L5	4296	PSU	O2-C2-N1	-3.02	119.68	122.79
2	L5	1860	PSU	O2-C2-N1	-3.01	119.68	122.79
2	L5	2839	PSU	O2-C2-N1	-3.01	119.68	122.79
82	S2	627	OMU	O4-C4-C5	-3.01	119.97	125.16
82	S2	27	A2M	O3'-C3'-C2'	3.01	119.61	111.19
82	S2	668	A2M	C1'-N9-C8	3.01	133.77	127.09
2	L5	4457	PSU	O2-C2-N1	-3.00	119.70	122.79
2	L5	1871	A2M	C4-N9-C1'	-2.99	119.64	126.63
2	L5	1862	PSU	O2-C2-N1	-2.99	119.71	122.79
82	S2	649	PSU	O2-C2-N1	-2.99	119.71	122.79
82	S2	468	A2M	C4-N9-C1'	-2.99	119.64	126.63
2	L5	2363	A2M	C3'-C2'-C1'	-2.99	97.09	102.81
2	L5	4571	A2M	C3'-C2'-C1'	-2.98	97.10	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	S2	1337	4AC	N4-C4-N3	2.98	118.70	113.87
2	L5	3853	PSU	O2-C2-N1	-2.97	119.72	122.79
2	L5	3920	PSU	O2-C2-N1	-2.97	119.73	122.79
4	L8	55	PSU	O2-C2-N1	-2.96	119.74	122.79
2	L5	4532	PSU	O2-C2-N1	-2.96	119.74	122.79
82	S2	668	A2M	O3'-C3'-C2'	2.96	119.46	111.19
82	S2	1326	OMU	O4-C4-C5	-2.95	120.07	125.16
2	L5	3925	OMU	O4-C4-C5	-2.95	120.07	125.16
2	L5	4227	OMU	O4-C4-C5	-2.95	120.08	125.16
82	S2	1832	6MZ	C4-N9-C8	2.94	108.82	105.74
2	L5	4552	PSU	O2-C2-N1	-2.93	119.76	122.79
82	S2	109	PSU	O2-C2-N1	-2.93	119.77	122.79
82	S2	1639	G7M	CN7-N7-C5	2.93	130.45	126.80
2	L5	3818	UY1	C6-N1-C2	-2.93	119.97	122.69
2	L5	2837	OMU	O4-C4-C5	-2.93	120.11	125.16
2	L5	1744	PSU	O2-C2-N1	-2.92	119.77	122.79
2	L5	4571	A2M	O3'-C3'-C2'	2.92	119.37	111.19
2	L5	4521	PSU	O2-C2-N1	-2.92	119.78	122.79
2	L5	3785	A2M	O3'-C3'-C2'	2.92	119.35	111.19
82	S2	166	A2M	C4-N9-C1'	-2.91	119.83	126.63
82	S2	1004	PSU	O2-C2-N1	-2.91	119.79	122.79
82	S2	121	OMU	O4-C4-C5	-2.91	120.15	125.16
82	S2	1177	PSU	O2-C2-N1	-2.90	119.80	122.79
2	L5	4220	6MZ	N3-C4-N9	2.89	132.09	127.17
2	L5	4220	6MZ	C5-N7-C8	2.89	107.99	103.45
2	L5	5010	PSU	O2-C2-N1	-2.89	119.81	122.79
2	L5	2401	A2M	C1'-N9-C8	2.88	133.50	127.09
2	L5	3825	A2M	C4-N9-C1'	-2.88	119.89	126.63
2	L5	4590	A2M	O3'-C3'-C2'	2.88	119.25	111.19
2	L5	3701	OMC	O2-C2-N3	-2.88	117.79	122.33
2	L5	4498	OMU	O4-C4-C5	-2.88	120.20	125.16
82	S2	1288	OMU	O4-C4-C5	-2.87	120.21	125.16
82	S2	172	OMU	O4-C4-C5	-2.87	120.21	125.16
82	S2	1244	PSU	O2-C2-N1	-2.87	119.83	122.79
82	S2	799	OMU	O4-C4-C5	-2.87	120.21	125.16
82	S2	1031	A2M	C4-N9-C1'	-2.87	119.93	126.63
2	L5	3695	PSU	O2-C2-N1	-2.86	119.83	122.79
2	L5	3867	A2M	C2'-C1'-N9	2.86	118.47	113.75
2	L5	4442	PSU	O2-C2-N1	-2.86	119.84	122.79
82	S2	1367	PSU	O2-C2-N1	-2.86	119.84	122.79
2	L5	398	A2M	C4-N9-C1'	-2.85	119.96	126.63
82	S2	354	OMU	O4-C4-C5	-2.85	120.25	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	4312	PSU	C6-N1-C2	-2.85	120.05	122.69
2	L5	2363	A2M	O3'-C3'-C2'	2.84	119.14	111.19
82	S2	1832	6MZ	N3-C4-N9	2.84	132.00	127.17
2	L5	4590	A2M	C4-N9-C1'	-2.84	120.00	126.63
82	S2	686	PSU	O2-C2-N1	-2.84	119.86	122.79
2	L5	4523	A2M	O3'-C3'-C2'	2.83	119.11	111.19
2	L5	2632	PSU	O2-C2-N1	-2.83	119.87	122.79
82	S2	1383	A2M	C4-N9-C1'	-2.83	120.01	126.63
2	L5	4312	PSU	O2-C2-N1	-2.83	119.87	122.79
2	L5	4293	PSU	O2-C2-N1	-2.83	119.87	122.79
82	S2	27	A2M	C4-N9-C1'	-2.83	120.02	126.63
82	S2	406	PSU	O2-C2-N1	-2.82	119.88	122.79
2	L5	4673	PSU	O2-C2-N1	-2.82	119.88	122.79
82	S2	99	A2M	C4-N9-C1'	-2.81	120.06	126.63
2	L5	2839	PSU	C6-N1-C2	-2.81	120.09	122.69
82	S2	651	PSU	O2-C2-N1	-2.81	119.89	122.79
82	S2	1232	PSU	O2-C2-N1	-2.81	119.89	122.79
2	L5	3844	PSU	C6-N1-C2	-2.80	120.09	122.69
2	L5	4403	PSU	O2-C2-N1	-2.80	119.90	122.79
82	S2	681	PSU	C6-N1-C2	-2.80	120.10	122.69
82	S2	159	A2M	C4-N9-C1'	-2.79	120.11	126.63
82	S2	668	A2M	O4'-C1'-C2'	2.78	111.38	106.59
2	L5	1871	A2M	C1'-N9-C8	2.78	133.26	127.09
2	L5	4431	PSU	O2-C2-N1	-2.77	119.94	122.79
2	L5	4500	PSU	C6-N1-C2	-2.77	120.12	122.69
82	S2	1045	PSU	O2-C2-N1	-2.76	119.94	122.79
82	S2	1081	PSU	O2-C2-N1	-2.76	119.94	122.79
2	L5	1326	A2M	O3'-C3'-C2'	2.76	118.91	111.19
82	S2	484	A2M	O3'-C3'-C2'	2.76	118.91	111.19
2	L5	1677	PSU	O2-C2-N1	-2.76	119.94	122.79
2	L5	4571	A2M	C4-N9-C1'	-2.75	120.19	126.63
82	S2	1046	PSU	O2-C2-N1	-2.75	119.95	122.79
82	S2	966	PSU	O2-C2-N1	-2.75	119.96	122.79
2	L5	3822	PSU	O2-C2-N1	-2.74	119.96	122.79
2	L5	3884	PSU	O2-C2-N1	-2.74	119.96	122.79
2	L5	4972	PSU	O2-C2-N1	-2.74	119.97	122.79
2	L5	4523	A2M	C4-N9-C1'	-2.73	120.24	126.63
2	L5	4353	PSU	O2-C2-N1	-2.73	119.97	122.79
82	S2	866	PSU	O2-C2-N1	-2.73	119.97	122.79
82	S2	468	A2M	C1'-N9-C8	2.73	133.15	127.09
2	L5	4973	PSU	O2-C2-N1	-2.72	119.98	122.79
82	S2	1832	6MZ	C4-C5-C6	2.72	119.04	116.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	1792	PSU	O2-C2-N1	-2.71	119.99	122.79
82	S2	484	A2M	C4-N9-C1'	-2.71	120.29	126.63
2	L5	1781	PSU	O2-C2-N1	-2.71	120.00	122.79
2	L5	398	A2M	C1'-N9-C8	2.71	133.10	127.09
2	L5	1582	PSU	O2-C2-N1	-2.71	120.00	122.79
82	S2	1031	A2M	C1'-N9-C8	2.70	133.09	127.09
2	L5	4361	PSU	O2-C2-N1	-2.70	120.00	122.79
2	L5	1326	A2M	C4-N9-C1'	-2.70	120.32	126.63
82	S2	576	A2M	C4-N9-C1'	-2.70	120.32	126.63
82	S2	166	A2M	C1'-N9-C8	2.69	133.07	127.09
82	S2	966	PSU	C6-N1-C2	-2.69	120.19	122.69
82	S2	159	A2M	C1'-N9-C8	2.69	133.07	127.09
2	L5	1524	A2M	C4'-O4'-C1'	-2.69	103.54	109.47
2	L5	3867	A2M	C4-N9-C1'	-2.69	120.35	126.63
2	L5	1683	PSU	C6-N1-C2	-2.68	120.20	122.69
2	L5	1326	A2M	C3'-C2'-C1'	-2.68	97.67	102.81
82	S2	1248	B8N	O4-C4-N3	-2.68	115.64	119.99
82	S2	27	A2M	C1'-N9-C8	2.67	133.03	127.09
82	S2	801	PSU	O2-C2-N1	-2.67	120.03	122.79
2	L5	4636	PSU	O2-C2-N1	-2.67	120.03	122.79
82	S2	863	PSU	O2-C2-N1	-2.67	120.03	122.79
2	L5	3825	A2M	C1'-N9-C8	2.67	133.02	127.09
82	S2	99	A2M	C1'-N9-C8	2.67	133.02	127.09
2	L5	2815	A2M	O3'-C3'-C2'	2.67	118.65	111.19
82	S2	484	A2M	C1'-N9-C8	2.67	133.01	127.09
82	S2	1056	PSU	O2-C2-N1	-2.67	120.04	122.79
2	L5	4620	OMU	O4-C4-C5	-2.66	120.58	125.16
2	L5	4353	PSU	C6-N1-C2	-2.66	120.22	122.69
2	L5	3818	UY1	O2-C2-N1	-2.65	120.05	122.79
2	L5	1524	A2M	O4'-C1'-C2'	2.65	111.15	106.59
2	L5	4590	A2M	C1'-N9-C8	2.65	132.97	127.09
2	L5	1782	PSU	O2-C2-N1	-2.64	120.07	122.79
2	L5	4552	PSU	C6-N1-C2	-2.63	120.25	122.69
2	L5	3718	A2M	C1'-N9-C8	2.63	132.94	127.09
2	L5	1782	PSU	C6-N1-C2	-2.63	120.25	122.69
2	L5	3830	A2M	C4-N9-C1'	-2.63	120.48	126.63
2	L5	4353	PSU	C6-C5-C4	2.63	119.95	118.17
2	L5	3785	A2M	C3'-C2'-C1'	-2.63	97.77	102.81
2	L5	2815	A2M	C3'-C2'-C1'	-2.63	97.77	102.81
2	L5	4628	PSU	O2-C2-N1	-2.63	120.08	122.79
2	L5	3822	PSU	C6-N1-C2	-2.63	120.25	122.69
2	L5	3785	A2M	C4-N9-C1'	-2.62	120.49	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	S2	159	A2M	C3'-C2'-C1'	-2.62	97.79	102.81
82	S2	105	PSU	O2-C2-N1	-2.62	120.09	122.79
2	L5	4220	6MZ	OP2-P-O5'	2.62	113.50	106.67
2	L5	3695	PSU	C6-N1-C2	-2.62	120.26	122.69
82	S2	1367	PSU	C6-N1-C2	-2.62	120.26	122.69
2	L5	2351	OMC	C1'-N1-C2	2.61	124.22	118.44
82	S2	1383	A2M	C1'-N9-C8	2.61	132.90	127.09
2	L5	4628	PSU	C6-N1-C2	-2.61	120.27	122.69
82	S2	93	PSU	O2-C2-N1	-2.61	120.09	122.79
82	S2	801	PSU	C6-N1-C2	-2.61	120.27	122.69
2	L5	3867	A2M	C1'-N9-C8	2.61	132.88	127.09
2	L5	4293	PSU	C6-N1-C2	-2.60	120.28	122.69
2	L5	3701	OMC	O2-C2-N1	2.60	124.00	118.90
2	L5	3920	PSU	C6-N1-C2	-2.60	120.28	122.69
2	L5	1323	A2M	C3'-C2'-C1'	-2.60	97.83	102.81
2	L5	3718	A2M	C4-N9-C1'	-2.60	120.55	126.63
2	L5	4471	PSU	C6-N1-C2	-2.60	120.28	122.69
2	L5	4576	PSU	C6-N1-C2	-2.60	120.28	122.69
2	L5	3639	PSU	C6-N1-C2	-2.59	120.28	122.69
4	L8	69	PSU	C6-N1-C2	-2.59	120.29	122.69
2	L5	2787	A2M	O4'-C1'-C2'	2.58	111.02	106.59
2	L5	1326	A2M	C1'-N9-C8	2.57	132.81	127.09
2	L5	4579	PSU	C6-N1-C2	-2.57	120.31	122.69
82	S2	1177	PSU	C6-N1-C2	-2.57	120.31	122.69
2	L5	400	A2M	C4-N9-C1'	-2.57	120.63	126.63
2	L5	2632	PSU	C6-N1-C2	-2.56	120.31	122.69
2	L5	4493	PSU	O2-C2-N1	-2.56	120.14	122.79
82	S2	681	PSU	O2-C2-N1	-2.56	120.14	122.79
2	L5	1744	PSU	C6-N1-C2	-2.56	120.31	122.69
2	L5	4471	PSU	O2-C2-N1	-2.56	120.15	122.79
82	S2	1232	PSU	C6-N1-C2	-2.56	120.32	122.69
82	S2	668	A2M	C2'-C1'-N9	2.56	117.96	113.75
2	L5	5001	PSU	O2-C2-N1	-2.56	120.15	122.79
2	L5	4442	PSU	C6-N1-C2	-2.55	120.32	122.69
2	L5	5010	PSU	C6-N1-C2	-2.55	120.32	122.69
2	L5	4220	6MZ	C4-C5-C6	2.55	118.90	116.78
2	L5	4673	PSU	C6-N1-C2	-2.55	120.32	122.69
2	L5	400	A2M	C2'-C1'-N9	2.55	117.95	113.75
82	S2	93	PSU	C6-N1-C2	-2.55	120.33	122.69
2	L5	3830	A2M	C1'-N9-C8	2.54	132.74	127.09
2	L5	1860	PSU	C6-N1-C2	-2.54	120.34	122.69
82	S2	651	PSU	C6-N1-C2	-2.54	120.34	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	S2	1046	PSU	C6-N1-C2	-2.53	120.34	122.69
82	S2	576	A2M	C1'-N9-C8	2.53	132.70	127.09
2	L5	2363	A2M	C2'-C1'-N9	2.52	117.90	113.75
4	L8	55	PSU	C6-N1-C2	-2.52	120.35	122.69
82	S2	649	PSU	C6-N1-C2	-2.51	120.36	122.69
2	L5	3853	PSU	C6-N1-C2	-2.51	120.36	122.69
82	S2	105	PSU	C6-N1-C2	-2.51	120.36	122.69
2	L5	4220	6MZ	C5-C6-N1	2.51	120.84	118.15
2	L5	2363	A2M	C4-N9-C1'	-2.50	120.77	126.63
82	S2	1004	PSU	C6-N1-C2	-2.50	120.37	122.69
2	L5	4571	A2M	C1'-N9-C8	2.50	132.64	127.09
2	L5	4521	PSU	C6-N1-C2	-2.50	120.37	122.69
82	S2	1174	PSU	C6-N1-C2	-2.49	120.38	122.69
2	L5	4973	PSU	C6-N1-C2	-2.49	120.38	122.69
2	L5	4299	PSU	O2-C2-N1	-2.49	120.22	122.79
2	L5	4523	A2M	C1'-N9-C8	2.48	132.61	127.09
82	S2	866	PSU	C6-C5-C4	2.48	119.85	118.17
2	L5	4500	PSU	C6-C5-C4	2.48	119.84	118.17
82	S2	354	OMU	O2-C2-N1	-2.47	119.58	122.80
2	L5	400	A2M	C1'-N9-C8	2.47	132.58	127.09
2	L5	1536	PSU	C6-N1-C2	-2.47	120.40	122.69
2	L5	5001	PSU	C6-N1-C2	-2.47	120.40	122.69
82	S2	814	PSU	O2-C2-N1	-2.47	120.25	122.79
2	L5	4442	PSU	C6-C5-C4	2.46	119.83	118.17
2	L5	3808	OMC	C1'-N1-C2	2.46	123.87	118.44
2	L5	2363	A2M	C1'-N9-C8	2.45	132.54	127.09
2	L5	4498	OMU	O2-C2-N1	-2.45	119.61	122.80
82	S2	109	PSU	C6-N1-C2	-2.45	120.42	122.69
2	L5	2787	A2M	C4-N9-C1'	-2.45	120.91	126.63
2	L5	4972	PSU	C6-N1-C2	-2.44	120.42	122.69
82	S2	1832	6MZ	C4-C5-N7	-2.44	107.79	110.58
2	L5	2815	A2M	C4-N9-C1'	-2.44	120.92	126.63
2	L5	1323	A2M	O4'-C1'-C2'	2.44	110.78	106.59
82	S2	1244	PSU	C6-N1-C2	-2.43	120.44	122.69
82	S2	1639	G7M	CN7-N7-C8	-2.43	121.11	124.79
82	S2	1272	OMC	C1'-N1-C2	2.43	123.81	118.44
2	L5	3639	PSU	C6-C5-C4	2.43	119.81	118.17
2	L5	3925	OMU	O2-C2-N1	-2.43	119.64	122.80
2	L5	3884	PSU	C6-N1-C2	-2.42	120.44	122.69
2	L5	3851	PSU	C6-N1-C2	-2.42	120.45	122.69
2	L5	4521	PSU	C6-C5-C4	2.41	119.80	118.17
2	L5	4431	PSU	C6-N1-C2	-2.40	120.46	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	2861	OMC	C1'-N1-C2	2.40	123.74	118.44
2	L5	1534	A2M	O3'-C3'-C4'	-2.40	104.19	111.08
82	S2	863	PSU	C6-N1-C2	-2.40	120.47	122.69
82	S2	406	PSU	C6-N1-C2	-2.39	120.48	122.69
2	L5	1582	PSU	C6-N1-C2	-2.38	120.48	122.69
82	S2	1045	PSU	C6-N1-C2	-2.38	120.48	122.69
82	S2	484	A2M	O4'-C1'-C2'	2.38	110.68	106.59
2	L5	3785	A2M	C2-N1-C6	-2.38	114.83	118.73
2	L5	3822	PSU	O4'-C1'-C2'	2.37	108.42	105.15
2	L5	2401	A2M	C6-C5-C4	-2.36	113.95	117.18
2	L5	1871	A2M	C6-C5-C4	-2.36	113.95	117.18
2	L5	1781	PSU	C6-N1-C2	-2.36	120.50	122.69
2	L5	4296	PSU	C6-N1-C2	-2.35	120.51	122.69
82	S2	686	PSU	C6-N1-C2	-2.35	120.51	122.69
82	S2	866	PSU	C6-N1-C2	-2.34	120.52	122.69
2	L5	2837	OMU	O2-C2-N1	-2.34	119.75	122.80
2	L5	4571	A2M	C2'-C1'-N9	2.34	117.60	113.75
2	L5	3637	PSU	C6-N1-C2	-2.34	120.52	122.69
2	L5	2815	A2M	C1'-N9-C8	2.34	132.28	127.09
2	L5	4299	PSU	C6-N1-C2	-2.33	120.53	122.69
2	L5	3785	A2M	C1'-N9-C8	2.33	132.27	127.09
2	L5	1524	A2M	C4-N9-C1'	-2.33	121.19	126.63
2	L5	4636	PSU	C6-C5-C4	2.33	119.74	118.17
82	S2	1639	G7M	N9-C8-N7	-2.32	106.84	112.48
2	L5	2787	A2M	C1'-N9-C8	2.32	132.25	127.09
82	S2	1056	PSU	C6-N1-C2	-2.32	120.54	122.69
2	L5	1323	A2M	C4-N9-C1'	-2.31	121.23	126.63
2	L5	4457	PSU	C6-N1-C2	-2.31	120.55	122.69
82	S2	1248	B8N	O4'-C1'-C2'	2.30	108.34	105.15
82	S2	1850	MA6	C1'-N9-C8	-2.30	121.99	127.09
2	L5	4361	PSU	C6-N1-C2	-2.29	120.56	122.69
2	L5	1683	PSU	C6-C5-C4	2.29	119.72	118.17
2	L5	4532	PSU	C6-N1-C2	-2.29	120.57	122.69
2	L5	2363	A2M	O4'-C1'-C2'	2.28	110.52	106.59
82	S2	668	A2M	C6-C5-C4	-2.28	114.06	117.18
2	L5	4590	A2M	C6-C5-C4	-2.27	114.07	117.18
82	S2	468	A2M	C6-C5-C4	-2.27	114.07	117.18
82	S2	428	OMU	O2-C2-N1	-2.27	119.84	122.80
2	L5	4523	A2M	C6-C5-C4	-2.27	114.08	117.18
82	S2	1288	OMU	C1'-N1-C2	2.27	121.67	117.59
2	L5	1744	PSU	C6-C5-C4	2.27	119.70	118.17
2	L5	1862	PSU	C6-N1-C2	-2.27	120.59	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	S2	1851	MA6	C1'-N9-C8	-2.26	122.07	127.09
4	L8	69	PSU	O4'-C1'-C2'	2.26	108.28	105.15
2	L5	1323	A2M	C1'-N9-C8	2.26	132.12	127.09
82	S2	172	OMU	O2-C2-N1	-2.26	119.85	122.80
82	S2	1326	OMU	O2-C2-N1	-2.26	119.85	122.80
2	L5	4571	A2M	O4'-C1'-C2'	2.26	110.48	106.59
2	L5	3785	A2M	C5-C6-N1	2.26	123.25	117.51
82	S2	1337	4AC	C5-C4-N4	-2.26	119.14	122.94
2	L5	2815	A2M	O4'-C1'-C2'	2.25	110.47	106.59
2	L5	3825	A2M	C6-C5-C4	-2.25	114.10	117.18
2	L5	3867	A2M	C6-C5-C4	-2.25	114.10	117.18
2	L5	1326	A2M	C2'-C1'-N9	2.25	117.46	113.75
82	S2	166	A2M	C6-C5-C4	-2.24	114.12	117.18
2	L5	1326	A2M	C6-C5-C4	-2.24	114.12	117.18
2	L5	4493	PSU	C6-N1-C2	-2.24	120.61	122.69
2	L5	1524	A2M	C1'-N9-C8	2.23	132.05	127.09
82	S2	27	A2M	C6-C5-C4	-2.23	114.13	117.18
2	L5	3867	A2M	O3'-C3'-C2'	2.23	117.43	111.19
2	L5	1326	A2M	O4'-C1'-C2'	2.23	110.43	106.59
82	S2	1031	A2M	C6-C5-C4	-2.23	114.13	117.18
2	L5	4571	A2M	C6-C5-C4	-2.22	114.15	117.18
2	L5	1322	1MA	N1-C6-N6	2.22	125.29	119.71
82	S2	406	PSU	C6-C5-C4	2.22	119.67	118.17
2	L5	4457	PSU	C6-C5-C4	2.21	119.66	118.17
82	S2	1056	PSU	C6-C5-C4	2.21	119.66	118.17
2	L5	1522	OMG	C2'-C1'-N9	-2.21	110.05	114.24
2	L5	3637	PSU	C6-C5-C4	2.21	119.66	118.17
2	L5	4227	OMU	O2-C2-N1	-2.20	119.93	122.80
2	L5	4403	PSU	O4'-C1'-C2'	2.20	108.20	105.15
82	S2	1383	A2M	C6-C5-C4	-2.20	114.18	117.18
82	S2	814	PSU	C6-N1-C2	-2.20	120.65	122.69
82	S2	1248	B8N	O4-C4-C5	-2.19	118.80	122.58
2	L5	2632	PSU	C6-C5-C4	2.18	119.65	118.17
2	L5	1792	PSU	C6-N1-C2	-2.18	120.67	122.69
82	S2	159	A2M	O4'-C1'-C2'	2.18	110.34	106.59
2	L5	398	A2M	C6-C5-C4	-2.17	114.21	117.18
2	L5	4636	PSU	O4'-C1'-C2'	2.17	108.15	105.15
82	S2	166	A2M	O4'-C1'-C2'	2.17	110.32	106.59
2	L5	400	A2M	C2-N1-C6	-2.17	115.17	118.73
2	L5	4523	A2M	C4'-O4'-C1'	-2.16	104.71	109.47
82	S2	116	OMU	O2-C2-N1	-2.16	119.99	122.80
2	L5	4552	PSU	C6-C5-C4	2.15	119.63	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	3830	A2M	C6-C5-C4	-2.15	114.24	117.18
2	L5	1534	A2M	O4'-C1'-C2'	2.15	110.29	106.59
4	L8	69	PSU	C6-C5-C4	2.15	119.63	118.17
2	L5	3782	5MC	C1'-N1-C6	-2.15	117.61	121.15
2	L5	4442	PSU	O4'-C1'-C2'	2.15	108.12	105.15
82	S2	649	PSU	C6-C5-C4	2.15	119.62	118.17
82	S2	99	A2M	C6-C5-C4	-2.15	114.25	117.18
2	L5	2839	PSU	C6-C5-C4	2.15	119.62	118.17
82	S2	576	A2M	C6-C5-C4	-2.15	114.25	117.18
82	S2	627	OMU	O2-C2-N1	-2.14	120.01	122.80
2	L5	1322	1MA	CM1-N1-C6	-2.14	116.83	120.15
2	L5	1534	A2M	C2-N1-C6	-2.14	115.22	118.73
2	L5	3785	A2M	C6-C5-C4	-2.13	114.26	117.18
2	L5	1534	A2M	C4-N9-C1'	-2.13	121.64	126.63
2	L5	400	A2M	C6-C5-C4	-2.13	114.28	117.18
2	L5	400	A2M	C5-C6-N1	2.12	122.90	117.51
2	L5	3785	A2M	O4'-C1'-N9	2.12	112.16	108.09
2	L5	3785	A2M	O4'-C4'-C3'	2.12	109.36	105.15
82	S2	1081	PSU	C6-N1-C2	-2.11	120.73	122.69
2	L5	3718	A2M	C6-C5-C4	-2.11	114.29	117.18
2	L5	2363	A2M	C2-N1-C6	-2.11	115.26	118.73
82	S2	1081	PSU	O4'-C1'-C2'	2.11	108.07	105.15
2	L5	1323	A2M	C2-N1-C6	-2.11	115.27	118.73
2	L5	398	A2M	C5-C6-N1	2.11	122.86	117.51
82	S2	99	A2M	C2-N1-C6	-2.11	115.27	118.73
2	L5	2401	A2M	O4'-C1'-C2'	2.11	110.21	106.59
2	L5	2363	A2M	C6-C5-C4	-2.10	114.31	117.18
82	S2	1383	A2M	C4'-O4'-C1'	-2.10	104.83	109.47
2	L5	3637	PSU	O2-C2-N1	-2.10	120.63	122.79
2	L5	2363	A2M	C5-C6-N1	2.09	122.83	117.51
2	L5	4523	A2M	C5-C6-N1	2.09	122.82	117.51
82	S2	468	A2M	O4'-C1'-C2'	2.09	110.18	106.59
2	L5	2787	A2M	C6-C5-C4	-2.09	114.33	117.18
2	L5	1524	A2M	C6-C5-C4	-2.09	114.33	117.18
82	S2	799	OMU	C1'-N1-C2	2.09	121.34	117.59
82	S2	484	A2M	O4'-C4'-C3'	2.09	109.29	105.15
2	L5	4306	OMU	O2-C2-N1	-2.08	120.08	122.80
2	L5	3867	A2M	C2-N1-C6	-2.08	115.31	118.73
2	L5	1323	A2M	C5-C6-N1	2.08	122.80	117.51
2	L5	1534	A2M	C1'-N9-C8	2.08	131.71	127.09
2	L5	1326	A2M	C5-C6-N1	2.08	122.80	117.51
2	L5	4636	PSU	C6-N1-C2	-2.08	120.76	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L5	4403	PSU	C6-N1-C2	-2.08	120.76	122.69
82	S2	484	A2M	C6-C5-C4	-2.08	114.34	117.18
82	S2	159	A2M	C6-C5-C4	-2.08	114.34	117.18
2	L5	2787	A2M	C5-C6-N1	2.08	122.79	117.51
2	L5	3825	A2M	C5-C6-N1	2.08	122.78	117.51
2	L5	3830	A2M	C5-C6-N1	2.07	122.78	117.51
2	L5	4403	PSU	C6-C5-C4	2.07	119.57	118.17
82	S2	99	A2M	C5-C6-N1	2.07	122.78	117.51
82	S2	1832	6MZ	OP2-P-OP1	2.07	118.91	110.83
2	L5	400	A2M	O4'-C1'-C2'	2.07	110.16	106.59
2	L5	398	A2M	C2-N1-C6	-2.07	115.33	118.73
2	L5	1871	A2M	C4'-O4'-C1'	-2.07	104.89	109.47
2	L5	1323	A2M	C6-C5-C4	-2.07	114.35	117.18
82	S2	121	OMU	O2-C2-N1	-2.07	120.11	122.80
2	L5	2401	A2M	C5-C6-N1	2.07	122.76	117.51
82	S2	166	A2M	C5-C6-N1	2.07	122.76	117.51
2	L5	4571	A2M	O3'-C3'-C4'	-2.06	105.15	111.08
2	L5	3867	A2M	C3'-C2'-C1'	-2.06	98.85	102.81
2	L5	4457	PSU	O4'-C1'-C2'	2.06	108.00	105.15
2	L5	2815	A2M	C6-C5-C4	-2.06	114.36	117.18
82	S2	468	A2M	C5-C6-N1	2.06	122.75	117.51
2	L5	3867	A2M	O4'-C1'-C2'	2.06	110.13	106.59
2	L5	4456	OMC	C1'-N1-C2	2.05	122.98	118.44
2	L5	4628	PSU	O4'-C1'-C2'	2.05	107.99	105.15
2	L5	4353	PSU	O4'-C1'-C2'	2.05	107.99	105.15
2	L5	2787	A2M	C2-N1-C6	-2.05	115.36	118.73
2	L5	3825	A2M	C2-N1-C6	-2.05	115.37	118.73
2	L5	3867	A2M	C5-C6-N1	2.05	122.71	117.51
82	S2	1383	A2M	C5-C6-N1	2.04	122.70	117.51
2	L5	1534	A2M	C5-C6-N1	2.04	122.69	117.51
82	S2	1442	OMU	O2-C2-N1	-2.04	120.14	122.80
2	L5	4571	A2M	C5-C6-N1	2.04	122.69	117.51
2	L5	4973	PSU	C6-C5-C4	2.04	119.55	118.17
82	S2	27	A2M	C5-C6-N1	2.04	122.68	117.51
2	L5	3825	A2M	O4'-C1'-C2'	2.03	110.09	106.59
2	L5	4972	PSU	C6-C5-C4	2.03	119.55	118.17
2	L5	2815	A2M	C5-C6-N1	2.03	122.66	117.51
82	S2	159	A2M	C5-C6-N1	2.02	122.65	117.51
2	L5	4523	A2M	C2-N1-C6	-2.02	115.41	118.73
2	L5	4521	PSU	O4'-C1'-C2'	2.02	107.94	105.15
82	S2	1031	A2M	C5-C6-N1	2.01	122.63	117.51
82	S2	1244	PSU	C6-C5-C4	2.01	119.53	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	S2	484	A2M	C5-C6-N1	2.01	122.61	117.51
2	L5	3920	PSU	C6-C5-C4	2.01	119.53	118.17
2	L5	1326	A2M	C2-N1-C6	-2.01	115.43	118.73
82	S2	27	A2M	O4'-C1'-C2'	2.01	110.05	106.59
82	S2	576	A2M	C5-C6-N1	2.01	122.61	117.51
2	L5	3718	A2M	C5-C6-N1	2.01	122.61	117.51
2	L5	4590	A2M	C5-C6-N1	2.01	122.60	117.51
2	L5	3695	PSU	O4'-C1'-C2'	2.00	107.92	105.15
82	S2	668	A2M	O3'-C3'-C4'	-2.00	105.34	111.08

There are no chirality outliers.

All (134) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L8	75	OMG	C1'-C2'-O2'-CM2
2	L5	1326	A2M	O4'-C4'-C5'-O5'
2	L5	1326	A2M	C1'-C2'-O2'-CM'
2	L5	1340	OMC	C1'-C2'-O2'-CM2
2	L5	1625	OMG	O4'-C4'-C5'-O5'
2	L5	2351	OMC	C1'-C2'-O2'-CM2
2	L5	2787	A2M	C1'-C2'-O2'-CM'
2	L5	3701	OMC	O4'-C4'-C5'-O5'
2	L5	3792	OMG	O4'-C4'-C5'-O5'
2	L5	4196	OMG	C1'-C2'-O2'-CM2
2	L5	4220	6MZ	C5'-O5'-P-OP1
2	L5	4220	6MZ	C5'-O5'-P-OP3
2	L5	4637	OMG	O4'-C4'-C5'-O5'
82	S2	27	A2M	C1'-C2'-O2'-CM'
82	S2	159	A2M	C1'-C2'-O2'-CM'
82	S2	601	OMG	C1'-C2'-O2'-CM2
82	S2	644	OMG	O4'-C4'-C5'-O5'
82	S2	1248	B8N	O4'-C4'-C5'-O5'
82	S2	1272	OMC	O4'-C4'-C5'-O5'
82	S2	1288	OMU	O4'-C4'-C5'-O5'
82	S2	1337	4AC	N3-C4-N4-C7
82	S2	1383	A2M	C1'-C2'-O2'-CM'
82	S2	1442	OMU	O4'-C4'-C5'-O5'
82	S2	1832	6MZ	C5-C6-N6-C9
82	S2	1832	6MZ	N1-C6-N6-C9
2	L5	3701	OMC	C2'-C1'-N1-C2
2	L5	2364	OMG	O4'-C4'-C5'-O5'
2	L5	3701	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	L5	4500	PSU	C3'-C4'-C5'-O5'
2	L5	4500	PSU	O4'-C4'-C5'-O5'
2	L5	4590	A2M	O4'-C4'-C5'-O5'
2	L5	4590	A2M	C3'-C4'-C5'-O5'
82	S2	436	OMG	O4'-C4'-C5'-O5'
82	S2	576	A2M	O4'-C4'-C5'-O5'
82	S2	576	A2M	C3'-C4'-C5'-O5'
82	S2	683	OMG	C3'-C4'-C5'-O5'
82	S2	799	OMU	C3'-C4'-C5'-O5'
82	S2	799	OMU	O4'-C4'-C5'-O5'
82	S2	801	PSU	C3'-C4'-C5'-O5'
82	S2	867	OMG	C3'-C4'-C5'-O5'
82	S2	1272	OMC	C3'-C4'-C5'-O5'
82	S2	1288	OMU	C3'-C4'-C5'-O5'
2	L5	1323	A2M	O4'-C4'-C5'-O5'
2	L5	1536	PSU	C3'-C4'-C5'-O5'
2	L5	1536	PSU	O4'-C4'-C5'-O5'
2	L5	1625	OMG	C3'-C4'-C5'-O5'
2	L5	2815	A2M	O4'-C4'-C5'-O5'
2	L5	3792	OMG	C3'-C4'-C5'-O5'
2	L5	3867	A2M	C3'-C4'-C5'-O5'
82	S2	99	A2M	O4'-C4'-C5'-O5'
82	S2	683	OMG	O4'-C4'-C5'-O5'
82	S2	1442	OMU	C3'-C4'-C5'-O5'
2	L5	3701	OMC	C2'-C1'-N1-C6
2	L5	1326	A2M	C3'-C4'-C5'-O5'
82	S2	644	OMG	C3'-C4'-C5'-O5'
2	L5	4447	5MC	C2'-C1'-N1-C6
2	L5	1677	PSU	C3'-C4'-C5'-O5'
2	L5	2364	OMG	C3'-C4'-C5'-O5'
2	L5	2876	OMG	C3'-C4'-C5'-O5'
2	L5	3899	OMG	C3'-C4'-C5'-O5'
2	L5	4637	OMG	C3'-C4'-C5'-O5'
82	S2	436	OMG	C3'-C4'-C5'-O5'
82	S2	517	OMC	C3'-C4'-C5'-O5'
82	S2	668	A2M	O4'-C4'-C5'-O5'
82	S2	668	A2M	C3'-C4'-C5'-O5'
82	S2	1248	B8N	C3'-C4'-C5'-O5'
82	S2	428	OMU	C2'-C1'-N1-C6
2	L5	1677	PSU	O4'-C4'-C5'-O5'
2	L5	2787	A2M	C3'-C4'-C5'-O5'
2	L5	2815	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
82	S2	801	PSU	O4'-C4'-C5'-O5'
82	S2	867	OMG	O4'-C4'-C5'-O5'
2	L5	1524	A2M	O4'-C4'-C5'-O5'
2	L5	1524	A2M	C3'-C4'-C5'-O5'
2	L5	3867	A2M	O4'-C4'-C5'-O5'
82	S2	517	OMC	O4'-C4'-C5'-O5'
2	L5	2787	A2M	C2'-C1'-N9-C8
2	L5	3899	OMG	O4'-C4'-C5'-O5'
2	L5	4618	OMG	C3'-C4'-C5'-O5'
2	L5	1323	A2M	C3'-C4'-C5'-O5'
2	L5	2876	OMG	O4'-C4'-C5'-O5'
82	S2	99	A2M	C3'-C4'-C5'-O5'
2	L5	4590	A2M	C4'-C5'-O5'-P
2	L5	2422	OMC	O4'-C4'-C5'-O5'
82	S2	1045	PSU	O4'-C4'-C5'-O5'
2	L5	3841	OMC	C1'-C2'-O2'-CM2
82	S2	166	A2M	C1'-C2'-O2'-CM'
82	S2	867	OMG	C1'-C2'-O2'-CM2
2	L5	2422	OMC	C3'-C4'-C5'-O5'
2	L5	3851	PSU	C3'-C4'-C5'-O5'
82	S2	428	OMU	O4'-C4'-C5'-O5'
82	S2	1248	B8N	C31-C32-C33-C34
82	S2	1045	PSU	C3'-C4'-C5'-O5'
82	S2	1248	B8N	N34-C33-C34-O36
82	S2	1639	G7M	C3'-C4'-C5'-O5'
2	L5	4447	5MC	O4'-C1'-N1-C6
82	S2	428	OMU	O4'-C1'-N1-C6
2	L5	4447	5MC	O4'-C1'-N1-C2
2	L5	3818	UY1	C4'-C5'-O5'-P
2	L5	4447	5MC	C2'-C1'-N1-C2
82	S2	1383	A2M	O4'-C4'-C5'-O5'
2	L5	3701	OMC	O4'-C1'-N1-C6
2	L5	1534	A2M	C4'-C5'-O5'-P
2	L5	4500	PSU	C4'-C5'-O5'-P
2	L5	3818	UY1	O4'-C1'-C5-C4
2	L5	2787	A2M	C2'-C1'-N9-C4
82	S2	428	OMU	C3'-C4'-C5'-O5'
82	S2	1383	A2M	C3'-C4'-C5'-O5'
82	S2	576	A2M	C4'-C5'-O5'-P
2	L5	1781	PSU	C3'-C4'-C5'-O5'
82	S2	428	OMU	C2'-C1'-N1-C2
2	L5	3887	OMC	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
82	S2	627	OMU	O4'-C4'-C5'-O5'
2	L5	3785	A2M	C3'-C2'-O2'-CM'
82	S2	1490	OMG	C4'-C5'-O5'-P
2	L5	3782	5MC	O4'-C4'-C5'-O5'
2	L5	4618	OMG	O4'-C4'-C5'-O5'
82	S2	1703	OMC	O4'-C4'-C5'-O5'
82	S2	644	OMG	C4'-C5'-O5'-P
82	S2	1851	MA6	C4'-C5'-O5'-P
2	L5	398	A2M	O4'-C4'-C5'-O5'
82	S2	428	OMU	O4'-C1'-N1-C2
2	L5	400	A2M	C1'-C2'-O2'-CM'
2	L5	3844	PSU	C4'-C5'-O5'-P
2	L5	1677	PSU	O4'-C1'-C5-C6
2	L5	3869	OMC	C3'-C2'-O2'-CM2
2	L5	3701	OMC	O4'-C1'-N1-C2
2	L5	1322	1MA	C2'-C1'-N9-C8
2	L5	2351	OMC	O4'-C4'-C5'-O5'
82	S2	1832	6MZ	O4'-C4'-C5'-O5'
2	L5	2787	A2M	O4'-C1'-N9-C8
82	S2	1639	G7M	O4'-C4'-C5'-O5'
2	L5	1326	A2M	C4'-C5'-O5'-P
2	L5	1322	1MA	C2'-C1'-N9-C4

There are no ring outliers.

67 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	S2	436	OMG	1	0
82	S2	681	PSU	1	0
82	S2	121	OMU	1	0
82	S2	159	A2M	2	0
2	L5	3884	PSU	1	0
2	L5	1683	PSU	2	0
2	L5	4620	OMU	2	0
2	L5	4227	OMU	1	0
82	S2	601	OMG	1	0
2	L5	2351	OMC	1	0
2	L5	1625	OMG	1	0
82	S2	1232	PSU	2	0
82	S2	1288	OMU	1	0
2	L5	4618	OMG	1	0
2	L5	1677	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	S2	1850	MA6	2	0
2	L5	2632	PSU	1	0
2	L5	398	A2M	1	0
82	S2	1639	G7M	3	0
2	L5	2876	OMG	1	0
2	L5	4571	A2M	1	0
2	L5	2422	OMC	1	0
82	S2	576	A2M	2	0
82	S2	509	OMG	2	0
2	L5	3818	UY1	1	0
82	S2	1328	OMG	1	0
2	L5	4447	5MC	1	0
82	S2	166	A2M	2	0
2	L5	1871	A2M	1	0
82	S2	1337	4AC	3	0
82	S2	867	OMG	1	0
82	S2	1383	A2M	1	0
2	L5	3785	A2M	1	0
2	L5	2424	OMG	1	0
82	S2	99	A2M	1	0
82	S2	484	A2M	1	0
2	L5	4456	OMC	1	0
2	L5	3822	PSU	1	0
2	L5	4457	PSU	1	0
2	L5	1340	OMC	2	0
2	L5	4293	PSU	1	0
2	L5	4579	PSU	1	0
2	L5	4590	A2M	1	0
2	L5	4536	OMC	2	0
2	L5	1326	A2M	3	0
2	L5	4220	6MZ	2	0
2	L5	3782	5MC	1	0
2	L5	3718	A2M	3	0
82	S2	468	A2M	1	0
2	L5	3701	OMC	1	0
2	L5	4196	OMG	1	0
2	L5	4431	PSU	1	0
2	L5	4392	OMG	1	0
2	L5	3867	A2M	3	0
2	L5	400	A2M	1	0
2	L5	4637	OMG	1	0
82	S2	462	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L5	4306	OMU	1	0
2	L5	3841	OMC	1	0
2	L5	4636	PSU	1	0
2	L5	2363	A2M	1	0
2	L5	2861	OMC	1	0
4	L8	75	OMG	2	0
82	S2	1046	PSU	1	0
82	S2	517	OMC	1	0
82	S2	27	A2M	1	0
82	S2	116	OMU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
88	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.82	0
87	SPM	L5	5258	-	13,13,13	0.35	0	12,12,12	0.99	0
88	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.91	0
88	SPD	LN	301	-	9,9,9	0.33	0	8,8,8	0.85	0
88	SPD	L5	5288	-	9,9,9	0.33	0	8,8,8	0.80	0
87	SPM	L5	5263	-	13,13,13	0.35	0	12,12,12	1.00	0
88	SPD	L5	5260	-	9,9,9	0.31	0	8,8,8	0.95	0
87	SPM	L5	5262	-	13,13,13	0.36	0	12,12,12	0.88	0
87	SPM	L5	5286	86	13,13,13	0.36	0	12,12,12	1.00	0
87	SPM	L5	5290	-	13,13,13	0.36	0	12,12,12	0.87	0
88	SPD	L5	5282	-	9,9,9	0.31	0	8,8,8	0.77	0
88	SPD	L5	5287	-	9,9,9	0.31	0	8,8,8	0.85	0
88	SPD	L8	202	-	9,9,9	0.33	0	8,8,8	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	SPD	L5	5281	-	9,9,9	0.33	0	8,8,8	0.84	0
87	SPM	L5	5266	-	13,13,13	0.37	0	12,12,12	1.12	0
88	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.84	0
87	SPM	L5	5289	-	13,13,13	0.36	0	12,12,12	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	SPD	L5	5284	-	-	0/7/7/7	-
87	SPM	L5	5258	-	-	2/11/11/11	-
88	SPD	L5	5283	-	-	4/7/7/7	-
88	SPD	LN	301	-	-	1/7/7/7	-
88	SPD	L5	5288	-	-	3/7/7/7	-
87	SPM	L5	5263	-	-	4/11/11/11	-
88	SPD	L5	5260	-	-	0/7/7/7	-
87	SPM	L5	5262	-	-	2/11/11/11	-
87	SPM	L5	5286	86	-	4/11/11/11	-
87	SPM	L5	5290	-	-	3/11/11/11	-
88	SPD	L5	5282	-	-	1/7/7/7	-
88	SPD	L5	5287	-	-	1/7/7/7	-
88	SPD	L8	202	-	-	3/7/7/7	-
88	SPD	L5	5281	-	-	1/7/7/7	-
87	SPM	L5	5266	-	-	5/11/11/11	-
88	SPD	L5	5285	-	-	1/7/7/7	-
87	SPM	L5	5289	-	-	3/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	L5	5283	SPD	C3-C4-C5-N6
87	L5	5289	SPM	C7-C8-C9-N10
88	L8	202	SPD	C3-C4-C5-N6

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Mol	Chain	Res	Type	Atoms
88	L5	5283	SPD	N6-C7-C8-C9
88	L5	5282	SPD	C3-C4-C5-N6
87	L5	5266	SPM	N10-C11-C12-C13
87	L5	5258	SPM	C3-C4-N5-C6
87	L5	5286	SPM	C12-C11-N10-C9
87	L5	5289	SPM	N10-C11-C12-C13
87	L5	5290	SPM	C8-C9-N10-C11
88	L5	5283	SPD	C4-C5-N6-C7
88	L5	5283	SPD	C2-C3-C4-C5
87	L5	5266	SPM	C7-C8-C9-N10
87	L5	5286	SPM	C7-C6-N5-C4
87	L5	5286	SPM	C8-C9-N10-C11
87	L5	5266	SPM	C2-C3-C4-N5
87	L5	5262	SPM	C6-C7-C8-C9
87	L5	5258	SPM	C6-C7-C8-C9
87	L5	5266	SPM	C6-C7-C8-C9
87	L5	5290	SPM	C6-C7-C8-C9
87	L5	5263	SPM	N5-C6-C7-C8
87	L5	5263	SPM	C7-C6-N5-C4
87	L5	5290	SPM	C7-C6-N5-C4
88	L5	5288	SPD	C4-C5-N6-C7
88	L5	5287	SPD	C2-C3-C4-C5
88	L5	5281	SPD	C2-C3-C4-C5
88	LN	301	SPD	C4-C5-N6-C7
87	L5	5263	SPM	N10-C11-C12-C13
87	L5	5286	SPM	N1-C2-C3-C4
88	L5	5288	SPD	C8-C7-N6-C5
87	L5	5266	SPM	N5-C6-C7-C8
88	L5	5288	SPD	N1-C2-C3-C4
87	L5	5263	SPM	C2-C3-C4-N5
88	L8	202	SPD	N6-C7-C8-C9
87	L5	5262	SPM	C3-C4-N5-C6
88	L8	202	SPD	C8-C7-N6-C5
87	L5	5289	SPM	N5-C6-C7-C8
88	L5	5285	SPD	C8-C7-N6-C5

There are no ring outliers.

8 monomers are involved in 9 short contacts:

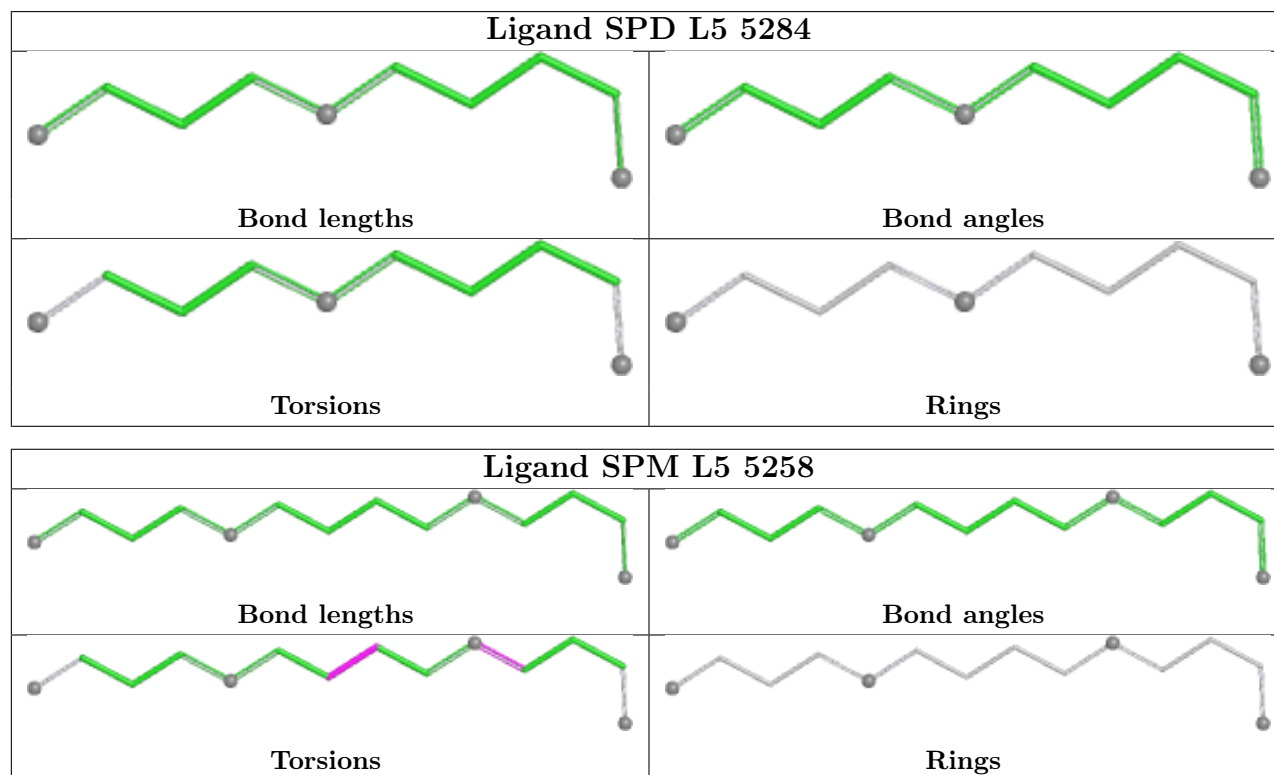
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5284	SPD	1	0
88	LN	301	SPD	1	0

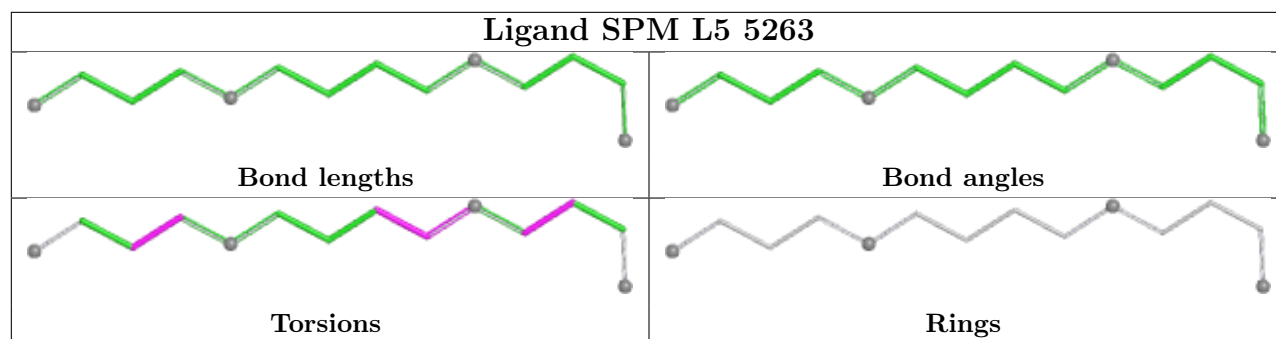
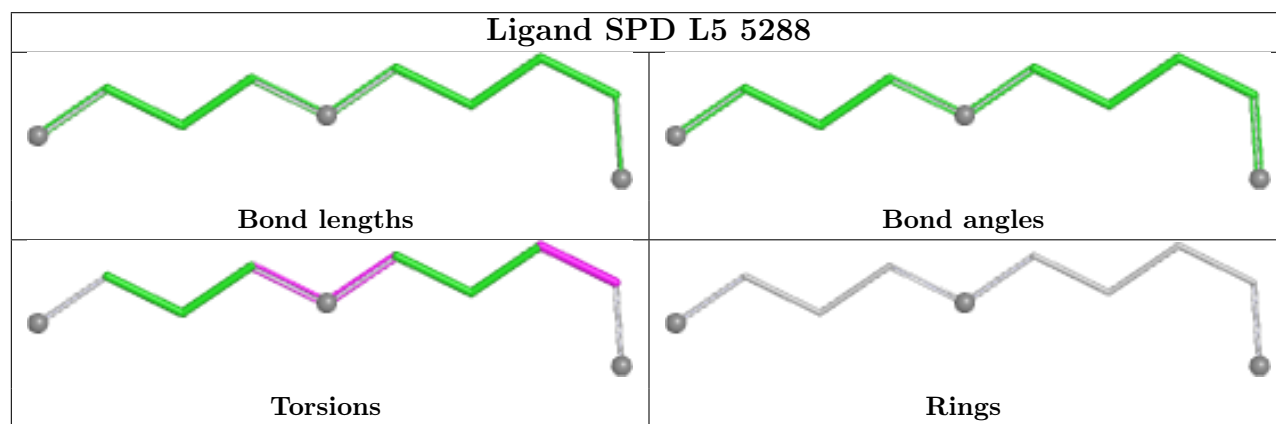
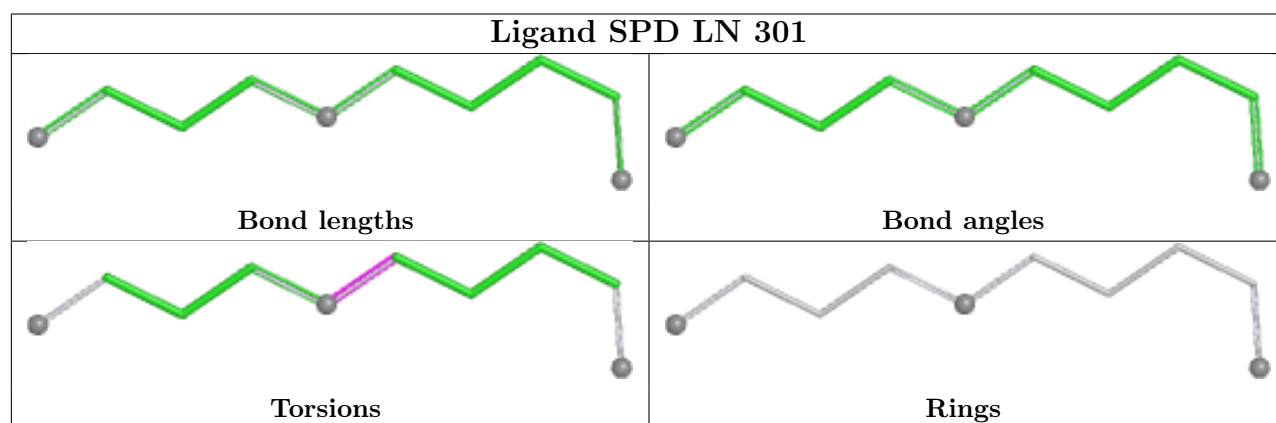
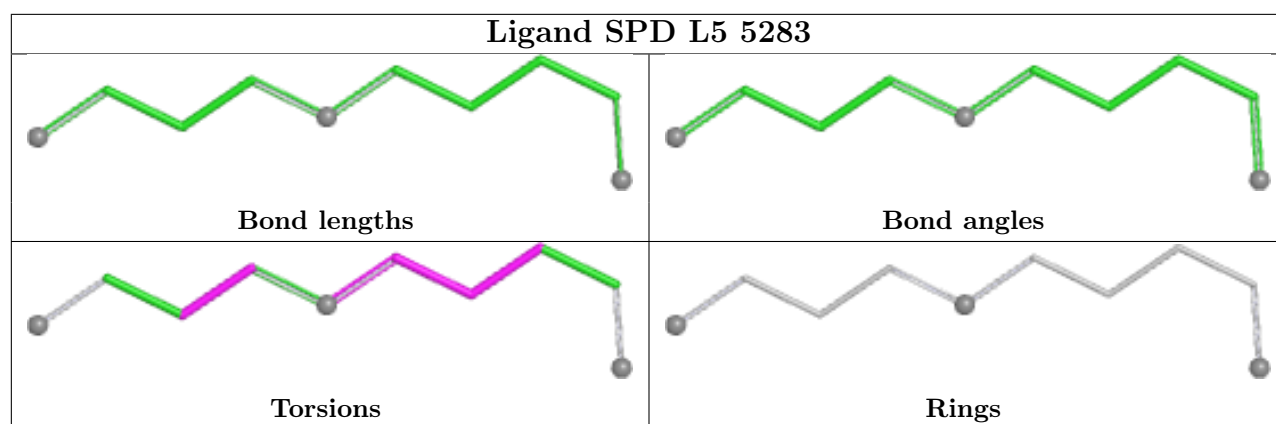
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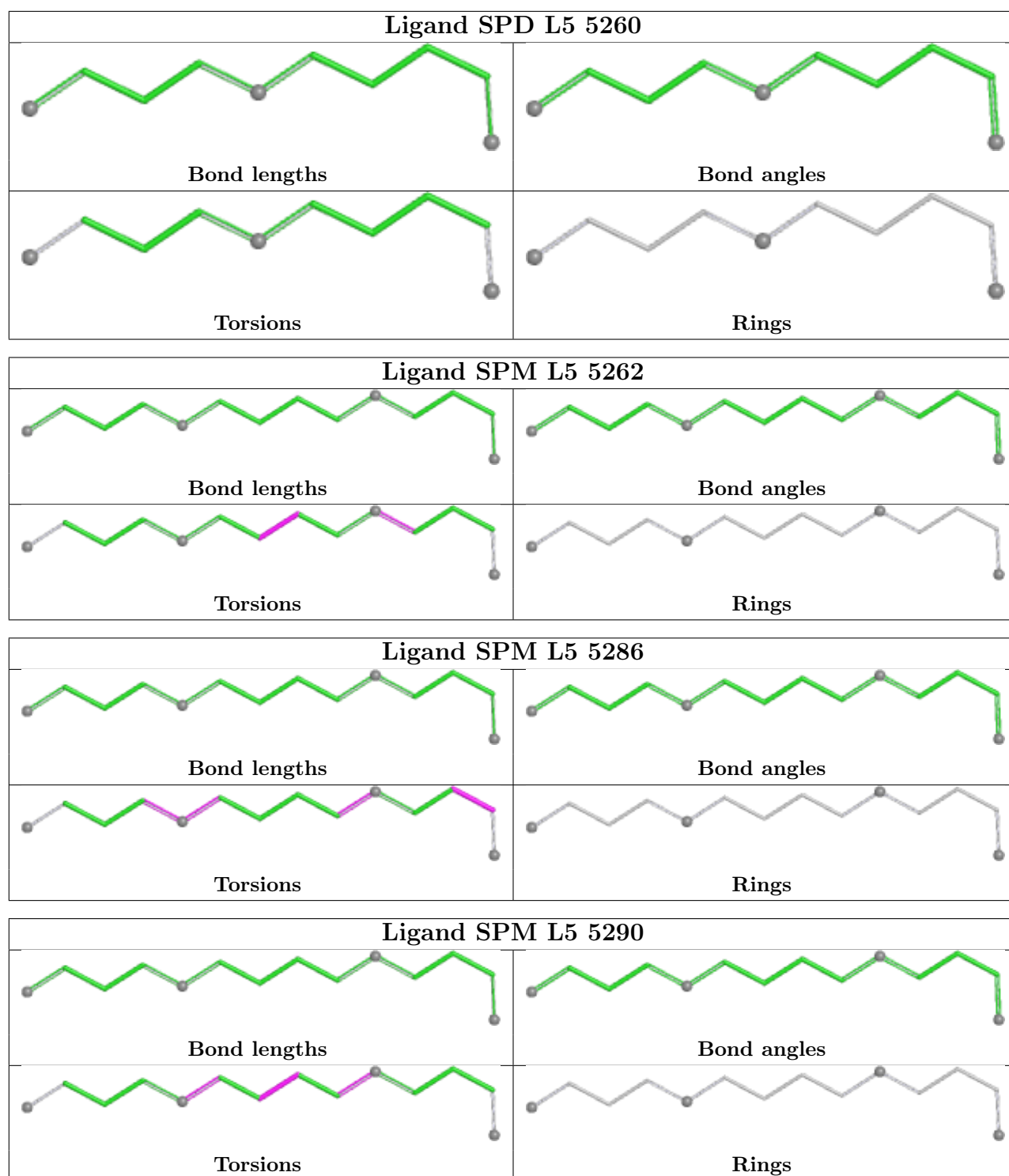
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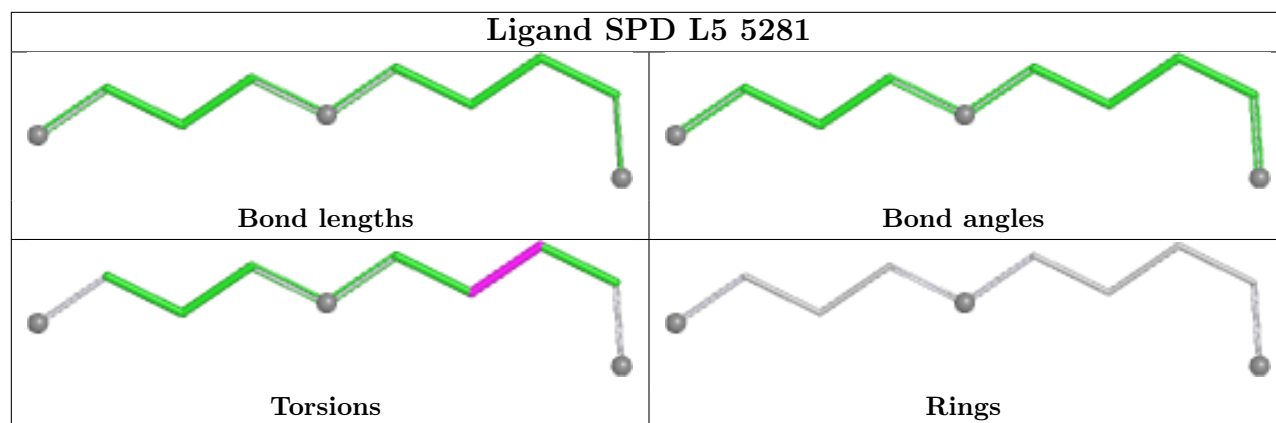
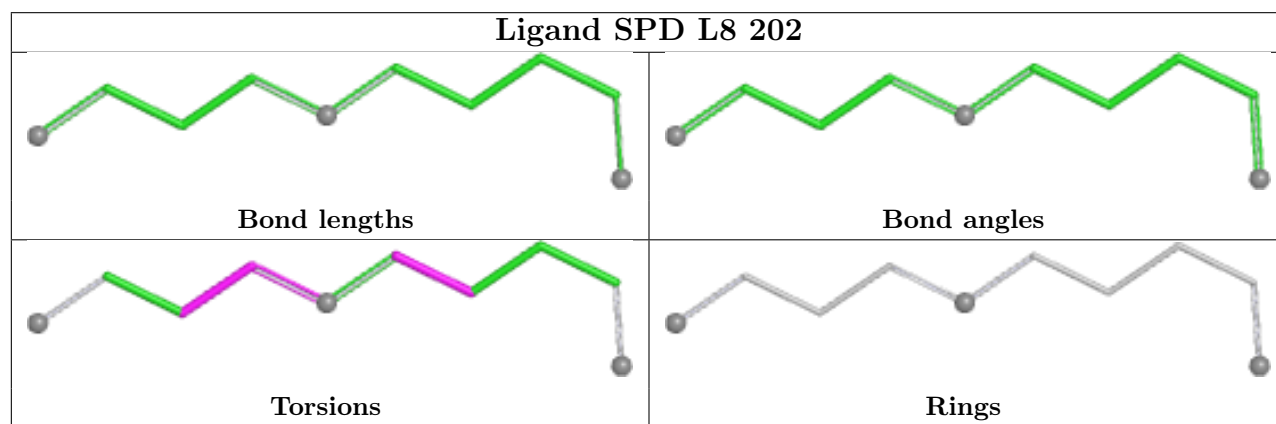
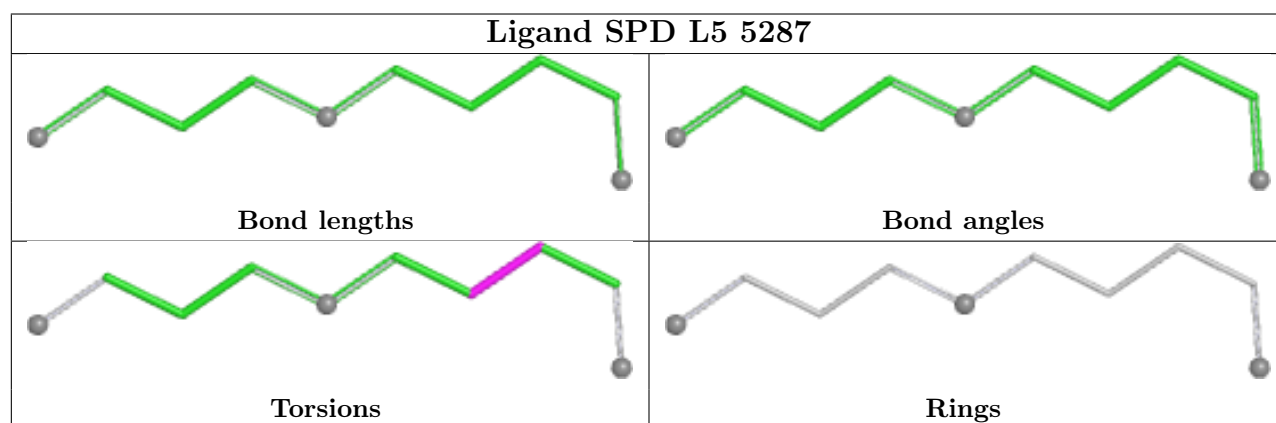
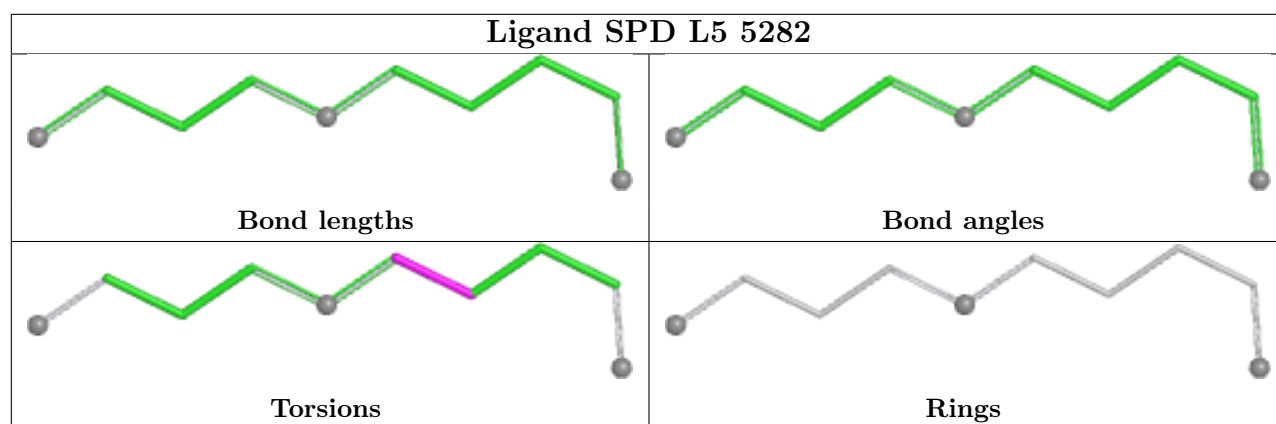
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	L5	5288	SPD	1	0
88	L5	5260	SPD	1	0
87	L5	5290	SPM	2	0
88	L5	5282	SPD	1	0
87	L5	5266	SPM	1	0
87	L5	5289	SPM	1	0

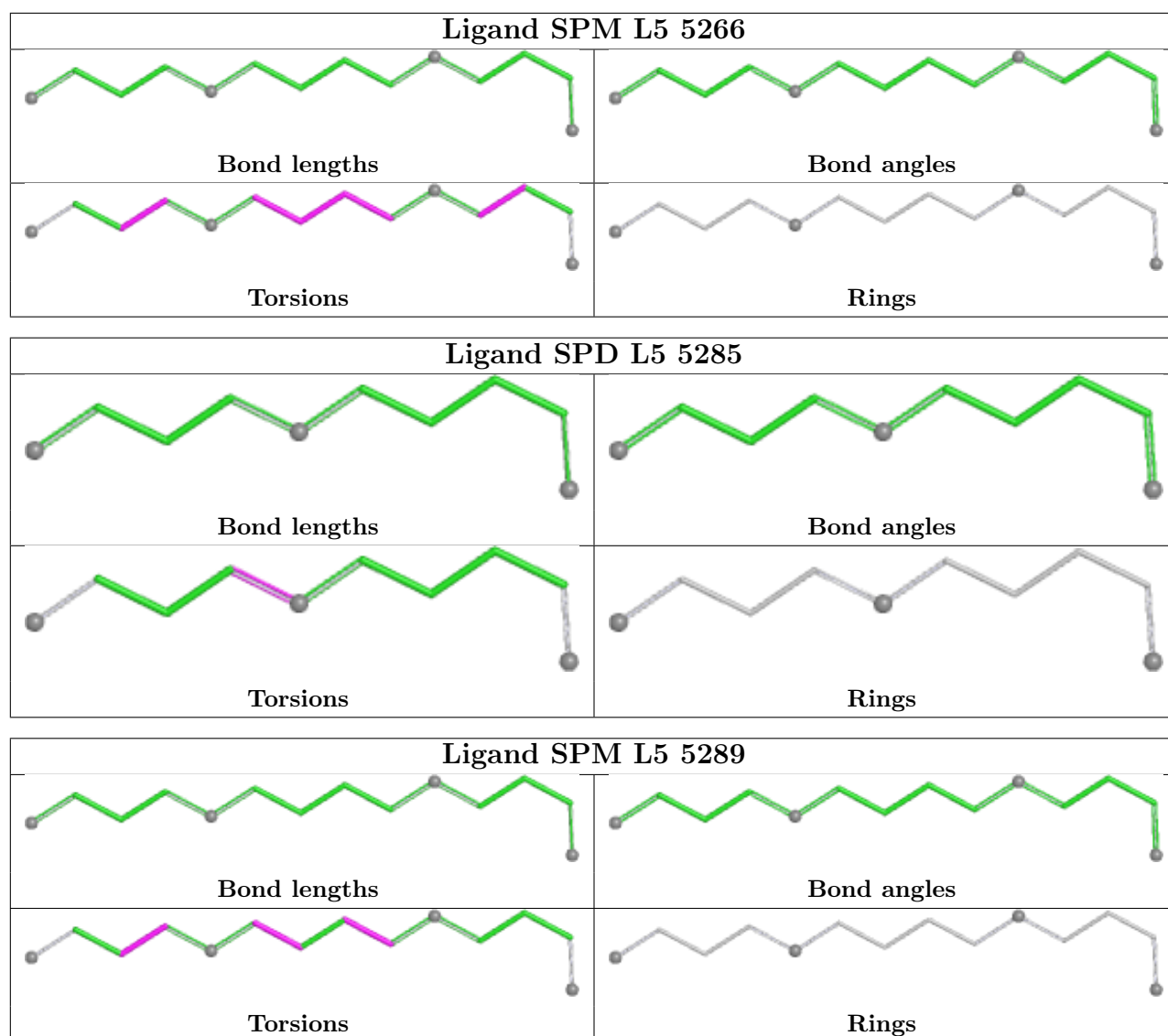
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [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
2	L5	8
82	S2	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	29.36
1	L5	2910:G	O3'	3584:C	P	21.20
1	L5	760:G	O3'	903:C	P	16.82
1	L5	519:C	O3'	642:G	P	15.80
1	L5	2112:G	O3'	2249:C	P	15.23
1	L5	4776:G	O3'	4858:C	P	15.05
1	S2	698:G	O3'	730:C	P	14.63
1	L5	3954:A	O3'	4056:A	P	13.42
1	S2	739:C	O3'	746:C	P	12.44
1	L5	990:C	O3'	1064:G	P	12.35
1	S2	225:G	O3'	287:U	P	7.53
1	L5	1100:U	O3'	1167:C	P	7.01
1	S2	1831:A	O3'	1832:6MZ	P	4.27

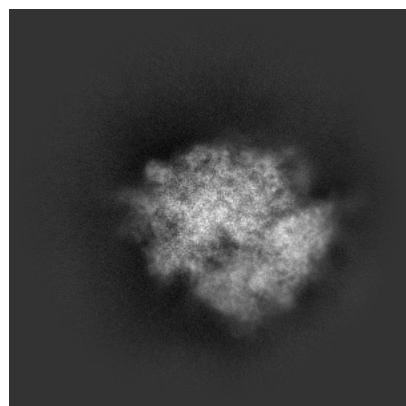
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71411. These allow visual inspection of the internal detail of the map and identification of artifacts.

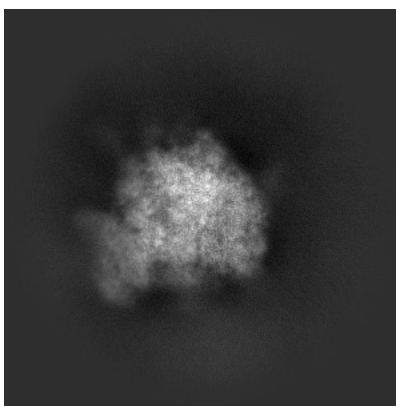
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

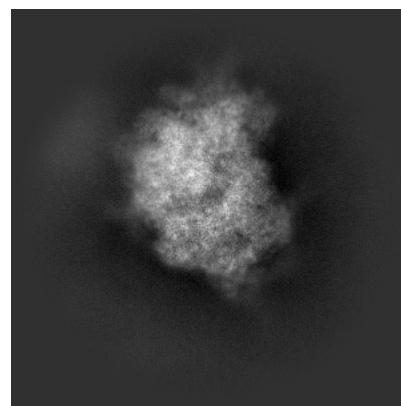
6.1.1 Primary map



X

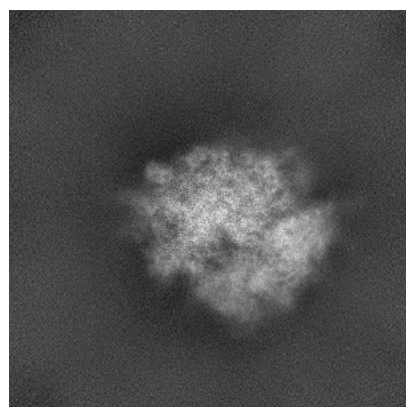


Y

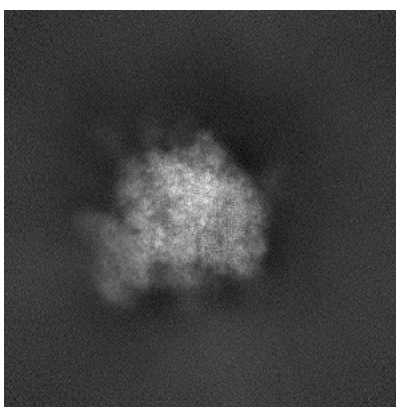


Z

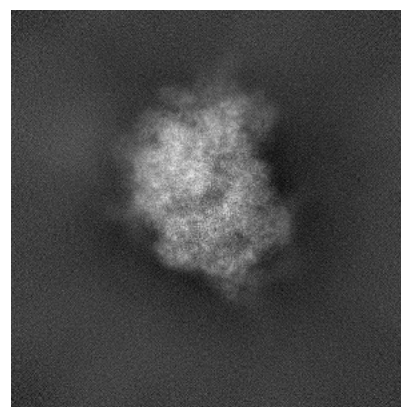
6.1.2 Raw map



X



Y

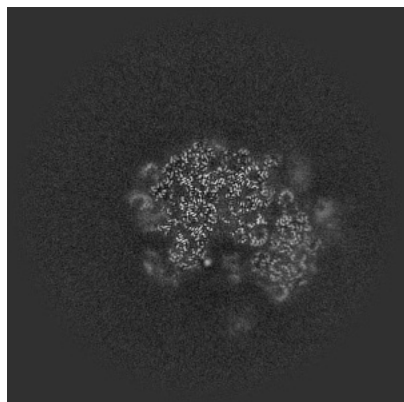


Z

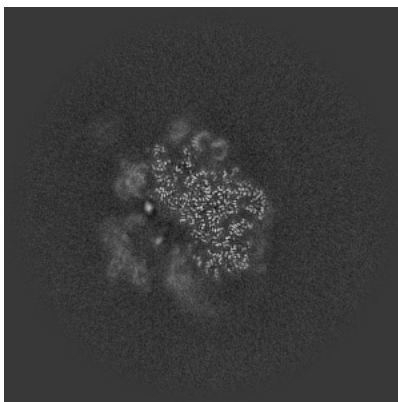
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

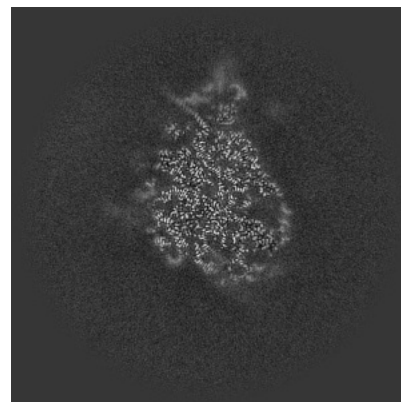
6.2.1 Primary map



X Index: 256

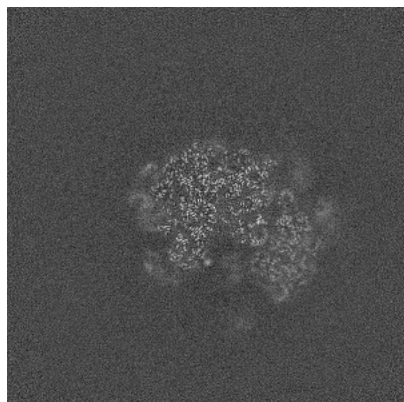


Y Index: 256

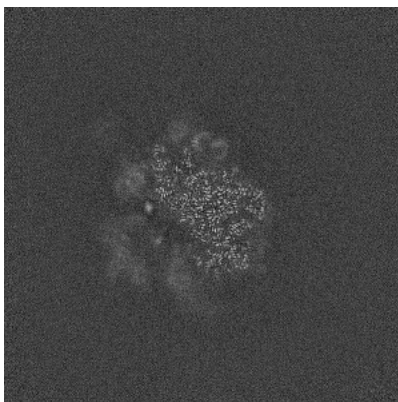


Z Index: 256

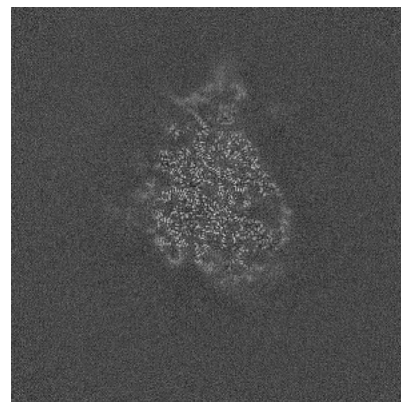
6.2.2 Raw map



X Index: 256



Y Index: 256

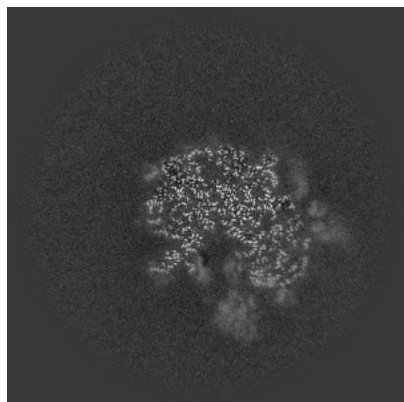


Z Index: 256

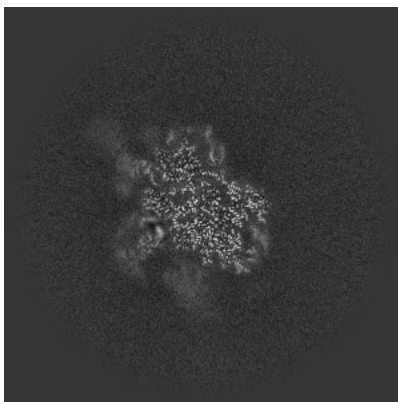
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

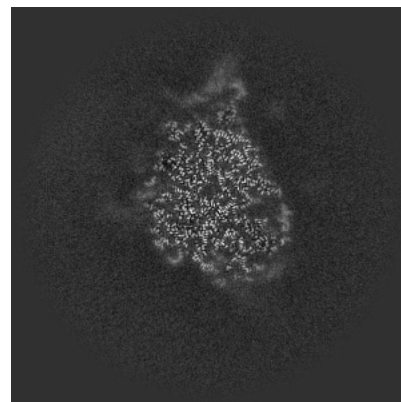
6.3.1 Primary map



X Index: 243

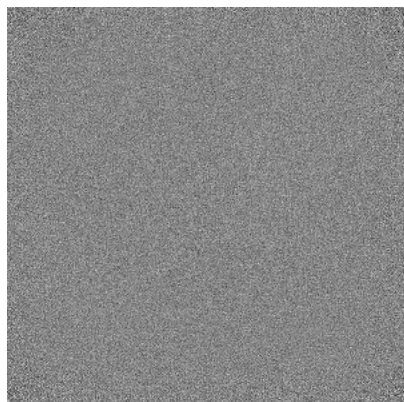


Y Index: 243

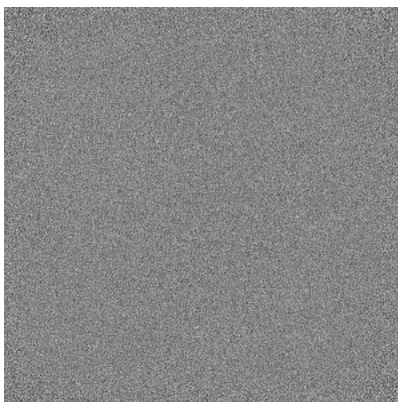


Z Index: 258

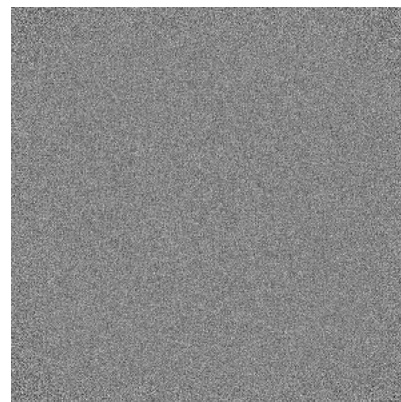
6.3.2 Raw map



X Index: 0



Y Index: 0

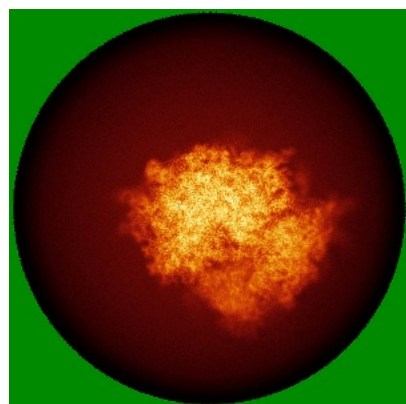


Z Index: 0

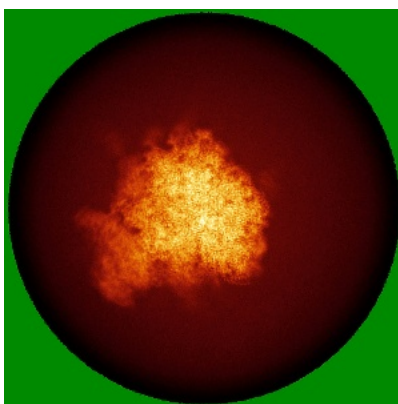
The images above show the largest variance slices of the map in three orthogonal directions.

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

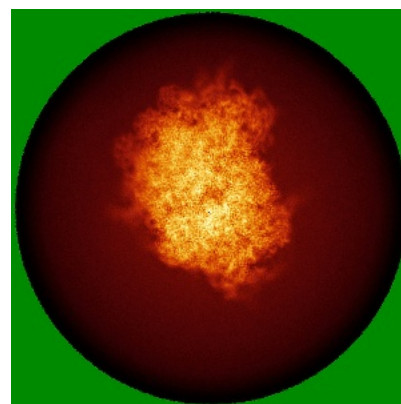
6.4.1 Primary map



X

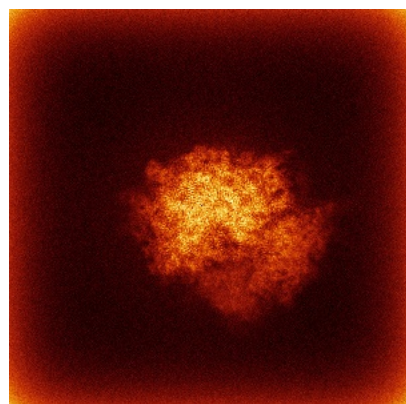


Y

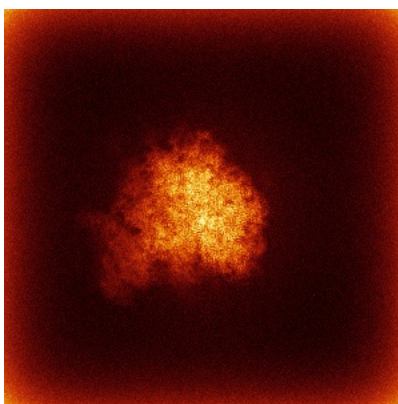


Z

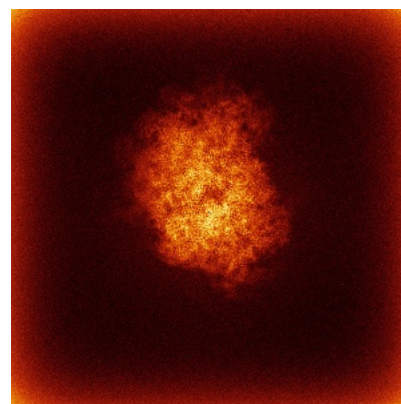
6.4.2 Raw map



X



Y

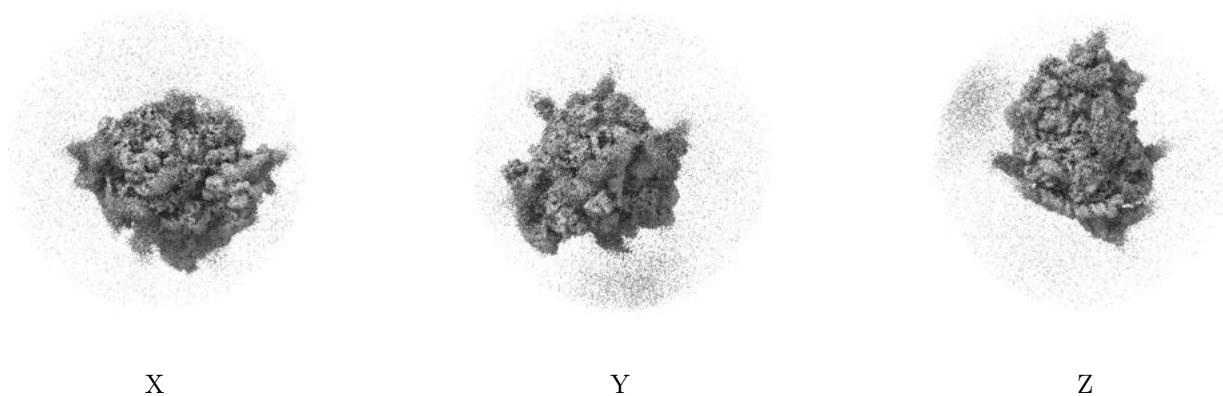


Z

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.

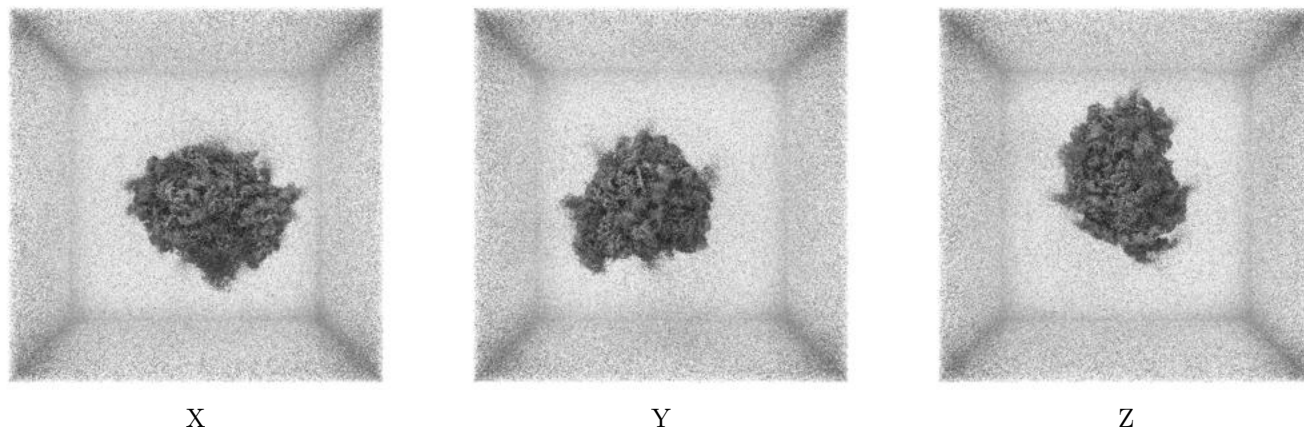
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0136. 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.

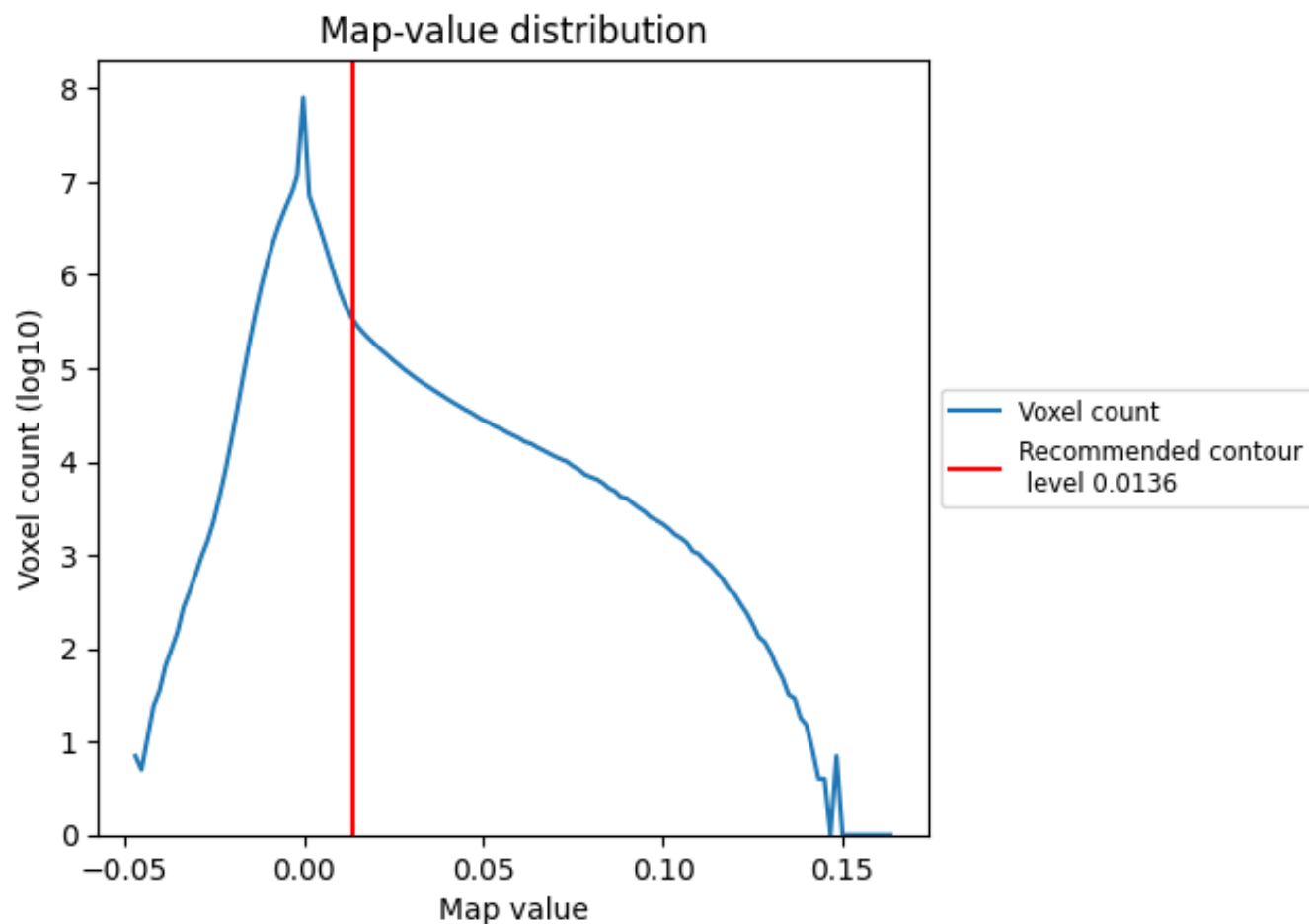
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

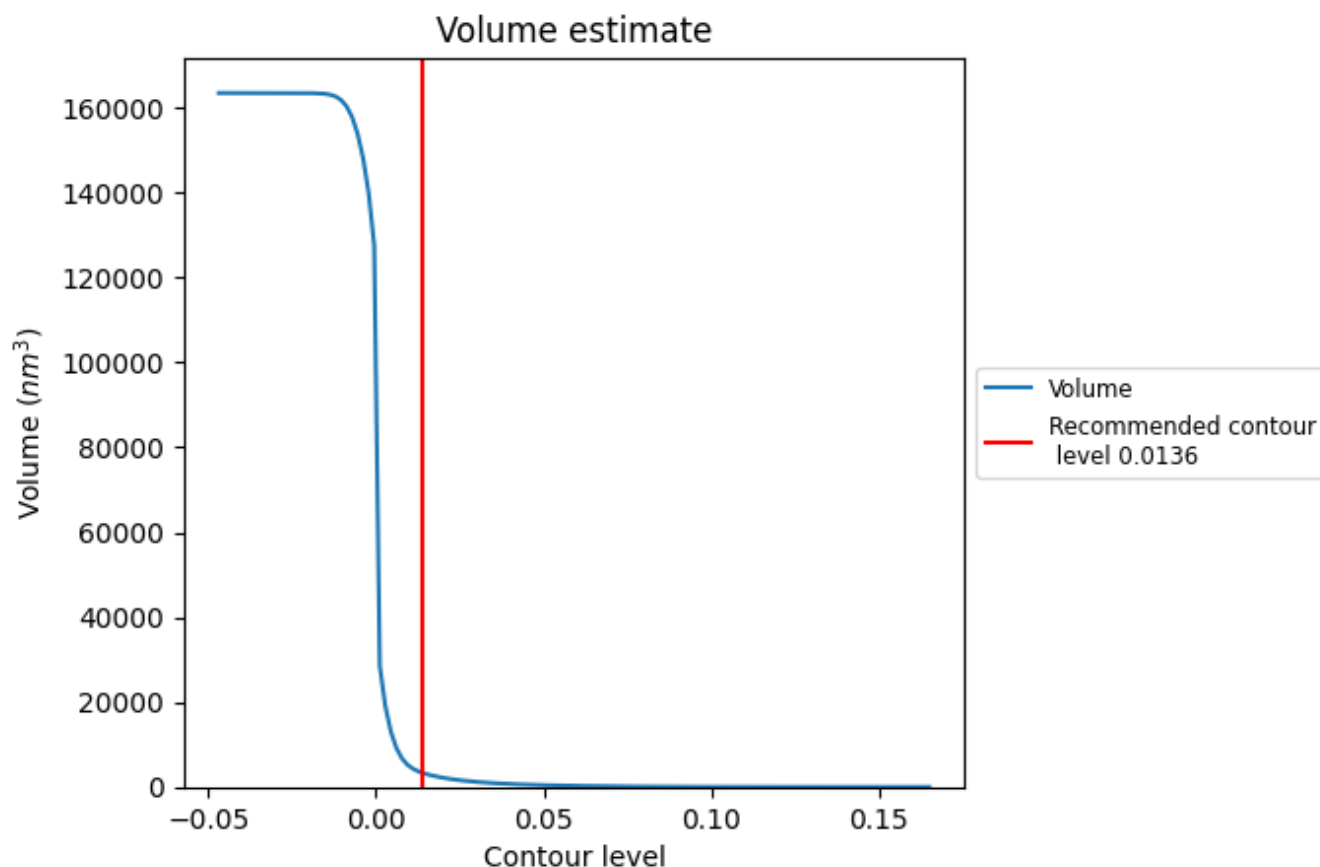
This section contains the results of statistical analysis of the map.

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.

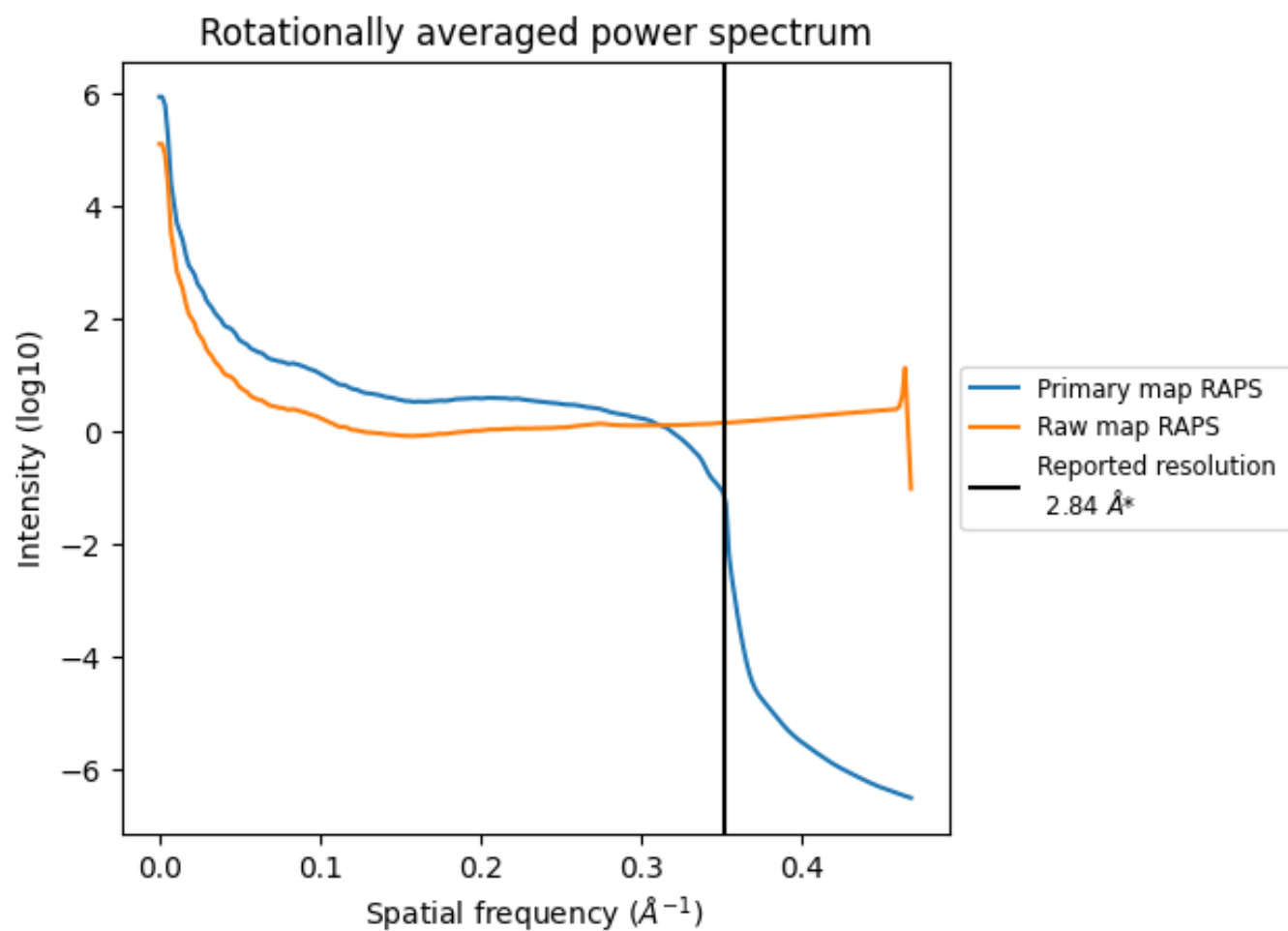
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3409 nm^3 ; this corresponds to an approximate mass of 3080 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 ⓘ

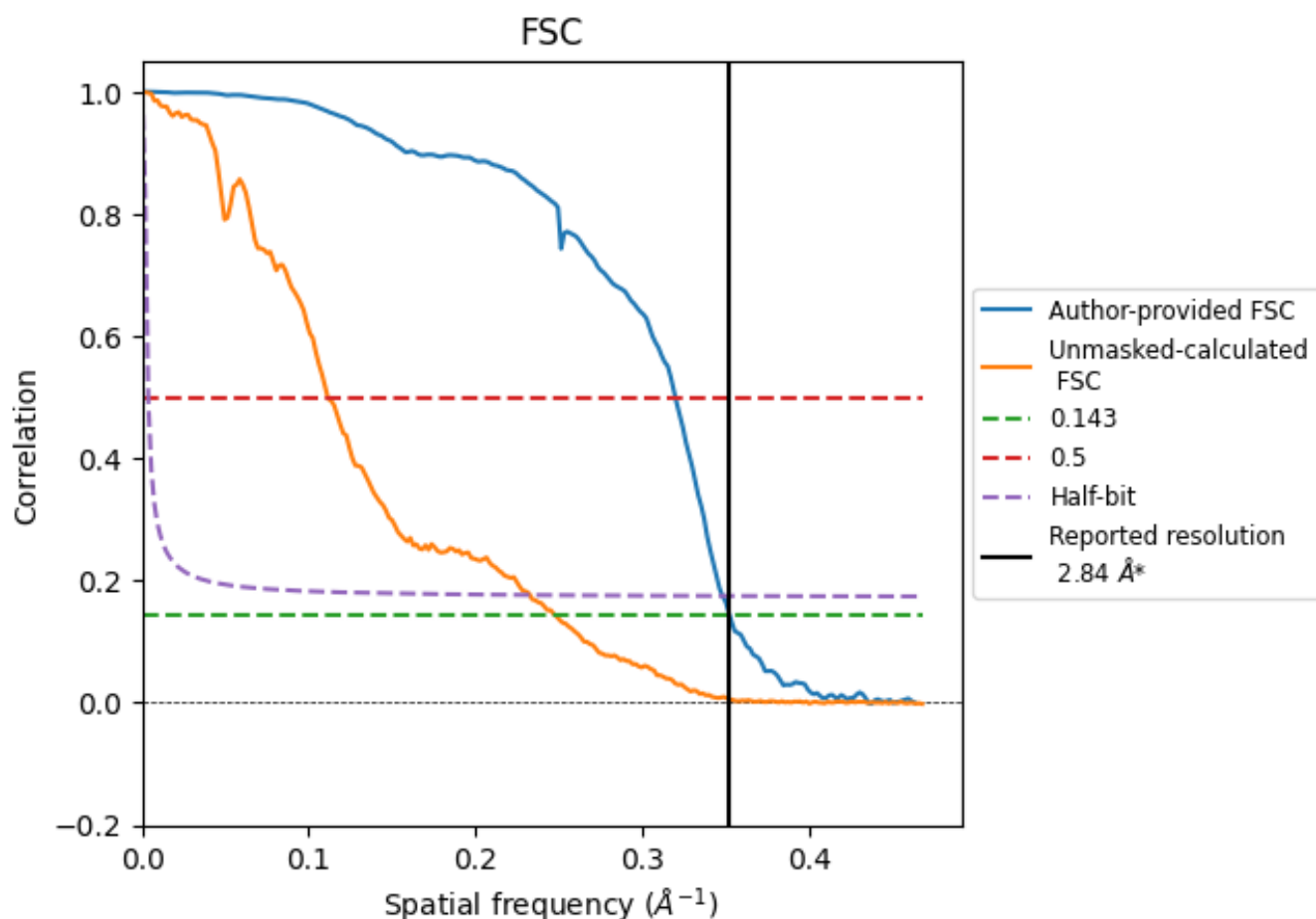


*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.352 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

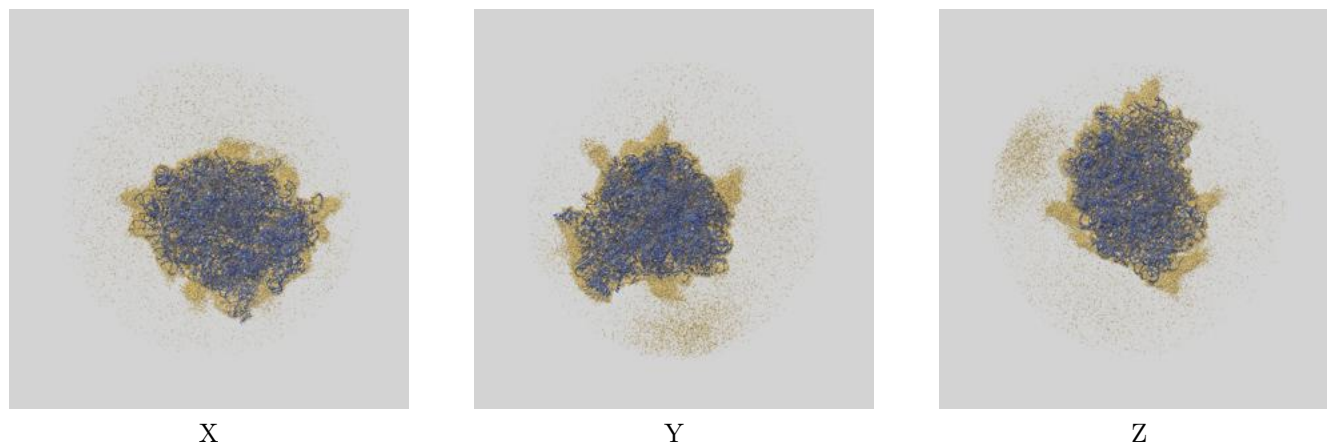
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.12	2.87
Unmasked-calculated*	4.03	8.98	4.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 2.84 by more than 10 %

9 Map-model fit [i](#)

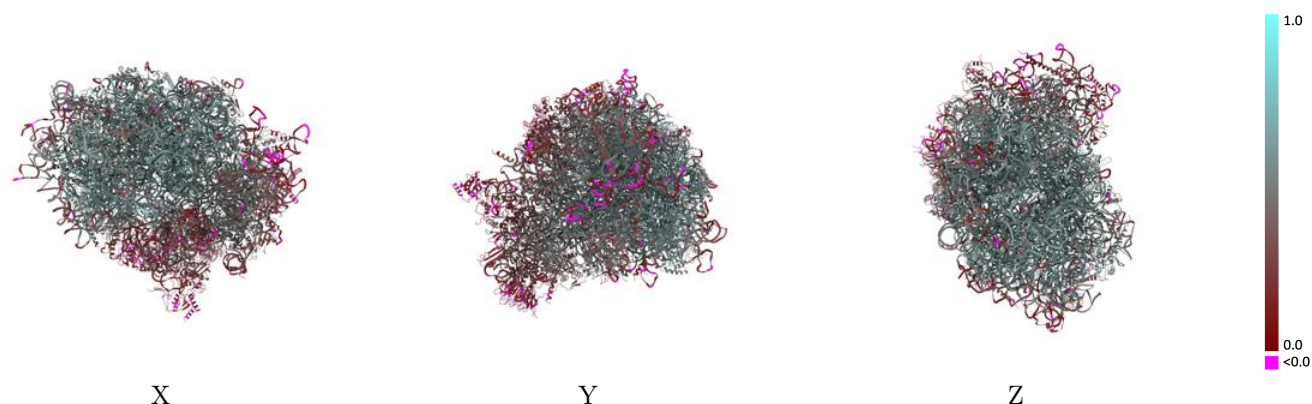
This section contains information regarding the fit between EMDB map EMD-71411 and PDB model 9P9H. Per-residue inclusion information can be found in section [3](#) on page [23](#).

9.1 Map-model overlay [i](#)



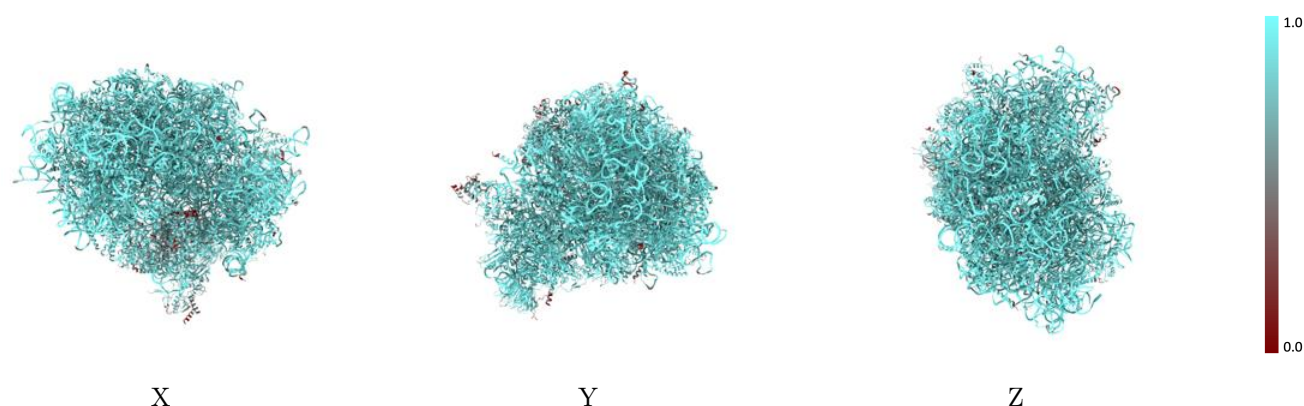
The images above show the 3D surface view of the map at the recommended contour level 0.0136 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



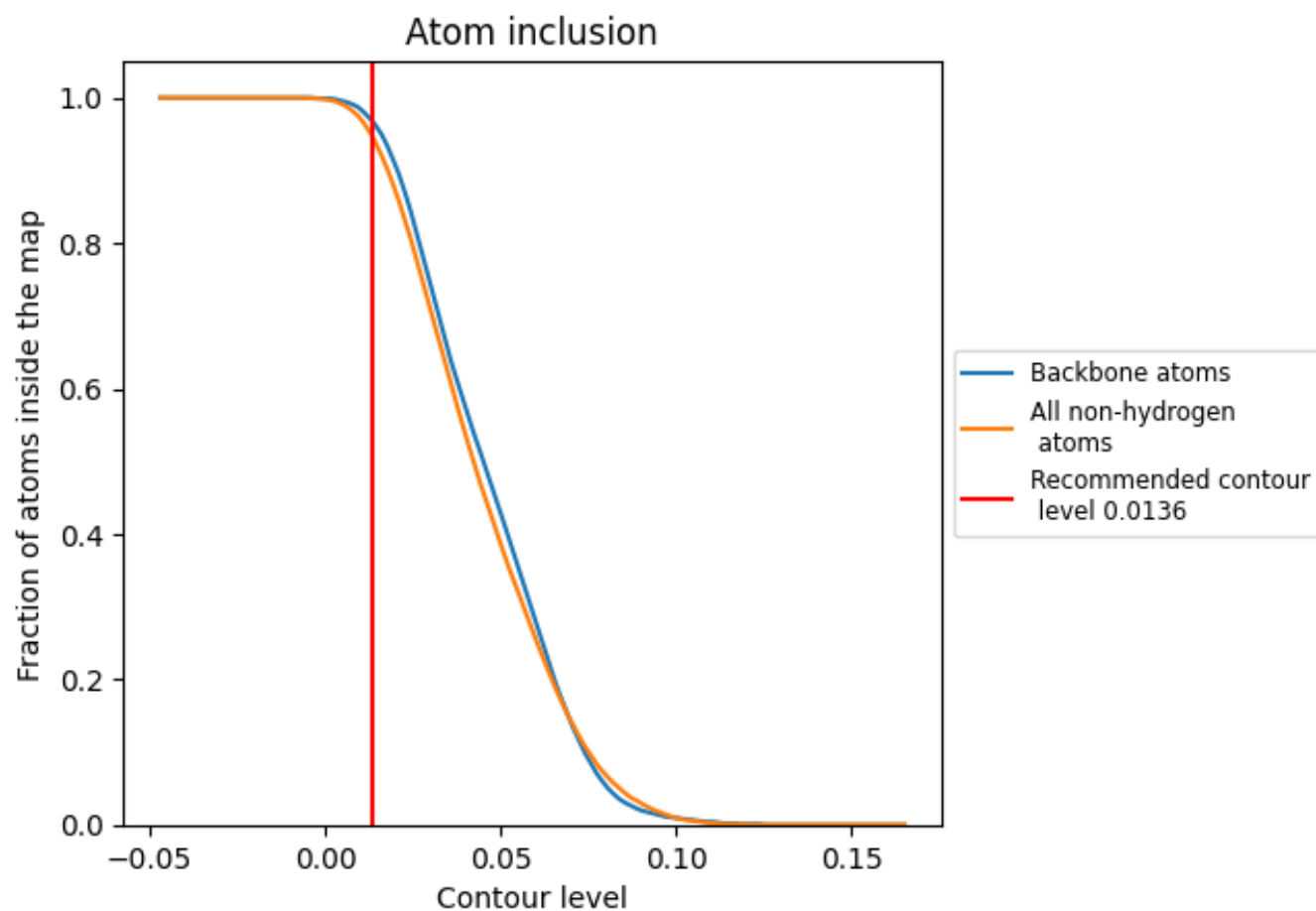
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0136).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% 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 (0.0136) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9460	 0.4620
CB	 0.6730	 0.2570
CE	 0.8260	 0.2460
CI	 0.7490	 0.3810
Et	 0.7460	 0.1930
L5	 0.9850	 0.5210
L7	 0.9980	 0.5680
L8	 0.9870	 0.5460
LA	 0.9880	 0.5860
LB	 0.9550	 0.5600
LC	 0.9560	 0.5570
LD	 0.9520	 0.5050
LE	 0.9090	 0.4830
LF	 0.9720	 0.5620
LG	 0.9040	 0.4920
LH	 0.9620	 0.5420
LI	 0.9460	 0.5470
LJ	 0.9110	 0.4550
LL	 0.9310	 0.5310
LM	 0.9650	 0.5450
LN	 0.9910	 0.6000
LO	 0.9650	 0.5620
LP	 0.9590	 0.5710
LQ	 0.9690	 0.5820
LR	 0.9140	 0.4990
LS	 0.9790	 0.5810
LT	 0.9430	 0.5400
LU	 0.9220	 0.4520
LV	 0.9650	 0.5710
LW	 0.8790	 0.3760
LX	 0.9470	 0.5380
LY	 0.9560	 0.5400
LZ	 0.9670	 0.5310
La	 0.9780	 0.5900
Lb	 0.9080	 0.4710



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Chain	Atom inclusion	Q-score
Lc	 0.9510	 0.5160
Ld	 0.9440	 0.5340
Le	 0.9730	 0.5760
Lf	 0.9750	 0.5880
Lg	 0.9610	 0.5540
Lh	 0.9510	 0.5340
Li	 0.9450	 0.5240
Lj	 0.9840	 0.5850
Lk	 0.9050	 0.4790
Ll	 0.9690	 0.5610
Lm	 0.9590	 0.5580
Ln	 0.9710	 0.5410
Lo	 0.9490	 0.5580
Lp	 0.9350	 0.5590
Lr	 0.9620	 0.5640
Ls	 0.7130	 0.1810
Lt	 0.6030	 0.0820
S2	 0.9840	 0.4110
SA	 0.9170	 0.4240
SB	 0.9090	 0.4480
SC	 0.9510	 0.4560
SD	 0.8940	 0.2670
SE	 0.9470	 0.4060
SF	 0.8540	 0.2930
SG	 0.8810	 0.2970
SH	 0.8880	 0.3550
SI	 0.9160	 0.4420
SJ	 0.9190	 0.3980
SK	 0.8770	 0.2060
SL	 0.9010	 0.4670
SM	 0.5390	 0.0760
SN	 0.9480	 0.5040
SO	 0.9190	 0.4540
SP	 0.7840	 0.2140
SQ	 0.9320	 0.2530
SR	 0.8800	 0.2970
SS	 0.8480	 0.2510
ST	 0.9050	 0.2460
SU	 0.8810	 0.2380
SV	 0.9500	 0.4440
SW	 0.9760	 0.5040
SX	 0.9320	 0.4620

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Chain	Atom inclusion	Q-score
SY	 0.8850	 0.3110
SZ	 0.8110	 0.2410
Sa	 0.9460	 0.4810
Sb	 0.9250	 0.4500
Sc	 0.8580	 0.3170
Sd	 0.9640	 0.2950
Se	 0.8470	 0.3160
Sf	 0.7580	 0.1350
Sg	 0.8490	 0.1650