



Full wwPDB EM Validation Report ⓘ

Jun 26, 2026 – 12:38 AM EDT

PDB ID : 9P72 / pdb_00009p72
EMDB ID : EMD-71331
Title : In situ human P-E state 80S ribosome
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-20
Resolution : 2.80 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

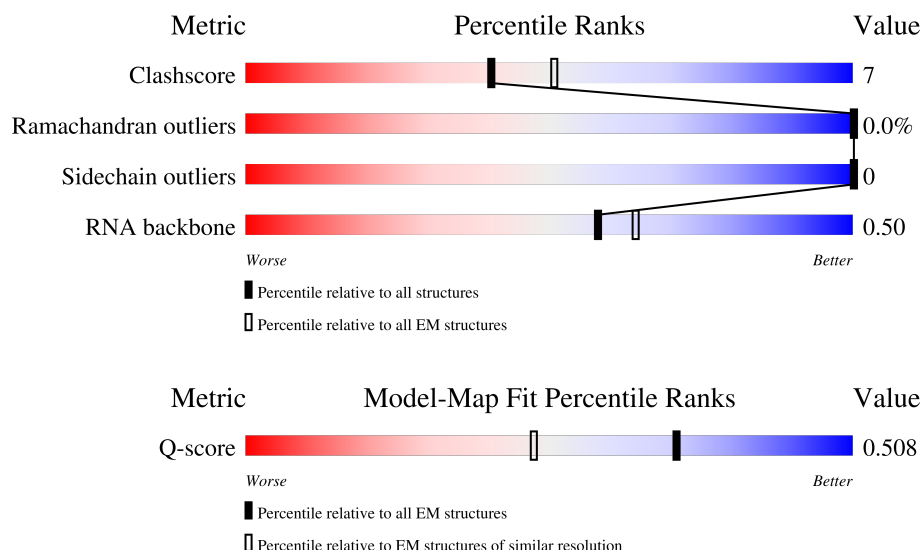
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.



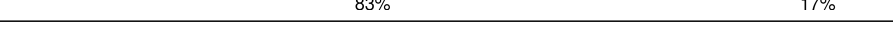
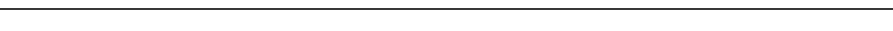
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	Pt	74	53% 45% .
2	Et	75	24% 63% 13%
3	L5	3655	56% 37% 7%

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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	156	
6	LA	248	
7	LB	402	
8	LC	368	
9	LD	293	
10	LE	240	
11	LF	225	
12	LG	241	
13	LH	190	
14	LI	213	
15	LJ	176	
16	LL	210	
17	LM	139	
18	LN	203	
19	LO	201	
20	LP	153	
21	LQ	187	
22	LR	187	
23	LS	175	
24	LT	159	
25	LU	101	
26	LV	131	
27	LW	118	
28	LX	120	

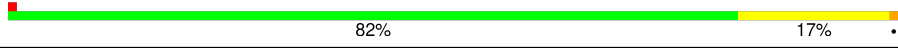
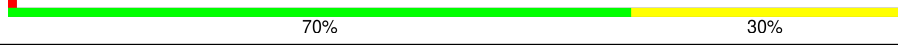
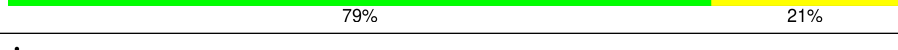
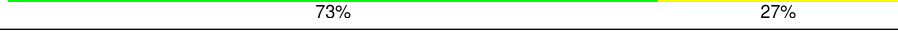
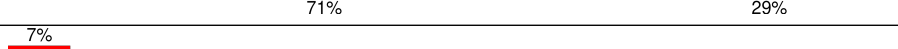
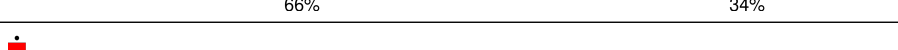
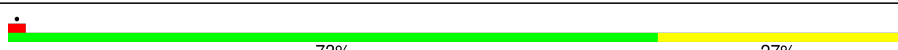
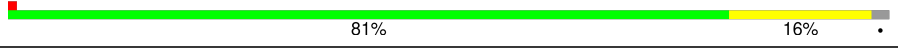
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Mol	Chain	Length	Quality of chain
29	LY	134	
30	LZ	135	
31	La	147	
32	Lb	109	
33	Lc	98	
34	Ld	107	
35	Le	128	
36	Lf	109	
37	Lg	114	
38	Lh	122	
39	Li	102	
40	Lj	86	
41	Lk	69	
42	Ll	50	
43	Lm	52	
44	Ln	24	
45	Lo	105	
46	Lp	91	
47	Lr	125	
48	Ls	196	
49	Lt	141	
50	SD	227	
51	SF	189	
52	SK	98	
53	SM	122	

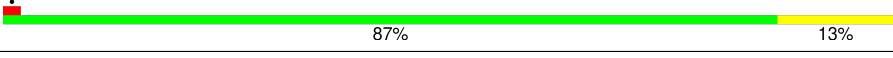
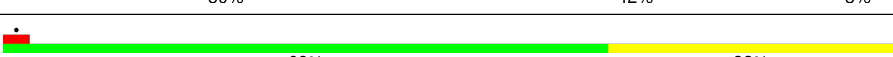
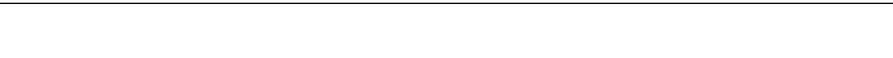
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Mol	Chain	Length	Quality of chain
54	SP	121	
55	SQ	144	
56	SR	135	
57	SS	145	
58	ST	143	
59	SU	104	
60	SZ	75	
61	Sc	64	
62	Sd	55	
63	Sf	67	
64	Sg	313	
65	SA	221	
66	SB	214	
67	SC	222	
68	SE	262	
69	SG	237	
70	SH	186	
71	SI	206	
72	SJ	185	
73	SL	153	
74	SN	150	
75	SO	140	
76	SV	83	
77	SW	129	
78	SX	141	

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Mol	Chain	Length	Quality of chain
79	SY	131	
80	Sa	102	
81	Sb	83	
82	Se	58	
83	S2	1740	
84	CI	31	

2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 219971 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 RNA chain called P site tRNA.

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

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

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

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

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

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

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

- Molecule 5 is a RNA chain called 5.8S rRNA [Homo sapiens].

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

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

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

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

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

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

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

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

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

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

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

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LE	?	-	SER	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	VAL	deletion	UNP Q02878
LE	?	-	GLU	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878
LE	?	-	GLU	deletion	UNP Q02878
LE	?	-	LYS	deletion	UNP Q02878

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 27 is a protein called Ribosomal protein L24.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LW	?	-	SER	deletion	UNP A0A994J4A5
LW	?	-	GLU	deletion	UNP A0A994J4A5
LW	?	-	GLU	deletion	UNP A0A994J4A5
LW	?	-	ILE	deletion	UNP A0A994J4A5
LW	?	-	GLN	deletion	UNP A0A994J4A5
LW	?	-	LYS	deletion	UNP A0A994J4A5

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

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

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

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

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

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

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

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

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

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

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	GLU	deletion	UNP P47914
Lb	?	-	VAL	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	ILE	deletion	UNP P47914
Lb	?	-	PRO	deletion	UNP P47914
Lb	?	-	LYS	deletion	UNP P47914
Lb	?	-	GLY	deletion	UNP P47914

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lt	?	-	PRO	deletion	UNP P30050
Lt	?	-	PRO	deletion	UNP P30050
Lt	?	-	ARG	deletion	UNP P30050
Lt	?	-	ASP	deletion	UNP P30050
Lt	?	-	ARG	deletion	UNP P30050
Lt	?	-	LYS	deletion	UNP P30050
Lt	?	-	LYS	deletion	UNP P30050
Lt	?	-	GLN	deletion	UNP P30050
Lt	?	-	LYS	deletion	UNP P30050
Lt	?	-	ASN	deletion	UNP P30050
Lt	?	-	ILE	deletion	UNP P30050
Lt	?	-	LYS	deletion	UNP P30050
Lt	?	-	HIS	deletion	UNP P30050
Lt	?	-	SER	deletion	UNP P30050
Lt	?	-	GLY	deletion	UNP P30050
Lt	?	-	ASN	deletion	UNP P30050

- Molecule 50 is a protein called Small ribosomal subunit protein uS3.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SH	?	-	SER	deletion	UNP P62081
SH	?	-	ARG	deletion	UNP P62081
SH	?	-	THR	deletion	UNP P62081

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

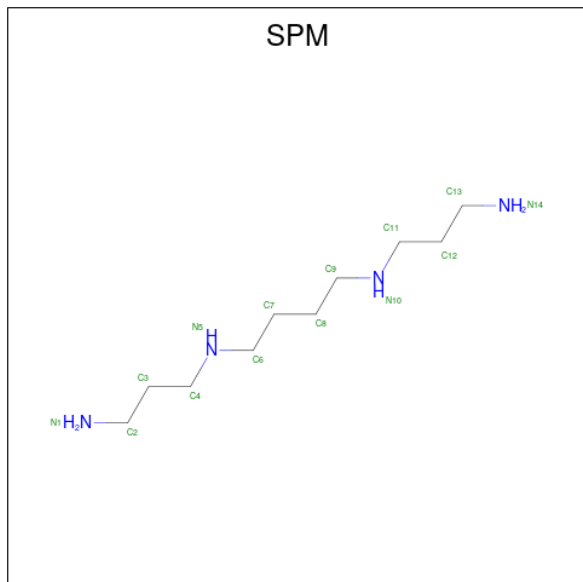
- Molecule 84 is a protein called Transcription factor BTF3.

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

- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

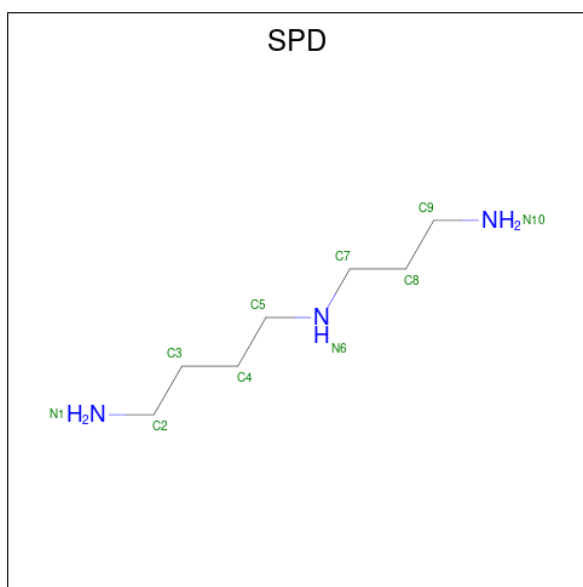
Mol	Chain	Residues	Atoms		AltConf
85	L5	179	Total	Mg	0
			179	179	
85	L7	3	Total	Mg	0
			3	3	
85	L8	5	Total	Mg	0
			5	5	
85	LA	1	Total	Mg	0
			1	1	
85	LP	1	Total	Mg	0
			1	1	
85	LV	1	Total	Mg	0
			1	1	
85	Le	1	Total	Mg	0
			1	1	
85	SS	1	Total	Mg	0
			1	1	
85	S2	27	Total	Mg	0
			27	27	

- Molecule 86 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 88 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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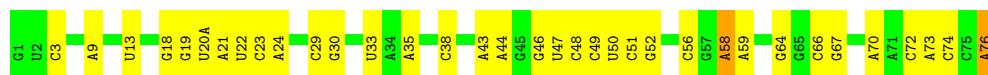
Mol	Chain	Residues	Atoms		AltConf
88	Lj	1	Total 1	Zn 1	0
88	Lm	1	Total 1	Zn 1	0
88	Lo	1	Total 1	Zn 1	0
88	Lp	1	Total 1	Zn 1	0
88	Sa	1	Total 1	Zn 1	0

3 Residue-property plots

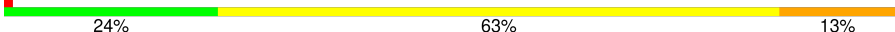
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

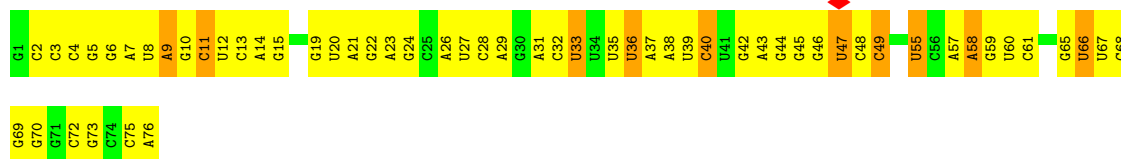
• Molecule 1: P site tRNA

Chain Pt: 



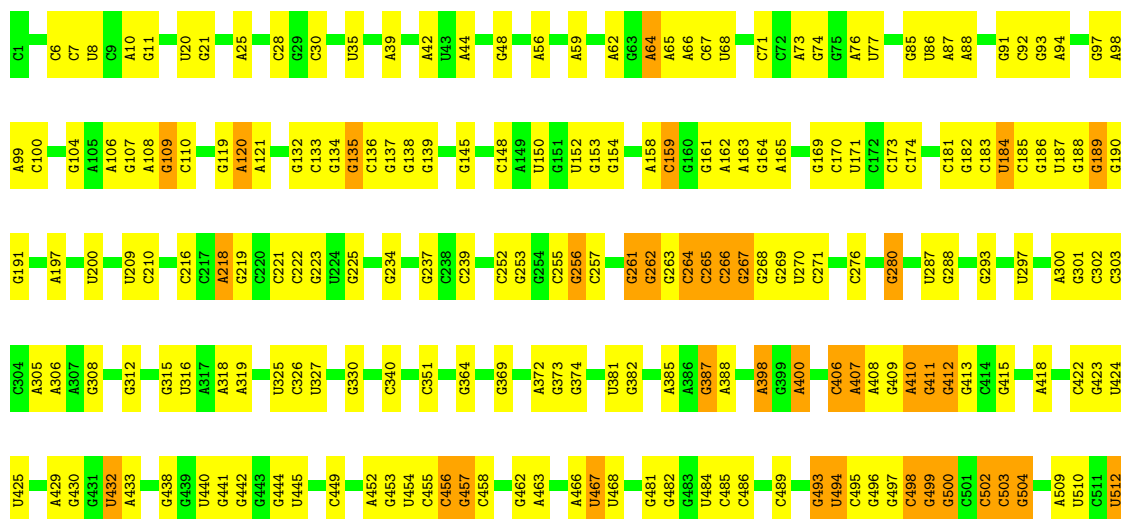
• Molecule 2: E site tRNA

Chain Et: 



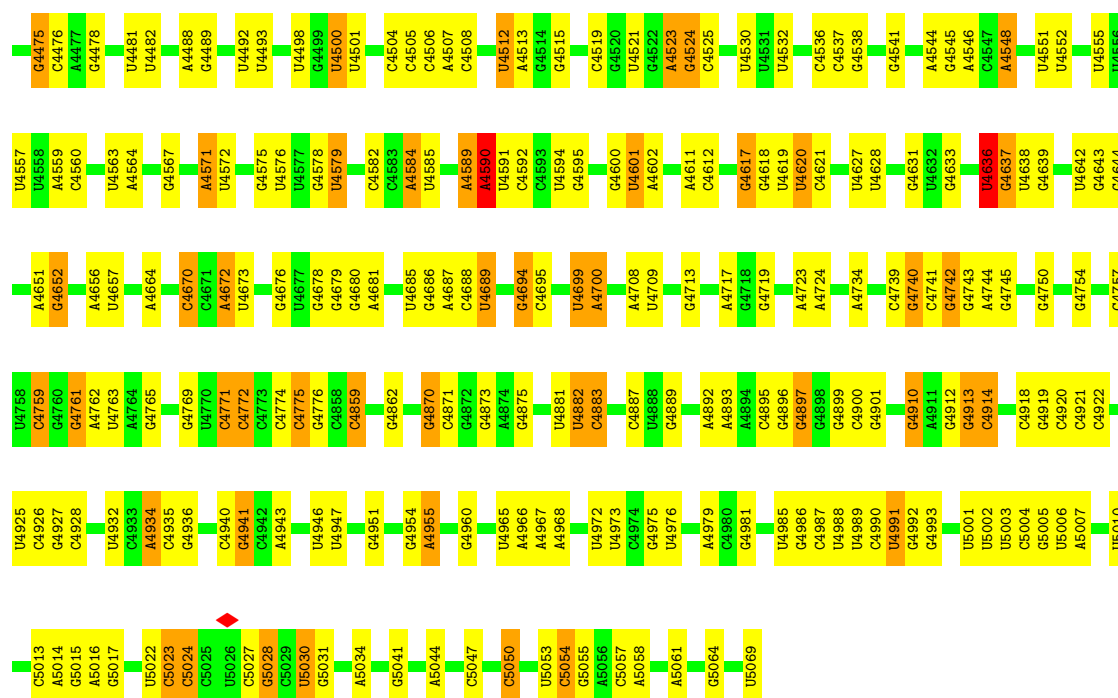
• Molecule 3: 28S rRNA

Chain L5: 



C2256	G2021	C1857	A1558	G1457	A1354	G1281	C1181	G957	U513
C2257	G2024	A1858	G1559	C1458	A1359	G1282	C1182	G958	U514
C2258	A2025	U1859	A1563	C1459	G1359	G1283	C1183	C959	C515
A2026	G2026	C1678	A1564	C1460	G1365	G1284	C1184	C960	C516
G2029	A2026	A1765	A1565	C1461	U1364	G1287	C1185	C961	C517
A2030	G2029	A1766	C1566	A1462	C1365	G1290	U1186	C962	G518
A2041	G2045	A1767	G1574	C1468	G1366	G1291	G1187	C963	C519
G2045	A2041	A1867	G1577	C1478	G1367	G1292	G1188	G964	G643
G2046	G2046	A1868	U1578	C1479	G1382	G1293	G1194	C967	G646
A2047	G2047	G1685	U1578	G1480	G1385	A1294	G1195	C968	G647
U2048	G2055	G1686	U1582	G1481	G1386	G1296	G1196	C969	
A2276	G2056	U1773	U1582	C1482	A1387	U1297	G1200	G970	
A2279	G2056	U1779	U1582	C1483	G1390	C1298	G1201	C979	C654
G2280	G2056	U1780	U1582	C1483	G1391	C1299	G1202	U980	C655
U2281	G2056	U1781	U1582	C1483	G1392	C1299	G1203	C981	C656
G2284	G2056	U1782	U1582	C1483	G1393	C1301	G1203	C982	C657
G2289	G2056	U1783	U1582	C1483	G1394	U1302	G1203	C983	G658
C2295	G2056	U1784	U1582	C1483	G1395	C1303	G1203	C984	G659
G2296	G2056	U1785	U1582	C1483	G1396	C1304	G1203	C985	C662
G2297	G2056	U1786	U1582	C1483	G1397	C1305	G1203	C986	G663
U2298	G2056	U1787	U1582	C1483	G1398	C1306	G1203	C987	G664
G2299	G2056	U1788	U1582	C1483	G1399	C1307	G1203	C988	G665
A2300	G2056	U1789	U1582	C1483	G1400	C1308	G1203	C989	G666
G2301	G2056	U1790	U1582	C1483	G1401	C1309	G1203	C990	G667
G2302	G2056	U1791	U1582	C1483	G1402	C1310	G1203	C991	G668
G2303	G2056	U1792	U1582	C1483	G1403	C1311	G1203	C992	G669
G2306	G2056	U1793	U1582	C1483	G1404	C1312	G1203	C993	C672
A2313	G2056	U1794	U1582	C1483	G1405	C1313	G1203	C994	C673
G2323	G2056	U1795	U1582	C1483	G1406	C1314	G1203	C995	G677
G2324	G2056	U1796	U1582	C1483	G1407	C1315	G1203	C996	G678
G2325	G2056	U1797	U1582	C1483	G1408	C1316	G1203	C997	G679
G2326	G2056	U1798	U1582	C1483	G1409	C1317	G1203	C998	G680
G2331	G2056	U1799	U1582	C1483	G1410	C1318	G1203	C999	G684
A2332	G2056	U1800	U1582	C1483	G1411	C1319	G1203	C1000	C685
G2333	G2056	U1801	U1582	C1483	G1412	C1320	G1203	C1001	U687
G2334	G2056	U1802	U1582	C1483	G1413	C1321	G1203	C1002	U688
C2101	G2056	U1803	U1582	C1483	G1414	C1322	G1203	C1003	U689
G2102	G2056	U1804	U1582	C1483	G1415	C1323	G1203	C1004	C690
G2103	G2056	U1805	U1582	C1483	G1416	C1324	G1203	C1005	C691
G2104	G2056	U1806	U1582	C1483	G1417	C1325	G1203	C1006	A692
A2105	G2056	U1807	U1582	C1483	G1418	C1326	G1203	C1007	G700
G2106	G2056	U1808	U1582	C1483	G1419	C1327	G1203	C1008	G701
C2107	G2056	U1809	U1582	C1483	G1420	C1328	G1203	C1009	U702
G2108	G2056	U1810	U1582	C1483	G1421	C1329	G1203	C1010	G703
G2109	G2056	U1811	U1582	C1483	G1422	C1330	G1203	C1011	G704
G2110	G2056	U1812	U1582	C1483	G1423	C1331	G1203	C1012	A711
G2111	G2056	U1813	U1582	C1483	G1424	C1332	G1203	C1013	C712
G2112	G2056	U1814	U1582	C1483	G1425	C1333	G1203	C1014	
G2113	G2056	U1815	U1582	C1483	G1426	C1334	G1203	C1015	
G2114	G2056	U1816	U1582	C1483	G1427	C1335	G1203	C1016	
G2115	G2056	U1817	U1582	C1483	G1428	C1336	G1203	C1017	
G2116	G2056	U1818	U1582	C1483	G1429	C1337	G1203	C1018	
G2117	G2056	U1819	U1582	C1483	G1430	C1338	G1203	C1019	
G2118	G2056	U1820	U1582	C1483	G1431	C1339	G1203	C1020	
G2119	G2056	U1821	U1582	C1483	G1432	C1340	G1203	C1021	
G2120	G2056	U1822	U1582	C1483	G1433	C1341	G1203	C1022	
G2121	G2056	U1823	U1582	C1483	G1434	C1342	G1203	C1023	
G2122	G2056	U1824	U1582	C1483	G1435	C1343	G1203	C1024	
G2123	G2056	U1825	U1582	C1483	G1436	C1344	G1203	C1025	
G2124	G2056	U1826	U1582	C1483	G1437	C1345	G1203	C1026	
G2125	G2056	U1827	U1582	C1483	G1438	C1346	G1203	C1027	
G2126	G2056	U1828	U1582	C1483	G1439	C1347	G1203	C1028	
G2127	G2056	U1829	U1582	C1483	G1440	C1348	G1203	C1029	
G2128	G2056	U1830	U1582	C1483	G1441	C1349	G1203	C1030	
G2129	G2056	U1831	U1582	C1483	G1442	C1350	G1203	C1031	
G2130	G2056	U1832	U1582	C1483	G1443	C1351	G1203	C1032	
G2131	G2056	U1833	U1582	C1483	G1444	C1352	G1203	C1033	
G2132	G2056	U1834	U1582	C1483	G1445	C1353	G1203	C1034	
G2133	G2056	U1835	U1582	C1483	G1446	C1354	G1203	C1035	
G2134	G2056	U1836	U1582	C1483	G1447	C1355	G1203	C1036	
G2135	G2056	U1837	U1582	C1483	G1448	C1356	G1203	C1037	
G2136	G2056	U1838	U1582	C1483	G1449	C1357	G1203	C1038	
G2137	G2056	U1839	U1582	C1483	G1450	C1358	G1203	C1039	
G2138	G2056	U1840	U1582	C1483	G1451	C1359	G1203	C1040	
G2139	G2056	U1841	U1582	C1483	G1452	C1360	G1203	C1041	
G2140	G2056	U1842	U1582	C1483	G1453	C1361	G1203	C1042	
G2141	G2056	U1843	U1582	C1483	G1454	C1362	G1203	C1043	
G2142	G2056	U1844	U1582	C1483	G1455	C1363	G1203	C1044	
G2143	G2056	U1845	U1582	C1483	G1456	C1364	G1203	C1045	
G2144	G2056	U1846	U1582	C1483	G1457	C1365	G1203	C1046	
G2145	G2056	U1847	U1582	C1483	G1458	C1366	G1203	C1047	
G2146	G2056	U1848	U1582	C1483	G1459	C1367	G1203	C1048	
G2147	G2056	U1849	U1582	C1483	G1460	C1368	G1203	C1049	
G2148	G2056	U1850	U1582	C1483	G1461	C1369	G1203	C1050	
G2149	G2056	U1851	U1582	C1483	G1462	C1370	G1203	C1051	
G2150	G2056	U1852	U1582	C1483	G1463	C1371	G1203	C1052	
G2151	G2056	U1853	U1582	C1483	G1464	C1372	G1203	C1053	
G2152	G2056	U1854	U1582	C1483	G1465	C1373	G1203	C1054	
G2153	G2056	U1855	U1582	C1483	G1466	C1374	G1203	C1055	
G2154	G2056	U1856	U1582	C1483	G1467	C1375	G1203	C1056	
G2155	G2056	U1857	U1582	C1483	G1468	C1376	G1203	C1057	
G2156	G2056	U1858	U1582	C1483	G1469	C1377	G1203	C1058	
G2157	G2056	U1859	U1582	C1483	G1470	C1378	G1203	C1059	
G2158	G2056	U1860	U1582	C1483	G1471	C1379	G1203	C1060	
G2159	G2056	U1861	U1582	C1483	G1472	C1380	G1203	C1061	
G2160	G2056	U1862	U1582	C1483	G1473	C1381	G1203	C1062	
G2161	G2056	U1863	U1582	C1483	G1474	C1382	G1203	C1063	
G2162	G2056	U1864	U1582	C1483	G1475	C1383	G1203	C1064	
G2163	G2056	U1865	U1582	C1483	G1476	C1384	G1203	C1065	
G2164	G2056	U1866	U1582	C1483	G1477	C1385	G1203	C1066	
G2165	G2056	U1867	U1582	C1483	G1478	C1386	G1203	C1067	
G2166	G2056	U1868	U1582	C1483	G1479	C1387	G1203	C1068	
G2167	G2056	U1869	U1582	C1483	G1480	C1388	G1203	C1069	
G2168	G2056	U1870	U1582	C1483	G1481	C1389	G1203	C1070	
G2169	G2056	U1871	U1582	C1483	G1482	C1390	G1203	C1071	
G2170	G2056	U1872	U1582	C1483	G1483	C1391	G1203	C1072	
G2171	G2056	U1873	U1582	C1483	G1484	C1392	G1203	C1073	
G2172	G2056	U1874	U1582	C1483	G1485	C1393	G1203	C1074	
G2173	G2056	U1875	U1582	C1483	G1486	C1394	G1203	C1075	
G2174	G2056	U1876	U1582	C1483	G1487	C1395	G1203	C1076	
G2175	G2056	U1877	U1582	C1483	G1488	C1396	G1203	C1077	
G2176	G2056	U1878	U1582	C1483	G1489	C1397	G1203	C1078	
G2177	G2056	U1879	U1582	C1483	G1490	C1398	G1203	C1079	
G2178	G2056	U1880	U1582	C1483	G1491	C1399	G1203	C1080	
G2179	G2056	U1881	U1582	C1483	G1492	C1400	G1203	C1081	
G2180	G2056	U1882	U1582	C1483	G1493	C1401	G1203	C1082	
G2181	G2056	U1883	U1582	C1483	G1494	C1402	G1203	C1083	
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G2187	G2056	U1889	U1582	C1483	G1500	C1408	G1203	C1089	
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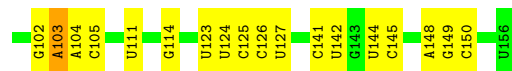
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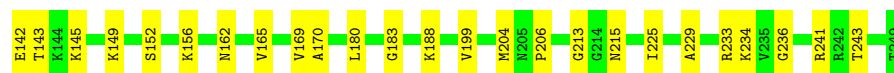
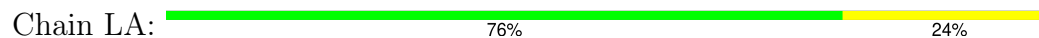
- Molecule 4: 5S rRNA



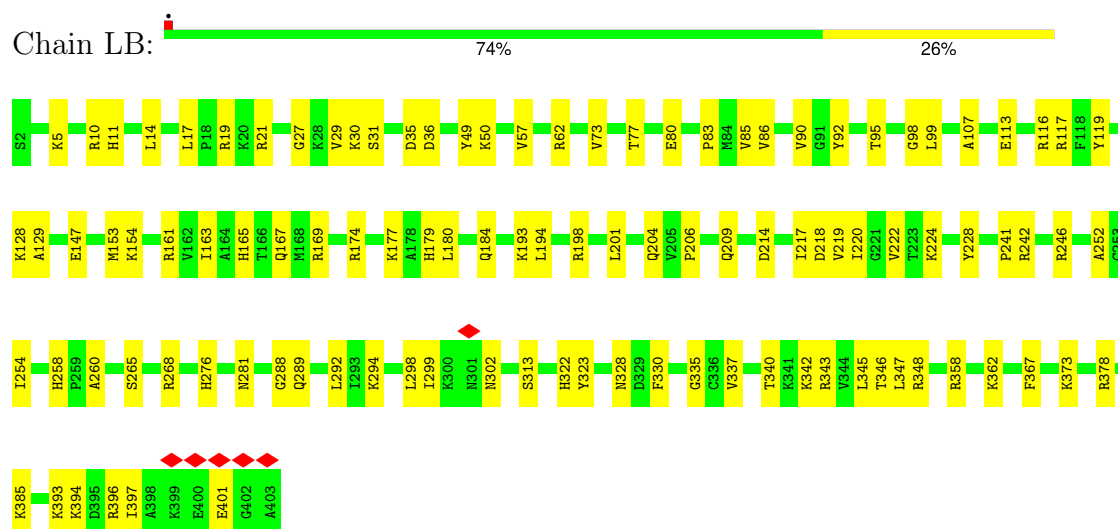
- Molecule 5: 5.8S rRNA [Homo sapiens]



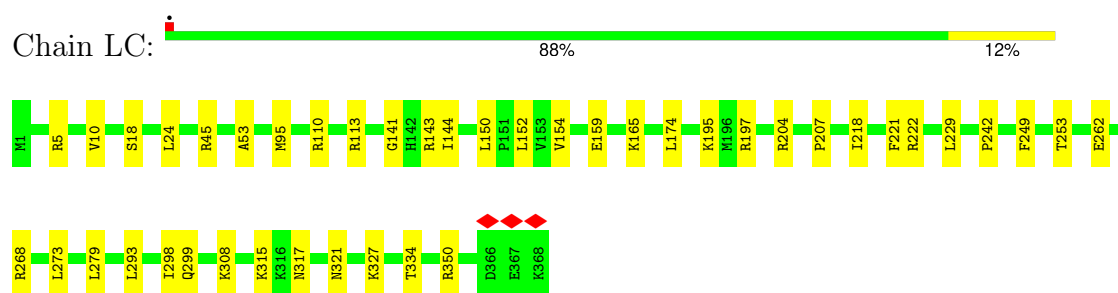
- Molecule 6: 60S ribosomal protein L8



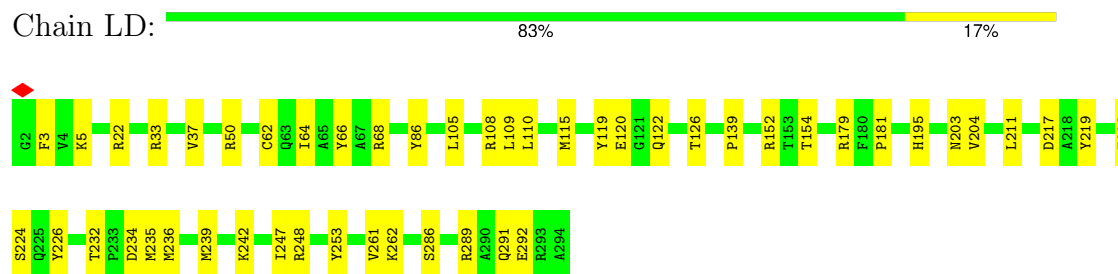
- Molecule 7: Large ribosomal subunit protein uL3



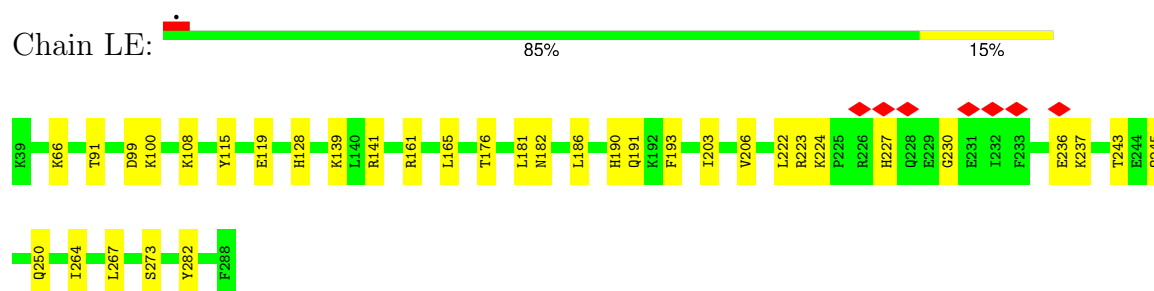
- Molecule 8: 60S ribosomal protein L4



- Molecule 9: Large ribosomal subunit protein uL18



- Molecule 10: Large ribosomal subunit protein eL6



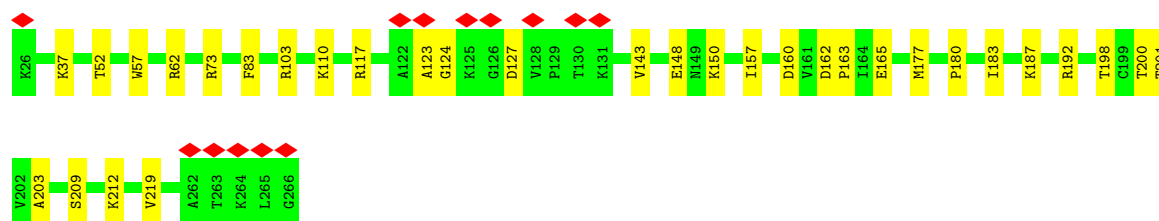
- Molecule 11: 60S ribosomal protein L7

Chain LF:  83% 17%



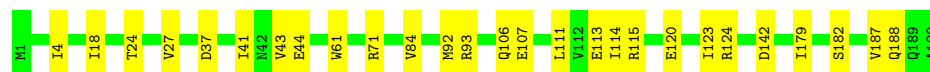
- Molecule 12: 60S ribosomal protein L7a

Chain LG:  5% 87% 13%



- Molecule 13: 60S ribosomal protein L9

Chain LH:  86% 14%



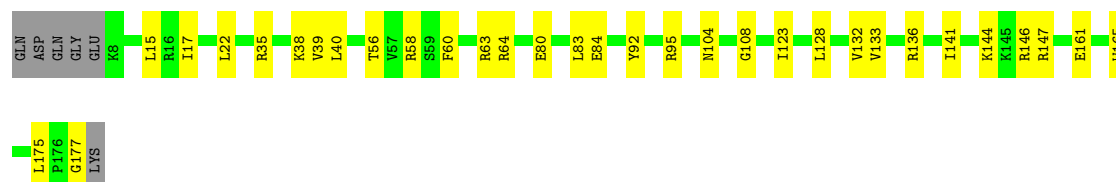
- Molecule 14: Ribosomal protein uL16-like

Chain LI:  87% 13%



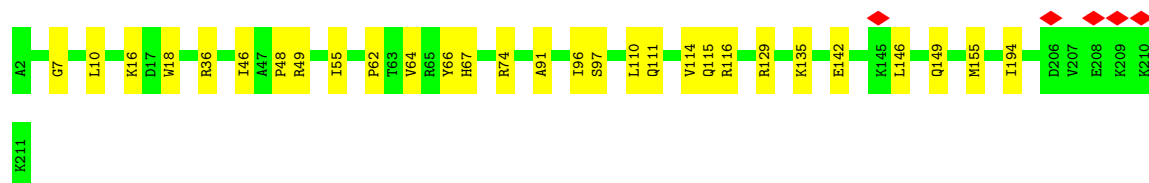
- Molecule 15: 60S ribosomal protein L11

Chain LJ:  78% 18% .



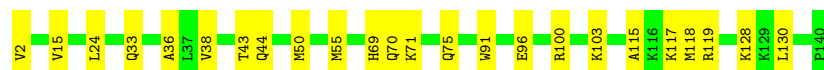
- Molecule 16: Large ribosomal subunit protein eL13

Chain LL:  86% 14%



- Molecule 17: 60S ribosomal protein L14

Chain LM: 83% 17%



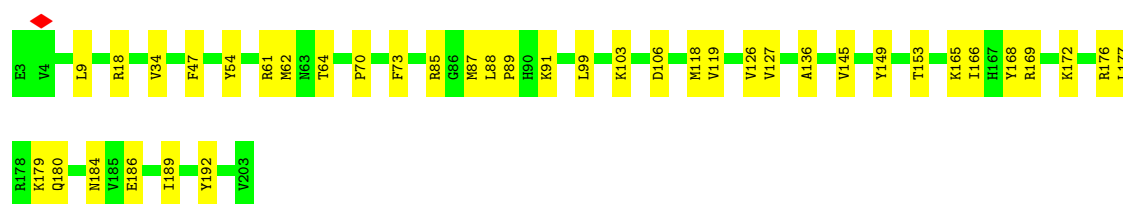
- Molecule 18: 60S ribosomal protein L15

Chain LN: 87% 13%



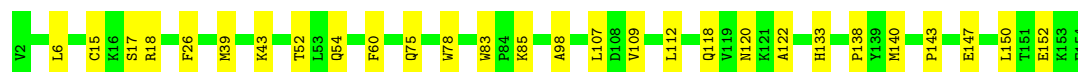
- Molecule 19: 60S ribosomal protein L13a

Chain LO: 81% 19%



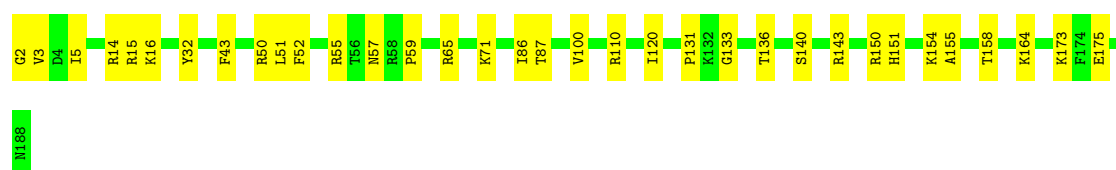
- Molecule 20: 60S ribosomal protein L17

Chain LP: 82% 18%



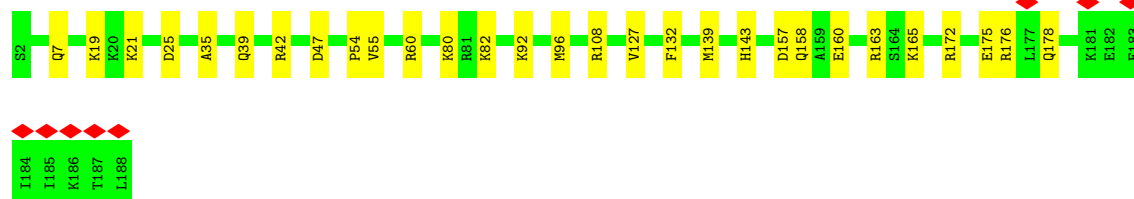
- Molecule 21: 60S ribosomal protein L18

Chain LQ: 82% 18%



- Molecule 22: 60S ribosomal protein L19

Chain LR:  84% 16%



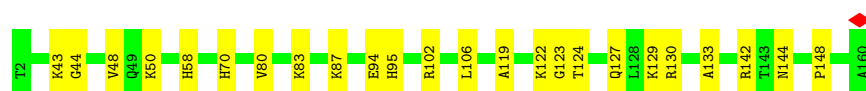
- Molecule 23: 60S ribosomal protein L18a

Chain LS:  86% 14%



- Molecule 24: 60S ribosomal protein L21

Chain LT:  85% 15%



- Molecule 25: Heparin-binding protein HBp15

Chain LU:  82% 18%



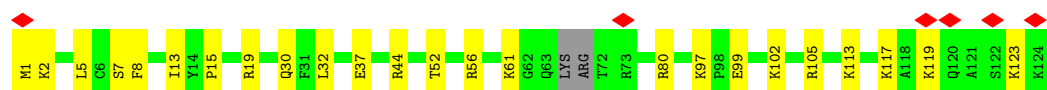
- Molecule 26: 60S ribosomal protein L23

Chain LV:  89% 11%



- Molecule 27: Ribosomal protein L24

Chain LW:  5% 78% 20%



- Molecule 28: 60S ribosomal protein L23a

Chain LX:  96%



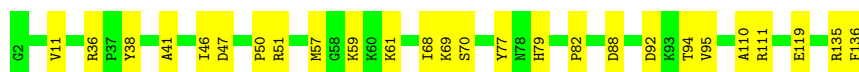
- Molecule 29: 60S ribosomal protein L26

Chain LY: 85% 15%



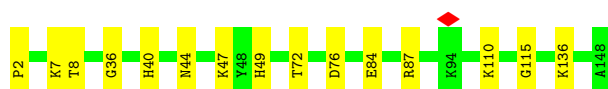
- Molecule 30: 60S ribosomal protein L27

Chain LZ: 81% 19%



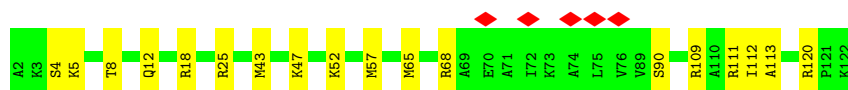
- Molecule 31: 60S ribosomal protein L27a

Chain La: 90% 10%



- Molecule 32: Large ribosomal subunit protein eL29

Chain Lb: 5% 83% 17%



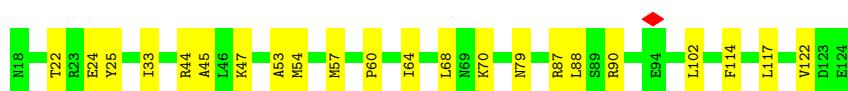
- Molecule 33: 60S ribosomal protein L30

Chain Lc: 77% 23%



- Molecule 34: 60S ribosomal protein L31

Chain Ld: 79% 21%



- Molecule 35: 60S ribosomal protein L32

Chain Le:  91% 9%



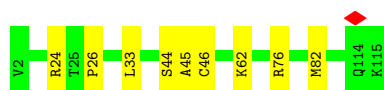
- Molecule 36: 60S ribosomal protein L35a

Chain Lf:  89% 11%



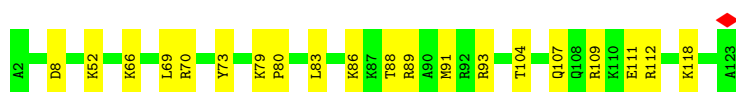
- Molecule 37: 60S ribosomal protein L34

Chain Lg:  92% 8%



- Molecule 38: 60S ribosomal protein L35

Chain Lh:  84% 16%



- Molecule 39: 60S ribosomal protein L36

Chain Li:  91% 9%



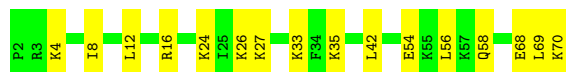
- Molecule 40: 60S ribosomal protein L37

Chain Lj:  80% 20%



- Molecule 41: 60S ribosomal protein L38

Chain Lk:  77% 23%



- Molecule 42: 60S ribosomal protein L39

Chain Ll:  88% 12%



- Molecule 43: Large ribosomal subunit protein eL40

Chain Lm:  90% 10%



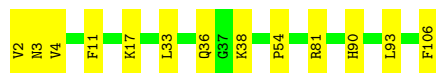
- Molecule 44: 60S ribosomal protein L41

Chain Ln:  92% 8%



- Molecule 45: 60S ribosomal protein L36a

Chain Lo:  88% 12%



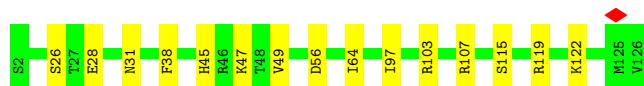
- Molecule 46: 60S ribosomal protein L37a

Chain Lp:  91% 9%



- Molecule 47: 60S ribosomal protein L28

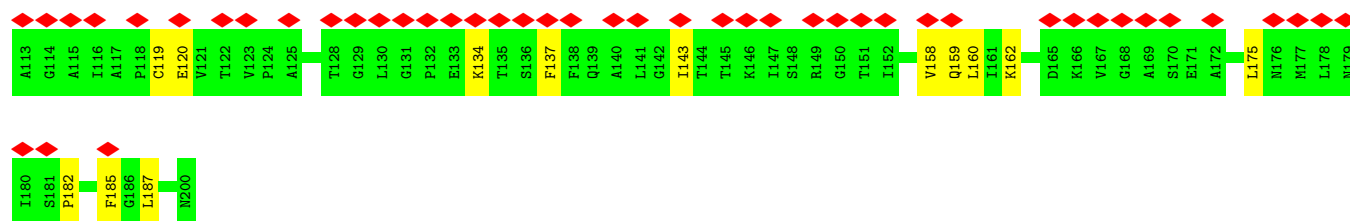
Chain Lr:  88% 12%



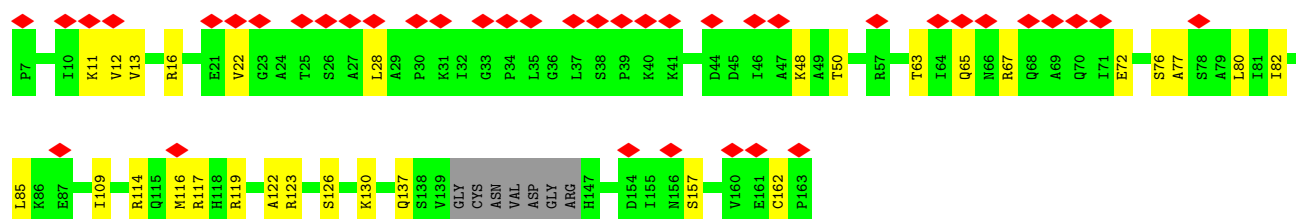
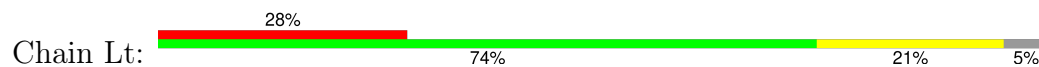
- Molecule 48: 60S acidic ribosomal protein P0

Chain Ls:  29% 81% 19%

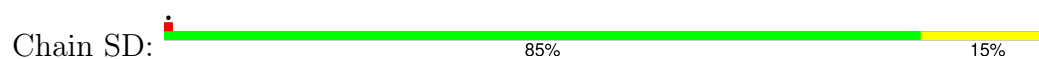




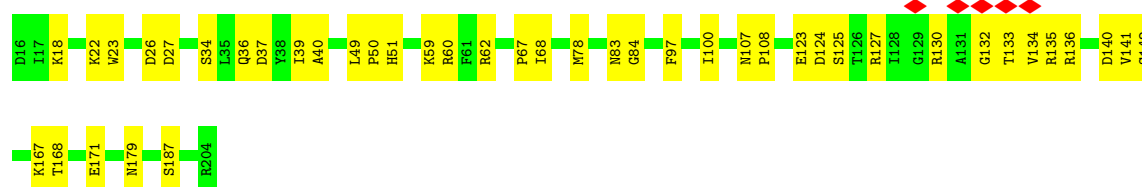
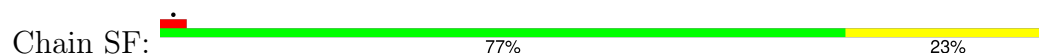
- Molecule 49: Large ribosomal subunit protein uL11



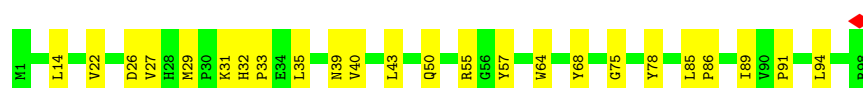
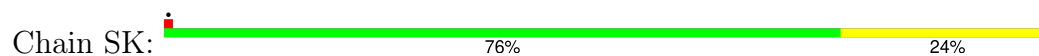
- Molecule 50: Small ribosomal subunit protein uS3



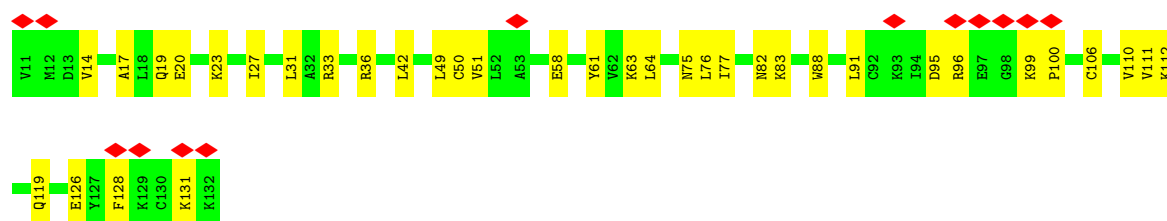
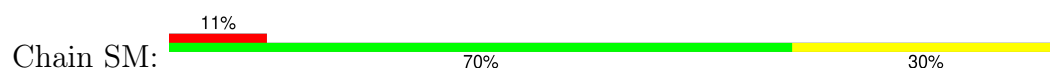
- Molecule 51: 40S ribosomal protein S5



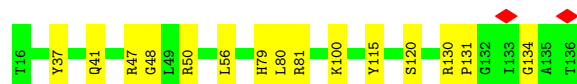
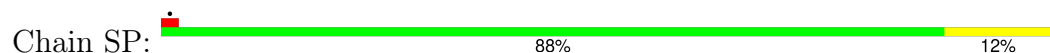
- Molecule 52: 40S ribosomal protein S10



- Molecule 53: Small ribosomal subunit protein eS12



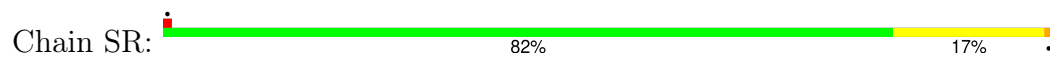
- Molecule 54: Small ribosomal subunit protein uS19



- Molecule 55: Small ribosomal subunit protein uS9



- Molecule 56: Small ribosomal subunit protein eS17

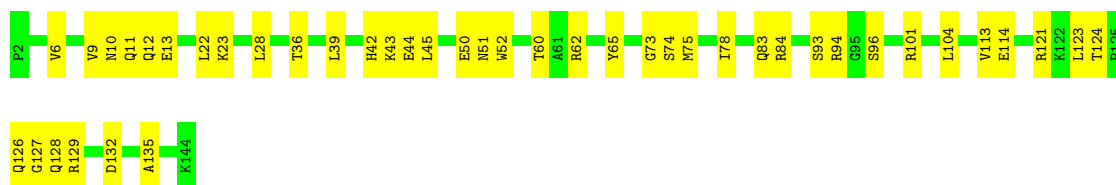


- Molecule 57: 40S ribosomal protein S18

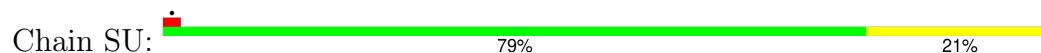


- Molecule 58: 40S ribosomal protein S19

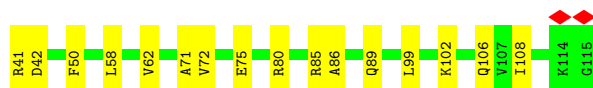
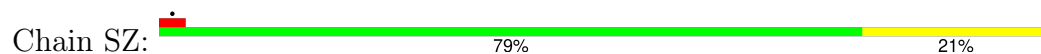




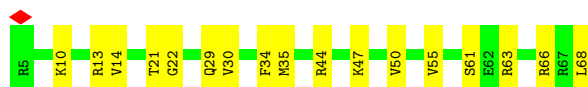
- Molecule 59: 40S ribosomal protein S20



- Molecule 60: Small ribosomal subunit protein eS25



- Molecule 61: 40S ribosomal protein S28



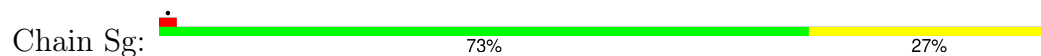
- Molecule 62: 40S ribosomal protein S29

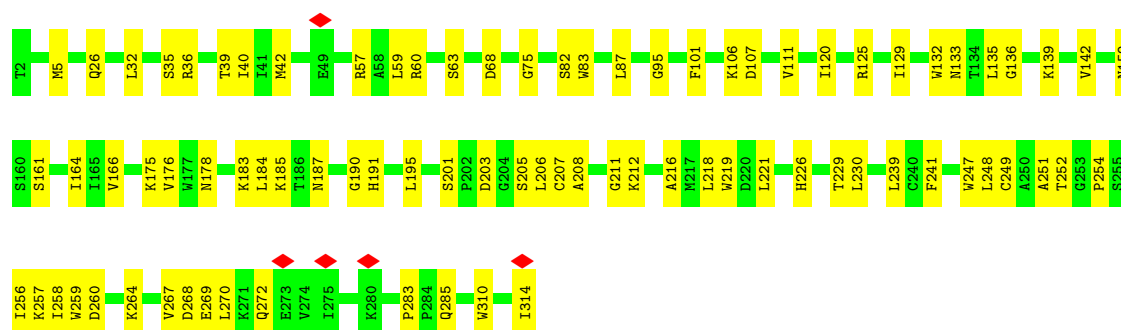


- Molecule 63: Ubiquitin-40S ribosomal protein S27a



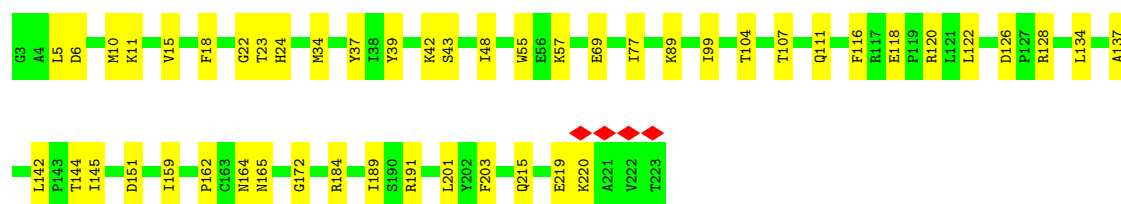
- Molecule 64: Receptor of activated protein C kinase 1





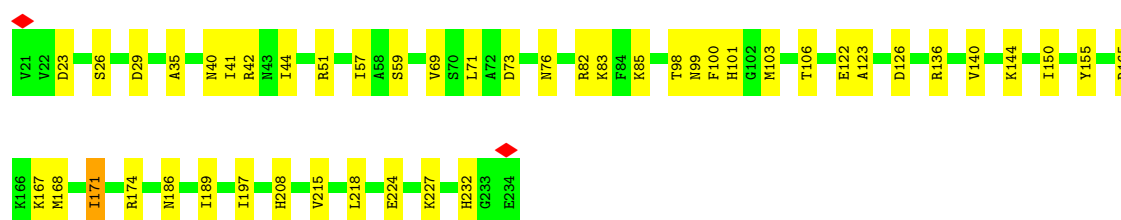
- Molecule 65: 40S ribosomal protein SA

Chain SA: 78% 22%



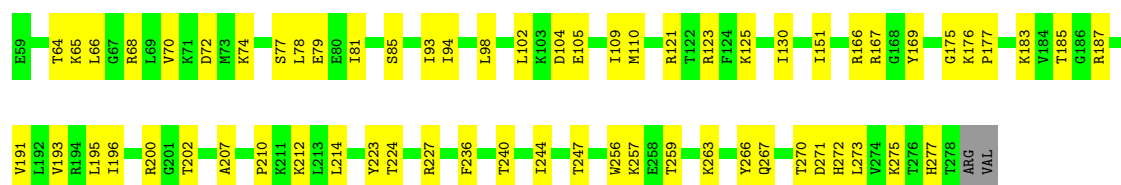
- Molecule 66: 40S ribosomal protein S3a

Chain SB: 79% 21%



- Molecule 67: 40S ribosomal protein S2

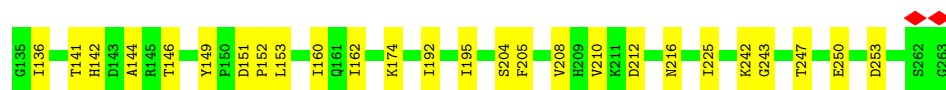
Chain SC: 71% 28%



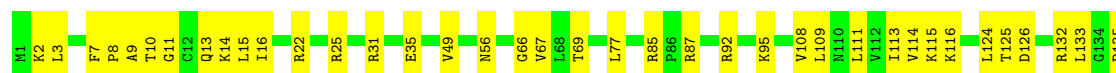
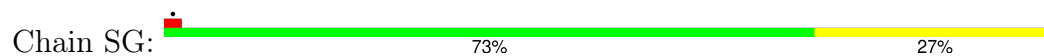
- Molecule 68: Small ribosomal subunit protein eS4, X isoform

Chain SE: 77% 23%

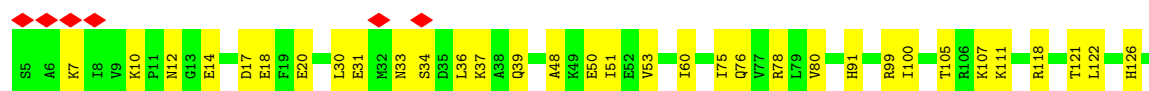
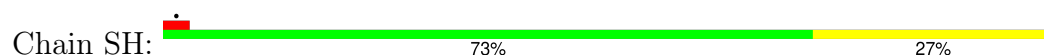




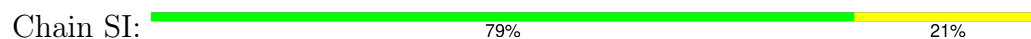
- Molecule 69: 40S ribosomal protein S6



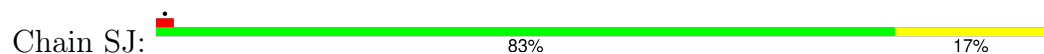
- Molecule 70: Small ribosomal subunit protein eS7



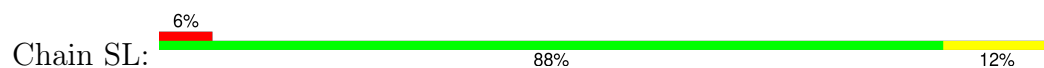
- Molecule 71: 40S ribosomal protein S8

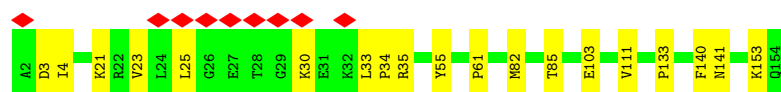


- Molecule 72: 40S ribosomal protein S9



- Molecule 73: 40S ribosomal protein S11





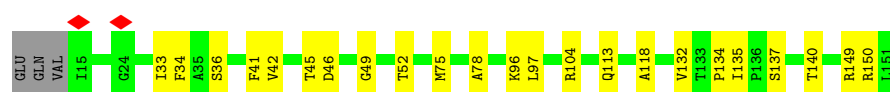
- Molecule 74: 40S ribosomal protein S13

Chain SN: 89% 11%



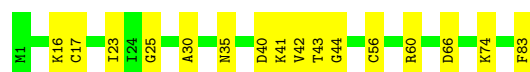
- Molecule 75: Small ribosomal subunit protein uS11

Chain SO: 81% 16%



- Molecule 76: Small ribosomal subunit protein eS21

Chain SV: 81% 19%



- Molecule 77: 40S ribosomal protein S15a

Chain SW: 79% 21%



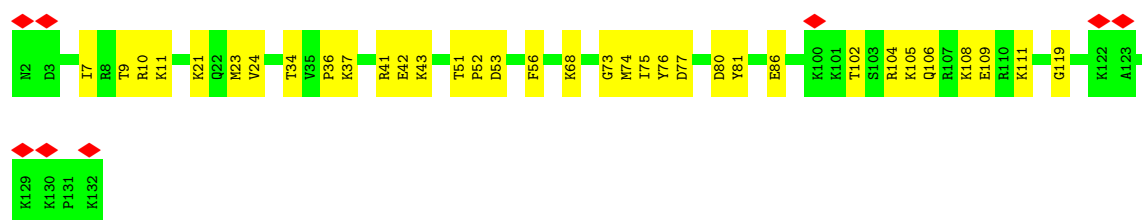
- Molecule 78: 40S ribosomal protein S23

Chain SX: 82% 18%

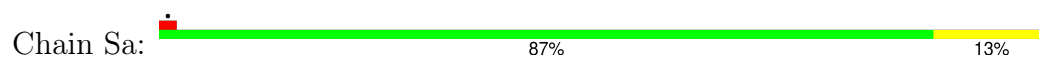


- Molecule 79: 40S ribosomal protein S24

Chain SY: 6% 74% 26%



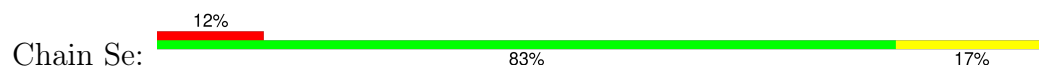
- Molecule 80: 40S ribosomal protein S26



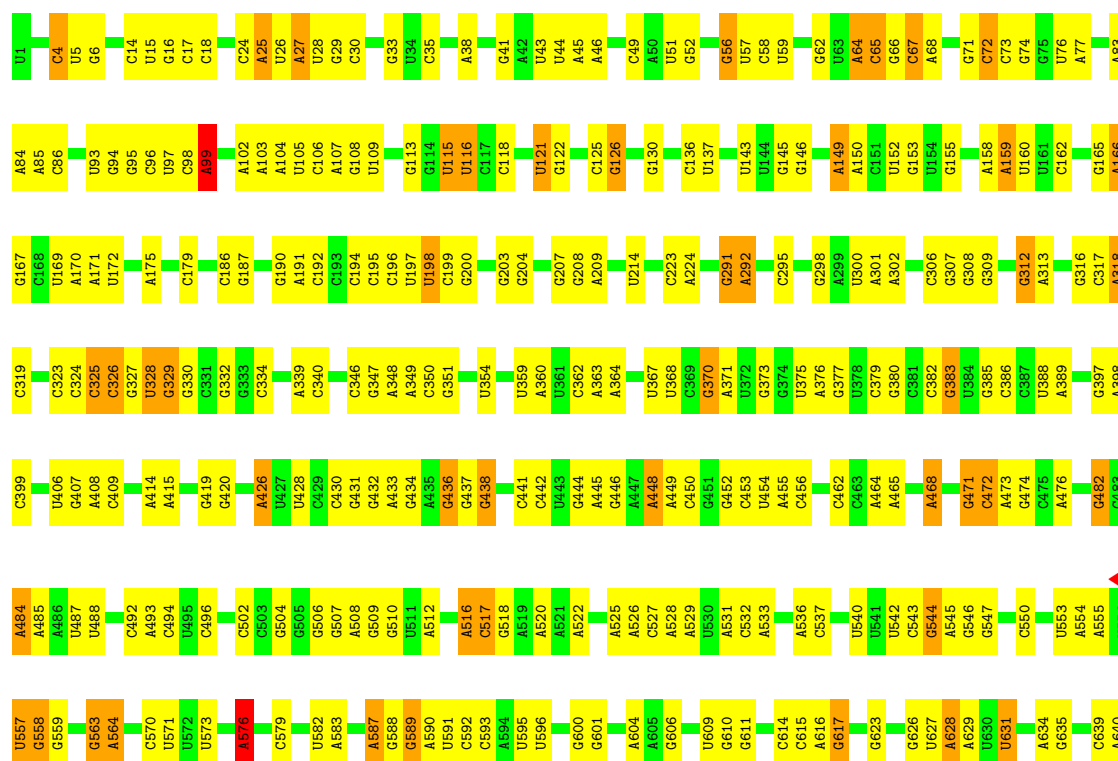
- Molecule 81: Small ribosomal subunit protein eS27

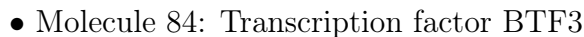


- Molecule 82: Small ribosomal subunit protein eS30



- Molecule 83: 18S rRNA







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67622	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	0.164	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0128	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: SPM, 5MC, 6MZ, UY1, 1MA, G7M, A2M, SPD, MG, ZN, PSU, B8N, 4AC, UR3, OMU, MA6, OMG, OMC

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	Pt	0.12	0/1761	0.26	0/2741
2	Et	0.14	0/1778	0.31	0/2767
3	L5	0.19	0/85098	0.30	0/132762
4	L7	0.16	0/2861	0.25	0/4459
5	L8	0.17	0/3631	0.28	0/5657
6	LA	0.20	0/1936	0.38	0/2596
7	LB	0.18	0/3306	0.36	0/4424
8	LC	0.18	0/2981	0.35	0/4002
9	LD	0.16	0/2428	0.33	0/3252
10	LE	0.17	0/1973	0.41	0/2645
11	LF	0.18	0/1905	0.32	0/2539
12	LG	0.17	0/1960	0.39	0/2637
13	LH	0.16	0/1537	0.34	0/2066
14	LI	0.17	0/1751	0.33	0/2340
15	LJ	0.16	0/1385	0.36	0/1852
16	LL	0.17	0/1732	0.32	0/2315
17	LM	0.18	0/1161	0.36	0/1554
18	LN	0.19	0/1746	0.33	0/2338
19	LO	0.20	0/1682	0.35	0/2250
20	LP	0.19	0/1268	0.39	0/1701
21	LQ	0.19	0/1537	0.35	0/2052
22	LR	0.17	0/1582	0.35	0/2091
23	LS	0.19	0/1493	0.33	0/2003
24	LT	0.18	0/1326	0.32	0/1770
25	LU	0.18	0/839	0.43	0/1126
26	LV	0.17	0/993	0.36	0/1332
27	LW	0.17	0/959	0.37	0/1270
28	LX	0.16	0/1002	0.33	0/1345
29	LY	0.17	0/1132	0.36	0/1504
30	LZ	0.16	0/1130	0.35	0/1507
31	La	0.17	0/1191	0.31	0/1591

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lb	0.16	0/889	0.40	0/1175
33	Lc	0.17	0/774	0.36	0/1038
34	Ld	0.17	0/903	0.34	0/1216
35	Le	0.18	0/1071	0.31	0/1429
36	Lf	0.19	0/895	0.35	0/1198
37	Lg	0.17	0/916	0.35	0/1220
38	Lh	0.15	0/1023	0.32	0/1351
39	Li	0.15	0/843	0.32	0/1115
40	Lj	0.19	0/720	0.36	0/952
41	Lk	0.16	0/575	0.42	0/761
42	Ll	0.17	0/454	0.29	0/599
43	Lm	0.16	0/435	0.33	0/575
44	Ln	0.18	0/231	0.31	0/294
45	Lo	0.18	0/876	0.33	0/1156
46	Lp	0.17	0/718	0.33	0/953
47	Lr	0.17	0/1017	0.32	0/1364
48	Ls	0.12	0/1519	0.33	0/2052
49	Lt	0.17	0/1009	0.50	0/1363
50	SD	0.13	0/1793	0.30	0/2414
51	SF	0.15	0/1516	0.36	0/2037
52	SK	0.14	0/851	0.43	0/1147
53	SM	0.13	0/950	0.37	0/1275
54	SP	0.15	0/1003	0.42	0/1342
55	SQ	0.15	0/1160	0.39	0/1553
56	SR	0.16	0/1105	0.42	0/1484
57	SS	0.15	0/1216	0.36	0/1628
58	ST	0.14	0/1131	0.39	0/1515
59	SU	0.17	0/831	0.44	0/1115
60	SZ	0.16	0/604	0.48	0/810
61	Sc	0.15	0/508	0.36	0/680
62	Sd	0.14	0/470	0.34	0/623
63	Sf	0.15	0/560	0.45	0/745
64	Sg	0.13	0/2493	0.36	0/3394
65	SA	0.14	0/1778	0.34	0/2416
66	SB	0.14	0/1765	0.35	0/2362
67	SC	0.15	0/1744	0.35	0/2357
68	SE	0.14	0/2118	0.35	0/2849
69	SG	0.15	0/1946	0.37	0/2590
70	SH	0.16	0/1519	0.41	0/2033
71	SI	0.16	0/1715	0.36	0/2287
72	SJ	0.13	0/1550	0.32	0/2069
73	SL	0.15	0/1268	0.31	0/1696
74	SN	0.13	0/1232	0.27	0/1656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
75	SO	0.17	0/1037	0.38	0/1391
76	SV	0.16	0/643	0.38	0/860
77	SW	0.17	0/1051	0.35	0/1406
78	SX	0.15	0/1116	0.36	0/1490
79	SY	0.15	0/1083	0.40	0/1438
80	Sa	0.17	0/836	0.33	0/1121
81	Sb	0.14	0/665	0.35	0/891
82	Se	0.14	0/465	0.41	0/612
83	S2	0.18	0/39756	0.28	0/61939
84	CI	0.16	0/247	0.30	0/323
All	All	0.17	0/231657	0.32	0/339847

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
55	SQ	0	1
66	SB	0	1
75	SO	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
66	SB	171	ILE	Peptide
75	SO	137	SER	Peptide
55	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	Pt	1576	0	803	20	0
2	Et	1593	0	810	37	0
3	L5	78444	0	39719	907	0
4	L7	2561	0	1295	21	0
5	L8	3315	0	1685	35	0
6	LA	1898	0	1993	45	0
7	LB	3238	0	3376	78	0
8	LC	2927	0	3104	32	0
9	LD	2382	0	2410	32	0
10	LE	1935	0	2096	25	0
11	LF	1870	0	1996	29	0
12	LG	1927	0	2074	21	0
13	LH	1518	0	1601	18	0
14	LI	1711	0	1749	21	0
15	LJ	1362	0	1399	22	0
16	LL	1701	0	1818	24	0
17	LM	1138	0	1204	20	0
18	LN	1701	0	1749	23	0
19	LO	1650	0	1794	29	0
20	LP	1242	0	1269	20	0
21	LQ	1513	0	1628	25	0
22	LR	1566	0	1729	21	0
23	LS	1453	0	1490	15	0
24	LT	1298	0	1366	17	0
25	LU	825	0	850	14	0
26	LV	979	0	1039	11	0
27	LW	945	0	1003	20	0
28	LX	985	0	1066	4	0
29	LY	1115	0	1205	13	0
30	LZ	1107	0	1182	18	0
31	La	1162	0	1213	12	0
32	Lb	876	0	948	17	0
33	Lc	764	0	804	13	0
34	Ld	888	0	930	17	0
35	Le	1053	0	1147	10	0
36	Lf	876	0	912	8	0
37	Lg	906	0	998	8	0
38	Lh	1015	0	1148	17	0
39	Li	832	0	917	7	0
40	Lj	705	0	737	16	0
41	Lk	569	0	637	14	0
42	Ll	444	0	483	5	0
43	Lm	429	0	465	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Ln	230	0	276	2	0
45	Lo	862	0	929	11	0
46	Lp	708	0	756	7	0
47	Lr	1002	0	1068	9	0
48	Ls	1496	0	1540	25	0
49	Lt	998	0	1032	20	0
50	SD	1765	0	1865	23	0
51	SF	1495	0	1549	38	0
52	SK	827	0	854	17	0
53	SM	940	0	965	23	0
54	SP	985	0	1031	13	0
55	SQ	1142	0	1213	29	0
56	SR	1090	0	1149	16	0
57	SS	1198	0	1261	32	0
58	ST	1112	0	1146	31	0
59	SU	821	0	883	16	0
60	SZ	598	0	656	15	0
61	Sc	506	0	536	11	0
62	Sd	459	0	452	16	0
63	Sf	548	0	551	19	0
64	Sg	2436	0	2393	58	0
65	SA	1741	0	1746	32	0
66	SB	1738	0	1809	29	0
67	SC	1707	0	1791	45	0
68	SE	2076	0	2177	41	0
69	SG	1923	0	2089	56	0
70	SH	1497	0	1590	32	0
71	SI	1686	0	1772	34	0
72	SJ	1525	0	1640	25	0
73	SL	1247	0	1323	14	0
74	SN	1208	0	1294	11	0
75	SO	1024	0	1050	15	0
76	SV	636	0	637	13	0
77	SW	1034	0	1080	25	0
78	SX	1098	0	1167	23	0
79	SY	1065	0	1142	26	0
80	Sa	821	0	870	10	0
81	Sb	651	0	672	16	0
82	Se	459	0	503	11	0
83	S2	36953	0	18679	529	0
84	CI	247	0	283	18	0
85	L5	179	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	L7	3	0	0	0	0
85	L8	5	0	0	0	0
85	LA	1	0	0	0	0
85	LP	1	0	0	0	0
85	LV	1	0	0	0	0
85	Le	1	0	0	0	0
85	S2	27	0	0	0	0
85	SS	1	0	0	0	0
86	L5	98	0	182	7	0
87	L5	90	0	171	5	0
87	LN	10	0	19	0	0
88	Lg	1	0	0	0	0
88	Lj	1	0	0	0	0
88	Lm	1	0	0	0	0
88	Lo	1	0	0	0	0
88	Lp	1	0	0	0	0
88	Sa	1	0	0	0	0
All	All	219971	0	163632	2637	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 (2637) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2708:U:O2'	84:CI:79:ARG:NH1	1.63	1.30
34:Ld:70:LYS:NZ	84:CI:66:GLY:HA3	1.81	0.96
83:S2:1033:G:H1	83:S2:1080:A:HO2'	1.07	0.95
83:S2:928:G:H1	83:S2:1013:U:H3	1.15	0.93
3:L5:1759:G:H1	3:L5:1773:U:H3	1.05	0.93
25:LU:116:GLN:O	84:CI:74:LYS:HA	1.66	0.93
2:Et:26:A:H61	2:Et:44:G:H1	1.04	0.92
2:Et:26:A:N6	2:Et:44:G:H1	1.67	0.92
3:L5:2007:G:H21	3:L5:2012:A:H62	0.96	0.90
3:L5:2007:G:N2	3:L5:2012:A:H62	1.69	0.89
83:S2:1656:G:H1	83:S2:1668:U:H3	1.19	0.89
83:S2:1748:G:H1	83:S2:1786:U:H3	0.92	0.89
16:LL:64:VAL:HA	16:LL:67:HIS:HD2	1.39	0.88
3:L5:3946:G:H1	3:L5:4067:U:H3	0.87	0.86
1:Pt:50:U:H3	1:Pt:64:G:H1	0.91	0.84
3:L5:2007:G:H21	3:L5:2012:A:N6	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1996:C:H42	3:L5:2000:G:H22	1.25	0.81
3:L5:1996:C:H42	3:L5:2000:G:N2	1.79	0.80
3:L5:2708:U:HO2'	84:CI:79:ARG:NH1	1.78	0.78
64:Sg:87:LEU:HB2	64:Sg:101:PHE:HB2	1.65	0.78
63:Sf:126:CYS:SG	63:Sf:144:CYS:N	2.54	0.77
83:S2:1776:G:N2	83:S2:1777:G:N7	2.32	0.77
66:SB:103:MET:HG3	66:SB:215:VAL:HG12	1.67	0.76
3:L5:1982:G:N2	3:L5:2009:A:O2'	2.19	0.76
3:L5:4774:C:O2'	3:L5:4775:C:O2	2.03	0.75
86:L5:5293:SPM:H112	19:LO:91:LYS:HD3	1.69	0.75
83:S2:925:G:H1	83:S2:1017:U:H3	1.34	0.75
49:Lt:12:VAL:HG11	49:Lt:65:GLN:H	1.51	0.74
7:LB:90:VAL:HG23	7:LB:163:ILE:HD11	1.68	0.74
2:Et:6:G:H1	2:Et:67:U:H3	1.36	0.73
3:L5:387:G:HO2'	3:L5:412:G:H1	1.33	0.73
83:S2:940:U:H3	83:S2:1002:U:H3	1.36	0.73
3:L5:5024:C:H41	3:L5:5028:G:H21	1.36	0.73
3:L5:2611:A:H5'	3:L5:2688:G:H4'	1.71	0.72
51:SF:134:VAL:HG12	51:SF:135:ARG:HG2	1.71	0.72
67:SC:210:PRO:HB3	67:SC:240:THR:HG21	1.70	0.72
3:L5:2520:C:O2	3:L5:2640:G:N2	2.22	0.72
55:SQ:72:VAL:HG11	55:SQ:80:GLN:HG3	1.71	0.72
70:SH:154:ILE:HB	70:SH:185:VAL:HG22	1.71	0.71
3:L5:3641:U:OP2	3:L5:3646:A:N6	2.23	0.71
3:L5:2103:G:N7	3:L5:2104:G:N2	2.38	0.71
3:L5:2702:C:OP1	25:LU:101:ARG:NH2	2.24	0.71
13:LH:106:GLN:HB2	13:LH:111:LEU:HB3	1.71	0.70
64:Sg:247:TRP:HB3	64:Sg:258:ILE:HD11	1.71	0.70
3:L5:184:U:O2	3:L5:253:G:N2	2.24	0.70
3:L5:1095:A:H2	3:L5:1200:G:H1	1.35	0.70
17:LM:15:VAL:HG22	17:LM:50:MET:HE1	1.74	0.70
78:SX:68:LYS:HB3	78:SX:91:LEU:HD13	1.74	0.70
3:L5:512:U:H3	3:L5:647:G:H1	1.40	0.70
25:LU:65:ARG:HG2	25:LU:67:LYS:H	1.57	0.69
3:L5:1366:G:H5''	16:LL:36:ARG:HH12	1.57	0.69
3:L5:664:G:N2	3:L5:666:G:O6	2.25	0.69
3:L5:1702:C:H4'	8:LC:308:LYS:HD2	1.75	0.69
7:LB:10:ARG:NH1	7:LB:11:HIS:O	2.24	0.69
15:LJ:146:ARG:HG2	15:LJ:147:ARG:HG3	1.74	0.69
3:L5:4910:G:H4'	7:LB:95:THR:HG22	1.75	0.69
34:Ld:70:LYS:HZ2	84:CI:66:GLY:HA3	1.54	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Sg:107:ASP:HB2	64:Sg:125:ARG:HG3	1.75	0.69
20:LP:39:MET:HG2	20:LP:43:LYS:HD3	1.75	0.69
6:LA:137:ILE:HD11	6:LA:149:LYS:HB2	1.75	0.68
70:SH:105:THR:HG23	70:SH:107:LYS:H	1.58	0.68
65:SA:89:LYS:HD2	65:SA:201:LEU:HG	1.76	0.68
83:S2:851:C:H5'	83:S2:852:G:H5'	1.76	0.68
26:LV:35:LYS:HB2	26:LV:67:LYS:HG3	1.75	0.68
3:L5:2351:OMC:HM22	8:LC:95:MET:HG3	1.76	0.68
20:LP:109:VAL:HA	20:LP:112:LEU:HD13	1.76	0.68
67:SC:193:VAL:HG11	67:SC:240:THR:HG22	1.76	0.68
83:S2:1658:G:OP2	83:S2:1660:C:N4	2.27	0.68
3:L5:137:G:H2'	3:L5:138:G:H8	1.59	0.68
3:L5:3954:A:H1'	3:L5:4058:U:H5'	1.75	0.68
3:L5:4413:C:O2	14:LI:158:LYS:NZ	2.27	0.68
71:SI:133:GLU:HA	71:SI:136:ILE:HG12	1.75	0.68
3:L5:1172:C:H42	3:L5:1188:C:H42	1.42	0.67
3:L5:2484:A:H62	3:L5:2494:U:H3	1.42	0.67
3:L5:2557:G:H1	3:L5:2570:U:H3	1.40	0.67
48:Ls:68:HIS:O	48:Ls:71:ASN:ND2	2.26	0.67
83:S2:1030:A:H2'	83:S2:1031:A2M:H8	1.74	0.67
83:S2:554:A:HO2'	83:S2:555:A:H8	1.40	0.67
2:Et:9:A:H2'	2:Et:11:C:H41	1.58	0.67
3:L5:1995:G:O2'	49:Lt:122:ALA:O	2.12	0.67
25:LU:114:TYR:CE2	84:CI:50:MET:HG3	2.29	0.67
58:ST:124:THR:HG23	58:ST:127:GLY:H	1.60	0.67
3:L5:2758:G:O2'	3:L5:2765:A:N3	2.28	0.67
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.77	0.67
47:Lr:28:GLU:OE2	47:Lr:31:ASN:ND2	2.26	0.67
69:SG:13:GLN:NE2	83:S2:153:G:N3	2.42	0.67
83:S2:587:A:H5'	83:S2:592:C:H41	1.60	0.67
3:L5:4618:OMG:H5'	26:LV:15:ARG:HB2	1.75	0.67
3:L5:1268:G:N7	32:Lb:111:ARG:NH2	2.43	0.67
3:L5:4546:A:N7	6:LA:215:ASN:ND2	2.43	0.67
69:SG:135:PRO:HG2	69:SG:141:ILE:HG22	1.77	0.67
6:LA:107:MET:HB3	6:LA:111:THR:HG21	1.75	0.66
3:L5:4242:U:H3	3:L5:4281:A:H2	1.43	0.66
41:Lk:26:LYS:HB2	41:Lk:69:LEU:HD12	1.77	0.66
67:SC:259:THR:HG23	76:SV:16:LYS:HZ3	1.61	0.66
3:L5:88:A:N7	21:LQ:173:LYS:NZ	2.43	0.66
3:L5:989:U:O2	3:L5:1064:G:N2	2.26	0.66
27:LW:80:ARG:NH2	69:SG:8:PRO:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78: SX:70: VAL: HG11	78: SX:94: ILE: HG21	1.78	0.66
3: L5:4098: A: N1	3: L5:4112: C: N4	2.42	0.66
3: L5:4594: U: H2'	3: L5:4595: G: H8	1.61	0.66
3: L5:1414: C: H2'	3: L5:1415: G: H8	1.61	0.65
3: L5:4910: G: N2	19: LO:106: ASP: O	2.28	0.65
27: LW:80: ARG: NH1	83: S2:167: G: O2'	2.28	0.65
66: SB:144: LYS: HD3	66: SB:208: HIS: HB3	1.78	0.65
69: SG:22: ARG: HG3	69: SG:25: ARG: HH12	1.59	0.65
34: Ld:64: ILE: HG23	34: Ld:68: LEU: HD23	1.77	0.65
78: SX:68: LYS: NZ	83: S2:616: A: OP1	2.29	0.65
3: L5:2093: A: N3	3: L5:2094: G: N1	2.44	0.65
50: SD:106: ARG: HG3	50: SD:175: VAL: HG22	1.79	0.65
3: L5:68: U: OP1	18: LN:178: HIS: ND1	2.29	0.65
3: L5:67: C: OP2	3: L5:312: G: N2	2.29	0.65
3: L5:3937: C: H1'	18: LN:125: SER: HB3	1.78	0.65
77: SW:2: VAL: N	83: S2:1091: C: HO2'	1.95	0.65
3: L5:1396: G: N7	31: La:110: LYS: NZ	2.43	0.65
3: L5:1499: C: OP1	21: LQ:150: ARG: NH2	2.30	0.65
74: SN:93: LYS: HE2	74: SN:151: ALA: HB2	1.78	0.65
83: S2:1854: U: H2'	83: S2:1855: G: H8	1.62	0.65
16: LL:64: VAL: HA	16: LL:67: HIS: CD2	2.28	0.64
27: LW:80: ARG: HH22	83: S2:167: G: H4'	1.62	0.64
69: SG:162: LEU: HG	69: SG:167: LYS: HE3	1.79	0.64
3: L5:748: G: O6	23: LS:98: ARG: NH2	2.30	0.64
6: LA:114: CYS: HB3	6: LA:165: VAL: HB	1.79	0.64
53: SM:128: PHE: HD1	53: SM:131: LYS: HZ3	1.44	0.64
55: SQ:19: ALA: HB2	55: SQ:75: GLY: HA3	1.80	0.64
83: S2:1228: A: H2'	83: S2:1229: G: H8	1.63	0.64
3: L5:2083: C: OP2	21: LQ:14: ARG: NH2	2.30	0.64
54: SP:130: ARG: HD3	54: SP:131: PRO: HD2	1.79	0.64
7: LB:222: VAL: O	7: LB:343: ARG: NH1	2.30	0.64
83: S2:1228: A: H2'	83: S2:1229: G: C8	2.33	0.64
3: L5:1994: C: H2'	3: L5:1995: G: C8	2.33	0.64
3: L5:2745: A: H2'	3: L5:2746: A: H8	1.62	0.64
47: Lr:38: PHE: O	47: Lr:45: HIS: NE2	2.26	0.64
71: SI:91: VAL: HG11	71: SI:205: ARG: HH12	1.61	0.64
11: LF:243: LEU: O	11: LF:247: MET: HB2	1.98	0.64
39: Li:2: ALA: N	39: Li:5: TYR: HH	1.96	0.64
65: SA:77: ILE: HG13	65: SA:99: ILE: HB	1.79	0.64
70: SH:51: ILE: HG21	70: SH:179: LYS: HG2	1.80	0.64
3: L5:305: A: OP2	18: LN:15: GLN: NE2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L7:38:U:N3	4:L7:41:G:OP2	2.31	0.64
2:Et:26:A:N1	2:Et:44:G:N2	2.46	0.63
3:L5:1996:C:N4	3:L5:2000:G:H22	1.95	0.63
64:Sg:40:ILE:HB	64:Sg:59:LEU:HB2	1.80	0.63
71:SI:22:HIS:HB3	83:S2:433:A:H5''	1.79	0.63
3:L5:4094:G:N2	3:L5:4115:G:OP2	2.32	0.63
3:L5:1739:G:N3	3:L5:1742:A:N6	2.46	0.63
69:SG:183:ARG:NH2	83:S2:316:G:OP2	2.30	0.63
3:L5:665:C:H4'	3:L5:666:G:H5'	1.78	0.63
31:La:72:THR:HG22	31:La:110:LYS:HB3	1.80	0.63
83:S2:533:A:H61	83:S2:550:C:H42	1.46	0.63
3:L5:1669:A:OP1	32:Lb:18:ARG:NH2	2.28	0.63
3:L5:4897:G:OP1	17:LM:128:LYS:NZ	2.32	0.63
64:Sg:252:THR:HG21	64:Sg:257:LYS:HD2	1.79	0.63
69:SG:176:ILE:HG12	69:SG:179:LEU:HD11	1.81	0.63
3:L5:1405:C:H2'	3:L5:1406:G:H8	1.64	0.63
32:Lb:109:ARG:HA	32:Lb:112:ILE:HG12	1.81	0.63
41:Lk:8:ILE:HD11	41:Lk:56:LEU:HD13	1.81	0.63
51:SF:168:THR:OG1	51:SF:171:GLU:OE1	2.16	0.63
3:L5:679:C:H2'	3:L5:680:G:H8	1.64	0.62
3:L5:2554:U:O2	3:L5:2764:A:N7	2.32	0.62
49:Lt:65:GLN:HG3	49:Lt:67:ARG:H	1.61	0.62
54:SP:37:TYR:O	57:SS:88:LYS:NZ	2.31	0.62
65:SA:10:MET:HE3	65:SA:55:TRP:HB2	1.80	0.62
83:S2:106:C:H2'	83:S2:107:A:H8	1.63	0.62
1:Pt:20(A):U:O4'	15:LJ:58:ARG:NH2	2.32	0.62
66:SB:171:ILE:HG22	66:SB:174:ARG:HE	1.64	0.62
74:SN:64:ARG:NH2	83:S2:919:A:OP2	2.31	0.62
2:Et:32:C:OP1	51:SF:135:ARG:NH2	2.31	0.62
49:Lt:114:ARG:NH2	49:Lt:126:SER:OG	2.32	0.62
50:SD:8:LYS:HG2	59:SU:61:LEU:HD11	1.81	0.62
68:SE:144:ALA:HB3	83:S2:121:OMU:HM23	1.81	0.62
68:SE:146:THR:HG21	83:S2:122:G:H21	1.64	0.62
83:S2:1422:G:H4'	83:S2:1423:C:H3'	1.82	0.62
69:SG:202:ASN:ND2	83:S2:125:C:OP1	2.31	0.62
15:LJ:141:ILE:HA	15:LJ:144:LYS:HD2	1.82	0.62
83:S2:1759:G:N2	83:S2:1760:G:O6	2.32	0.62
3:L5:1857:C:H2'	3:L5:1858:A:H8	1.65	0.62
9:LD:232:THR:OG1	9:LD:234:ASP:OD1	2.18	0.62
83:S2:1536:G:H2'	83:S2:1537:A:H8	1.63	0.62
58:ST:12:GLN:NE2	83:S2:1593:C:O2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4431:PSU:OP2	14:LI:3:ARG:NH2	2.31	0.62
6:LA:29:LEU:O	6:LA:123:ARG:NH1	2.32	0.62
62:Sd:19:ARG:NH2	83:S2:1661:A:OP1	2.33	0.62
69:SG:7:PHE:HD2	69:SG:10:THR:HG22	1.64	0.62
67:SC:72:ASP:OD2	67:SC:272:HIS:NE2	2.29	0.62
72:SJ:136:ARG:NH1	72:SJ:159:PHE:O	2.31	0.62
77:SW:107:SER:HB2	83:S2:860:G:H21	1.65	0.62
83:S2:1277:C:H2'	83:S2:1278:A:H8	1.63	0.62
3:L5:121:A:H62	3:L5:152:U:H3	1.48	0.62
3:L5:308:G:OP2	3:L5:308:G:N2	2.27	0.62
3:L5:327:U:O2'	39:Li:30:ARG:NH1	2.32	0.62
7:LB:107:ALA:HB2	7:LB:201:LEU:HD22	1.82	0.62
54:SP:48:GLY:O	54:SP:50:ARG:NH1	2.32	0.62
71:SI:106:SER:HB3	71:SI:171:LEU:HG	1.81	0.62
81:Sb:20:LYS:NZ	83:S2:1016:U:OP2	2.32	0.62
83:S2:94:G:O2'	83:S2:508:A:O2'	2.16	0.62
3:L5:2601:A:N6	3:L5:2744:A:OP2	2.29	0.61
3:L5:4525:C:OP1	7:LB:246:ARG:NH2	2.33	0.61
72:SJ:121:LYS:HD3	83:S2:527:C:H4'	1.80	0.61
83:S2:1010:G:H2'	83:S2:1011:A:H8	1.65	0.61
4:L7:23:A:N3	4:L7:118:C:O2'	2.31	0.61
77:SW:111:MET:HE3	77:SW:116:ALA:HA	1.81	0.61
83:S2:889:U:OP2	83:S2:896:U:N3	2.33	0.61
83:S2:1536:G:H2'	83:S2:1537:A:C8	2.35	0.61
3:L5:62:A:N3	3:L5:77:U:O2'	2.29	0.61
3:L5:4251:A:H5''	15:LJ:108:GLY:HA3	1.83	0.61
20:LP:52:THR:HG23	20:LP:85:LYS:HG3	1.80	0.61
68:SE:10:LYS:NZ	83:S2:95:G:OP1	2.34	0.61
83:S2:1203:G:H2'	83:S2:1204:A:C8	2.35	0.61
3:L5:4088:C:OP1	6:LA:37:ARG:NH1	2.33	0.61
6:LA:108:PRO:HB2	46:Lp:86:LEU:HD23	1.83	0.61
52:SK:85:LEU:HD21	52:SK:89:ILE:HB	1.83	0.61
63:Sf:144:CYS:HB2	63:Sf:146:LEU:HD23	1.83	0.61
83:S2:628:A:N6	83:S2:1500:G:O2'	2.31	0.61
3:L5:1726:U:H5'	11:LF:135:ILE:HD11	1.82	0.61
75:SO:104:ARG:NH2	83:S2:959:G:OP1	2.33	0.61
83:S2:165:G:OP2	83:S2:165:G:N2	2.29	0.61
3:L5:121:A:OP1	12:LG:110:LYS:NZ	2.27	0.61
55:SQ:58:LEU:HB3	55:SQ:62:ARG:HD2	1.81	0.61
22:LR:172:ARG:NH1	83:S2:909:G:OP1	2.33	0.61
41:Lk:27:LYS:O	41:Lk:70:LYS:NZ	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SA:118:GLU:HG3	67:SC:65:LYS:HE2	1.82	0.61
59:SU:70:CYS:SG	83:S2:1491:G:O2'	2.56	0.61
3:L5:4472:G:O2'	43:Lm:100:TYR:O	2.19	0.61
63:Sf:99:LYS:NZ	83:S2:1287:A:OP1	2.28	0.61
3:L5:1480:C:O2'	3:L5:1482:G:OP2	2.18	0.60
60:SZ:58:LEU:HD12	60:SZ:62:VAL:HG21	1.81	0.60
3:L5:4992:G:H2'	3:L5:4993:G:C8	2.36	0.60
71:SI:150:ASP:HA	71:SI:153:LYS:HG2	1.83	0.60
34:Ld:90:ARG:HD3	34:Ld:102:LEU:HD13	1.82	0.60
77:SW:71:LYS:NZ	83:S2:1156:U:OP1	2.35	0.60
83:S2:695:C:N4	83:S2:736:C:O2'	2.34	0.60
50:SD:32:ASP:OD1	50:SD:57:ASN:ND2	2.34	0.60
83:S2:874:G:H2'	83:S2:875:A:H8	1.66	0.60
6:LA:104:VAL:HA	6:LA:107:MET:HE3	1.83	0.60
22:LR:176:ARG:NH2	83:S2:910:G:OP1	2.32	0.60
50:SD:161:GLY:HA3	83:S2:1388:A:H61	1.67	0.60
53:SM:91:LEU:HD12	53:SM:106:CYS:HB2	1.83	0.60
78:SX:107:ARG:HG3	78:SX:110:HIS:HB3	1.83	0.60
83:S2:747:U:O2	83:S2:796:G:N2	2.35	0.60
3:L5:5064:G:H21	20:LP:75:GLN:HE22	1.48	0.60
53:SM:63:LYS:HD3	53:SM:64:LEU:HD22	1.84	0.60
55:SQ:8:GLN:HG3	55:SQ:27:ARG:HE	1.66	0.60
73:SL:85:THR:HG21	83:S2:373:G:H4'	1.84	0.60
83:S2:609:U:H2'	83:S2:610:G:H8	1.67	0.60
3:L5:4076:G:OP1	12:LG:73:ARG:NE	2.34	0.60
12:LG:165:GLU:OE2	18:LN:26:ARG:NH1	2.34	0.60
69:SG:2:LYS:HD3	69:SG:15:LEU:HD21	1.84	0.60
78:SX:9:THR:HG22	83:S2:681:PSU:H4'	1.82	0.60
3:L5:513:U:N3	3:L5:516:C:OP2	2.33	0.60
3:L5:1703:C:O2'	3:L5:1704:C:O4'	2.18	0.60
3:L5:2899:C:OP1	22:LR:108:ARG:NH2	2.32	0.60
19:LO:34:VAL:HG22	19:LO:103:LYS:HB2	1.83	0.60
50:SD:40:ARG:NH2	59:SU:106:ILE:O	2.34	0.60
3:L5:2458:C:H5''	18:LN:67:ARG:HD2	1.83	0.60
25:LU:28:PRO:HB2	25:LU:34:MET:HG3	1.84	0.60
41:Lk:54:GLU:OE2	41:Lk:58:GLN:NE2	2.32	0.60
64:Sg:164:ILE:HG22	64:Sg:178:ASN:HA	1.84	0.60
3:L5:1390:G:N2	3:L5:1393:G:OP2	2.34	0.59
3:L5:3664:G:H2'	3:L5:3665:G:H8	1.67	0.59
3:L5:3701:OMC:H5	3:L5:3748:A:H62	1.47	0.59
3:L5:1563:A:N6	83:S2:1028:A:N1	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LP:118:GLN:OE1	20:LP:120:ASN:ND2	2.35	0.59
23:LS:76:LYS:NZ	23:LS:100:LEU:O	2.35	0.59
70:SH:165:ASN:O	70:SH:169:LYS:NZ	2.34	0.59
3:L5:109:G:OP2	16:LL:74:ARG:NH2	2.34	0.59
3:L5:935:A:O2'	17:LM:44:GLN:O	2.20	0.59
81:Sb:14:GLU:HA	81:Sb:17:ARG:HG2	1.84	0.59
83:S2:508:A:H3'	83:S2:509:OMG:H8	1.67	0.59
51:SF:171:GLU:OE2	60:SZ:106:GLN:NE2	2.36	0.59
71:SI:141:ARG:HD3	71:SI:145:ILE:HG21	1.83	0.59
83:S2:747:U:N3	83:S2:796:G:N1	2.50	0.59
3:L5:3611:A:H2	3:L5:5016:A:H8	1.50	0.59
7:LB:299:ILE:HB	7:LB:313:SER:HB3	1.85	0.59
40:Lj:14:LYS:NZ	42:Ll:51:LEU:OXT	2.35	0.59
56:SR:99:ASP:OD2	65:SA:42:LYS:NZ	2.25	0.59
64:Sg:68:ASP:HB3	64:Sg:111:VAL:HG22	1.84	0.59
71:SI:70:GLU:OE2	73:SL:21:LYS:NZ	2.32	0.59
3:L5:1996:C:O3'	48:Ls:44:ARG:NH1	2.35	0.59
11:LF:105:VAL:HG13	11:LF:136:VAL:HG12	1.84	0.59
57:SS:109:GLU:HA	57:SS:112:GLU:HG2	1.84	0.59
83:S2:888:U:H4'	83:S2:889:U:H5'	1.83	0.59
3:L5:4084:G:O6	6:LA:72:ARG:NH2	2.35	0.59
67:SC:102:LEU:HD22	67:SC:130:ILE:HD12	1.83	0.59
69:SG:92:ARG:O	83:S2:453:C:O2'	2.20	0.59
3:L5:3822:PSU:OP1	86:L5:5292:SPM:N5	2.33	0.59
9:LD:204:VAL:HB	9:LD:236:MET:HE1	1.83	0.59
55:SQ:131:LYS:HB2	55:SQ:140:ARG:HH22	1.66	0.59
59:SU:51:LYS:HB3	59:SU:90:ASP:HB2	1.84	0.59
83:S2:1562:C:H2'	83:S2:1563:G:H8	1.65	0.59
3:L5:300:A:H2'	3:L5:301:G:H8	1.68	0.59
3:L5:989:U:H3	3:L5:1064:G:H1	1.49	0.59
3:L5:1326:A2M:H2'	3:L5:1327:C:C6	2.38	0.59
3:L5:2300:A:N7	8:LC:143:ARG:NH1	2.50	0.59
3:L5:2708:U:H1'	84:CI:79:ARG:HH22	1.68	0.59
5:L8:75:OMG:OP2	29:LY:74:TYR:OH	2.20	0.59
7:LB:83:PRO:O	7:LB:167:GLN:NE2	2.35	0.59
51:SF:36:GLN:NE2	51:SF:37:ASP:OD1	2.36	0.59
51:SF:127:ARG:HG2	51:SF:136:ARG:HE	1.68	0.59
69:SG:85:ARG:O	69:SG:87:ARG:NH1	2.36	0.59
3:L5:1704:C:O3'	11:LF:46:ARG:NH1	2.36	0.58
15:LJ:22:LEU:HD22	15:LJ:128:LEU:HD12	1.85	0.58
44:Ln:1:MET:HG3	83:S2:1706:G:H5'	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:SC:200:ARG:O	72:SJ:54:ARG:NH2	2.33	0.58
73:SL:133:PRO:HG2	83:S2:383:G:H21	1.68	0.58
79:SY:105:LYS:NZ	83:S2:507:G:O6	2.31	0.58
3:L5:4098:A:H2'	3:L5:4099:G:H4'	1.84	0.58
38:Lh:80:PRO:HD2	38:Lh:83:LEU:HD12	1.85	0.58
45:Lo:2:VAL:N	45:Lo:90:HIS:O	2.36	0.58
48:Ls:17:ILE:HD12	48:Ls:54:LEU:HD21	1.83	0.58
3:L5:268:G:H2'	3:L5:269:G:H8	1.68	0.58
58:ST:22:LEU:HG	58:ST:28:LEU:HD21	1.85	0.58
67:SC:257:LYS:O	76:SV:16:LYS:NZ	2.32	0.58
3:L5:3823:G:OP2	3:L5:3823:G:N2	2.30	0.58
69:SG:133:LEU:HD12	83:S2:65:C:C4	2.38	0.58
78:SX:105:PHE:HD1	78:SX:121:LYS:HB3	1.66	0.58
3:L5:1890:G:N2	3:L5:1890:G:OP2	2.32	0.58
3:L5:2335:C:H2'	3:L5:2336:G:H8	1.68	0.58
19:LO:9:LEU:HD23	19:LO:118:MET:HB2	1.85	0.58
50:SD:172:VAL:HG22	50:SD:185:LYS:HG2	1.85	0.58
83:S2:1288:OMU:HN3	83:S2:1311:C:H42	1.51	0.58
18:LN:146:PRO:HB2	38:Lh:104:THR:HG23	1.86	0.58
65:SA:128:ARG:NH2	65:SA:151:ASP:O	2.36	0.58
68:SE:29:PRO:HA	83:S2:496:C:H5'	1.86	0.58
3:L5:2613:C:OP1	37:Lg:24:ARG:NH2	2.37	0.58
9:LD:62:CYS:HB3	9:LD:105:LEU:HD22	1.84	0.58
25:LU:44:GLN:HB2	25:LU:56:LEU:HD21	1.84	0.58
59:SU:61:LEU:HB2	59:SU:82:MET:HB3	1.86	0.58
83:S2:981:A:H2'	83:S2:982:G:C8	2.39	0.58
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.68	0.58
3:L5:4986:G:H1'	7:LB:174:ARG:NH2	2.19	0.58
51:SF:124:ASP:OD1	51:SF:125:SER:N	2.27	0.58
83:S2:948:C:H2'	83:S2:949:G:H8	1.69	0.58
33:Lc:99:PRO:HG3	33:Lc:104:ILE:HB	1.86	0.58
51:SF:142:SER:HB3	61:Sc:50:VAL:HG22	1.85	0.58
10:LE:227:HIS:HE1	10:LE:230:GLY:HA2	1.68	0.57
66:SB:26:SER:O	66:SB:51:ARG:NH2	2.37	0.57
68:SE:73:ASP:OD2	68:SE:122:LYS:NZ	2.37	0.57
69:SG:198:ARG:NH1	83:S2:126:G:OP2	2.36	0.57
83:S2:928:G:H2'	83:S2:929:G:C8	2.39	0.57
3:L5:1283:G:N1	3:L5:2076:G:OP1	2.33	0.57
3:L5:2658:G:N2	3:L5:2676:A:OP2	2.37	0.57
3:L5:3946:G:N2	3:L5:4067:U:O2	2.29	0.57
9:LD:64:ILE:HD13	9:LD:109:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:SY:41:ARG:NH2	79:SY:52:PRO:O	2.37	0.57
3:L5:4279:A:H5'	3:L5:4281:A:H1'	1.86	0.57
40:Lj:2:THR:HB	40:Lj:6:SER:HB2	1.86	0.57
3:L5:2624:G:OP2	25:LU:97:ARG:NH2	2.36	0.57
6:LA:101:VAL:HG22	6:LA:165:VAL:HG22	1.87	0.57
7:LB:394:LYS:HA	7:LB:397:ILE:HG12	1.86	0.57
75:SO:45:THR:HA	75:SO:52:THR:HA	1.86	0.57
4:L7:7:G:OP1	9:LD:33:ARG:NH1	2.37	0.57
5:L8:150:C:N4	12:LG:52:THR:O	2.38	0.57
8:LC:298:ILE:HD13	21:LQ:131:PRO:HB3	1.87	0.57
51:SF:127:ARG:HG2	51:SF:136:ARG:HB2	1.86	0.57
57:SS:85:ASN:OD1	57:SS:97:GLN:NE2	2.34	0.57
71:SI:88:ASN:OD1	71:SI:205:ARG:NH2	2.38	0.57
3:L5:4077:A:N1	3:L5:4171:C:N4	2.52	0.57
5:L8:87:G:O6	29:LY:113:LYS:NZ	2.35	0.57
15:LJ:63:ARG:HH11	45:Lo:106:PHE:HB2	1.68	0.57
66:SB:186:ASN:HA	66:SB:189:ILE:HD12	1.85	0.57
83:S2:1528:G:O2'	83:S2:1666:C:OP1	2.21	0.57
5:L8:21:C:OP1	8:LC:195:LYS:NZ	2.32	0.57
15:LJ:104:ASN:HD22	15:LJ:133:VAL:HG13	1.69	0.57
57:SS:130:ARG:NH2	83:S2:1230:C:OP1	2.37	0.57
63:Sf:95:ARG:HH12	83:S2:1291:A:H62	1.51	0.57
64:Sg:260:ASP:O	64:Sg:264:LYS:N	2.38	0.57
80:Sa:8:ASN:ND2	83:S2:1861:G:OP1	2.37	0.57
83:S2:640:A:H2'	83:S2:641:A:C8	2.40	0.57
3:L5:1500:A:H5''	3:L5:1501:C:H5''	1.87	0.57
3:L5:5002:U:OP2	7:LB:385:LYS:NZ	2.33	0.57
29:LY:67:ILE:O	29:LY:84:ARG:NH2	2.38	0.57
64:Sg:107:ASP:OD2	64:Sg:125:ARG:NH1	2.38	0.57
64:Sg:254:PRO:O	64:Sg:272:GLN:NE2	2.38	0.57
66:SB:40:ASN:HD21	66:SB:76:ASN:HB2	1.70	0.57
3:L5:2848:G:O2'	3:L5:3838:U:O4	2.21	0.57
3:L5:3811:G:O2'	3:L5:3814:U:OP2	2.20	0.57
3:L5:4617:G:OP1	7:LB:62:ARG:NH1	2.32	0.57
3:L5:2017:A:O2'	3:L5:2018:C:H6	1.87	0.57
3:L5:2017:A:O2'	3:L5:2018:C:O5'	2.20	0.57
3:L5:4451:G:N2	3:L5:4452:U:O4	2.34	0.57
20:LP:17:SER:HB2	20:LP:98:ALA:HB2	1.87	0.57
45:Lo:11:PHE:O	45:Lo:81:ARG:NH2	2.38	0.57
3:L5:1969:G:H4'	48:Ls:36:GLY:HA2	1.87	0.56
7:LB:17:LEU:O	7:LB:19:ARG:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SM:110:VAL:O	53:SM:112:LYS:NZ	2.37	0.56
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.40	0.56
22:LR:92:LYS:HG2	22:LR:96:MET:HE3	1.86	0.56
27:LW:119:LYS:O	27:LW:123:LYS:HB2	2.04	0.56
48:Ls:91:THR:OG1	48:Ls:93:GLU:OE1	2.23	0.56
3:L5:1971:C:O2	48:Ls:41:GLN:NE2	2.38	0.56
3:L5:2362:U:H2'	3:L5:2363:A2M:H8	1.87	0.56
3:L5:4092:G:N7	3:L5:4114:C:N4	2.53	0.56
3:L5:4775:C:H41	3:L5:4859:C:N4	2.03	0.56
3:L5:4940:C:H5'	3:L5:4941:G:H5''	1.85	0.56
52:SK:50:GLN:HE22	83:S2:1276:A:H1'	1.70	0.56
60:SZ:80:ARG:O	83:S2:1598:G:O2'	2.19	0.56
64:Sg:176:VAL:HG23	64:Sg:185:LYS:HB2	1.87	0.56
66:SB:122:GLU:HG2	66:SB:140:VAL:HG12	1.86	0.56
83:S2:1754:G:N7	83:S2:1779:G:N2	2.53	0.56
3:L5:518:G:H1	3:L5:643:C:H2'	1.70	0.56
3:L5:667:A:H5''	3:L5:668:C:H5''	1.86	0.56
3:L5:1754:U:H1'	9:LD:3:PHE:HZ	1.71	0.56
3:L5:2407:G:O6	42:L1:2:SER:N	2.38	0.56
3:L5:4097:G:O6	3:L5:4098:A:N6	2.38	0.56
6:LA:229:ALA:HB3	6:LA:234:LYS:HB3	1.87	0.56
9:LD:223:PHE:HB3	9:LD:226:TYR:HB2	1.88	0.56
21:LQ:15:ARG:NH1	21:LQ:52:PHE:O	2.39	0.56
34:Ld:70:LYS:HZ1	84:CI:66:GLY:HA3	1.70	0.56
48:Ls:31:GLY:HA2	48:Ls:86:VAL:HG12	1.87	0.56
73:SL:33:LEU:HD12	73:SL:34:PRO:HD2	1.87	0.56
75:SO:149:ARG:NH2	83:S2:961:G:OP1	2.39	0.56
3:L5:1214:C:N3	32:Lb:90:SER:OG	2.38	0.56
3:L5:4107:G:N2	3:L5:4108:G:O6	2.38	0.56
10:LE:222:LEU:HB2	10:LE:237:LYS:HD2	1.87	0.56
17:LM:100:ARG:HA	17:LM:103:LYS:HG2	1.88	0.56
68:SE:49:ARG:NH2	83:S2:496:C:OP1	2.31	0.56
83:S2:1112:U:O2	83:S2:1121:G:O6	2.23	0.56
83:S2:1736:G:H2'	83:S2:1737:G:H8	1.70	0.56
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.40	0.56
83:S2:64:A:N6	83:S2:83:A:OP2	2.39	0.56
3:L5:1100:U:O3'	3:L5:1167:C:N4	2.38	0.56
3:L5:3619:G:H22	3:L5:3624:A:H1'	1.70	0.56
3:L5:4873:G:N7	19:LO:179:LYS:NZ	2.50	0.56
64:Sg:206:LEU:HD12	64:Sg:218:LEU:HD12	1.88	0.56
71:SI:56:ARG:NH2	83:S2:380:G:OP1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SS:48:ALA:O	57:SS:66:ARG:NH2	2.39	0.56
83:S2:84:A:N3	83:S2:150:A:O2'	2.38	0.56
83:S2:1777:G:H2'	83:S2:1778:C:H6	1.71	0.56
3:L5:97:G:OP1	16:LL:16:LYS:NZ	2.37	0.56
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.42	0.56
83:S2:1010:G:H2'	83:S2:1011:A:C8	2.40	0.56
3:L5:1516:G:O2'	16:LL:18:TRP:NE1	2.36	0.55
3:L5:1785:C:OP1	14:LI:133:GLN:NE2	2.39	0.55
15:LJ:136:ARG:NH2	15:LJ:161:GLU:OE2	2.32	0.55
28:LX:64:SER:HB2	38:Lh:69:LEU:HD13	1.89	0.55
48:Ls:34:ASN:HB3	48:Ls:185:PHE:HE1	1.71	0.55
3:L5:4093:G:H1	3:L5:4114:C:H2'	1.71	0.55
3:L5:4363:A:H5''	45:Lo:36:GLN:HG2	1.89	0.55
3:L5:4694:G:H4'	13:LH:71:ARG:HH12	1.72	0.55
64:Sg:32:LEU:HA	64:Sg:42:MET:HA	1.88	0.55
75:SO:135:ILE:O	83:S2:943:U:O2'	2.24	0.55
7:LB:292:LEU:HB2	7:LB:298:LEU:HD12	1.88	0.55
13:LH:18:ILE:HG12	13:LH:27:VAL:HG22	1.88	0.55
43:Lm:79:GLU:OE2	43:Lm:81:SER:OG	2.24	0.55
61:Sc:66:ARG:HH12	61:Sc:68:LEU:HD23	1.71	0.55
73:SL:61:PRO:HG3	73:SL:141:ASN:HB3	1.89	0.55
76:SV:42:VAL:HG23	76:SV:43:THR:HG23	1.88	0.55
83:S2:1748:G:O6	83:S2:1786:U:O4	2.25	0.55
3:L5:700:G:N1	3:L5:701:G:C6	2.74	0.55
7:LB:10:ARG:NH2	7:LB:265:SER:O	2.38	0.55
18:LN:157:LYS:O	18:LN:162:ARG:NH1	2.39	0.55
52:SK:55:ARG:NH1	52:SK:78:TYR:OH	2.39	0.55
59:SU:68:THR:O	62:Sd:40:ARG:NH1	2.39	0.55
6:LA:13:GLY:O	6:LA:17:ARG:HG3	2.07	0.55
15:LJ:83:LEU:HD22	15:LJ:132:VAL:HG11	1.88	0.55
50:SD:32:ASP:OD2	50:SD:65:ARG:NH1	2.39	0.55
59:SU:79:ARG:NH2	83:S2:1669:G:OP1	2.36	0.55
67:SC:121:ARG:NH1	67:SC:123:ARG:HE	2.04	0.55
67:SC:191:VAL:HG11	67:SC:236:PHE:HA	1.88	0.55
79:SY:80:ASP:OD1	79:SY:81:TYR:N	2.40	0.55
83:S2:1513:C:H2'	83:S2:1514:G:H8	1.71	0.55
3:L5:1591:U:OP2	3:L5:2856:C:O2'	2.19	0.55
3:L5:2764:A:H2'	3:L5:2765:A:H8	1.71	0.55
5:L8:67:U:H2'	5:L8:68:G:H8	1.71	0.55
68:SE:151:ASP:HA	69:SG:212:LEU:HD21	1.88	0.55
77:SW:111:MET:HE1	77:SW:119:LYS:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:557:U:H2'	83:S2:558:G:C8	2.42	0.55
83:S2:1550:G:H3'	83:S2:1579:A:H61	1.71	0.55
3:L5:1895:G:OP1	11:LF:96:ARG:NH2	2.40	0.55
3:L5:2516:G:O2'	37:Lg:62:LYS:NZ	2.40	0.55
14:LI:87:MET:HG2	14:LI:138:ILE:HG12	1.88	0.55
27:LW:56:ARG:HH21	27:LW:61:LYS:HB3	1.72	0.55
64:Sg:120:ILE:HB	64:Sg:132:TRP:HB2	1.88	0.55
68:SE:45:ILE:HG13	68:SE:61:VAL:HG11	1.88	0.55
83:S2:43:U:OP2	83:S2:485:A:N6	2.38	0.55
3:L5:512:U:O4	3:L5:647:G:O6	2.24	0.55
3:L5:1683:PSU:OP1	31:La:44:ASN:ND2	2.37	0.55
15:LJ:84:GLU:OE2	15:LJ:92:TYR:OH	2.20	0.55
50:SD:60:GLY:HA3	50:SD:65:ARG:H	1.72	0.55
67:SC:121:ARG:HH12	67:SC:123:ARG:HE	1.55	0.55
67:SC:267:GLN:OE1	76:SV:35:ASN:ND2	2.39	0.55
70:SH:12:ASN:ND2	70:SH:14:GLU:OE2	2.39	0.55
72:SJ:164:PRO:HB3	72:SJ:170:PRO:HA	1.88	0.55
79:SY:36:PRO:HG3	83:S2:570:C:H4'	1.88	0.55
82:Se:31:ARG:NH2	83:S2:525:A:O3'	2.40	0.55
5:L8:62:A:OP1	38:Lh:52:LYS:NZ	2.37	0.55
10:LE:119:GLU:HG3	35:Le:7:LEU:HD22	1.88	0.55
3:L5:364:G:O6	40:Lj:55:ARG:NH2	2.40	0.55
3:L5:1396:G:HO2'	3:L5:1468:C:HO2'	1.50	0.55
3:L5:4220:6MZ:O5'	3:L5:4220:6MZ:H8	2.07	0.55
7:LB:95:THR:OG1	7:LB:98:GLY:O	2.20	0.55
19:LO:126:VAL:HG13	19:LO:127:VAL:HG13	1.89	0.55
48:Ls:58:ASN:ND2	48:Ls:84:GLY:O	2.31	0.55
3:L5:1100:U:H3	3:L5:1194:G:H1	1.55	0.54
3:L5:2084:C:O2	21:LQ:16:LYS:NZ	2.38	0.54
3:L5:4478:G:O2'	3:L5:4602:A:N1	2.37	0.54
7:LB:80:GLU:OE1	7:LB:323:TYR:OH	2.25	0.54
51:SF:78:MET:HE3	83:S2:1222:G:H5''	1.87	0.54
74:SN:5:HIS:HB3	74:SN:117:LEU:HD13	1.89	0.54
3:L5:1646:A:O2'	40:Lj:49:TRP:O	2.21	0.54
3:L5:2486:G:O6	3:L5:2493:G:O6	2.26	0.54
3:L5:4987:C:OP2	7:LB:116:ARG:NH2	2.41	0.54
10:LE:165:LEU:HD11	10:LE:176:THR:HG22	1.89	0.54
12:LG:103:ARG:NH2	12:LG:192:ARG:O	2.40	0.54
49:Lt:85:LEU:HD13	49:Lt:109:ILE:HD12	1.89	0.54
55:SQ:140:ARG:HB2	83:S2:1644:C:H4'	1.89	0.54
66:SB:99:ASN:OD1	66:SB:100:PHE:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:5:U:H2'	83:S2:6:G:H8	1.72	0.54
83:S2:525:A:H2'	83:S2:526:A:C8	2.42	0.54
1:Pt:56:C:OP1	15:LJ:64:ARG:NH2	2.40	0.54
3:L5:4274:A:H2'	3:L5:4275:G:H8	1.73	0.54
17:LM:119:ARG:HG3	19:LO:189:ILE:HG23	1.87	0.54
51:SF:84:GLY:O	83:S2:1673:U:O2'	2.18	0.54
55:SQ:3:SER:OG	55:SQ:4:LYS:N	2.40	0.54
55:SQ:78:VAL:HG12	83:S2:1673:U:H5''	1.89	0.54
71:SI:25:ARG:HA	83:S2:448:A:H5''	1.87	0.54
3:L5:184:U:H3	3:L5:253:G:H1	1.53	0.54
23:LS:173:ASN:ND2	23:LS:175:PHE:O	2.40	0.54
60:SZ:99:LEU:HD21	60:SZ:102:LYS:HB2	1.89	0.54
67:SC:227:ARG:NH2	83:S2:663:C:O2'	2.40	0.54
75:SO:134:PRO:HB3	83:S2:944:A:H5''	1.88	0.54
82:Se:41:ARG:HG3	82:Se:42:PHE:HD1	1.73	0.54
83:S2:1265:A:O2'	83:S2:1327:G:OP2	2.19	0.54
3:L5:1259:G:H2'	3:L5:1260:G:H8	1.73	0.54
3:L5:4967:A:H2'	3:L5:4968:A:H8	1.72	0.54
13:LH:106:GLN:NE2	13:LH:113:GLU:OE2	2.37	0.54
37:Lg:45:ALA:HB3	37:Lg:82:MET:HE2	1.89	0.54
39:Li:55:ARG:O	39:Li:59:GLU:HG2	2.08	0.54
63:Sf:97:LYS:NZ	83:S2:1289:U:OP2	2.39	0.54
67:SC:109:ILE:HD11	67:SC:151:ILE:HD11	1.88	0.54
73:SL:103:GLU:HG3	78:SX:11:ARG:HB2	1.88	0.54
83:S2:629:A:O2'	83:S2:631:U:OP1	2.25	0.54
3:L5:2568:C:H2'	3:L5:2569:G:H8	1.71	0.54
7:LB:258:HIS:HA	7:LB:260:ALA:H	1.72	0.54
8:LC:262:GLU:HB3	8:LC:273:LEU:HD13	1.90	0.54
12:LG:117:ARG:NH2	12:LG:127:ASP:O	2.41	0.54
24:LT:44:GLY:HA2	24:LT:95:HIS:HB3	1.90	0.54
36:Lf:43:LEU:O	36:Lf:109:ARG:NH2	2.41	0.54
57:SS:120:HIS:ND1	83:S2:1622:U:OP1	2.40	0.54
83:S2:367:U:H4'	83:S2:371:A:C8	2.42	0.54
83:S2:1171:G:O2'	83:S2:1187:G:O6	2.23	0.54
83:S2:1845:A:H2'	83:S2:1846:G:C8	2.42	0.54
3:L5:1241:C:O2'	32:Lb:120:ARG:O	2.25	0.54
3:L5:1548:G:O2'	3:L5:2812:A:N3	2.37	0.54
3:L5:2092:G:O2'	3:L5:2262:G:N2	2.40	0.54
3:L5:2568:C:H2'	3:L5:2569:G:C8	2.43	0.54
41:Lk:24:LYS:HD3	41:Lk:69:LEU:HD21	1.90	0.54
60:SZ:85:ARG:NH2	83:S2:1597:C:OP2	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:SI:3:ILE:O	71:SI:30:GLY:N	2.40	0.54
83:S2:864:A:H2'	83:S2:865:A:H8	1.71	0.54
3:L5:3615:G:H1'	27:LW:44:ARG:HD3	1.90	0.54
3:L5:4501:U:OP1	7:LB:5:LYS:NZ	2.41	0.54
6:LA:140:ASN:ND2	6:LA:143:THR:OG1	2.41	0.54
32:Lb:43:MET:HE2	32:Lb:47:LYS:HZ1	1.72	0.54
48:Ls:143:ILE:HD12	48:Ls:158:VAL:HG11	1.90	0.54
67:SC:187:ARG:NH2	83:S2:1143:A:OP2	2.40	0.54
3:L5:2579:G:N2	3:L5:2582:A:OP2	2.36	0.54
3:L5:5047:C:O2'	3:L5:5050:C:OP2	2.22	0.54
30:LZ:11:VAL:HG12	30:LZ:82:PRO:HA	1.90	0.54
33:Lc:48:LEU:HD13	33:Lc:57:LYS:HG3	1.89	0.54
68:SE:100:ARG:HB2	68:SE:114:ILE:HD13	1.88	0.54
2:Et:6:G:H2'	2:Et:7:A:C8	2.43	0.54
3:L5:261:G:H2'	3:L5:262:G:C8	2.43	0.54
3:L5:1095:A:N1	3:L5:1200:G:O6	2.41	0.54
3:L5:1802:A:N3	24:LT:130:ARG:NH2	2.55	0.54
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.43	0.54
3:L5:2809:G:O2'	3:L5:4644:G:OP1	2.22	0.54
3:L5:4620:OMU:OP2	3:L5:4670:C:N4	2.41	0.54
3:L5:5006:U:H4'	3:L5:5007:A:H5'	1.89	0.54
24:LT:43:LYS:O	24:LT:58:HIS:ND1	2.40	0.54
33:Lc:51:ASN:HB2	33:Lc:77:ASN:HB2	1.89	0.54
33:Lc:82:GLY:HA2	33:Lc:91:VAL:HG12	1.90	0.54
38:Lh:73:TYR:HB3	38:Lh:79:LYS:HG2	1.89	0.54
51:SF:83:ASN:OD1	83:S2:1651:A:O2'	2.25	0.54
75:SO:42:VAL:HG11	75:SO:78:ALA:HA	1.90	0.54
83:S2:885:U:O2	83:S2:901:G:O6	2.26	0.54
3:L5:4946:U:HO2'	36:Lf:2:SER:N	2.05	0.53
43:Lm:99:CYS:HB2	43:Lm:114:LYS:HE3	1.91	0.53
74:SN:29:THR:OG1	74:SN:31:ASP:OD1	2.24	0.53
83:S2:1337:4AC:H2'	83:S2:1338:G:H8	1.73	0.53
83:S2:1589:A:N3	83:S2:1653:U:O2'	2.41	0.53
3:L5:956:A:H1'	3:L5:2076:G:H5''	1.90	0.53
4:L7:26:C:O2'	15:LJ:147:ARG:NH1	2.39	0.53
7:LB:219:VAL:HG11	7:LB:337:VAL:HG13	1.90	0.53
19:LO:62:MET:HE2	19:LO:64:THR:HB	1.90	0.53
53:SM:36:ARG:NH1	83:S2:1310:U:OP1	2.42	0.53
70:SH:99:ARG:NH1	83:S2:913:A:OP2	2.42	0.53
71:SI:116:HIS:O	71:SI:152:ARG:NH2	2.39	0.53
81:Sb:49:HIS:ND1	81:Sb:69:GLY:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2693:G:OP2	41:Lk:33:LYS:NZ	2.37	0.53
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.42	0.53
3:L5:4769:G:H5''	19:LO:176:ARG:HD3	1.90	0.53
10:LE:141:ARG:NH2	36:Lf:110:ILE:O	2.41	0.53
48:Ls:13:TYR:O	48:Ls:17:ILE:HG12	2.08	0.53
64:Sg:82:SER:OG	64:Sg:83:TRP:N	2.41	0.53
70:SH:142:LYS:HB3	77:SW:54:ASP:HB3	1.91	0.53
83:S2:5:U:H2'	83:S2:6:G:C8	2.43	0.53
3:L5:702:U:H2'	3:L5:703:G:O4'	2.07	0.53
3:L5:3732:A:H2'	3:L5:3733:A:H8	1.73	0.53
56:SR:7:LYS:HB3	56:SR:11:LYS:HE2	1.89	0.53
3:L5:1258:G:H2'	3:L5:1259:G:C8	2.44	0.53
3:L5:2083:C:P	21:LQ:14:ARG:HH22	2.32	0.53
3:L5:2284:G:OP1	31:La:7:LYS:NZ	2.35	0.53
3:L5:2580:U:OP1	30:LZ:36:ARG:NH1	2.37	0.53
3:L5:3868:G:H22	3:L5:3900:G:H1'	1.72	0.53
51:SF:60:ARG:HD2	83:S2:1679:A:H2'	1.91	0.53
83:S2:159:A2M:O5'	83:S2:159:A2M:H8	2.08	0.53
83:S2:795:A:H2'	83:S2:796:G:C8	2.43	0.53
83:S2:1221:G:O2'	83:S2:1676:U:O2	2.25	0.53
83:S2:1417:C:O2	83:S2:1422:G:O6	2.27	0.53
3:L5:1328:G:O2'	3:L5:2349:A:OP1	2.26	0.53
3:L5:1759:G:N2	3:L5:1773:U:O2	2.27	0.53
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.44	0.53
3:L5:2745:A:H2'	3:L5:2746:A:C8	2.41	0.53
3:L5:3867:A2M:H2'	3:L5:3868:G:O4'	2.08	0.53
3:L5:4769:G:OP1	19:LO:176:ARG:NH1	2.37	0.53
3:L5:4954:G:H2'	3:L5:4955:A:C8	2.44	0.53
4:L7:120:U:H4'	9:LD:262:LYS:HG2	1.89	0.53
51:SF:141:VAL:HG12	61:Sc:47:LYS:HG2	1.90	0.53
65:SA:120:ARG:HD2	67:SC:266:TYR:HB3	1.90	0.53
67:SC:207:ALA:HB2	83:S2:4:C:H4'	1.91	0.53
83:S2:98:C:OP2	83:S2:426:A:O2'	2.22	0.53
3:L5:150:U:OP2	12:LG:200:THR:OG1	2.23	0.53
27:LW:19:ARG:NH2	27:LW:37:GLU:OE2	2.42	0.53
69:SG:49:VAL:HB	69:SG:115:LYS:HG2	1.90	0.53
77:SW:3:ARG:HH22	77:SW:28:ARG:HH21	1.56	0.53
78:SX:105:PHE:CD1	78:SX:121:LYS:HB3	2.43	0.53
3:L5:4775:C:H41	3:L5:4859:C:H42	1.56	0.53
10:LE:161:ARG:NH1	10:LE:273:SER:OG	2.42	0.53
25:LU:23:LEU:HD23	25:LU:110:TYR:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SG:116:LYS:HE3	69:SG:125:THR:HG21	1.90	0.53
77:SW:30:CYS:SG	77:SW:31:SER:N	2.81	0.53
83:S2:28:U:H2'	83:S2:29:G:H8	1.72	0.53
83:S2:528:A:H2'	83:S2:529:A:C8	2.44	0.53
83:S2:671:A:H4'	83:S2:672:A:H5''	1.91	0.53
83:S2:1347:U:H2'	83:S2:1348:G:N3	2.24	0.53
3:L5:1327:C:H2'	3:L5:1328:G:C8	2.43	0.53
10:LE:243:THR:HG22	10:LE:245:GLN:H	1.74	0.53
19:LO:186:GLU:OE1	19:LO:186:GLU:N	2.42	0.53
56:SR:60:ARG:HA	56:SR:63:ARG:HG2	1.91	0.53
83:S2:1115:U:O2'	83:S2:1117:C:OP2	2.24	0.53
3:L5:1700:G:H5''	3:L5:1704:C:H42	1.74	0.53
7:LB:14:LEU:HD22	7:LB:17:LEU:HD11	1.91	0.53
7:LB:165:HIS:HB3	7:LB:180:LEU:HD23	1.90	0.53
10:LE:91:THR:HA	10:LE:108:LYS:HA	1.90	0.53
31:La:84:GLU:OE1	31:La:87:ARG:NH2	2.41	0.53
66:SB:167:LYS:O	66:SB:171:ILE:HG12	2.08	0.53
67:SC:196:ILE:HB	67:SC:223:TYR:HB2	1.89	0.53
83:S2:656:G:N2	83:S2:663:C:H5''	2.24	0.53
2:Et:2:C:H2'	2:Et:3:C:C6	2.44	0.52
3:L5:1094:G:O6	3:L5:1201:U:O2	2.27	0.52
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.92	0.52
3:L5:1552:G:O2'	3:L5:1574:G:N2	2.31	0.52
3:L5:2588:C:OP1	3:L5:2768:C:O2'	2.22	0.52
3:L5:4163:U:H5'	3:L5:4164:C:H5''	1.91	0.52
3:L5:4305:G:N7	24:LT:87:LYS:NZ	2.50	0.52
12:LG:209:SER:HA	12:LG:212:LYS:HG3	1.91	0.52
54:SP:115:TYR:OH	83:S2:1620:A:OP1	2.25	0.52
58:ST:96:SER:OG	83:S2:1568:C:OP1	2.27	0.52
62:Sd:14:PHE:HB2	83:S2:1661:A:H8	1.75	0.52
70:SH:30:LEU:O	70:SH:33:ASN:ND2	2.42	0.52
1:Pt:35:A:OP2	55:SQ:146:ARG:NH2	2.42	0.52
3:L5:1306:C:H2'	3:L5:1307:A:H8	1.74	0.52
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.44	0.52
3:L5:4260:U:H2'	3:L5:4261:C:C6	2.45	0.52
7:LB:50:LYS:HB2	7:LB:345:LEU:HD11	1.91	0.52
27:LW:7:SER:OG	27:LW:8:PHE:N	2.43	0.52
81:Sb:68:GLY:O	83:S2:928:G:N2	2.39	0.52
83:S2:543:C:H3'	83:S2:544:G:H8	1.74	0.52
83:S2:1337:4AC:H2'	83:S2:1338:G:C8	2.44	0.52
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2832:A:OP1	34:Ld:47:LYS:NZ	2.33	0.52
3:L5:4122:G:O2'	30:LZ:136:PHE:OXT	2.23	0.52
23:LS:5:GLY:O	23:LS:111:ARG:NH2	2.42	0.52
68:SE:31:PRO:HA	68:SE:81:THR:HB	1.91	0.52
69:SG:132:ARG:NH2	83:S2:152:U:O4'	2.42	0.52
79:SY:21:LYS:HE2	79:SY:75:ILE:HD11	1.91	0.52
83:S2:1324:G:HO2'	83:S2:1510:G:HO2'	1.54	0.52
3:L5:1857:C:H2'	3:L5:1858:A:C8	2.45	0.52
3:L5:2706:G:N7	84:CI:78:HIS:NE2	2.57	0.52
3:L5:2765:A:H2'	3:L5:2766:A:C8	2.44	0.52
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.45	0.52
13:LH:187:VAL:HG12	13:LH:188:GLN:HG3	1.91	0.52
19:LO:168:TYR:CE2	19:LO:172:LYS:HD2	2.44	0.52
26:LV:112:MET:SD	26:LV:135:ASN:ND2	2.75	0.52
36:Lf:78:HIS:HB3	36:Lf:83:MET:HB3	1.92	0.52
77:SW:57:ARG:HG2	83:S2:920:A:H4'	1.92	0.52
83:S2:1203:G:H2'	83:S2:1204:A:H8	1.75	0.52
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.39	0.52
7:LB:29:VAL:HG12	7:LB:31:SER:H	1.75	0.52
55:SQ:80:GLN:O	55:SQ:84:ILE:HG13	2.10	0.52
55:SQ:139:ALA:HB2	83:S2:1650:A:H5''	1.90	0.52
59:SU:80:PHE:HB3	62:Sd:52:PHE:HB3	1.91	0.52
62:Sd:2:GLY:N	83:S2:1271:C:O2	2.42	0.52
83:S2:1101:U:H2'	83:S2:1102:G:H8	1.74	0.52
83:S2:1736:G:H2'	83:S2:1737:G:C8	2.44	0.52
3:L5:93:G:H2'	3:L5:94:A:C8	2.45	0.52
3:L5:2583:C:OP2	37:Lg:76:ARG:NH1	2.40	0.52
3:L5:3932:U:H2'	3:L5:3933:G:H8	1.74	0.52
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.74	0.52
9:LD:120:GLU:O	9:LD:248:ARG:NH1	2.43	0.52
19:LO:54:TYR:OH	19:LO:73:PHE:O	2.27	0.52
55:SQ:53:GLU:OE1	55:SQ:85:ARG:NH2	2.43	0.52
59:SU:40:ILE:O	59:SU:44:LYS:HG2	2.10	0.52
69:SG:147:LEU:HD12	69:SG:151:ASP:HB2	1.91	0.52
83:S2:1829:G:H1'	83:S2:1850:MA6:H2	1.90	0.52
2:Et:23:A:H2'	2:Et:24:G:C8	2.43	0.52
3:L5:2018:C:H2'	3:L5:2019:C:C6	2.44	0.52
3:L5:2543:A:H2	3:L5:2773:G:H22	1.58	0.52
3:L5:4991:U:H2'	3:L5:4992:G:H8	1.75	0.52
51:SF:40:ALA:HB3	51:SF:67:PRO:HA	1.91	0.52
52:SK:85:LEU:HD12	52:SK:86:PRO:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1348:G:H2'	83:S2:1349:G:H8	1.75	0.52
83:S2:1773:C:H2'	83:S2:1774:C:H5''	1.92	0.52
3:L5:717:U:H2'	3:L5:718:C:C6	2.45	0.52
3:L5:4301:U:OP2	3:L5:4303:C:N4	2.42	0.52
33:Lc:47:ILE:HD12	33:Lc:94:LEU:HD11	1.92	0.52
49:Lt:82:ILE:HG12	49:Lt:137:GLN:HG2	1.92	0.52
50:SD:142:LEU:HD13	50:SD:150:MET:HE2	1.91	0.52
56:SR:29:HIS:CD2	64:Sg:36:ARG:HH21	2.28	0.52
58:ST:83:GLN:OE1	58:ST:93:SER:OG	2.21	0.52
64:Sg:205:SER:HA	64:Sg:221:LEU:HB2	1.91	0.52
65:SA:18:PHE:HD1	65:SA:23:THR:HG21	1.74	0.52
68:SE:208:VAL:HG11	68:SE:225:ILE:HG13	1.91	0.52
77:SW:6:VAL:HG12	77:SW:34:ILE:HD11	1.92	0.52
83:S2:106:C:OP1	83:S2:431:G:O2'	2.25	0.52
3:L5:1942:A:N3	3:L5:4432:C:O2'	2.40	0.52
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.45	0.52
3:L5:4589:A:N1	3:L5:4621:C:O2'	2.38	0.52
5:L8:141:C:H2'	5:L8:142:U:C6	2.45	0.52
50:SD:114:ALA:HB3	50:SD:117:ARG:HG3	1.90	0.52
53:SM:96:ARG:NH2	53:SM:100:PRO:O	2.43	0.52
61:Sc:29:GLN:NE2	61:Sc:66:ARG:O	2.36	0.52
63:Sf:102:VAL:HG22	63:Sf:104:LYS:HG2	1.90	0.52
63:Sf:107:LYS:NZ	63:Sf:108:VAL:O	2.42	0.52
71:SI:49:ARG:HE	83:S2:446:G:H5''	1.75	0.52
74:SN:14:SER:HB3	83:S2:1016:U:H5''	1.92	0.52
3:L5:2520:C:H2'	3:L5:2521:G:H8	1.75	0.52
3:L5:2846:G:O2'	26:LV:19:GLY:O	2.27	0.52
3:L5:4991:U:H2'	3:L5:4992:G:C8	2.46	0.52
22:LR:127:VAL:HG12	22:LR:132:PHE:HD2	1.75	0.52
26:LV:92:ASP:O	27:LW:2:LYS:NZ	2.43	0.52
51:SF:59:LYS:HB3	51:SF:62:ARG:HG3	1.92	0.52
52:SK:31:LYS:NZ	52:SK:40:VAL:H	2.08	0.52
55:SQ:100:VAL:HG22	55:SQ:101:ASP:H	1.75	0.52
64:Sg:129:ILE:HB	64:Sg:142:VAL:HB	1.92	0.52
64:Sg:129:ILE:O	64:Sg:142:VAL:N	2.40	0.52
64:Sg:208:ALA:HB2	64:Sg:218:LEU:HD13	1.92	0.52
72:SJ:29:LEU:HD23	82:Se:41:ARG:HD2	1.92	0.52
79:SY:76:TYR:OH	79:SY:86:GLU:OE1	2.19	0.52
83:S2:1533:A:H2	83:S2:1536:G:N3	2.08	0.52
3:L5:1333:A:H2'	3:L5:1334:A:C8	2.45	0.51
3:L5:1514:U:H2'	3:L5:1515:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2521:G:H4'	37:Lg:26:PRO:HD2	1.92	0.51
3:L5:2749:C:H2'	3:L5:2750:G:H8	1.74	0.51
3:L5:3697:U:H5''	3:L5:3698:G:H5'	1.92	0.51
3:L5:4761:G:H2'	3:L5:4762:A:C8	2.45	0.51
5:L8:67:U:H2'	5:L8:68:G:C8	2.45	0.51
19:LO:180:GLN:NE2	19:LO:184:ASN:OD1	2.43	0.51
42:LI:28:ARG:HA	42:LI:33:ASN:ND2	2.25	0.51
57:SS:5:ILE:N	60:SZ:50:PHE:O	2.40	0.51
79:SY:34:THR:O	83:S2:570:C:O2'	2.19	0.51
83:S2:1360:U:O2'	83:S2:1379:A:OP2	2.25	0.51
3:L5:2749:C:H2'	3:L5:2750:G:C8	2.45	0.51
3:L5:4246:G:H2'	3:L5:4247:G:H8	1.75	0.51
11:LF:41:MET:HE2	32:Lb:113:ALA:HB2	1.91	0.51
14:LI:101:LYS:NZ	14:LI:102:MET:O	2.41	0.51
22:LR:25:ASP:OD2	84:CI:72:ARG:NH2	2.38	0.51
83:S2:955:A:N1	83:S2:968:U:O2'	2.40	0.51
3:L5:735:G:H5''	17:LM:70:GLN:HG3	1.93	0.51
3:L5:2021:G:OP1	48:Ls:58:ASN:N	2.38	0.51
7:LB:258:HIS:HA	7:LB:260:ALA:N	2.24	0.51
64:Sg:249:CYS:HB3	64:Sg:258:ILE:HD13	1.93	0.51
69:SG:136:LYS:HB2	83:S2:65:C:H41	1.76	0.51
83:S2:26:U:H2'	83:S2:27:A2M:H8	1.91	0.51
3:L5:3661:G:N7	6:LA:152:SER:OG	2.41	0.51
11:LF:157:ARG:HD2	11:LF:213:LEU:HD23	1.92	0.51
12:LG:180:PRO:HG3	12:LG:219:VAL:HG13	1.93	0.51
22:LR:54:PRO:HG3	84:CI:70:ALA:HB2	1.91	0.51
33:Lc:30:GLY:O	33:Lc:34:THR:OG1	2.25	0.51
51:SF:133:THR:HG22	51:SF:134:VAL:HG23	1.93	0.51
68:SE:125:LYS:O	68:SE:142:HIS:N	2.44	0.51
69:SG:11:GLY:HA2	83:S2:166:A2M:HM'1	1.91	0.51
83:S2:656:G:H21	83:S2:663:C:H5''	1.75	0.51
83:S2:941:C:H2'	83:S2:942:G:H8	1.76	0.51
3:L5:1305:C:OP1	5:L8:7:U:O2'	2.28	0.51
3:L5:2303:C:H5''	35:Le:104:SER:HB3	1.93	0.51
8:LC:293:LEU:O	8:LC:299:GLN:NE2	2.41	0.51
11:LF:96:ARG:HH12	11:LF:224:THR:HG22	1.75	0.51
72:SJ:5:ARG:HB3	83:S2:38:A:H5''	1.93	0.51
1:Pt:33:U:OP2	55:SQ:146:ARG:NH1	2.43	0.51
3:L5:444:G:H2'	3:L5:445:U:C6	2.45	0.51
3:L5:1727:U:OP1	11:LF:131:ASN:ND2	2.43	0.51
3:L5:3911:C:H2'	3:L5:3912:U:H6	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LC:110:ARG:O	8:LC:113:ARG:NH1	2.39	0.51
57:SS:39:ARG:NH1	58:ST:36:THR:O	2.40	0.51
69:SG:3:LEU:HD23	69:SG:109:LEU:HB3	1.91	0.51
83:S2:693:A:H2'	83:S2:694:G:C8	2.45	0.51
83:S2:996:A:H2'	83:S2:997:A:C8	2.46	0.51
3:L5:267:G:OP1	38:Lh:109:ARG:NH2	2.43	0.51
3:L5:2045:G:O6	3:L5:3870:C:O2'	2.29	0.51
3:L5:3720:G:H22	3:L5:3733:A:H2	1.59	0.51
3:L5:5064:G:N2	20:LP:75:GLN:HE22	2.08	0.51
65:SA:126:ASP:OD1	65:SA:165:ASN:ND2	2.43	0.51
79:SY:11:LYS:HB2	79:SY:24:VAL:HG12	1.93	0.51
83:S2:888:U:O2'	83:S2:898:U:N3	2.43	0.51
3:L5:965:G:H21	3:L5:2092:G:H1'	1.76	0.51
6:LA:206:PRO:HG3	6:LA:213:GLY:HA3	1.93	0.51
26:LV:87:SER:OG	27:LW:19:ARG:NH1	2.44	0.51
62:Sd:8:TRP:HZ3	83:S2:1512:C:H5''	1.75	0.51
69:SG:7:PHE:HD1	69:SG:113:ILE:HB	1.74	0.51
75:SO:113:GLN:OE1	80:Sa:46:GLU:N	2.42	0.51
3:L5:729:G:H5''	11:LF:76:ARG:HD2	1.93	0.51
3:L5:1973:G:O2'	49:Lt:117:ARG:NH2	2.44	0.51
3:L5:1998:A:N6	48:Ls:40:MET:SD	2.84	0.51
7:LB:92:TYR:HB3	7:LB:99:LEU:HD22	1.92	0.51
14:LI:207:ASP:OD1	14:LI:210:ARG:NH1	2.44	0.51
25:LU:114:TYR:CD2	84:CI:50:MET:HG3	2.46	0.51
55:SQ:130:LYS:NZ	55:SQ:131:LYS:O	2.42	0.51
62:Sd:7:TYR:OH	83:S2:1274:G:N7	2.39	0.51
70:SH:162:GLN:HE22	70:SH:166:VAL:HB	1.75	0.51
1:Pt:50:U:O2	1:Pt:64:G:N2	2.24	0.51
3:L5:493:G:HO2'	3:L5:494:U:P	2.34	0.51
3:L5:2101:C:H2'	3:L5:2102:G:C8	2.45	0.51
3:L5:2296:G:O2'	8:LC:242:PRO:O	2.25	0.51
3:L5:4088:C:H2'	3:L5:4089:G:C8	2.46	0.51
3:L5:4986:G:H1'	7:LB:174:ARG:HH21	1.75	0.51
45:Lo:33:LEU:HA	45:Lo:38:LYS:HG2	1.92	0.51
72:SJ:136:ARG:HD3	72:SJ:160:SER:HA	1.92	0.51
83:S2:1144:A:H2'	83:S2:1145:A:C8	2.46	0.51
3:L5:1396:G:O2'	3:L5:1468:C:O2'	2.23	0.50
3:L5:2275:G:H2'	3:L5:2276:A:C8	2.46	0.50
3:L5:3659:G:OP1	6:LA:241:ARG:NH1	2.44	0.50
3:L5:4238:G:H2'	3:L5:4239:A:H8	1.76	0.50
12:LG:157:ILE:HA	12:LG:201:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:ST:65:TYR:HE1	58:ST:128:GLN:HG3	1.75	0.50
68:SE:204:SER:OG	68:SE:205:PHE:N	2.43	0.50
79:SY:102:THR:OG1	79:SY:106:GLN:OE1	2.29	0.50
81:Sb:67:THR:OG1	81:Sb:70:LYS:O	2.20	0.50
83:S2:1845:A:H2'	83:S2:1846:G:H8	1.76	0.50
1:Pt:56:C:O4'	15:LJ:64:ARG:NE	2.41	0.50
3:L5:303:C:OP2	18:LN:68:ARG:NH2	2.41	0.50
3:L5:1308:C:H2'	3:L5:1309:C:C6	2.46	0.50
3:L5:1339:U:H2'	3:L5:1340:OMC:C6	2.46	0.50
3:L5:2765:A:H2'	3:L5:2766:A:H8	1.75	0.50
3:L5:3848:U:H2'	3:L5:3849:A:H8	1.77	0.50
3:L5:4239:A:H2'	3:L5:4240:G:C8	2.46	0.50
3:L5:4419:U:OP1	3:L5:4475:G:N2	2.43	0.50
83:S2:436:OMG:OP2	83:S2:471:G:O2'	2.25	0.50
83:S2:1372:U:OP1	83:S2:1385:G:N2	2.37	0.50
2:Et:37:A:H3'	2:Et:38:A:H8	1.76	0.50
3:L5:173:C:OP1	16:LL:129:ARG:NH1	2.44	0.50
3:L5:679:C:H2'	3:L5:680:G:C8	2.45	0.50
3:L5:730:G:OP2	11:LF:76:ARG:NE	2.41	0.50
3:L5:1628:C:OP1	6:LA:14:SER:OG	2.30	0.50
3:L5:1645:C:H2'	3:L5:1646:A:C8	2.45	0.50
3:L5:3732:A:H2'	3:L5:3733:A:C8	2.47	0.50
3:L5:4088:C:H2'	3:L5:4089:G:H8	1.76	0.50
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.45	0.50
21:LQ:32:TYR:HD2	21:LQ:51:LEU:HD11	1.76	0.50
23:LS:161:ARG:HD2	23:LS:164:LYS:HB2	1.93	0.50
62:Sd:17:GLY:O	62:Sd:27:ARG:NH1	2.44	0.50
67:SC:78:LEU:HD12	67:SC:81:ILE:HD12	1.93	0.50
74:SN:66:VAL:HG13	74:SN:67:THR:HG23	1.93	0.50
3:L5:729:G:O6	23:LS:70:LYS:NZ	2.44	0.50
5:L8:39:G:OP1	38:Lh:86:LYS:NZ	2.44	0.50
7:LB:217:ILE:HD12	7:LB:347:LEU:HB3	1.92	0.50
11:LF:214:SER:OG	11:LF:215:SER:N	2.42	0.50
51:SF:26:ASP:OD1	51:SF:26:ASP:N	2.45	0.50
53:SM:51:VAL:HG12	53:SM:77:ILE:HB	1.93	0.50
63:Sf:123:SER:HG	63:Sf:126:CYS:H	1.59	0.50
83:S2:1595:U:H2'	83:S2:1596:U:C6	2.47	0.50
3:L5:1194:G:H2'	3:L5:1195:G:H8	1.76	0.50
3:L5:1760:G:N2	3:L5:1761:G:O6	2.45	0.50
59:SU:20:ILE:HG22	59:SU:116:ILE:HG22	1.92	0.50
71:SI:10:LYS:NZ	83:S2:370:G:O2'	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78: SX:52: LEU: HD11	78: SX:73: GLN: HB2	1.93	0.50
82: Se:56: ASN: ND2	83: S2:606: G: O4'	2.43	0.50
83: S2:1226: G: N1	83: S2:1639: G7M: OP2	2.37	0.50
83: S2:1277: C: H2'	83: S2:1278: A: C8	2.45	0.50
1: Pt:23: C: H2'	1: Pt:24: A: H8	1.77	0.50
3: L5:1601: A: OP1	40: Lj:5: THR: OG1	2.22	0.50
3: L5:3886: G: OP1	19: LO:85: ARG: NH2	2.44	0.50
3: L5:3898: G: H5'	7: LB:254: ILE: HG13	1.94	0.50
3: L5:4887: C: H42	3: L5:4932: U: H3	1.60	0.50
19: LO:54: TYR: CD1	19: LO:145: VAL: HG21	2.46	0.50
31: La:36: GLY: HA3	31: La:40: HIS: CE1	2.47	0.50
51: SF:34: SER: HA	61: Sc:55: VAL: HG23	1.94	0.50
83: S2:907: G: H2'	83: S2:908: A: C8	2.46	0.50
3: L5:502: C: H3'	3: L5:503: C: H3'	1.94	0.50
3: L5:1867: A: H2'	3: L5:1868: A: C8	2.47	0.50
3: L5:2298: U: OP1	8: LC:204: ARG: NE	2.45	0.50
3: L5:2756: G: O6	30: LZ:51: ARG: NH2	2.30	0.50
3: L5:4149: C: OP1	30: LZ:59: LYS: N	2.43	0.50
6: LA:118: GLU: OE2	6: LA:156: LYS: NZ	2.45	0.50
69: SG:31: ARG: NH1	83: S2:1745: A: O3'	2.44	0.50
71: SI:98: LYS: HG3	71: SI:178: ARG: HG2	1.94	0.50
77: SW:4: MET: SD	83: S2:682: U: O2'	2.65	0.50
83: S2:942: G: H2'	83: S2:943: U: C6	2.47	0.50
83: S2:1731: A: H2'	83: S2:1732: G: C8	2.46	0.50
3: L5:500: G: OP1	3: L5:504: G: N2	2.45	0.50
3: L5:1459: A: OP1	21: LQ:65: ARG: NH1	2.44	0.50
3: L5:4459: U: H2'	3: L5:4460: U: C6	2.47	0.50
3: L5:4759: C: O2	19: LO:165: LYS: NZ	2.38	0.50
60: SZ:106: GLN: HG3	60: SZ:108: ILE: HD11	1.93	0.50
83: S2:149: A: H3'	83: S2:150: A: H8	1.77	0.50
83: S2:980: A: H2'	83: S2:981: A: C8	2.47	0.50
83: S2:1758: G: O6	83: S2:1772: C: N4	2.45	0.50
1: Pt:73: A: N3	14: LI:110: ARG: NH1	2.60	0.50
3: L5:1317: U: H2'	3: L5:1318: C: C6	2.46	0.50
3: L5:1320: U: O2'	3: L5:1891: A: N1	2.41	0.50
3: L5:1984: A: N6	3: L5:2010: A: O2'	2.44	0.50
3: L5:2539: C: H2'	3: L5:2540: C: C6	2.47	0.50
3: L5:4601: U: H2'	3: L5:4602: A: H8	1.77	0.50
7: LB:86: VAL: HG12	7: LB:201: LEU: HD23	1.94	0.50
55: SQ:98: LYS: O	64: Sg:57: ARG: NH1	2.37	0.50
83: S2:484: A2M: H8	83: S2:484: A2M: O5'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Pt:23:C:H2'	1:Pt:24:A:C8	2.47	0.49
3:L5:519:C:H1'	3:L5:643:C:C2	2.47	0.49
3:L5:691:C:H2'	3:L5:692:A:C8	2.47	0.49
3:L5:1364:U:OP2	16:LL:36:ARG:NH2	2.29	0.49
3:L5:1413:C:H2'	3:L5:1414:C:C6	2.46	0.49
3:L5:4153:C:H5''	28:LX:38:LYS:HD2	1.93	0.49
3:L5:4489:G:H4'	87:L5:5290:SPD:H91	1.94	0.49
83:S2:751:G:H1'	83:S2:793:G:H21	1.77	0.49
83:S2:1801:A:H2'	83:S2:1802:C:C6	2.47	0.49
3:L5:382:G:N1	3:L5:385:A:OP2	2.40	0.49
3:L5:1669:A:H4'	3:L5:1685:G:N2	2.27	0.49
3:L5:2049:G:HO2'	3:L5:3884:PSU:HO2'	1.56	0.49
3:L5:4347:G:H2'	3:L5:4348:A:C8	2.47	0.49
3:L5:4582:C:O2'	7:LB:99:LEU:O	2.26	0.49
9:LD:211:LEU:HB3	9:LD:219:TYR:HB2	1.94	0.49
16:LL:46:ILE:HB	16:LL:49:ARG:HB2	1.94	0.49
16:LL:111:GLN:O	16:LL:115:GLN:HG2	2.13	0.49
34:Ld:24:GLU:OE2	34:Ld:87:ARG:NH2	2.40	0.49
58:ST:62:ARG:NH2	83:S2:1543:U:OP2	2.40	0.49
62:Sd:54:LYS:NZ	83:S2:1482:C:OP1	2.44	0.49
63:Sf:124:ASP:OD1	63:Sf:124:ASP:N	2.44	0.49
69:SG:135:PRO:HA	83:S2:169:U:H5''	1.94	0.49
71:SI:141:ARG:NH2	83:S2:192:C:OP2	2.45	0.49
83:S2:1129:G:H3'	83:S2:1130:G:H21	1.76	0.49
3:L5:500:G:H1'	3:L5:504:G:H3'	1.93	0.49
3:L5:1824:G:H2'	3:L5:1825:A:C8	2.47	0.49
3:L5:2614:C:O2'	3:L5:2808:G:OP1	2.28	0.49
3:L5:4095:G:N7	3:L5:4096:C:N4	2.60	0.49
3:L5:4260:U:H2'	3:L5:4261:C:H6	1.77	0.49
7:LB:161:ARG:HG2	7:LB:184:GLN:HA	1.95	0.49
27:LW:7:SER:HB2	27:LW:13:ILE:HD11	1.95	0.49
48:Ls:29:ILE:HG22	48:Ls:88:PHE:CD1	2.48	0.49
49:Lt:11:LYS:HG3	49:Lt:13:VAL:HG23	1.94	0.49
50:SD:77:PHE:HB2	50:SD:79:PHE:CE1	2.48	0.49
51:SF:18:LYS:HD2	51:SF:22:LYS:HA	1.94	0.49
52:SK:27:VAL:HB	52:SK:43:LEU:HD12	1.94	0.49
55:SQ:15:ARG:HH22	83:S2:1444:U:P	2.35	0.49
58:ST:74:SER:O	58:ST:78:ILE:HD12	2.12	0.49
68:SE:124:CYS:HB3	68:SE:141:THR:HB	1.93	0.49
78:SX:90:CYS:HA	78:SX:93:PHE:HD2	1.77	0.49
2:Et:43:A:H2'	2:Et:44:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:153:G:H2'	3:L5:154:G:H8	1.77	0.49
3:L5:654:C:O3'	8:LC:268:ARG:NH1	2.44	0.49
3:L5:1084:C:H2'	3:L5:1085:C:C6	2.47	0.49
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.47	0.49
3:L5:1509:C:H5''	31:La:2:PRO:HD3	1.94	0.49
3:L5:1734:G:N2	3:L5:1735:U:O4	2.31	0.49
3:L5:2638:G:H22	3:L5:2719:C:P	2.35	0.49
3:L5:4126:C:OP1	12:LG:37:LYS:NZ	2.46	0.49
67:SC:77:SER:OG	67:SC:79:GLU:OE1	2.31	0.49
83:S2:49:C:H2'	83:S2:472:C:H41	1.78	0.49
3:L5:325:U:H2'	3:L5:326:C:C6	2.47	0.49
3:L5:374:G:OP2	40:Lj:56:ARG:NH1	2.38	0.49
3:L5:2459:G:N2	3:L5:2462:C:OP2	2.38	0.49
3:L5:3736:A:H2'	3:L5:3737:A:H8	1.78	0.49
10:LE:223:ARG:NH2	10:LE:236:GLU:O	2.46	0.49
49:Lt:114:ARG:NH2	49:Lt:162:CYS:SG	2.86	0.49
63:Sf:117:LEU:HD12	63:Sf:118:ARG:HD3	1.94	0.49
65:SA:184:ARG:HG2	65:SA:189:ILE:HB	1.94	0.49
69:SG:172:LYS:NZ	83:S2:67:C:OP2	2.40	0.49
79:SY:108:LYS:NZ	83:S2:506:G:OP1	2.42	0.49
83:S2:57:U:OP1	83:S2:504:G:O2'	2.29	0.49
83:S2:1652:G:H1	83:S2:1672:U:H3	1.58	0.49
2:Et:13:C:H2'	2:Et:14:A:H8	1.77	0.49
3:L5:158:A:H5''	3:L5:159:C:H2'	1.95	0.49
3:L5:3610:A:H2'	3:L5:3611:A:C8	2.47	0.49
3:L5:3932:U:H2'	3:L5:3933:G:C8	2.47	0.49
4:L7:119:U:C2	9:LD:261:VAL:HG11	2.47	0.49
41:Lk:24:LYS:HB2	41:Lk:35:LYS:HB2	1.95	0.49
48:Ls:134:LYS:HD2	48:Ls:137:PHE:HE2	1.78	0.49
57:SS:145:THR:OG1	83:S2:1523:C:OP1	2.27	0.49
58:ST:104:LEU:HD22	58:ST:121:ARG:HD2	1.94	0.49
58:ST:121:ARG:HH21	83:S2:1563:G:H5''	1.77	0.49
59:SU:19:ARG:HB3	59:SU:92:HIS:CE1	2.47	0.49
64:Sg:63:SER:HB2	83:S2:1398:G:H1'	1.94	0.49
70:SH:39:GLN:HG3	70:SH:75:ILE:HG21	1.95	0.49
78:SX:17:ARG:HH22	83:S2:659:G:H21	1.61	0.49
83:S2:1098:C:H2'	83:S2:1099:G:C8	2.48	0.49
83:S2:1201:U:H2'	83:S2:1202:U:C6	2.48	0.49
83:S2:1221:G:H2'	83:S2:1222:G:C8	2.48	0.49
3:L5:318:A:H2'	3:L5:319:A:C8	2.48	0.49
3:L5:1461:C:H2'	3:L5:1462:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1494:U:H2'	3:L5:1495:G:H8	1.76	0.49
3:L5:2870:A:H2'	3:L5:2871:A:C8	2.48	0.49
7:LB:393:LYS:HG3	7:LB:396:ARG:HH21	1.77	0.49
55:SQ:110:ASP:N	55:SQ:110:ASP:OD1	2.44	0.49
63:Sf:103:LEU:HB2	63:Sf:105:TYR:CE2	2.47	0.49
65:SA:22:GLY:O	65:SA:24:HIS:ND1	2.45	0.49
83:S2:1101:U:H2'	83:S2:1102:G:C8	2.48	0.49
83:S2:1568:C:H2'	83:S2:1569:A:C8	2.47	0.49
3:L5:1070:G:O2'	3:L5:1071:C:O5'	2.29	0.49
3:L5:1802:A:H5''	3:L5:1803:G:H5'	1.93	0.49
3:L5:2492:C:H2'	3:L5:2493:G:H8	1.77	0.49
9:LD:108:ARG:CZ	9:LD:253:TYR:HB2	2.43	0.49
10:LE:161:ARG:O	10:LE:182:ASN:ND2	2.46	0.49
26:LV:37:LEU:HD23	26:LV:65:VAL:HG12	1.94	0.49
78:SX:22:TRP:NE1	83:S2:359:U:OP1	2.41	0.49
2:Et:32:C:H5'	51:SF:134:VAL:HG13	1.94	0.49
3:L5:1503:A:H1'	3:L5:1504:G:C8	2.48	0.49
3:L5:4763:U:O2'	23:LS:174:THR:OG1	2.25	0.49
15:LJ:95:ARG:HD3	15:LJ:175:LEU:HB2	1.95	0.49
55:SQ:97:GLN:HB2	55:SQ:105:LYS:HG3	1.93	0.49
71:SI:10:LYS:O	71:SI:18:ARG:NH1	2.46	0.49
83:S2:107:A:H2'	83:S2:108:G:C8	2.48	0.49
83:S2:639:C:H2'	83:S2:640:A:C8	2.48	0.49
3:L5:424:U:H2'	3:L5:425:U:C6	2.47	0.49
3:L5:4966:A:H5''	7:LB:128:LYS:HG3	1.95	0.49
5:L8:19:C:H2'	5:L8:20:A:C8	2.47	0.49
9:LD:217:ASP:N	9:LD:217:ASP:OD1	2.41	0.49
10:LE:186:LEU:N	10:LE:250:GLN:OE1	2.44	0.49
12:LG:143:VAL:HG22	12:LG:203:ALA:HB2	1.95	0.49
35:Le:99:ILE:HD13	35:Le:108:ARG:HB2	1.94	0.49
83:S2:51:U:H2'	83:S2:52:G:H8	1.77	0.49
83:S2:595:U:H2'	83:S2:596:U:C6	2.48	0.49
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.48	0.48
3:L5:4638:U:OP1	3:L5:5044:A:O2'	2.30	0.48
57:SS:46:ARG:NH1	58:ST:50:GLU:OE2	2.45	0.48
58:ST:44:GLU:HG3	58:ST:45:LEU:HD12	1.95	0.48
68:SE:212:ASP:OD1	68:SE:216:ASN:N	2.46	0.48
69:SG:191:ARG:HH12	83:S2:312:G:H2'	1.77	0.48
70:SH:30:LEU:HG	70:SH:33:ASN:HD22	1.78	0.48
71:SI:98:LYS:HB3	83:S2:377:G:H5'	1.94	0.48
72:SJ:40:LYS:NZ	83:S2:641:A:OP1	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:118:C:H1'	83:S2:445:A:C5	2.48	0.48
83:S2:414:A:H2'	83:S2:415:A:H8	1.78	0.48
83:S2:553:U:O4	83:S2:554:A:N6	2.43	0.48
83:S2:866:PSU:H2'	83:S2:867:OMG:C8	2.48	0.48
3:L5:387:G:O2'	3:L5:412:G:N1	2.36	0.48
3:L5:4095:G:H2'	3:L5:4096:C:C6	2.48	0.48
7:LB:220:ILE:HB	7:LB:346:THR:HB	1.96	0.48
21:LQ:151:HIS:ND1	21:LQ:164:LYS:O	2.44	0.48
34:Ld:22:THR:HG23	34:Ld:122:VAL:HG13	1.94	0.48
50:SD:51:LEU:HD12	50:SD:91:VAL:HG12	1.94	0.48
50:SD:160:SER:OG	83:S2:1386:A:OP2	2.27	0.48
82:Se:41:ARG:HG3	82:Se:42:PHE:CD1	2.48	0.48
83:S2:1240:A:N3	83:S2:1267:C:O2'	2.37	0.48
83:S2:1393:G:H2'	83:S2:1394:G:C8	2.47	0.48
3:L5:495:C:H2'	3:L5:496:G:C8	2.49	0.48
3:L5:1270:A:H8	3:L5:2106:G:H21	1.60	0.48
3:L5:1558:A:H2'	3:L5:1559:G:H8	1.79	0.48
3:L5:1837:A:OP2	24:LT:130:ARG:NH1	2.43	0.48
3:L5:2407:G:H2'	42:Ll:13:LEU:HD22	1.96	0.48
3:L5:2743:A:H2'	3:L5:2744:A:C8	2.48	0.48
3:L5:2803:U:H2'	3:L5:2804:OMC:H6	1.79	0.48
3:L5:3689:G:O2'	3:L5:3818:UY1:OP2	2.28	0.48
11:LF:171:ASP:OD1	11:LF:172:ASN:N	2.46	0.48
63:Sf:108:VAL:HG12	63:Sf:114:ILE:HA	1.95	0.48
68:SE:100:ARG:NH2	68:SE:118:GLU:OE2	2.46	0.48
70:SH:53:VAL:HG12	70:SH:175:GLY:HA3	1.95	0.48
83:S2:525:A:H2'	83:S2:526:A:H8	1.79	0.48
83:S2:1779:G:H2'	83:S2:1780:G:C8	2.48	0.48
3:L5:2638:G:N1	3:L5:2718:U:H2'	2.28	0.48
3:L5:3777:G:O2'	3:L5:3815:G:O6	2.27	0.48
5:L8:39:G:O2'	5:L8:104:A:N1	2.43	0.48
7:LB:85:VAL:HG22	7:LB:204:GLN:HG2	1.95	0.48
12:LG:57:TRP:O	12:LG:62:ARG:NH1	2.46	0.48
49:Lt:22:VAL:HA	49:Lt:48:LYS:HG2	1.95	0.48
53:SM:82:ASN:OD1	53:SM:83:LYS:N	2.46	0.48
57:SS:121:ARG:HG3	57:SS:131:VAL:HB	1.94	0.48
58:ST:60:THR:HG22	58:ST:75:MET:HE2	1.95	0.48
72:SJ:60:LEU:HD22	72:SJ:70:ARG:HA	1.96	0.48
72:SJ:142:VAL:HG12	72:SJ:144:ILE:H	1.77	0.48
72:SJ:162:ARG:NH1	83:S2:582:U:OP1	2.46	0.48
83:S2:1457:U:H2'	83:S2:1458:G:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:498:C:C4	3:L5:499:G:H1'	2.48	0.48
3:L5:1398:A:N1	3:L5:1419:G:O2'	2.44	0.48
3:L5:1993:C:H2'	3:L5:1994:C:C6	2.49	0.48
3:L5:2626:U:O4	25:LU:97:ARG:NH1	2.47	0.48
3:L5:3867:A2M:H8	3:L5:3867:A2M:H5''	1.94	0.48
3:L5:4636:PSU:N1	34:Ld:79:ASN:OD1	2.46	0.48
13:LH:4:ILE:HG12	13:LH:61:TRP:CH2	2.49	0.48
18:LN:46:ASP:OD1	18:LN:47:LYS:N	2.45	0.48
32:Lb:65:MET:HG3	32:Lb:68:ARG:HH12	1.78	0.48
34:Ld:54:MET:HE3	34:Ld:60:PRO:HA	1.95	0.48
34:Ld:57:MET:HG2	34:Ld:88:LEU:HD23	1.95	0.48
57:SS:137:LYS:NZ	83:S2:1236:G:O6	2.47	0.48
62:Sd:16:GLN:NE2	62:Sd:27:ARG:O	2.45	0.48
65:SA:42:LYS:HD2	65:SA:48:ILE:HD11	1.94	0.48
66:SB:123:ALA:HB2	66:SB:165:ARG:HG2	1.94	0.48
67:SC:259:THR:HG21	76:SV:16:LYS:H	1.78	0.48
68:SE:104:ASP:HB3	68:SE:110:ALA:HB2	1.96	0.48
72:SJ:145:PRO:HD2	83:S2:522:A:H5''	1.95	0.48
79:SY:119:GLY:O	83:S2:84:A:O2'	2.26	0.48
2:Et:55:U:H2'	2:Et:57:A:N7	2.29	0.48
3:L5:684:G:H5''	10:LE:100:LYS:HE3	1.94	0.48
3:L5:2041:A:N7	3:L5:4434:C:O2'	2.45	0.48
3:L5:3717:A:OP2	3:L5:3735:G:N2	2.38	0.48
3:L5:4063:U:H2'	3:L5:4064:C:C6	2.49	0.48
3:L5:4591:U:H2'	3:L5:4592:C:C6	2.48	0.48
3:L5:4743:G:H2'	3:L5:4744:A:C8	2.49	0.48
7:LB:29:VAL:HA	7:LB:220:ILE:HD13	1.96	0.48
8:LC:218:ILE:HA	8:LC:229:LEU:HD22	1.95	0.48
12:LG:150:LYS:NZ	12:LG:177:MET:O	2.43	0.48
13:LH:107:GLU:N	13:LH:107:GLU:OE1	2.47	0.48
29:LY:23:SER:HA	29:LY:26:ARG:HB2	1.95	0.48
60:SZ:42:ASP:OD1	60:SZ:42:ASP:N	2.43	0.48
1:Pt:51:C:H2'	1:Pt:52:G:H8	1.78	0.48
3:L5:369:G:N2	3:L5:372:A:OP2	2.40	0.48
3:L5:441:G:H2'	3:L5:442:G:H8	1.79	0.48
3:L5:711:A:H2'	3:L5:712:C:C6	2.48	0.48
3:L5:1084:C:H2'	3:L5:1085:C:H6	1.77	0.48
3:L5:1326:A2M:HM'3	3:L5:1326:A2M:H1'	1.69	0.48
3:L5:1695:U:O2'	3:L5:1719:A:N3	2.41	0.48
3:L5:4281:A:H2'	3:L5:4282:A:H2'	1.95	0.48
3:L5:4680:G:H2'	3:L5:4681:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LM:71:LYS:O	17:LM:75:GLN:HG3	2.13	0.48
27:LW:97:LYS:O	27:LW:99:GLU:N	2.45	0.48
58:ST:126:GLN:HB2	58:ST:129:ARG:HH21	1.79	0.48
67:SC:110:MET:HG2	67:SC:125:LYS:HB3	1.95	0.48
73:SL:35:ARG:NH2	73:SL:55:TYR:O	2.47	0.48
83:S2:102:A:H4'	83:S2:104:A:C8	2.49	0.48
3:L5:907:C:H2'	3:L5:908:G:H8	1.79	0.48
3:L5:1175:A:H2	3:L5:1185:G:H1	1.62	0.48
3:L5:1340:OMC:HM23	3:L5:1340:OMC:H1'	1.72	0.48
3:L5:2580:U:O2'	30:LZ:79:HIS:ND1	2.43	0.48
3:L5:4069:U:H2'	3:L5:4070:U:C6	2.48	0.48
14:LI:73:ASN:HB2	14:LI:87:MET:HE1	1.96	0.48
45:Lo:4:VAL:HG23	45:Lo:93:LEU:HD23	1.95	0.48
55:SQ:90:LYS:HA	55:SQ:93:VAL:HG22	1.95	0.48
59:SU:22:ILE:HG23	59:SU:114:VAL:HG22	1.94	0.48
63:Sf:85:TYR:OH	83:S2:1509:U:OP1	2.17	0.48
83:S2:1588:A:H2'	83:S2:1589:A:C8	2.48	0.48
2:Et:22:G:H2'	2:Et:23:A:C8	2.49	0.48
3:L5:4238:G:H2'	3:L5:4239:A:C8	2.48	0.48
3:L5:4476:C:O2'	3:L5:4478:G:OP2	2.27	0.48
22:LR:39:GLN:OE1	22:LR:42:ARG:NH1	2.46	0.48
35:Le:108:ARG:HD2	35:Le:128:ARG:HB2	1.95	0.48
51:SF:168:THR:OG1	60:SZ:106:GLN:OE1	2.24	0.48
56:SR:29:HIS:HA	56:SR:32:LYS:HG2	1.96	0.48
66:SB:23:ASP:N	66:SB:23:ASP:OD1	2.47	0.48
69:SG:227:GLN:HB3	69:SG:231:ARG:HH21	1.79	0.48
83:S2:325:C:N3	83:S2:326:C:O2'	2.46	0.48
3:L5:2295:C:O2'	8:LC:45:ARG:NH2	2.47	0.48
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.49	0.48
3:L5:3910:C:H2'	3:L5:3911:C:H6	1.79	0.48
5:L8:39:G:H1'	5:L8:103:A:N6	2.29	0.48
55:SQ:110:ASP:OD1	55:SQ:111:ILE:HD12	2.14	0.48
57:SS:63:GLU:O	57:SS:67:VAL:HG23	2.14	0.48
3:L5:408:A:O2'	3:L5:411:G:OP2	2.25	0.47
3:L5:1086:C:H2'	3:L5:1087:A:H8	1.78	0.47
3:L5:1733:G:N3	3:L5:4214:A:H2'	2.28	0.47
3:L5:3825:A2M:H2'	3:L5:3826:C:O4'	2.14	0.47
15:LJ:17:ILE:HD12	15:LJ:80:GLU:HG2	1.95	0.47
22:LR:157:ASP:OD1	22:LR:158:GLN:N	2.47	0.47
23:LS:27:LEU:HB3	24:LT:148:PRO:HB3	1.96	0.47
69:SG:190:ARG:NH2	83:S2:334:C:OP2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:198:U:H2'	83:S2:199:C:H2'	1.95	0.47
3:L5:85:G:O2'	3:L5:97:G:O6	2.23	0.47
3:L5:2764:A:H2'	3:L5:2765:A:C8	2.49	0.47
3:L5:3664:G:H2'	3:L5:3665:G:C8	2.47	0.47
3:L5:3718:A2M:H2'	3:L5:3719:A:O4'	2.14	0.47
23:LS:15:ARG:HD2	23:LS:25:PRO:HG2	1.96	0.47
26:LV:43:LYS:HE2	26:LV:62:MET:HE3	1.96	0.47
38:Lh:89:ARG:O	38:Lh:93:ARG:HG2	2.15	0.47
51:SF:49:LEU:HD12	51:SF:50:PRO:HD2	1.95	0.47
54:SP:79:HIS:HD2	83:S2:1298:G:C4	2.32	0.47
60:SZ:86:ALA:HA	60:SZ:89:GLN:HE21	1.79	0.47
66:SB:168:MET:HB2	66:SB:197:ILE:HD13	1.96	0.47
78:SX:28:LYS:O	78:SX:32:LEU:HB2	2.13	0.47
83:S2:683:OMG:N1	83:S2:1022:U:OP2	2.38	0.47
83:S2:1004:PSU:H2'	83:S2:1005:G:H8	1.78	0.47
83:S2:1348:G:OP2	83:S2:1348:G:N2	2.43	0.47
3:L5:965:G:N2	3:L5:2092:G:H1'	2.29	0.47
3:L5:1175:A:H2	3:L5:1185:G:H22	1.62	0.47
3:L5:1382:G:OP1	16:LL:66:TYR:OH	2.30	0.47
3:L5:1538:U:H2'	3:L5:1539:G:H8	1.79	0.47
3:L5:1749:A:H2'	3:L5:1750:G:C8	2.49	0.47
3:L5:2808:G:O3'	22:LR:60:ARG:NH1	2.47	0.47
3:L5:4345:C:H2'	3:L5:4346:U:C6	2.49	0.47
16:LL:91:ALA:HB1	16:LL:96:ILE:HB	1.97	0.47
36:Lf:25:THR:HB	36:Lf:87:LYS:HD3	1.96	0.47
57:SS:36:VAL:HG21	57:SS:71:MET:HE3	1.95	0.47
68:SE:153:LEU:O	68:SE:174:LYS:NZ	2.45	0.47
81:Sb:42:LYS:HE3	81:Sb:57:VAL:HG22	1.95	0.47
83:S2:145:G:H2'	83:S2:146:G:C8	2.49	0.47
83:S2:588:G:H4'	83:S2:589:G:H5'	1.96	0.47
83:S2:1130:G:OP2	83:S2:1130:G:N2	2.39	0.47
83:S2:1550:G:O2'	83:S2:1558:C:O2	2.24	0.47
3:L5:1097:C:H2'	3:L5:1098:G:C8	2.50	0.47
3:L5:1818:G:O2'	3:L5:1820:C:OP2	2.27	0.47
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.48	0.47
3:L5:2537:A:OP1	41:Lk:42:LEU:N	2.46	0.47
3:L5:4457:PSU:H1'	7:LB:252:ALA:HB3	1.96	0.47
19:LO:119:VAL:N	23:LS:168:THR:O	2.46	0.47
33:Lc:38:ILE:HD11	33:Lc:46:VAL:HG21	1.95	0.47
64:Sg:239:LEU:HD11	64:Sg:248:LEU:HD21	1.96	0.47
83:S2:962:A:N1	83:S2:1055:A:O2'	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:993:G:OP1	83:S2:1131:G:N2	2.39	0.47
3:L5:3861:A:H2'	3:L5:3862:A:H8	1.78	0.47
3:L5:3917:A:H2'	3:L5:3918:G:H8	1.79	0.47
27:LW:102:LYS:HA	27:LW:105:ARG:HG2	1.96	0.47
30:LZ:41:ALA:HB2	30:LZ:77:TYR:HE1	1.78	0.47
51:SF:39:ILE:HG23	51:SF:68:ILE:HD13	1.96	0.47
54:SP:134:GLY:H	83:S2:1236:G:H4'	1.80	0.47
70:SH:100:ILE:HG21	70:SH:122:LEU:HD12	1.97	0.47
83:S2:136:C:H5''	83:S2:137:U:H5''	1.97	0.47
83:S2:750:C:O2	83:S2:752:G:C2	2.68	0.47
83:S2:1405:A:H2'	83:S2:1406:G:O4'	2.14	0.47
1:Pt:29:C:H2'	1:Pt:30:G:H8	1.80	0.47
3:L5:7:C:H2'	3:L5:8:U:C6	2.50	0.47
3:L5:64:A:H1'	3:L5:76:A:H1'	1.94	0.47
3:L5:423:G:H21	20:LP:118:GLN:NE2	2.11	0.47
3:L5:3641:U:H5	3:L5:3646:A:N7	2.12	0.47
3:L5:3870:C:H2'	3:L5:3871:A:H8	1.79	0.47
3:L5:4584:A:H2'	3:L5:4585:U:O4'	2.15	0.47
3:L5:4935:C:H2'	3:L5:4936:G:C8	2.50	0.47
6:LA:225:ILE:HG12	6:LA:234:LYS:HA	1.97	0.47
9:LD:66:TYR:HE2	9:LD:68:ARG:HE	1.62	0.47
68:SE:152:PRO:HG2	69:SG:216:ARG:HG3	1.95	0.47
73:SL:133:PRO:O	83:S2:383:G:O2'	2.31	0.47
83:S2:17:C:O2'	83:S2:1194:A:N1	2.43	0.47
83:S2:419:G:N2	83:S2:661:U:O2	2.48	0.47
2:Et:22:G:H2'	2:Et:23:A:H8	1.79	0.47
3:L5:71:C:H1'	16:LL:62:PRO:O	2.15	0.47
3:L5:190:G:H2'	3:L5:191:G:H8	1.80	0.47
3:L5:293:G:OP1	86:L5:5264:SPM:N1	2.36	0.47
3:L5:308:G:O6	18:LN:12:ARG:NH1	2.46	0.47
3:L5:425:U:H4'	20:LP:6:LEU:HD21	1.95	0.47
3:L5:1351:G:O6	21:LQ:55:ARG:NH1	2.46	0.47
3:L5:1414:C:H2'	3:L5:1415:G:C8	2.46	0.47
3:L5:1545:G:H2'	3:L5:1546:C:C6	2.50	0.47
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.30	0.47
3:L5:1670:G:OP1	32:Lb:12:GLN:NE2	2.36	0.47
3:L5:2411:C:H2'	3:L5:2412:A:H8	1.78	0.47
3:L5:3607:U:H2'	3:L5:3608:A:C8	2.50	0.47
3:L5:3708:C:H2'	3:L5:3709:U:C6	2.50	0.47
3:L5:3856:A:H5''	20:LP:83:TRP:O	2.15	0.47
3:L5:3916:G:H2'	3:L5:3917:A:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4642:U:H2'	3:L5:4643:G:H8	1.79	0.47
3:L5:4717:A:OP2	7:LB:30:LYS:NZ	2.32	0.47
3:L5:4883:C:N4	10:LE:181:LEU:O	2.38	0.47
3:L5:4954:G:H2'	3:L5:4955:A:H8	1.79	0.47
5:L8:30:U:H2'	5:L8:31:G:C8	2.49	0.47
7:LB:27:GLY:HA2	7:LB:276:HIS:CD2	2.50	0.47
7:LB:77:THR:OG1	7:LB:335:GLY:O	2.30	0.47
7:LB:113:GLU:OE2	7:LB:169:ARG:NH1	2.47	0.47
8:LC:141:GLY:O	8:LC:204:ARG:NH1	2.30	0.47
9:LD:179:ARG:HD3	9:LD:179:ARG:HA	1.76	0.47
10:LE:223:ARG:HA	10:LE:224:LYS:HA	1.71	0.47
11:LF:127:LYS:HB2	24:LT:133:ALA:HB3	1.97	0.47
14:LI:36:LEU:HD11	14:LI:69:ARG:HD2	1.97	0.47
16:LL:142:GLU:HA	16:LL:146:LEU:HD12	1.97	0.47
17:LM:24:LEU:HB2	17:LM:43:THR:HG21	1.97	0.47
33:Lc:38:ILE:HG21	33:Lc:63:TYR:HB3	1.95	0.47
57:SS:60:THR:OG1	57:SS:62:ASP:OD1	2.25	0.47
57:SS:88:LYS:H	57:SS:95:TYR:HD1	1.62	0.47
58:ST:101:ARG:NH1	83:S2:1566:G:O6	2.37	0.47
67:SC:104:ASP:OD1	67:SC:105:GLU:N	2.47	0.47
69:SG:66:GLY:HA2	83:S2:1745:A:H1'	1.97	0.47
69:SG:191:ARG:HH22	83:S2:312:G:H2'	1.80	0.47
75:SO:33:ILE:HB	75:SO:97:LEU:HD23	1.95	0.47
75:SO:34:PHE:HB3	75:SO:41:PHE:HB2	1.96	0.47
79:SY:51:THR:OG1	79:SY:53:ASP:OD1	2.25	0.47
83:S2:15:U:H2'	83:S2:16:G:O4'	2.13	0.47
83:S2:941:C:H2'	83:S2:942:G:C8	2.49	0.47
83:S2:1272:OMC:H1'	83:S2:1272:OMC:HM23	1.69	0.47
2:Et:23:A:H2'	2:Et:24:G:H8	1.80	0.47
3:L5:1195:G:H2'	3:L5:1196:G:C8	2.50	0.47
3:L5:1326:A2M:H2'	3:L5:1327:C:H6	1.79	0.47
3:L5:1942:A:H2'	3:L5:1943:A:H8	1.80	0.47
3:L5:2279:A:O2'	35:Le:48:ARG:NH2	2.48	0.47
3:L5:3633:C:H2'	3:L5:3634:G:C8	2.49	0.47
3:L5:4327:C:OP1	24:LT:70:HIS:NE2	2.48	0.47
11:LF:241:ASN:O	11:LF:245:ARG:HG2	2.14	0.47
24:LT:102:ARG:O	24:LT:106:LEU:HG	2.14	0.47
49:Lt:50:THR:OG1	49:Lt:72:GLU:OE1	2.23	0.47
53:SM:23:LYS:O	53:SM:27:ILE:HG12	2.15	0.47
58:ST:39:LEU:HD21	58:ST:52:TRP:CZ3	2.50	0.47
67:SC:169:TYR:OH	67:SC:175:GLY:O	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Sb:23:ARG:NH1	81:Sb:27:SER:O	2.48	0.47
83:S2:1610:G:H2'	83:S2:1611:G:H8	1.80	0.47
83:S2:1616:U:O2'	83:S2:1661:A:N3	2.38	0.47
2:Et:43:A:H2'	2:Et:44:G:H8	1.80	0.47
3:L5:716:C:OP1	8:LC:317:ASN:HB2	2.15	0.47
3:L5:2691:U:O2'	41:Lk:4:LYS:NZ	2.46	0.47
3:L5:4523:A2M:HM'3	3:L5:4523:A2M:H1'	1.76	0.47
7:LB:322:HIS:O	7:LB:342:LYS:NZ	2.39	0.47
17:LM:96:GLU:O	17:LM:100:ARG:HG2	2.15	0.47
22:LR:7:GLN:NE2	22:LR:35:ALA:O	2.33	0.47
52:SK:31:LYS:HZ3	52:SK:40:VAL:H	1.61	0.47
57:SS:15:VAL:HG12	57:SS:16:LEU:HG	1.97	0.47
58:ST:6:VAL:HG12	58:ST:135:ALA:HB2	1.96	0.47
63:Sf:138:ARG:NH2	83:S2:1292:C:N3	2.50	0.47
83:S2:106:C:H2'	83:S2:107:A:C8	2.48	0.47
83:S2:382:C:H2'	83:S2:383:G:C8	2.50	0.47
83:S2:634:A:H2'	83:S2:635:G:H8	1.80	0.47
83:S2:1692:U:H2'	83:S2:1693:G:C8	2.49	0.47
83:S2:1731:A:H2'	83:S2:1732:G:H8	1.80	0.47
3:L5:92:C:OP1	87:L5:5261:SPD:N10	2.38	0.47
3:L5:455:C:O2'	3:L5:456:C:H5'	2.15	0.47
3:L5:1684:A:OP1	31:La:47:LYS:NZ	2.45	0.47
3:L5:2389:A:H4'	34:Ld:70:LYS:HG3	1.97	0.47
3:L5:2550:G:O2'	3:L5:2587:A:N1	2.48	0.47
3:L5:4196:OMG:HM23	3:L5:4196:OMG:H1'	1.67	0.47
3:L5:4481:U:H2'	3:L5:4482:U:H6	1.79	0.47
13:LH:93:ARG:NE	13:LH:142:ASP:O	2.46	0.47
13:LH:115:ARG:HD3	13:LH:123:ILE:HD12	1.96	0.47
18:LN:140:LYS:HD3	18:LN:140:LYS:HA	1.69	0.47
29:LY:22:PRO:HD2	29:LY:25:ILE:HD11	1.97	0.47
48:Ls:91:THR:HG21	48:Ls:98:ILE:HG13	1.96	0.47
66:SB:98:THR:O	66:SB:232:HIS:NE2	2.47	0.47
68:SE:26:VAL:HG22	72:SJ:4:ALA:HB2	1.97	0.47
71:SI:126:GLY:O	71:SI:128:LYS:NZ	2.46	0.47
74:SN:37:ILE:HG23	74:SN:50:ILE:HG21	1.96	0.47
78:SX:88:ASP:HA	83:S2:617:G:H4'	1.97	0.47
79:SY:119:GLY:HA2	83:S2:85:A:H5'	1.96	0.47
83:S2:455:A:H2'	83:S2:456:C:C6	2.50	0.47
2:Et:8:U:N3	2:Et:15:G:O6	2.48	0.46
3:L5:1504:G:H2'	3:L5:1505:C:C6	2.50	0.46
3:L5:2347:A:C4	35:Le:31:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4272:G:OP2	3:L5:4272:G:N2	2.29	0.46
4:L7:49:A:H5''	9:LD:224:SER:HB2	1.96	0.46
5:L8:5:U:H2'	5:L8:6:C:H6	1.80	0.46
5:L8:58:G:N7	40:Lj:63:ARG:NH2	2.48	0.46
6:LA:48:ILE:HG22	46:Lp:54:ILE:HG12	1.97	0.46
18:LN:184:ILE:O	18:LN:194:ARG:NH1	2.30	0.46
39:Li:35:LYS:HE3	39:Li:35:LYS:HB3	1.79	0.46
71:SI:139:LYS:HE2	71:SI:139:LYS:HB2	1.71	0.46
80:Sa:13:LYS:HD3	80:Sa:13:LYS:HA	1.71	0.46
82:Se:32:ALA:HB2	83:S2:525:A:H5''	1.97	0.46
83:S2:24:C:O2'	83:S2:25:A:H8	1.97	0.46
83:S2:1221:G:H2'	83:S2:1222:G:H8	1.81	0.46
3:L5:407:A:O2'	3:L5:410:A:OP1	2.30	0.46
3:L5:2739:C:O2	6:LA:188:LYS:NZ	2.46	0.46
3:L5:3654:G:O2'	3:L5:3693:U:OP1	2.25	0.46
3:L5:3785:A2M:H2	3:L5:4551:U:O2	2.16	0.46
3:L5:4676:G:OP1	7:LB:281:ASN:ND2	2.43	0.46
5:L8:8:U:H2'	5:L8:9:A:C8	2.51	0.46
15:LJ:56:THR:OG1	15:LJ:64:ARG:N	2.45	0.46
25:LU:98:ASP:OD2	84:CI:59:GLN:HG2	2.15	0.46
66:SB:126:ASP:OD2	66:SB:136:ARG:NH2	2.47	0.46
74:SN:15:ALA:HB2	81:Sb:20:LYS:HD3	1.97	0.46
74:SN:20:ARG:HH21	77:SW:56:HIS:HB3	1.80	0.46
76:SV:17:CYS:HB2	76:SV:56:CYS:HB3	1.97	0.46
77:SW:76:SER:HB2	83:S2:1158:G:H5''	1.96	0.46
82:Se:8:ARG:HG2	82:Se:11:LYS:HD3	1.97	0.46
3:L5:1178:G:H2'	9:LD:286:SER:HB3	1.96	0.46
3:L5:1281:G:N1	10:LE:128:HIS:HB2	2.31	0.46
3:L5:2910:G:N2	3:L5:3585:G:O2'	2.49	0.46
3:L5:4364:G:H2'	3:L5:4365:C:H6	1.80	0.46
6:LA:180:LEU:HD21	46:Lp:22:LEU:HB3	1.96	0.46
9:LD:181:PRO:HD2	9:LD:195:HIS:CD2	2.50	0.46
13:LH:24:THR:HA	13:LH:37:ASP:HA	1.96	0.46
17:LM:38:VAL:HG21	17:LM:50:MET:HB3	1.97	0.46
18:LN:116:LEU:HD22	18:LN:135:ILE:HD11	1.97	0.46
52:SK:64:TRP:HB3	62:Sd:23:VAL:HA	1.98	0.46
66:SB:71:LEU:HD22	66:SB:82:ARG:HD2	1.97	0.46
69:SG:3:LEU:HD22	69:SG:111:LEU:HD11	1.98	0.46
69:SG:67:VAL:HG12	69:SG:69:THR:HG22	1.98	0.46
70:SH:20:GLU:HG2	70:SH:48:ALA:HB3	1.96	0.46
83:S2:659:G:O2'	83:S2:662:G:O2'	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1438:A:H2'	83:S2:1439:A:C8	2.50	0.46
3:L5:4739:C:H2'	3:L5:4740:G:H5'	1.97	0.46
11:LF:222:LYS:N	11:LF:232:ASP:OD1	2.46	0.46
23:LS:69:GLU:HG3	23:LS:71:SER:H	1.80	0.46
38:Lh:107:GLN:O	38:Lh:111:GLU:HG3	2.16	0.46
49:Lt:119:ARG:NH2	49:Lt:123:ARG:HH12	2.13	0.46
79:SY:105:LYS:O	79:SY:109:GLU:HG2	2.16	0.46
3:L5:161:G:H2'	3:L5:162:A:H8	1.81	0.46
3:L5:280:G:H5''	18:LN:14:LYS:HE2	1.96	0.46
3:L5:418:A:C2	5:L8:17:A:H1'	2.51	0.46
3:L5:462:G:H2'	3:L5:463:A:C8	2.50	0.46
3:L5:2249:C:H2'	3:L5:2250:C:H5	1.80	0.46
3:L5:2777:G:H5''	3:L5:2778:G:H5'	1.97	0.46
3:L5:4184:G:H5'	6:LA:233:ARG:HB2	1.97	0.46
3:L5:4340:U:O2	87:L5:5261:SPD:N10	2.48	0.46
3:L5:4563:U:H2'	3:L5:4564:A:H8	1.81	0.46
3:L5:4571:A2M:H2'	3:L5:4572:U:H6	1.79	0.46
3:L5:4882:U:OP1	17:LM:117:LYS:NZ	2.48	0.46
9:LD:234:ASP:OD1	9:LD:235:MET:N	2.49	0.46
57:SS:13:LEU:HD22	57:SS:20:ILE:HD11	1.97	0.46
58:ST:114:GLU:OE1	58:ST:114:GLU:N	2.47	0.46
64:Sg:166:VAL:HG12	64:Sg:176:VAL:HG12	1.97	0.46
64:Sg:175:LYS:HB3	64:Sg:184:LEU:HD11	1.97	0.46
65:SA:145:ILE:HG23	65:SA:159:ILE:HB	1.97	0.46
67:SC:166:ARG:HB3	67:SC:247:THR:HB	1.98	0.46
67:SC:167:ARG:HB3	67:SC:177:PRO:HB2	1.97	0.46
83:S2:27:A2M:H2'	83:S2:28:U:O4'	2.16	0.46
83:S2:35:C:H5''	83:S2:579:C:H5''	1.97	0.46
83:S2:482:G:N1	83:S2:485:A:OP2	2.47	0.46
3:L5:268:G:H2'	3:L5:269:G:C8	2.48	0.46
3:L5:1253:G:H2'	3:L5:1256:G:H5'	1.97	0.46
3:L5:1392:A:H2'	3:L5:1393:G:C8	2.50	0.46
3:L5:1751:A:H2'	3:L5:1752:G:C8	2.51	0.46
3:L5:2491:C:O2'	3:L5:2492:C:O4'	2.28	0.46
3:L5:2656:U:H5''	30:LZ:38:TYR:HB3	1.97	0.46
3:L5:2671:C:H2'	3:L5:2672:C:C6	2.51	0.46
3:L5:2856:C:O2	7:LB:242:ARG:NH2	2.39	0.46
3:L5:3610:A:H2'	3:L5:3611:A:H8	1.80	0.46
3:L5:4322:G:N2	3:L5:4325:A:OP2	2.41	0.46
3:L5:4504:C:H2'	3:L5:4505:C:C6	2.51	0.46
14:LI:152:LEU:HB3	14:LI:165:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LO:47:PHE:HA	19:LO:136:ALA:HB2	1.97	0.46
22:LR:175:GLU:O	22:LR:178:GLN:HG3	2.16	0.46
46:Lp:75:SER:O	46:Lp:79:VAL:HG23	2.16	0.46
48:Ls:159:GLN:NE2	48:Ls:162:LYS:HG3	2.31	0.46
59:SU:56:MET:HB2	59:SU:86:LYS:HG3	1.97	0.46
63:Sf:110:GLU:HG2	63:Sf:113:LYS:HD3	1.97	0.46
67:SC:202:THR:HG23	72:SJ:54:ARG:HH22	1.81	0.46
70:SH:31:GLU:HA	70:SH:37:LYS:HG3	1.97	0.46
70:SH:126:HIS:CE1	70:SH:181:THR:HG23	2.50	0.46
80:Sa:36:ILE:HD11	80:Sa:75:VAL:HG12	1.97	0.46
83:S2:327:G:H5''	83:S2:328:U:C2	2.50	0.46
83:S2:750:C:H42	83:S2:793:G:H1'	1.80	0.46
83:S2:1004:PSU:H2'	83:S2:1005:G:C8	2.51	0.46
3:L5:10:A:H2'	3:L5:11:G:C8	2.51	0.46
3:L5:1787:A:O5'	86:L5:5259:SPM:N14	2.47	0.46
3:L5:2634:C:H2'	3:L5:2635:U:H6	1.81	0.46
5:L8:8:U:H2'	5:L8:9:A:H8	1.80	0.46
7:LB:36:ASP:N	7:LB:36:ASP:OD1	2.49	0.46
13:LH:114:ILE:HB	13:LH:124:ARG:HB2	1.98	0.46
55:SQ:42:ILE:HG23	55:SQ:44:PRO:HD2	1.98	0.46
68:SE:80:ILE:HG23	68:SE:81:THR:HG23	1.96	0.46
68:SE:242:LYS:HD3	68:SE:242:LYS:HA	1.75	0.46
69:SG:224:ARG:HH21	69:SG:227:GLN:HG3	1.81	0.46
83:S2:454:U:H2'	83:S2:455:A:H8	1.80	0.46
83:S2:649:PSU:H2'	83:S2:650:A:H8	1.81	0.46
83:S2:1428:G:N1	83:S2:1585:U:O4'	2.49	0.46
3:L5:2845:A:H61	3:L5:3843:C:H42	1.63	0.46
3:L5:4291:G:H5'	3:L5:4293:PSU:C6	2.51	0.46
3:L5:4524:G:OP1	3:L5:4559:A:N6	2.37	0.46
10:LE:264:ILE:HD11	10:LE:267:LEU:HD22	1.97	0.46
29:LY:2:LYS:HD2	29:LY:7:VAL:HG23	1.96	0.46
36:Lf:45:LYS:HA	36:Lf:107:PRO:HD2	1.96	0.46
67:SC:271:ASP:O	67:SC:275:LYS:HG3	2.16	0.46
68:SE:79:ASP:HB3	68:SE:82:TYR:HB2	1.98	0.46
83:S2:1617:G:N1	83:S2:1620:A:OP2	2.48	0.46
83:S2:1670:C:H2'	83:S2:1671:G:C8	2.50	0.46
3:L5:1461:C:H2'	3:L5:1462:A:H8	1.80	0.46
3:L5:1478:C:H2'	3:L5:1479:G:H8	1.81	0.46
3:L5:2611:A:H2'	3:L5:2612:G:C8	2.51	0.46
20:LP:107:LEU:HD13	20:LP:152:GLU:HG3	1.97	0.46
34:Ld:53:ALA:HA	34:Ld:88:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ls:110:ALA:HA	48:Ls:182:PRO:HG2	1.97	0.46
52:SK:14:LEU:HD22	52:SK:35:LEU:HD23	1.97	0.46
53:SM:14:VAL:HG21	53:SM:126:GLU:HG3	1.98	0.46
55:SQ:125:ARG:HB2	83:S2:1648:G:H5''	1.97	0.46
61:Sc:14:VAL:HG13	61:Sc:30:VAL:HB	1.98	0.46
65:SA:184:ARG:NE	65:SA:191:ARG:HD3	2.31	0.46
76:SV:16:LYS:HG2	76:SV:23:ILE:HD13	1.97	0.46
83:S2:1139:C:H2'	83:S2:1140:G:O4'	2.16	0.46
3:L5:1244:G:H2'	3:L5:1245:C:H6	1.81	0.46
3:L5:1683:PSU:H2'	3:L5:1684:A:C8	2.51	0.46
3:L5:2622:G:O6	25:LU:81:ARG:NH2	2.49	0.46
3:L5:4070:U:H2'	3:L5:4071:U:C6	2.51	0.46
13:LH:41:ILE:HG22	13:LH:43:VAL:HG13	1.97	0.46
24:LT:48:VAL:HG21	24:LT:94:GLU:HG2	1.96	0.46
56:SR:108:LEU:HD12	65:SA:39:TYR:HE1	1.81	0.46
68:SE:192:ILE:HG12	68:SE:243:GLY:HA3	1.98	0.46
82:Se:41:ARG:NH2	83:S2:639:C:OP1	2.49	0.46
83:S2:1279:C:H2'	83:S2:1280:G:H8	1.81	0.46
3:L5:1411:C:H2'	3:L5:1412:G:C8	2.51	0.45
3:L5:1878:G:H2'	3:L5:1879:C:C6	2.52	0.45
3:L5:2072:C:OP1	21:LQ:2:GLY:N	2.49	0.45
3:L5:2831:G:H2'	3:L5:2832:A:H8	1.80	0.45
3:L5:3841:OMC:HM23	3:L5:3841:OMC:H1'	1.74	0.45
3:L5:4246:G:H2'	3:L5:4247:G:C8	2.51	0.45
3:L5:4611:A:H2'	3:L5:4612:C:H6	1.82	0.45
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.98	0.45
7:LB:153:MET:HB3	7:LB:194:LEU:HD11	1.98	0.45
51:SF:60:ARG:NH2	83:S2:1679:A:OP1	2.46	0.45
54:SP:56:LEU:HD22	54:SP:80:LEU:HD11	1.99	0.45
65:SA:215:GLN:O	65:SA:219:GLU:HG2	2.16	0.45
70:SH:51:ILE:HD11	70:SH:176:VAL:HG12	1.98	0.45
71:SI:44:HIS:ND1	83:S2:1740:C:OP1	2.32	0.45
83:S2:16:G:H2'	83:S2:17:C:C6	2.51	0.45
83:S2:1217:A:H2'	83:S2:1218:C:C6	2.49	0.45
3:L5:1558:A:H2'	3:L5:1559:G:C8	2.51	0.45
3:L5:1960:A:C8	48:Ls:63:LYS:HE2	2.51	0.45
3:L5:2763:U:H4'	3:L5:2764:A:H5''	1.98	0.45
3:L5:3595:U:H5''	3:L5:3597:G:OP2	2.16	0.45
3:L5:3726:A:H2'	3:L5:3727:A:C8	2.51	0.45
3:L5:3848:U:H2'	3:L5:3849:A:C8	2.51	0.45
3:L5:3893:C:H2'	3:L5:3894:A:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4439:U:O2'	14:LI:105:CYS:O	2.34	0.45
3:L5:4672:A:OP1	26:LV:15:ARG:NH2	2.37	0.45
3:L5:5057:C:H2'	3:L5:5058:A:C8	2.51	0.45
4:L7:58:A:H2'	4:L7:59:G:H8	1.81	0.45
16:LL:55:ILE:O	16:LL:97:SER:OG	2.31	0.45
21:LQ:57:ASN:HA	21:LQ:143:ARG:HD2	1.97	0.45
22:LR:139:MET:HG2	22:LR:143:HIS:CE1	2.51	0.45
32:Lb:5:LYS:HE2	32:Lb:8:THR:HB	1.98	0.45
49:Lt:77:ALA:HB3	49:Lt:80:LEU:HB2	1.96	0.45
56:SR:22:THR:O	64:Sg:212:LYS:NZ	2.49	0.45
57:SS:38:ARG:HD2	58:ST:45:LEU:HD11	1.98	0.45
59:SU:96:GLU:OE2	59:SU:98:VAL:N	2.48	0.45
64:Sg:35:SER:OG	64:Sg:36:ARG:N	2.49	0.45
65:SA:104:THR:O	65:SA:107:THR:OG1	2.32	0.45
77:SW:44:HIS:NE2	77:SW:112:ASP:OD2	2.40	0.45
83:S2:116:OMU:HM23	83:S2:116:OMU:H1'	1.77	0.45
83:S2:186:C:H2'	83:S2:187:G:C8	2.51	0.45
83:S2:517:OMC:H2'	83:S2:518:G:O4'	2.16	0.45
83:S2:808:A:H2	83:S2:855:G:H22	1.65	0.45
3:L5:287:U:H2'	3:L5:288:G:C8	2.51	0.45
3:L5:1912:G:N2	19:LO:87:MET:HE2	2.31	0.45
3:L5:2521:G:H5'	3:L5:2640:G:H1'	1.98	0.45
3:L5:4113:U:H4'	3:L5:4115:G:C5	2.51	0.45
3:L5:4619:U:H2'	3:L5:4620:OMU:H6	1.97	0.45
5:L8:102:G:H5''	40:Lj:39:TYR:HE1	1.81	0.45
7:LB:17:LEU:HD23	7:LB:17:LEU:HA	1.79	0.45
14:LI:51:HIS:CD2	14:LI:168:SER:HB3	2.52	0.45
30:LZ:68:ILE:HD12	30:LZ:119:GLU:HG2	1.97	0.45
51:SF:97:PHE:HA	51:SF:100:ILE:HG12	1.97	0.45
53:SM:19:GLN:HE22	53:SM:88:TRP:CG	2.34	0.45
57:SS:15:VAL:HG13	57:SS:68:ILE:HD11	1.99	0.45
64:Sg:133:ASN:HB3	64:Sg:139:LYS:HD2	1.98	0.45
65:SA:6:ASP:OD1	65:SA:6:ASP:N	2.49	0.45
79:SY:7:ILE:HG12	79:SY:43:LYS:HD3	1.98	0.45
83:S2:317:C:H2'	83:S2:318:A:C4	2.51	0.45
3:L5:400:A2M:HM'3	3:L5:400:A2M:H1'	1.52	0.45
3:L5:433:A:C2	3:L5:3867:A2M:H4'	2.51	0.45
3:L5:2693:G:OP1	41:Lk:35:LYS:HE2	2.17	0.45
3:L5:4239:A:H2'	3:L5:4240:G:H8	1.81	0.45
3:L5:4288:C:O2'	3:L5:4321:U:OP1	2.35	0.45
3:L5:4345:C:H2'	3:L5:4346:U:H6	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L8:102:G:OP2	5:L8:104:A:O2'	2.27	0.45
14:LI:39:LYS:HE3	14:LI:39:LYS:HB2	1.81	0.45
30:LZ:46:ILE:HA	30:LZ:70:SER:HA	1.99	0.45
48:Ls:29:ILE:HG22	48:Ls:88:PHE:HD1	1.81	0.45
49:Lt:76:SER:OG	49:Lt:116:MET:SD	2.73	0.45
53:SM:49:LEU:HB2	53:SM:111:VAL:HB	1.99	0.45
58:ST:132:ASP:OD2	83:S2:1415:C:O2'	2.26	0.45
64:Sg:101:PHE:CE2	64:Sg:136:GLY:HA2	2.52	0.45
69:SG:14:LYS:HD3	69:SG:124:LEU:HD12	1.98	0.45
75:SO:96:LYS:HD3	75:SO:132:VAL:HG11	1.97	0.45
83:S2:1243:U:OP2	83:S2:1518:C:O2'	2.26	0.45
83:S2:1259:A:N6	83:S2:1519:U:O5'	2.49	0.45
3:L5:1510:G:H2'	3:L5:1511:U:C6	2.51	0.45
3:L5:2468:U:O2'	3:L5:2506:G:N2	2.49	0.45
3:L5:2824:OMC:HM23	3:L5:2824:OMC:H1'	1.66	0.45
3:L5:2875:C:OP1	46:Lp:23:ARG:NH2	2.50	0.45
3:L5:3910:C:H2'	3:L5:3911:C:C6	2.51	0.45
3:L5:4093:G:H3'	3:L5:4094:G:H8	1.81	0.45
3:L5:4113:U:H4'	3:L5:4115:G:C6	2.52	0.45
3:L5:4305:G:O5'	24:LT:83:LYS:NZ	2.49	0.45
3:L5:4642:U:H2'	3:L5:4643:G:C8	2.52	0.45
12:LG:83:PHE:HA	12:LG:183:ILE:HD13	1.98	0.45
20:LP:18:ARG:NH2	20:LP:147:GLU:OE1	2.50	0.45
20:LP:138:PRO:HB3	20:LP:140:MET:HE2	1.97	0.45
56:SR:32:LYS:NZ	83:S2:1452:A:OP2	2.50	0.45
57:SS:62:ASP:OD1	57:SS:62:ASP:N	2.49	0.45
59:SU:19:ARG:HH11	59:SU:92:HIS:HB3	1.81	0.45
70:SH:33:ASN:ND2	70:SH:36:LEU:HB3	2.31	0.45
70:SH:111:LYS:HE3	83:S2:796:G:H21	1.82	0.45
2:Et:7:A:O2'	2:Et:49:C:O4'	2.33	0.45
3:L5:1725:U:H2'	3:L5:1726:U:H6	1.82	0.45
3:L5:2306:G:H1'	3:L5:2332:A:N6	2.31	0.45
3:L5:2558:C:H2'	3:L5:2559:G:H8	1.82	0.45
3:L5:2577:C:OP1	30:LZ:111:ARG:NH2	2.49	0.45
10:LE:139:LYS:O	10:LE:191:GLN:NE2	2.39	0.45
40:Lj:85:LYS:HB3	40:Lj:85:LYS:HE3	1.72	0.45
51:SF:27:ASP:OD1	51:SF:107:ASN:ND2	2.50	0.45
57:SS:27:ALA:HB2	57:SS:52:LEU:HD12	1.99	0.45
64:Sg:230:LEU:HD21	64:Sg:259:TRP:CE2	2.52	0.45
65:SA:164:ASN:OD1	65:SA:165:ASN:N	2.50	0.45
69:SG:7:PHE:CE2	69:SG:9:ALA:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:SI:84:ASN:HD22	71:SI:100:CYS:HB3	1.81	0.45
79:SY:77:ASP:OD1	79:SY:77:ASP:N	2.49	0.45
83:S2:17:C:H2'	83:S2:18:C:C6	2.51	0.45
83:S2:809:A:H2'	83:S2:810:A:O4'	2.17	0.45
83:S2:1716:C:H2'	83:S2:1717:C:H6	1.82	0.45
83:S2:1797:U:H2'	83:S2:1798:C:C6	2.52	0.45
3:L5:158:A:N1	3:L5:276:C:O2'	2.35	0.45
3:L5:422:C:H2'	3:L5:423:G:H8	1.81	0.45
3:L5:1194:G:H2'	3:L5:1195:G:C8	2.51	0.45
3:L5:3946:G:O6	3:L5:4067:U:O4	2.35	0.45
8:LC:327:LYS:O	11:LF:47:ARG:NH1	2.42	0.45
29:LY:4:ASN:HB3	29:LY:7:VAL:HG22	1.97	0.45
30:LZ:47:ASP:N	30:LZ:69:LYS:O	2.47	0.45
51:SF:167:LYS:HA	60:SZ:71:ALA:HB1	1.98	0.45
57:SS:125:HIS:CD2	57:SS:131:VAL:HG11	2.52	0.45
67:SC:185:THR:OG1	83:S2:1155:U:OP1	2.30	0.45
67:SC:256:TRP:CD2	77:SW:68:ARG:HD3	2.51	0.45
68:SE:122:LYS:HE2	68:SE:124:CYS:SG	2.56	0.45
78:SX:90:CYS:HA	78:SX:93:PHE:CD2	2.52	0.45
83:S2:674:C:H2'	83:S2:675:U:C6	2.52	0.45
83:S2:1345:G:OP1	83:S2:1688:C:O2'	2.35	0.45
83:S2:1562:C:H2'	83:S2:1563:G:C8	2.49	0.45
83:S2:1856:C:H2'	83:S2:1857:G:H8	1.82	0.45
2:Et:66:U:H2'	2:Et:67:U:H6	1.82	0.45
2:Et:68:C:H2'	2:Et:69:G:H8	1.81	0.45
3:L5:264:C:H2'	3:L5:265:C:C4	2.52	0.45
3:L5:429:A:H2'	3:L5:430:G:C8	2.52	0.45
3:L5:1866:U:OP1	14:LI:4:ARG:NH1	2.41	0.45
3:L5:4590:A2M:HM'3	3:L5:4590:A2M:H1'	1.76	0.45
4:L7:58:A:H2'	4:L7:59:G:C8	2.52	0.45
12:LG:187:LYS:HB2	12:LG:198:THR:HG23	1.98	0.45
34:Ld:44:ARG:HA	34:Ld:47:LYS:HE3	1.98	0.45
72:SJ:28:GLU:OE2	72:SJ:44:TRP:NE1	2.37	0.45
72:SJ:111:GLN:HE21	72:SJ:123:ILE:HG13	1.82	0.45
83:S2:223:C:H2'	83:S2:224:A:C8	2.52	0.45
83:S2:1217:A:H2'	83:S2:1218:C:H6	1.81	0.45
2:Et:75:C:O2'	45:Lo:54:PRO:O	2.28	0.45
3:L5:662:C:H2'	3:L5:663:G:H8	1.82	0.45
3:L5:1982:G:H2'	3:L5:1983:A:O4'	2.15	0.45
3:L5:2706:G:N7	84:CI:78:HIS:CD2	2.85	0.45
3:L5:3873:G:H2'	3:L5:3874:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LB:147:GLU:OE2	7:LB:198:ARG:NH2	2.34	0.45
7:LB:302:ASN:HB2	7:LB:313:SER:HA	1.99	0.45
16:LL:48:PRO:HG3	38:Lh:118:LYS:HE2	1.99	0.45
21:LQ:133:GLY:O	21:LQ:136:THR:OG1	2.26	0.45
65:SA:111:GLN:HA	65:SA:116:PHE:CG	2.51	0.45
66:SB:44:ILE:HG23	66:SB:69:VAL:HG11	1.98	0.45
66:SB:85:LYS:HB2	66:SB:101:HIS:HB3	1.99	0.45
70:SH:53:VAL:HG21	70:SH:172:THR:HG22	1.99	0.45
70:SH:143:ARG:HB2	70:SH:155:LYS:HB2	1.98	0.45
83:S2:948:C:H2'	83:S2:949:G:C8	2.51	0.45
83:S2:1581:C:H5'	83:S2:1582:C:H5	1.81	0.45
3:L5:1359:G:H4'	18:LN:203:TYR:HB2	1.99	0.45
3:L5:1696:C:H5'	3:L5:1719:A:H1'	1.99	0.45
3:L5:1994:C:H2'	3:L5:1995:G:H8	1.80	0.45
3:L5:4456:OMC:HM21	7:LB:241:PRO:HD3	1.99	0.45
3:L5:4633:G:N2	3:L5:4664:A:N7	2.64	0.45
4:L7:63:C:H5'	4:L7:64:G:H5''	1.99	0.45
7:LB:35:ASP:OD2	7:LB:193:LYS:NZ	2.50	0.45
7:LB:378:ARG:HE	27:LW:32:LEU:HD21	1.82	0.45
17:LM:36:ALA:HB3	17:LM:55:MET:HE1	1.99	0.45
17:LM:118:MET:HG2	19:LO:192:TYR:CZ	2.52	0.45
49:Lt:16:ARG:CZ	49:Lt:63:THR:HB	2.47	0.45
64:Sg:270:LEU:HD13	64:Sg:310:TRP:CD2	2.52	0.45
83:S2:1383:A2M:H1'	83:S2:1383:A2M:HM'3	1.57	0.45
83:S2:1648:G:O2'	83:S2:1674:G:O6	2.31	0.45
3:L5:10:A:H2'	3:L5:11:G:H8	1.82	0.44
3:L5:190:G:H2'	3:L5:191:G:C8	2.52	0.44
3:L5:1309:C:H2'	3:L5:1310:C:C6	2.52	0.44
3:L5:2730:U:H2'	3:L5:2731:C:C6	2.52	0.44
3:L5:4541:G:N2	3:L5:4544:A:OP2	2.43	0.44
4:L7:4:U:H2'	4:L7:5:A:H8	1.82	0.44
7:LB:206:PRO:HG2	7:LB:209:GLN:HG3	1.97	0.44
8:LC:150:LEU:O	8:LC:152:LEU:N	2.50	0.44
9:LD:86:TYR:HE1	9:LD:247:ILE:HG13	1.81	0.44
17:LM:130:LEU:HB3	19:LO:177:LEU:HD11	1.98	0.44
33:Lc:23:LYS:HE3	33:Lc:23:LYS:HB3	1.86	0.44
66:SB:40:ASN:OD1	66:SB:41:ILE:HD12	2.17	0.44
68:SE:59:ASP:O	68:SE:63:LYS:HG3	2.17	0.44
69:SG:183:ARG:HH22	83:S2:316:G:H5''	1.83	0.44
73:SL:111:VAL:HG12	73:SL:140:PHE:HB2	1.99	0.44
79:SY:10:ARG:HA	83:S2:839:C:H41	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1189:A:H2'	83:S2:1190:A:H8	1.82	0.44
83:S2:1667:U:H2'	83:S2:1668:U:C6	2.51	0.44
3:L5:223:G:OP2	8:LC:165:LYS:NZ	2.49	0.44
3:L5:481:G:H2'	3:L5:482:G:C8	2.53	0.44
3:L5:1348:U:H2'	3:L5:1349:G:H8	1.82	0.44
3:L5:1875:C:H2'	3:L5:1876:U:C6	2.52	0.44
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.53	0.44
3:L5:3923:A:H2'	3:L5:3924:C:C6	2.53	0.44
3:L5:4178:A:H2'	3:L5:4179:G:C8	2.52	0.44
3:L5:4305:G:C6	24:LT:80:VAL:HG21	2.53	0.44
3:L5:4637:OMG:HM23	3:L5:4637:OMG:H1'	1.68	0.44
5:L8:66:A:H2'	5:L8:67:U:C6	2.52	0.44
14:LI:54:SER:HB3	14:LI:135:ILE:HD11	1.99	0.44
22:LR:21:LYS:HE3	22:LR:55:VAL:HA	1.98	0.44
27:LW:5:LEU:HD12	27:LW:30:GLN:NE2	2.32	0.44
30:LZ:95:VAL:HG12	30:LZ:110:ALA:HA	1.99	0.44
47:Lr:119:ARG:HA	47:Lr:122:LYS:HE3	2.00	0.44
50:SD:73:VAL:HG11	50:SD:86:LEU:HD11	2.00	0.44
51:SF:127:ARG:H	51:SF:135:ARG:HD2	1.81	0.44
62:Sd:56:ASP:OXT	83:S2:1480:A:O2'	2.30	0.44
68:SE:89:VAL:HG11	68:SE:119:ALA:HB1	1.98	0.44
80:Sa:79:ILE:HD11	83:S2:1864:U:H5'	2.00	0.44
83:S2:51:U:H2'	83:S2:52:G:C8	2.52	0.44
83:S2:1410:C:H2'	83:S2:1411:G:H8	1.81	0.44
3:L5:1324:A:O2'	3:L5:1326:A2M:OP1	2.30	0.44
3:L5:1995:G:H2'	3:L5:1996:C:C6	2.53	0.44
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.53	0.44
3:L5:2634:C:H2'	3:L5:2635:U:C6	2.53	0.44
3:L5:2667:C:O4'	22:LR:96:MET:HG2	2.17	0.44
3:L5:3727:A:H2'	3:L5:3728:A:C8	2.51	0.44
3:L5:3866:C:H2'	3:L5:3867:A2M:O4'	2.18	0.44
3:L5:4742:G:H2'	3:L5:4743:G:H8	1.81	0.44
13:LH:93:ARG:HG2	13:LH:182:SER:HB3	1.99	0.44
27:LW:56:ARG:HE	27:LW:61:LYS:CB	2.31	0.44
54:SP:37:TYR:HB3	54:SP:41:GLN:HB2	1.98	0.44
56:SR:35:CYS:HA	56:SR:38:ILE:HG12	1.98	0.44
61:Sc:21:THR:OG1	61:Sc:22:GLY:N	2.50	0.44
67:SC:85:SER:OG	76:SV:25:GLY:O	2.27	0.44
71:SI:26:LYS:HE3	83:S2:444:G:O6	2.17	0.44
78:SX:105:PHE:CE2	78:SX:112:VAL:HB	2.52	0.44
79:SY:68:LYS:HE2	79:SY:68:LYS:HB3	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Sb:22:LYS:HE3	83:S2:1129:G:H5''	1.98	0.44
83:S2:512:A:H4'	83:S2:576:A2M:H2	2.00	0.44
83:S2:1856:C:H2'	83:S2:1857:G:C8	2.53	0.44
2:Et:68:C:H2'	2:Et:69:G:C8	2.52	0.44
3:L5:44:A:H5''	86:L5:5264:SPM:H81	1.98	0.44
3:L5:318:A:H2'	3:L5:319:A:H8	1.83	0.44
3:L5:457:G:H2'	3:L5:458:C:H6	1.83	0.44
3:L5:513:U:H3'	3:L5:514:U:H4'	1.99	0.44
3:L5:1662:C:H2'	3:L5:1663:C:H6	1.83	0.44
3:L5:1979:A:N6	3:L5:1984:A:OP1	2.51	0.44
3:L5:4306:OMU:HM23	3:L5:4306:OMU:H1'	1.77	0.44
5:L8:90:C:H2'	5:L8:91:A:C8	2.53	0.44
52:SK:31:LYS:HZ3	52:SK:39:ASN:N	2.16	0.44
56:SR:16:ILE:HD11	56:SR:54:VAL:HG21	1.98	0.44
64:Sg:135:LEU:HD23	64:Sg:135:LEU:HA	1.88	0.44
65:SA:37:TYR:OH	65:SA:57:LYS:NZ	2.46	0.44
83:S2:159:A2M:HM'3	83:S2:159:A2M:H1'	1.59	0.44
83:S2:420:G:O2'	83:S2:660:C:N3	2.46	0.44
83:S2:433:A:H2'	83:S2:434:G:C8	2.53	0.44
83:S2:750:C:C2	83:S2:752:G:N2	2.86	0.44
83:S2:867:OMG:HM23	83:S2:867:OMG:H1'	1.82	0.44
83:S2:1320:G:H2'	83:S2:1321:G:O4'	2.16	0.44
83:S2:1390:U:H2'	83:S2:1391:OMC:C6	2.53	0.44
3:L5:950:G:H2'	3:L5:951:G:H8	1.82	0.44
3:L5:966:A:OP2	3:L5:2092:G:N2	2.49	0.44
3:L5:1431:C:H2'	3:L5:1432:G:O4'	2.17	0.44
3:L5:3660:C:OP1	6:LA:241:ARG:NH2	2.42	0.44
3:L5:4507:A:H2'	3:L5:4508:C:C6	2.52	0.44
5:L8:148:A:H2'	5:L8:149:G:C8	2.53	0.44
7:LB:73:VAL:O	26:LV:89:ARG:NH2	2.50	0.44
8:LC:315:LYS:HD2	11:LF:168:ALA:HB1	1.99	0.44
11:LF:182:TYR:CZ	11:LF:203:GLU:HG2	2.52	0.44
14:LI:205:PRO:HD2	14:LI:208:LYS:HE2	1.99	0.44
16:LL:110:LEU:O	16:LL:114:VAL:HG13	2.17	0.44
27:LW:2:LYS:HE3	27:LW:15:PRO:HB3	2.00	0.44
53:SM:31:LEU:HG	53:SM:33:ARG:HG3	1.98	0.44
64:Sg:251:ALA:HA	64:Sg:256:ILE:HD13	2.00	0.44
65:SA:37:TYR:OH	76:SV:66:ASP:OD2	2.22	0.44
65:SA:69:GLU:HB2	67:SC:270:THR:HG21	1.99	0.44
71:SI:56:ARG:HH22	83:S2:380:G:P	2.40	0.44
83:S2:71:G:H2'	83:S2:72:C:H4'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1610:G:H2'	83:S2:1611:G:C8	2.53	0.44
83:S2:1720:U:H5''	83:S2:1721:U:H5''	2.00	0.44
3:L5:1346:C:H2'	3:L5:1347:G:H8	1.82	0.44
3:L5:1756:U:O2'	3:L5:1758:G:OP2	2.25	0.44
3:L5:1846:G:H2'	3:L5:1847:C:C6	2.52	0.44
3:L5:2385:U:H2'	3:L5:2386:U:H6	1.83	0.44
3:L5:3911:C:H2'	3:L5:3912:U:C6	2.51	0.44
6:LA:22:HIS:O	6:LA:24:LYS:NZ	2.48	0.44
6:LA:142:GLU:O	6:LA:143:THR:OG1	2.34	0.44
13:LH:27:VAL:HG12	13:LH:84:VAL:HG21	2.00	0.44
17:LM:115:ALA:HB1	19:LO:192:TYR:HB3	1.99	0.44
20:LP:54:GLN:HA	20:LP:83:TRP:CD1	2.51	0.44
47:Lr:49:VAL:HG23	47:Lr:64:ILE:HG22	1.97	0.44
58:ST:39:LEU:HA	58:ST:39:LEU:HD23	1.72	0.44
60:SZ:99:LEU:HD11	60:SZ:102:LYS:HB2	2.00	0.44
63:Sf:97:LYS:HE2	83:S2:1289:U:C5	2.53	0.44
64:Sg:268:ASP:OD1	64:Sg:269:GLU:N	2.51	0.44
68:SE:149:TYR:CD2	69:SG:205:GLU:HB3	2.52	0.44
69:SG:56:ASN:HB2	69:SG:108:VAL:HG22	2.00	0.44
69:SG:183:ARG:HH12	83:S2:316:G:H5''	1.83	0.44
83:S2:886:A:N6	83:S2:901:G:N3	2.66	0.44
83:S2:946:U:H2'	83:S2:947:G:C8	2.53	0.44
83:S2:1232:PSU:H2'	83:S2:1233:G:C8	2.53	0.44
83:S2:1683:C:H2'	83:S2:1684:C:H6	1.83	0.44
83:S2:1752:C:H41	83:S2:1755:C:N4	2.15	0.44
3:L5:20:U:H3'	3:L5:21:G:H8	1.82	0.44
3:L5:92:C:OP2	3:L5:4341:C:O2'	2.29	0.44
3:L5:457:G:H2'	3:L5:458:C:C6	2.53	0.44
3:L5:689:U:H2'	3:L5:690:C:C6	2.53	0.44
3:L5:1100:U:O4	3:L5:1194:G:O6	2.36	0.44
3:L5:2376:A:H2'	3:L5:2377:C:C6	2.53	0.44
3:L5:2415:U:H2'	3:L5:2416:G:C8	2.53	0.44
3:L5:3597:G:H2'	3:L5:3598:C:H6	1.83	0.44
3:L5:3690:U:H2'	3:L5:3691:G:O4'	2.18	0.44
3:L5:3805:U:H2'	3:L5:3806:G:H8	1.83	0.44
3:L5:4920:C:H2'	3:L5:4921:C:C6	2.52	0.44
25:LU:66:SER:HB3	25:LU:69:LYS:HB2	2.00	0.44
30:LZ:50:PRO:HD3	30:LZ:68:ILE:HG12	2.00	0.44
48:Ls:54:LEU:HG	48:Ls:61:MET:HE1	1.99	0.44
51:SF:51:HIS:O	55:SQ:50:LYS:NZ	2.42	0.44
51:SF:60:ARG:HE	83:S2:1679:A:P	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Sg:216:ALA:N	64:Sg:230:LEU:O	2.51	0.44
69:SG:14:LYS:HE2	69:SG:16:ILE:HD11	2.00	0.44
69:SG:181:THR:HG22	69:SG:183:ARG:H	1.83	0.44
75:SO:75:MET:HG3	75:SO:118:ALA:HB2	1.98	0.44
83:S2:375:U:H2'	83:S2:376:A:C8	2.53	0.44
83:S2:432:G:H2'	83:S2:433:A:C8	2.53	0.44
83:S2:1351:G:O2'	83:S2:1378:A:N1	2.46	0.44
1:Pt:38:C:O2'	83:S2:1058:A:OP1	2.33	0.44
3:L5:690:C:H2'	3:L5:691:C:C6	2.53	0.44
3:L5:1294:A:H1'	3:L5:1296:G:C2	2.53	0.44
3:L5:1534:A2M:N3	40:Lj:11:ARG:HB2	2.32	0.44
3:L5:1563:A:H2'	3:L5:1564:A:C8	2.52	0.44
3:L5:1631:A:C8	6:LA:199:VAL:HG21	2.52	0.44
3:L5:1855:G:OP1	32:Lb:4:SER:HB2	2.18	0.44
3:L5:1881:C:H5'	3:L5:2281:U:H1'	2.00	0.44
3:L5:2109:G:H2'	3:L5:2110:C:C6	2.53	0.44
3:L5:2811:G:N1	3:L5:2814:C:OP2	2.45	0.44
3:L5:3870:C:H2'	3:L5:3871:A:C8	2.52	0.44
3:L5:4775:C:H2'	3:L5:4776:G:H8	1.83	0.44
49:Lt:12:VAL:HG11	49:Lt:65:GLN:N	2.27	0.44
66:SB:57:ILE:HG22	66:SB:59:SER:H	1.83	0.44
67:SC:271:ASP:OD1	67:SC:272:HIS:N	2.50	0.44
70:SH:18:GLU:OE1	70:SH:18:GLU:N	2.51	0.44
71:SI:57:ALA:HB2	71:SI:183:GLY:HA2	2.00	0.44
83:S2:24:C:HO2'	83:S2:25:A:P	2.41	0.44
83:S2:866:PSU:H2'	83:S2:867:OMG:H8	1.83	0.44
83:S2:1036:A:H4'	83:S2:1855:G:N2	2.33	0.44
1:Pt:29:C:H2'	1:Pt:30:G:C8	2.53	0.44
3:L5:138:G:H2'	3:L5:139:G:H8	1.83	0.44
3:L5:223:G:H4'	3:L5:225:G:C8	2.52	0.44
3:L5:1290:G:H2'	3:L5:1291:G:C8	2.53	0.44
3:L5:2323:C:H2'	3:L5:2324:C:C6	2.53	0.44
3:L5:3867:A2M:HM'3	3:L5:3867:A2M:H1'	1.59	0.44
3:L5:4627:U:H4'	7:LB:373:LYS:HE2	2.00	0.44
9:LD:152:ARG:HG3	9:LD:154:THR:HG23	1.99	0.44
13:LH:61:TRP:CZ3	17:LM:33:GLN:HG3	2.53	0.44
26:LV:42:VAL:HB	26:LV:45:ILE:HG13	1.98	0.44
51:SF:22:LYS:HG3	51:SF:23:TRP:CD2	2.53	0.44
65:SA:137:ALA:HB1	65:SA:142:LEU:HB3	1.98	0.44
66:SB:29:ASP:OD1	66:SB:29:ASP:N	2.51	0.44
67:SC:212:LYS:HE2	67:SC:212:LYS:HB3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SG:87:ARG:HD3	69:SG:87:ARG:HA	1.77	0.44
70:SH:17:ASP:OD1	70:SH:17:ASP:N	2.50	0.44
75:SO:150:ARG:NH2	83:S2:1854:U:OP1	2.38	0.44
77:SW:55:ASP:HB3	81:Sb:25:VAL:HG13	2.00	0.44
83:S2:17:C:H2'	83:S2:18:C:H6	1.83	0.44
83:S2:291:G:H2'	83:S2:292:A:C8	2.53	0.44
83:S2:399:C:H5	83:S2:680:G:H5''	1.83	0.44
83:S2:544:G:H2'	83:S2:545:A:C8	2.53	0.44
83:S2:857:U:H2'	83:S2:858:A:C8	2.52	0.44
83:S2:1128:C:H2'	83:S2:1129:G:H8	1.82	0.44
83:S2:1409:A:H2'	83:S2:1410:C:C6	2.52	0.44
83:S2:1441:U:O2	83:S2:1443:C:N4	2.46	0.44
3:L5:161:G:H2'	3:L5:162:A:C8	2.53	0.43
3:L5:381:U:H4'	3:L5:415:G:H5'	2.00	0.43
3:L5:677:G:H2'	3:L5:678:C:C6	2.53	0.43
3:L5:1338:G:H4'	3:L5:1339:U:H6	1.83	0.43
3:L5:1403:G:N7	3:L5:1408:G:N2	2.66	0.43
3:L5:1977:C:O2'	3:L5:1978:C:OP1	2.36	0.43
3:L5:4742:G:H2'	3:L5:4743:G:C8	2.53	0.43
3:L5:4965:U:H4'	3:L5:4966:A:H5'	2.00	0.43
3:L5:5027:C:OP2	71:SI:77:ARG:NH2	2.51	0.43
6:LA:65:ASP:OD2	6:LA:72:ARG:NE	2.37	0.43
15:LJ:15:LEU:HD12	15:LJ:165:TRP:HB2	2.00	0.43
22:LR:160:GLU:OE1	22:LR:163:ARG:NH2	2.40	0.43
38:Lh:52:LYS:HA	38:Lh:52:LYS:HD3	1.78	0.43
40:Lj:67:LEU:HD23	40:Lj:67:LEU:HA	1.84	0.43
52:SK:64:TRP:CD2	62:Sd:23:VAL:HG22	2.52	0.43
63:Sf:103:LEU:HD12	63:Sf:105:TYR:CZ	2.53	0.43
69:SG:170:ARG:HA	83:S2:72:C:H42	1.81	0.43
69:SG:170:ARG:HG3	83:S2:72:C:N3	2.33	0.43
83:S2:516:A:N1	83:S2:643:A:O2'	2.47	0.43
83:S2:639:C:H2'	83:S2:640:A:H8	1.81	0.43
3:L5:1177:U:O4	3:L5:1183:C:N4	2.49	0.43
3:L5:1847:C:H2'	3:L5:1848:C:C6	2.53	0.43
3:L5:3945:A:H2'	3:L5:3946:G:C8	2.53	0.43
3:L5:4536:OMC:HM22	3:L5:4537:C:O4'	2.18	0.43
3:L5:4761:G:H2'	3:L5:4762:A:H8	1.82	0.43
5:L8:144:U:H2'	5:L8:145:C:C6	2.53	0.43
7:LB:289:GLN:HE22	7:LB:292:LEU:HD11	1.81	0.43
21:LQ:86:ILE:HD11	21:LQ:100:VAL:HG11	2.00	0.43
63:Sf:119:ARG:HB3	63:Sf:132:MET:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SA:220:LYS:HA	65:SA:220:LYS:HD3	1.86	0.43
76:SV:74:LYS:NZ	76:SV:83:PHE:HB3	2.33	0.43
83:S2:573:U:O2	83:S2:576:A2M:H8	2.17	0.43
3:L5:1282:G:OP2	10:LE:128:HIS:NE2	2.52	0.43
3:L5:1613:A:H5''	6:LA:183:GLY:CA	2.49	0.43
3:L5:3606:U:H2'	3:L5:3607:U:C6	2.53	0.43
3:L5:3723:A:H2'	3:L5:3724:A:C8	2.53	0.43
3:L5:3880:G:H2'	3:L5:3881:G:C8	2.53	0.43
3:L5:4253:A:H5'	3:L5:4254:G:C8	2.53	0.43
3:L5:4578:G:H2'	3:L5:4579:PSU:H6	1.84	0.43
3:L5:4612:C:C2	13:LH:120:GLU:HB2	2.54	0.43
4:L7:35:U:O2	4:L7:45:U:O2'	2.33	0.43
4:L7:37:G:H2'	4:L7:38:U:O4'	2.18	0.43
6:LA:114:CYS:N	6:LA:165:VAL:O	2.46	0.43
9:LD:110:LEU:HB3	9:LD:115:MET:O	2.19	0.43
19:LO:88:LEU:HD12	19:LO:99:LEU:HD13	2.00	0.43
67:SC:214:LEU:HD22	67:SC:244:ILE:HD11	2.00	0.43
68:SE:38:LEU:HD23	83:S2:346:C:H5''	2.00	0.43
76:SV:40:ASP:OD1	76:SV:44:GLY:N	2.51	0.43
79:SY:23:MET:O	79:SY:73:GLY:N	2.46	0.43
79:SY:56:PHE:HB2	79:SY:74:MET:HB2	2.00	0.43
83:S2:165:G:H2'	83:S2:166:A2M:H8	1.99	0.43
83:S2:1215:C:O2'	83:S2:1645:C:OP2	2.33	0.43
83:S2:1702:G:H2'	83:S2:1703:OMC:O4'	2.17	0.43
3:L5:700:G:C6	3:L5:701:G:O6	2.72	0.43
3:L5:1494:U:H2'	3:L5:1495:G:C8	2.53	0.43
3:L5:1705:G:H2'	3:L5:1706:A:O4'	2.18	0.43
3:L5:1751:A:H2'	3:L5:1752:G:H8	1.83	0.43
3:L5:1858:A:H2'	3:L5:1859:C:H6	1.82	0.43
3:L5:2017:A:HO2'	3:L5:2018:C:C5'	2.31	0.43
3:L5:2102:G:H1'	3:L5:2103:G:C8	2.53	0.43
3:L5:2413:U:H2'	3:L5:2414:G:H8	1.84	0.43
3:L5:3599:A:H2'	3:L5:3600:G:C8	2.52	0.43
3:L5:4481:U:H2'	3:L5:4482:U:C6	2.53	0.43
3:L5:4670:C:O2'	3:L5:4672:A:OP2	2.29	0.43
3:L5:5004:C:H2'	3:L5:5005:G:O4'	2.17	0.43
6:LA:20:VAL:HA	6:LA:23:ARG:HG3	1.98	0.43
12:LG:52:THR:HG22	28:LX:41:ARG:HG3	2.00	0.43
18:LN:200:LEU:HD22	18:LN:204:ARG:NH1	2.33	0.43
29:LY:126:ARG:HG2	29:LY:130:LYS:HE2	2.00	0.43
47:Lr:26:SER:OG	47:Lr:28:GLU:OE1	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Sg:230:LEU:HD11	64:Sg:259:TRP:CD1	2.53	0.43
67:SC:94:ILE:O	67:SC:98:LEU:N	2.39	0.43
67:SC:263:LYS:HA	67:SC:267:GLN:HE21	1.82	0.43
68:SE:57:THR:HG21	83:S2:494:C:H5''	2.00	0.43
69:SG:126:ASP:OD1	69:SG:126:ASP:N	2.48	0.43
71:SI:114:GLU:HB3	71:SI:136:ILE:HD12	2.01	0.43
81:Sb:33:MET:HE3	81:Sb:48:SER:HA	2.00	0.43
83:S2:194:C:H2'	83:S2:195:C:H6	1.84	0.43
83:S2:437:G:H2'	83:S2:438:G:O4'	2.19	0.43
83:S2:468:A2M:HM'3	83:S2:468:A2M:H1'	1.67	0.43
83:S2:737:G:H8	83:S2:738:C:H4'	1.83	0.43
2:Et:12:U:H2'	2:Et:13:C:C6	2.53	0.43
3:L5:197:A:N3	3:L5:222:C:O2'	2.46	0.43
3:L5:907:C:H2'	3:L5:908:G:C8	2.53	0.43
3:L5:2095:A:H4'	3:L5:2096:G:H5'	1.99	0.43
3:L5:2683:C:H2'	3:L5:2684:C:H6	1.84	0.43
3:L5:3687:A:O2'	6:LA:236:GLY:N	2.51	0.43
3:L5:3865:A:H61	3:L5:3881:G:H1	1.65	0.43
3:L5:4139:G:H1'	3:L5:4146:G:N1	2.34	0.43
67:SC:65:LYS:HD2	67:SC:273:LEU:HD13	2.01	0.43
70:SH:7:LYS:HD3	70:SH:10:LYS:HB3	1.99	0.43
77:SW:106:THR:OG1	77:SW:111:MET:HE2	2.19	0.43
80:Sa:6:ARG:NH1	83:S2:1147:C:OP1	2.52	0.43
83:S2:388:U:H2'	83:S2:389:A:C8	2.54	0.43
83:S2:454:U:H2'	83:S2:455:A:C8	2.54	0.43
83:S2:1279:C:H2'	83:S2:1280:G:C8	2.54	0.43
83:S2:1653:U:H2'	83:S2:1654:G:C8	2.53	0.43
3:L5:138:G:H2'	3:L5:139:G:C8	2.54	0.43
3:L5:1326:A2M:OP2	3:L5:4445:U:O2'	2.31	0.43
3:L5:1906:U:H2'	3:L5:1907:A:H8	1.83	0.43
3:L5:2020:U:H2'	3:L5:2021:G:H8	1.84	0.43
3:L5:2706:G:C8	84:CI:78:HIS:NE2	2.82	0.43
3:L5:4318:C:H4'	45:Lo:17:LYS:HA	1.99	0.43
3:L5:4524:G:C2	7:LB:252:ALA:HB1	2.54	0.43
6:LA:117:GLU:O	6:LA:162:ASN:ND2	2.42	0.43
8:LC:10:VAL:O	8:LC:18:SER:OG	2.25	0.43
11:LF:162:ILE:HD12	11:LF:167:ILE:HB	2.00	0.43
12:LG:162:ASP:HB3	12:LG:163:PRO:HD3	1.99	0.43
29:LY:10:ASP:HB3	29:LY:13:LYS:HB2	2.00	0.43
35:Le:30:LYS:HG3	35:Le:31:ILE:HG12	2.00	0.43
38:Lh:70:ARG:HG2	38:Lh:83:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SA:5:LEU:HD11	76:SV:41:LYS:HD2	2.01	0.43
66:SB:224:GLU:HB2	66:SB:227:LYS:HD3	2.01	0.43
73:SL:3:ASP:OD1	73:SL:4:ILE:N	2.50	0.43
81:Sb:11:SER:OG	81:Sb:14:GLU:OE1	2.36	0.43
83:S2:329:G:H2'	83:S2:330:G:C8	2.54	0.43
83:S2:462:OMC:HM23	83:S2:462:OMC:H1'	1.74	0.43
2:Et:32:C:H2'	2:Et:33:U:C2	2.54	0.43
3:L5:1806:G:H2'	3:L5:1807:C:H6	1.83	0.43
3:L5:3722:G:H2'	3:L5:3723:A:H8	1.83	0.43
3:L5:5023:C:OP2	71:SI:124:LYS:NZ	2.51	0.43
16:LL:7:GLY:O	31:La:49:HIS:NE2	2.40	0.43
31:La:76:ASP:HB3	31:La:115:GLY:HA3	2.01	0.43
35:Le:91:CYS:HB3	35:Le:95:TYR:HD2	1.84	0.43
53:SM:58:GLU:HB3	53:SM:61:TYR:HB2	2.01	0.43
57:SS:64:VAL:O	57:SS:68:ILE:HG12	2.18	0.43
57:SS:102:GLY:HA2	57:SS:105:ASN:HD21	1.84	0.43
57:SS:129:LEU:HA	57:SS:144:ARG:NH2	2.34	0.43
64:Sg:57:ARG:HE	64:Sg:95:GLY:HA3	1.83	0.43
68:SE:75:LYS:NZ	83:S2:122:G:OP1	2.37	0.43
81:Sb:26:GLN:NE2	83:S2:921:G:OP2	2.50	0.43
83:S2:656:G:H5'	83:S2:662:G:N2	2.33	0.43
83:S2:1102:G:H2'	83:S2:1103:C:C6	2.54	0.43
83:S2:1199:A:H2'	83:S2:1200:A:C8	2.53	0.43
3:L5:173:C:H2'	3:L5:174:C:C6	2.53	0.43
3:L5:184:U:O2'	3:L5:189:G:O4'	2.37	0.43
3:L5:724:C:OP1	8:LC:350:ARG:HD3	2.19	0.43
3:L5:755:C:H2'	3:L5:756:G:H8	1.84	0.43
3:L5:1327:C:H2'	3:L5:1328:G:H8	1.83	0.43
3:L5:1344:C:H1'	16:LL:10:LEU:HD11	2.01	0.43
3:L5:1426:G:N1	3:L5:1458:C:OP2	2.40	0.43
3:L5:1628:C:H5''	6:LA:15:VAL:HG21	2.01	0.43
3:L5:1787:A:N3	3:L5:4210:U:O2'	2.52	0.43
3:L5:3896:C:H1'	7:LB:268:ARG:NH2	2.33	0.43
3:L5:4934:A:H2'	3:L5:4935:C:H6	1.83	0.43
3:L5:5002:U:H2'	3:L5:5003:U:C6	2.53	0.43
87:L5:5284:SPD:H82	87:L5:5284:SPD:H51	1.78	0.43
4:L7:15:C:H2'	4:L7:16:A:H8	1.84	0.43
8:LC:144:ILE:HG13	8:LC:144:ILE:O	2.19	0.43
10:LE:190:HIS:HB3	10:LE:193:PHE:HD2	1.84	0.43
20:LP:15:CYS:SG	20:LP:150:LEU:HB2	2.59	0.43
22:LR:47:ASP:HB3	84:CI:76:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LY:76:LYS:HE2	42:L1:31:THR:HB	2.01	0.43
51:SF:100:ILE:HD11	51:SF:108:PRO:HB3	2.00	0.43
55:SQ:89:SER:OG	55:SQ:119:LEU:O	2.35	0.43
57:SS:73:ASN:HB3	57:SS:76:GLN:OE1	2.19	0.43
58:ST:10:ASN:HB3	58:ST:13:GLU:OE2	2.19	0.43
67:SC:183:LYS:HA	67:SC:195:LEU:O	2.18	0.43
70:SH:76:GLN:O	70:SH:80:VAL:HG23	2.19	0.43
73:SL:23:VAL:HG23	73:SL:25:LEU:HG	2.00	0.43
78:SX:17:ARG:HH12	83:S2:659:G:N2	2.17	0.43
83:S2:348:A:H2'	83:S2:349:A:C8	2.54	0.43
83:S2:834:C:H42	83:S2:839:C:H42	1.64	0.43
83:S2:1093:A:H2'	83:S2:1094:C:H6	1.83	0.43
83:S2:1401:A:H2'	83:S2:1402:A:C8	2.54	0.43
3:L5:252:C:H2'	3:L5:253:G:H8	1.83	0.43
3:L5:1269:G:O2'	3:L5:1270:A:O4'	2.27	0.43
3:L5:1307:A:H2'	3:L5:1308:C:C6	2.52	0.43
3:L5:1589:C:H2'	3:L5:1590:C:C6	2.54	0.43
3:L5:2683:C:H2'	3:L5:2684:C:C6	2.54	0.43
3:L5:4638:U:H2'	3:L5:4639:G:N3	2.34	0.43
4:L7:92:C:H2'	4:L7:93:G:H8	1.84	0.43
5:L8:26:C:O2'	8:LC:53:ALA:O	2.36	0.43
5:L8:58:G:O6	40:Lj:63:ARG:NH1	2.50	0.43
7:LB:288:GLY:HA3	7:LB:330:PHE:CE1	2.53	0.43
10:LE:99:ASP:OD1	10:LE:99:ASP:N	2.52	0.43
27:LW:113:LYS:O	27:LW:117:LYS:HG2	2.18	0.43
72:SJ:38:ARG:N	72:SJ:42:GLU:OE2	2.35	0.43
72:SJ:121:LYS:NZ	83:S2:528:A:H5'	2.34	0.43
77:SW:77:PRO:HG2	77:SW:79:PHE:CE2	2.54	0.43
79:SY:42:GLU:HA	79:SY:52:PRO:HB3	2.00	0.43
80:Sa:60:ASP:OD1	80:Sa:60:ASP:N	2.43	0.43
83:S2:1457:U:H2'	83:S2:1458:G:C8	2.53	0.43
83:S2:1643:U:H2'	83:S2:1644:C:C6	2.54	0.43
1:Pt:50:U:H2'	1:Pt:51:C:C6	2.54	0.43
2:Et:58:A:O2'	2:Et:59:G:H5''	2.19	0.43
3:L5:170:C:H42	3:L5:266:C:H42	1.67	0.43
3:L5:1281:G:C6	10:LE:128:HIS:HB2	2.54	0.43
3:L5:1503:A:H62	21:LQ:87:THR:HG21	1.83	0.43
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	2.01	0.43
3:L5:2864:A:H2'	3:L5:2865:U:C6	2.53	0.43
3:L5:3748:A:H5''	6:LA:243:THR:HB	2.01	0.43
3:L5:4492:U:O2'	3:L5:4512:U:O2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LF:37:PHE:HZ	32:Lb:113:ALA:HB1	1.83	0.43
14:LI:207:ASP:HA	14:LI:210:ARG:HG2	2.01	0.43
15:LJ:95:ARG:HD2	15:LJ:177:GLY:HA3	2.01	0.43
23:LS:93:MET:HE1	23:LS:117:HIS:CE1	2.54	0.43
40:Lj:2:THR:HG22	40:Lj:4:GLY:H	1.84	0.43
41:Lk:12:LEU:HD12	41:Lk:16:ARG:HH12	1.83	0.43
50:SD:225:GLU:N	64:Sg:187:ASN:O	2.49	0.43
53:SM:112:LYS:HE2	53:SM:112:LYS:HB2	1.78	0.43
54:SP:47:ARG:NE	83:S2:1619:A:OP1	2.39	0.43
58:ST:73:GLY:O	58:ST:94:ARG:NH2	2.50	0.43
60:SZ:72:VAL:HA	60:SZ:75:GLU:HG2	2.00	0.43
64:Sg:201:SER:OG	64:Sg:203:ASP:OD1	2.26	0.43
64:Sg:226:HIS:NE2	64:Sg:229:THR:OG1	2.47	0.43
67:SC:176:LYS:O	67:SC:200:ARG:NH2	2.52	0.43
69:SG:195:LYS:HD3	83:S2:126:G:H5'	2.01	0.43
82:Se:8:ARG:NH1	83:S2:615:C:O3'	2.51	0.43
83:S2:27:A2M:HM'3	83:S2:27:A2M:H1'	1.65	0.43
83:S2:520:A:O2'	83:S2:825:A:N3	2.48	0.43
83:S2:747:U:O2	83:S2:796:G:C2	2.71	0.43
83:S2:964:A:H2'	83:S2:965:U:H6	1.83	0.43
83:S2:1259:A:H1'	83:S2:1264:C:N4	2.33	0.43
3:L5:6:C:H2'	3:L5:7:C:H6	1.84	0.42
3:L5:423:G:H2'	3:L5:424:U:C6	2.54	0.42
3:L5:494:U:H2'	3:L5:495:C:C6	2.54	0.42
3:L5:737:C:C5	3:L5:739:G:H5''	2.54	0.42
3:L5:966:A:H5''	3:L5:2092:G:H22	1.85	0.42
3:L5:1280:C:O2'	8:LC:321:ASN:OD1	2.21	0.42
3:L5:2610:G:H2'	3:L5:2611:A:C8	2.54	0.42
3:L5:4344:U:H2'	3:L5:4345:C:C6	2.54	0.42
3:L5:4392:OMG:HM21	3:L5:4394:A:H2'	2.00	0.42
3:L5:4723:A:H2'	3:L5:4724:A:C8	2.53	0.42
3:L5:4771:C:H2'	3:L5:4772:C:C6	2.54	0.42
3:L5:4913:G:H4'	3:L5:4914:C:O5'	2.18	0.42
4:L7:57:C:H2'	4:L7:58:A:H8	1.84	0.42
24:LT:119:ALA:O	24:LT:123:GLY:N	2.52	0.42
53:SM:19:GLN:HE22	53:SM:88:TRP:CD1	2.36	0.42
54:SP:81:ARG:NH1	54:SP:120:SER:OG	2.52	0.42
58:ST:84:ARG:HH12	83:S2:1605:G:P	2.42	0.42
64:Sg:283:PRO:O	64:Sg:285:GLN:NE2	2.52	0.42
66:SB:155:TYR:OH	83:S2:989:C:OP2	2.25	0.42
81:Sb:62:VAL:HG23	81:Sb:74:THR:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:692:G:N7	83:S2:693:A:N6	2.67	0.42
2:Et:4:C:H2'	2:Et:5:G:C8	2.54	0.42
2:Et:9:A:O2'	2:Et:45:G:N3	2.47	0.42
3:L5:239:C:OP1	29:LY:46:SER:OG	2.37	0.42
3:L5:267:G:H2'	3:L5:268:G:C8	2.54	0.42
3:L5:1398:A:OP1	31:La:136:LYS:NZ	2.52	0.42
5:L8:96:C:H5''	38:Lh:66:LYS:HG2	2.01	0.42
9:LD:291:GLN:NE2	14:LI:213:HIS:O	2.33	0.42
15:LJ:38:LYS:HD2	15:LJ:123:ILE:HD11	2.02	0.42
37:Lg:44:SER:OG	37:Lg:46:CYS:SG	2.69	0.42
47:Lr:97:ILE:HD13	47:Lr:107:ARG:HA	2.01	0.42
50:SD:46:THR:HG21	50:SD:79:PHE:CE2	2.54	0.42
50:SD:138:VAL:HG13	50:SD:182:LEU:HD21	2.01	0.42
50:SD:205:PRO:HB3	83:S2:1389:C:H4'	2.00	0.42
56:SR:44:LYS:HG3	56:SR:47:ARG:HH21	1.83	0.42
66:SB:136:ARG:HB2	66:SB:218:LEU:HD11	2.01	0.42
71:SI:165:GLN:HB3	71:SI:171:LEU:HD23	2.00	0.42
83:S2:115:U:H2'	83:S2:116:OMU:C6	2.49	0.42
83:S2:194:C:H2'	83:S2:195:C:C6	2.53	0.42
83:S2:363:A:N1	83:S2:397:G:O2'	2.46	0.42
83:S2:1093:A:H2'	83:S2:1094:C:C6	2.53	0.42
83:S2:1724:A:H2'	83:S2:1725:U:C6	2.54	0.42
2:Et:28:C:H2'	2:Et:29:A:H8	1.84	0.42
3:L5:99:A:H5''	18:LN:184:ILE:HD12	2.01	0.42
3:L5:221:C:H2'	3:L5:222:C:C6	2.54	0.42
3:L5:270:U:H2'	3:L5:271:C:C6	2.54	0.42
3:L5:1081:C:C2'	3:L5:1082:C:H5'	2.49	0.42
3:L5:1298:C:H2'	3:L5:1299:G:C8	2.54	0.42
3:L5:2876:OMG:HM22	3:L5:2877:G:H5'	2.00	0.42
3:L5:5053:U:H3'	3:L5:5054:C:C6	2.53	0.42
4:L7:112:U:H2'	4:L7:113:G:H8	1.84	0.42
6:LA:75:LEU:HD12	6:LA:75:LEU:HA	1.91	0.42
7:LB:49:TYR:OH	7:LB:179:HIS:ND1	2.49	0.42
8:LC:207:PRO:HB3	8:LC:249:PHE:CD2	2.55	0.42
8:LC:221:PHE:O	8:LC:222:ARG:HG2	2.20	0.42
9:LD:33:ARG:O	9:LD:37:VAL:HG22	2.20	0.42
22:LR:19:LYS:HB2	22:LR:19:LYS:HE2	1.85	0.42
22:LR:82:LYS:HA	22:LR:82:LYS:HD2	1.83	0.42
23:LS:83:ARG:HG3	23:LS:125:GLN:HB2	2.01	0.42
28:LX:80:PRO:HA	28:LX:98:PHE:HA	2.01	0.42
65:SA:11:LYS:O	65:SA:15:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SG:174:PRO:HB3	83:S2:65:C:C6	2.53	0.42
72:SJ:41:ARG:N	83:S2:642:U:OP1	2.51	0.42
74:SN:55:ARG:HD3	83:S2:1017:U:H5'	2.02	0.42
78:SX:22:TRP:HE3	78:SX:28:LYS:HD2	1.83	0.42
82:Se:58:ASN:ND2	83:S2:606:G:H1'	2.34	0.42
83:S2:349:A:H2'	83:S2:350:C:C6	2.53	0.42
83:S2:441:C:H2'	83:S2:442:C:C6	2.54	0.42
83:S2:600:G:H2'	83:S2:601:OMG:H8	1.83	0.42
83:S2:943:U:C2	83:S2:944:A:C8	3.07	0.42
83:S2:1084:A:OP1	83:S2:1858:G:O2'	2.29	0.42
83:S2:1407:U:H2'	83:S2:1408:U:C6	2.54	0.42
3:L5:264:C:H1'	38:Lh:112:ARG:HH21	1.85	0.42
3:L5:438:G:OP1	35:Le:16:ARG:NH1	2.43	0.42
3:L5:1294:A:H1'	3:L5:1296:G:N1	2.34	0.42
3:L5:1806:G:H2'	3:L5:1807:C:C6	2.54	0.42
3:L5:2378:G:N2	3:L5:2381:A:OP2	2.49	0.42
3:L5:2708:U:O2'	84:CI:79:ARG:CZ	2.55	0.42
3:L5:3772:U:H3	3:L5:3776:G:H22	1.66	0.42
3:L5:4115:G:O2'	3:L5:4116:C:O5'	2.35	0.42
3:L5:4678:G:N2	3:L5:4713:G:H1'	2.34	0.42
11:LF:29:LYS:HD2	11:LF:32:ARG:HH21	1.84	0.42
12:LG:148:GLU:OE2	18:LN:6:TYR:OH	2.35	0.42
16:LL:111:GLN:HA	16:LL:114:VAL:HG22	2.00	0.42
54:SP:100:LYS:HB2	83:S2:1240:A:C5	2.54	0.42
56:SR:52:GLY:O	56:SR:55:THR:OG1	2.37	0.42
64:Sg:183:LYS:HA	64:Sg:183:LYS:HD2	1.83	0.42
65:SA:34:MET:HE1	65:SA:162:PRO:HB3	2.01	0.42
70:SH:18:GLU:C	70:SH:20:GLU:H	2.28	0.42
72:SJ:176:LYS:HA	72:SJ:179:LYS:HG2	2.01	0.42
83:S2:1273:C:O2'	83:S2:1506:A:N1	2.50	0.42
83:S2:1620:A:H1'	83:S2:1624:U:OP2	2.19	0.42
3:L5:444:G:H2'	3:L5:445:U:H6	1.84	0.42
3:L5:493:G:O2'	3:L5:494:U:OP1	2.32	0.42
3:L5:728:U:H5''	11:LF:76:ARG:NH1	2.35	0.42
3:L5:1346:C:H2'	3:L5:1347:G:C8	2.55	0.42
3:L5:1631:A:C2	6:LA:204:MET:HG2	2.54	0.42
3:L5:1779:U:H2'	3:L5:1780:A:C8	2.55	0.42
3:L5:1895:G:H2'	3:L5:1896:A:O4'	2.18	0.42
3:L5:2385:U:H2'	3:L5:2386:U:C6	2.54	0.42
3:L5:2739:C:OP2	46:Lp:33:GLN:NE2	2.53	0.42
3:L5:4981:G:O6	7:LB:21:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LF:238:ASP:O	11:LF:241:ASN:ND2	2.51	0.42
18:LN:178:HIS:HA	18:LN:181:HIS:NE2	2.34	0.42
21:LQ:50:ARG:HH21	21:LQ:140:SER:HB2	1.84	0.42
24:LT:122:LYS:NZ	24:LT:124:THR:HB	2.34	0.42
48:Ls:58:ASN:C	48:Ls:62:ARG:HE	2.27	0.42
53:SM:17:ALA:O	53:SM:20:GLU:HG3	2.18	0.42
53:SM:91:LEU:HD23	53:SM:91:LEU:HA	1.85	0.42
53:SM:95:ASP:HB3	53:SM:99:LYS:HB3	2.01	0.42
64:Sg:5:MET:HB3	64:Sg:270:LEU:HD21	2.01	0.42
68:SE:126:VAL:HA	68:SE:141:THR:HA	2.02	0.42
77:SW:76:SER:OG	83:S2:1158:G:O3'	2.27	0.42
83:S2:29:G:H2'	83:S2:30:C:C6	2.55	0.42
83:S2:874:G:H2'	83:S2:875:A:C8	2.51	0.42
83:S2:1289:U:O4	83:S2:1311:C:N4	2.52	0.42
3:L5:2079:G:H2'	3:L5:2080:U:C6	2.54	0.42
3:L5:4304:A:OP2	3:L5:4305:G:N2	2.52	0.42
3:L5:4458:C:H2'	3:L5:4459:U:C6	2.54	0.42
3:L5:4460:U:H2'	3:L5:4461:C:H6	1.84	0.42
3:L5:4651:A:H2'	3:L5:4652:G:O4'	2.19	0.42
6:LA:80:GLU:HB2	6:LA:170:ALA:HA	2.00	0.42
9:LD:37:VAL:HG12	9:LD:50:ARG:HD3	2.00	0.42
23:LS:99:ASP:OD1	23:LS:100:LEU:N	2.51	0.42
51:SF:179:ASN:HB2	51:SF:187:SER:HB3	2.02	0.42
56:SR:114:LEU:HB2	56:SR:117:LEU:HG	2.01	0.42
76:SV:30:ALA:O	76:SV:60:ARG:HD3	2.20	0.42
80:Sa:12:LYS:HG3	80:Sa:15:ARG:HB2	2.02	0.42
3:L5:256:G:H2'	3:L5:257:C:C6	2.55	0.42
3:L5:330:G:N7	87:L5:5284:SPD:N1	2.67	0.42
3:L5:481:G:H2'	3:L5:482:G:H8	1.84	0.42
3:L5:1339:U:OP1	31:La:8:THR:OG1	2.32	0.42
3:L5:1523:A:N3	3:L5:4389:C:O2'	2.51	0.42
3:L5:1591:U:N3	3:L5:4555:U:OP1	2.44	0.42
3:L5:2558:C:H2'	3:L5:2559:G:C8	2.53	0.42
3:L5:4113:U:H3'	3:L5:4114:C:H4'	2.02	0.42
3:L5:4153:C:H2'	3:L5:4154:G:C8	2.55	0.42
3:L5:5002:U:H2'	3:L5:5003:U:H6	1.85	0.42
86:L5:5263:SPM:H111	86:L5:5263:SPM:H82	1.87	0.42
4:L7:7:G:H5''	9:LD:22:ARG:HD3	2.00	0.42
38:Lh:8:ASP:OD1	38:Lh:8:ASP:N	2.52	0.42
39:Li:76:ARG:HD3	39:Li:76:ARG:HA	1.81	0.42
60:SZ:41:ARG:HA	60:SZ:41:ARG:HD2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:Sg:39:THR:HG22	64:Sg:60:ARG:HG2	2.02	0.42
72:SJ:121:LYS:HZ1	83:S2:528:A:H5'	1.85	0.42
77:SW:62:VAL:HG11	81:Sb:8:LEU:HG	2.01	0.42
83:S2:96:C:H2'	83:S2:97:U:C6	2.55	0.42
83:S2:455:A:H2'	83:S2:456:C:H6	1.83	0.42
83:S2:601:OMG:H1'	83:S2:601:OMG:HM23	1.77	0.42
83:S2:876:C:H2'	83:S2:877:C:C6	2.54	0.42
83:S2:902:G:O2'	83:S2:903:A:O4'	2.38	0.42
3:L5:163:A:H2'	3:L5:164:G:H8	1.84	0.42
3:L5:441:G:H2'	3:L5:442:G:C8	2.55	0.42
3:L5:1779:U:OP2	9:LD:5:LYS:NZ	2.45	0.42
3:L5:2056:G:H4'	19:LO:18:ARG:HH22	1.84	0.42
3:L5:2090:U:H4'	3:L5:2091:C:H3'	2.01	0.42
3:L5:2561:C:H2'	3:L5:2562:G:O4'	2.19	0.42
3:L5:3600:G:H2'	3:L5:3601:C:C6	2.55	0.42
3:L5:4578:G:H2'	3:L5:4579:PSU:C6	2.55	0.42
3:L5:5015:G:H2'	3:L5:5016:A:C2	2.55	0.42
5:L8:41:A:H4'	40:Lj:59:THR:HG23	2.01	0.42
9:LD:289:ARG:O	9:LD:292:GLU:HG3	2.18	0.42
10:LE:203:ILE:O	10:LE:206:VAL:HG22	2.20	0.42
20:LP:60:PHE:O	20:LP:78:TRP:NE1	2.50	0.42
20:LP:122:ALA:HB3	20:LP:143:PRO:HG2	2.01	0.42
21:LQ:3:VAL:HG13	21:LQ:5:ILE:HG12	2.02	0.42
32:Lb:43:MET:HE2	32:Lb:47:LYS:NZ	2.34	0.42
34:Ld:25:TYR:CD1	34:Ld:88:LEU:HD13	2.55	0.42
36:Lf:45:LYS:NZ	36:Lf:108:SER:HA	2.35	0.42
37:Lg:33:LEU:HD23	37:Lg:33:LEU:HA	1.89	0.42
51:SF:123:GLU:OE1	61:Sc:63:ARG:NH2	2.53	0.42
58:ST:9:VAL:O	58:ST:11:GLN:NE2	2.48	0.42
58:ST:42:HIS:NE2	58:ST:43:LYS:HE3	2.34	0.42
68:SE:72:ILE:HD12	68:SE:77:ARG:HB2	2.02	0.42
78:SX:107:ARG:HG2	78:SX:112:VAL:HG22	2.02	0.42
79:SY:9:THR:H	83:S2:837:A:N6	2.18	0.42
83:S2:509:OMG:H2'	83:S2:510:G:H8	1.85	0.42
83:S2:853:C:C2	83:S2:854:A:C8	3.08	0.42
83:S2:1013:U:C2	83:S2:1014:G:C8	3.08	0.42
83:S2:1112:U:H2'	83:S2:1113:A:C8	2.55	0.42
1:Pt:22:U:H2'	1:Pt:23:C:H6	1.85	0.42
3:L5:99:A:H2'	3:L5:100:C:O2	2.20	0.42
3:L5:406:C:O2'	3:L5:407:A:OP1	2.33	0.42
3:L5:700:G:C6	3:L5:701:G:C6	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:919:C:OP1	17:LM:69:HIS:ND1	2.31	0.42
3:L5:5030:U:H2'	3:L5:5031:G:H8	1.85	0.42
6:LA:145:LYS:HD3	6:LA:145:LYS:HA	1.83	0.42
30:LZ:92:ASP:OD1	30:LZ:94:THR:OG1	2.34	0.42
30:LZ:135:ARG:HD2	30:LZ:135:ARG:HA	1.82	0.42
34:Ld:33:ILE:HD11	34:Ld:45:ALA:HA	2.01	0.42
53:SM:128:PHE:HA	53:SM:131:LYS:HG2	2.02	0.42
56:SR:126:MET:HG2	65:SA:43:SER:HB2	2.02	0.42
57:SS:132:ARG:HD3	83:S2:1623:A:N6	2.34	0.42
58:ST:23:LYS:HD3	58:ST:51:ASN:HD22	1.85	0.42
83:S2:28:U:H2'	83:S2:29:G:C8	2.53	0.42
83:S2:223:C:H2'	83:S2:224:A:H8	1.85	0.42
84:CI:63:ARG:HD2	84:CI:63:ARG:HA	1.85	0.42
3:L5:21:G:H1'	5:L8:103:A:N3	2.34	0.42
3:L5:120:A:N1	3:L5:148:C:O2'	2.45	0.42
3:L5:351:C:OP2	8:LC:197:ARG:NH1	2.35	0.42
3:L5:1677:PSU:H4'	3:L5:1680:G:C2	2.55	0.42
3:L5:1872:G:O2'	3:L5:4219:A:N3	2.42	0.42
3:L5:2295:C:H2'	3:L5:2296:G:H8	1.83	0.42
3:L5:2519:U:H1'	3:L5:2520:C:C6	2.55	0.42
3:L5:4061:G:C5	3:L5:4062:A:C8	3.07	0.42
3:L5:4208:U:OP1	3:L5:4334:U:O2'	2.32	0.42
3:L5:4232:U:H5'	45:Lo:3:ASN:HB3	2.02	0.42
6:LA:7:GLY:HA2	6:LA:10:LYS:HG3	2.02	0.42
7:LB:224:LYS:HD2	7:LB:340:THR:HG22	2.02	0.42
15:LJ:35:ARG:O	15:LJ:39:VAL:HG23	2.20	0.42
19:LO:61:ARG:HA	19:LO:70:PRO:HD2	2.00	0.42
30:LZ:88:ASP:OD1	30:LZ:88:ASP:N	2.40	0.42
47:Lr:47:LYS:O	47:Lr:103:ARG:HD2	2.20	0.42
53:SM:42:LEU:HD21	53:SM:50:CYS:SG	2.59	0.42
65:SA:134:LEU:HD21	65:SA:144:THR:HG21	2.02	0.42
66:SB:83:LYS:HD3	66:SB:106:THR:HG22	2.02	0.42
69:SG:92:ARG:NH1	83:S2:1738:C:OP1	2.39	0.42
70:SH:34:SER:OG	70:SH:78:ARG:NH2	2.50	0.42
71:SI:132:GLU:O	71:SI:136:ILE:HG23	2.20	0.42
77:SW:28:ARG:HB3	77:SW:29:PRO:HD3	2.01	0.42
83:S2:1129:G:H3'	83:S2:1130:G:N2	2.35	0.42
83:S2:1174:PSU:H2'	83:S2:1175:G:H8	1.85	0.42
83:S2:1324:G:H1	83:S2:1504:U:H3	1.68	0.42
83:S2:1442:OMU:HM23	83:S2:1442:OMU:H1'	1.90	0.42
83:S2:1708:C:H2'	83:S2:1709:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:86:U:H2'	3:L5:87:A:C8	2.54	0.41
3:L5:106:A:H2'	3:L5:107:G:O4'	2.19	0.41
3:L5:135:G:N3	3:L5:135:G:H2'	2.35	0.41
3:L5:423:G:H5'	20:LP:26:PHE:HZ	1.84	0.41
3:L5:982:U:H2'	3:L5:983:C:C6	2.55	0.41
3:L5:1978:C:H2'	3:L5:1979:A:O4'	2.20	0.41
3:L5:2422:OMC:HM23	3:L5:2422:OMC:H1'	1.91	0.41
3:L5:2481:G:H2'	3:L5:2482:C:C6	2.55	0.41
3:L5:2542:G:H2'	3:L5:2543:A:C8	2.55	0.41
3:L5:3893:C:O2'	3:L5:4979:A:N1	2.51	0.41
3:L5:4524:G:N3	7:LB:252:ALA:HB1	2.35	0.41
4:L7:75:G:N2	4:L7:100:A:OP2	2.42	0.41
5:L8:75:OMG:HM23	5:L8:75:OMG:H1'	1.79	0.41
7:LB:154:LYS:HE2	7:LB:154:LYS:HB2	1.72	0.41
11:LF:182:TYR:HB3	11:LF:200:ARG:HG3	2.02	0.41
13:LH:92:MET:HE2	13:LH:179:ILE:HG22	2.02	0.41
16:LL:194:ILE:HD12	16:LL:194:ILE:HA	1.88	0.41
19:LO:166:ILE:HG12	19:LO:169:ARG:HH21	1.85	0.41
21:LQ:43:PHE:CD2	21:LQ:133:GLY:HA3	2.55	0.41
30:LZ:57:MET:HG2	30:LZ:61:LYS:HD3	2.02	0.41
33:Lc:78:ASN:OD1	33:Lc:78:ASN:N	2.53	0.41
49:Lt:28:LEU:HD23	49:Lt:28:LEU:H	1.85	0.41
50:SD:55:THR:HA	50:SD:58:VAL:HG12	2.02	0.41
53:SM:20:GLU:HG2	53:SM:119:GLN:HB2	2.01	0.41
57:SS:24:ARG:H	57:SS:24:ARG:HG2	1.69	0.41
63:Sf:103:LEU:HG	63:Sf:104:LYS:H	1.85	0.41
64:Sg:159:ASN:HD21	64:Sg:161:SER:HB2	1.84	0.41
64:Sg:207:CYS:SG	64:Sg:219:TRP:HB2	2.60	0.41
64:Sg:230:LEU:HD21	64:Sg:259:TRP:CZ2	2.55	0.41
68:SE:195:ILE:HD13	68:SE:210:VAL:HG22	2.01	0.41
69:SG:77:LEU:HD12	69:SG:95:LYS:HD3	2.02	0.41
69:SG:133:LEU:HB2	83:S2:65:C:C2	2.55	0.41
81:Sb:34:ASP:O	81:Sb:79:PHE:HA	2.20	0.41
1:Pt:3:C:H42	1:Pt:70:A:H61	1.68	0.41
3:L5:252:C:H2'	3:L5:253:G:C8	2.55	0.41
3:L5:1172:C:O2'	3:L5:1173:G:H8	2.03	0.41
3:L5:1333:A:H2'	3:L5:1334:A:H8	1.84	0.41
3:L5:1510:G:H2'	3:L5:1511:U:H6	1.84	0.41
3:L5:1697:G:H2'	3:L5:1698:C:O4'	2.20	0.41
3:L5:1826:G:H4'	32:Lb:43:MET:HE3	2.01	0.41
3:L5:1979:A:H1'	3:L5:1988:G:N2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L8:36:G:C5	38:Lh:89:ARG:HD3	2.55	0.41
10:LE:282:TYR:HE1	36:Lf:31:GLU:HG2	1.84	0.41
24:LT:50:LYS:HB3	24:LT:50:LYS:HE2	1.79	0.41
24:LT:142:ARG:NH1	24:LT:144:ASN:OD1	2.53	0.41
29:LY:59:ARG:HB2	29:LY:103:LYS:HD2	2.02	0.41
48:Ls:119:CYS:SG	48:Ls:120:GLU:N	2.93	0.41
50:SD:136:VAL:HG12	50:SD:186:VAL:HG22	2.01	0.41
65:SA:122:LEU:HD22	65:SA:137:ALA:HB2	2.02	0.41
67:SC:74:LYS:HA	67:SC:74:LYS:HD3	1.88	0.41
83:S2:85:A:H2'	83:S2:86:C:H6	1.85	0.41
83:S2:1468:C:H2'	83:S2:1469:A:C8	2.55	0.41
83:S2:1733:U:H2'	83:S2:1734:G:O4'	2.20	0.41
3:L5:86:U:H2'	3:L5:87:A:H8	1.86	0.41
3:L5:327:U:HO2'	39:Li:30:ARG:HH11	1.63	0.41
3:L5:1844:G:H5''	32:Lb:25:ARG:NH2	2.35	0.41
3:L5:2696:A:H62	41:Lk:35:LYS:NZ	2.17	0.41
3:L5:2732:G:H2'	3:L5:2733:C:C6	2.55	0.41
3:L5:3799:A:N3	3:L5:4506:C:O2'	2.43	0.41
3:L5:3855:C:H2'	3:L5:3856:A:H8	1.85	0.41
3:L5:3930:U:H3	3:L5:4180:G:H1	1.69	0.41
4:L7:110:G:H2'	4:L7:111:C:C6	2.54	0.41
5:L8:19:C:H2'	5:L8:20:A:H8	1.85	0.41
33:Lc:60:ILE:HD13	33:Lc:93:THR:HG21	2.01	0.41
38:Lh:88:THR:HB	38:Lh:91:MET:HB2	2.03	0.41
44:Ln:2:ARG:NE	83:S2:1842:4AC:OP2	2.38	0.41
52:SK:26:ASP:HB3	52:SK:29:MET:HB2	2.02	0.41
61:Sc:44:ARG:NH1	61:Sc:61:SER:O	2.53	0.41
69:SG:149:LYS:HD2	69:SG:149:LYS:HA	1.93	0.41
70:SH:160:LYS:HD3	70:SH:189:PHE:HB3	2.00	0.41
71:SI:99:ASN:HB2	83:S2:377:G:O5'	2.21	0.41
73:SL:82:MET:HE3	73:SL:82:MET:HB2	1.95	0.41
78:SX:28:LYS:NZ	83:S2:1189:A:OP1	2.43	0.41
79:SY:111:LYS:NZ	83:S2:56:G:OP1	2.43	0.41
83:S2:1802:C:H2'	83:S2:1803:U:C6	2.55	0.41
3:L5:6:C:H2'	3:L5:7:C:C6	2.55	0.41
3:L5:171:U:H5'	16:LL:135:LYS:HD3	2.01	0.41
3:L5:466:A:H2'	3:L5:467:U:C6	2.56	0.41
3:L5:2264:C:H2'	3:L5:2265:G:O4'	2.20	0.41
3:L5:2404:A:O2'	40:Lj:12:ARG:O	2.32	0.41
7:LB:367:PHE:HB2	27:LW:1:MET:HB2	2.02	0.41
19:LO:149:TYR:O	19:LO:153:THR:OG1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Ls:160:LEU:HD11	48:Ls:175:LEU:HD21	2.02	0.41
56:SR:24:LEU:HD23	56:SR:34:VAL:HG21	2.03	0.41
66:SB:73:ASP:OD1	66:SB:73:ASP:N	2.53	0.41
68:SE:160:ILE:HD12	68:SE:162:ILE:HD11	2.02	0.41
68:SE:253:ASP:OD1	68:SE:253:ASP:N	2.54	0.41
75:SO:34:PHE:CE1	75:SO:36:SER:HB3	2.55	0.41
77:SW:57:ARG:HD2	83:S2:919:A:H4'	2.00	0.41
83:S2:626:G:N2	83:S2:626:G:OP2	2.52	0.41
83:S2:649:PSU:H2'	83:S2:650:A:C8	2.54	0.41
83:S2:1174:PSU:H2'	83:S2:1175:G:C8	2.55	0.41
83:S2:1304:U:H2'	83:S2:1305:C:C6	2.55	0.41
1:Pt:76:A:N7	3:L5:4548:A:N6	2.69	0.41
3:L5:169:G:O6	3:L5:170:C:N4	2.53	0.41
3:L5:432:U:H1'	86:L5:5293:SPM:H82	2.02	0.41
3:L5:1248:C:H2'	3:L5:1249:C:C6	2.56	0.41
3:L5:2326:G:H5''	35:Le:127:ALA:HB1	2.03	0.41
3:L5:3660:C:P	6:LA:241:ARG:HH22	2.43	0.41
3:L5:4460:U:H2'	3:L5:4461:C:C6	2.56	0.41
3:L5:4920:C:H2'	3:L5:4921:C:H6	1.85	0.41
8:LC:5:ARG:NE	8:LC:24:LEU:O	2.37	0.41
21:LQ:154:LYS:HB3	21:LQ:154:LYS:HE2	1.82	0.41
33:Lc:31:TYR:OH	33:Lc:59:GLU:OE1	2.28	0.41
45:Lo:33:LEU:HD12	45:Lo:38:LYS:HE3	2.02	0.41
49:Lt:11:LYS:HD2	49:Lt:11:LYS:HA	1.94	0.41
52:SK:57:TYR:HB3	52:SK:75:GLY:HA2	2.03	0.41
75:SO:140:THR:HB	83:S2:1046:PSU:H1'	2.02	0.41
79:SY:37:LYS:HG3	83:S2:571:U:H5''	2.02	0.41
83:S2:300:U:H2'	83:S2:301:A:C8	2.56	0.41
83:S2:588:G:OP2	83:S2:588:G:N2	2.39	0.41
83:S2:1047:C:H2'	83:S2:1048:G:O4'	2.21	0.41
83:S2:1128:C:H2'	83:S2:1129:G:C8	2.56	0.41
83:S2:1755:C:H2'	83:S2:1756:C:C6	2.55	0.41
2:Et:39:U:H2'	2:Et:40:C:C6	2.56	0.41
3:L5:267:G:H2'	3:L5:268:G:H8	1.85	0.41
3:L5:1307:A:H2'	3:L5:1308:C:H6	1.86	0.41
3:L5:1687:U:H2'	3:L5:1688:G:C8	2.56	0.41
3:L5:2412:A:H2'	3:L5:2413:U:C6	2.56	0.41
3:L5:2570:U:H2'	3:L5:2571:C:C6	2.56	0.41
3:L5:2890:C:H2'	3:L5:2891:U:C6	2.56	0.41
5:L8:78:G:H2'	5:L8:79:G:C8	2.56	0.41
7:LB:119:TYR:OH	7:LB:129:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LF:155:TYR:OH	11:LF:188:GLU:OE2	2.31	0.41
22:LR:80:LYS:HA	22:LR:80:LYS:HD2	1.87	0.41
23:LS:95:ARG:NH2	23:LS:112:ASP:OD2	2.53	0.41
34:Ld:114:PHE:HA	34:Ld:117:LEU:HD12	2.02	0.41
68:SE:247:THR:N	68:SE:250:GLU:OE2	2.51	0.41
70:SH:50:GLU:HG2	70:SH:60:ILE:HD13	2.03	0.41
72:SJ:150:ARG:HG3	83:S2:821:G:C6	2.56	0.41
83:S2:1681:U:H2'	83:S2:1682:C:C6	2.56	0.41
2:Et:27:U:H2'	2:Et:28:C:C6	2.56	0.41
2:Et:35:U:O4	51:SF:130:ARG:NH2	2.42	0.41
3:L5:429:A:H2'	3:L5:430:G:H8	1.86	0.41
3:L5:499:G:H2'	3:L5:499:G:N3	2.35	0.41
3:L5:979:C:OP2	10:LE:66:LYS:HD3	2.20	0.41
3:L5:980:U:H2'	3:L5:981:C:C6	2.55	0.41
3:L5:1702:C:H42	11:LF:36:LYS:NZ	2.19	0.41
3:L5:2018:C:H2'	3:L5:2019:C:H6	1.83	0.41
3:L5:2608:G:H2'	3:L5:2609:G:H8	1.85	0.41
3:L5:2696:A:OP1	41:Lk:26:LYS:NZ	2.42	0.41
3:L5:3933:G:H2'	3:L5:3934:G:H8	1.85	0.41
3:L5:4870:G:H5''	17:LM:91:TRP:CD2	2.55	0.41
6:LA:115:CYS:SG	6:LA:124:GLY:HA3	2.60	0.41
6:LA:131:GLY:H	6:LA:169:VAL:HG13	1.85	0.41
7:LB:397:ILE:O	7:LB:401:GLU:HG2	2.21	0.41
16:LL:49:ARG:O	16:LL:149:GLN:NE2	2.53	0.41
16:LL:116:ARG:NH2	16:LL:155:MET:O	2.49	0.41
21:LQ:59:PRO:HG3	21:LQ:143:ARG:HA	2.02	0.41
50:SD:15:GLY:HA3	62:Sd:50:ILE:HG23	2.03	0.41
50:SD:222:PRO:HB3	64:Sg:190:GLY:HA3	2.03	0.41
54:SP:120:SER:OG	54:SP:120:SER:O	2.38	0.41
64:Sg:241:PHE:CE2	64:Sg:248:LEU:HD12	2.55	0.41
64:Sg:314:ILE:HD12	64:Sg:314:ILE:HA	1.92	0.41
70:SH:118:ARG:HD3	70:SH:121:THR:HG21	2.02	0.41
72:SJ:38:ARG:NH2	83:S2:522:A:N7	2.69	0.41
77:SW:42:MET:HB3	77:SW:42:MET:HE2	1.86	0.41
83:S2:186:C:H2'	83:S2:187:G:H8	1.84	0.41
83:S2:376:A:H2'	83:S2:377:G:O4'	2.21	0.41
83:S2:1417:C:N3	83:S2:1422:G:N1	2.66	0.41
83:S2:1628:C:H2'	83:S2:1629:C:C6	2.55	0.41
3:L5:223:G:H4'	3:L5:225:G:N7	2.36	0.41
3:L5:1867:A:OP1	14:LI:13:LYS:NZ	2.50	0.41
3:L5:2448:G:H2'	3:L5:2449:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4934:A:H2'	3:L5:4935:C:C6	2.55	0.41
7:LB:80:GLU:OE2	7:LB:328:ASN:ND2	2.49	0.41
8:LC:279:LEU:HD23	8:LC:279:LEU:HA	1.89	0.41
9:LD:119:TYR:OH	9:LD:139:PRO:O	2.31	0.41
10:LE:115:TYR:CD1	47:Lr:115:SER:HB3	2.55	0.41
18:LN:155:VAL:O	18:LN:162:ARG:NH2	2.53	0.41
21:LQ:110:ARG:HG3	21:LQ:120:ILE:HD12	2.02	0.41
24:LT:127:GLN:NE2	24:LT:129:LYS:O	2.53	0.41
27:LW:52:THR:O	27:LW:56:ARG:HG2	2.21	0.41
29:LY:56:GLN:HB3	29:LY:67:ILE:HD13	2.03	0.41
57:SS:62:ASP:O	57:SS:65:GLU:HG3	2.21	0.41
64:Sg:106:LYS:HB3	64:Sg:125:ARG:HB2	2.01	0.41
68:SE:134:LYS:N	83:S2:298:G:OP1	2.40	0.41
70:SH:91:HIS:ND1	70:SH:169:LYS:HG2	2.35	0.41
83:S2:563:G:HO2'	83:S2:564:A:P	2.44	0.41
83:S2:1531:A:H2'	83:S2:1532:C:C6	2.55	0.41
83:S2:1570:G:O2'	83:S2:1614:A:O2'	2.36	0.41
2:Et:35:U:H2'	2:Et:36:U:C6	2.56	0.41
3:L5:302:C:H2'	3:L5:303:C:H6	1.86	0.41
3:L5:398:A2M:O5'	3:L5:398:A2M:H8	2.21	0.41
3:L5:1306:C:H2'	3:L5:1307:A:C8	2.53	0.41
3:L5:1405:C:N4	3:L5:1408:G:N3	2.43	0.41
3:L5:1413:C:H2'	3:L5:1414:C:H6	1.85	0.41
3:L5:1600:A:H5'	20:LP:133:HIS:HA	2.03	0.41
3:L5:1703:C:O2'	3:L5:1704:C:O5'	2.39	0.41
3:L5:1811:G:H2'	3:L5:1812:C:C6	2.56	0.41
3:L5:1914:C:H4'	19:LO:89:PRO:HD3	2.03	0.41
3:L5:2424:OMG:HM23	3:L5:2424:OMG:H1'	1.93	0.41
3:L5:2517:A:H5'	37:Lg:62:LYS:HD3	2.02	0.41
3:L5:3925:OMU:HM23	3:L5:3925:OMU:H1'	1.83	0.41
3:L5:4257:A:C2	15:LJ:60:PHE:HB3	2.56	0.41
3:L5:4364:G:H2'	3:L5:4365:C:C6	2.55	0.41
3:L5:4688:C:H2'	3:L5:4689:PSU:C6	2.56	0.41
3:L5:4892:A:H2'	3:L5:4893:A:O4'	2.20	0.41
3:L5:4979:A:OP1	7:LB:228:TYR:HB2	2.21	0.41
5:L8:39:G:H1'	5:L8:103:A:H61	1.85	0.41
6:LA:112:ILE:HG22	6:LA:135:THR:HG23	2.02	0.41
7:LB:337:VAL:HG11	7:LB:345:LEU:HD13	2.02	0.41
8:LC:159:GLU:HG3	8:LC:253:THR:HG21	2.01	0.41
8:LC:334:THR:HG21	11:LF:51:TYR:OH	2.21	0.41
14:LI:187:LYS:HE3	14:LI:189:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LJ:40:LEU:HD23	15:LJ:40:LEU:HA	1.91	0.41
17:LM:33:GLN:O	17:LM:33:GLN:HG2	2.20	0.41
18:LN:75:VAL:HG21	18:LN:80:THR:HG22	2.02	0.41
20:LP:112:LEU:HD23	20:LP:150:LEU:HD13	2.03	0.41
25:LU:22:THR:HA	25:LU:71:THR:HA	2.03	0.41
49:Lt:130:LYS:NZ	49:Lt:157:SER:O	2.53	0.41
51:SF:140:ASP:N	51:SF:140:ASP:OD1	2.54	0.41
54:SP:100:LYS:HD3	83:S2:1240:A:C8	2.56	0.41
55:SQ:31:LEU:HD12	55:SQ:33:LYS:HE2	2.03	0.41
57:SS:132:ARG:NH1	83:S2:1623:A:N1	2.69	0.41
64:Sg:205:SER:C	64:Sg:221:LEU:HD23	2.46	0.41
66:SB:35:ALA:O	66:SB:42:ARG:NE	2.53	0.41
67:SC:68:ARG:HG2	67:SC:277:HIS:HB2	2.02	0.41
68:SE:36:HIS:ND1	68:SE:85:GLY:HA3	2.36	0.41
69:SG:35:GLU:HG2	69:SG:114:VAL:HG21	2.03	0.41
69:SG:174:PRO:O	83:S2:77:A:O2'	2.31	0.41
69:SG:193:ALA:O	69:SG:196:LYS:N	2.53	0.41
70:SH:140:VAL:HG12	74:SN:19:ARG:HD3	2.02	0.41
71:SI:5:ARG:NE	83:S2:379:C:O2	2.54	0.41
80:Sa:32:LYS:NZ	83:S2:989:C:O2	2.54	0.41
82:Se:39:ASN:HA	82:Se:43:VAL:HG12	2.03	0.41
83:S2:688:U:H1'	83:S2:689:U:OP2	2.21	0.41
83:S2:1088:U:H4'	83:S2:1089:G:OP2	2.21	0.41
83:S2:1354:G:N2	83:S2:1357:A:OP2	2.38	0.41
83:S2:1671:G:H2'	83:S2:1672:U:H6	1.85	0.41
1:Pt:43:A:H2'	1:Pt:44:A:C8	2.56	0.41
2:Et:9:A:H4'	2:Et:47:U:P	2.61	0.41
3:L5:1350:C:H2'	3:L5:1351:G:C8	2.56	0.41
3:L5:1497:A:N6	21:LQ:175:GLU:O	2.54	0.41
3:L5:1727:U:H2'	3:L5:1728:U:C6	2.56	0.41
3:L5:2864:A:H2'	3:L5:2865:U:H6	1.85	0.41
3:L5:4617:G:OP2	7:LB:358:ARG:NH2	2.54	0.41
3:L5:4685:U:H2'	3:L5:4686:G:C8	2.56	0.41
4:L7:11:A:N1	4:L7:66:G:O2'	2.51	0.41
7:LB:117:ARG:HA	7:LB:177:LYS:HD2	2.03	0.41
14:LI:87:MET:HE3	14:LI:87:MET:HB2	1.93	0.41
22:LR:165:LYS:NZ	83:S2:908:A:OP2	2.46	0.41
52:SK:22:VAL:HG22	52:SK:68:TYR:HD1	1.84	0.41
66:SB:150:ILE:HG12	83:S2:1124:C:H5''	2.02	0.41
75:SO:46:ASP:OD1	75:SO:49:GLY:N	2.51	0.41
78:SX:123:VAL:HG12	78:SX:124:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:Sa:41:ILE:HD12	80:Sa:68:TYR:CD2	2.56	0.41
83:S2:66:G:H2'	83:S2:67:C:H4'	2.03	0.41
2:Et:39:U:H1'	51:SF:132:GLY:O	2.21	0.40
3:L5:305:A:P	18:LN:15:GLN:HE22	2.39	0.40
3:L5:1251:C:H2'	3:L5:1252:C:C6	2.56	0.40
3:L5:1259:G:H2'	3:L5:1260:G:C8	2.54	0.40
3:L5:1309:C:H2'	3:L5:1310:C:H6	1.86	0.40
3:L5:1354:A:N1	3:L5:1385:G:O2'	2.46	0.40
3:L5:4186:A:H2'	3:L5:4187:G:C8	2.56	0.40
7:LB:218:ASP:OD2	7:LB:348:ARG:NH2	2.41	0.40
12:LG:160:ASP:OD1	12:LG:160:ASP:N	2.54	0.40
48:Ls:102:LEU:HD11	48:Ls:187:LEU:HD23	2.02	0.40
50:SD:10:LYS:NZ	59:SU:111:GLU:HG3	2.36	0.40
53:SM:75:ASN:OD1	53:SM:76:LEU:N	2.54	0.40
55:SQ:67:ASP:OD2	55:SQ:69:ARG:NH1	2.54	0.40
61:Sc:13:ARG:CZ	61:Sc:35:MET:HE1	2.51	0.40
66:SB:167:LYS:HB2	66:SB:167:LYS:HE2	1.84	0.40
67:SC:195:LEU:HD23	67:SC:224:THR:HG23	2.03	0.40
72:SJ:114:VAL:HG23	72:SJ:126:ALA:HB1	2.03	0.40
78:SX:128:VAL:HG23	78:SX:138:LYS:HD2	2.03	0.40
79:SY:104:ARG:HG2	79:SY:108:LYS:HE2	2.02	0.40
83:S2:1144:A:H5'	83:S2:1355:C:H5	1.85	0.40
83:S2:1259:A:H1'	83:S2:1264:C:H42	1.86	0.40
3:L5:28:C:P	18:LN:193:ARG:HH22	2.44	0.40
3:L5:919:C:H2'	3:L5:920:C:H6	1.86	0.40
3:L5:1661:C:H2'	3:L5:1662:C:H6	1.86	0.40
3:L5:1811:G:H21	32:Lb:57:MET:HE2	1.86	0.40
3:L5:2732:G:H2'	3:L5:2733:C:H6	1.86	0.40
3:L5:2844:A:O2'	3:L5:4631:G:H4'	2.22	0.40
9:LD:203:ASN:OD1	9:LD:203:ASN:N	2.52	0.40
11:LF:147:LEU:O	11:LF:151:ASN:ND2	2.46	0.40
13:LH:44:GLU:OE2	17:LM:2:VAL:N	2.54	0.40
47:Lr:56:ASP:OD1	47:Lr:56:ASP:N	2.48	0.40
52:SK:64:TRP:CE3	62:Sd:23:VAL:HG22	2.56	0.40
55:SQ:34:VAL:HG11	55:SQ:84:ILE:HD13	2.03	0.40
55:SQ:90:LYS:HB3	55:SQ:90:LYS:HE2	1.86	0.40
64:Sg:207:CYS:HB3	64:Sg:221:LEU:HD21	2.03	0.40
73:SL:30:LYS:HA	73:SL:30:LYS:HD2	1.97	0.40
77:SW:28:ARG:NH2	83:S2:1093:A:H5''	2.36	0.40
79:SY:41:ARG:HH21	79:SY:53:ASP:HA	1.86	0.40
83:S2:430:C:H2'	83:S2:431:G:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
83:S2:1103:C:H2'	83:S2:1104:G:H8	1.86	0.40
83:S2:1269:G:H2'	83:S2:1270:G:C8	2.56	0.40
83:S2:1438:A:H2'	83:S2:1439:A:H8	1.84	0.40
1:Pt:18:G:H21	1:Pt:58:A:H5'	1.85	0.40
3:L5:218:A:H1'	3:L5:219:G:C8	2.56	0.40
3:L5:1419:G:H5''	21:LQ:71:LYS:NZ	2.36	0.40
3:L5:2364:OMG:HM23	3:L5:2364:OMG:H1'	1.94	0.40
3:L5:3758:U:H2'	3:L5:3765:G:N2	2.37	0.40
3:L5:4228:OMG:H5''	3:L5:4229:U:O4'	2.22	0.40
3:L5:4232:U:H5''	45:Lo:3:ASN:O	2.21	0.40
3:L5:4390:A:H2'	3:L5:4391:G:O4'	2.22	0.40
3:L5:4523:A2M:H5''	3:L5:4524:G:H5'	2.04	0.40
7:LB:294:LYS:HD3	7:LB:298:LEU:HD11	2.04	0.40
8:LC:154:VAL:HG11	8:LC:174:LEU:HD11	2.04	0.40
9:LD:122:GLN:NE2	9:LD:126:THR:HG22	2.36	0.40
12:LG:123:ALA:HA	12:LG:124:GLY:HA2	1.79	0.40
33:Lc:17:ARG:O	33:Lc:21:VAL:HG23	2.22	0.40
39:Li:90:LEU:HA	39:Li:93:VAL:HG22	2.03	0.40
56:SR:128:PHE:CD2	56:SR:129:LYS:HG3	2.57	0.40
58:ST:78:ILE:HD11	83:S2:1587:G:C5	2.56	0.40
62:Sd:22:ARG:HH21	62:Sd:37:ASN:HB2	1.87	0.40
64:Sg:191:HIS:CG	64:Sg:195:LEU:HD21	2.56	0.40
65:SA:172:GLY:HA3	65:SA:203:PHE:HD1	1.86	0.40
66:SB:136:ARG:O	66:SB:215:VAL:HA	2.22	0.40
67:SC:64:THR:HG22	67:SC:66:LEU:H	1.86	0.40
71:SI:81:VAL:HG22	71:SI:102:VAL:HG12	2.02	0.40
73:SL:153:LYS:HA	73:SL:153:LYS:HD3	1.86	0.40
83:S2:508:A:H3'	83:S2:509:OMG:C8	2.53	0.40
83:S2:929:G:H2'	83:S2:930:C:O4'	2.21	0.40
83:S2:1491:G:H2'	83:S2:1492:U:C6	2.57	0.40
3:L5:35:U:H4'	3:L5:1525:A:C2	2.57	0.40
3:L5:1095:A:N1	3:L5:1200:G:C6	2.90	0.40
3:L5:1628:C:OP2	6:LA:9:ARG:HD2	2.22	0.40
3:L5:1664:U:H2'	3:L5:1665:C:C6	2.56	0.40
3:L5:1982:G:H5'	49:Lt:28:LEU:HD13	2.03	0.40
3:L5:4918:C:H2'	3:L5:4919:G:C8	2.56	0.40
9:LD:239:MET:HA	9:LD:242:LYS:NZ	2.37	0.40
21:LQ:155:ALA:O	21:LQ:158:THR:OG1	2.35	0.40
41:Lk:68:GLU:HG3	41:Lk:70:LYS:H	1.86	0.40
52:SK:91:PRO:HB2	52:SK:94:LEU:HD23	2.03	0.40
58:ST:11:GLN:HB2	83:S2:1542:C:H4'	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SZ:102:LYS:HA	60:SZ:102:LYS:HD3	1.74	0.40
64:Sg:26:GLN:NE2	64:Sg:75:GLY:HA3	2.36	0.40
64:Sg:195:LEU:HA	64:Sg:211:GLY:HA3	2.04	0.40
68:SE:45:ILE:HD12	68:SE:80:ILE:HD11	2.04	0.40
68:SE:136:ILE:HD12	68:SE:149:TYR:CE1	2.57	0.40
72:SJ:11:LYS:NZ	83:S2:24:C:OP1	2.41	0.40
83:S2:99:A2M:HM'3	83:S2:99:A2M:H1'	1.64	0.40
83:S2:747:U:C2	83:S2:796:G:N1	2.89	0.40
83:S2:871:U:O2'	83:S2:873:G:OP1	2.30	0.40
83:S2:1227:G:C2	83:S2:1228:A:C8	3.09	0.40
83:S2:1231:C:O2'	83:S2:1253:A:N6	2.54	0.40
83:S2:1705:C:H2'	83:S2:1706:G:C8	2.56	0.40
2:Et:4:C:H2'	2:Et:5:G:H8	1.87	0.40
3:L5:1408:G:O2'	3:L5:1411:C:N4	2.54	0.40
3:L5:1410:U:H3	32:Lb:52:LYS:NZ	2.19	0.40
3:L5:1505:C:H2'	3:L5:1506:G:C8	2.56	0.40
3:L5:1554:A:OP1	46:Lp:5:THR:OG1	2.26	0.40
3:L5:1700:G:H5'	3:L5:1702:C:OP2	2.22	0.40
3:L5:1908:A:H2'	3:L5:1909:G:O4'	2.22	0.40
3:L5:3893:C:H2'	3:L5:3894:A:H8	1.87	0.40
3:L5:4237:C:H2'	3:L5:4238:G:C8	2.56	0.40
3:L5:4237:C:H2'	3:L5:4238:G:H8	1.87	0.40
3:L5:4563:U:C2	3:L5:4564:A:C8	3.09	0.40
7:LB:57:VAL:HG22	7:LB:73:VAL:HG22	2.03	0.40
7:LB:214:ASP:OD2	7:LB:362:LYS:HA	2.21	0.40
40:Lj:27:TYR:HA	40:Lj:34:CYS:HA	2.03	0.40
52:SK:32:HIS:ND1	52:SK:33:PRO:HD2	2.37	0.40
57:SS:10:GLN:HE21	57:SS:13:LEU:HG	1.86	0.40
58:ST:113:VAL:HG22	58:ST:123:LEU:HD23	2.03	0.40
61:Sc:10:LYS:HE2	61:Sc:34:PHE:HD2	1.86	0.40
64:Sg:258:ILE:HG23	64:Sg:267:VAL:HG23	2.04	0.40
67:SC:70:VAL:HG21	67:SC:93:ILE:HG23	2.04	0.40
71:SI:23:LYS:HG2	83:S2:434:G:OP1	2.21	0.40
77:SW:28:ARG:HH22	83:S2:1093:A:H5''	1.86	0.40
78:SX:46:HIS:CD2	78:SX:103:ALA:HB2	2.56	0.40
83:S2:1162:C:H2'	83:S2:1163:C:O4'	2.21	0.40
83:S2:1446:A:O2'	83:S2:1447:G:H5''	2.21	0.40
83:S2:1801:A:H2'	83:S2:1802:C:H6	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	LA	246/248 (99%)	230 (94%)	16 (6%)	0	100	100
7	LB	400/402 (100%)	386 (96%)	14 (4%)	0	100	100
8	LC	366/368 (100%)	354 (97%)	12 (3%)	0	100	100
9	LD	291/293 (99%)	282 (97%)	9 (3%)	0	100	100
10	LE	236/240 (98%)	221 (94%)	15 (6%)	0	100	100
11	LF	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
12	LG	239/241 (99%)	224 (94%)	15 (6%)	0	100	100
13	LH	188/190 (99%)	183 (97%)	5 (3%)	0	100	100
14	LI	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
15	LJ	168/176 (96%)	161 (96%)	7 (4%)	0	100	100
16	LL	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
17	LM	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
18	LN	201/203 (99%)	199 (99%)	2 (1%)	0	100	100
19	LO	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
20	LP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
21	LQ	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
22	LR	185/187 (99%)	180 (97%)	5 (3%)	0	100	100
23	LS	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
24	LT	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
25	LU	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
26	LV	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
27	LW	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
28	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
29	LY	132/134 (98%)	127 (96%)	5 (4%)	0	100	100
30	LZ	133/135 (98%)	125 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	La	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
32	Lb	105/109 (96%)	100 (95%)	5 (5%)	0	100	100
33	Lc	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
34	Ld	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
35	Le	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
36	Lf	107/109 (98%)	107 (100%)	0	0	100	100
37	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
38	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
39	Li	100/102 (98%)	100 (100%)	0	0	100	100
40	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
41	Lk	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
42	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
43	Lm	50/52 (96%)	50 (100%)	0	0	100	100
44	Ln	22/24 (92%)	22 (100%)	0	0	100	100
45	Lo	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
46	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
47	Lr	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
48	Ls	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
49	Lt	128/141 (91%)	112 (88%)	16 (12%)	0	100	100
50	SD	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
51	SF	187/189 (99%)	174 (93%)	13 (7%)	0	100	100
52	SK	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
53	SM	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
54	SP	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
55	SQ	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
56	SR	133/135 (98%)	125 (94%)	7 (5%)	1 (1%)	16	44
57	SS	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
58	ST	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
59	SU	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
60	SZ	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
61	Sc	62/64 (97%)	60 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	Sd	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
63	Sf	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
64	Sg	311/313 (99%)	295 (95%)	16 (5%)	0	100	100
65	SA	219/221 (99%)	206 (94%)	13 (6%)	0	100	100
66	SB	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
67	SC	218/222 (98%)	207 (95%)	11 (5%)	0	100	100
68	SE	260/262 (99%)	251 (96%)	9 (4%)	0	100	100
69	SG	235/237 (99%)	225 (96%)	10 (4%)	0	100	100
70	SH	182/186 (98%)	169 (93%)	13 (7%)	0	100	100
71	SI	204/206 (99%)	197 (97%)	7 (3%)	0	100	100
72	SJ	183/185 (99%)	175 (96%)	7 (4%)	1 (0%)	24	55
73	SL	151/153 (99%)	147 (97%)	4 (3%)	0	100	100
74	SN	148/150 (99%)	147 (99%)	1 (1%)	0	100	100
75	SO	135/140 (96%)	126 (93%)	9 (7%)	0	100	100
76	SV	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
77	SW	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
78	SX	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
79	SY	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
80	Sa	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
81	Sb	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
82	Se	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
84	CI	29/31 (94%)	29 (100%)	0	0	100	100
All	All	11672/11860 (98%)	11194 (96%)	476 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	LA	190/190 (100%)	190 (100%)	0	100	100
7	LB	348/348 (100%)	348 (100%)	0	100	100
8	LC	306/306 (100%)	306 (100%)	0	100	100
9	LD	246/247 (100%)	246 (100%)	0	100	100
10	LE	212/212 (100%)	212 (100%)	0	100	100
11	LF	194/194 (100%)	194 (100%)	0	100	100
12	LG	203/205 (99%)	203 (100%)	0	100	100
13	LH	169/169 (100%)	169 (100%)	0	100	100
14	LI	180/180 (100%)	180 (100%)	0	100	100
15	LJ	143/148 (97%)	143 (100%)	0	100	100
16	LL	176/176 (100%)	176 (100%)	0	100	100
17	LM	118/118 (100%)	118 (100%)	0	100	100
18	LN	171/171 (100%)	171 (100%)	0	100	100
19	LO	173/173 (100%)	173 (100%)	0	100	100
20	LP	134/134 (100%)	134 (100%)	0	100	100
21	LQ	164/164 (100%)	164 (100%)	0	100	100
22	LR	166/166 (100%)	166 (100%)	0	100	100
23	LS	156/156 (100%)	156 (100%)	0	100	100
24	LT	139/139 (100%)	139 (100%)	0	100	100
25	LU	91/91 (100%)	91 (100%)	0	100	100
26	LV	101/101 (100%)	101 (100%)	0	100	100
27	LW	95/97 (98%)	95 (100%)	0	100	100
28	LX	108/108 (100%)	108 (100%)	0	100	100
29	LY	124/124 (100%)	124 (100%)	0	100	100
30	LZ	117/117 (100%)	117 (100%)	0	100	100
31	La	120/120 (100%)	120 (100%)	0	100	100
32	Lb	88/90 (98%)	88 (100%)	0	100	100
33	Lc	83/83 (100%)	83 (100%)	0	100	100
34	Ld	98/98 (100%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	Le	114/114 (100%)	114 (100%)	0	100	100
36	Lf	88/88 (100%)	88 (100%)	0	100	100
37	Lg	98/98 (100%)	98 (100%)	0	100	100
38	Lh	109/109 (100%)	109 (100%)	0	100	100
39	Li	86/86 (100%)	86 (100%)	0	100	100
40	Lj	73/73 (100%)	73 (100%)	0	100	100
41	Lk	64/64 (100%)	64 (100%)	0	100	100
42	Ll	47/47 (100%)	47 (100%)	0	100	100
43	Lm	48/48 (100%)	48 (100%)	0	100	100
44	Ln	23/23 (100%)	23 (100%)	0	100	100
45	Lo	93/93 (100%)	93 (100%)	0	100	100
46	Lp	74/74 (100%)	74 (100%)	0	100	100
47	Lr	109/109 (100%)	109 (100%)	0	100	100
48	Ls	162/164 (99%)	162 (100%)	0	100	100
49	Lt	107/115 (93%)	107 (100%)	0	100	100
50	SD	190/190 (100%)	190 (100%)	0	100	100
51	SF	159/159 (100%)	159 (100%)	0	100	100
52	SK	89/89 (100%)	89 (100%)	0	100	100
53	SM	102/104 (98%)	102 (100%)	0	100	100
54	SP	107/107 (100%)	107 (100%)	0	100	100
55	SQ	119/119 (100%)	119 (100%)	0	100	100
56	SR	122/122 (100%)	122 (100%)	0	100	100
57	SS	126/126 (100%)	126 (100%)	0	100	100
58	ST	113/113 (100%)	113 (100%)	0	100	100
59	SU	94/94 (100%)	94 (100%)	0	100	100
60	SZ	66/66 (100%)	66 (100%)	0	100	100
61	Sc	57/57 (100%)	57 (100%)	0	100	100
62	Sd	48/48 (100%)	48 (100%)	0	100	100
63	Sf	60/60 (100%)	60 (100%)	0	100	100
64	Sg	272/272 (100%)	272 (100%)	0	100	100
65	SA	183/183 (100%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	SB	195/195 (100%)	195 (100%)	0	100	100
67	SC	186/188 (99%)	186 (100%)	0	100	100
68	SE	224/224 (100%)	224 (100%)	0	100	100
69	SG	207/207 (100%)	207 (100%)	0	100	100
70	SH	166/166 (100%)	166 (100%)	0	100	100
71	SI	178/178 (100%)	178 (100%)	0	100	100
72	SJ	161/161 (100%)	161 (100%)	0	100	100
73	SL	137/137 (100%)	137 (100%)	0	100	100
74	SN	130/130 (100%)	130 (100%)	0	100	100
75	SO	107/110 (97%)	107 (100%)	0	100	100
76	SV	67/67 (100%)	67 (100%)	0	100	100
77	SW	112/112 (100%)	112 (100%)	0	100	100
78	SX	113/113 (100%)	113 (100%)	0	100	100
79	SY	113/113 (100%)	113 (100%)	0	100	100
80	Sa	89/89 (100%)	89 (100%)	0	100	100
81	Sb	75/75 (100%)	75 (100%)	0	100	100
82	Se	47/47 (100%)	47 (100%)	0	100	100
84	CI	25/25 (100%)	25 (100%)	0	100	100
All	All	10147/10176 (100%)	10147 (100%)	0	100	100

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

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

Mol	Chain	Res	Type
6	LA	38	HIS
6	LA	97	ASN
7	LB	68	ASN
7	LB	145	GLN
7	LB	184	GLN
7	LB	203	GLN
7	LB	204	GLN
7	LB	209	GLN
7	LB	289	GLN
8	LC	329	ASN

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Mol	Chain	Res	Type
8	LC	347	HIS
9	LD	202	GLN
10	LE	227	HIS
11	LF	39	GLN
12	LG	64	GLN
12	LG	112	GLN
13	LH	78	GLN
13	LH	98	HIS
13	LH	138	GLN
13	LH	163	GLN
14	LI	59	GLN
15	LJ	110	GLN
17	LM	34	ASN
17	LM	66	HIS
18	LN	87	HIS
18	LN	109	HIS
18	LN	117	ASN
19	LO	50	ASN
20	LP	75	GLN
20	LP	97	ASN
20	LP	116	HIS
23	LS	23	HIS
23	LS	50	GLN
23	LS	125	GLN
25	LU	94	ASN
26	LV	77	HIS
27	LW	50	ASN
27	LW	79	GLN
29	LY	61	HIS
31	La	34	ASN
31	La	67	GLN
31	La	120	GLN
33	Lc	19	GLN
33	Lc	72	HIS
35	Le	52	GLN
36	Lf	99	HIS
43	Lm	117	HIS
43	Lm	120	ASN
48	Ls	179	ASN
49	Lt	65	GLN
49	Lt	115	GLN
49	Lt	149	HIS

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Mol	Chain	Res	Type
51	SF	29	GLN
51	SF	79	HIS
52	SK	28	HIS
52	SK	32	HIS
52	SK	50	GLN
53	SM	19	GLN
55	SQ	77	HIS
57	SS	87	GLN
59	SU	81	GLN
62	Sd	37	ASN
63	Sf	93	HIS
64	Sg	119	GLN
64	Sg	159	ASN
64	Sg	272	GLN
64	Sg	285	GLN
65	SA	9	GLN
65	SA	50	ASN
65	SA	84	GLN
65	SA	141	ASN
66	SB	76	ASN
66	SB	101	HIS
66	SB	202	GLN
67	SC	267	GLN
67	SC	277	HIS
68	SE	50	ASN
70	SH	76	GLN
70	SH	165	ASN
71	SI	35	ASN
71	SI	181	GLN
73	SL	11	GLN
74	SN	105	ASN
76	SV	35	ASN
77	SW	5	ASN
77	SW	90	GLN
78	SX	16	HIS
79	SY	89	HIS
81	Sb	51	GLN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Pt	72/74 (97%)	15 (20%)	0
2	Et	73/75 (97%)	25 (34%)	0
3	L5	3643/3655 (99%)	726 (19%)	16 (0%)
4	L7	119/120 (99%)	9 (7%)	0
5	L8	155/156 (99%)	21 (13%)	0
83	S2	1714/1740 (98%)	369 (21%)	3 (0%)
All	All	5776/5820 (99%)	1165 (20%)	19 (0%)

All (1165) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Pt	9	A
1	Pt	13	U
1	Pt	19	G
1	Pt	21	A
1	Pt	46	G
1	Pt	47	U
1	Pt	48	C
1	Pt	49	C
1	Pt	58	A
1	Pt	59	A
1	Pt	66	C
1	Pt	67	G
1	Pt	72	C
1	Pt	74	C
1	Pt	76	A
2	Et	9	A
2	Et	10	G
2	Et	11	C
2	Et	19	G
2	Et	20	U
2	Et	21	A
2	Et	31	A
2	Et	33	U
2	Et	36	U
2	Et	40	C
2	Et	42	G
2	Et	46	G
2	Et	47	U
2	Et	48	C
2	Et	49	C

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Mol	Chain	Res	Type
2	Et	55	U
2	Et	58	A
2	Et	60	U
2	Et	61	C
2	Et	65	G
2	Et	66	U
2	Et	70	G
2	Et	72	C
2	Et	73	G
2	Et	76	A
3	L5	25	A
3	L5	30	C
3	L5	39	A
3	L5	42	A
3	L5	48	G
3	L5	56	A
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	66	A
3	L5	73	A
3	L5	74	G
3	L5	91	G
3	L5	98	A
3	L5	104	G
3	L5	108	A
3	L5	109	G
3	L5	110	C
3	L5	119	G
3	L5	120	A
3	L5	132	G
3	L5	133	C
3	L5	134	G
3	L5	135	G
3	L5	136	C
3	L5	145	G
3	L5	159	C
3	L5	165	A
3	L5	181	C
3	L5	182	G
3	L5	183	C
3	L5	184	U

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Mol	Chain	Res	Type
3	L5	185	C
3	L5	186	G
3	L5	187	U
3	L5	188	G
3	L5	189	G
3	L5	200	U
3	L5	209	U
3	L5	210	C
3	L5	216	C
3	L5	218	A
3	L5	234	G
3	L5	237	G
3	L5	255	C
3	L5	256	G
3	L5	261	G
3	L5	262	G
3	L5	263	G
3	L5	264	C
3	L5	265	C
3	L5	266	C
3	L5	267	G
3	L5	280	G
3	L5	297	U
3	L5	306	A
3	L5	315	G
3	L5	316	U
3	L5	340	C
3	L5	373	G
3	L5	387	G
3	L5	388	A
3	L5	407	A
3	L5	409	G
3	L5	410	A
3	L5	411	G
3	L5	412	G
3	L5	413	G
3	L5	432	U
3	L5	440	U
3	L5	449	C
3	L5	452	A
3	L5	453	G
3	L5	454	U

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Mol	Chain	Res	Type
3	L5	456	C
3	L5	457	G
3	L5	467	U
3	L5	468	U
3	L5	484	U
3	L5	485	C
3	L5	486	C
3	L5	489	C
3	L5	493	G
3	L5	494	U
3	L5	497	G
3	L5	498	C
3	L5	499	G
3	L5	500	G
3	L5	502	C
3	L5	503	C
3	L5	504	G
3	L5	509	A
3	L5	510	U
3	L5	512	U
3	L5	513	U
3	L5	514	U
3	L5	518	G
3	L5	643	C
3	L5	646	G
3	L5	654	C
3	L5	655	C
3	L5	656	C
3	L5	657	C
3	L5	659	G
3	L5	666	G
3	L5	667	A
3	L5	668	C
3	L5	669	C
3	L5	672	C
3	L5	673	C
3	L5	685	C
3	L5	686	A
3	L5	687	U
3	L5	704	C
3	L5	730	G
3	L5	731	G

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Mol	Chain	Res	Type
3	L5	738	C
3	L5	739	G
3	L5	742	G
3	L5	746	A
3	L5	759	G
3	L5	904	C
3	L5	905	C
3	L5	910	G
3	L5	913	U
3	L5	914	U
3	L5	915	A
3	L5	917	A
3	L5	923	C
3	L5	924	C
3	L5	932	A
3	L5	933	G
3	L5	935	A
3	L5	936	C
3	L5	941	C
3	L5	943	A
3	L5	944	A
3	L5	945	U
3	L5	956	A
3	L5	958	G
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	962	C
3	L5	965	G
3	L5	966	A
3	L5	967	C
3	L5	969	C
3	L5	970	G
3	L5	982	U
3	L5	985	C
3	L5	1070	G
3	L5	1071	C
3	L5	1072	C
3	L5	1075	G
3	L5	1082	C
3	L5	1083	U
3	L5	1168	G

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Mol	Chain	Res	Type
3	L5	1171	G
3	L5	1172	C
3	L5	1173	G
3	L5	1179	U
3	L5	1180	C
3	L5	1181	C
3	L5	1182	C
3	L5	1183	C
3	L5	1184	A
3	L5	1187	G
3	L5	1202	C
3	L5	1203	G
3	L5	1210	C
3	L5	1211	G
3	L5	1214	C
3	L5	1215	C
3	L5	1219	G
3	L5	1222	A
3	L5	1241	C
3	L5	1246	G
3	L5	1253	G
3	L5	1254	A
3	L5	1257	A
3	L5	1258	G
3	L5	1266	G
3	L5	1267	C
3	L5	1269	G
3	L5	1271	G
3	L5	1272	C
3	L5	1273	G
3	L5	1275	G
3	L5	1280	C
3	L5	1284	G
3	L5	1287	G
3	L5	1293	G
3	L5	1294	A
3	L5	1295	C
3	L5	1296	G
3	L5	1301	C
3	L5	1302	U
3	L5	1314	C
3	L5	1326	A2M

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Mol	Chain	Res	Type
3	L5	1337	A
3	L5	1354	A
3	L5	1359	G
3	L5	1365	C
3	L5	1366	G
3	L5	1367	C
3	L5	1387	A
3	L5	1394	G
3	L5	1397	A
3	L5	1403	G
3	L5	1404	G
3	L5	1407	C
3	L5	1409	C
3	L5	1410	U
3	L5	1411	C
3	L5	1414	C
3	L5	1415	G
3	L5	1417	C
3	L5	1420	A
3	L5	1437	C
3	L5	1439	C
3	L5	1442	C
3	L5	1443	A
3	L5	1444	G
3	L5	1446	C
3	L5	1447	C
3	L5	1457	G
3	L5	1482	G
3	L5	1483	C
3	L5	1497	A
3	L5	1498	G
3	L5	1502	G
3	L5	1504	G
3	L5	1517	G
3	L5	1524	A2M
3	L5	1534	A2M
3	L5	1535	C
3	L5	1537	A
3	L5	1547	A
3	L5	1566	C
3	L5	1578	U
3	L5	1591	U

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Mol	Chain	Res	Type
3	L5	1596	U
3	L5	1621	A
3	L5	1624	G
3	L5	1625	OMG
3	L5	1631	A
3	L5	1633	G
3	L5	1634	A
3	L5	1638	A
3	L5	1640	C
3	L5	1641	G
3	L5	1642	A
3	L5	1654	G
3	L5	1661	C
3	L5	1676	C
3	L5	1677	PSU
3	L5	1678	C
3	L5	1697	G
3	L5	1699	A
3	L5	1700	G
3	L5	1701	A
3	L5	1702	C
3	L5	1704	C
3	L5	1705	G
3	L5	1717	C
3	L5	1718	C
3	L5	1719	A
3	L5	1726	U
3	L5	1731	C
3	L5	1734	G
3	L5	1742	A
3	L5	1750	G
3	L5	1753	G
3	L5	1755	C
3	L5	1757	U
3	L5	1758	G
3	L5	1761	G
3	L5	1762	C
3	L5	1763	C
3	L5	1764	G
3	L5	1765	A
3	L5	1766	A
3	L5	1767	A

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Mol	Chain	Res	Type
3	L5	1768	C
3	L5	1770	A
3	L5	1787	A
3	L5	1804	A
3	L5	1806	G
3	L5	1810	G
3	L5	1815	G
3	L5	1821	G
3	L5	1822	U
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1855	G
3	L5	1869	G
3	L5	1882	U
3	L5	1892	A
3	L5	1893	C
3	L5	1897	A
3	L5	1917	A
3	L5	1918	U
3	L5	1919	G
3	L5	1920	C
3	L5	1921	C
3	L5	1922	G
3	L5	1925	G
3	L5	1931	C
3	L5	1932	A
3	L5	1936	C
3	L5	1948	G
3	L5	1951	G
3	L5	1961	G
3	L5	1962	A
3	L5	1974	U
3	L5	1975	G
3	L5	1978	C
3	L5	1980	U
3	L5	1981	G
3	L5	1982	G
3	L5	1983	A
3	L5	1984	A
3	L5	1985	G
3	L5	1986	U

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Mol	Chain	Res	Type
3	L5	1990	A
3	L5	1991	A
3	L5	1993	C
3	L5	1997	U
3	L5	1998	A
3	L5	1999	A
3	L5	2001	G
3	L5	2002	A
3	L5	2003	G
3	L5	2004	U
3	L5	2005	G
3	L5	2007	G
3	L5	2011	C
3	L5	2014	C
3	L5	2017	A
3	L5	2018	C
3	L5	2024	G
3	L5	2026	A
3	L5	2046	G
3	L5	2048	U
3	L5	2055	G
3	L5	2056	G
3	L5	2069	A
3	L5	2084	C
3	L5	2085	G
3	L5	2092	G
3	L5	2093	A
3	L5	2095	A
3	L5	2096	G
3	L5	2097	U
3	L5	2098	G
3	L5	2101	C
3	L5	2102	G
3	L5	2107	C
3	L5	2110	C
3	L5	2111	G
3	L5	2112	G
3	L5	2250	C
3	L5	2252	G
3	L5	2253	A
3	L5	2256	C
3	L5	2258	C

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Mol	Chain	Res	Type
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2313	A
3	L5	2331	G
3	L5	2333	G
3	L5	2345	G
3	L5	2348	G
3	L5	2351	OMC
3	L5	2360	A
3	L5	2364	OMG
3	L5	2395	A
3	L5	2397	G
3	L5	2417	A
3	L5	2425	U
3	L5	2450	G
3	L5	2453	A
3	L5	2464	C
3	L5	2465	C
3	L5	2469	C
3	L5	2471	G
3	L5	2474	G
3	L5	2475	G
3	L5	2478	C
3	L5	2479	G
3	L5	2483	G
3	L5	2484	A
3	L5	2485	U
3	L5	2486	G
3	L5	2487	G
3	L5	2488	C
3	L5	2489	C
3	L5	2490	U
3	L5	2494	U
3	L5	2504	C
3	L5	2505	C
3	L5	2506	G
3	L5	2513	A
3	L5	2519	U
3	L5	2520	C
3	L5	2529	A
3	L5	2537	A

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Mol	Chain	Res	Type
3	L5	2544	G
3	L5	2546	G
3	L5	2547	G
3	L5	2554	U
3	L5	2555	G
3	L5	2556	G
3	L5	2559	G
3	L5	2560	C
3	L5	2565	A
3	L5	2573	A
3	L5	2583	C
3	L5	2587	A
3	L5	2589	C
3	L5	2627	C
3	L5	2653	C
3	L5	2662	G
3	L5	2669	C
3	L5	2670	C
3	L5	2675	G
3	L5	2676	A
3	L5	2687	U
3	L5	2694	G
3	L5	2695	A
3	L5	2696	A
3	L5	2706	G
3	L5	2707	U
3	L5	2708	U
3	L5	2709	C
3	L5	2710	C
3	L5	2711	G
3	L5	2712	G
3	L5	2721	G
3	L5	2724	G
3	L5	2726	G
3	L5	2738	C
3	L5	2739	C
3	L5	2742	G
3	L5	2743	A
3	L5	2746	A
3	L5	2761	U
3	L5	2762	G
3	L5	2763	U

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Mol	Chain	Res	Type
3	L5	2769	U
3	L5	2770	C
3	L5	2788	U
3	L5	2790	U
3	L5	2806	A
3	L5	2814	C
3	L5	2815	A2M
3	L5	2826	U
3	L5	2827	G
3	L5	2838	G
3	L5	2855	G
3	L5	2867	C
3	L5	2877	G
3	L5	2894	A
3	L5	2895	A
3	L5	2900	U
3	L5	2902	G
3	L5	2903	G
3	L5	2904	U
3	L5	2905	C
3	L5	2907	G
3	L5	2908	U
3	L5	3590	G
3	L5	3591	C
3	L5	3594	C
3	L5	3595	U
3	L5	3596	A
3	L5	3597	G
3	L5	3604	A
3	L5	3605	C
3	L5	3626	G
3	L5	3635	A
3	L5	3644	U
3	L5	3646	A
3	L5	3648	A
3	L5	3662	A
3	L5	3664	G
3	L5	3670	C
3	L5	3673	C
3	L5	3674	G
3	L5	3701	OMC
3	L5	3710	G

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Mol	Chain	Res	Type
3	L5	3711	A
3	L5	3713	U
3	L5	3726	A
3	L5	3727	A
3	L5	3748	A
3	L5	3753	G
3	L5	3760	A
3	L5	3770	U
3	L5	3774	A
3	L5	3775	A
3	L5	3776	G
3	L5	3777	G
3	L5	3785	A2M
3	L5	3786	U
3	L5	3792	OMG
3	L5	3811	G
3	L5	3812	C
3	L5	3814	U
3	L5	3817	A
3	L5	3819	G
3	L5	3824	A
3	L5	3838	U
3	L5	3839	G
3	L5	3840	U
3	L5	3867	A2M
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3880	G
3	L5	3885	G
3	L5	3892	U
3	L5	3897	G
3	L5	3901	A
3	L5	3906	A
3	L5	3907	G
3	L5	3908	A
3	L5	3915	U
3	L5	3923	A
3	L5	3938	G
3	L5	3939	G
3	L5	3942	A
3	L5	3944	G

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Mol	Chain	Res	Type
3	L5	3947	A
3	L5	3949	A
3	L5	3950	U
3	L5	3953	G
3	L5	4057	C
3	L5	4058	U
3	L5	4059	C
3	L5	4060	U
3	L5	4061	G
3	L5	4062	A
3	L5	4064	C
3	L5	4068	U
3	L5	4076	G
3	L5	4084	G
3	L5	4093	G
3	L5	4095	G
3	L5	4097	G
3	L5	4098	A
3	L5	4099	G
3	L5	4101	C
3	L5	4104	G
3	L5	4108	G
3	L5	4111	U
3	L5	4114	C
3	L5	4115	G
3	L5	4116	C
3	L5	4117	U
3	L5	4122	G
3	L5	4127	A
3	L5	4141	G
3	L5	4142	C
3	L5	4143	G
3	L5	4144	C
3	L5	4146	G
3	L5	4149	C
3	L5	4150	G
3	L5	4162	C
3	L5	4163	U
3	L5	4168	G
3	L5	4170	A
3	L5	4177	C
3	L5	4183	G

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Mol	Chain	Res	Type
3	L5	4184	G
3	L5	4191	G
3	L5	4203	A
3	L5	4212	A
3	L5	4222	G
3	L5	4225	G
3	L5	4229	U
3	L5	4233	A
3	L5	4242	U
3	L5	4251	A
3	L5	4254	G
3	L5	4257	A
3	L5	4258	C
3	L5	4265	U
3	L5	4268	A
3	L5	4273	A
3	L5	4281	A
3	L5	4282	A
3	L5	4291	G
3	L5	4296	PSU
3	L5	4304	A
3	L5	4305	G
3	L5	4314	C
3	L5	4319	C
3	L5	4329	G
3	L5	4330	G
3	L5	4332	C
3	L5	4349	C
3	L5	4350	C
3	L5	4354	U
3	L5	4373	G
3	L5	4376	A
3	L5	4377	G
3	L5	4378	A
3	L5	4379	A
3	L5	4387	C
3	L5	4391	G
3	L5	4394	A
3	L5	4405	G
3	L5	4420	U
3	L5	4421	C
3	L5	4422	A

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Mol	Chain	Res	Type
3	L5	4438	U
3	L5	4448	G
3	L5	4449	A
3	L5	4452	U
3	L5	4464	A
3	L5	4466	C
3	L5	4475	G
3	L5	4488	A
3	L5	4500	PSU
3	L5	4512	U
3	L5	4513	A
3	L5	4515	G
3	L5	4519	C
3	L5	4524	G
3	L5	4545	G
3	L5	4548	A
3	L5	4557	U
3	L5	4560	C
3	L5	4567	G
3	L5	4575	G
3	L5	4584	A
3	L5	4589	A
3	L5	4590	A2M
3	L5	4601	U
3	L5	4617	G
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4652	G
3	L5	4656	A
3	L5	4657	U
3	L5	4670	C
3	L5	4672	A
3	L5	4679	G
3	L5	4687	A
3	L5	4694	G
3	L5	4695	C
3	L5	4700	A
3	L5	4708	A
3	L5	4709	U
3	L5	4719	G
3	L5	4734	A
3	L5	4740	G

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Mol	Chain	Res	Type
3	L5	4741	C
3	L5	4742	G
3	L5	4745	G
3	L5	4750	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4765	G
3	L5	4771	C
3	L5	4772	C
3	L5	4775	C
3	L5	4859	C
3	L5	4862	G
3	L5	4870	G
3	L5	4871	C
3	L5	4875	G
3	L5	4881	U
3	L5	4882	U
3	L5	4883	C
3	L5	4889	G
3	L5	4895	C
3	L5	4896	G
3	L5	4897	G
3	L5	4899	G
3	L5	4900	C
3	L5	4901	G
3	L5	4910	G
3	L5	4912	G
3	L5	4914	C
3	L5	4922	C
3	L5	4925	U
3	L5	4926	C
3	L5	4927	G
3	L5	4928	C
3	L5	4934	A
3	L5	4941	G
3	L5	4943	A
3	L5	4947	U
3	L5	4951	G
3	L5	4955	A
3	L5	4960	G

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Mol	Chain	Res	Type
3	L5	4975	G
3	L5	4976	U
3	L5	4985	U
3	L5	4988	U
3	L5	4989	U
3	L5	4990	C
3	L5	4991	U
3	L5	5013	C
3	L5	5014	A
3	L5	5017	G
3	L5	5022	U
3	L5	5023	C
3	L5	5024	C
3	L5	5028	G
3	L5	5030	U
3	L5	5034	A
3	L5	5041	G
3	L5	5050	C
3	L5	5054	C
3	L5	5055	G
3	L5	5061	A
3	L5	5069	U
4	L7	22	A
4	L7	33	U
4	L7	38	U
4	L7	53	U
4	L7	54	A
4	L7	64	G
4	L7	97	G
4	L7	100	A
4	L7	110	G
5	L8	25	G
5	L8	34	U
5	L8	35	C
5	L8	59	A
5	L8	62	A
5	L8	63	U
5	L8	80	A
5	L8	82	A
5	L8	84	A
5	L8	85	U
5	L8	87	G

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Mol	Chain	Res	Type
5	L8	94	G
5	L8	103	A
5	L8	105	C
5	L8	111	U
5	L8	114	G
5	L8	123	U
5	L8	124	U
5	L8	125	C
5	L8	126	C
5	L8	127	U
83	S2	4	C
83	S2	14	C
83	S2	25	A
83	S2	33	G
83	S2	41	G
83	S2	44	U
83	S2	45	A
83	S2	46	A
83	S2	56	G
83	S2	58	C
83	S2	59	U
83	S2	62	G
83	S2	64	A
83	S2	65	C
83	S2	67	C
83	S2	68	A
83	S2	72	C
83	S2	73	C
83	S2	74	G
83	S2	76	U
83	S2	99	A2M
83	S2	103	A
83	S2	113	G
83	S2	115	U
83	S2	126	G
83	S2	130	G
83	S2	143	U
83	S2	149	A
83	S2	155	G
83	S2	158	A
83	S2	160	U
83	S2	162	C

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Mol	Chain	Res	Type
83	S2	170	A
83	S2	171	A
83	S2	175	A
83	S2	179	C
83	S2	190	G
83	S2	191	A
83	S2	196	C
83	S2	197	U
83	S2	198	U
83	S2	200	G
83	S2	203	G
83	S2	204	G
83	S2	207	G
83	S2	208	G
83	S2	209	A
83	S2	214	U
83	S2	291	G
83	S2	292	A
83	S2	295	C
83	S2	302	A
83	S2	306	C
83	S2	307	G
83	S2	308	G
83	S2	309	G
83	S2	312	G
83	S2	313	A
83	S2	318	A
83	S2	319	C
83	S2	323	C
83	S2	324	C
83	S2	325	C
83	S2	326	C
83	S2	328	U
83	S2	329	G
83	S2	332	G
83	S2	339	A
83	S2	340	C
83	S2	347	G
83	S2	351	G
83	S2	360	A
83	S2	362	C
83	S2	364	A

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Mol	Chain	Res	Type
83	S2	368	U
83	S2	370	G
83	S2	383	G
83	S2	385	G
83	S2	386	C
83	S2	398	A
83	S2	407	G
83	S2	408	A
83	S2	409	C
83	S2	426	A
83	S2	436	OMG
83	S2	438	G
83	S2	448	A
83	S2	449	A
83	S2	450	C
83	S2	452	G
83	S2	464	A
83	S2	465	A
83	S2	471	G
83	S2	472	C
83	S2	473	A
83	S2	474	G
83	S2	476	A
83	S2	482	G
83	S2	487	U
83	S2	488	U
83	S2	492	C
83	S2	493	A
83	S2	502	C
83	S2	516	A
83	S2	517	OMC
83	S2	531	A
83	S2	532	C
83	S2	536	A
83	S2	537	C
83	S2	540	U
83	S2	542	U
83	S2	544	G
83	S2	546	G
83	S2	547	G
83	S2	557	U
83	S2	558	G

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Mol	Chain	Res	Type
83	S2	559	G
83	S2	563	G
83	S2	564	A
83	S2	576	A2M
83	S2	583	A
83	S2	587	A
83	S2	589	G
83	S2	590	A
83	S2	591	U
83	S2	593	C
83	S2	604	A
83	S2	611	G
83	S2	614	C
83	S2	617	G
83	S2	623	G
83	S2	628	A
83	S2	631	U
83	S2	643	A
83	S2	644	OMG
83	S2	655	A
83	S2	660	C
83	S2	664	A
83	S2	668	A2M
83	S2	669	A
83	S2	671	A
83	S2	672	A
83	S2	673	G
83	S2	683	OMG
83	S2	688	U
83	S2	689	U
83	S2	692	G
83	S2	695	C
83	S2	696	G
83	S2	697	G
83	S2	698	G
83	S2	732	U
83	S2	733	C
83	S2	736	C
83	S2	737	G
83	S2	738	C
83	S2	749	U
83	S2	750	C

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Mol	Chain	Res	Type
83	S2	751	G
83	S2	752	G
83	S2	753	C
83	S2	788	G
83	S2	791	C
83	S2	792	C
83	S2	798	G
83	S2	799	OMU
83	S2	801	PSU
83	S2	821	G
83	S2	822	U
83	S2	823	U
83	S2	824	C
83	S2	830	A
83	S2	834	C
83	S2	835	C
83	S2	836	G
83	S2	837	A
83	S2	838	G
83	S2	839	C
83	S2	842	C
83	S2	847	A
83	S2	867	OMG
83	S2	870	A
83	S2	874	G
83	S2	877	C
83	S2	880	G
83	S2	888	U
83	S2	889	U
83	S2	891	G
83	S2	893	U
83	S2	894	G
83	S2	896	U
83	S2	897	U
83	S2	898	U
83	S2	899	U
83	S2	900	C
83	S2	901	G
83	S2	903	A
83	S2	904	A
83	S2	913	A
83	S2	919	A

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Mol	Chain	Res	Type
83	S2	920	A
83	S2	933	G
83	S2	934	G
83	S2	943	U
83	S2	963	A
83	S2	969	U
83	S2	970	G
83	S2	971	G
83	S2	972	A
83	S2	985	G
83	S2	990	A
83	S2	992	A
83	S2	999	G
83	S2	1008	A
83	S2	1017	U
83	S2	1023	A
83	S2	1027	A
83	S2	1060	A
83	S2	1061	U
83	S2	1062	A
83	S2	1080	A
83	S2	1083	A
83	S2	1085	C
83	S2	1109	C
83	S2	1113	A
83	S2	1114	U
83	S2	1116	C
83	S2	1121	G
83	S2	1123	C
83	S2	1133	A
83	S2	1138	C
83	S2	1148	A
83	S2	1153	C
83	S2	1154	U
83	S2	1170	A
83	S2	1195	A
83	S2	1207	G
83	S2	1208	A
83	S2	1215	C
83	S2	1216	C
83	S2	1217	A
83	S2	1224	G

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Mol	Chain	Res	Type
83	S2	1227	G
83	S2	1242	U
83	S2	1243	U
83	S2	1248	B8N
83	S2	1251	A
83	S2	1253	A
83	S2	1256	G
83	S2	1257	G
83	S2	1259	A
83	S2	1271	C
83	S2	1272	OMC
83	S2	1274	G
83	S2	1275	G
83	S2	1283	C
83	S2	1286	G
83	S2	1288	OMU
83	S2	1290	G
83	S2	1294	G
83	S2	1295	A
83	S2	1301	A
83	S2	1302	G
83	S2	1303	C
83	S2	1308	U
83	S2	1342	U
83	S2	1357	A
83	S2	1371	U
83	S2	1372	U
83	S2	1373	C
83	S2	1376	A
83	S2	1378	A
83	S2	1382	A
83	S2	1401	A
83	S2	1402	A
83	S2	1413	G
83	S2	1418	C
83	S2	1419	C
83	S2	1420	G
83	S2	1421	A
83	S2	1422	G
83	S2	1423	C
83	S2	1432	U
83	S2	1433	C

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Mol	Chain	Res	Type
83	S2	1435	C
83	S2	1437	C
83	S2	1438	A
83	S2	1439	A
83	S2	1442	OMU
83	S2	1449	G
83	S2	1454	A
83	S2	1455	A
83	S2	1463	U
83	S2	1480	A
83	S2	1489	A
83	S2	1490	OMG
83	S2	1492	U
83	S2	1494	U
83	S2	1495	G
83	S2	1497	G
83	S2	1498	A
83	S2	1521	C
83	S2	1522	A
83	S2	1531	A
83	S2	1533	A
83	S2	1544	C
83	S2	1546	G
83	S2	1552	G
83	S2	1553	C
83	S2	1556	A
83	S2	1558	C
83	S2	1575	G
83	S2	1580	A
83	S2	1581	C
83	S2	1585	U
83	S2	1587	G
83	S2	1588	A
83	S2	1600	G
83	S2	1604	G
83	S2	1621	U
83	S2	1623	A
83	S2	1631	U
83	S2	1633	A
83	S2	1634	A
83	S2	1637	A
83	S2	1648	G

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Mol	Chain	Res	Type
83	S2	1654	G
83	S2	1663	A
83	S2	1665	G
83	S2	1683	C
83	S2	1686	G
83	S2	1695	A
83	S2	1698	C
83	S2	1699	A
83	S2	1715	A
83	S2	1721	U
83	S2	1722	G
83	S2	1744	G
83	S2	1745	A
83	S2	1752	C
83	S2	1753	C
83	S2	1754	G
83	S2	1755	C
83	S2	1757	G
83	S2	1759	G
83	S2	1761	U
83	S2	1772	C
83	S2	1773	C
83	S2	1774	C
83	S2	1777	G
83	S2	1782	G
83	S2	1783	C
83	S2	1784	G
83	S2	1786	U
83	S2	1798	C
83	S2	1810	U
83	S2	1821	U
83	S2	1825	A
83	S2	1829	G
83	S2	1831	A
83	S2	1835	A
83	S2	1838	U
83	S2	1849	G
83	S2	1851	MA6
83	S2	1861	G
83	S2	1862	G
83	S2	1863	A
83	S2	1864	U

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Mol	Chain	Res	Type
83	S2	1865	C

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	406	C
3	L5	493	G
3	L5	914	U
3	L5	1082	C
3	L5	1590	C
3	L5	1633	G
3	L5	1703	C
3	L5	1977	C
3	L5	2416	G
3	L5	2485	U
3	L5	2675	G
3	L5	2760	G
3	L5	3673	C
3	L5	4600	G
3	L5	4699	U
3	L5	4913	G
83	S2	291	G
83	S2	563	G
83	S2	688	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	A2M	L5	2363	85,3	22,25,26	1.24	2 (9%)	30,36,39	1.50	6 (20%)
83	OMG	S2	509	83	23,26,27	0.47	0	32,38,41	0.50	0
3	OMC	L5	1340	3	19,22,23	0.55	0	25,31,34	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	1744	85,3	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
3	OMU	L5	3925	3	19,22,23	3.31	7 (36%)	25,31,34	1.85	5 (20%)
3	PSU	L5	4673	85,3	18,21,22	1.08	1 (5%)	21,30,33	1.89	4 (19%)
83	PSU	S2	93	83	18,21,22	1.11	1 (5%)	21,30,33	1.74	4 (19%)
3	PSU	L5	4552	3	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
83	PSU	S2	1004	83	18,21,22	1.14	1 (5%)	21,30,33	1.89	4 (19%)
3	PSU	L5	4689	3	18,21,22	1.08	1 (5%)	21,30,33	1.93	4 (19%)
3	OMU	L5	2837	3	19,22,23	3.37	7 (36%)	25,31,34	1.85	4 (16%)
83	OMC	S2	1391	83	19,22,23	0.50	0	25,31,34	0.69	0
83	OMG	S2	1490	83	23,26,27	0.52	0	32,38,41	0.49	0
3	PSU	L5	3853	85,3	18,21,22	1.05	1 (5%)	21,30,33	1.79	4 (19%)
3	PSU	L5	4431	3	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	1862	3	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
3	A2M	L5	3785	85,3	22,25,26	1.16	1 (4%)	30,36,39	1.62	9 (30%)
3	OMC	L5	3808	3	19,22,23	0.58	0	25,31,34	0.85	1 (4%)
83	OMU	S2	1288	83	19,22,23	3.37	7 (36%)	25,31,34	1.78	5 (20%)
3	PSU	L5	3844	3	18,21,22	1.14	1 (5%)	21,30,33	1.81	4 (19%)
3	PSU	L5	1782	3	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
83	4AC	S2	1842	83	21,24,25	0.37	0	28,34,37	0.46	0
3	OMG	L5	1316	3	23,26,27	0.51	0	32,38,41	0.57	0
3	UR3	L5	4530	3	19,22,23	2.73	7 (36%)	26,32,35	1.57	3 (11%)
83	PSU	S2	801	83	18,21,22	1.12	1 (5%)	21,30,33	1.87	4 (19%)
83	A2M	S2	484	83	22,25,26	1.21	1 (4%)	30,36,39	1.47	6 (20%)
3	PSU	L5	1683	3	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
3	PSU	L5	2839	3	18,21,22	1.09	1 (5%)	21,30,33	1.84	4 (19%)
83	OMU	S2	1442	83	19,22,23	3.39	7 (36%)	25,31,34	1.76	4 (16%)
3	PSU	L5	1781	3	18,21,22	1.05	1 (5%)	21,30,33	1.75	4 (19%)
83	A2M	S2	576	83	22,25,26	1.26	2 (9%)	30,36,39	1.54	5 (16%)
3	PSU	L5	4442	3	18,21,22	1.14	1 (5%)	21,30,33	1.89	5 (23%)
3	A2M	L5	4571	3	22,25,26	1.31	2 (9%)	30,36,39	1.56	6 (20%)
3	OMU	L5	4306	3	19,22,23	3.33	7 (36%)	25,31,34	1.82	4 (16%)
83	PSU	S2	814	83	18,21,22	1.12	1 (5%)	21,30,33	1.82	4 (19%)
83	PSU	S2	1244	83	18,21,22	1.12	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L5	3920	85,3	18,21,22	1.09	1 (5%)	21,30,33	1.89	4 (19%)
83	OMU	S2	354	83	19,22,23	3.34	7 (36%)	25,31,34	1.84	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	400	3	22,25,26	1.31	1 (4%)	30,36,39	1.54	6 (20%)
3	A2M	L5	3830	3	22,25,26	1.24	1 (4%)	30,36,39	1.59	5 (16%)
83	OMU	S2	116	83	19,22,23	3.35	7 (36%)	25,31,34	1.73	4 (16%)
83	OMU	S2	1326	83	19,22,23	3.35	7 (36%)	25,31,34	1.85	5 (20%)
3	PSU	L5	3639	3	18,21,22	1.12	1 (5%)	21,30,33	1.90	5 (23%)
3	PSU	L5	4493	3	18,21,22	1.09	1 (5%)	21,30,33	1.88	4 (19%)
83	PSU	S2	105	83	18,21,22	1.12	1 (5%)	21,30,33	1.83	4 (19%)
3	OMC	L5	2422	85,3	19,22,23	0.53	0	25,31,34	0.71	0
3	A2M	L5	3867	3	22,25,26	1.27	1 (4%)	30,36,39	1.43	6 (20%)
83	OMG	S2	644	83	23,26,27	0.46	0	32,38,41	0.50	0
3	OMG	L5	4499	3	23,26,27	0.47	0	32,38,41	0.49	0
3	A2M	L5	2401	3	22,25,26	1.25	1 (4%)	30,36,39	1.56	6 (20%)
83	A2M	S2	668	85,83	22,25,26	1.34	2 (9%)	30,36,39	1.54	6 (20%)
3	1MA	L5	1322	85,3	21,25,26	0.56	0	30,37,40	0.78	1 (3%)
3	OMG	L5	2424	3	23,26,27	0.50	0	32,38,41	0.48	0
83	OMG	S2	683	83	23,26,27	0.50	0	32,38,41	0.47	0
3	OMG	L5	4637	3	23,26,27	0.49	0	32,38,41	0.50	0
5	PSU	L8	69	5	18,21,22	1.10	1 (5%)	21,30,33	1.87	5 (23%)
3	PSU	L5	4457	3	18,21,22	1.08	1 (5%)	21,30,33	1.88	5 (23%)
3	PSU	L5	4576	3	18,21,22	1.10	1 (5%)	21,30,33	1.81	4 (19%)
3	A2M	L5	1534	85,3	22,25,26	1.21	1 (4%)	30,36,39	1.43	7 (23%)
3	PSU	L5	4299	3	18,21,22	1.05	1 (5%)	21,30,33	1.91	5 (23%)
83	OMG	S2	1328	83	23,26,27	0.45	0	32,38,41	0.46	0
83	PSU	S2	863	83	18,21,22	1.12	1 (5%)	21,30,33	1.87	4 (19%)
3	OMC	L5	2861	3	19,22,23	0.54	0	25,31,34	0.86	1 (4%)
3	OMC	L5	4456	3	19,22,23	0.59	0	25,31,34	0.91	1 (4%)
3	PSU	L5	1860	3	18,21,22	1.09	1 (5%)	21,30,33	1.91	4 (19%)
83	PSU	S2	1367	83	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
3	A2M	L5	2815	3	22,25,26	1.26	1 (4%)	30,36,39	1.46	6 (20%)
3	PSU	L5	4521	85,3	18,21,22	1.10	1 (5%)	21,30,33	2.01	5 (23%)
83	PSU	S2	109	83	18,21,22	1.12	1 (5%)	21,30,33	1.89	4 (19%)
83	PSU	S2	406	83	18,21,22	1.10	1 (5%)	21,30,33	1.98	5 (23%)
83	A2M	S2	99	85,83	22,25,26	1.25	1 (4%)	30,36,39	1.54	5 (16%)
3	A2M	L5	3718	3	22,25,26	1.18	1 (4%)	30,36,39	1.48	5 (16%)
5	OMG	L8	75	5	23,26,27	0.47	0	32,38,41	0.52	0
3	PSU	L5	4636	3	18,21,22	1.13	1 (5%)	21,30,33	2.04	6 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4973	3	18,21,22	1.11	1 (5%)	21,30,33	1.90	4 (19%)
83	PSU	S2	1177	83	18,21,22	1.08	1 (5%)	21,30,33	1.84	4 (19%)
83	PSU	S2	866	83	18,21,22	1.11	1 (5%)	21,30,33	1.86	5 (23%)
83	OMC	S2	517	83	19,22,23	0.50	0	25,31,34	0.65	0
3	PSU	L5	5001	3	18,21,22	1.12	1 (5%)	21,30,33	1.88	4 (19%)
3	PSU	L5	4500	3	18,21,22	1.13	1 (5%)	21,30,33	2.01	5 (23%)
3	OMU	L5	4620	3	19,22,23	3.28	7 (36%)	25,31,34	1.72	4 (16%)
3	OMG	L5	3792	3	23,26,27	0.49	0	32,38,41	0.51	0
3	PSU	L5	4579	3	18,21,22	1.07	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	4296	3	18,21,22	1.11	1 (5%)	21,30,33	1.90	4 (19%)
3	OMG	L5	3744	3	23,26,27	0.49	0	32,38,41	0.51	0
3	OMC	L5	3701	3	19,22,23	0.65	0	25,31,34	1.70	4 (16%)
83	MA6	S2	1851	83	23,26,27	1.27	2 (8%)	33,38,41	3.38	13 (39%)
3	OMG	L5	3627	3	23,26,27	0.47	0	32,38,41	0.56	0
3	OMG	L5	1522	3	23,26,27	0.49	0	32,38,41	0.60	0
3	PSU	L5	1792	3	18,21,22	1.07	1 (5%)	21,30,33	1.80	4 (19%)
3	OMU	L5	4498	3	19,22,23	3.33	7 (36%)	25,31,34	1.83	5 (20%)
83	PSU	S2	651	83	18,21,22	1.12	1 (5%)	21,30,33	1.91	4 (19%)
3	5MC	L5	3782	85,3	19,22,23	0.59	0	26,32,35	0.71	0
3	OMG	L5	4494	3	23,26,27	0.50	0	32,38,41	0.53	0
3	OMG	L5	1625	3	23,26,27	0.48	0	32,38,41	0.48	0
83	PSU	S2	686	83	18,21,22	1.13	1 (5%)	21,30,33	1.92	4 (19%)
3	A2M	L5	1524	3	22,25,26	1.33	2 (9%)	30,36,39	1.51	6 (20%)
3	OMC	L5	2351	85,3	19,22,23	0.60	0	25,31,34	1.19	2 (8%)
3	OMC	L5	3869	3	19,22,23	0.55	0	25,31,34	0.72	0
83	B8N	S2	1248	83	25,29,30	3.27	6 (24%)	28,42,45	1.99	7 (25%)
3	OMU	L5	4227	3	19,22,23	3.36	7 (36%)	25,31,34	1.83	4 (16%)
83	A2M	S2	27	83	22,25,26	1.25	1 (4%)	30,36,39	1.53	6 (20%)
3	PSU	L5	4293	3	18,21,22	1.11	1 (5%)	21,30,33	1.98	4 (19%)
3	A2M	L5	4590	3	22,25,26	1.23	1 (4%)	30,36,39	1.52	5 (16%)
5	PSU	L8	55	5	18,21,22	1.07	1 (5%)	21,30,33	1.94	5 (23%)
83	OMC	S2	1703	83	19,22,23	0.52	0	25,31,34	0.60	0
83	OMG	S2	867	83	23,26,27	0.49	0	32,38,41	0.47	0
83	PSU	S2	649	83	18,21,22	1.12	1 (5%)	21,30,33	1.91	4 (19%)
83	PSU	S2	1046	83	18,21,22	1.11	1 (5%)	21,30,33	1.83	4 (19%)
3	PSU	L5	4471	3	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
83	PSU	S2	681	83	18,21,22	1.08	1 (5%)	21,30,33	1.81	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L5	2804	3	19,22,23	0.59	0	25,31,34	0.97	1 (4%)
3	A2M	L5	1871	85,3	22,25,26	1.31	1 (4%)	30,36,39	1.63	6 (20%)
3	6MZ	L5	4220	3	22,25,26	3.94	11 (50%)	29,36,39	2.43	10 (34%)
3	OMG	L5	4370	3	23,26,27	0.48	0	32,38,41	0.53	0
83	OMU	S2	627	83	19,22,23	3.40	7 (36%)	25,31,34	1.79	5 (20%)
83	OMC	S2	174	83	19,22,23	0.49	0	25,31,34	0.64	0
3	OMC	L5	2365	85,3	19,22,23	0.53	0	25,31,34	0.62	0
3	OMC	L5	3887	3	19,22,23	0.54	0	25,31,34	0.77	0
83	PSU	S2	1174	83	18,21,22	1.12	1 (5%)	21,30,33	1.86	4 (19%)
3	PSU	L5	4532	3	18,21,22	1.10	1 (5%)	21,30,33	1.81	4 (19%)
83	MA6	S2	1850	83	23,26,27	1.27	2 (8%)	33,38,41	3.32	12 (36%)
3	PSU	L5	4972	3	18,21,22	1.08	1 (5%)	21,30,33	1.87	4 (19%)
83	PSU	S2	1045	83	18,21,22	1.08	1 (5%)	21,30,33	1.82	4 (19%)
3	PSU	L5	4361	3	18,21,22	1.08	1 (5%)	21,30,33	1.79	4 (19%)
3	OMG	L5	3899	3	23,26,27	0.53	0	32,38,41	0.55	0
83	A2M	S2	159	83	22,25,26	1.22	2 (9%)	30,36,39	1.50	6 (20%)
3	PSU	L5	1582	3	18,21,22	1.12	1 (5%)	21,30,33	1.85	4 (19%)
83	OMG	S2	436	83	23,26,27	0.48	0	32,38,41	0.53	0
83	6MZ	S2	1832	85,83	26,26,26	2.83	4 (15%)	36,39,39	2.10	11 (30%)
3	PSU	L5	3822	3	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
3	PSU	L5	3637	3	18,21,22	1.11	1 (5%)	21,30,33	1.97	4 (19%)
83	OMC	S2	1272	83	19,22,23	0.56	0	25,31,34	1.05	2 (8%)
83	OMU	S2	121	83	19,22,23	3.36	7 (36%)	25,31,34	1.81	5 (20%)
83	A2M	S2	1031	83	22,25,26	1.23	1 (4%)	30,36,39	1.54	5 (16%)
83	A2M	S2	468	83	22,25,26	1.28	1 (4%)	30,36,39	1.53	6 (20%)
3	PSU	L5	4403	3	18,21,22	1.09	1 (5%)	21,30,33	1.97	6 (28%)
3	PSU	L5	3851	3	18,21,22	1.11	1 (5%)	21,30,33	1.86	4 (19%)
83	OMU	S2	172	83	19,22,23	3.36	7 (36%)	25,31,34	1.85	5 (20%)
3	OMC	L5	4536	3	19,22,23	0.55	0	25,31,34	0.71	0
3	PSU	L5	3695	3	18,21,22	1.09	1 (5%)	21,30,33	1.90	5 (23%)
3	A2M	L5	1326	3	22,25,26	1.25	1 (4%)	30,36,39	1.43	6 (20%)
83	PSU	S2	1081	83	18,21,22	1.08	1 (5%)	21,30,33	1.88	5 (23%)
3	UY1	L5	3818	3	19,22,23	4.93	10 (52%)	21,31,34	2.02	6 (28%)
3	OMC	L5	3841	3	19,22,23	0.54	0	25,31,34	0.65	0
3	5MC	L5	4447	3	19,22,23	0.72	0	26,32,35	0.62	0
3	PSU	L5	4312	3	18,21,22	1.10	1 (5%)	21,30,33	1.91	4 (19%)
3	OMG	L5	4392	3	23,26,27	0.47	0	32,38,41	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	4523	85,3	22,25,26	1.32	2 (9%)	30,36,39	1.57	6 (20%)
3	PSU	L5	1536	3	18,21,22	1.09	1 (5%)	21,30,33	1.90	4 (19%)
3	A2M	L5	398	3	22,25,26	1.26	1 (4%)	30,36,39	1.60	5 (16%)
83	OMC	S2	462	83	19,22,23	0.53	0	25,31,34	0.73	0
83	A2M	S2	166	83	22,25,26	1.30	1 (4%)	30,36,39	1.54	6 (20%)
3	PSU	L5	1677	3	18,21,22	1.08	1 (5%)	21,30,33	2.01	5 (23%)
3	A2M	L5	1323	3	22,25,26	1.32	3 (13%)	30,36,39	1.57	7 (23%)
3	OMG	L5	4196	1,3	23,26,27	0.46	0	32,38,41	0.48	0
3	OMG	L5	2364	85,3	23,26,27	0.49	0	32,38,41	0.51	0
3	OMG	L5	4228	3	23,26,27	0.48	0	32,38,41	0.58	0
3	PSU	L5	5010	3	18,21,22	1.12	1 (5%)	21,30,33	1.88	4 (19%)
83	PSU	S2	1232	83	18,21,22	1.15	1 (5%)	21,30,33	1.92	4 (19%)
3	OMG	L5	2876	3	23,26,27	0.49	0	32,38,41	0.49	0
3	PSU	L5	4628	3	18,21,22	1.09	1 (5%)	21,30,33	1.84	5 (23%)
83	OMU	S2	799	83	19,22,23	3.40	7 (36%)	25,31,34	1.80	4 (16%)
83	OMG	S2	601	83	23,26,27	0.47	0	32,38,41	0.47	0
83	OMU	S2	428	83	19,22,23	3.37	7 (36%)	25,31,34	1.83	5 (20%)
3	PSU	L5	2632	3	18,21,22	1.07	1 (5%)	21,30,33	1.84	4 (19%)
3	PSU	L5	3884	3	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
83	G7M	S2	1639	1,83	23,26,27	2.66	9 (39%)	34,39,42	2.59	11 (32%)
3	OMG	L5	4623	3	23,26,27	0.49	0	32,38,41	0.57	0
83	A2M	S2	1383	83	22,25,26	1.24	1 (4%)	30,36,39	1.59	5 (16%)
83	PSU	S2	966	85,83	18,21,22	1.09	1 (5%)	21,30,33	1.83	4 (19%)
3	A2M	L5	2787	3	22,25,26	1.22	1 (4%)	30,36,39	1.49	6 (20%)
83	4AC	S2	1337	83	21,24,25	0.39	0	28,34,37	0.74	1 (3%)
3	A2M	L5	3825	3	22,25,26	1.26	1 (4%)	30,36,39	1.54	5 (16%)
83	PSU	S2	1056	83	18,21,22	1.11	1 (5%)	21,30,33	1.89	4 (19%)
3	PSU	L5	4353	3	18,21,22	1.10	1 (5%)	21,30,33	1.89	4 (19%)
3	OMC	L5	2824	3	19,22,23	0.55	0	25,31,34	0.72	0
3	OMG	L5	4618	3	23,26,27	0.50	0	32,38,41	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	2363	85,3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	OMG	S2	509	83	-	0/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	1744	85,3	-	0/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4673	85,3	-	0/7/25/26	0/2/2/2
83	PSU	S2	93	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1004	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
83	OMC	S2	1391	83	-	0/9/27/28	0/2/2/2
83	OMG	S2	1490	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	3853	85,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3785	85,3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
83	OMU	S2	1288	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	3844	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	1782	3	-	0/7/25/26	0/2/2/2
83	4AC	S2	1842	83	-	0/11/29/30	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	801	83	-	2/7/25/26	0/2/2/2
83	A2M	S2	484	83	-	0/9/27/28	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	1442	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	1781	3	-	2/7/25/26	0/2/2/2
83	A2M	S2	576	83	-	3/9/27/28	0/3/3/3
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	4306	3	-	1/9/27/28	0/2/2/2
83	PSU	S2	814	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	1244	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	3920	85,3	-	0/7/25/26	0/2/2/2
83	OMU	S2	354	83	-	0/9/27/28	0/2/2/2
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3
83	OMU	S2	116	83	-	1/9/27/28	0/2/2/2
83	OMU	S2	1326	83	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	105	83	-	0/7/25/26	0/2/2/2
3	OMC	L5	2422	85,3	-	2/9/27/28	0/2/2/2
3	A2M	L5	3867	3	-	3/9/27/28	0/3/3/3
83	OMG	S2	644	83	-	3/9/27/28	0/3/3/3
3	OMG	L5	4499	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	2401	3	-	0/9/27/28	0/3/3/3
83	A2M	S2	668	85,83	-	2/9/27/28	0/3/3/3
3	1MA	L5	1322	85,3	-	2/7/25/26	0/3/3/3
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
83	OMG	S2	683	83	-	2/9/27/28	0/3/3/3
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1534	85,3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
83	OMG	S2	1328	83	-	1/9/27/28	0/3/3/3
83	PSU	S2	863	83	-	0/7/25/26	0/2/2/2
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1367	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	2815	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4521	85,3	-	0/7/25/26	0/2/2/2
83	PSU	S2	109	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	406	83	-	0/7/25/26	0/2/2/2
83	A2M	S2	99	85,83	-	3/9/27/28	0/3/3/3
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
5	OMG	L8	75	5	-	0/9/27/28	0/3/3/3
3	PSU	L5	4636	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	4973	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1177	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	866	83	-	0/7/25/26	0/2/2/2
83	OMC	S2	517	83	-	2/9/27/28	0/2/2/2
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	1/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	3792	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3701	3	-	6/9/27/28	0/2/2/2
83	MA6	S2	1851	83	-	1/11/29/30	0/3/3/3
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
83	PSU	S2	651	83	-	0/7/25/26	0/2/2/2
3	5MC	L5	3782	85,3	-	1/7/25/26	0/2/2/2
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1625	3	-	2/9/27/28	0/3/3/3
83	PSU	S2	686	83	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	3/9/27/28	0/3/3/3
3	OMC	L5	2351	85,3	-	3/9/27/28	0/2/2/2
3	OMC	L5	3869	3	-	1/9/27/28	0/2/2/2
83	B8N	S2	1248	83	-	4/16/34/35	0/2/2/2
3	OMU	L5	4227	3	-	0/9/27/28	0/2/2/2
83	A2M	S2	27	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4590	3	-	3/9/27/28	0/3/3/3
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
83	OMC	S2	1703	83	-	1/9/27/28	0/2/2/2
83	OMG	S2	867	83	-	2/9/27/28	0/3/3/3
83	PSU	S2	649	83	-	0/7/25/26	0/2/2/2
83	PSU	S2	1046	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	681	83	-	0/7/25/26	0/2/2/2
3	OMC	L5	2804	3	-	1/9/27/28	0/2/2/2
3	A2M	L5	1871	85,3	-	0/9/27/28	0/3/3/3
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
83	OMU	S2	627	83	-	4/9/27/28	0/2/2/2
83	OMC	S2	174	83	-	0/9/27/28	0/2/2/2
3	OMC	L5	2365	85,3	-	0/9/27/28	0/2/2/2
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
83	PSU	S2	1174	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	MA6	S2	1850	83	-	0/11/29/30	0/3/3/3
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1045	83	-	2/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3899	3	-	3/9/27/28	0/3/3/3
83	A2M	S2	159	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	1582	3	-	0/7/25/26	0/2/2/2
83	OMG	S2	436	83	-	2/9/27/28	0/3/3/3
83	6MZ	S2	1832	85,83	-	3/12/28/28	0/3/3/3
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3637	3	-	0/7/25/26	0/2/2/2
83	OMC	S2	1272	83	-	5/9/27/28	0/2/2/2
83	OMU	S2	121	83	-	0/9/27/28	0/2/2/2
83	A2M	S2	1031	83	-	0/9/27/28	0/3/3/3
83	A2M	S2	468	83	-	1/9/27/28	0/3/3/3
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	1/7/25/26	0/2/2/2
83	OMU	S2	172	83	-	0/9/27/28	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	4/9/27/28	0/3/3/3
83	PSU	S2	1081	83	-	0/7/25/26	0/2/2/2
3	UY1	L5	3818	3	-	2/9/27/28	0/2/2/2
3	OMC	L5	3841	3	-	1/9/27/28	0/2/2/2
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	4523	85,3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1536	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
83	OMC	S2	462	83	-	1/9/27/28	0/2/2/2
83	A2M	S2	166	83	-	0/9/27/28	0/3/3/3
3	PSU	L5	1677	3	-	4/7/25/26	0/2/2/2
3	A2M	L5	1323	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	4196	1,3	-	1/9/27/28	0/3/3/3
3	OMG	L5	2364	85,3	-	2/9/27/28	0/3/3/3
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
83	PSU	S2	1232	83	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	2876	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
83	OMU	S2	799	83	-	2/9/27/28	0/2/2/2
83	OMG	S2	601	83	-	1/9/27/28	0/3/3/3
83	OMU	S2	428	83	-	4/9/27/28	0/2/2/2
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3884	3	-	0/7/25/26	0/2/2/2
83	G7M	S2	1639	1,83	-	0/7/25/26	0/3/3/3
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
83	A2M	S2	1383	83	-	1/9/27/28	0/3/3/3
83	PSU	S2	966	85,83	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	3	-	5/9/27/28	0/3/3/3
83	4AC	S2	1337	83	-	1/11/29/30	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
83	PSU	S2	1056	83	-	0/7/25/26	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2824	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	4618	3	-	1/9/27/28	0/3/3/3

All (273) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	C6-C5	12.91	1.49	1.35
83	S2	1832	6MZ	C6-N6	12.80	1.48	1.34
3	L5	4220	6MZ	C6-N6	12.11	1.48	1.34
3	L5	3818	UY1	C2-N1	11.87	1.52	1.36
83	S2	799	OMU	C2-N1	8.50	1.51	1.38
3	L5	2837	OMU	C2-N1	8.38	1.51	1.38
83	S2	1442	OMU	C2-N1	8.38	1.51	1.38
83	S2	627	OMU	C2-N1	8.36	1.51	1.38
3	L5	4227	OMU	C2-N1	8.36	1.51	1.38
3	L5	4220	6MZ	C3'-C2'	-8.32	1.30	1.53
83	S2	354	OMU	C2-N1	8.24	1.51	1.38
83	S2	1288	OMU	C2-N1	8.23	1.51	1.38
83	S2	121	OMU	C2-N1	8.21	1.51	1.38
83	S2	428	OMU	C2-N1	8.21	1.51	1.38
3	L5	4306	OMU	C2-N1	8.19	1.51	1.38
83	S2	116	OMU	C2-N1	8.18	1.51	1.38
83	S2	172	OMU	C2-N1	8.18	1.51	1.38
3	L5	3925	OMU	C2-N1	8.16	1.51	1.38
83	S2	1326	OMU	C2-N1	8.13	1.51	1.38
3	L5	4498	OMU	C2-N1	8.11	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4620	OMU	C2-N1	8.00	1.51	1.38
83	S2	1248	B8N	C6-N1	7.87	1.55	1.36
83	S2	1248	B8N	C4-N3	-7.86	1.26	1.40
3	L5	3818	UY1	C2-N3	7.71	1.50	1.37
83	S2	1248	B8N	C4-C5	7.04	1.63	1.47
83	S2	116	OMU	C2-N3	6.98	1.50	1.38
83	S2	1442	OMU	C2-N3	6.97	1.50	1.38
83	S2	627	OMU	C2-N3	6.96	1.50	1.38
83	S2	172	OMU	C2-N3	6.93	1.50	1.38
83	S2	121	OMU	C2-N3	6.91	1.50	1.38
83	S2	799	OMU	C2-N3	6.89	1.50	1.38
83	S2	428	OMU	C2-N3	6.86	1.49	1.38
83	S2	1288	OMU	C2-N3	6.85	1.49	1.38
83	S2	1326	OMU	C2-N3	6.84	1.49	1.38
3	L5	2837	OMU	C2-N3	6.81	1.49	1.38
3	L5	4498	OMU	C2-N3	6.80	1.49	1.38
3	L5	4227	OMU	C2-N3	6.78	1.49	1.38
83	S2	354	OMU	C2-N3	6.78	1.49	1.38
3	L5	4306	OMU	C2-N3	6.78	1.49	1.38
3	L5	4620	OMU	C2-N3	6.71	1.49	1.38
3	L5	3925	OMU	C2-N3	6.67	1.49	1.38
83	S2	1639	G7M	C4-N3	6.63	1.49	1.34
3	L5	4530	UR3	C2-N1	6.44	1.47	1.38
3	L5	4530	UR3	C6-C5	6.29	1.49	1.35
83	S2	1248	B8N	C2-N1	5.92	1.56	1.39
83	S2	1288	OMU	C6-C5	5.91	1.48	1.35
83	S2	1326	OMU	C6-C5	5.90	1.48	1.35
83	S2	627	OMU	C6-C5	5.90	1.48	1.35
83	S2	428	OMU	C6-C5	5.88	1.48	1.35
83	S2	172	OMU	C6-C5	5.88	1.48	1.35
83	S2	121	OMU	C6-C5	5.86	1.48	1.35
83	S2	1442	OMU	C6-C5	5.85	1.48	1.35
3	L5	2837	OMU	C6-C5	5.83	1.48	1.35
83	S2	799	OMU	C6-C5	5.83	1.48	1.35
3	L5	4227	OMU	C6-C5	5.82	1.48	1.35
83	S2	116	OMU	C6-C5	5.81	1.48	1.35
3	L5	4498	OMU	C6-C5	5.80	1.48	1.35
3	L5	3925	OMU	C6-C5	5.79	1.48	1.35
83	S2	354	OMU	C6-C5	5.77	1.48	1.35
3	L5	4306	OMU	C6-C5	5.77	1.48	1.35
3	L5	4620	OMU	C6-C5	5.73	1.48	1.35
3	L5	4530	UR3	C2-N3	5.69	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2837	OMU	O4-C4	-5.53	1.13	1.24
3	L5	3925	OMU	O4-C4	-5.51	1.13	1.24
3	L5	4227	OMU	O4-C4	-5.50	1.13	1.24
3	L5	4306	OMU	O4-C4	-5.49	1.13	1.24
83	S2	428	OMU	O4-C4	-5.49	1.13	1.24
3	L5	4620	OMU	O4-C4	-5.48	1.13	1.24
3	L5	4498	OMU	O4-C4	-5.48	1.13	1.24
83	S2	799	OMU	O4-C4	-5.46	1.13	1.24
83	S2	1326	OMU	O4-C4	-5.46	1.13	1.24
83	S2	1639	G7M	C2-N3	5.44	1.46	1.33
83	S2	116	OMU	O4-C4	-5.44	1.13	1.24
83	S2	627	OMU	O4-C4	-5.44	1.13	1.24
83	S2	172	OMU	O4-C4	-5.43	1.13	1.24
83	S2	354	OMU	O4-C4	-5.42	1.13	1.24
83	S2	1288	OMU	O4-C4	-5.41	1.14	1.24
3	L5	3818	UY1	C6-N1	5.40	1.45	1.36
83	S2	121	OMU	O4-C4	-5.40	1.14	1.24
83	S2	1442	OMU	O4-C4	-5.37	1.14	1.24
83	S2	1248	B8N	C6-C5	5.33	1.42	1.35
83	S2	1639	G7M	C2-N2	4.93	1.45	1.34
83	S2	1639	G7M	C5-N7	-4.80	1.33	1.39
3	L5	4220	6MZ	O4'-C4'	4.77	1.55	1.45
3	L5	4220	6MZ	O4'-C1'	-4.71	1.31	1.42
83	S2	627	OMU	C4-N3	4.51	1.46	1.38
83	S2	428	OMU	C4-N3	4.48	1.46	1.38
83	S2	1288	OMU	C4-N3	4.45	1.46	1.38
3	L5	3818	UY1	C4-N3	4.44	1.47	1.38
83	S2	172	OMU	C4-N3	4.43	1.46	1.38
83	S2	1442	OMU	C4-N3	4.41	1.46	1.38
83	S2	116	OMU	C4-N3	4.38	1.46	1.38
3	L5	4498	OMU	C4-N3	4.33	1.46	1.38
83	S2	1326	OMU	C4-N3	4.32	1.46	1.38
83	S2	354	OMU	C4-N3	4.31	1.46	1.38
3	L5	4220	6MZ	C5'-C4'	-4.31	1.38	1.51
83	S2	121	OMU	C4-N3	4.31	1.46	1.38
83	S2	799	OMU	C4-N3	4.30	1.46	1.38
3	L5	2837	OMU	C4-N3	4.27	1.45	1.38
3	L5	4306	OMU	C4-N3	4.19	1.45	1.38
3	L5	4227	OMU	C4-N3	4.16	1.45	1.38
3	L5	4620	OMU	C4-N3	4.13	1.45	1.38
3	L5	3925	OMU	C4-N3	4.09	1.45	1.38
83	S2	1232	PSU	C6-C5	3.84	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	1639	G7M	C5-C6	3.83	1.54	1.43
3	L5	3844	PSU	C6-C5	3.80	1.39	1.35
83	S2	93	PSU	C6-C5	3.79	1.39	1.35
83	S2	1004	PSU	C6-C5	3.77	1.39	1.35
83	S2	814	PSU	C6-C5	3.75	1.39	1.35
83	S2	863	PSU	C6-C5	3.75	1.39	1.35
83	S2	1367	PSU	C6-C5	3.74	1.39	1.35
83	S2	686	PSU	C6-C5	3.73	1.39	1.35
83	S2	801	PSU	C6-C5	3.73	1.39	1.35
83	S2	1244	PSU	C6-C5	3.73	1.39	1.35
83	S2	1174	PSU	C6-C5	3.71	1.39	1.35
83	S2	1248	B8N	C1'-C5	3.71	1.58	1.50
3	L5	1582	PSU	C6-C5	3.70	1.39	1.35
83	S2	651	PSU	C6-C5	3.70	1.39	1.35
3	L5	5010	PSU	C6-C5	3.70	1.39	1.35
83	S2	649	PSU	C6-C5	3.68	1.39	1.35
83	S2	105	PSU	C6-C5	3.68	1.39	1.35
3	L5	3637	PSU	C6-C5	3.64	1.39	1.35
3	L5	3851	PSU	C6-C5	3.64	1.39	1.35
3	L5	3822	PSU	C6-C5	3.64	1.39	1.35
83	S2	866	PSU	C6-C5	3.64	1.39	1.35
3	L5	1862	PSU	C6-C5	3.64	1.39	1.35
3	L5	4442	PSU	C6-C5	3.64	1.39	1.35
3	L5	4296	PSU	C6-C5	3.64	1.39	1.35
3	L5	4532	PSU	C6-C5	3.63	1.39	1.35
83	S2	109	PSU	C6-C5	3.63	1.39	1.35
83	S2	1046	PSU	C6-C5	3.62	1.39	1.35
3	L5	5001	PSU	C6-C5	3.62	1.39	1.35
3	L5	4471	PSU	C6-C5	3.61	1.39	1.35
3	L5	4493	PSU	C6-C5	3.61	1.39	1.35
3	L5	4576	PSU	C6-C5	3.60	1.39	1.35
83	S2	966	PSU	C6-C5	3.60	1.39	1.35
3	L5	4312	PSU	C6-C5	3.60	1.39	1.35
3	L5	1782	PSU	C6-C5	3.60	1.39	1.35
3	L5	4500	PSU	C6-C5	3.59	1.39	1.35
3	L5	4552	PSU	C6-C5	3.59	1.39	1.35
3	L5	4973	PSU	C6-C5	3.59	1.39	1.35
3	L5	1860	PSU	C6-C5	3.59	1.39	1.35
83	S2	1045	PSU	C6-C5	3.59	1.39	1.35
3	L5	2632	PSU	C6-C5	3.58	1.39	1.35
83	S2	1056	PSU	C6-C5	3.58	1.39	1.35
3	L5	4293	PSU	C6-C5	3.58	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	O4-C4	-3.58	1.16	1.23
3	L5	1683	PSU	C6-C5	3.57	1.39	1.35
3	L5	1792	PSU	C6-C5	3.56	1.39	1.35
3	L5	1744	PSU	C6-C5	3.56	1.39	1.35
3	L5	3639	PSU	C6-C5	3.56	1.39	1.35
3	L5	4361	PSU	C6-C5	3.55	1.39	1.35
3	L5	4431	PSU	C6-C5	3.55	1.39	1.35
3	L5	4636	PSU	C6-C5	3.55	1.39	1.35
3	L5	4353	PSU	C6-C5	3.55	1.39	1.35
5	L8	69	PSU	C6-C5	3.55	1.39	1.35
83	S2	406	PSU	C6-C5	3.54	1.39	1.35
3	L5	4628	PSU	C6-C5	3.54	1.39	1.35
83	S2	1081	PSU	C6-C5	3.53	1.39	1.35
83	S2	1177	PSU	C6-C5	3.53	1.39	1.35
3	L5	4972	PSU	C6-C5	3.53	1.39	1.35
3	L5	1536	PSU	C6-C5	3.53	1.39	1.35
3	L5	2839	PSU	C6-C5	3.52	1.39	1.35
3	L5	1781	PSU	C6-C5	3.51	1.39	1.35
3	L5	3920	PSU	C6-C5	3.50	1.39	1.35
5	L8	55	PSU	C6-C5	3.50	1.39	1.35
3	L5	3695	PSU	C6-C5	3.50	1.39	1.35
3	L5	3884	PSU	C6-C5	3.48	1.39	1.35
3	L5	4579	PSU	C6-C5	3.47	1.39	1.35
83	S2	681	PSU	C6-C5	3.47	1.39	1.35
3	L5	4673	PSU	C6-C5	3.46	1.39	1.35
3	L5	1871	A2M	O5'-C5'	-3.45	1.34	1.44
3	L5	4457	PSU	C6-C5	3.45	1.39	1.35
3	L5	3853	PSU	C6-C5	3.45	1.39	1.35
3	L5	3825	A2M	O5'-C5'	-3.45	1.34	1.44
3	L5	1323	A2M	O5'-C5'	-3.44	1.34	1.44
3	L5	4521	PSU	C6-C5	3.44	1.39	1.35
3	L5	400	A2M	O5'-C5'	-3.43	1.34	1.44
3	L5	3785	A2M	O5'-C5'	-3.43	1.34	1.44
83	S2	99	A2M	O5'-C5'	-3.43	1.34	1.44
83	S2	576	A2M	O5'-C5'	-3.43	1.34	1.44
3	L5	1524	A2M	O5'-C5'	-3.41	1.34	1.44
3	L5	4689	PSU	C6-C5	3.40	1.39	1.35
3	L5	2815	A2M	O5'-C5'	-3.40	1.34	1.44
3	L5	3830	A2M	O5'-C5'	-3.40	1.34	1.44
3	L5	4299	PSU	C6-C5	3.39	1.39	1.35
3	L5	2401	A2M	O5'-C5'	-3.38	1.34	1.44
83	S2	166	A2M	O5'-C5'	-3.38	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	668	A2M	O5'-C5'	-3.37	1.34	1.44
83	S2	468	A2M	O5'-C5'	-3.37	1.34	1.44
83	S2	1383	A2M	O5'-C5'	-3.36	1.34	1.44
3	L5	2787	A2M	O5'-C5'	-3.35	1.34	1.44
3	L5	4571	A2M	O5'-C5'	-3.35	1.34	1.44
83	S2	1031	A2M	O5'-C5'	-3.33	1.34	1.44
3	L5	4403	PSU	C6-C5	3.33	1.39	1.35
3	L5	4220	6MZ	C5-C4	-3.33	1.33	1.39
3	L5	3867	A2M	O5'-C5'	-3.32	1.34	1.44
3	L5	2363	A2M	O5'-C5'	-3.32	1.34	1.44
3	L5	1326	A2M	O5'-C5'	-3.31	1.34	1.44
3	L5	3718	A2M	O5'-C5'	-3.30	1.34	1.44
3	L5	3818	UY1	C1'-C5	3.27	1.57	1.50
83	S2	1851	MA6	C6-N6	3.25	1.45	1.36
3	L5	3818	UY1	O2-C2	-3.25	1.16	1.23
3	L5	398	A2M	O5'-C5'	-3.25	1.34	1.44
83	S2	1850	MA6	C6-N6	3.23	1.45	1.36
3	L5	1677	PSU	C6-C5	3.23	1.38	1.35
3	L5	4523	A2M	O5'-C5'	-3.22	1.34	1.44
3	L5	4220	6MZ	C5-N7	-3.22	1.33	1.39
83	S2	484	A2M	O5'-C5'	-3.21	1.34	1.44
3	L5	4590	A2M	O5'-C5'	-3.19	1.34	1.44
83	S2	27	A2M	O5'-C5'	-3.15	1.35	1.44
3	L5	1534	A2M	O5'-C5'	-3.12	1.35	1.44
83	S2	159	A2M	O5'-C5'	-3.10	1.35	1.44
3	L5	4220	6MZ	C2'-C1'	3.09	1.63	1.53
83	S2	1832	6MZ	C5-C4	-3.00	1.33	1.39
83	S2	1832	6MZ	C5-N7	-2.98	1.33	1.39
83	S2	627	OMU	C5-C4	2.94	1.50	1.43
83	S2	1288	OMU	C5-C4	2.90	1.50	1.43
83	S2	799	OMU	C5-C4	2.90	1.50	1.43
83	S2	1326	OMU	C5-C4	2.88	1.50	1.43
83	S2	172	OMU	C5-C4	2.87	1.49	1.43
83	S2	1639	G7M	C2-N1	2.84	1.44	1.37
3	L5	4227	OMU	C5-C4	2.84	1.49	1.43
83	S2	1442	OMU	C5-C4	2.83	1.49	1.43
83	S2	428	OMU	C5-C4	2.82	1.49	1.43
83	S2	354	OMU	C5-C4	2.81	1.49	1.43
3	L5	4220	6MZ	C8-N9	-2.79	1.32	1.37
3	L5	3925	OMU	C5-C4	2.79	1.49	1.43
83	S2	121	OMU	C5-C4	2.78	1.49	1.43
83	S2	1832	6MZ	C8-N9	-2.78	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2837	OMU	C5-C4	2.76	1.49	1.43
3	L5	4306	OMU	C5-C4	2.75	1.49	1.43
3	L5	4498	OMU	C5-C4	2.74	1.49	1.43
83	S2	1288	OMU	C6-N1	2.72	1.44	1.38
83	S2	1442	OMU	C6-N1	2.72	1.44	1.38
83	S2	799	OMU	C6-N1	2.72	1.44	1.38
3	L5	4220	6MZ	O3'-C3'	2.72	1.49	1.43
83	S2	121	OMU	C6-N1	2.70	1.44	1.38
83	S2	354	OMU	C6-N1	2.69	1.44	1.38
3	L5	2837	OMU	C6-N1	2.69	1.44	1.38
83	S2	1326	OMU	C6-N1	2.68	1.44	1.38
83	S2	627	OMU	C6-N1	2.67	1.44	1.38
83	S2	116	OMU	C5-C4	2.67	1.49	1.43
83	S2	428	OMU	C6-N1	2.67	1.44	1.38
3	L5	4498	OMU	C6-N1	2.66	1.44	1.38
3	L5	4530	UR3	C6-N1	2.66	1.44	1.38
83	S2	116	OMU	C6-N1	2.66	1.44	1.38
3	L5	4306	OMU	C6-N1	2.65	1.44	1.38
3	L5	4227	OMU	C6-N1	2.64	1.44	1.38
3	L5	4620	OMU	C5-C4	2.63	1.49	1.43
83	S2	172	OMU	C6-N1	2.62	1.44	1.38
3	L5	4620	OMU	C6-N1	2.61	1.44	1.38
3	L5	3925	OMU	C6-N1	2.61	1.44	1.38
3	L5	4530	UR3	O2-C2	-2.57	1.17	1.22
83	S2	1639	G7M	O6-C6	-2.48	1.18	1.23
3	L5	1524	A2M	O4'-C4'	-2.47	1.39	1.45
83	S2	1639	G7M	C6-N1	2.46	1.43	1.38
83	S2	668	A2M	O4'-C4'	-2.44	1.39	1.45
83	S2	1851	MA6	C5-C4	-2.40	1.34	1.39
3	L5	1323	A2M	O4'-C4'	-2.33	1.39	1.45
83	S2	1850	MA6	C5-C4	-2.32	1.34	1.39
3	L5	4530	UR3	C5-C4	2.26	1.49	1.43
3	L5	4220	6MZ	C6-N1	-2.24	1.31	1.35
3	L5	3818	UY1	O4'-C1'	-2.19	1.40	1.43
3	L5	4530	UR3	C3U-N3	2.16	1.50	1.47
3	L5	1323	A2M	O3'-C3'	-2.14	1.37	1.43
3	L5	3818	UY1	C4-C5	2.14	1.50	1.44
3	L5	4571	A2M	O4'-C4'	-2.10	1.40	1.45
83	S2	576	A2M	C5-C4	2.10	1.42	1.39
83	S2	159	A2M	C5-C4	2.08	1.42	1.39
3	L5	2363	A2M	O4'-C4'	-2.06	1.40	1.45
3	L5	4523	A2M	O3'-C3'	-2.02	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	S2	1639	G7M	C4-N9	-2.01	1.33	1.38

All (637) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1851	MA6	N1-C6-N6	-11.87	102.39	116.86
83	S2	1850	MA6	N1-C6-N6	-11.57	102.75	116.86
83	S2	1851	MA6	C5-C6-N6	7.95	137.92	125.33
83	S2	1850	MA6	C5-C6-N6	7.74	137.58	125.33
83	S2	1639	G7M	C1'-N9-C4	7.62	148.99	126.49
83	S2	1639	G7M	C1'-N9-C8	-7.41	101.72	126.74
3	L5	4220	6MZ	N1-C2-N3	-5.89	119.66	128.58
83	S2	1832	6MZ	N1-C2-N3	-5.85	119.72	128.58
83	S2	1326	OMU	C4-N3-C2	-5.78	119.43	126.61
3	L5	3925	OMU	C4-N3-C2	-5.75	119.48	126.61
83	S2	172	OMU	C4-N3-C2	-5.73	119.50	126.61
83	S2	1851	MA6	N1-C2-N3	-5.72	119.92	128.58
83	S2	428	OMU	C4-N3-C2	-5.71	119.52	126.61
3	L5	4227	OMU	C4-N3-C2	-5.69	119.55	126.61
3	L5	4498	OMU	C4-N3-C2	-5.69	119.55	126.61
83	S2	1850	MA6	N1-C2-N3	-5.68	119.98	128.58
83	S2	799	OMU	C4-N3-C2	-5.63	119.62	126.61
3	L5	4306	OMU	C4-N3-C2	-5.61	119.65	126.61
83	S2	627	OMU	C4-N3-C2	-5.59	119.67	126.61
83	S2	354	OMU	C4-N3-C2	-5.56	119.71	126.61
83	S2	1288	OMU	C4-N3-C2	-5.54	119.73	126.61
3	L5	2837	OMU	C4-N3-C2	-5.54	119.73	126.61
83	S2	1851	MA6	N9-C8-N7	-5.45	106.20	113.94
3	L5	4530	UR3	C4-N3-C2	-5.44	120.20	124.58
83	S2	1442	OMU	C4-N3-C2	-5.39	119.92	126.61
83	S2	121	OMU	C4-N3-C2	-5.38	119.93	126.61
83	S2	1850	MA6	N9-C8-N7	-5.33	106.38	113.94
3	L5	3637	PSU	N1-C2-N3	5.27	120.73	115.17
83	S2	1248	B8N	C5-C4-N3	5.26	125.70	116.15
83	S2	116	OMU	C4-N3-C2	-5.20	120.15	126.61
3	L5	3701	OMC	C1'-N1-C2	5.11	129.73	118.44
3	L5	1677	PSU	N1-C2-N3	5.08	120.52	115.17
3	L5	4293	PSU	N1-C2-N3	5.07	120.52	115.17
3	L5	4636	PSU	N1-C2-N3	5.04	120.49	115.17
3	L5	4500	PSU	N1-C2-N3	5.02	120.47	115.17
3	L5	4620	OMU	C4-N3-C2	-5.01	120.39	126.61
3	L5	4521	PSU	N1-C2-N3	5.00	120.45	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1677	PSU	C4-N3-C2	-5.00	119.48	126.37
3	L5	4689	PSU	N1-C2-N3	4.97	120.41	115.17
5	L8	55	PSU	N1-C2-N3	4.96	120.40	115.17
83	S2	406	PSU	N1-C2-N3	4.95	120.39	115.17
3	L5	3818	UY1	C4-N3-C2	-4.94	119.57	126.37
3	L5	4636	PSU	C4-N3-C2	-4.93	119.58	126.37
3	L5	4299	PSU	N1-C2-N3	4.92	120.36	115.17
3	L5	1860	PSU	N1-C2-N3	4.90	120.33	115.17
83	S2	406	PSU	C4-N3-C2	-4.88	119.64	126.37
3	L5	4312	PSU	N1-C2-N3	4.88	120.32	115.17
3	L5	4521	PSU	C4-N3-C2	-4.88	119.65	126.37
3	L5	1862	PSU	N1-C2-N3	4.88	120.31	115.17
3	L5	4403	PSU	N1-C2-N3	4.87	120.30	115.17
83	S2	651	PSU	N1-C2-N3	4.87	120.30	115.17
3	L5	3920	PSU	N1-C2-N3	4.86	120.30	115.17
3	L5	1536	PSU	N1-C2-N3	4.85	120.28	115.17
3	L5	4293	PSU	C4-N3-C2	-4.84	119.70	126.37
83	S2	1232	PSU	N1-C2-N3	4.84	120.27	115.17
83	S2	1832	6MZ	N9-C8-N7	-4.84	107.07	113.94
83	S2	1232	PSU	C4-N3-C2	-4.83	119.72	126.37
3	L5	3822	PSU	N1-C2-N3	4.83	120.26	115.17
83	S2	649	PSU	N1-C2-N3	4.83	120.26	115.17
3	L5	1782	PSU	N1-C2-N3	4.83	120.26	115.17
83	S2	686	PSU	N1-C2-N3	4.82	120.25	115.17
3	L5	1683	PSU	N1-C2-N3	4.82	120.25	115.17
83	S2	863	PSU	N1-C2-N3	4.81	120.24	115.17
3	L5	4403	PSU	C4-N3-C2	-4.81	119.75	126.37
3	L5	4493	PSU	N1-C2-N3	4.81	120.24	115.17
3	L5	4673	PSU	N1-C2-N3	4.81	120.24	115.17
3	L5	4552	PSU	N1-C2-N3	4.81	120.24	115.17
3	L5	4500	PSU	C4-N3-C2	-4.80	119.75	126.37
3	L5	4973	PSU	N1-C2-N3	4.80	120.23	115.17
3	L5	4471	PSU	N1-C2-N3	4.80	120.23	115.17
3	L5	4973	PSU	C4-N3-C2	-4.80	119.77	126.37
83	S2	686	PSU	C4-N3-C2	-4.79	119.77	126.37
3	L5	4972	PSU	N1-C2-N3	4.79	120.22	115.17
83	S2	801	PSU	N1-C2-N3	4.79	120.22	115.17
3	L5	5010	PSU	N1-C2-N3	4.78	120.21	115.17
3	L5	3639	PSU	N1-C2-N3	4.78	120.21	115.17
83	S2	1004	PSU	N1-C2-N3	4.78	120.21	115.17
83	S2	1056	PSU	N1-C2-N3	4.77	120.20	115.17
83	S2	1244	PSU	N1-C2-N3	4.77	120.20	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1832	6MZ	C5-C4-N3	-4.77	120.16	126.72
3	L5	1582	PSU	N1-C2-N3	4.76	120.19	115.17
3	L5	3695	PSU	N1-C2-N3	4.76	120.19	115.17
3	L5	4353	PSU	N1-C2-N3	4.76	120.19	115.17
3	L5	2632	PSU	N1-C2-N3	4.76	120.19	115.17
3	L5	3637	PSU	C4-N3-C2	-4.75	119.83	126.37
3	L5	5001	PSU	N1-C2-N3	4.75	120.18	115.17
5	L8	55	PSU	C4-N3-C2	-4.75	119.83	126.37
3	L5	3884	PSU	N1-C2-N3	4.75	120.17	115.17
3	L5	3851	PSU	N1-C2-N3	4.74	120.17	115.17
3	L5	4220	6MZ	N9-C8-N7	-4.73	107.22	113.94
3	L5	4552	PSU	C4-N3-C2	-4.73	119.86	126.37
83	S2	1081	PSU	N1-C2-N3	4.73	120.15	115.17
3	L5	3695	PSU	C4-N3-C2	-4.72	119.87	126.37
3	L5	4296	PSU	C4-N3-C2	-4.72	119.87	126.37
3	L5	4628	PSU	N1-C2-N3	4.72	120.14	115.17
3	L5	4353	PSU	C4-N3-C2	-4.72	119.87	126.37
83	S2	651	PSU	C4-N3-C2	-4.72	119.87	126.37
3	L5	4296	PSU	N1-C2-N3	4.72	120.14	115.17
3	L5	4457	PSU	N1-C2-N3	4.71	120.14	115.17
5	L8	69	PSU	N1-C2-N3	4.71	120.14	115.17
83	S2	109	PSU	N1-C2-N3	4.71	120.14	115.17
83	S2	1081	PSU	C4-N3-C2	-4.71	119.88	126.37
3	L5	4457	PSU	C4-N3-C2	-4.71	119.89	126.37
83	S2	649	PSU	C4-N3-C2	-4.70	119.89	126.37
3	L5	1862	PSU	C4-N3-C2	-4.70	119.90	126.37
3	L5	1744	PSU	N1-C2-N3	4.69	120.12	115.17
3	L5	4431	PSU	N1-C2-N3	4.69	120.12	115.17
83	S2	1177	PSU	N1-C2-N3	4.69	120.11	115.17
3	L5	5001	PSU	C4-N3-C2	-4.69	119.91	126.37
83	S2	1244	PSU	C4-N3-C2	-4.69	119.91	126.37
83	S2	1367	PSU	C4-N3-C2	-4.69	119.91	126.37
3	L5	4579	PSU	N1-C2-N3	4.69	120.11	115.17
3	L5	3884	PSU	C4-N3-C2	-4.69	119.92	126.37
83	S2	1174	PSU	N1-C2-N3	4.68	120.11	115.17
3	L5	3844	PSU	N1-C2-N3	4.68	120.10	115.17
83	S2	105	PSU	N1-C2-N3	4.68	120.10	115.17
83	S2	1367	PSU	N1-C2-N3	4.67	120.09	115.17
3	L5	1782	PSU	C4-N3-C2	-4.67	119.94	126.37
3	L5	1860	PSU	C4-N3-C2	-4.67	119.94	126.37
83	S2	863	PSU	C4-N3-C2	-4.66	119.95	126.37
3	L5	4442	PSU	C4-N3-C2	-4.66	119.95	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3639	PSU	C4-N3-C2	-4.66	119.95	126.37
3	L5	5010	PSU	C4-N3-C2	-4.66	119.95	126.37
3	L5	4493	PSU	C4-N3-C2	-4.66	119.95	126.37
83	S2	1177	PSU	C4-N3-C2	-4.66	119.95	126.37
83	S2	1046	PSU	N1-C2-N3	4.66	120.08	115.17
3	L5	4312	PSU	C4-N3-C2	-4.66	119.96	126.37
3	L5	4431	PSU	C4-N3-C2	-4.65	119.96	126.37
3	L5	4673	PSU	C4-N3-C2	-4.65	119.96	126.37
83	S2	866	PSU	N1-C2-N3	4.65	120.08	115.17
83	S2	814	PSU	C4-N3-C2	-4.65	119.96	126.37
3	L5	4442	PSU	N1-C2-N3	4.65	120.07	115.17
83	S2	966	PSU	N1-C2-N3	4.65	120.07	115.17
3	L5	4299	PSU	C4-N3-C2	-4.64	119.97	126.37
3	L5	1536	PSU	C4-N3-C2	-4.64	119.97	126.37
83	S2	109	PSU	C4-N3-C2	-4.64	119.97	126.37
3	L5	1683	PSU	C4-N3-C2	-4.64	119.98	126.37
3	L5	2839	PSU	N1-C2-N3	4.63	120.06	115.17
83	S2	1056	PSU	C4-N3-C2	-4.63	119.99	126.37
3	L5	1582	PSU	C4-N3-C2	-4.63	120.00	126.37
83	S2	1004	PSU	C4-N3-C2	-4.63	120.00	126.37
83	S2	866	PSU	C4-N3-C2	-4.62	120.00	126.37
5	L8	69	PSU	C4-N3-C2	-4.62	120.01	126.37
3	L5	4579	PSU	C4-N3-C2	-4.62	120.01	126.37
3	L5	4220	6MZ	C9-N6-C6	-4.61	118.57	122.85
83	S2	1046	PSU	C4-N3-C2	-4.61	120.02	126.37
3	L5	3822	PSU	C4-N3-C2	-4.61	120.02	126.37
3	L5	4532	PSU	N1-C2-N3	4.61	120.03	115.17
3	L5	1744	PSU	C4-N3-C2	-4.60	120.03	126.37
83	S2	681	PSU	N1-C2-N3	4.60	120.02	115.17
3	L5	4972	PSU	C4-N3-C2	-4.59	120.05	126.37
3	L5	1792	PSU	N1-C2-N3	4.59	120.00	115.17
83	S2	801	PSU	C4-N3-C2	-4.58	120.06	126.37
83	S2	1045	PSU	C4-N3-C2	-4.58	120.06	126.37
83	S2	1174	PSU	C4-N3-C2	-4.58	120.06	126.37
83	S2	814	PSU	N1-C2-N3	4.58	120.00	115.17
83	S2	1045	PSU	N1-C2-N3	4.57	119.99	115.17
83	S2	966	PSU	C4-N3-C2	-4.57	120.08	126.37
83	S2	105	PSU	C4-N3-C2	-4.56	120.08	126.37
3	L5	4576	PSU	C4-N3-C2	-4.56	120.09	126.37
3	L5	3851	PSU	C4-N3-C2	-4.55	120.10	126.37
3	L5	4689	PSU	C4-N3-C2	-4.55	120.10	126.37
3	L5	3853	PSU	N1-C2-N3	4.55	119.97	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3920	PSU	C4-N3-C2	-4.55	120.10	126.37
3	L5	4532	PSU	C4-N3-C2	-4.55	120.11	126.37
83	S2	681	PSU	C4-N3-C2	-4.54	120.11	126.37
3	L5	4361	PSU	N1-C2-N3	4.54	119.96	115.17
3	L5	3818	UY1	N1-C2-N3	4.54	119.95	115.17
83	S2	1248	B8N	C4-N3-C2	-4.53	120.04	125.62
3	L5	4576	PSU	N1-C2-N3	4.52	119.94	115.17
83	S2	1850	MA6	C5-C4-N3	-4.52	120.49	126.72
3	L5	1781	PSU	N1-C2-N3	4.52	119.93	115.17
3	L5	2839	PSU	C4-N3-C2	-4.52	120.15	126.37
3	L5	1792	PSU	C4-N3-C2	-4.52	120.15	126.37
3	L5	4471	PSU	C4-N3-C2	-4.52	120.15	126.37
83	S2	1639	G7M	C2-N3-C4	4.51	120.06	112.30
3	L5	4361	PSU	C4-N3-C2	-4.50	120.17	126.37
3	L5	4628	PSU	C4-N3-C2	-4.50	120.17	126.37
3	L5	2632	PSU	C4-N3-C2	-4.49	120.19	126.37
3	L5	4220	6MZ	C5-C4-N3	-4.48	120.55	126.72
83	S2	93	PSU	N1-C2-N3	4.48	119.89	115.17
3	L5	3853	PSU	C4-N3-C2	-4.47	120.22	126.37
83	S2	1851	MA6	C5-C4-N3	-4.44	120.60	126.72
83	S2	93	PSU	C4-N3-C2	-4.38	120.34	126.37
3	L5	3844	PSU	C4-N3-C2	-4.35	120.38	126.37
3	L5	1781	PSU	C4-N3-C2	-4.32	120.42	126.37
3	L5	3830	A2M	C3'-C2'-C1'	-4.20	94.76	102.81
83	S2	1851	MA6	C4-N9-C8	4.18	110.12	105.74
3	L5	1871	A2M	C3'-C2'-C1'	-4.16	94.83	102.81
83	S2	121	OMU	N3-C2-N1	4.12	120.25	114.89
3	L5	3925	OMU	N3-C2-N1	4.11	120.24	114.89
83	S2	1639	G7M	C5-C4-N3	-4.08	120.44	128.15
3	L5	3701	OMC	C1'-N1-C6	-4.07	112.08	120.78
83	S2	1850	MA6	C4-N9-C8	4.07	110.01	105.74
83	S2	1383	A2M	C3'-C2'-C1'	-4.06	95.04	102.81
3	L5	4498	OMU	N3-C2-N1	4.04	120.15	114.89
3	L5	4523	A2M	C3'-C2'-C1'	-4.00	95.16	102.81
3	L5	2837	OMU	N3-C2-N1	3.97	120.06	114.89
3	L5	398	A2M	C3'-C2'-C1'	-3.97	95.21	102.81
83	S2	354	OMU	N3-C2-N1	3.96	120.04	114.89
83	S2	1326	OMU	N3-C2-N1	3.95	120.03	114.89
3	L5	4306	OMU	N3-C2-N1	3.92	119.99	114.89
83	S2	172	OMU	N3-C2-N1	3.89	119.95	114.89
3	L5	4227	OMU	N3-C2-N1	3.88	119.94	114.89
83	S2	1639	G7M	C5-C6-N1	3.87	119.84	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1248	B8N	C1'-C5-C4	3.87	123.47	117.61
83	S2	799	OMU	N3-C2-N1	3.80	119.84	114.89
3	L5	4227	OMU	C5-C4-N3	3.77	120.08	114.80
83	S2	428	OMU	C5-C4-N3	3.77	120.08	114.80
83	S2	1031	A2M	C3'-C2'-C1'	-3.76	95.60	102.81
83	S2	428	OMU	N3-C2-N1	3.75	119.77	114.89
83	S2	1326	OMU	C5-C4-N3	3.73	120.03	114.80
83	S2	1288	OMU	N3-C2-N1	3.73	119.75	114.89
83	S2	1442	OMU	N3-C2-N1	3.73	119.74	114.89
83	S2	116	OMU	N3-C2-N1	3.71	119.73	114.89
83	S2	799	OMU	C5-C4-N3	3.70	119.98	114.80
3	L5	4530	UR3	C5-C4-N3	3.69	119.90	115.04
83	S2	627	OMU	C5-C4-N3	3.67	119.95	114.80
3	L5	4306	OMU	C5-C4-N3	3.67	119.94	114.80
83	S2	1288	OMU	C5-C4-N3	3.65	119.91	114.80
3	L5	3925	OMU	C5-C4-N3	3.62	119.87	114.80
83	S2	627	OMU	N3-C2-N1	3.62	119.61	114.89
3	L5	4590	A2M	C3'-C2'-C1'	-3.62	95.88	102.81
83	S2	354	OMU	C5-C4-N3	3.61	119.86	114.80
3	L5	4620	OMU	N3-C2-N1	3.59	119.57	114.89
83	S2	1850	MA6	C4-C5-C6	3.59	119.62	115.91
3	L5	3825	A2M	C3'-C2'-C1'	-3.59	95.94	102.81
83	S2	172	OMU	C5-C4-N3	3.58	119.81	114.80
83	S2	1851	MA6	C2-N1-C6	3.57	120.55	111.83
83	S2	1850	MA6	C2-N1-C6	3.56	120.52	111.83
3	L5	2837	OMU	C5-C4-N3	3.55	119.78	114.80
3	L5	4498	OMU	C5-C4-N3	3.54	119.76	114.80
83	S2	576	A2M	O3'-C3'-C2'	3.54	121.10	111.19
83	S2	1442	OMU	C5-C4-N3	3.53	119.74	114.80
83	S2	1832	6MZ	C2-N3-C4	3.53	120.44	111.83
3	L5	398	A2M	O3'-C3'-C2'	3.50	121.00	111.19
83	S2	1851	MA6	C4-C5-C6	3.50	119.53	115.91
83	S2	116	OMU	C5-C4-N3	3.44	119.62	114.80
83	S2	99	A2M	C3'-C2'-C1'	-3.44	96.21	102.81
3	L5	2351	OMC	C1'-N1-C2	3.44	126.04	118.44
3	L5	4620	OMU	C5-C4-N3	3.42	119.59	114.80
83	S2	166	A2M	O3'-C3'-C2'	3.42	120.76	111.19
3	L5	2787	A2M	O3'-C3'-C2'	3.39	120.68	111.19
3	L5	4220	6MZ	C2-N3-C4	3.37	120.07	111.83
83	S2	121	OMU	C5-C4-N3	3.35	119.50	114.80
83	S2	99	A2M	O3'-C3'-C2'	3.33	120.50	111.19
83	S2	27	A2M	C3'-C2'-C1'	-3.31	96.47	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	1832	6MZ	C5-N7-C8	3.31	108.65	103.45
83	S2	1639	G7M	O6-C6-C5	-3.30	120.63	128.01
83	S2	1248	B8N	N3-C2-N1	3.30	120.75	116.72
83	S2	1850	MA6	N3-C4-N9	3.30	132.78	127.17
83	S2	1851	MA6	C5-N7-C8	3.30	108.63	103.45
83	S2	1639	G7M	CN7-N7-C5	3.29	130.90	126.80
3	L5	3830	A2M	O3'-C3'-C2'	3.29	120.40	111.19
83	S2	576	A2M	C3'-C2'-C1'	-3.27	96.55	102.81
3	L5	4689	PSU	C6-N1-C2	-3.26	119.66	122.69
83	S2	1850	MA6	C5-N7-C8	3.25	108.56	103.45
83	S2	1383	A2M	O3'-C3'-C2'	3.25	120.28	111.19
3	L5	2401	A2M	C3'-C2'-C1'	-3.24	96.60	102.81
3	L5	3718	A2M	O3'-C3'-C2'	3.23	120.24	111.19
83	S2	1850	MA6	C2-N3-C4	3.23	119.72	111.83
83	S2	1851	MA6	C2-N3-C4	3.23	119.72	111.83
83	S2	1639	G7M	N9-C4-N3	3.22	132.39	125.95
83	S2	1851	MA6	N3-C4-N9	3.21	132.63	127.17
3	L5	3818	UY1	C6-C5-C4	3.21	120.34	118.17
3	L5	4220	6MZ	C4-N9-C8	3.20	109.09	105.74
83	S2	468	A2M	O3'-C3'-C2'	3.19	120.12	111.19
3	L5	2401	A2M	O3'-C3'-C2'	3.17	120.06	111.19
83	S2	159	A2M	O3'-C3'-C2'	3.16	120.03	111.19
3	L5	1871	A2M	C4-N9-C1'	-3.15	119.27	126.63
83	S2	166	A2M	C3'-C2'-C1'	-3.13	96.80	102.81
83	S2	1832	6MZ	C4-N9-C8	3.12	109.01	105.74
83	S2	1272	OMC	C1'-N1-C2	3.11	125.30	118.44
3	L5	3785	A2M	O3'-C3'-C2'	3.11	119.88	111.19
83	S2	468	A2M	C3'-C2'-C1'	-3.10	96.87	102.81
83	S2	1832	6MZ	N3-C4-N9	3.09	132.43	127.17
3	L5	1323	A2M	C2'-C1'-N9	3.09	118.84	113.75
3	L5	1871	A2M	O3'-C3'-C2'	3.09	119.83	111.19
3	L5	4220	6MZ	N3-C4-N9	3.08	132.41	127.17
3	L5	3818	UY1	C6-N1-C2	-3.08	119.83	122.69
83	S2	1031	A2M	O3'-C3'-C2'	3.07	119.78	111.19
3	L5	1677	PSU	O2-C2-N1	-3.05	119.64	122.79
3	L5	1536	PSU	O2-C2-N1	-3.05	119.65	122.79
3	L5	4571	A2M	O3'-C3'-C2'	3.04	119.71	111.19
3	L5	1524	A2M	O3'-C3'-C2'	3.04	119.70	111.19
3	L5	3825	A2M	O3'-C3'-C2'	3.04	119.70	111.19
3	L5	1534	A2M	C3'-C2'-C1'	-3.04	96.99	102.81
83	S2	428	OMU	O4-C4-C5	-3.04	119.92	125.16
3	L5	2401	A2M	C4-N9-C1'	-3.01	119.59	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	627	OMU	O4-C4-C5	-3.00	119.98	125.16
83	S2	116	OMU	O4-C4-C5	-2.98	120.02	125.16
83	S2	1442	OMU	O4-C4-C5	-2.98	120.03	125.16
3	L5	4500	PSU	O2-C2-N1	-2.97	119.72	122.79
83	S2	1832	6MZ	C4-C5-C6	2.97	119.25	116.78
3	L5	400	A2M	O3'-C3'-C2'	2.97	119.50	111.19
83	S2	484	A2M	O3'-C3'-C2'	2.97	119.49	111.19
83	S2	668	A2M	O3'-C3'-C2'	2.96	119.46	111.19
3	L5	4620	OMU	O4-C4-C5	-2.95	120.07	125.16
3	L5	3718	A2M	C3'-C2'-C1'	-2.95	97.16	102.81
3	L5	4523	A2M	C4-N9-C1'	-2.95	119.73	126.63
3	L5	4521	PSU	O2-C2-N1	-2.95	119.75	122.79
3	L5	4306	OMU	O4-C4-C5	-2.95	120.08	125.16
3	L5	4571	A2M	C3'-C2'-C1'	-2.95	97.17	102.81
3	L5	4689	PSU	O2-C2-N1	-2.94	119.75	122.79
3	L5	4227	OMU	O4-C4-C5	-2.93	120.10	125.16
83	S2	1174	PSU	O2-C2-N1	-2.93	119.77	122.79
3	L5	1860	PSU	O2-C2-N1	-2.92	119.77	122.79
83	S2	172	OMU	O4-C4-C5	-2.92	120.12	125.16
83	S2	354	OMU	O4-C4-C5	-2.92	120.13	125.16
83	S2	668	A2M	C4-N9-C1'	-2.92	119.81	126.63
3	L5	3925	OMU	O4-C4-C5	-2.92	120.13	125.16
83	S2	1326	OMU	O4-C4-C5	-2.90	120.16	125.16
83	S2	1288	OMU	O4-C4-C5	-2.90	120.16	125.16
83	S2	799	OMU	O4-C4-C5	-2.89	120.18	125.16
83	S2	27	A2M	O3'-C3'-C2'	2.88	119.25	111.19
3	L5	4220	6MZ	C5-N7-C8	2.87	107.97	103.45
3	L5	4293	PSU	C6-N1-C2	-2.87	120.03	122.69
3	L5	4498	OMU	O4-C4-C5	-2.86	120.22	125.16
83	S2	1639	G7M	C2-N1-C6	-2.86	119.92	125.11
3	L5	2837	OMU	O4-C4-C5	-2.86	120.22	125.16
3	L5	2815	A2M	O3'-C3'-C2'	2.86	119.20	111.19
3	L5	1323	A2M	C3'-C2'-C1'	-2.85	97.34	102.81
3	L5	3844	PSU	C6-N1-C2	-2.85	120.05	122.69
83	S2	121	OMU	O4-C4-C5	-2.84	120.26	125.16
83	S2	27	A2M	C4-N9-C1'	-2.84	120.00	126.63
83	S2	1248	B8N	O4-C4-N3	-2.84	115.39	119.99
83	S2	1383	A2M	C4-N9-C1'	-2.83	120.02	126.63
3	L5	4571	A2M	C4-N9-C1'	-2.83	120.03	126.63
3	L5	400	A2M	C3'-C2'-C1'	-2.82	97.40	102.81
83	S2	109	PSU	O2-C2-N1	-2.82	119.88	122.79
3	L5	3701	OMC	O2-C2-N1	2.82	124.42	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4296	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L5	3830	A2M	C4-N9-C1'	-2.81	120.06	126.63
83	S2	1004	PSU	O2-C2-N1	-2.81	119.89	122.79
3	L5	4523	A2M	O3'-C3'-C2'	2.81	119.05	111.19
3	L5	398	A2M	C4-N9-C1'	-2.81	120.07	126.63
3	L5	3637	PSU	C6-N1-C2	-2.80	120.09	122.69
83	S2	468	A2M	C4-N9-C1'	-2.80	120.09	126.63
83	S2	1056	PSU	O2-C2-N1	-2.79	119.91	122.79
3	L5	1677	PSU	C6-C5-C4	2.79	120.06	118.17
3	L5	4500	PSU	C6-N1-C2	-2.79	120.10	122.69
83	S2	686	PSU	O2-C2-N1	-2.79	119.91	122.79
83	S2	649	PSU	O2-C2-N1	-2.79	119.91	122.79
3	L5	1871	A2M	C1'-N9-C8	2.79	133.28	127.09
3	L5	3701	OMC	O2-C2-N3	-2.79	117.94	122.33
3	L5	4403	PSU	O2-C2-N1	-2.79	119.92	122.79
83	S2	406	PSU	O2-C2-N1	-2.77	119.93	122.79
3	L5	3785	A2M	C4-N9-C1'	-2.77	120.14	126.63
3	L5	3853	PSU	O2-C2-N1	-2.77	119.93	122.79
3	L5	4628	PSU	C6-N1-C2	-2.77	120.12	122.69
83	S2	801	PSU	O2-C2-N1	-2.77	119.93	122.79
83	S2	1031	A2M	C4-N9-C1'	-2.77	120.16	126.63
3	L5	4293	PSU	O2-C2-N1	-2.77	119.93	122.79
83	S2	99	A2M	C4-N9-C1'	-2.76	120.17	126.63
3	L5	3920	PSU	C6-N1-C2	-2.76	120.13	122.69
83	S2	1367	PSU	O2-C2-N1	-2.76	119.94	122.79
3	L5	4312	PSU	C6-N1-C2	-2.76	120.13	122.69
83	S2	1004	PSU	C6-N1-C2	-2.76	120.13	122.69
3	L5	1536	PSU	C6-N1-C2	-2.76	120.13	122.69
3	L5	1683	PSU	O2-C2-N1	-2.75	119.95	122.79
83	S2	1045	PSU	O2-C2-N1	-2.75	119.95	122.79
3	L5	1323	A2M	O3'-C3'-C2'	2.75	118.89	111.19
3	L5	2401	A2M	C1'-N9-C8	2.75	133.19	127.09
3	L5	1524	A2M	C4'-O4'-C1'	-2.75	103.40	109.47
3	L5	4579	PSU	O2-C2-N1	-2.74	119.96	122.79
3	L5	4590	A2M	C4-N9-C1'	-2.74	120.22	126.63
3	L5	4471	PSU	C6-N1-C2	-2.74	120.15	122.69
3	L5	4673	PSU	C6-N1-C2	-2.74	120.15	122.69
3	L5	3851	PSU	O2-C2-N1	-2.74	119.97	122.79
83	S2	159	A2M	C3'-C2'-C1'	-2.74	97.57	102.81
83	S2	166	A2M	C4-N9-C1'	-2.73	120.24	126.63
3	L5	2632	PSU	C6-N1-C2	-2.73	120.16	122.69
83	S2	484	A2M	C4-N9-C1'	-2.73	120.24	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3785	A2M	C4'-O4'-C1'	-2.73	103.44	109.47
3	L5	4220	6MZ	C4-C5-C6	2.72	119.04	116.78
3	L5	4493	PSU	O2-C2-N1	-2.72	119.98	122.79
3	L5	2363	A2M	O3'-C3'-C2'	2.72	118.80	111.19
83	S2	1056	PSU	C6-N1-C2	-2.71	120.17	122.69
3	L5	5010	PSU	O2-C2-N1	-2.71	119.99	122.79
3	L5	2804	OMC	C1'-N1-C2	2.71	124.43	118.44
3	L5	4636	PSU	O2-C2-N1	-2.71	119.99	122.79
83	S2	801	PSU	C6-N1-C2	-2.71	120.18	122.69
3	L5	3825	A2M	C4-N9-C1'	-2.71	120.30	126.63
3	L5	4312	PSU	O2-C2-N1	-2.71	120.00	122.79
83	S2	649	PSU	C6-N1-C2	-2.71	120.18	122.69
3	L5	4636	PSU	C6-C5-C4	2.71	120.00	118.17
83	S2	1046	PSU	O2-C2-N1	-2.70	120.00	122.79
3	L5	5001	PSU	O2-C2-N1	-2.70	120.01	122.79
3	L5	2787	A2M	O4'-C1'-C2'	2.69	111.23	106.59
3	L5	3822	PSU	O2-C2-N1	-2.69	120.01	122.79
3	L5	3785	A2M	C3'-C2'-C1'	-2.69	97.66	102.81
3	L5	4471	PSU	O2-C2-N1	-2.69	120.01	122.79
3	L5	4590	A2M	O3'-C3'-C2'	2.69	118.70	111.19
3	L5	2839	PSU	O2-C2-N1	-2.68	120.02	122.79
3	L5	3884	PSU	C6-N1-C2	-2.68	120.20	122.69
83	S2	866	PSU	O2-C2-N1	-2.68	120.02	122.79
83	S2	1337	4AC	N4-C4-N3	2.68	118.22	113.87
83	S2	159	A2M	C4-N9-C1'	-2.68	120.36	126.63
3	L5	1524	A2M	O4'-C1'-C2'	2.68	111.20	106.59
3	L5	1683	PSU	C6-N1-C2	-2.67	120.21	122.69
3	L5	1323	A2M	O4'-C1'-C2'	2.67	111.19	106.59
5	L8	55	PSU	O2-C2-N1	-2.67	120.04	122.79
3	L5	3867	A2M	C2'-C1'-N9	2.67	118.14	113.75
3	L5	4628	PSU	O2-C2-N1	-2.67	120.04	122.79
83	S2	1244	PSU	O2-C2-N1	-2.67	120.04	122.79
3	L5	2363	A2M	C2'-C1'-N9	2.67	118.14	113.75
5	L8	55	PSU	C6-N1-C2	-2.66	120.22	122.69
3	L5	3695	PSU	O2-C2-N1	-2.66	120.04	122.79
83	S2	484	A2M	C1'-N9-C8	2.66	132.99	127.09
83	S2	668	A2M	C1'-N9-C8	2.66	132.99	127.09
3	L5	3822	PSU	C6-N1-C2	-2.65	120.23	122.69
83	S2	1174	PSU	C6-N1-C2	-2.65	120.23	122.69
3	L5	4673	PSU	O2-C2-N1	-2.65	120.05	122.79
3	L5	1782	PSU	O2-C2-N1	-2.65	120.06	122.79
3	L5	3920	PSU	O2-C2-N1	-2.65	120.06	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	651	PSU	O2-C2-N1	-2.65	120.06	122.79
83	S2	27	A2M	C1'-N9-C8	2.65	132.97	127.09
83	S2	966	PSU	O2-C2-N1	-2.64	120.06	122.79
3	L5	1781	PSU	C6-N1-C2	-2.64	120.24	122.69
83	S2	1232	PSU	O2-C2-N1	-2.64	120.07	122.79
3	L5	398	A2M	C1'-N9-C8	2.64	132.95	127.09
3	L5	4442	PSU	O2-C2-N1	-2.64	120.07	122.79
3	L5	3639	PSU	O2-C2-N1	-2.63	120.07	122.79
3	L5	4299	PSU	C6-N1-C2	-2.63	120.25	122.69
83	S2	668	A2M	O4'-C1'-C2'	2.63	111.12	106.59
3	L5	4523	A2M	C1'-N9-C8	2.63	132.93	127.09
83	S2	576	A2M	C4-N9-C1'	-2.63	120.49	126.63
83	S2	863	PSU	C6-N1-C2	-2.63	120.25	122.69
3	L5	2632	PSU	O2-C2-N1	-2.63	120.08	122.79
3	L5	4579	PSU	C6-N1-C2	-2.63	120.25	122.69
3	L5	4576	PSU	O2-C2-N1	-2.62	120.08	122.79
83	S2	681	PSU	C6-N1-C2	-2.62	120.26	122.69
3	L5	4972	PSU	O2-C2-N1	-2.62	120.08	122.79
3	L5	4552	PSU	C6-N1-C2	-2.62	120.26	122.69
3	L5	4552	PSU	O2-C2-N1	-2.62	120.09	122.79
3	L5	2839	PSU	C6-N1-C2	-2.62	120.26	122.69
83	S2	1639	G7M	CN7-N7-C8	-2.62	120.83	124.79
3	L5	3884	PSU	O2-C2-N1	-2.62	120.09	122.79
83	S2	159	A2M	C1'-N9-C8	2.62	132.90	127.09
3	L5	4972	PSU	C6-N1-C2	-2.61	120.27	122.69
3	L5	1860	PSU	C6-N1-C2	-2.61	120.27	122.69
83	S2	1383	A2M	C1'-N9-C8	2.61	132.89	127.09
3	L5	4431	PSU	C6-N1-C2	-2.61	120.27	122.69
3	L5	1326	A2M	O3'-C3'-C2'	2.60	118.46	111.19
83	S2	468	A2M	C1'-N9-C8	2.59	132.85	127.09
83	S2	1081	PSU	O2-C2-N1	-2.59	120.11	122.79
83	S2	109	PSU	C6-N1-C2	-2.59	120.28	122.69
3	L5	3639	PSU	C6-N1-C2	-2.59	120.29	122.69
83	S2	1031	A2M	C1'-N9-C8	2.59	132.84	127.09
3	L5	4521	PSU	C6-N1-C2	-2.59	120.29	122.69
3	L5	1744	PSU	C6-N1-C2	-2.59	120.29	122.69
3	L5	5010	PSU	C6-N1-C2	-2.59	120.29	122.69
3	L5	1782	PSU	C6-N1-C2	-2.59	120.29	122.69
83	S2	99	A2M	C1'-N9-C8	2.59	132.84	127.09
3	L5	3830	A2M	C1'-N9-C8	2.59	132.83	127.09
3	L5	5001	PSU	C6-N1-C2	-2.59	120.29	122.69
3	L5	3695	PSU	C6-N1-C2	-2.58	120.30	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	651	PSU	C6-N1-C2	-2.58	120.30	122.69
3	L5	4431	PSU	O2-C2-N1	-2.57	120.13	122.79
3	L5	4636	PSU	C6-N1-C2	-2.57	120.31	122.69
3	L5	1792	PSU	O2-C2-N1	-2.57	120.14	122.79
3	L5	4532	PSU	O2-C2-N1	-2.57	120.14	122.79
3	L5	2861	OMC	C1'-N1-C2	2.57	124.11	118.44
83	S2	1046	PSU	C6-N1-C2	-2.56	120.31	122.69
83	S2	863	PSU	O2-C2-N1	-2.56	120.14	122.79
3	L5	3844	PSU	O2-C2-N1	-2.56	120.15	122.79
3	L5	2815	A2M	C2'-C1'-N9	2.56	117.96	113.75
3	L5	3718	A2M	C1'-N9-C8	2.56	132.77	127.09
5	L8	69	PSU	O2-C2-N1	-2.56	120.15	122.79
83	S2	93	PSU	C6-N1-C2	-2.56	120.32	122.69
83	S2	686	PSU	C6-N1-C2	-2.56	120.32	122.69
83	S2	1244	PSU	C6-N1-C2	-2.55	120.32	122.69
5	L8	69	PSU	C6-N1-C2	-2.55	120.32	122.69
3	L5	4571	A2M	C1'-N9-C8	2.55	132.75	127.09
83	S2	966	PSU	C6-N1-C2	-2.55	120.33	122.69
83	S2	105	PSU	C6-N1-C2	-2.55	120.33	122.69
3	L5	1781	PSU	O2-C2-N1	-2.55	120.16	122.79
3	L5	1862	PSU	C6-N1-C2	-2.54	120.33	122.69
3	L5	1582	PSU	C6-N1-C2	-2.54	120.33	122.69
3	L5	4500	PSU	C6-C5-C4	2.54	119.89	118.17
3	L5	2363	A2M	C3'-C2'-C1'	-2.54	97.94	102.81
3	L5	2363	A2M	C4-N9-C1'	-2.54	120.69	126.63
83	S2	1232	PSU	C6-N1-C2	-2.54	120.34	122.69
3	L5	1862	PSU	O2-C2-N1	-2.53	120.17	122.79
3	L5	3718	A2M	C4-N9-C1'	-2.53	120.70	126.63
3	L5	3851	PSU	C6-N1-C2	-2.53	120.34	122.69
3	L5	4299	PSU	O2-C2-N1	-2.53	120.18	122.79
3	L5	4457	PSU	O2-C2-N1	-2.53	120.18	122.79
3	L5	4361	PSU	C6-N1-C2	-2.53	120.34	122.69
83	S2	866	PSU	C6-N1-C2	-2.53	120.34	122.69
3	L5	4493	PSU	C6-N1-C2	-2.53	120.35	122.69
3	L5	2787	A2M	C4-N9-C1'	-2.53	120.73	126.63
3	L5	3818	UY1	O2-C2-N1	-2.52	120.19	122.79
3	L5	4973	PSU	O2-C2-N1	-2.52	120.19	122.79
83	S2	681	PSU	O2-C2-N1	-2.52	120.19	122.79
3	L5	3785	A2M	C1'-N9-C8	2.52	132.69	127.09
3	L5	4973	PSU	C6-N1-C2	-2.52	120.36	122.69
3	L5	4456	OMC	C1'-N1-C2	2.51	123.99	118.44
83	S2	166	A2M	C1'-N9-C8	2.51	132.67	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	400	A2M	C4-N9-C1'	-2.51	120.77	126.63
3	L5	3808	OMC	C1'-N1-C2	2.51	123.98	118.44
3	L5	2363	A2M	O4'-C1'-C2'	2.51	110.90	106.59
83	S2	105	PSU	O2-C2-N1	-2.50	120.21	122.79
83	S2	406	PSU	C6-N1-C2	-2.50	120.37	122.69
3	L5	1326	A2M	C4-N9-C1'	-2.49	120.80	126.63
3	L5	4353	PSU	O2-C2-N1	-2.49	120.22	122.79
3	L5	4590	A2M	C1'-N9-C8	2.49	132.62	127.09
3	L5	1323	A2M	C4-N9-C1'	-2.49	120.81	126.63
3	L5	4353	PSU	C6-N1-C2	-2.49	120.38	122.69
3	L5	2351	OMC	C1'-N1-C6	-2.48	115.48	120.78
3	L5	4457	PSU	C6-N1-C2	-2.48	120.39	122.69
83	S2	1177	PSU	C6-N1-C2	-2.48	120.39	122.69
3	L5	4521	PSU	C6-C5-C4	2.48	119.85	118.17
3	L5	3825	A2M	C1'-N9-C8	2.47	132.58	127.09
83	S2	93	PSU	O2-C2-N1	-2.47	120.24	122.79
83	S2	814	PSU	O2-C2-N1	-2.47	120.24	122.79
83	S2	576	A2M	C1'-N9-C8	2.47	132.57	127.09
3	L5	1744	PSU	O2-C2-N1	-2.47	120.24	122.79
3	L5	4361	PSU	O2-C2-N1	-2.47	120.25	122.79
3	L5	1792	PSU	C6-N1-C2	-2.45	120.41	122.69
3	L5	4442	PSU	C6-N1-C2	-2.45	120.41	122.69
3	L5	4530	UR3	C6-N1-C2	-2.45	119.79	121.80
3	L5	3867	A2M	C4-N9-C1'	-2.45	120.90	126.63
3	L5	1677	PSU	C6-N1-C2	-2.45	120.42	122.69
83	S2	1367	PSU	C6-N1-C2	-2.45	120.42	122.69
3	L5	4532	PSU	C6-N1-C2	-2.45	120.42	122.69
83	S2	1851	MA6	C1'-N9-C8	-2.44	121.68	127.09
3	L5	4576	PSU	C6-N1-C2	-2.44	120.43	122.69
3	L5	4403	PSU	C6-N1-C2	-2.43	120.44	122.69
3	L5	4296	PSU	C6-N1-C2	-2.43	120.44	122.69
83	S2	1045	PSU	C6-N1-C2	-2.43	120.44	122.69
83	S2	1177	PSU	O2-C2-N1	-2.42	120.29	122.79
83	S2	1272	OMC	C1'-N1-C6	-2.40	115.65	120.78
3	L5	2363	A2M	C1'-N9-C8	2.40	132.42	127.09
3	L5	4220	6MZ	C5-C6-N1	2.39	120.71	118.15
83	S2	1081	PSU	C6-N1-C2	-2.38	120.48	122.69
83	S2	1832	6MZ	C4-C5-N7	-2.38	107.86	110.58
3	L5	1534	A2M	C4-N9-C1'	-2.37	121.09	126.63
3	L5	3853	PSU	C6-N1-C2	-2.36	120.50	122.69
3	L5	1534	A2M	C1'-N9-C8	2.36	132.33	127.09
3	L5	1582	PSU	O2-C2-N1	-2.36	120.36	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3867	A2M	C1'-N9-C8	2.35	132.32	127.09
3	L5	400	A2M	C2'-C1'-N9	2.35	117.62	113.75
3	L5	4442	PSU	O4'-C1'-C2'	2.35	108.40	105.15
83	S2	814	PSU	C6-N1-C2	-2.35	120.52	122.69
3	L5	3867	A2M	O3'-C3'-C2'	2.34	117.74	111.19
3	L5	400	A2M	C1'-N9-C8	2.34	132.28	127.09
83	S2	1850	MA6	C1'-N9-C8	-2.34	121.91	127.09
3	L5	1326	A2M	O4'-C1'-C2'	2.33	110.60	106.59
3	L5	4403	PSU	O4'-C1'-C2'	2.33	108.38	105.15
3	L5	1326	A2M	C1'-N9-C8	2.32	132.25	127.09
83	S2	406	PSU	C6-C5-C4	2.32	119.74	118.17
3	L5	1322	1MA	N1-C6-N6	2.32	125.53	119.71
3	L5	2787	A2M	C1'-N9-C8	2.32	132.24	127.09
3	L5	1524	A2M	C4-N9-C1'	-2.30	121.24	126.63
83	S2	1248	B8N	O4'-C1'-C2'	2.30	108.33	105.15
3	L5	1871	A2M	C6-C5-C4	-2.28	114.06	117.18
3	L5	4403	PSU	C6-C5-C4	2.28	119.71	118.17
3	L5	3867	A2M	C3'-C2'-C1'	-2.28	98.45	102.81
3	L5	3822	PSU	O4'-C1'-C2'	2.27	108.28	105.15
3	L5	2815	A2M	C4-N9-C1'	-2.26	121.35	126.63
5	L8	69	PSU	O4'-C1'-C2'	2.25	108.26	105.15
3	L5	1323	A2M	C1'-N9-C8	2.25	132.08	127.09
3	L5	4571	A2M	O4'-C1'-C2'	2.24	110.45	106.59
83	S2	1326	OMU	O2-C2-N1	-2.24	119.88	122.80
3	L5	400	A2M	O4'-C1'-C2'	2.24	110.44	106.59
83	S2	484	A2M	O4'-C1'-C2'	2.24	110.44	106.59
3	L5	3785	A2M	O4'-C4'-C3'	2.23	109.59	105.15
3	L5	4636	PSU	O4'-C1'-C2'	2.23	108.23	105.15
3	L5	2815	A2M	C3'-C2'-C1'	-2.22	98.56	102.81
3	L5	3785	A2M	C2-N1-C6	-2.20	115.11	118.73
83	S2	468	A2M	O4'-C1'-C2'	2.20	110.38	106.59
83	S2	27	A2M	O4'-C1'-C2'	2.20	110.38	106.59
3	L5	2787	A2M	O4'-C4'-C3'	2.20	109.52	105.15
83	S2	172	OMU	O2-C2-N1	-2.20	119.94	122.80
83	S2	1081	PSU	O4'-C1'-C2'	2.19	108.19	105.15
3	L5	2815	A2M	C1'-N9-C8	2.19	131.96	127.09
3	L5	1326	A2M	C3'-C2'-C1'	-2.19	98.61	102.81
3	L5	1524	A2M	C1'-N9-C8	2.17	131.91	127.09
3	L5	4523	A2M	C6-C5-C4	-2.16	114.22	117.18
83	S2	468	A2M	C6-C5-C4	-2.16	114.23	117.18
3	L5	4571	A2M	C6-C5-C4	-2.15	114.24	117.18
3	L5	2401	A2M	C6-C5-C4	-2.15	114.24	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	S2	866	PSU	O4'-C1'-C2'	2.15	108.13	105.15
83	S2	668	A2M	C6-C5-C4	-2.15	114.25	117.18
83	S2	1639	G7M	N9-C8-N7	-2.14	107.28	112.48
83	S2	668	A2M	C2'-C1'-N9	2.14	117.28	113.75
3	L5	398	A2M	C6-C5-C4	-2.14	114.25	117.18
3	L5	2401	A2M	O4'-C1'-C2'	2.14	110.28	106.59
83	S2	27	A2M	C6-C5-C4	-2.14	114.26	117.18
3	L5	4498	OMU	O2-C2-N1	-2.14	120.01	122.80
3	L5	3830	A2M	C6-C5-C4	-2.13	114.28	117.18
83	S2	166	A2M	C6-C5-C4	-2.13	114.28	117.18
3	L5	4590	A2M	C6-C5-C4	-2.12	114.28	117.18
83	S2	1248	B8N	O4-C4-C5	-2.12	118.91	122.58
83	S2	484	A2M	C3'-C2'-C1'	-2.12	98.74	102.81
3	L5	3785	A2M	C5-C6-N1	2.12	122.89	117.51
83	S2	1383	A2M	C6-C5-C4	-2.12	114.29	117.18
3	L5	1534	A2M	C2-N1-C6	-2.11	115.27	118.73
83	S2	354	OMU	O2-C2-N1	-2.11	120.05	122.80
3	L5	4299	PSU	C6-C5-C4	2.11	119.59	118.17
83	S2	1031	A2M	C6-C5-C4	-2.10	114.31	117.18
83	S2	166	A2M	O4'-C1'-C2'	2.10	110.20	106.59
3	L5	1871	A2M	C4'-O4'-C1'	-2.10	104.83	109.47
3	L5	4457	PSU	O4'-C1'-C2'	2.09	108.04	105.15
3	L5	3637	PSU	C6-C5-C4	2.09	119.58	118.17
83	S2	484	A2M	C6-C5-C4	-2.08	114.33	117.18
83	S2	428	OMU	O2-C2-N1	-2.08	120.09	122.80
3	L5	4523	A2M	C4'-O4'-C1'	-2.07	104.89	109.47
83	S2	159	A2M	O4'-C1'-C2'	2.07	110.16	106.59
5	L8	55	PSU	C6-C5-C4	2.07	119.57	118.17
3	L5	2815	A2M	O4'-C1'-C2'	2.07	110.15	106.59
3	L5	1534	A2M	O4'-C1'-C2'	2.06	110.14	106.59
83	S2	1832	6MZ	C5-C6-N1	2.06	120.36	118.15
3	L5	3785	A2M	C6-C5-C4	-2.06	114.36	117.18
83	S2	1288	OMU	O2-C2-N1	-2.05	120.12	122.80
3	L5	1534	A2M	O3'-C3'-C2'	2.05	116.93	111.19
83	S2	576	A2M	C6-C5-C4	-2.05	114.37	117.18
3	L5	3825	A2M	C6-C5-C4	-2.05	114.38	117.18
83	S2	1832	6MZ	OP2-P-OP1	2.05	118.83	110.83
3	L5	3695	PSU	O4'-C1'-C2'	2.05	107.98	105.15
3	L5	1326	A2M	C6-C5-C4	-2.05	114.39	117.18
83	S2	121	OMU	O2-C2-N1	-2.04	120.14	122.80
83	S2	99	A2M	C6-C5-C4	-2.04	114.40	117.18
3	L5	1323	A2M	C6-C5-C4	-2.03	114.40	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1524	A2M	C2-N1-C6	-2.03	115.39	118.73
83	S2	159	A2M	C6-C5-C4	-2.03	114.40	117.18
3	L5	1534	A2M	C2'-C1'-N9	2.02	117.08	113.75
83	S2	1851	MA6	C4-C5-N7	-2.02	108.27	110.58
3	L5	3818	UY1	O4'-C1'-C2'	2.02	108.10	104.56
3	L5	2787	A2M	C6-C5-C4	-2.02	114.42	117.18
83	S2	627	OMU	O2-C2-N1	-2.02	120.17	122.80
3	L5	3925	OMU	O2-C2-N1	-2.01	120.17	122.80
3	L5	3867	A2M	C2-N1-C6	-2.01	115.42	118.73
3	L5	4628	PSU	O4'-C1'-C2'	2.01	107.93	105.15
3	L5	3718	A2M	C6-C5-C4	-2.01	114.43	117.18
3	L5	3639	PSU	O4'-C1'-C2'	2.00	107.92	105.15

There are no chirality outliers.

All (145) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L5	400	A2M	C1'-C2'-O2'-CM'
3	L5	1326	A2M	O4'-C4'-C5'-O5'
3	L5	1340	OMC	C1'-C2'-O2'-CM2
3	L5	1625	OMG	O4'-C4'-C5'-O5'
3	L5	2351	OMC	C1'-C2'-O2'-CM2
3	L5	2364	OMG	O4'-C4'-C5'-O5'
3	L5	2787	A2M	C1'-C2'-O2'-CM'
3	L5	2824	OMC	C1'-C2'-O2'-CM2
3	L5	3701	OMC	O4'-C4'-C5'-O5'
3	L5	3792	OMG	O4'-C4'-C5'-O5'
3	L5	3841	OMC	C1'-C2'-O2'-CM2
3	L5	3867	A2M	C1'-C2'-O2'-CM'
3	L5	4196	OMG	C1'-C2'-O2'-CM2
3	L5	4306	OMU	C1'-C2'-O2'-CM2
3	L5	4500	PSU	O4'-C4'-C5'-O5'
3	L5	4590	A2M	O4'-C4'-C5'-O5'
3	L5	4620	OMU	C1'-C2'-O2'-CM2
3	L5	4637	OMG	O4'-C4'-C5'-O5'
3	L5	4637	OMG	C1'-C2'-O2'-CM2
83	S2	27	A2M	C1'-C2'-O2'-CM'
83	S2	99	A2M	C1'-C2'-O2'-CM'
83	S2	159	A2M	C1'-C2'-O2'-CM'
83	S2	436	OMG	O4'-C4'-C5'-O5'
83	S2	462	OMC	C1'-C2'-O2'-CM2
83	S2	601	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
83	S2	644	OMG	O4'-C4'-C5'-O5'
83	S2	1248	B8N	O4'-C4'-C5'-O5'
83	S2	1272	OMC	C1'-C2'-O2'-CM2
83	S2	1272	OMC	O4'-C4'-C5'-O5'
83	S2	1288	OMU	C3'-C4'-C5'-O5'
83	S2	1288	OMU	O4'-C4'-C5'-O5'
83	S2	1337	4AC	N3-C4-N4-C7
83	S2	1383	A2M	C1'-C2'-O2'-CM'
83	S2	1442	OMU	O4'-C4'-C5'-O5'
83	S2	1832	6MZ	C5-C6-N6-C9
83	S2	1832	6MZ	N1-C6-N6-C9
3	L5	3701	OMC	C2'-C1'-N1-C2
3	L5	1326	A2M	C3'-C4'-C5'-O5'
3	L5	1536	PSU	O4'-C4'-C5'-O5'
3	L5	2815	A2M	O4'-C4'-C5'-O5'
3	L5	3701	OMC	C3'-C4'-C5'-O5'
3	L5	3867	A2M	C3'-C4'-C5'-O5'
3	L5	4500	PSU	C3'-C4'-C5'-O5'
3	L5	4590	A2M	C3'-C4'-C5'-O5'
83	S2	99	A2M	O4'-C4'-C5'-O5'
83	S2	576	A2M	O4'-C4'-C5'-O5'
83	S2	576	A2M	C3'-C4'-C5'-O5'
83	S2	683	OMG	C3'-C4'-C5'-O5'
83	S2	799	OMU	C3'-C4'-C5'-O5'
83	S2	799	OMU	O4'-C4'-C5'-O5'
83	S2	801	PSU	C3'-C4'-C5'-O5'
83	S2	867	OMG	C3'-C4'-C5'-O5'
83	S2	1272	OMC	C3'-C4'-C5'-O5'
3	L5	1323	A2M	O4'-C4'-C5'-O5'
3	L5	1536	PSU	C3'-C4'-C5'-O5'
3	L5	1625	OMG	C3'-C4'-C5'-O5'
3	L5	3867	A2M	O4'-C4'-C5'-O5'
83	S2	517	OMC	C3'-C4'-C5'-O5'
83	S2	517	OMC	O4'-C4'-C5'-O5'
83	S2	801	PSU	O4'-C4'-C5'-O5'
83	S2	867	OMG	O4'-C4'-C5'-O5'
83	S2	1442	OMU	C3'-C4'-C5'-O5'
3	L5	3701	OMC	C2'-C1'-N1-C6
3	L5	4447	5MC	C2'-C1'-N1-C6
3	L5	2364	OMG	C3'-C4'-C5'-O5'
3	L5	2815	A2M	C3'-C4'-C5'-O5'
3	L5	3792	OMG	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	L5	4637	OMG	C3'-C4'-C5'-O5'
83	S2	436	OMG	C3'-C4'-C5'-O5'
83	S2	644	OMG	C3'-C4'-C5'-O5'
3	L5	1524	A2M	C3'-C4'-C5'-O5'
83	S2	668	A2M	O4'-C4'-C5'-O5'
83	S2	1248	B8N	C3'-C4'-C5'-O5'
83	S2	1248	B8N	N34-C33-C34-O36
3	L5	1677	PSU	O4'-C4'-C5'-O5'
3	L5	1781	PSU	C3'-C4'-C5'-O5'
83	S2	99	A2M	C3'-C4'-C5'-O5'
83	S2	668	A2M	C3'-C4'-C5'-O5'
83	S2	683	OMG	O4'-C4'-C5'-O5'
83	S2	627	OMU	C2'-C1'-N1-C6
3	L5	1524	A2M	O4'-C4'-C5'-O5'
3	L5	1677	PSU	C3'-C4'-C5'-O5'
3	L5	2422	OMC	O4'-C4'-C5'-O5'
3	L5	4296	PSU	O4'-C4'-C5'-O5'
3	L5	2787	A2M	C3'-C4'-C5'-O5'
3	L5	4296	PSU	C3'-C4'-C5'-O5'
3	L5	4590	A2M	C4'-C5'-O5'-P
83	S2	428	OMU	C2'-C1'-N1-C6
3	L5	4447	5MC	C2'-C1'-N1-C2
3	L5	1323	A2M	C3'-C4'-C5'-O5'
3	L5	2422	OMC	C3'-C4'-C5'-O5'
3	L5	2787	A2M	C2'-C1'-N9-C8
83	S2	116	OMU	C1'-C2'-O2'-CM2
83	S2	468	A2M	C1'-C2'-O2'-CM'
83	S2	1328	OMG	C1'-C2'-O2'-CM2
83	S2	1045	PSU	C3'-C4'-C5'-O5'
3	L5	3899	OMG	C3'-C4'-C5'-O5'
3	L5	398	A2M	O4'-C4'-C5'-O5'
83	S2	1045	PSU	O4'-C4'-C5'-O5'
83	S2	1703	OMC	O4'-C4'-C5'-O5'
3	L5	3701	OMC	O4'-C1'-N1-C6
3	L5	4447	5MC	O4'-C1'-N1-C6
83	S2	428	OMU	O4'-C1'-N1-C6
83	S2	627	OMU	O4'-C1'-N1-C6
3	L5	4447	5MC	O4'-C1'-N1-C2
3	L5	3869	OMC	C3'-C2'-O2'-CM2
3	L5	3818	UY1	C4'-C5'-O5'-P
3	L5	3818	UY1	O4'-C1'-C5-C4
3	L5	2787	A2M	C2'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	3844	PSU	C4'-C5'-O5'-P
3	L5	4500	PSU	C4'-C5'-O5'-P
83	S2	1851	MA6	C4'-C5'-O5'-P
3	L5	1781	PSU	O4'-C4'-C5'-O5'
3	L5	4618	OMG	C3'-C4'-C5'-O5'
83	S2	576	A2M	C4'-C5'-O5'-P
3	L5	4499	OMG	C3'-C2'-O2'-CM2
3	L5	3887	OMC	C4'-C5'-O5'-P
83	S2	644	OMG	C4'-C5'-O5'-P
3	L5	3851	PSU	C3'-C4'-C5'-O5'
3	L5	3701	OMC	O4'-C1'-N1-C2
83	S2	627	OMU	C2'-C1'-N1-C2
83	S2	1490	OMG	C4'-C5'-O5'-P
83	S2	627	OMU	O4'-C1'-N1-C2
3	L5	1322	1MA	C2'-C1'-N9-C8
3	L5	1326	A2M	C1'-C2'-O2'-CM'
3	L5	1322	1MA	C2'-C1'-N9-C4
3	L5	1677	PSU	O4'-C1'-C5-C6
3	L5	4636	PSU	O4'-C1'-C5-C6
3	L5	2351	OMC	C2'-C1'-N1-C6
83	S2	428	OMU	C2'-C1'-N1-C2
3	L5	1524	A2M	C3'-C2'-O2'-CM'
3	L5	3899	OMG	C3'-C2'-O2'-CM2
83	S2	428	OMU	O4'-C1'-N1-C2
3	L5	1677	PSU	C2'-C1'-C5-C6
3	L5	2787	A2M	O4'-C1'-N9-C8
83	S2	1832	6MZ	O4'-C4'-C5'-O5'
3	L5	1326	A2M	C4'-C5'-O5'-P
83	S2	1272	OMC	C4'-C5'-O5'-P
3	L5	2804	OMC	C2'-C1'-N1-C2
83	S2	1272	OMC	C2'-C1'-N1-C2
83	S2	1248	B8N	N34-C33-C34-O35
3	L5	2351	OMC	O4'-C4'-C5'-O5'
3	L5	3782	5MC	O4'-C4'-C5'-O5'
3	L5	3899	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

80 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	2363	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	S2	509	OMG	3	0
3	L5	1340	OMC	2	0
3	L5	3925	OMU	1	0
83	S2	1004	PSU	2	0
3	L5	4689	PSU	1	0
83	S2	1391	OMC	1	0
3	L5	4431	PSU	1	0
3	L5	3785	A2M	1	0
83	S2	1288	OMU	1	0
83	S2	1842	4AC	1	0
83	S2	484	A2M	1	0
3	L5	1683	PSU	2	0
83	S2	1442	OMU	1	0
83	S2	576	A2M	2	0
3	L5	4571	A2M	1	0
3	L5	4306	OMU	1	0
3	L5	400	A2M	1	0
83	S2	116	OMU	2	0
3	L5	2422	OMC	1	0
3	L5	3867	A2M	5	0
3	L5	2424	OMG	1	0
83	S2	683	OMG	1	0
3	L5	4637	OMG	1	0
3	L5	4457	PSU	1	0
3	L5	1534	A2M	1	0
3	L5	4456	OMC	1	0
83	S2	99	A2M	1	0
3	L5	3718	A2M	3	0
5	L8	75	OMG	2	0
3	L5	4636	PSU	1	0
83	S2	866	PSU	2	0
83	S2	517	OMC	1	0
3	L5	4620	OMU	2	0
3	L5	4579	PSU	2	0
3	L5	3701	OMC	1	0
3	L5	2351	OMC	1	0
83	S2	27	A2M	3	0
3	L5	4293	PSU	1	0
3	L5	4590	A2M	1	0
83	S2	1703	OMC	1	0
83	S2	867	OMG	3	0
83	S2	649	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	S2	1046	PSU	1	0
83	S2	681	PSU	1	0
3	L5	2804	OMC	1	0
3	L5	1871	A2M	1	0
3	L5	4220	6MZ	1	0
83	S2	1174	PSU	2	0
83	S2	1850	MA6	1	0
83	S2	159	A2M	2	0
83	S2	436	OMG	1	0
3	L5	3822	PSU	1	0
83	S2	1272	OMC	1	0
83	S2	121	OMU	1	0
83	S2	1031	A2M	1	0
83	S2	468	A2M	1	0
3	L5	4536	OMC	1	0
3	L5	1326	A2M	5	0
3	L5	3818	UY1	1	0
3	L5	3841	OMC	1	0
3	L5	4392	OMG	1	0
3	L5	4523	A2M	2	0
3	L5	398	A2M	1	0
83	S2	462	OMC	1	0
83	S2	166	A2M	2	0
3	L5	1677	PSU	1	0
3	L5	4196	OMG	1	0
3	L5	2364	OMG	1	0
3	L5	4228	OMG	1	0
83	S2	1232	PSU	1	0
3	L5	2876	OMG	1	0
83	S2	601	OMG	2	0
3	L5	3884	PSU	1	0
83	S2	1639	G7M	1	0
83	S2	1383	A2M	1	0
83	S2	1337	4AC	2	0
3	L5	3825	A2M	1	0
3	L5	2824	OMC	1	0
3	L5	4618	OMG	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
87	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.84	0
86	SPM	L5	5293	-	13,13,13	0.36	0	12,12,12	0.87	0
87	SPD	L5	5261	-	9,9,9	0.32	0	8,8,8	0.94	0
87	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.88	0
86	SPM	L5	5259	-	13,13,13	0.35	0	12,12,12	0.99	0
86	SPM	L5	5263	-	13,13,13	0.34	0	12,12,12	0.98	0
87	SPD	L5	5288	-	9,9,9	0.31	0	8,8,8	0.83	0
87	SPD	LN	301	-	9,9,9	0.31	0	8,8,8	0.91	0
87	SPD	L5	5283	-	9,9,9	0.34	0	8,8,8	0.86	0
87	SPD	L5	5291	-	9,9,9	0.31	0	8,8,8	0.81	0
86	SPM	L5	5267	-	13,13,13	0.36	0	12,12,12	1.09	0
87	SPD	L5	5284	-	9,9,9	0.31	0	8,8,8	0.79	0
87	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.85	0
87	SPD	L5	5290	-	9,9,9	0.33	0	8,8,8	0.85	0
86	SPM	L5	5264	-	13,13,13	0.34	0	12,12,12	1.01	0
86	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.90	0
86	SPM	L5	5289	-	13,13,13	0.37	0	12,12,12	1.01	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPD	L5	5286	-	-	0/7/7/7	-
86	SPM	L5	5293	-	-	5/11/11/11	-
87	SPD	L5	5261	-	-	1/7/7/7	-
87	SPD	L5	5285	-	-	4/7/7/7	-
86	SPM	L5	5259	-	-	2/11/11/11	-
86	SPM	L5	5263	-	-	2/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPD	L5	5288	-	-	3/7/7/7	-
87	SPD	LN	301	-	-	1/7/7/7	-
87	SPD	L5	5283	-	-	1/7/7/7	-
87	SPD	L5	5291	-	-	4/7/7/7	-
86	SPM	L5	5267	-	-	4/11/11/11	-
87	SPD	L5	5284	-	-	1/7/7/7	-
87	SPD	L5	5287	-	-	3/7/7/7	-
87	SPD	L5	5290	-	-	2/7/7/7	-
86	SPM	L5	5264	-	-	4/11/11/11	-
86	SPM	L5	5292	-	-	4/11/11/11	-
86	SPM	L5	5289	-	-	5/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (46) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
87	L5	5287	SPD	N6-C7-C8-C9
87	L5	5284	SPD	C3-C4-C5-N6
86	L5	5264	SPM	C12-C11-N10-C9
86	L5	5267	SPM	N10-C11-C12-C13
86	L5	5289	SPM	N1-C2-C3-C4
86	L5	5293	SPM	C11-C12-C13-N14
86	L5	5293	SPM	N10-C11-C12-C13
86	L5	5267	SPM	C6-C7-C8-C9
86	L5	5293	SPM	C7-C6-N5-C4
86	L5	5289	SPM	N10-C11-C12-C13
86	L5	5263	SPM	C11-C12-C13-N14
87	L5	5288	SPD	C7-C8-C9-N10
87	L5	5291	SPD	C8-C7-N6-C5
87	L5	5291	SPD	N6-C7-C8-C9
87	L5	5285	SPD	C4-C5-N6-C7
87	LN	301	SPD	C4-C5-N6-C7
86	L5	5292	SPM	C7-C6-N5-C4
86	L5	5292	SPM	C8-C9-N10-C11
86	L5	5264	SPM	C8-C9-N10-C11
87	L5	5288	SPD	C8-C7-N6-C5
86	L5	5289	SPM	C7-C8-C9-N10
87	L5	5291	SPD	C3-C4-C5-N6
87	L5	5261	SPD	C7-C8-C9-N10
87	L5	5283	SPD	C7-C8-C9-N10
87	L5	5290	SPD	N6-C7-C8-C9

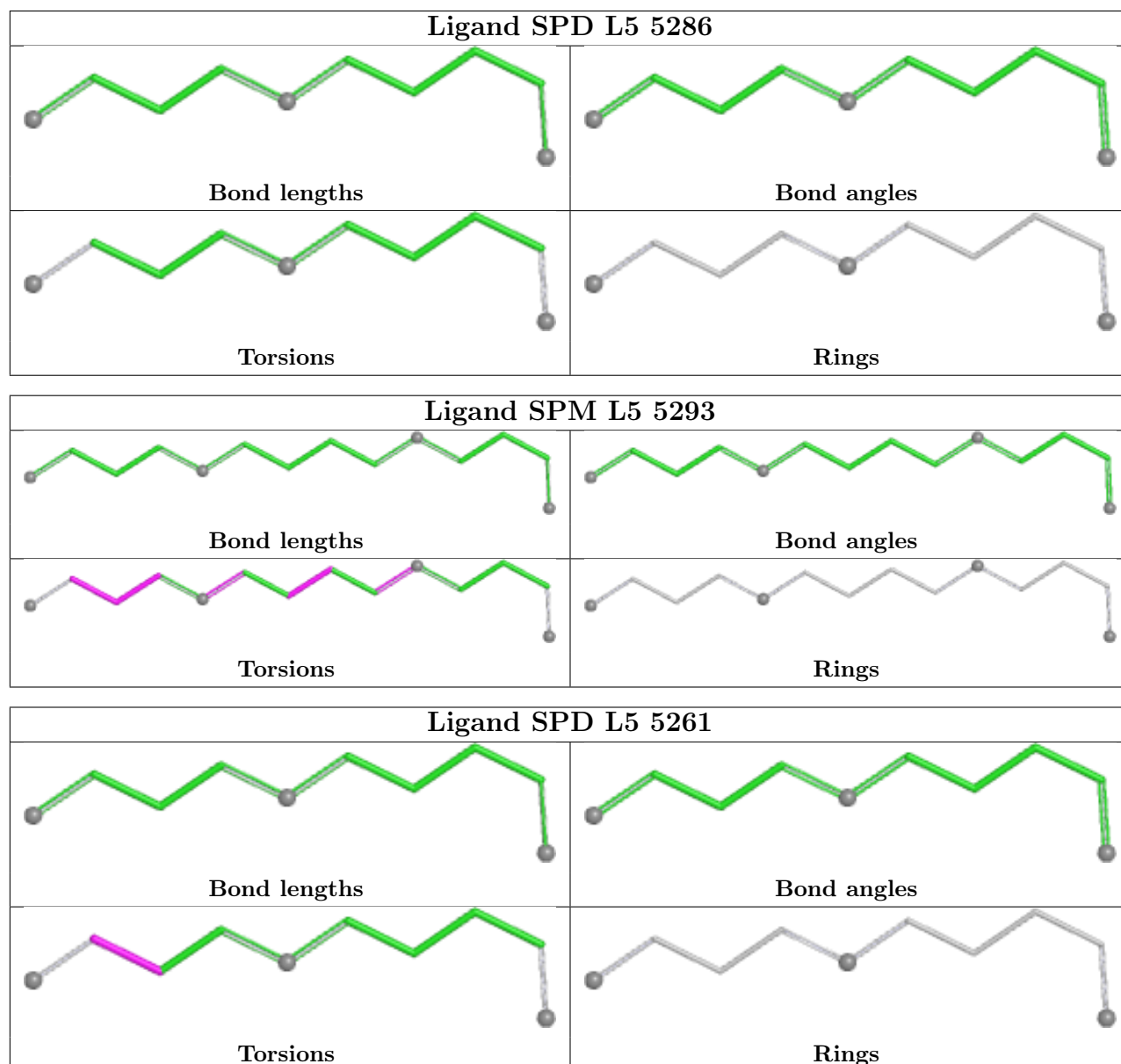
There are no ring outliers.

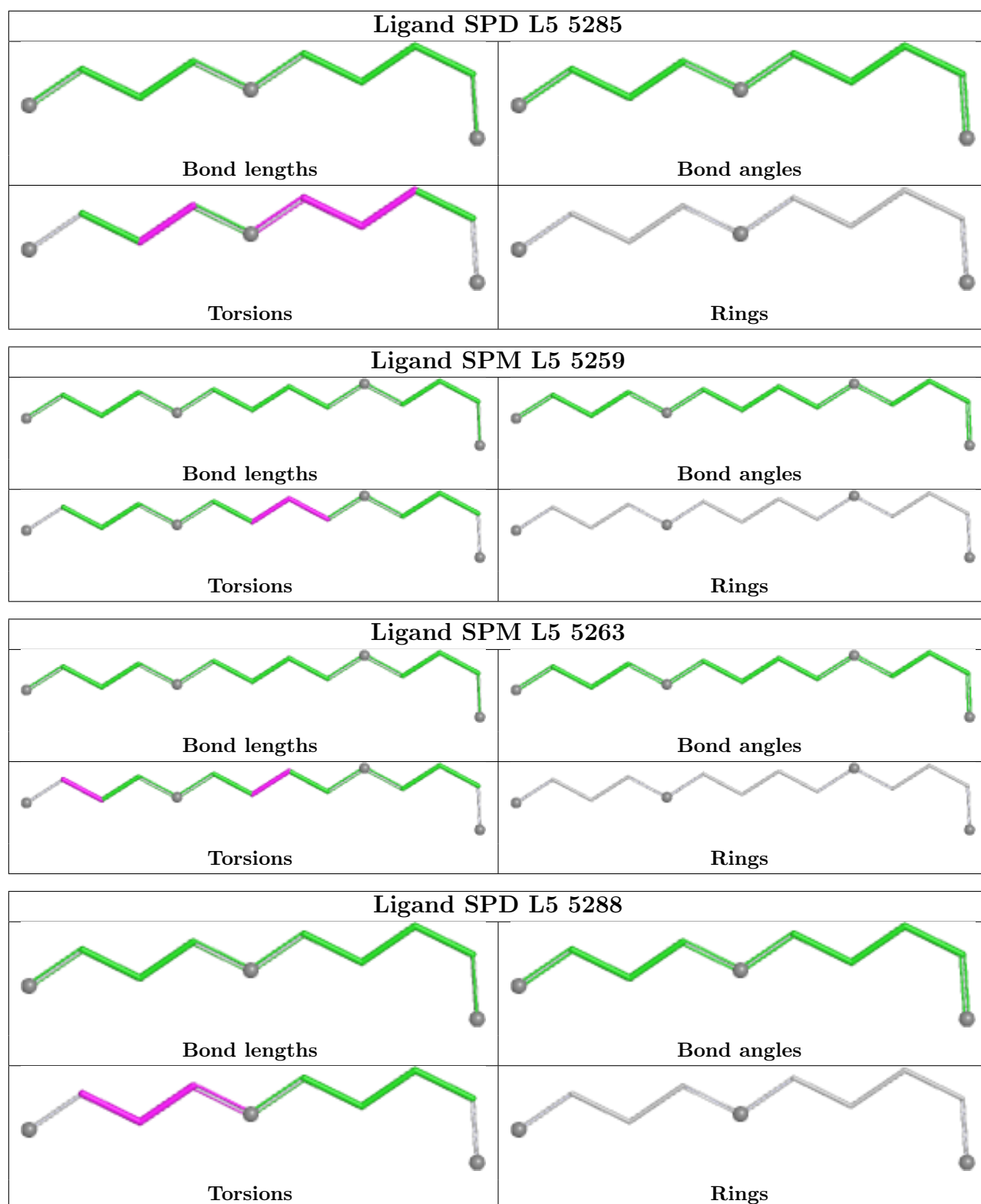
8 monomers are involved in 12 short contacts:

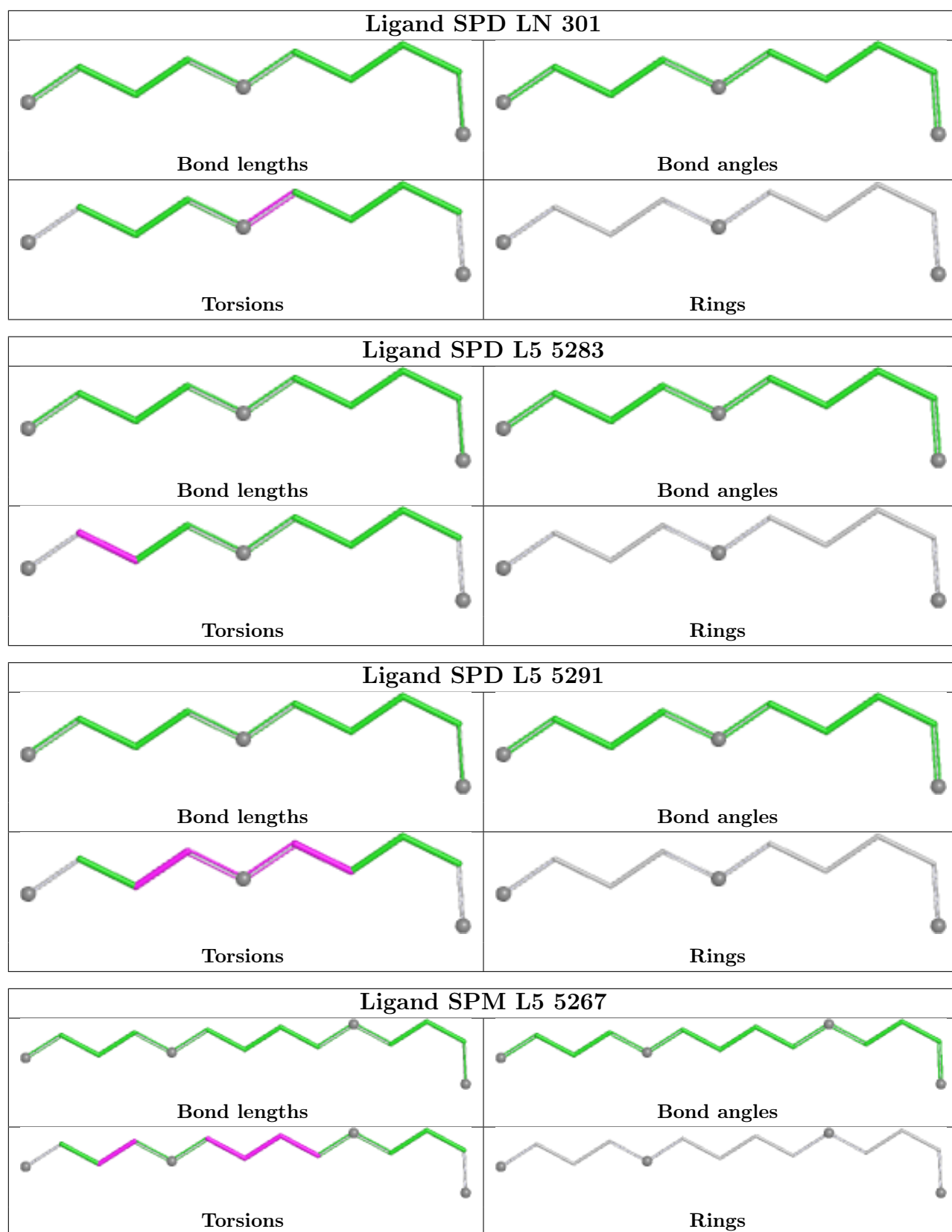
Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	L5	5293	SPM	2	0
87	L5	5261	SPD	2	0
86	L5	5259	SPM	1	0
86	L5	5263	SPM	1	0
87	L5	5284	SPD	2	0
87	L5	5290	SPD	1	0
86	L5	5264	SPM	2	0
86	L5	5292	SPM	1	0

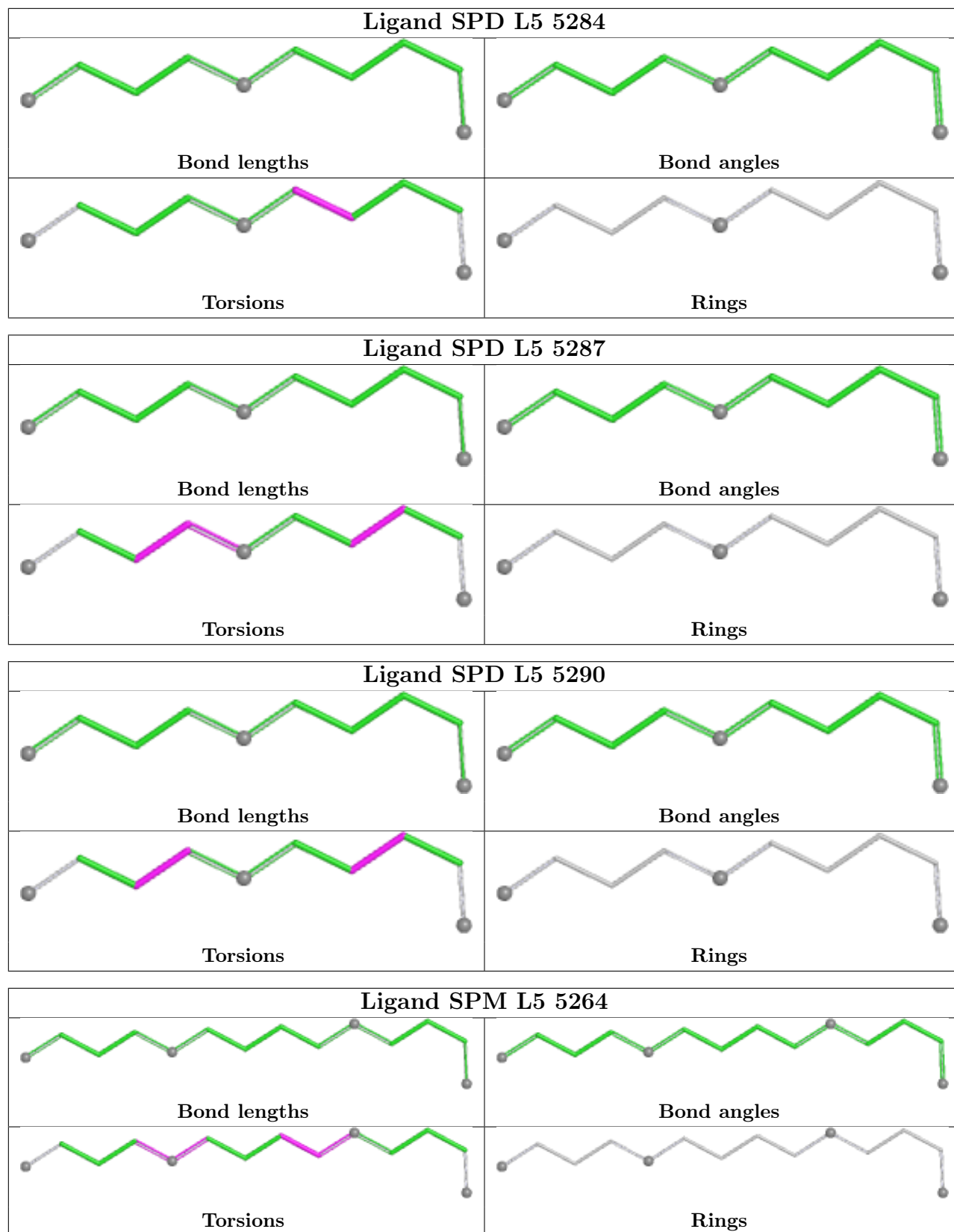
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

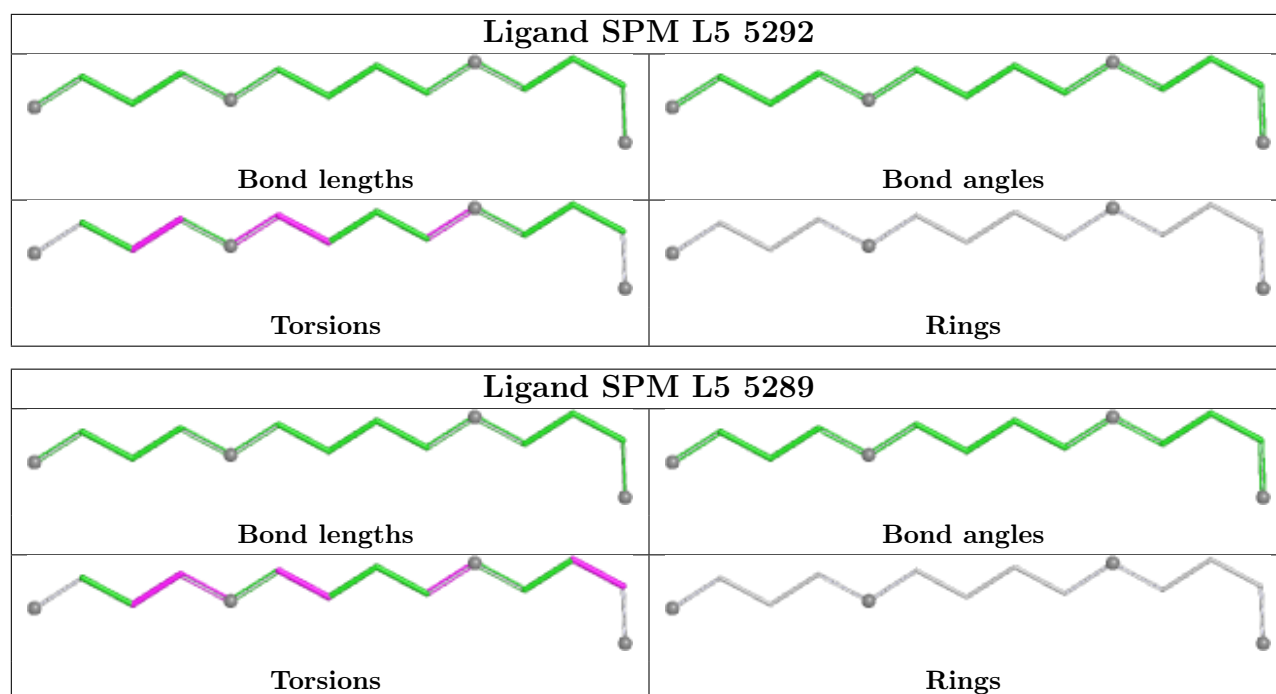
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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
3	L5	10
83	S2	5
32	Lb	1
10	LE	1
49	Lt	1
70	SH	1
1	Pt	1
2	Et	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lb	76:VAL	C	89:VAL	N	35.06
1	S2	753:C	O3'	785:C	P	29.06
1	LE	76:ALA	C	87:LYS	N	21.90
1	L5	2910:G	O3'	3584:C	P	21.12

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L5	1706:A	O3'	1716:G	P	20.98
1	L5	760:G	O3'	903:C	P	16.74
1	L5	519:C	O3'	642:G	P	15.41
1	S2	698:G	O3'	730:C	P	15.10
1	L5	2112:G	O3'	2249:C	P	15.05
1	L5	4776:G	O3'	4858:C	P	15.05
1	Lt	87:GLU	C	104:ILE	N	13.36
1	L5	3954:A	O3'	4056:A	P	13.15
1	S2	739:C	O3'	746:C	P	12.53
1	L5	990:C	O3'	1064:G	P	12.05
1	L5	1222:A	O3'	1234:G	P	10.97
1	SH	107:LYS	C	111:LYS	N	10.88
1	Pt	15:G	O3'	18:G	P	10.02
1	S2	225:G	O3'	287:U	P	7.34
1	L5	1100:U	O3'	1167:C	P	7.25
1	Et	16:C	O3'	18:U	P	6.28
1	S2	1831:A	O3'	1832:6MZ	P	4.47

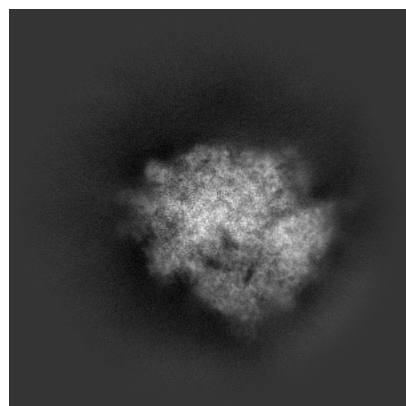
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71331. These allow visual inspection of the internal detail of the map and identification of artifacts.

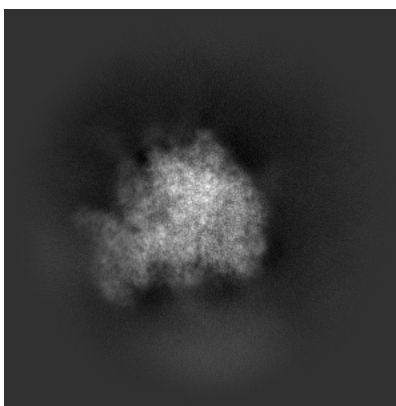
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

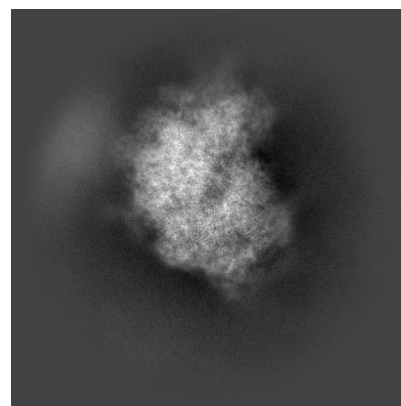
6.1.1 Primary map



X

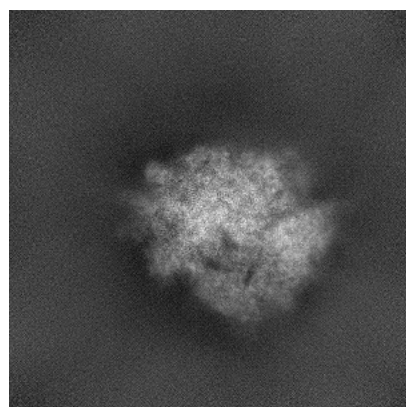


Y

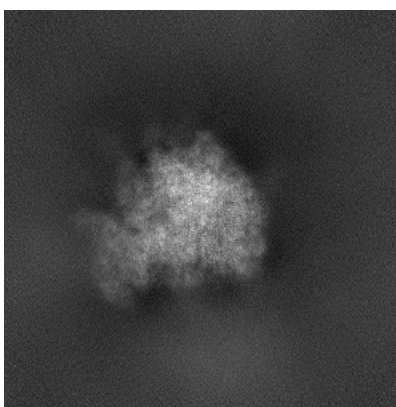


Z

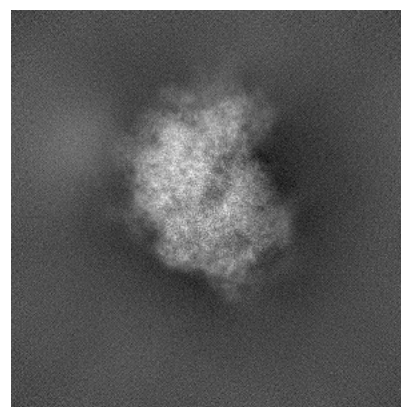
6.1.2 Raw map



X



Y

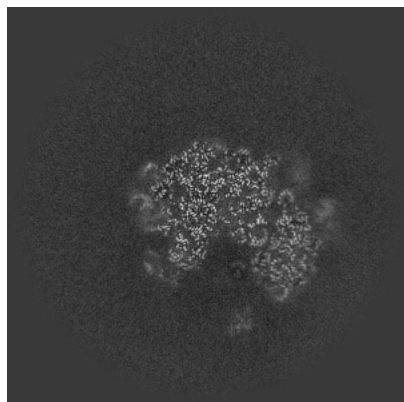


Z

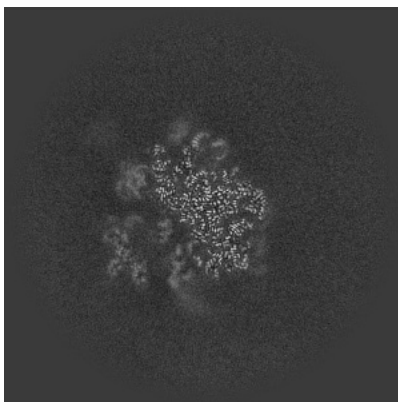
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

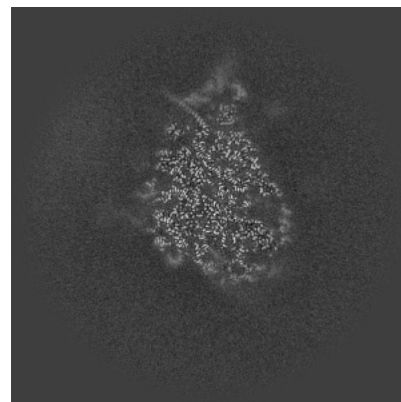
6.2.1 Primary map



X Index: 256

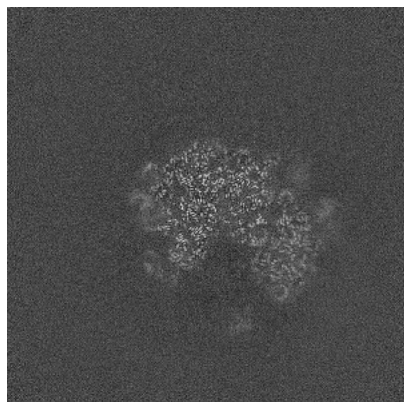


Y Index: 256

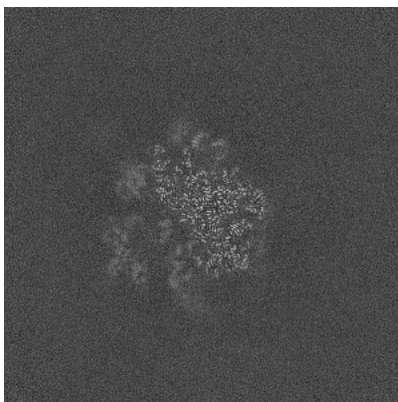


Z Index: 256

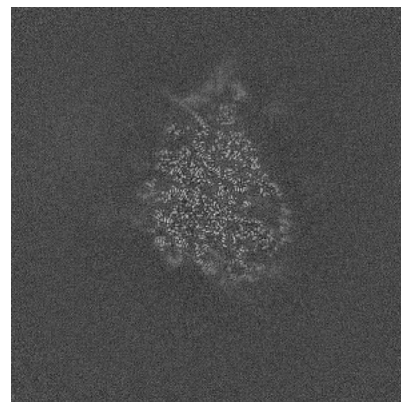
6.2.2 Raw map



X Index: 256



Y Index: 256

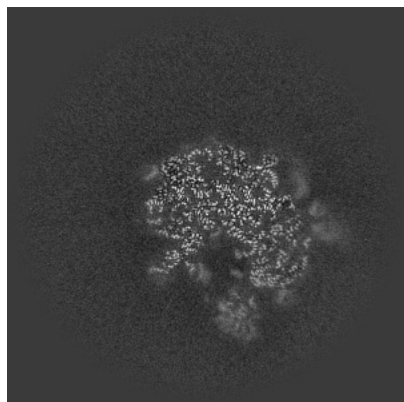


Z Index: 256

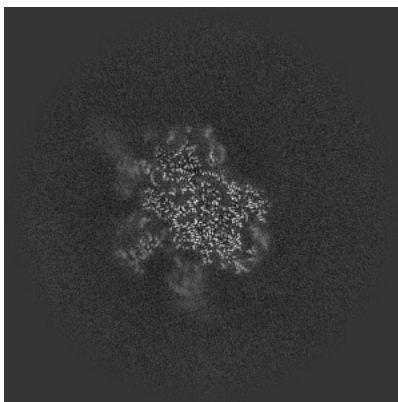
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

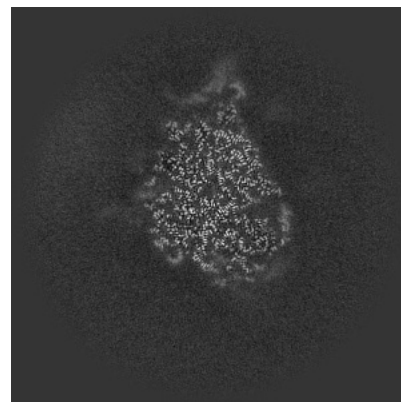
6.3.1 Primary map



X Index: 243

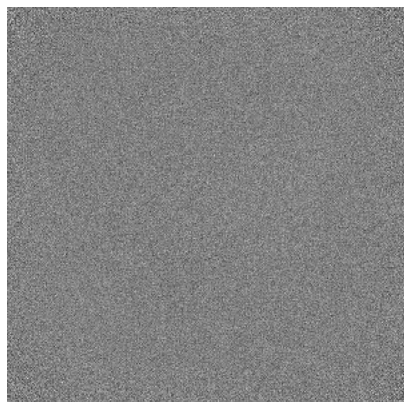


Y Index: 243

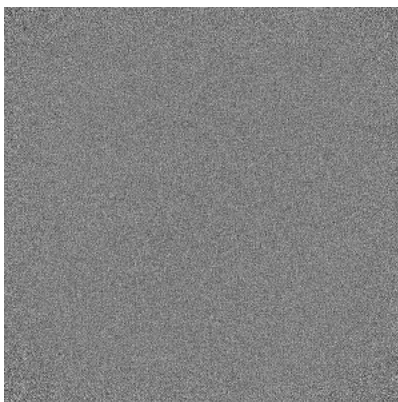


Z Index: 258

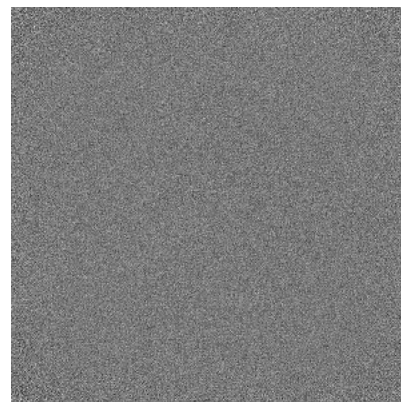
6.3.2 Raw map



X Index: 0



Y Index: 0

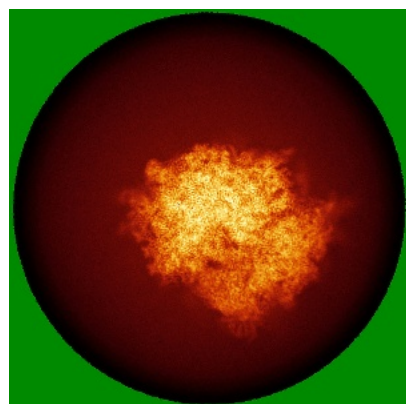


Z Index: 0

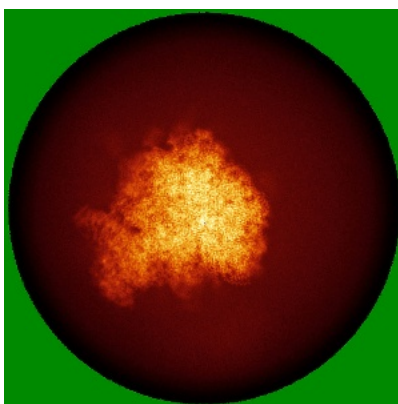
The images above show the largest variance slices of the map in three orthogonal directions.

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

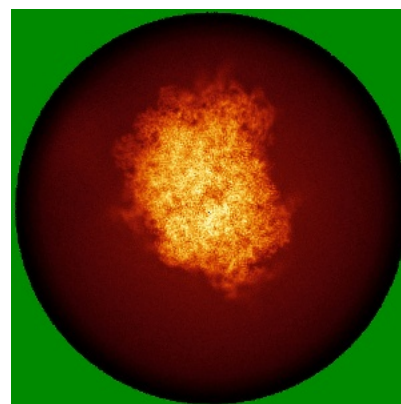
6.4.1 Primary map



X

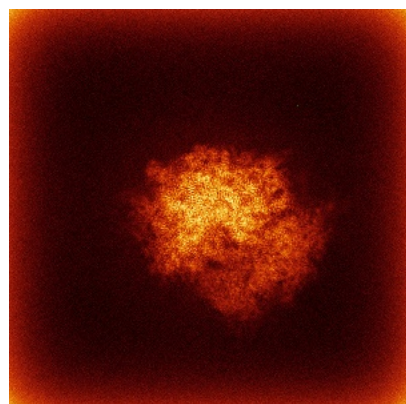


Y

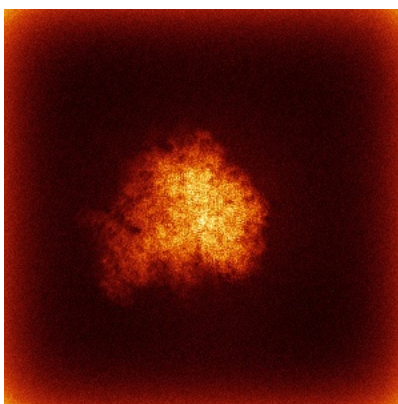


Z

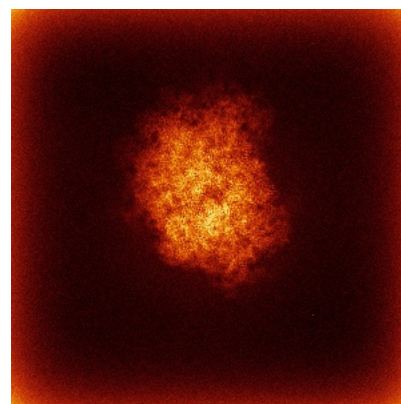
6.4.2 Raw map



X



Y

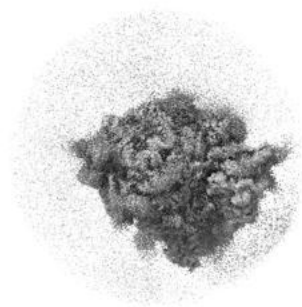


Z

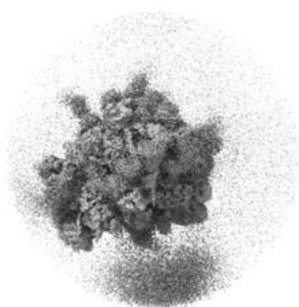
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

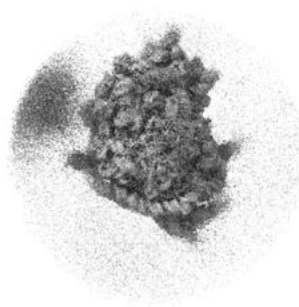
6.5.1 Primary map



X



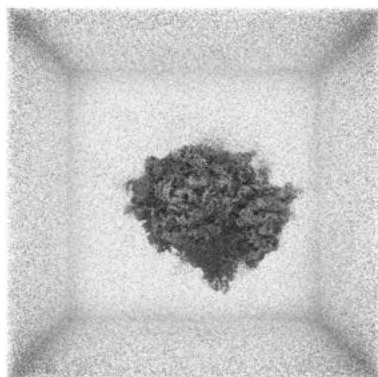
Y



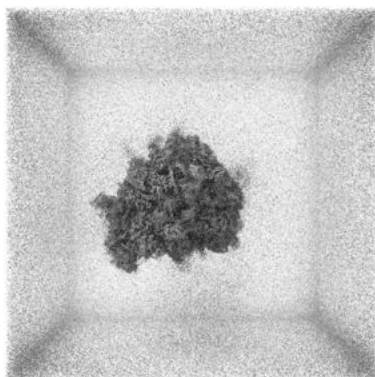
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0128. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

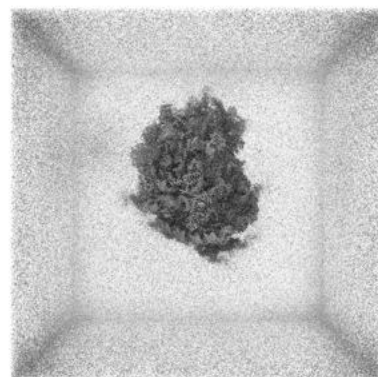
6.5.2 Raw map



X



Y



Z

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.

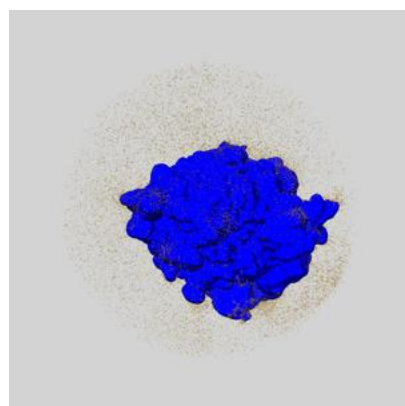
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

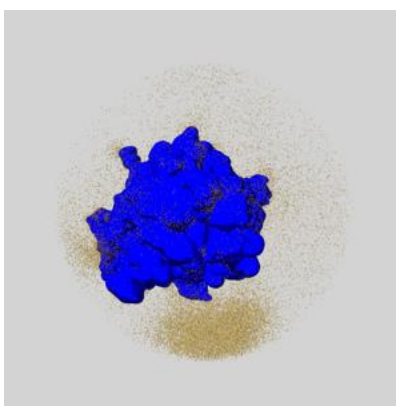
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

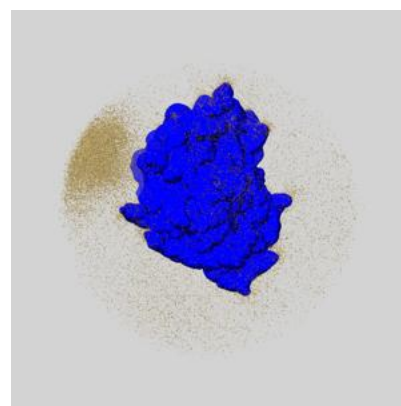
6.6.1 emd_71331_msk_1.map [i](#)



X



Y

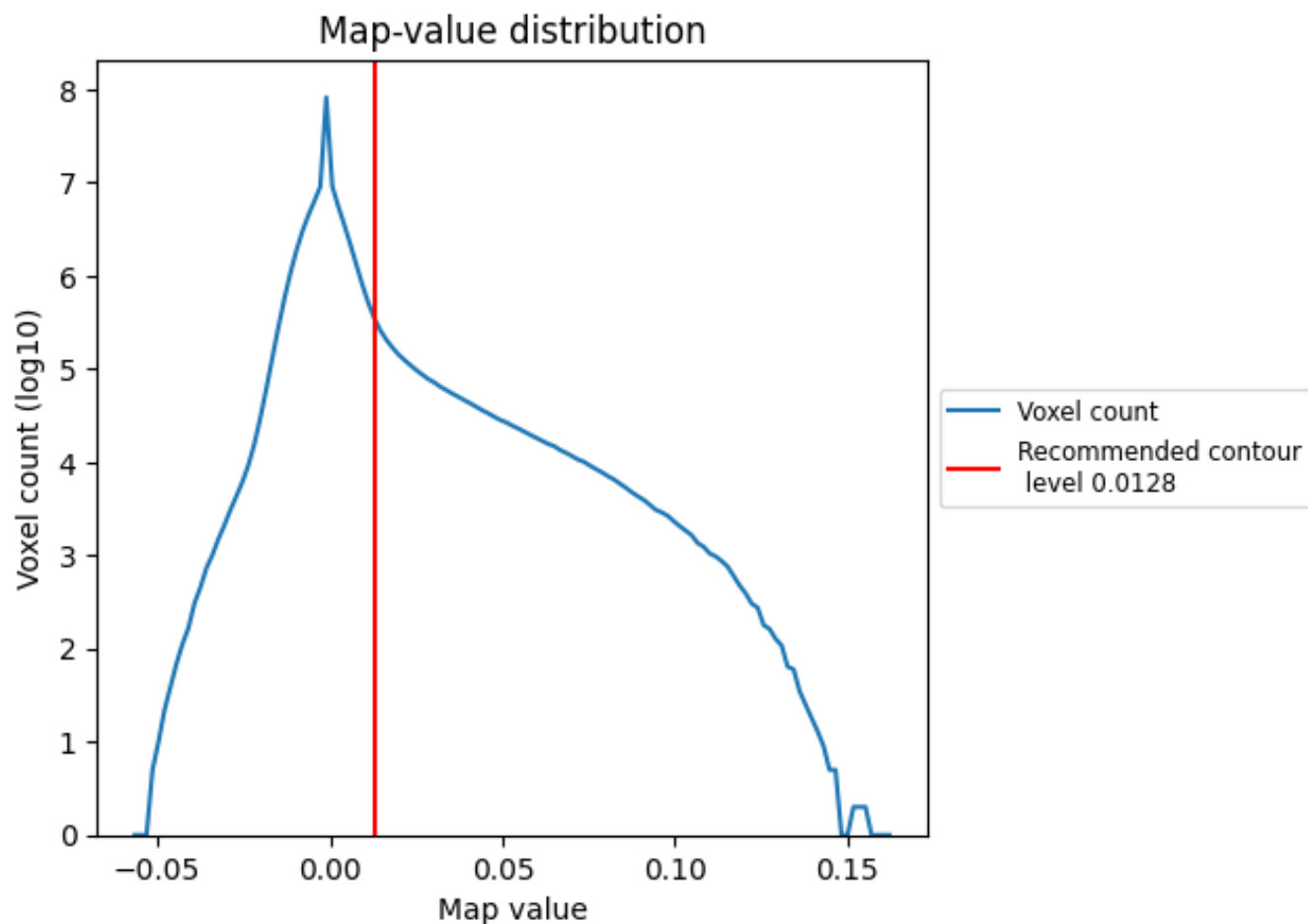


Z

7 Map analysis [i](#)

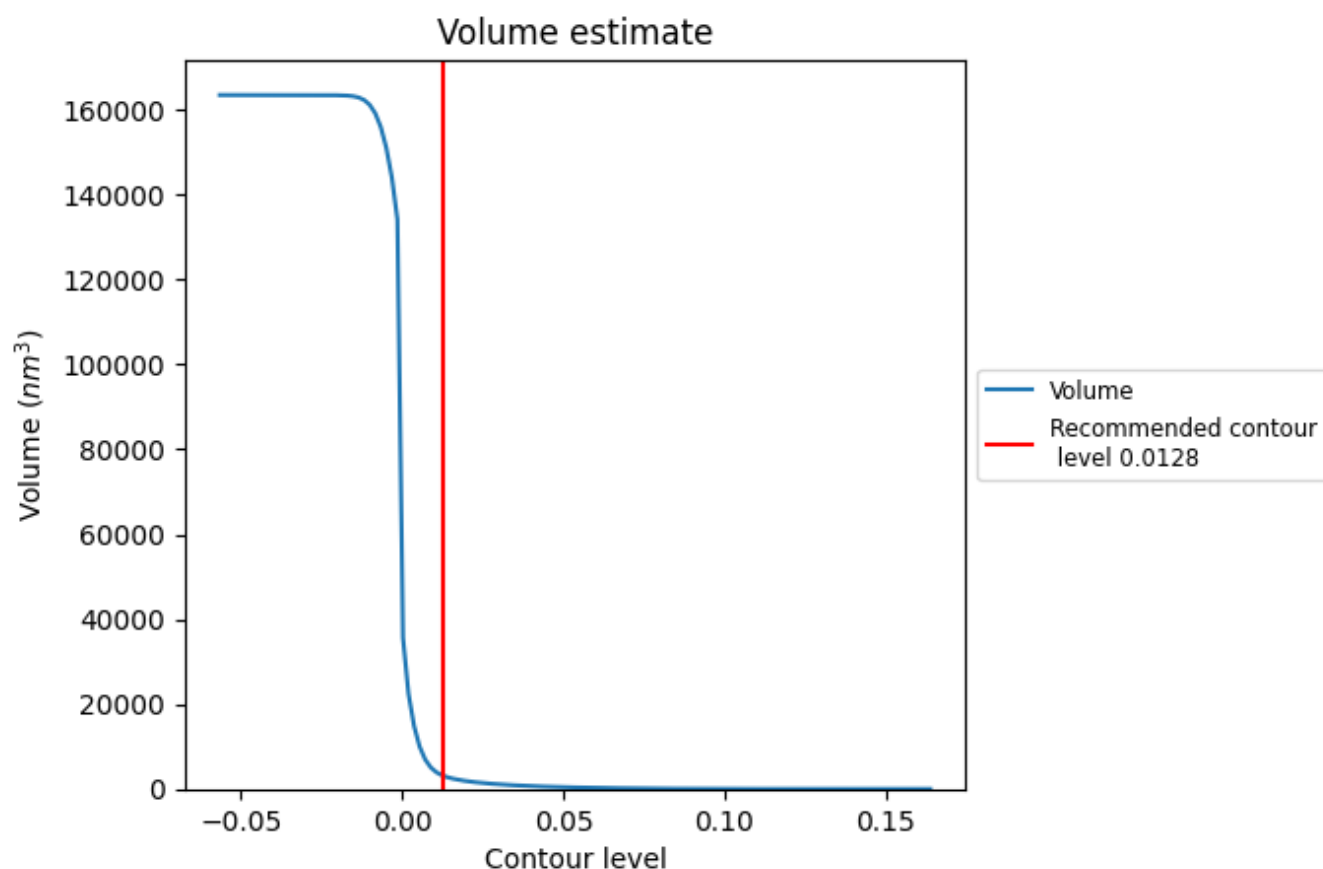
This section contains the results of statistical analysis of the map.

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.

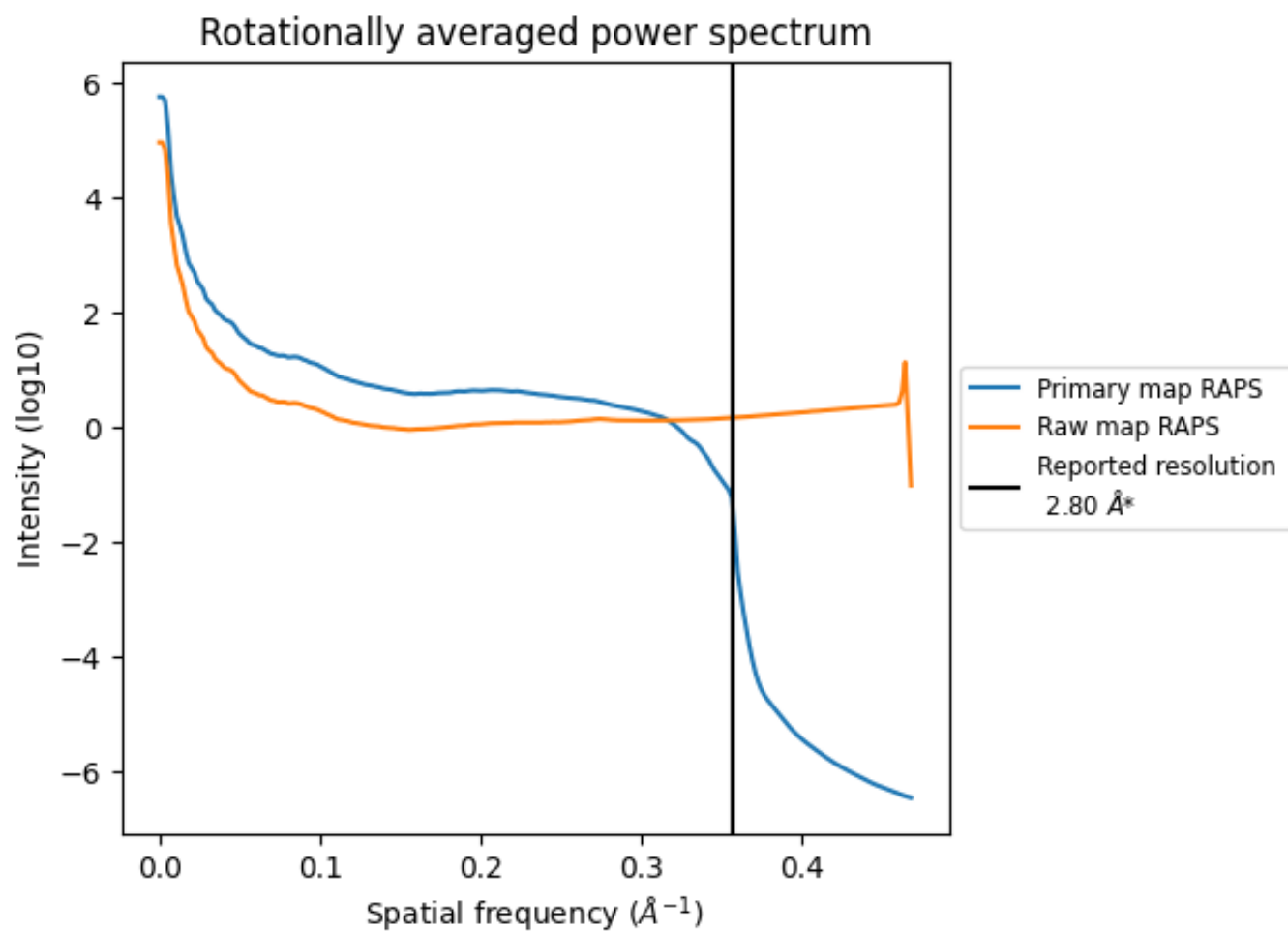
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3105 nm^3 ; this corresponds to an approximate mass of 2804 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 ⓘ

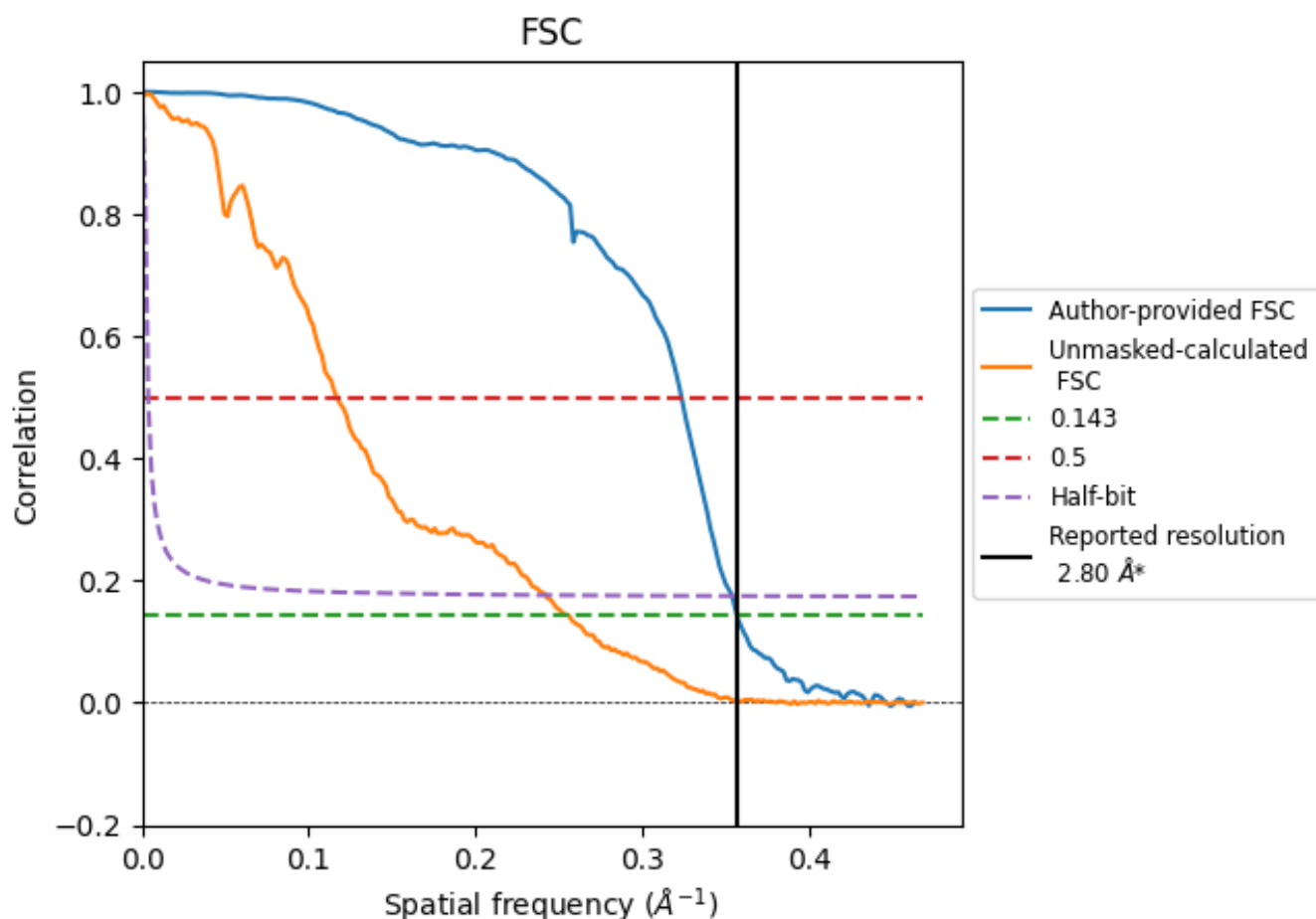


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

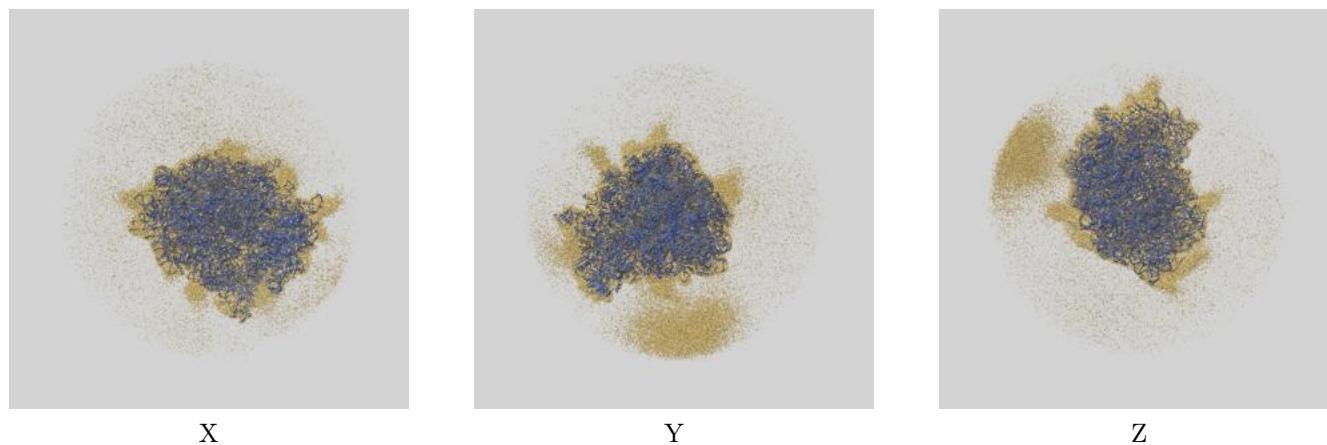
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.09	2.82
Unmasked-calculated*	3.91	8.56	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

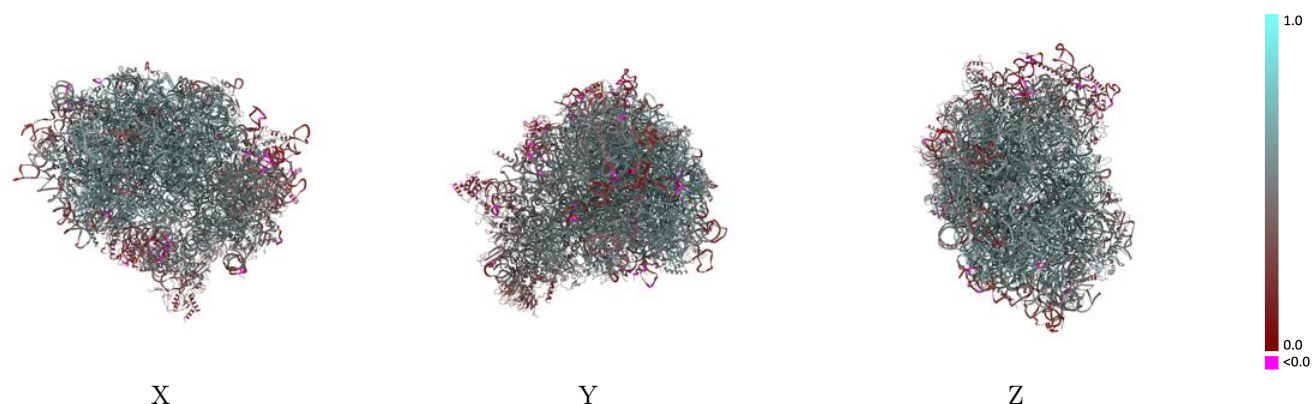
This section contains information regarding the fit between EMDB map EMD-71331 and PDB model 9P72. Per-residue inclusion information can be found in section 3 on page 24.

9.1 Map-model overlay [i](#)



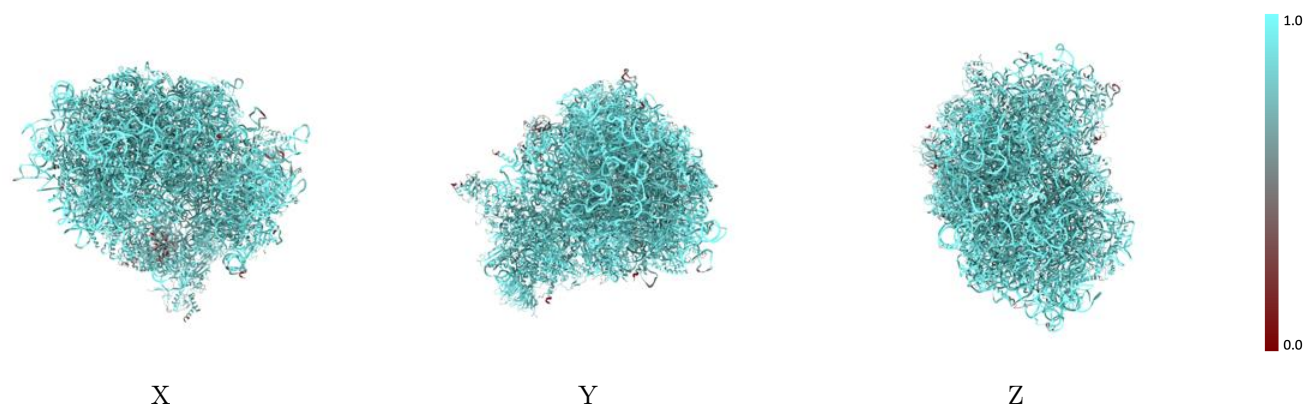
The images above show the 3D surface view of the map at the recommended contour level 0.0128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



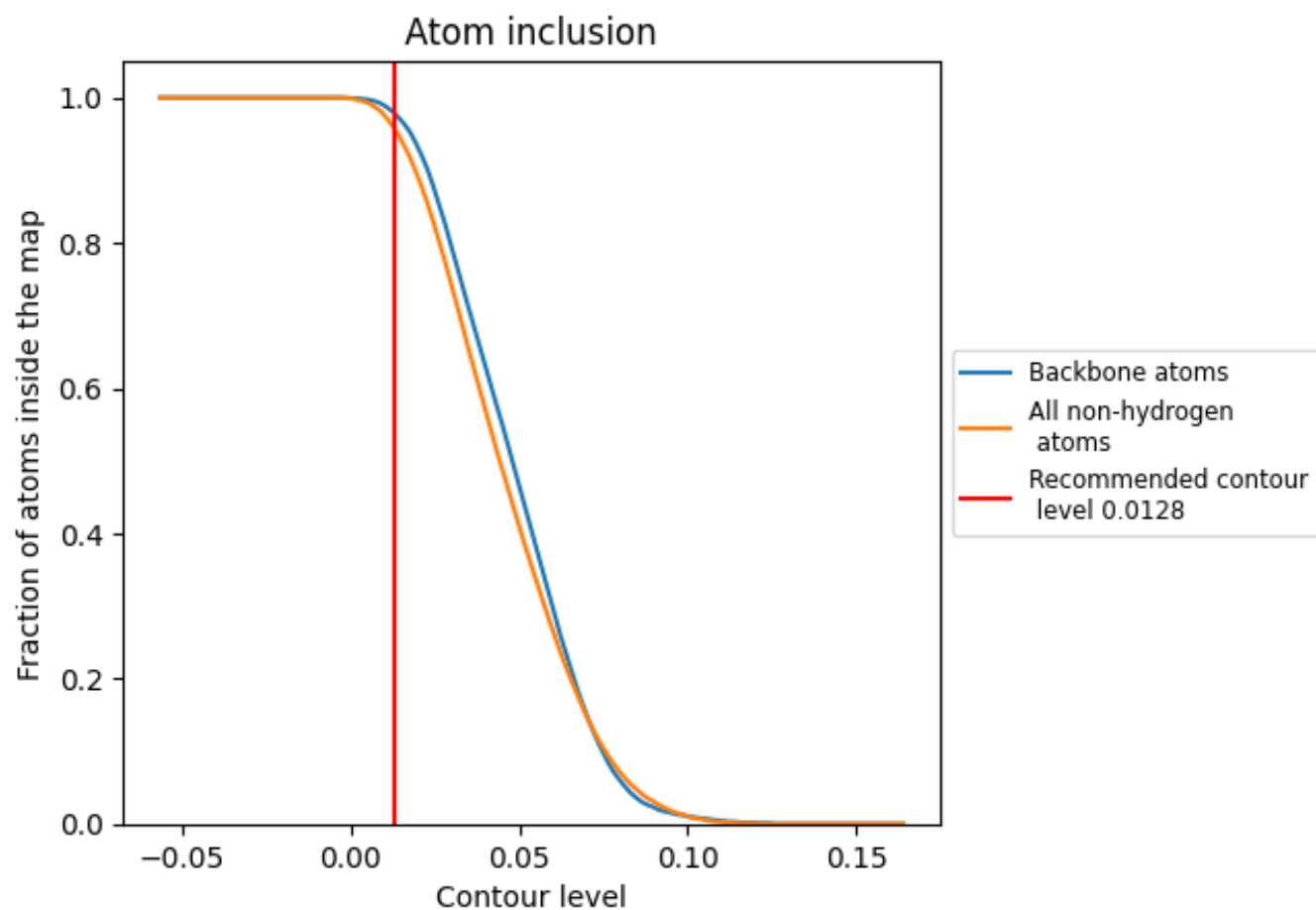
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0128).

9.4 Atom inclusion ⓘ



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9580	 0.5080
CI	 0.8160	 0.4450
Et	 0.9350	 0.2290
L5	 0.9820	 0.5310
L7	 0.9980	 0.5770
L8	 0.9880	 0.5580
LA	 0.9790	 0.5940
LB	 0.9580	 0.5730
LC	 0.9580	 0.5710
LD	 0.9480	 0.5330
LE	 0.9200	 0.5110
LF	 0.9770	 0.5740
LG	 0.9110	 0.5130
LH	 0.9570	 0.5630
LI	 0.9550	 0.5640
LJ	 0.9390	 0.5100
LL	 0.9360	 0.5470
LM	 0.9670	 0.5530
LN	 0.9910	 0.6080
LO	 0.9700	 0.5700
LP	 0.9710	 0.5830
LQ	 0.9790	 0.5950
LR	 0.9130	 0.5200
LS	 0.9840	 0.5940
LT	 0.9530	 0.5570
LU	 0.9460	 0.4940
LV	 0.9650	 0.5810
LW	 0.8710	 0.4130
LX	 0.9500	 0.5530
LY	 0.9530	 0.5540
LZ	 0.9640	 0.5460
La	 0.9760	 0.6000
Lb	 0.9130	 0.4960
Lc	 0.9650	 0.5450
Ld	 0.9480	 0.5610



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Chain	Atom inclusion	Q-score
Le	 0.9780	 0.5940
Lf	 0.9850	 0.5990
Lg	 0.9630	 0.5700
Lh	 0.9450	 0.5470
Li	 0.9590	 0.5480
Lj	 0.9900	 0.5940
Lk	 0.9080	 0.5030
Ll	 0.9810	 0.5800
Lm	 0.9590	 0.5700
Ln	 0.9860	 0.5700
Lo	 0.9570	 0.5690
Lp	 0.9670	 0.5720
Lr	 0.9710	 0.5780
Ls	 0.6350	 0.2060
Lt	 0.5870	 0.1380
Pt	 0.9680	 0.4760
S2	 0.9840	 0.4850
SA	 0.9120	 0.4780
SB	 0.9200	 0.5060
SC	 0.9530	 0.5110
SD	 0.8970	 0.4140
SE	 0.9520	 0.4840
SF	 0.9110	 0.4370
SG	 0.8790	 0.3930
SH	 0.8590	 0.4030
SI	 0.9170	 0.4900
SJ	 0.9230	 0.4660
SK	 0.8920	 0.3600
SL	 0.9070	 0.5120
SM	 0.7000	 0.1900
SN	 0.9520	 0.5360
SO	 0.9370	 0.5230
SP	 0.8710	 0.3920
SQ	 0.9070	 0.4350
SR	 0.8660	 0.4110
SS	 0.9050	 0.4280
ST	 0.9310	 0.4340
SU	 0.8950	 0.3700
SV	 0.9490	 0.4870
SW	 0.9720	 0.5350
SX	 0.9470	 0.5250
SY	 0.8710	 0.3920

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Chain	Atom inclusion	Q-score
SZ	 0.8490	 0.4040
Sa	 0.9400	 0.5230
Sb	 0.9190	 0.4810
Sc	 0.8870	 0.4320
Sd	 0.9500	 0.4760
Se	 0.8110	 0.4000
Sf	 0.7790	 0.2470
Sg	 0.8920	 0.3480