



Full wwPDB EM Validation Report ⓘ

Jun 27, 2026 – 12:56 PM EDT

PDB ID : 9PA7 / pdb_00009pa7
EMDB ID : EMD-71435
Title : In situ human 80S consensus ribosome with EBP1
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-25
Resolution : 2.67 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

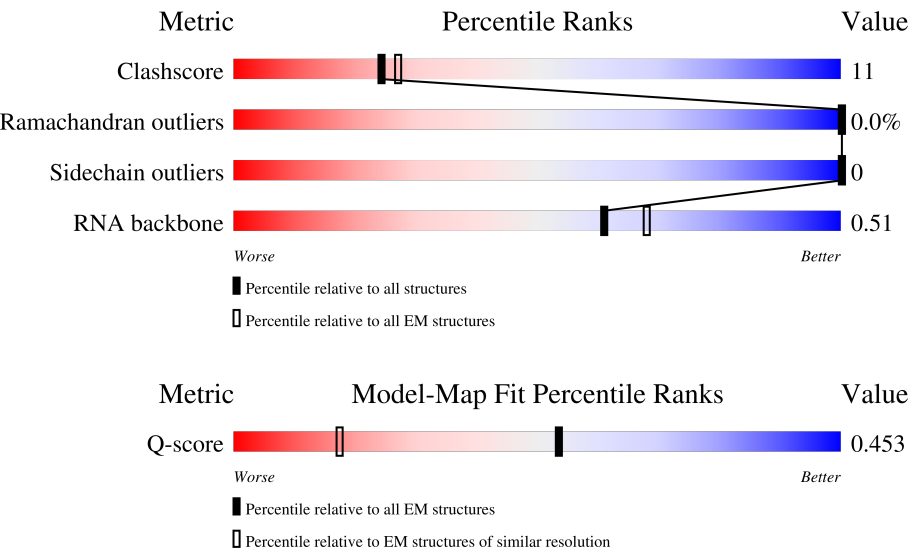
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.67 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.



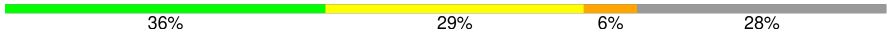
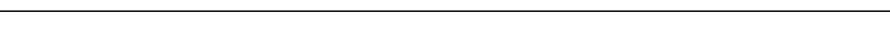
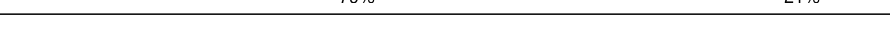
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9182 (2.17 - 3.17)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	CD	36	8% 69% 31%
2	CI	31	65% 35%
3	CF	441	13% 64% 36%

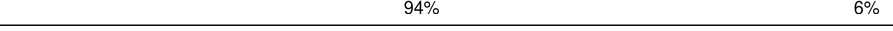
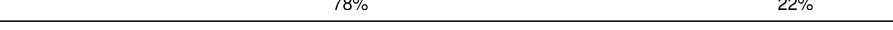
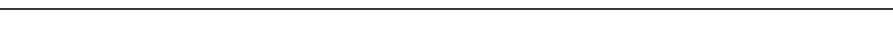
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Mol	Chain	Length	Quality of chain
4	L5	5070	
5	L7	120	
6	L8	156	
7	LA	248	
8	LB	402	
9	LC	368	
10	LD	293	
11	LE	250	
12	LF	225	
13	LG	241	
14	LH	190	
15	LI	213	
16	LJ	176	
17	LL	210	
18	LM	139	
19	LN	203	
20	LO	201	
21	LP	153	
22	LQ	187	
23	LR	187	
24	LS	175	
25	LT	159	
26	LU	101	
27	LV	131	
28	LW	118	

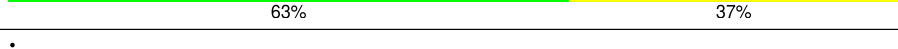
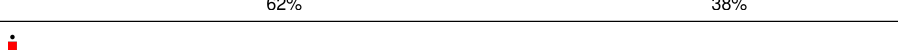
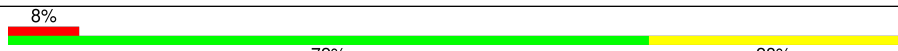
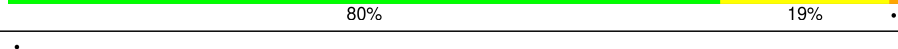
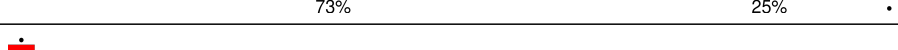
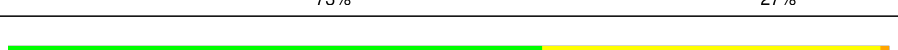
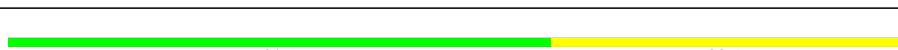
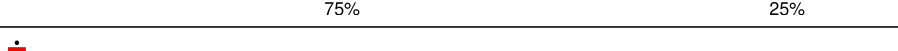
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Mol	Chain	Length	Quality of chain
29	LX	120	
30	LY	134	
31	LZ	135	
32	La	147	
33	Lb	109	
34	Lc	98	
35	Ld	107	
36	Le	128	
37	Lf	109	
38	Lg	114	
39	Lh	122	
40	Li	102	
41	Lj	86	
42	Lk	69	
43	Ll	50	
44	Lm	52	
45	Ln	24	
46	Lo	105	
47	Lp	91	
48	Lr	125	
49	Ls	196	
50	Lt	141	
51	Pt	74	
52	S2	1740	
53	SA	221	

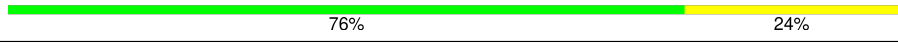
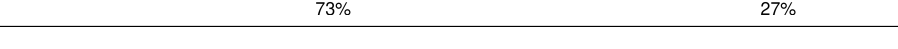
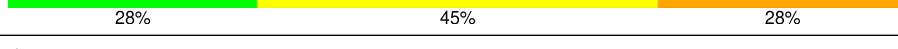
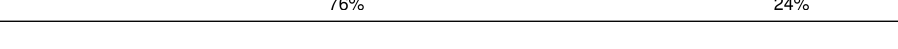
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Mol	Chain	Length	Quality of chain
54	SB	214	
55	SC	222	
56	SD	227	
57	SE	262	
58	SF	189	
59	SG	237	
60	SH	186	
61	SI	206	
62	SJ	185	
63	SK	98	
64	SL	153	
65	SM	122	
66	SN	150	
67	SO	140	
68	SP	121	
69	SQ	144	
70	SR	135	
71	SS	145	
72	ST	143	
73	SU	104	
74	SV	83	
75	SW	129	
76	SX	141	
77	SY	131	
78	SZ	75	

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Mol	Chain	Length	Quality of chain
79	Sa	102	
80	Sb	83	
81	Sc	64	
82	Sd	55	
83	Se	58	
84	Sf	67	
85	Sg	313	
86	AT	76	
87	CA	354	

2 Entry composition [i](#)

There are 94 unique types of molecules in this entry. The entry contains 231160 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SERPINE1 mRNA-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CD	36	Total	C	N	O	S	0	0
			285	179	47	58	1		

- Molecule 2 is a protein called Transcription factor BTF3.

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

- Molecule 3 is a protein called Elongation factor 1-alpha 1.

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

- Molecule 4 is a RNA chain called 28S rRNA.

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

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

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

- Molecule 6 is a RNA chain called 5.8S rRNA.

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

- Molecule 7 is a protein called 60S ribosomal protein L8.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 9 is a protein called 60S ribosomal protein L4.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 11 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 12 is a protein called 60S ribosomal protein L7.

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

- Molecule 13 is a protein called 60S ribosomal protein L7a.

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

- Molecule 14 is a protein called 60S ribosomal protein L9.

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

- Molecule 15 is a protein called Ribosomal protein uL16-like.

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

- Molecule 16 is a protein called 60S ribosomal protein L11.

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

- Molecule 17 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 18 is a protein called 60S ribosomal protein L14.

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

- Molecule 19 is a protein called 60S ribosomal protein L15.

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

- Molecule 20 is a protein called 60S ribosomal protein L13a.

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

- Molecule 21 is a protein called 60S ribosomal protein L17.

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

- Molecule 22 is a protein called 60S ribosomal protein L18.

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

- Molecule 23 is a protein called 60S ribosomal protein L19.

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

- Molecule 24 is a protein called 60S ribosomal protein L18a.

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

- Molecule 25 is a protein called 60S ribosomal protein L21.

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

- Molecule 26 is a protein called Heparin-binding protein HBp15.

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

- Molecule 27 is a protein called 60S ribosomal protein L23.

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

- Molecule 28 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	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 29 is a protein called 60S ribosomal protein L23a.

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

- Molecule 30 is a protein called 60S ribosomal protein L26.

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

- Molecule 31 is a protein called 60S ribosomal protein L27.

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

- Molecule 32 is a protein called 60S ribosomal protein L27a.

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

- Molecule 33 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	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 34 is a protein called 60S ribosomal protein L30.

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

- Molecule 35 is a protein called 60S ribosomal protein L31.

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

- Molecule 36 is a protein called 60S ribosomal protein L32.

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

- Molecule 37 is a protein called 60S ribosomal protein L35a.

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

- Molecule 38 is a protein called 60S ribosomal protein L34.

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

- Molecule 39 is a protein called 60S ribosomal protein L35.

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

- Molecule 40 is a protein called 60S ribosomal protein L36.

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

- Molecule 41 is a protein called 60S ribosomal protein L37.

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

- Molecule 42 is a protein called 60S ribosomal protein L38.

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

- Molecule 43 is a protein called 60S ribosomal protein L39.

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

- Molecule 44 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 45 is a protein called 60S ribosomal protein L41.

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

- Molecule 46 is a protein called 60S ribosomal protein L36a.

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

- Molecule 47 is a protein called 60S ribosomal protein L37a.

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

- Molecule 48 is a protein called 60S ribosomal protein L28.

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

- Molecule 49 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 50 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 51 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Pt	74	Total	C	N	O	P	0	0
			1576	705	285	513	73		

- Molecule 52 is a RNA chain called 18S rRNA.

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

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

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

- Molecule 54 is a protein called 40S ribosomal protein S3a.

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

- Molecule 55 is a protein called 40S ribosomal protein S2.

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

- Molecule 56 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 57 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 58 is a protein called 40S ribosomal protein S5.

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

- Molecule 59 is a protein called 40S ribosomal protein S6.

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

- Molecule 60 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	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 61 is a protein called 40S ribosomal protein S8.

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

- Molecule 62 is a protein called 40S ribosomal protein S9.

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

- Molecule 63 is a protein called 40S ribosomal protein S10.

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

- Molecule 64 is a protein called 40S ribosomal protein S11.

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

- Molecule 65 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 66 is a protein called 40S ribosomal protein S13.

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

- Molecule 67 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 68 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 69 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 70 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 71 is a protein called 40S ribosomal protein S18.

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

- Molecule 72 is a protein called 40S ribosomal protein S19.

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

- Molecule 73 is a protein called 40S ribosomal protein S20.

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

- Molecule 74 is a protein called Small ribosomal subunit protein eS21.

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

- Molecule 75 is a protein called 40S ribosomal protein S15a.

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

- Molecule 76 is a protein called 40S ribosomal protein S23.

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

- Molecule 77 is a protein called 40S ribosomal protein S24.

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

- Molecule 78 is a protein called Small ribosomal subunit protein eS25.

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

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

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

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

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

- Molecule 81 is a protein called 40S ribosomal protein S28.

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

- Molecule 82 is a protein called 40S ribosomal protein S29.

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

- Molecule 83 is a protein called Small ribosomal subunit protein eS30.

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

- Molecule 84 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 85 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 86 is a RNA chain called A/T site tRNA.

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

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AT	3	C	U	conflict	GB 28626602
AT	16	C	U	conflict	GB 28626602
AT	51	U	C	conflict	GB 28626602
AT	76	C	A	conflict	GB 28626602
AT	77	A	C	conflict	GB 28626602

- Molecule 87 is a protein called Proliferation-associated protein 2G4.

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

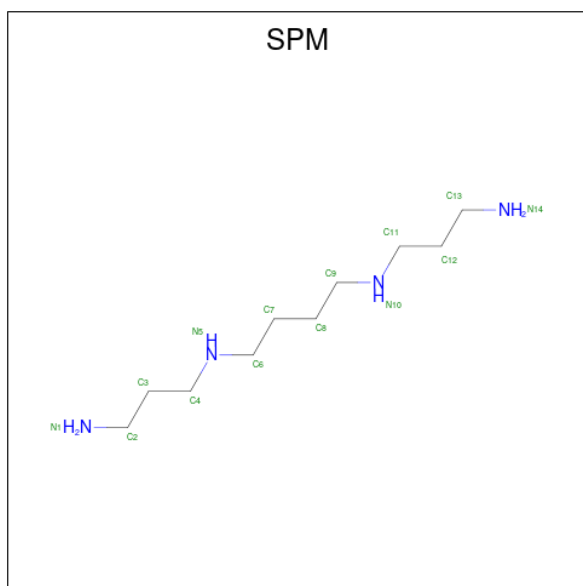
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	?	-	GLU	deletion	UNP Q9UQ80
CA	?	-	ASP	deletion	UNP Q9UQ80

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
88	L5	185	Total	Mg	0
			185	185	
88	L7	3	Total	Mg	0
			3	3	
88	L8	5	Total	Mg	0
			5	5	
88	LA	1	Total	Mg	0
			1	1	
88	LP	1	Total	Mg	0
			1	1	
88	LV	1	Total	Mg	0
			1	1	
88	Le	1	Total	Mg	0
			1	1	
88	S2	28	Total	Mg	0
			28	28	

- Molecule 89 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of Interest" by depositor).



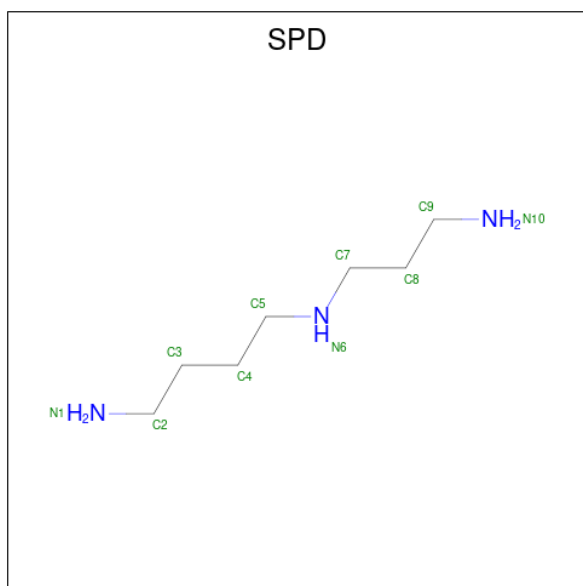
Mol	Chain	Residues	Atoms			AltConf
89	L5	1	Total	C	N	0
			14	10	4	
89	L5	1	Total	C	N	0
			14	10	4	

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Mol	Chain	Residues	Atoms			AltConf
89	L5	1	Total	C	N	0
			14	10	4	
89	L5	1	Total	C	N	0
			14	10	4	
89	L5	1	Total	C	N	0
			14	10	4	
89	L5	1	Total	C	N	0
			14	10	4	
89	L5	1	Total	C	N	0
			14	10	4	
89	S2	1	Total	C	N	0
			14	10	4	

- Molecule 90 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms			AltConf
90	L5	1	Total	C	N	0
			10	7	3	
90	L5	1	Total	C	N	0
			10	7	3	
90	L5	1	Total	C	N	0
			10	7	3	
90	L8	1	Total	C	N	0
			10	7	3	
90	LN	1	Total	C	N	0
			10	7	3	
90	S2	1	Total	C	N	0
			10	7	3	
90	S2	1	Total	C	N	0
			10	7	3	

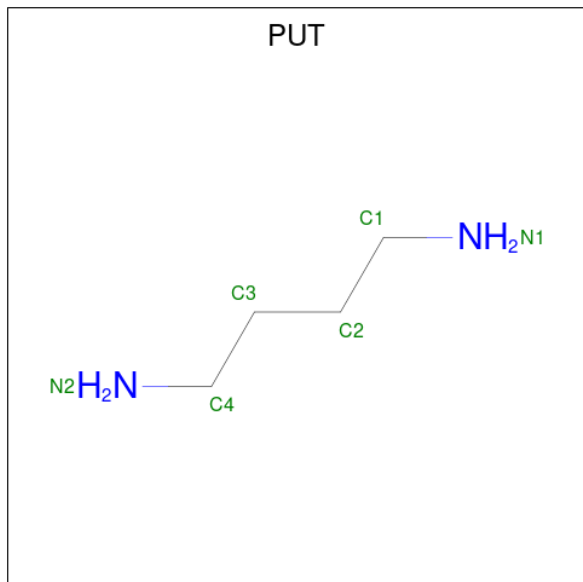
- Molecule 91 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
91	L5	74	Total	K	0
			74	74	
91	Lg	1	Total	K	0
			1	1	

- Molecule 92 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 93 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
93	S2	1	Total	C	N	0
			6	4	2	

- Molecule 94 is water.

Mol	Chain	Residues	Atoms		AltConf
94	CF	1	Total	O	0
			1	1	
94	L5	3310	Total	O	0
			3310	3310	
94	L7	16	Total	O	0
			16	16	
94	L8	118	Total	O	0
			118	118	
94	LA	43	Total	O	0
			43	43	
94	LB	66	Total	O	0
			66	66	
94	LC	45	Total	O	0
			45	45	
94	LD	1	Total	O	0
			1	1	
94	LG	13	Total	O	0
			13	13	

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Mol	Chain	Residues	Atoms		AltConf
94	LH	1	Total 1	O 1	0
94	LI	7	Total 7	O 7	0
94	LL	33	Total 33	O 33	0
94	LN	99	Total 99	O 99	0
94	LO	58	Total 58	O 58	0
94	LP	38	Total 38	O 38	0
94	LQ	21	Total 21	O 21	0
94	LR	12	Total 12	O 12	0
94	LS	2	Total 2	O 2	0
94	LT	9	Total 9	O 9	0
94	LU	1	Total 1	O 1	0
94	LV	41	Total 41	O 41	0
94	LW	15	Total 15	O 15	0
94	LX	10	Total 10	O 10	0
94	La	38	Total 38	O 38	0
94	Lb	14	Total 14	O 14	0
94	Ld	1	Total 1	O 1	0
94	Le	50	Total 50	O 50	0
94	Lf	13	Total 13	O 13	0
94	Lg	2	Total 2	O 2	0
94	Lh	8	Total 8	O 8	0

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Mol	Chain	Residues	Atoms		AltConf
94	Li	10	Total 10	O 10	0
94	Lj	29	Total 29	O 29	0
94	Ll	5	Total 5	O 5	0
94	Ln	2	Total 2	O 2	0
94	Lo	37	Total 37	O 37	0
94	Lp	4	Total 4	O 4	0
94	Lr	3	Total 3	O 3	0
94	Pt	6	Total 6	O 6	0
94	S2	340	Total 340	O 340	0
94	SE	12	Total 12	O 12	0
94	SF	5	Total 5	O 5	0
94	SH	1	Total 1	O 1	0
94	SI	14	Total 14	O 14	0
94	SJ	1	Total 1	O 1	0
94	SL	22	Total 22	O 22	0
94	SP	1	Total 1	O 1	0
94	SQ	7	Total 7	O 7	0
94	SS	8	Total 8	O 8	0
94	ST	2	Total 2	O 2	0
94	SU	3	Total 3	O 3	0
94	SX	8	Total 8	O 8	0

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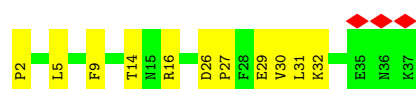
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Mol	Chain	Residues	Atoms		AltConf
94	SZ	1	Total 1	O 1	0
94	Sc	1	Total 1	O 1	0
94	Sd	3	Total 3	O 3	0

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.

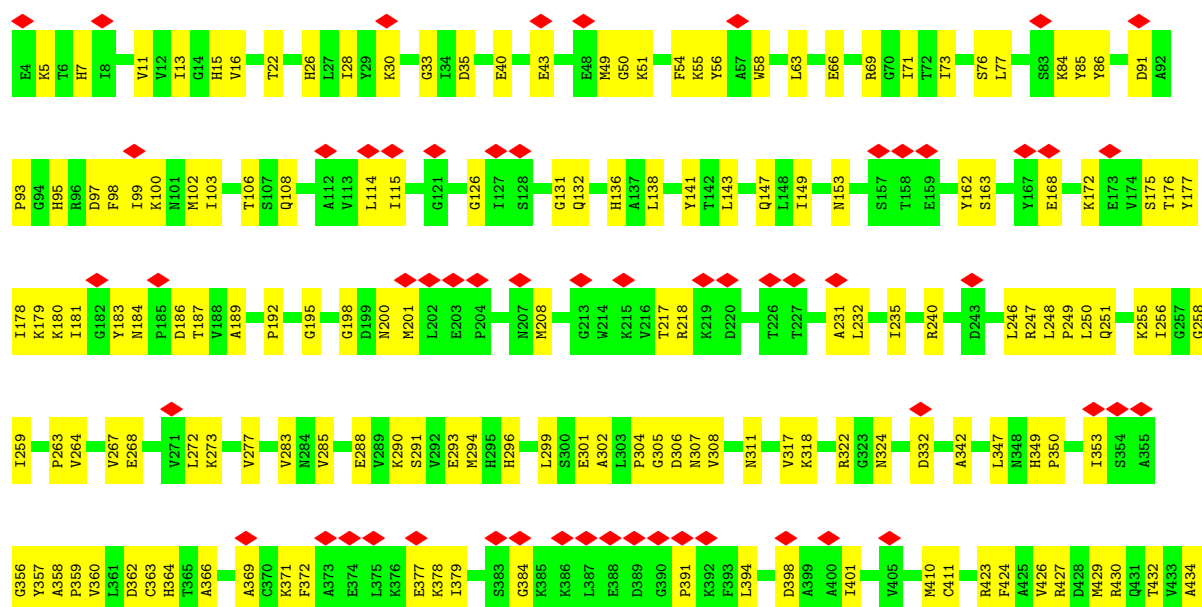
- Molecule 1: SERPINE1 mRNA-binding protein 1

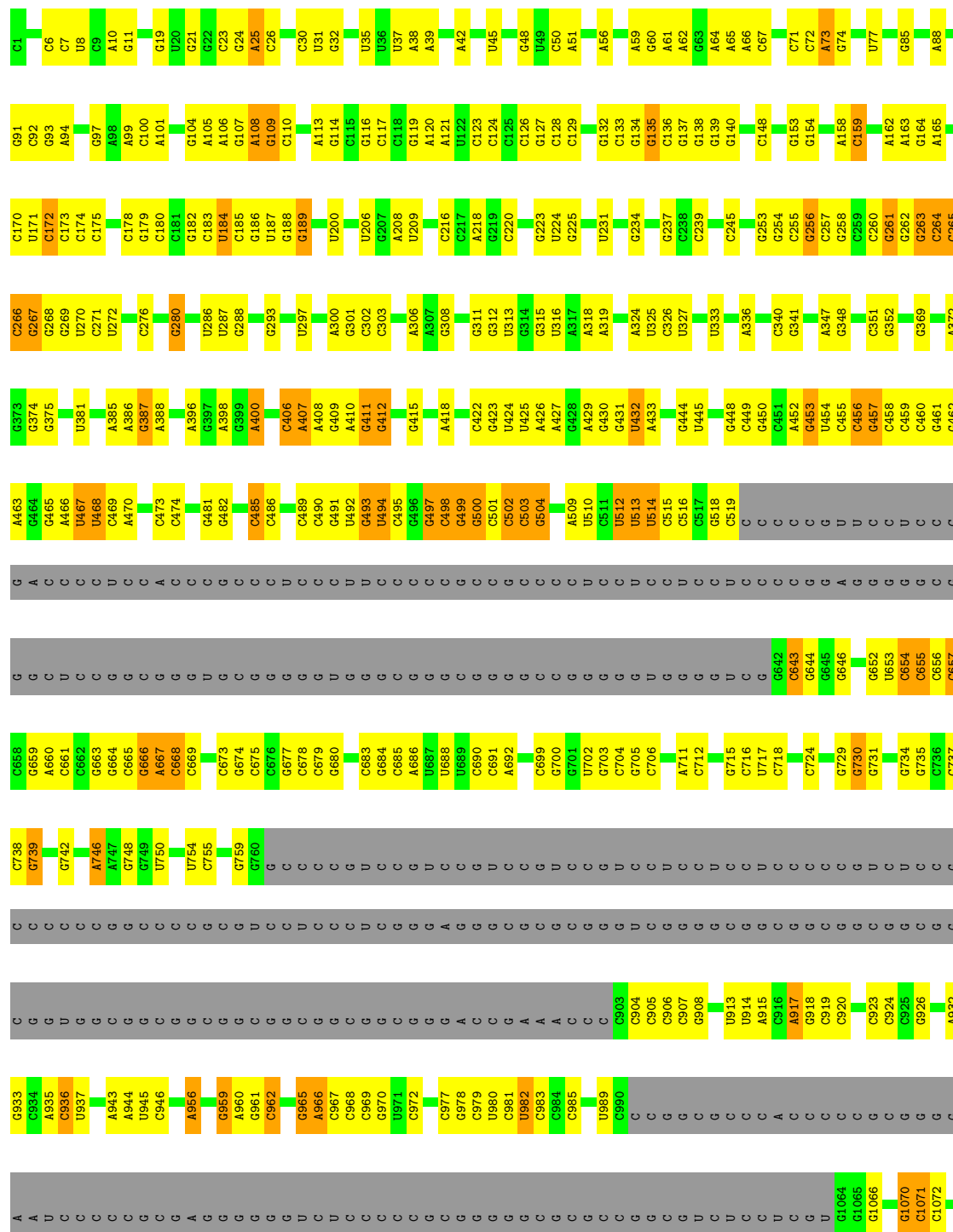


- Molecule 2: Transcription factor BTF3



- Molecule 3: Elongation factor 1-alpha 1





G2092	A1990	G1895	G1792	C	A1632	A1534	C1436	G1349	C1276	G1199	A	G1075
A2093	A1991	A1896	U1792	G1716	G1633	A1535	C1437	C1350	C1278	G1200	C	C1076
G2094	U1992	A1897	A1802	C1717	A1634	U1536	U1438	G1351	A1279	U1201	G	A1077
A2095	C1993	C1898	C1803	C1718	A1635	A1537	C1439	C1352	C1280	C1202	G	C1078
G2096	C1994	G1899	G1804	A1719	U1638	U1538	U1440	G1353	G1281	G1203	G	C1079
U2097	G1995	A1805	A1804	C1720	A1639	G1539	C1441	A1354	G1282		G	C1080
G2098	C1996	A1907	A1805	G1721	C1640	G1544	C1442	G1355	G1283	C1210	G	C1081
U1997	A1908	A1908	C1806	G1721	C1641	G1544	A1443	U1356	G1284	G1211	G	C1082
A2100	A1998	G1909	C1807	U1725	A1642	A1547	A1443	C1357	C1285		G	C1083
C2101	A1999	G1910	C1807	U1726	G1645	A1548	U1445	G1358	C1286	C1214	G	C1084
G2102	G2000	G1810	G1810	U1727	C1646	U1727	C1446	C1357	C1287	C1215	U	C1085
C2103	A2001	G1915	G1820	U1728	A1646	G1582	C1447	G1359	G1287	C1216	G	C1086
G2104	G2003	G1916	G1821	C1731	U1647	A1583	G1448	C1365	G1293	G1217	C	C1087
A2105		A1917	G1822	C1732	G1654	A1584	C1449	G1366	A1294	G1218	C	C1088
C2106	U2008	U1918	U1823	G1733	U1654	A1585		C1367	C1295	G1219	G	C1091
G2107	C2009	G1919	G1824	C1734	C1661	C1556	C1458	A1368	G1296	G1220	C	C1092
C2108	A2010	C1920	A1824	U1735	C1662	C1557	A1459	C1369	U1297	G1221	G	C1093
G2109	G2011	C1921	A1825	U1736	C1663	A1558	C1460	G1370	C1298	A1222	C	C1094
C2110		G1922		G1739	U1664	G1559	C1461		G1299	G	C	A1095
G2111	A2017	U1925	U1834	C1740	C1665	G1562	A1462	C1378	C1300	U	C	A1096
A2017	C2018	G1835	G1835	G1741	U1669	A1562	C1468	C1379	C1301	U	G	C1097
C2018	C2019	G1836	A1837	A1741	A1669	A1563	C1469	A1387	A1302	U	G	C1098
U2020	G2021	A1837	A1837	A1742	U1672	A1564			A1303	C	G	C1099
G2021		G1842		U1743	U1673	C1565	G1475	G1390	C1304	U	C	C1099
		G1842		U1744	U1673	C1566	C1476	A1391	C1305	U	C	U1100
		G1842		G1745	C1674	U1567		A1392	C1306	U	C	
		G1846		G1745	C1675	C1568	C1480	G1393	A1307	C	G	U
		C1847		G1750	C1676	C1568	C1481	G1394	C1308	G	G	C
		C1848		A1751	U1677	G1574	G1482	U1395	C1309	G	G	C
		C1848		G1752	U1677	G1574	C1483	G1396	C1310	G	G	C
		C1855			U1683	G1577		A1397		G1234	G	A
		C1855		U1757	U1683	G1577		A1398		G1235		C
		C1856		G1758	A1684	U1578	U1494	C1399	C1314			C
		C1856		G1759	G1685	C1579	G1495	G1400	C1315	C1239		C
		C1859		C1760	C1686	U1591	G1496	G1399	C1316	G1240		C
		C1859		U1687	C1686	U1591	C1505	G1407	U1317	C1241		C
		C1860		C1761	G1687	U1596	C1506	G1408	C1318	G1242		U
		C1861		G1762	G1688	U1596	C1507	C1409		G1243		U
		C1862		C1763	U1693	A1601	C1508	U1410	A1322	G1244		C
		C1865		G1764	U1693	A1601	A1508	C1411	A1323	C1245		C
		C1866		A1765	C1694	G1604	G1509	C1414	A1324	G1246		U
		A1867		A1765	C1694	G1604	G1510	C1415	A1325			C
		A1867		A1766	C1695	G1605	U1511	G1416	C1327	C1251		C
		A1868		A1767	C1696	G1605	U1512	G1416	C1328	C1252		C
		A1869		C1768	C1697	U1596	U1513	C1417	G1329	G1253		G
		C1870		G1769	C1698	U1596	U1514			A1254		C
		A1871		U1770	C1699	A1601	A1515	A1420	C1332			G
		G1872		U1771	A1699	A1601	G1517	G1426	A1333			C
		G1872		U1771	A1700	G1604	G1517	G1426	A1334			C
		C1875		G1772	A1701	G1604	U1511	C1414	A1337	A1257		C
		U1876		U1773	C1702	G1605	U1512	G1415	G1258	G1259		C
		C1877		C1774	C1703	G1605	U1513	G1416	U1338			C
		C1878		U1779	C1704	G1612	U1514	C1417	U1339			C
		G1879		U1780	G1705	A1613	A1515		C1340	G1266		G
		C1880		U1781	A1706	G1617	G1516	A1420	U1341	C1267		C
		G1880		U1782	C	G1617	G1517		A1342	G1268		C
		C1881		U1782	C	G1624	G1517		G1269	C1269		C
		U1882		U1782	C	G1624	G1517		A1270			C
		C1883		C1785	A	G1625			C1343			C
		C1883		A1786	C	G1625			G1271	G1194		C
		A1892		A1787	C	C1628	A1524	G1431	C1272	G1195		G
		C1893		A1788	C	C1628	A1525	G1432	C1273	G1196		G
		C1894		C1789	C	A1631		G1435	A1274	C1197		C
		C1894		C1789	C	A1631			G1275	G1198		G







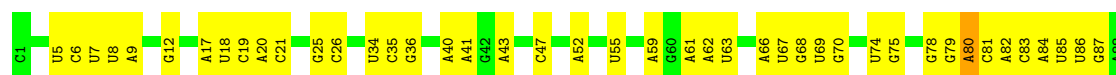
• Molecule 5: 5S rRNA

Chain L7: 74% 21% 5%



• Molecule 6: 5.8S rRNA

Chain L8: 53% 44% 3%



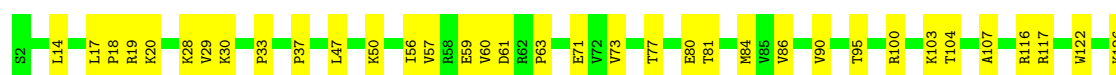
• Molecule 7: 60S ribosomal protein L8

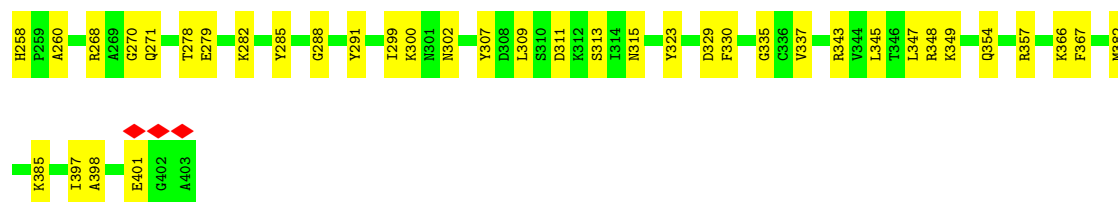
Chain LA: 70% 29% 1%



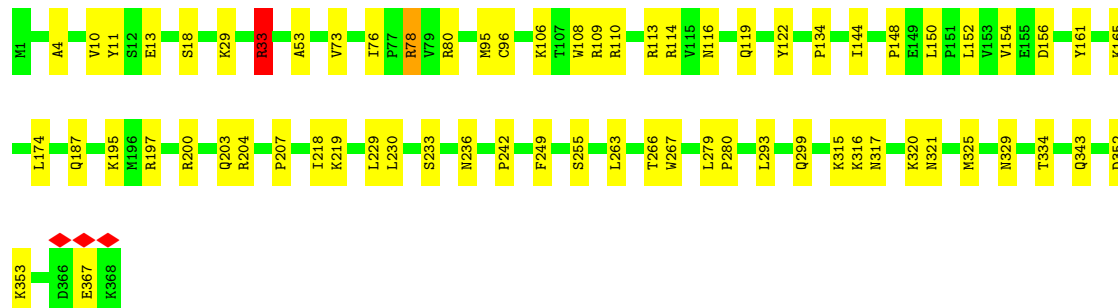
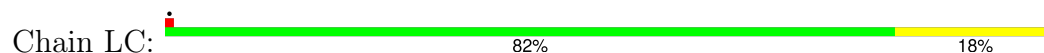
• Molecule 8: Large ribosomal subunit protein uL3

Chain LB: 73% 27% 0%

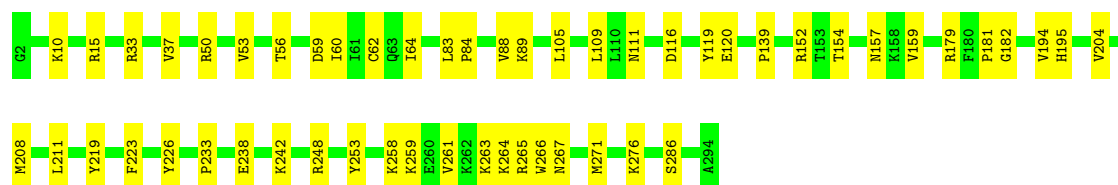
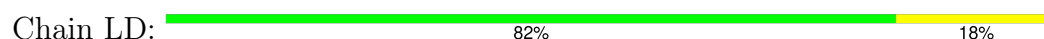




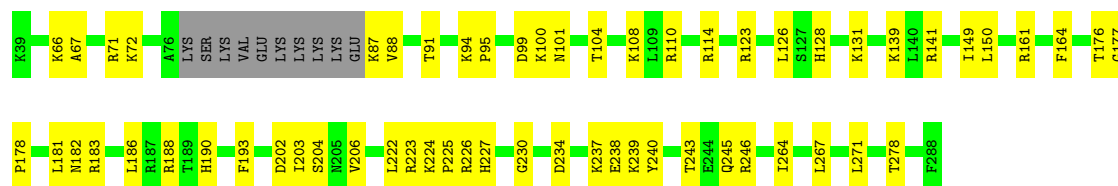
• Molecule 9: 60S ribosomal protein L4



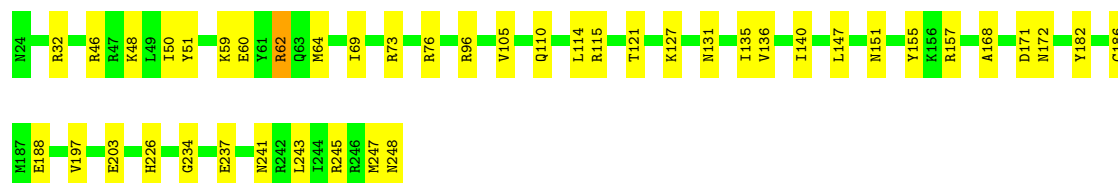
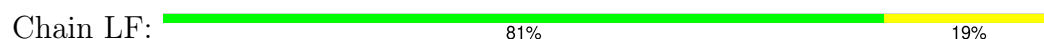
• Molecule 10: Large ribosomal subunit protein uL18



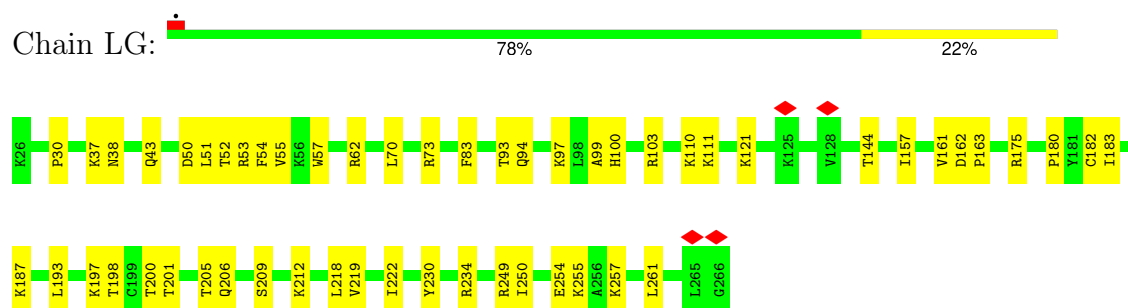
• Molecule 11: Large ribosomal subunit protein eL6



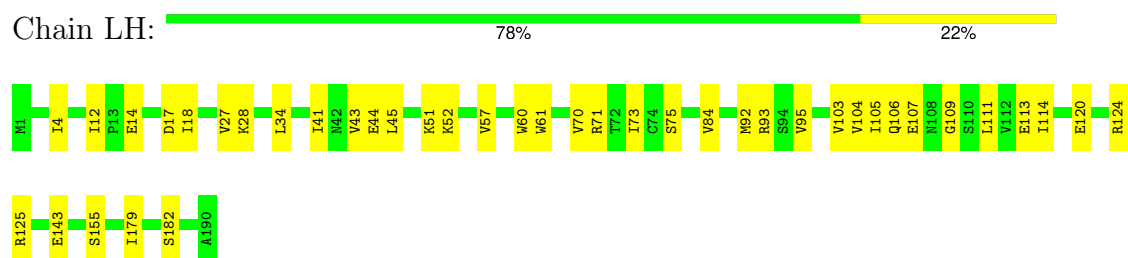
• Molecule 12: 60S ribosomal protein L7



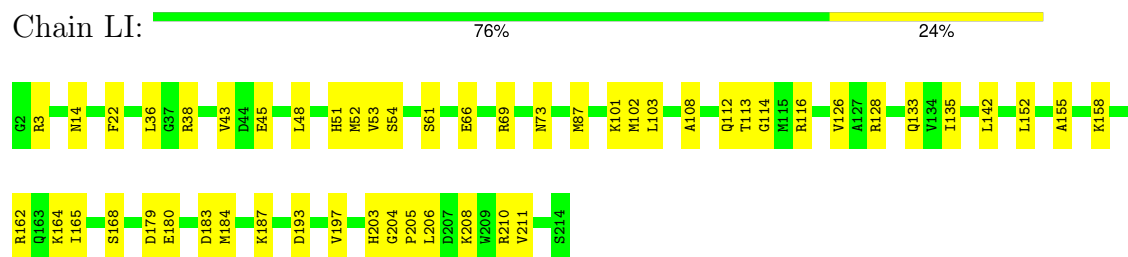
- Molecule 13: 60S ribosomal protein L7a



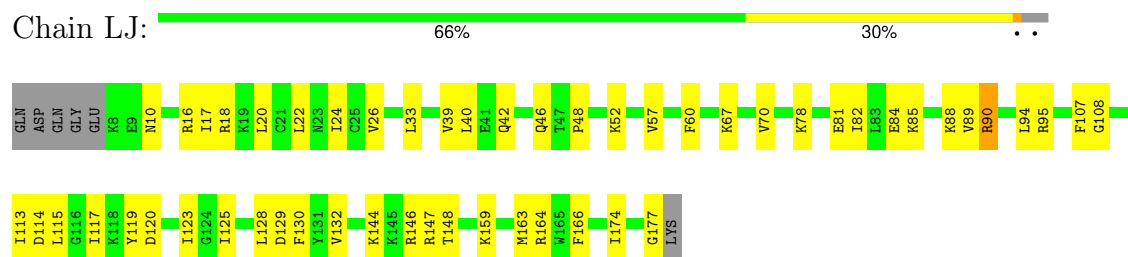
- Molecule 14: 60S ribosomal protein L9



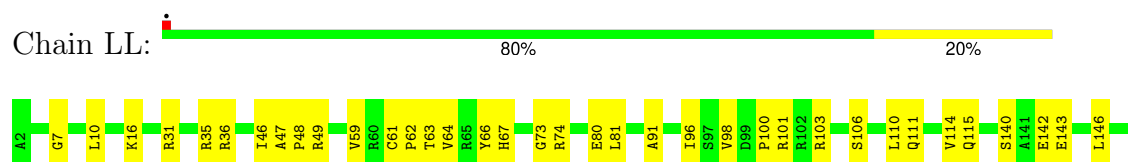
- Molecule 15: Ribosomal protein uL16-like



- Molecule 16: 60S ribosomal protein L11



- Molecule 17: Large ribosomal subunit protein eL13





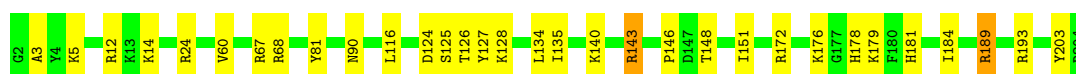
- Molecule 18: 60S ribosomal protein L14

Chain LM: 79% 21%



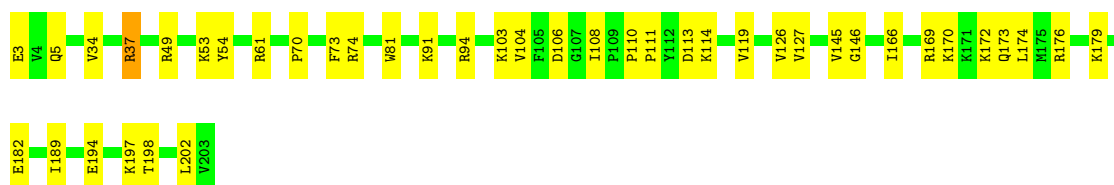
- Molecule 19: 60S ribosomal protein L15

Chain LN: 84% 15%



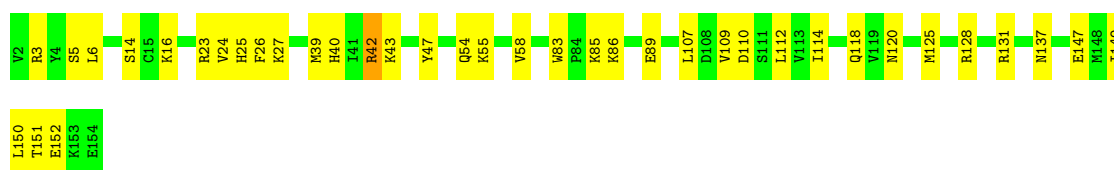
- Molecule 20: 60S ribosomal protein L13a

Chain LO: 80% 20%



- Molecule 21: 60S ribosomal protein L17

Chain LP: 75% 24%



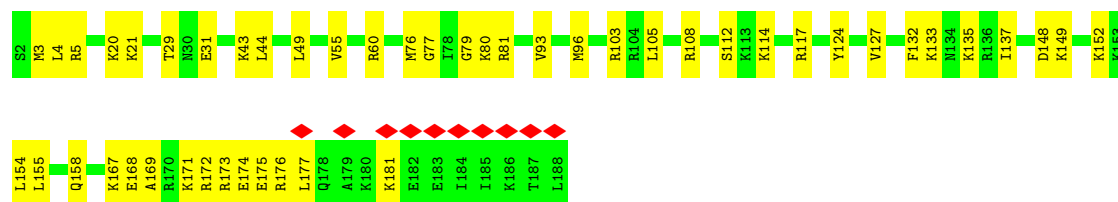
- Molecule 22: 60S ribosomal protein L18

Chain LQ: 88% 12%



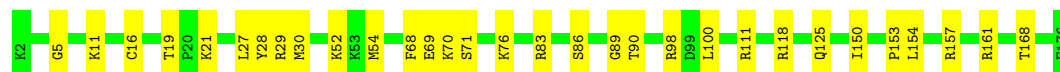
- Molecule 23: 60S ribosomal protein L19

Chain LR: 5% 74% 26%



- Molecule 24: 60S ribosomal protein L18a

Chain LS: 82% 18%



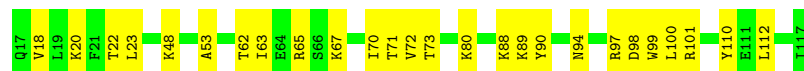
- Molecule 25: 60S ribosomal protein L21

Chain LT: 78% 22%



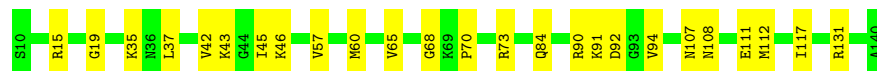
- Molecule 26: Heparin-binding protein HBp15

Chain LU: 74% 26%



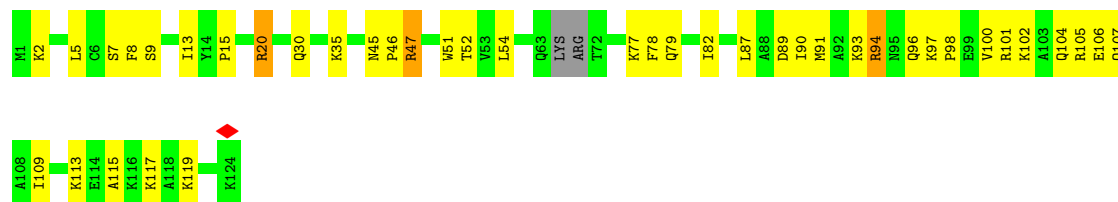
- Molecule 27: 60S ribosomal protein L23

Chain LV: 81% 19%



- Molecule 28: Ribosomal protein L24

Chain LW: 64% 32%



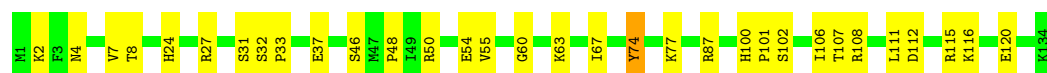
- Molecule 29: 60S ribosomal protein L23a

Chain LX:  88% 12%



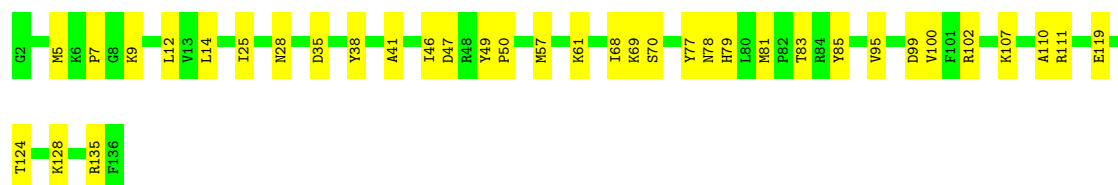
- Molecule 30: 60S ribosomal protein L26

Chain LY:  76% 23%



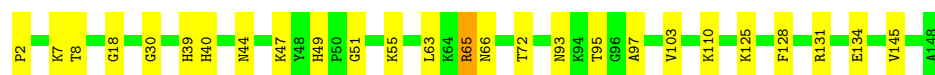
- Molecule 31: 60S ribosomal protein L27

Chain LZ:  73% 27%



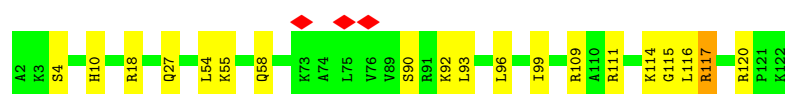
- Molecule 32: 60S ribosomal protein L27a

Chain La:  82% 17%



- Molecule 33: Large ribosomal subunit protein eL29

Chain Lb:  83% 17%



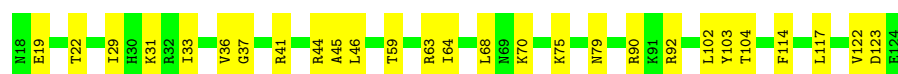
- Molecule 34: 60S ribosomal protein L30

Chain Lc:  76% 24%



- Molecule 35: 60S ribosomal protein L31

Chain Ld:  75% 25%



- Molecule 36: 60S ribosomal protein L32

Chain Le:  88% 12%



- Molecule 37: 60S ribosomal protein L35a

Chain Lf:  86% 14%



- Molecule 38: 60S ribosomal protein L34

Chain Lg:  87% 13%



- Molecule 39: 60S ribosomal protein L35

Chain Lh:  84% 16%



- Molecule 40: 60S ribosomal protein L36

Chain Li:  94% 6%



- Molecule 41: 60S ribosomal protein L37

Chain Lj:  77% 23%



- Molecule 42: 60S ribosomal protein L38

Chain Lk:  78% 22%



- Molecule 43: 60S ribosomal protein L39

Chain Ll:  70% 28% .



- Molecule 44: Large ribosomal subunit protein eL40

Chain Lm:  79% 21%



- Molecule 45: 60S ribosomal protein L41

Chain Ln:  75% 21% .



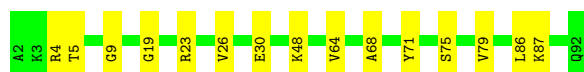
- Molecule 46: 60S ribosomal protein L36a

Chain Lo:  78% 22%



- Molecule 47: 60S ribosomal protein L37a

Chain Lp:  84% 16%



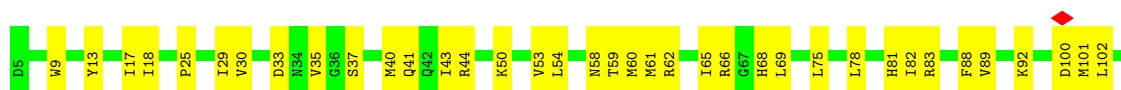
- Molecule 48: 60S ribosomal protein L28

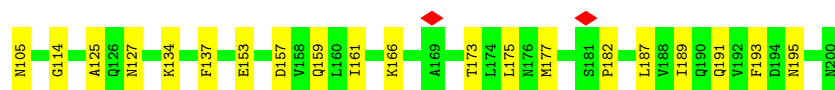
Chain Lr:  88% 12%



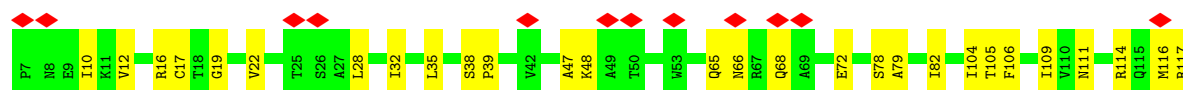
- Molecule 49: 60S acidic ribosomal protein P0

Chain Ls:  71% 29%





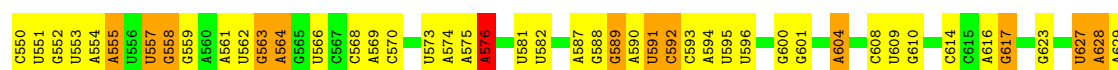
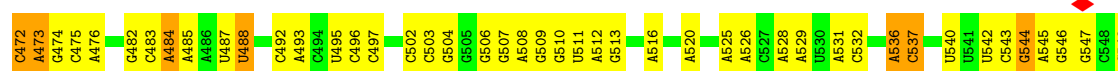
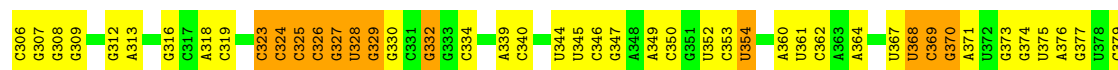
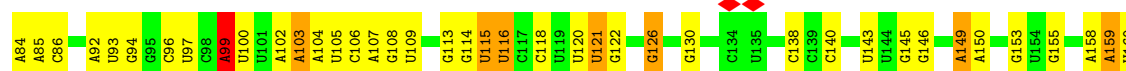
- Molecule 50: Large ribosomal subunit protein uL11



- Molecule 51: P site tRNA



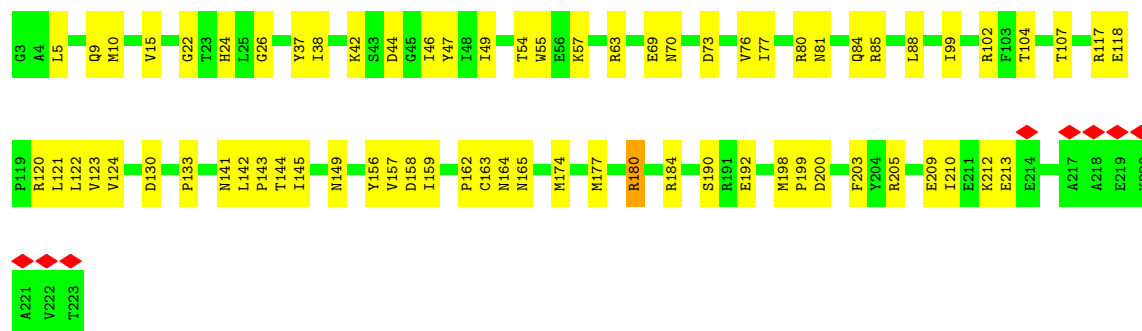
- Molecule 52: 18S rRNA





- Molecule 53: 40S ribosomal protein SA

Chain SA:



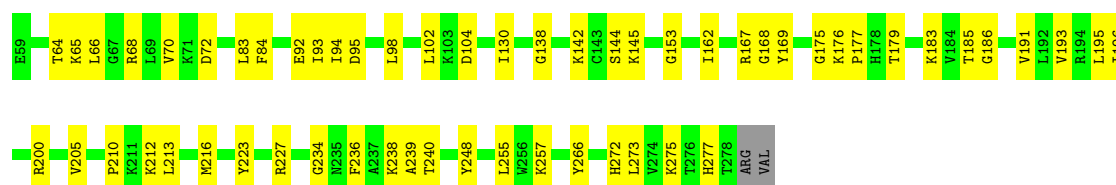
- Molecule 54: 40S ribosomal protein S3a

Chain SB:



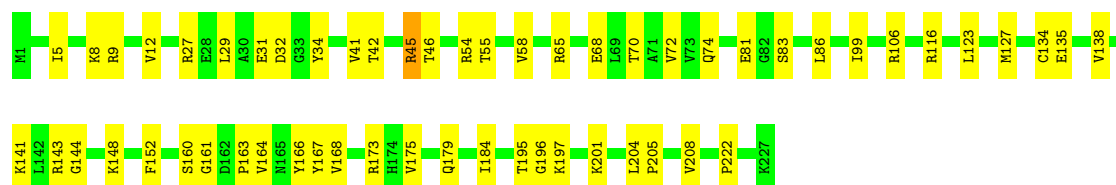
- Molecule 55: 40S ribosomal protein S2

Chain SC:



- Molecule 56: Small ribosomal subunit protein uS3

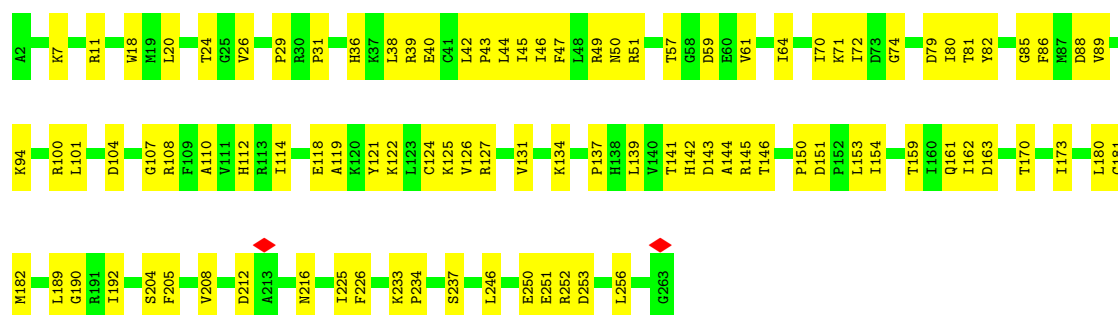
Chain SD:



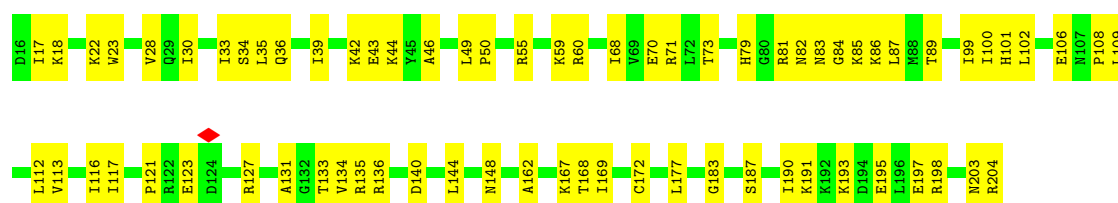
- Molecule 57: Small ribosomal subunit protein eS4, X isoform

Chain SE:

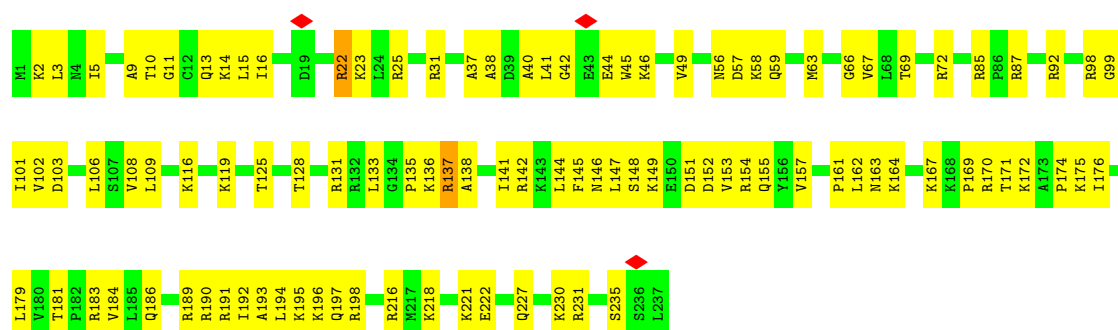




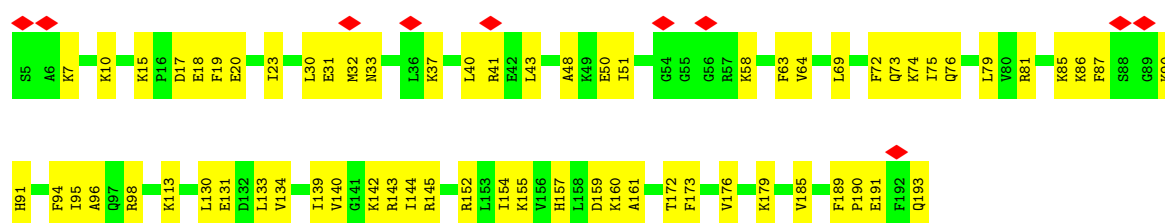
- Molecule 58: 40S ribosomal protein S5



- Molecule 59: 40S ribosomal protein S6

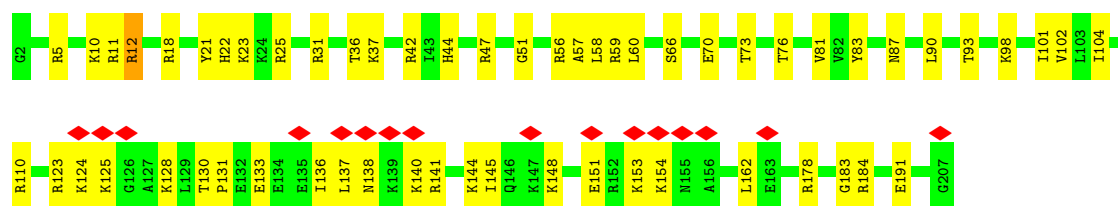


- Molecule 60: Small ribosomal subunit protein eS7

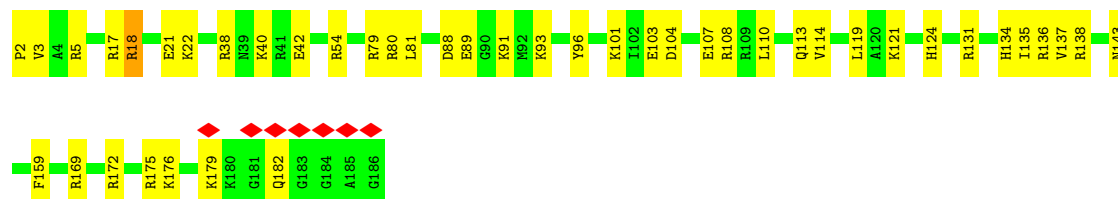
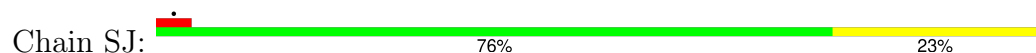


- Molecule 61: 40S ribosomal protein S8





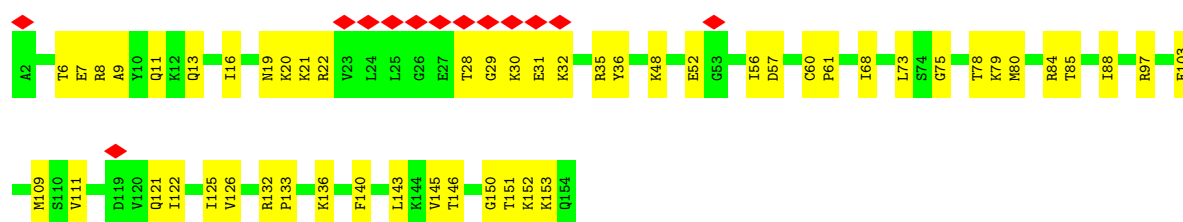
- Molecule 62: 40S ribosomal protein S9



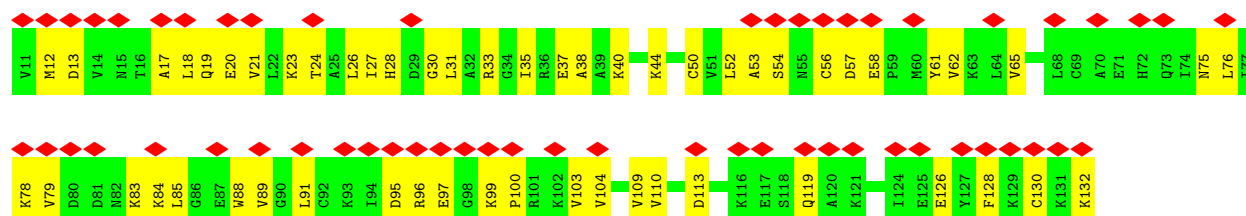
- Molecule 63: 40S ribosomal protein S10



- Molecule 64: 40S ribosomal protein S11



- Molecule 65: Small ribosomal subunit protein eS12



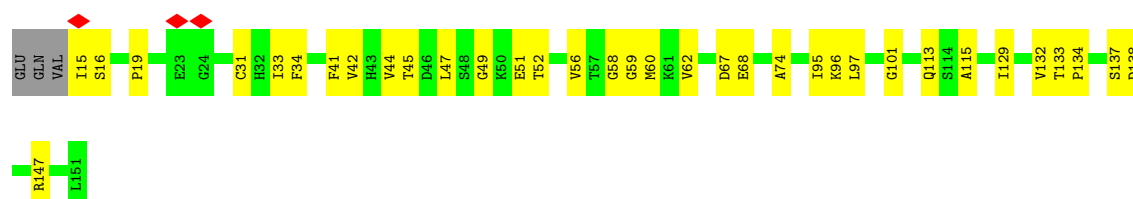
- Molecule 66: 40S ribosomal protein S13

Chain SN:  80% 19%



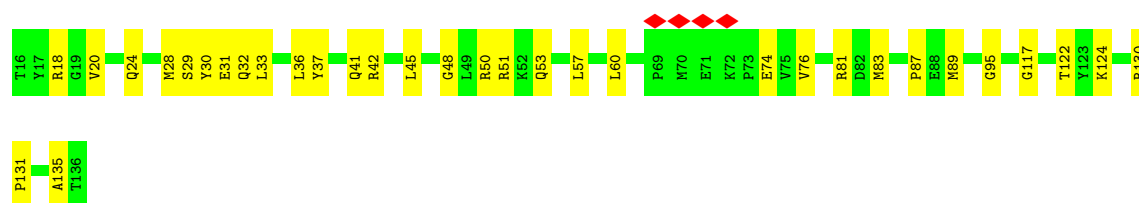
- Molecule 67: Small ribosomal subunit protein uS11

Chain SO:  73% 25%



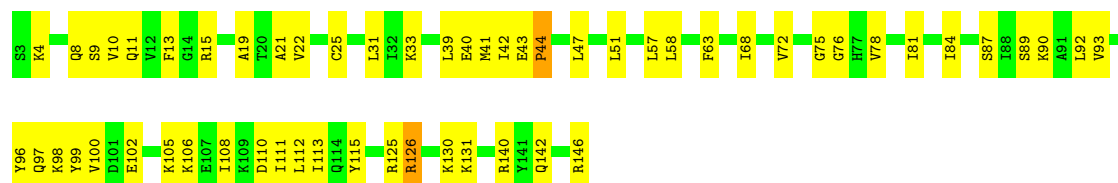
- Molecule 68: Small ribosomal subunit protein uS19

Chain SP:  73% 27%



- Molecule 69: Small ribosomal subunit protein uS9

Chain SQ:  60% 38%



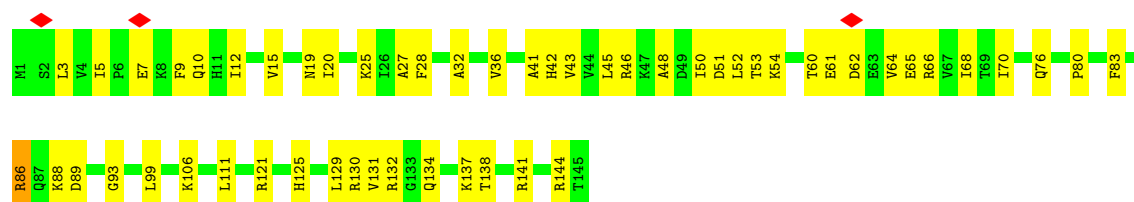
- Molecule 70: Small ribosomal subunit protein eS17

Chain SR:  61% 39%

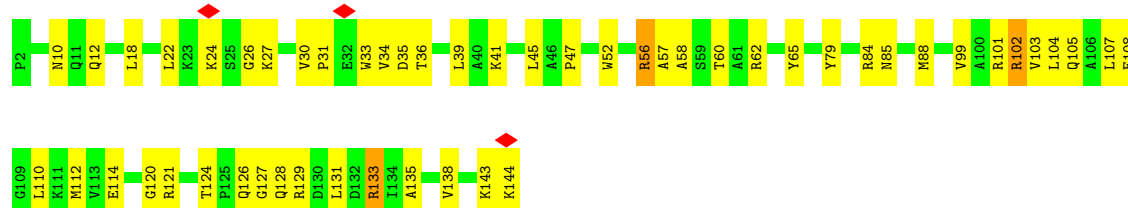


- Molecule 71: 40S ribosomal protein S18

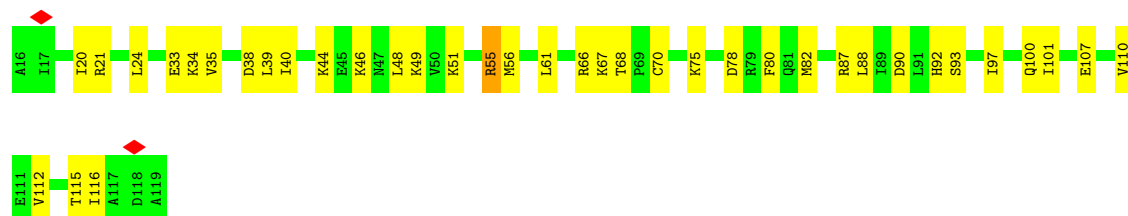
Chain SS:  63% 37%



- Molecule 72: 40S ribosomal protein S19



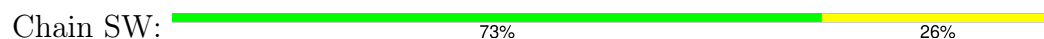
- Molecule 73: 40S ribosomal protein S20



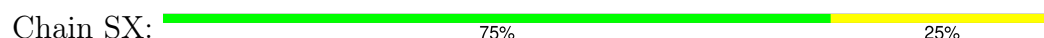
- Molecule 74: Small ribosomal subunit protein eS21



- Molecule 75: 40S ribosomal protein S15a



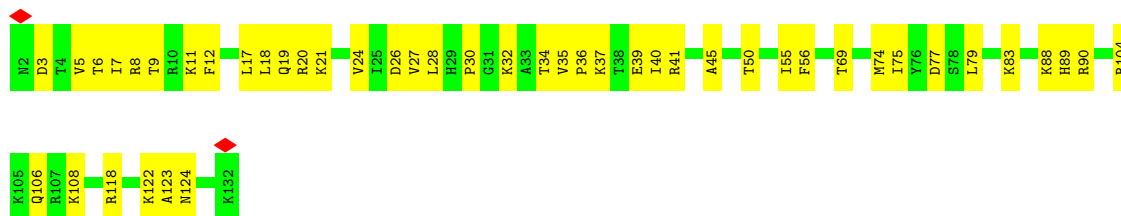
- Molecule 76: 40S ribosomal protein S23



R142

- Molecule 77: 40S ribosomal protein S24

Chain SY:  65% 35%



- Molecule 78: Small ribosomal subunit protein eS25

Chain SZ:  5% 67% 33%



- Molecule 79: 40S ribosomal protein S26

Chain Sa:  81% 19%



- Molecule 80: Small ribosomal subunit protein eS27

Chain Sb:  76% 24%



- Molecule 81: 40S ribosomal protein S28

Chain Sc:  73% 27%



- Molecule 82: 40S ribosomal protein S29

Chain Sd:  58% 42%



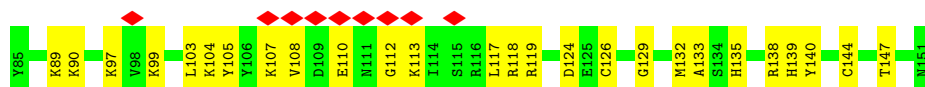
- Molecule 83: Small ribosomal subunit protein eS30

Chain Se:  88% 12%



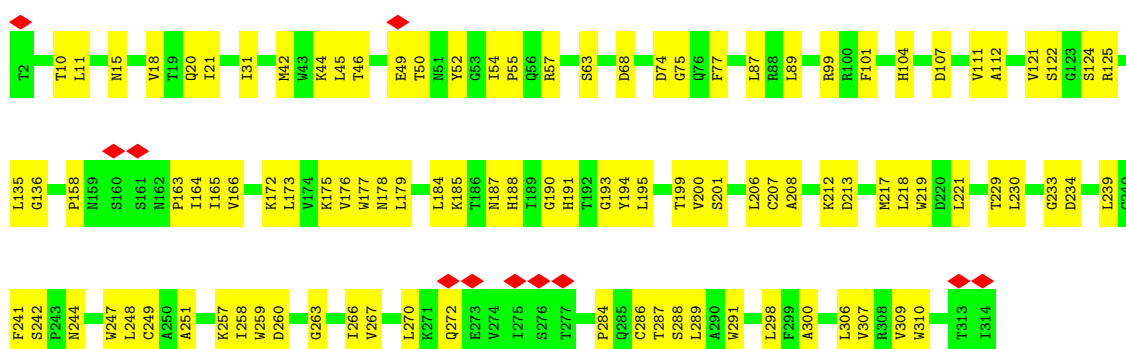
- Molecule 84: Ubiquitin-40S ribosomal protein S27a

Chain Sf:  13% 61% 39%

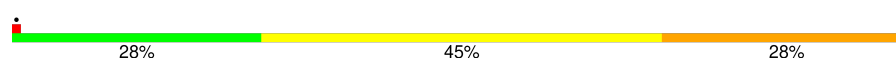


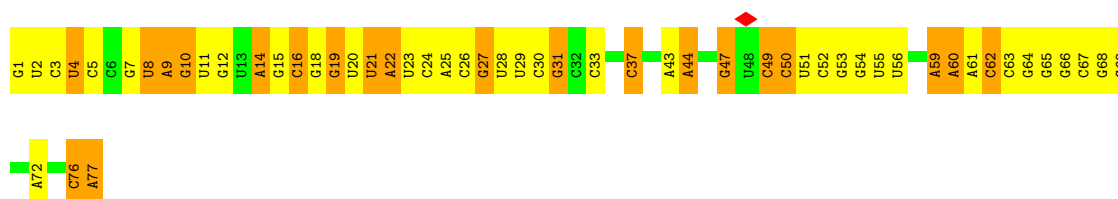
- Molecule 85: Receptor of activated protein C kinase 1

Chain Sg:  67% 33%



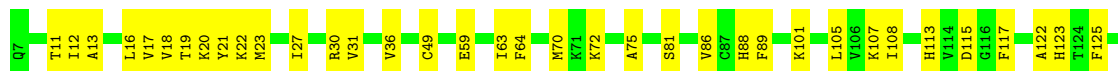
- Molecule 86: A/T site tRNA

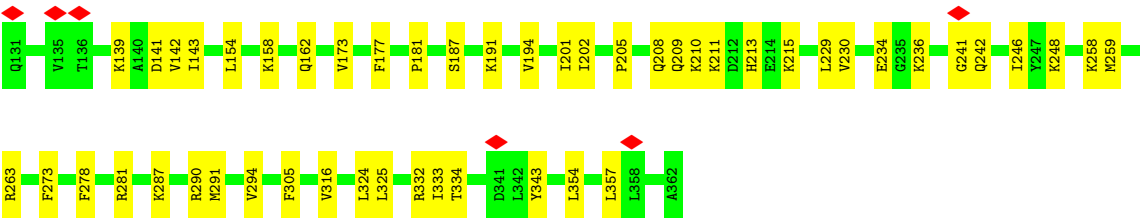
Chain AT:  28% 45% 28%



- Molecule 87: Proliferation-associated protein 2G4

Chain CA:  76% 24%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	221164	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	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	1.017	Depositor
Minimum map value	-0.302	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.0575	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: 4AC, SPD, SPM, 5MC, 6MZ, 1MA, K, SEP, OMU, MA6, PSU, UY1, A2M, ZN, UR3, MG, B8N, G7M, OMC, OMG, PUT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	CD	0.14	0/291	0.39	0/391
2	CI	0.16	0/247	0.44	0/323
3	CF	0.16	0/3442	0.40	0/4656
4	L5	0.16	0/85098	0.30	0/132762
5	L7	0.12	0/2861	0.23	0/4459
6	L8	0.13	0/3631	0.26	0/5657
7	LA	0.20	0/1936	0.39	0/2596
8	LB	0.18	0/3306	0.42	0/4424
9	LC	0.21	0/2981	0.45	1/4002 (0.0%)
10	LD	0.18	0/2428	0.36	0/3252
11	LE	0.19	0/1973	0.43	0/2645
12	LF	0.16	0/1905	0.31	0/2539
13	LG	0.21	0/1960	0.42	0/2637
14	LH	0.18	0/1537	0.39	0/2066
15	LI	0.16	0/1751	0.37	0/2340
16	LJ	0.19	0/1385	0.44	0/1852
17	LL	0.16	0/1732	0.36	0/2315
18	LM	0.18	0/1161	0.35	0/1554
19	LN	0.16	0/1746	0.37	1/2338 (0.0%)
20	LO	0.18	0/1682	0.36	0/2250
21	LP	0.19	0/1268	0.38	0/1701
22	LQ	0.16	0/1537	0.33	0/2052
23	LR	0.17	0/1582	0.38	0/2091
24	LS	0.14	0/1493	0.31	0/2003
25	LT	0.19	0/1326	0.43	0/1770
26	LU	0.21	0/839	0.53	0/1126
27	LV	0.21	0/993	0.40	0/1332
28	LW	0.18	0/959	0.48	1/1270 (0.1%)
29	LX	0.16	0/1002	0.33	0/1345
30	LY	0.19	0/1132	0.46	0/1504
31	LZ	0.18	0/1130	0.38	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	La	0.17	0/1191	0.38	0/1591
33	Lb	0.17	0/889	0.38	0/1175
34	Lc	0.17	0/774	0.39	0/1038
35	Ld	0.18	0/903	0.35	0/1216
36	Le	0.15	0/1071	0.35	0/1429
37	Lf	0.18	0/895	0.37	0/1198
38	Lg	0.15	0/916	0.36	0/1220
39	Lh	0.18	0/1023	0.34	0/1351
40	Li	0.17	0/843	0.40	0/1115
41	Lj	0.17	0/720	0.41	0/952
42	Lk	0.17	0/575	0.46	0/761
43	Ll	0.18	0/454	0.39	0/599
44	Lm	0.15	0/435	0.36	0/575
45	Ln	0.18	0/231	0.32	0/294
46	Lo	0.22	0/876	0.43	0/1156
47	Lp	0.16	0/718	0.39	0/953
48	Lr	0.19	0/1017	0.35	0/1364
49	Ls	0.20	0/1519	0.44	0/2052
50	Lt	0.20	0/1009	0.55	0/1363
51	Pt	0.10	0/1761	0.24	0/2741
52	S2	0.17	0/39755	0.28	0/61935
53	SA	0.18	0/1778	0.41	0/2416
54	SB	0.20	0/1765	0.45	0/2362
55	SC	0.18	0/1744	0.42	0/2357
56	SD	0.17	0/1793	0.40	0/2414
57	SE	0.19	0/2118	0.42	0/2849
58	SF	0.21	0/1516	0.43	0/2037
59	SG	0.19	0/1946	0.42	0/2590
60	SH	0.22	0/1519	0.46	0/2033
61	SI	0.18	0/1715	0.44	0/2287
62	SJ	0.16	0/1550	0.38	0/2069
63	SK	0.19	0/851	0.41	0/1147
64	SL	0.17	0/1268	0.40	0/1696
65	SM	0.20	0/950	0.52	0/1275
66	SN	0.16	0/1232	0.33	0/1656
67	SO	0.19	0/1037	0.41	0/1391
68	SP	0.23	0/1003	0.48	0/1342
69	SQ	0.22	0/1160	0.46	0/1553
70	SR	0.18	0/1105	0.48	0/1484
71	SS	0.20	0/1216	0.44	0/1628
72	ST	0.19	0/1131	0.53	0/1515
73	SU	0.21	0/831	0.48	0/1115
74	SV	0.21	0/643	0.46	0/860

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	SW	0.22	0/1051	0.40	0/1406
76	SX	0.16	0/1116	0.39	0/1490
77	SY	0.19	0/1083	0.43	0/1438
78	SZ	0.22	0/604	0.47	0/810
79	Sa	0.21	0/836	0.47	0/1121
80	Sb	0.18	0/665	0.40	0/891
81	Sc	0.21	0/508	0.46	0/680
82	Sd	0.18	0/470	0.43	0/623
83	Se	0.19	0/465	0.40	0/612
84	Sf	0.34	0/560	0.60	0/745
85	Sg	0.17	0/2493	0.40	0/3394
86	AT	0.13	0/1805	0.28	0/2809
87	CA	0.18	0/2810	0.40	0/3780
All	All	0.17	0/238226	0.34	3/348712 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	LA	0	2
9	LC	0	2
12	LF	0	1
16	LJ	0	1
19	LN	0	1
20	LO	0	1
21	LP	0	1
28	LW	0	2
30	LY	0	1
31	LZ	0	1
32	La	0	1
33	Lb	0	1
36	Le	0	1
43	Ll	0	1
45	Ln	0	1
53	SA	0	1
54	SB	0	1
56	SD	0	1
59	SG	0	3
61	SI	0	2
62	SJ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
63	SK	0	1
66	SN	0	1
69	SQ	0	1
71	SS	0	1
72	ST	0	3
73	SU	0	1
74	SV	0	1
75	SW	0	1
83	Se	0	1
All	All	0	38

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	LN	143	ARG	CG-CD-NE	5.86	124.89	112.00
9	LC	33	ARG	CB-CA-C	5.44	118.43	110.87
28	LW	47	ARG	CB-CG-CD	5.18	123.22	111.30

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	LA	147	ARG	Sidechain
7	LA	245	ARG	Sidechain
9	LC	33	ARG	Sidechain
9	LC	78	ARG	Sidechain
12	LF	62	ARG	Sidechain
16	LJ	90	ARG	Sidechain
19	LN	189	ARG	Sidechain
20	LO	37	ARG	Sidechain
21	LP	42	ARG	Sidechain
28	LW	20	ARG	Sidechain
28	LW	94	ARG	Sidechain
30	LY	74	TYR	Sidechain
31	LZ	111	ARG	Sidechain
32	La	65	ARG	Sidechain
33	Lb	117	ARG	Sidechain
36	Le	128	ARG	Sidechain
43	Ll	46	ARG	Sidechain
45	Ln	18	ARG	Sidechain

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Mol	Chain	Res	Type	Group
53	SA	180	ARG	Sidechain
54	SB	51	ARG	Sidechain
56	SD	45	ARG	Sidechain
59	SG	137	ARG	Sidechain
59	SG	191	ARG	Sidechain
59	SG	22	ARG	Sidechain
61	SI	12	ARG	Sidechain
61	SI	178	ARG	Sidechain
62	SJ	18	ARG	Sidechain
63	SK	96	ARG	Sidechain
66	SN	99	ARG	Sidechain
69	SQ	126	ARG	Sidechain
71	SS	86	ARG	Sidechain
72	ST	102	ARG	Sidechain
72	ST	133	ARG	Sidechain
72	ST	56	ARG	Sidechain
73	SU	55	ARG	Sidechain
74	SV	22	ARG	Sidechain
75	SW	57	ARG	Sidechain
83	Se	13	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CD	285	0	260	10	0
2	CI	247	0	283	8	0
3	CF	3383	0	3431	154	0
4	L5	78445	0	39700	1215	0
5	L7	2561	0	1295	24	0
6	L8	3315	0	1685	49	0
7	LA	1898	0	1993	59	0
8	LB	3238	0	3375	101	0
9	LC	2927	0	3104	56	0
10	LD	2382	0	2410	36	0
11	LE	1935	0	2096	50	0
12	LF	1870	0	1996	33	0
13	LG	1927	0	2074	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	LH	1518	0	1601	30	0
15	LI	1711	0	1749	37	0
16	LJ	1362	0	1399	40	0
17	LL	1701	0	1818	35	0
18	LM	1138	0	1204	25	0
19	LN	1701	0	1749	28	0
20	LO	1650	0	1794	33	0
21	LP	1242	0	1269	30	0
22	LQ	1513	0	1628	20	0
23	LR	1566	0	1729	36	0
24	LS	1453	0	1490	21	0
25	LT	1298	0	1366	32	0
26	LU	825	0	850	24	0
27	LV	979	0	1039	23	0
28	LW	945	0	1003	34	0
29	LX	985	0	1066	27	0
30	LY	1115	0	1205	26	0
31	LZ	1107	0	1182	25	0
32	La	1162	0	1213	24	0
33	Lb	876	0	948	22	0
34	Lc	764	0	804	16	0
35	Ld	888	0	930	19	0
36	Le	1053	0	1147	12	0
37	Lf	876	0	912	11	0
38	Lg	906	0	998	15	0
39	Lh	1015	0	1148	21	0
40	Li	832	0	917	8	0
41	Lj	705	0	737	17	0
42	Lk	569	0	637	17	0
43	Ll	444	0	483	13	0
44	Lm	429	0	465	9	0
45	Ln	230	0	276	7	0
46	Lo	862	0	929	16	0
47	Lp	708	0	756	13	0
48	Lr	1002	0	1068	11	0
49	Ls	1496	0	1540	41	0
50	Lt	998	0	1032	32	0
51	Pt	1576	0	802	20	0
52	S2	36953	0	18679	728	0
53	SA	1741	0	1746	66	0
54	SB	1738	0	1809	49	0
55	SC	1707	0	1791	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	SD	1765	0	1865	36	0
57	SE	2076	0	2177	76	0
58	SF	1495	0	1549	58	0
59	SG	1923	0	2089	94	0
60	SH	1497	0	1590	52	0
61	SI	1686	0	1772	54	0
62	SJ	1525	0	1640	37	0
63	SK	827	0	854	29	0
64	SL	1247	0	1323	44	0
65	SM	940	0	965	47	0
66	SN	1208	0	1294	24	0
67	SO	1024	0	1050	27	0
68	SP	985	0	1031	28	0
69	SQ	1142	0	1213	50	0
70	SR	1090	0	1149	48	0
71	SS	1198	0	1261	46	0
72	ST	1112	0	1146	42	0
73	SU	821	0	883	43	0
74	SV	636	0	637	28	0
75	SW	1034	0	1080	38	0
76	SX	1098	0	1167	26	0
77	SY	1065	0	1142	45	0
78	SZ	598	0	656	22	0
79	Sa	821	0	870	16	0
80	Sb	651	0	672	16	0
81	Sc	506	0	536	22	0
82	Sd	459	0	448	23	0
83	Se	459	0	503	7	0
84	Sf	548	0	551	27	0
85	Sg	2436	0	2393	77	0
86	AT	1616	0	823	94	0
87	CA	2764	0	2779	72	0
88	L5	185	0	0	0	0
88	L7	3	0	0	0	0
88	L8	5	0	0	0	0
88	LA	1	0	0	0	0
88	LP	1	0	0	0	0
88	LV	1	0	0	0	0
88	Le	1	0	0	0	0
88	S2	28	0	0	0	0
89	L5	98	0	182	10	0
89	S2	14	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	L5	80	0	151	3	0
90	L8	10	0	19	0	0
90	LN	10	0	19	0	0
90	S2	20	0	38	0	0
91	L5	74	0	0	0	0
91	Lg	1	0	0	0	0
92	Lg	1	0	0	0	0
92	Lj	1	0	0	0	0
92	Lm	1	0	0	0	0
92	Lo	1	0	0	0	0
92	Lp	1	0	0	0	0
92	Sa	1	0	0	0	0
92	Sd	1	0	0	0	0
93	S2	6	0	12	0	0
94	CF	1	0	0	0	0
94	L5	3310	0	0	17	0
94	L7	16	0	0	0	0
94	L8	118	0	0	0	0
94	LA	43	0	0	0	0
94	LB	66	0	0	1	0
94	LC	45	0	0	0	0
94	LD	1	0	0	0	0
94	LG	13	0	0	0	0
94	LH	1	0	0	0	0
94	LI	7	0	0	0	0
94	LL	33	0	0	0	0
94	LN	99	0	0	2	0
94	LO	58	0	0	1	0
94	LP	38	0	0	2	0
94	LQ	21	0	0	0	0
94	LR	12	0	0	0	0
94	LS	2	0	0	0	0
94	LT	9	0	0	0	0
94	LU	1	0	0	0	0
94	LV	41	0	0	3	0
94	LW	15	0	0	0	0
94	LX	10	0	0	0	0
94	La	38	0	0	0	0
94	Lb	14	0	0	0	0
94	Ld	1	0	0	0	0
94	Le	50	0	0	0	0
94	Lf	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
94	Lg	2	0	0	0	0
94	Lh	8	0	0	1	0
94	Li	10	0	0	1	0
94	Lj	29	0	0	0	0
94	Ll	5	0	0	0	0
94	Ln	2	0	0	0	0
94	Lo	37	0	0	1	0
94	Lp	4	0	0	0	0
94	Lr	3	0	0	0	0
94	Pt	6	0	0	1	0
94	S2	340	0	0	5	0
94	SE	12	0	0	2	0
94	SF	5	0	0	1	0
94	SH	1	0	0	0	0
94	SI	14	0	0	4	0
94	SJ	1	0	0	0	0
94	SL	22	0	0	0	0
94	SP	1	0	0	0	0
94	SQ	7	0	0	0	0
94	SS	8	0	0	0	0
94	ST	2	0	0	0	0
94	SU	3	0	0	0	0
94	SX	8	0	0	0	0
94	SZ	1	0	0	1	0
94	Sc	1	0	0	0	0
94	Sd	3	0	0	0	0
All	All	231160	0	170165	4176	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 11.

All (4176) 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:CF:358:ALA:CB	86:AT:52:C:H4'	1.43	1.47
3:CF:358:ALA:HB3	86:AT:52:C:C4'	1.59	1.30
3:CF:358:ALA:CB	86:AT:52:C:C4'	2.10	1.30
3:CF:358:ALA:H	86:AT:52:C:C3'	1.58	1.17
3:CF:358:ALA:HB3	86:AT:52:C:O4'	1.42	1.16
29:LX:156:ILE:HD11	87:CA:291:MET:HB2	1.11	1.08
3:CF:358:ALA:HB2	86:AT:52:C:H4'	1.26	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LX:156:ILE:HD11	87:CA:291:MET:CB	1.83	1.07
3:CF:358:ALA:N	86:AT:52:C:O3'	1.82	1.03
86:AT:51:U:H3	86:AT:65:G:H1	1.04	0.96
50:Lt:16:ARG:HH12	50:Lt:28:LEU:HB3	1.31	0.94
29:LX:87:MET:HB2	87:CA:259:MET:HE1	1.50	0.94
50:Lt:16:ARG:HE	50:Lt:17:CYS:H	1.12	0.93
69:SQ:43:GLU:HG3	69:SQ:44:PRO:HD3	1.49	0.93
3:CF:358:ALA:CA	86:AT:52:C:H4'	1.98	0.91
4:L5:2017:A:HO2'	4:L5:2018:C:H6	0.96	0.91
3:CF:290:LYS:HE3	52:S2:488:U:H5''	1.52	0.90
60:SH:144:ILE:HD13	60:SH:154:ILE:HG13	1.54	0.90
73:SU:48:LEU:HG	73:SU:93:SER:HB3	1.52	0.89
55:SC:68:ARG:HG2	55:SC:277:HIS:HB2	1.54	0.89
4:L5:1175:A:H2	4:L5:1185:G:H1	1.20	0.89
58:SF:34:SER:HA	81:Sc:55:VAL:HG13	1.55	0.87
3:CF:371:LYS:HZ2	86:AT:52:C:H5''	1.40	0.87
4:L5:1273:G:N7	33:Lb:117:ARG:NH1	2.23	0.86
3:CF:358:ALA:N	86:AT:52:C:H4'	1.90	0.86
52:S2:925:G:H1	52:S2:1017:U:H3	1.23	0.85
18:LM:15:VAL:HG22	18:LM:50:MET:HE1	1.58	0.85
52:S2:1543:U:O2'	69:SQ:43:GLU:OE1	1.92	0.85
52:S2:1289:U:H4'	63:SK:2:LEU:HD21	1.56	0.84
72:ST:85:ASN:HB3	72:ST:88:MET:HB2	1.59	0.84
28:LW:82:ILE:HG22	59:SG:131:ARG:HB2	1.60	0.84
51:Pt:50:U:H3	51:Pt:64:G:H1	1.26	0.84
65:SM:26:LEU:HA	65:SM:31:LEU:HD21	1.58	0.84
3:CF:358:ALA:N	86:AT:52:C:C3'	2.36	0.83
70:SR:32:LYS:HE2	70:SR:47:ARG:HH12	1.42	0.83
45:Ln:15:ARG:HG3	45:Ln:18:ARG:HH21	1.40	0.83
15:LI:14:ASN:O	15:LI:128:ARG:NH2	2.12	0.82
54:SB:144:LYS:HD3	54:SB:208:HIS:HB3	1.60	0.82
3:CF:429:MET:HE1	86:AT:53:G:N3	1.94	0.82
29:LX:151:ASN:HD22	87:CA:287:LYS:HD3	1.44	0.82
4:L5:2557:G:H1	4:L5:2570:U:H3	1.25	0.81
3:CF:358:ALA:HB3	86:AT:52:C:C1'	2.09	0.81
4:L5:2708:U:H5'	87:CA:263:ARG:HG2	1.62	0.81
4:L5:3717:A:H2'	4:L5:3718:A2M:H8	1.62	0.81
53:SA:118:GLU:HG2	55:SC:65:LYS:HE2	1.59	0.81
61:SI:87:ASN:HB3	61:SI:90:LEU:HD23	1.63	0.80
3:CF:293:GLU:HB2	86:AT:77:A:N3	1.96	0.80
3:CF:430:ARG:HD3	86:AT:65:G:H5'	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:2702:C:OP1	26:LU:101:ARG:NH2	2.15	0.80
4:L5:2611:A:H5'	4:L5:2688:G:H4'	1.65	0.79
52:S2:952:G:H21	67:SO:52:THR:HG21	1.47	0.79
66:SN:99:ARG:HH12	66:SN:143:SER:HB3	1.46	0.79
3:CF:259:ILE:HD13	86:AT:77:A:N6	1.97	0.79
4:L5:1972:G:N2	4:L5:1994:C:O2	2.14	0.79
23:LR:133:LYS:H	23:LR:137:ILE:HD11	1.47	0.79
27:LV:94:VAL:HG11	28:LW:20:ARG:HH21	1.46	0.79
78:SZ:62:VAL:HA	78:SZ:65:TYR:HE1	1.46	0.79
13:LG:205:THR:HG22	13:LG:206:GLN:H	1.47	0.78
3:CF:349:HIS:NE2	86:AT:54:G:H5'	1.98	0.78
4:L5:4546:A:N7	7:LA:215:ASN:ND2	2.31	0.78
85:Sg:31:ILE:HG12	85:Sg:45:LEU:HD21	1.63	0.78
60:SH:7:LYS:HE2	60:SH:10:LYS:HB3	1.65	0.78
53:SA:10:MET:HE2	53:SA:15:VAL:HG22	1.65	0.78
3:CF:100:LYS:HE2	86:AT:66:G:OP1	1.83	0.78
60:SH:154:ILE:HB	60:SH:185:VAL:HG22	1.65	0.78
61:SI:57:ALA:HB1	61:SI:60:LEU:HD21	1.66	0.78
82:Sd:3:HIS:ND1	82:Sd:5:GLN:OE1	2.17	0.78
81:Sc:44:ARG:NH1	81:Sc:61:SER:O	2.17	0.78
3:CF:356:GLY:O	86:AT:53:G:OP2	2.02	0.77
63:SK:14:LEU:HD22	63:SK:35:LEU:HD13	1.66	0.77
69:SQ:102:GLU:HA	69:SQ:105:LYS:HB3	1.65	0.77
67:SO:95:ILE:HB	67:SO:129:ILE:HG22	1.65	0.77
69:SQ:43:GLU:CG	69:SQ:44:PRO:HD3	2.13	0.77
58:SF:70:GLU:OE2	58:SF:86:LYS:NZ	2.18	0.77
59:SG:164:LYS:HB2	59:SG:167:LYS:HG2	1.67	0.77
52:S2:921:G:H2'	75:SW:28:ARG:NH1	2.00	0.76
57:SE:161:GLN:HG3	57:SE:170:THR:HB	1.67	0.76
4:L5:1402:C:O2	4:L5:1415:G:N2	2.13	0.76
52:S2:570:C:O2'	77:SY:34:THR:O	2.03	0.76
52:S2:346:C:H5''	57:SE:38:LEU:HD22	1.66	0.76
53:SA:77:ILE:HG22	53:SA:99:ILE:HB	1.68	0.76
78:SZ:68:ILE:HG23	78:SZ:109:TYR:HB2	1.68	0.76
60:SH:144:ILE:HD11	60:SH:152:ARG:HB3	1.67	0.76
50:Lt:16:ARG:HE	50:Lt:17:CYS:N	1.84	0.76
65:SM:79:VAL:HG11	65:SM:85:LEU:HB2	1.68	0.76
21:LP:23:ARG:HD3	21:LP:125:MET:HE1	1.67	0.76
86:AT:21:U:H5'	86:AT:49:C:H42	1.51	0.76
53:SA:99:ILE:HD11	53:SA:117:ARG:HH12	1.49	0.75
77:SY:56:PHE:HB2	77:SY:74:MET:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:3947:A:N1	4:L5:4068:U:O2'	2.20	0.75
57:SE:42:LEU:HD22	57:SE:46:ILE:HD11	1.67	0.75
58:SF:28:VAL:O	58:SF:42:LYS:NZ	2.19	0.75
4:L5:2351:OMC:HM22	9:LC:95:MET:HG3	1.68	0.75
35:Ld:19:GLU:OE2	35:Ld:92:ARG:NH1	2.20	0.75
4:L5:1402:C:N3	4:L5:1415:G:N1	2.28	0.75
4:L5:4242:U:H3	4:L5:4281:A:H2	1.35	0.74
85:Sg:107:ASP:HB2	85:Sg:125:ARG:HD2	1.68	0.74
66:SN:99:ARG:NH1	66:SN:143:SER:HB3	2.02	0.74
29:LX:80:PRO:HG2	29:LX:155:ILE:HG21	1.69	0.74
37:Lf:71:TRP:HB2	37:Lf:89:ARG:NH1	2.03	0.74
3:CF:358:ALA:N	86:AT:52:C:C4'	2.50	0.74
21:LP:109:VAL:HA	21:LP:112:LEU:HD13	1.70	0.74
52:S2:1433:C:H42	73:SU:92:HIS:HD2	1.36	0.74
53:SA:198:MET:HE3	70:SR:85:VAL:HG13	1.67	0.74
4:L5:1326:A2M:H2'	4:L5:1327:C:C6	2.24	0.73
4:L5:2601:A:N6	4:L5:2744:A:OP2	2.22	0.73
4:L5:3945:A:H2'	4:L5:3946:G:C8	2.24	0.73
3:CF:350:PRO:HB2	86:AT:55:U:OP1	1.89	0.73
4:L5:1996:C:H42	4:L5:2000:G:H22	1.35	0.73
4:L5:1095:A:H2	4:L5:1200:G:H1	1.32	0.72
48:Lr:26:SER:OG	48:Lr:28:GLU:OE1	2.06	0.72
52:S2:588:G:H4'	52:S2:589:G:H5'	1.70	0.72
3:CF:350:PRO:CB	86:AT:55:U:OP1	2.37	0.72
52:S2:1228:A:H2'	52:S2:1229:G:C8	2.24	0.72
57:SE:44:LEU:HD11	57:SE:72:ILE:HD11	1.71	0.72
8:LB:222:VAL:O	8:LB:343:ARG:NH1	2.23	0.72
42:Lk:35:LYS:HB3	42:Lk:42:LEU:HD21	1.71	0.72
63:SK:14:LEU:HD23	63:SK:21:MET:HE1	1.72	0.72
54:SB:224:GLU:HB3	54:SB:227:LYS:HE3	1.72	0.72
3:CF:358:ALA:H	86:AT:52:C:C2'	2.02	0.72
4:L5:513:U:N3	4:L5:516:C:OP2	2.23	0.72
30:LY:74:TYR:CE2	30:LY:77:LYS:HD3	2.25	0.72
52:S2:628:A:N6	52:S2:1500:G:O2'	2.22	0.72
65:SM:61:TYR:HD1	84:Sf:104:LYS:HZ1	1.37	0.72
4:L5:1996:C:H42	4:L5:2000:G:N2	1.88	0.72
52:S2:1756:C:N4	52:S2:1775:U:O4	2.23	0.72
4:L5:2324:C:O2'	36:Le:98:GLU:OE2	2.08	0.71
3:CF:356:GLY:O	86:AT:52:C:H5''	1.91	0.71
3:CF:356:GLY:C	86:AT:53:G:OP2	2.33	0.71
25:LT:119:ALA:HA	25:LT:122:LYS:HE3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:1230:C:OP1	71:SS:130:ARG:NH2	2.23	0.71
8:LB:300:LYS:HD2	8:LB:311:ASP:HA	1.72	0.71
19:LN:124:ASP:OD1	19:LN:125:SER:N	2.23	0.71
72:ST:65:TYR:HE1	72:ST:128:GLN:HG3	1.54	0.71
4:L5:1268:G:N7	33:Lb:111:ARG:NH2	2.39	0.71
52:S2:223:C:OP1	64:SL:20:LYS:NZ	2.24	0.71
52:S2:928:G:H1	52:S2:1013:U:H3	1.39	0.71
87:CA:75:ALA:HB2	87:CA:113:HIS:HB3	1.72	0.71
3:CF:358:ALA:N	86:AT:52:C:O2'	2.24	0.71
52:S2:1598:G:O2'	78:SZ:80:ARG:O	2.08	0.71
62:SJ:88:ASP:HB3	62:SJ:91:LYS:HB2	1.70	0.71
67:SO:113:GLN:OE1	79:Sa:46:GLU:N	2.24	0.71
82:Sd:3:HIS:CD2	82:Sd:6:LEU:HD22	2.25	0.71
67:SO:74:ALA:HB1	67:SO:115:ALA:HB2	1.71	0.71
85:Sg:247:TRP:HB3	85:Sg:258:ILE:HD11	1.71	0.71
4:L5:3937:C:H1'	19:LN:125:SER:HB3	1.72	0.71
50:Lt:111:ASN:ND2	50:Lt:161:GLU:OE2	2.23	0.71
4:L5:1480:C:O2'	4:L5:1482:G:OP2	2.08	0.70
15:LI:36:LEU:HD21	15:LI:69:ARG:HH11	1.56	0.70
59:SG:116:LYS:HE3	59:SG:125:THR:HG21	1.71	0.70
85:Sg:87:LEU:HB2	85:Sg:101:PHE:HB2	1.72	0.70
4:L5:2520:C:O2	4:L5:2640:G:N2	2.23	0.70
18:LM:104:MET:HG3	18:LM:108:ASP:HB2	1.73	0.70
4:L5:500:G:OP1	4:L5:504:G:N2	2.24	0.70
52:S2:860:G:H21	75:SW:107:SER:HB2	1.55	0.70
66:SN:26:LEU:HD21	66:SN:60:VAL:HG12	1.72	0.70
4:L5:2739:C:O2	7:LA:188:LYS:NZ	2.24	0.70
87:CA:154:LEU:HD11	87:CA:332:ARG:HD2	1.72	0.70
4:L5:1503:A:H62	22:LQ:87:THR:HG21	1.57	0.70
61:SI:57:ALA:HB2	61:SI:183:GLY:HA2	1.74	0.70
4:L5:2758:G:O2'	4:L5:2765:A:N3	2.23	0.70
30:LY:2:LYS:HD2	30:LY:7:VAL:HG13	1.73	0.70
45:Ln:1:MET:HG3	52:S2:1706:G:H5'	1.74	0.70
87:CA:27:ILE:HD11	87:CA:59:GLU:HG3	1.74	0.70
7:LA:29:LEU:O	7:LA:123:ARG:NH1	2.24	0.70
52:S2:94:G:HO2'	52:S2:508:A:HO2'	1.39	0.70
52:S2:1424:G:H2'	52:S2:1425:G:H8	1.57	0.70
55:SC:193:VAL:HG11	55:SC:240:THR:HG22	1.72	0.69
75:SW:111:MET:HE3	75:SW:116:ALA:HA	1.74	0.69
52:S2:1512:C:H5''	82:Sd:8:TRP:HZ3	1.57	0.69
52:S2:1648:G:H5''	69:SQ:125:ARG:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:SZ:62:VAL:HA	78:SZ:65:TYR:CE1	2.27	0.69
4:L5:4992:G:H2'	4:L5:4993:G:C8	2.27	0.69
52:S2:1729:U:H3	52:S2:1805:G:H1	1.40	0.69
86:AT:61:A:OP1	86:AT:63:C:N4	2.25	0.69
29:LX:151:ASN:ND2	87:CA:287:LYS:HD3	2.06	0.69
58:SF:135:ARG:O	58:SF:203:ASN:ND2	2.26	0.69
58:SF:102:LEU:HD21	78:SZ:110:THR:HB	1.74	0.69
52:S2:377:G:H5'	61:SI:98:LYS:HB3	1.73	0.69
3:CF:426:VAL:HB	3:CF:434:ALA:HB3	1.74	0.69
4:L5:1408:G:O2'	4:L5:1411:C:N3	2.26	0.69
4:L5:2486:G:O6	4:L5:2493:G:O6	2.11	0.69
4:L5:2554:U:O2	4:L5:2764:A:N7	2.26	0.69
17:LL:64:VAL:HA	17:LL:67:HIS:CD2	2.28	0.69
55:SC:210:PRO:HB3	55:SC:240:THR:HG21	1.74	0.69
58:SF:68:ILE:HD11	58:SF:116:ILE:HG13	1.73	0.69
69:SQ:31:LEU:HD11	69:SQ:33:LYS:HE3	1.75	0.69
71:SS:25:LYS:HD3	71:SS:27:ALA:H	1.58	0.69
79:Sa:7:ASN:ND2	79:Sa:10:ARG:O	2.26	0.69
4:L5:3701:OMC:H5	4:L5:3748:A:H62	1.40	0.69
61:SI:70:GLU:OE2	64:SL:21:LYS:NZ	2.25	0.69
4:L5:3641:U:OP2	4:L5:3646:A:N6	2.24	0.69
52:S2:1562:C:H2'	52:S2:1563:G:H8	1.56	0.69
58:SF:30:ILE:HG23	58:SF:117:ILE:HD11	1.73	0.69
75:SW:37:PHE:HE1	75:SW:103:VAL:HB	1.58	0.69
3:CF:371:LYS:NZ	86:AT:52:C:H5''	2.09	0.68
4:L5:1435:G:N2	4:L5:1449:C:O2	2.17	0.68
27:LV:111:GLU:HG3	27:LV:131:ARG:HD3	1.74	0.68
52:S2:928:G:H2'	52:S2:929:G:C8	2.29	0.68
55:SC:102:LEU:HD23	55:SC:130:ILE:HD12	1.74	0.68
56:SD:138:VAL:HG22	56:SD:184:ILE:HG12	1.74	0.68
54:SB:144:LYS:HB2	54:SB:206:PRO:HB2	1.75	0.68
65:SM:56:CYS:SG	65:SM:61:TYR:HD2	2.16	0.68
11:LE:243:THR:HG22	11:LE:245:GLN:H	1.59	0.68
85:Sg:163:PRO:HB2	85:Sg:179:LEU:HB2	1.75	0.68
9:LC:218:ILE:HA	9:LC:229:LEU:HD22	1.74	0.68
34:Lc:28:VAL:HG11	34:Lc:37:MET:HG3	1.76	0.68
52:S2:1491:G:O2'	73:SU:70:CYS:SG	2.51	0.68
53:SA:80:ARG:NH2	53:SA:165:ASN:O	2.25	0.68
65:SM:31:LEU:HD12	65:SM:89:VAL:HG23	1.75	0.68
4:L5:1994:C:H2'	4:L5:1995:G:C8	2.29	0.68
56:SD:208:VAL:HG21	70:SR:12:ALA:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:SR:76:GLU:HA	70:SR:79:GLU:HG2	1.73	0.68
3:CF:247:ARG:NH2	3:CF:332:ASP:O	2.27	0.68
4:L5:4103:C:H1'	4:L5:4106:G:H1	1.59	0.68
7:LA:107:MET:HB3	7:LA:111:THR:HG21	1.75	0.68
52:S2:373:G:H4'	64:SL:85:THR:HG21	1.76	0.68
73:SU:67:LYS:HG3	73:SU:78:ASP:HB2	1.76	0.68
4:L5:1270:A:H8	4:L5:2106:G:H21	1.40	0.67
4:L5:3717:A:H2'	4:L5:3718:A2M:C8	2.24	0.67
8:LB:107:ALA:HB2	8:LB:201:LEU:HD22	1.75	0.67
53:SA:163:CYS:SG	53:SA:164:ASN:N	2.67	0.67
71:SS:45:LEU:HD13	71:SS:50:ILE:HD11	1.75	0.67
52:S2:694:G:H2'	52:S2:695:C:O4'	1.94	0.67
52:S2:1285:G:N1	65:SM:57:ASP:OD1	2.25	0.67
4:L5:1994:C:H2'	4:L5:1995:G:H8	1.57	0.67
52:S2:1423:C:H5	69:SQ:4:LYS:HE3	1.59	0.67
56:SD:196:GLY:HA3	56:SD:201:LYS:HG2	1.75	0.67
4:L5:3680:U:OP1	7:LA:54:ARG:NH2	2.28	0.67
28:LW:79:GLN:HB3	28:LW:87:LEU:HD11	1.75	0.67
57:SE:80:ILE:HG23	57:SE:81:THR:HG23	1.77	0.67
81:Sc:62:GLU:OE1	81:Sc:62:GLU:N	2.27	0.67
3:CF:192:PRO:O	3:CF:200:ASN:ND2	2.27	0.67
3:CF:358:ALA:HB2	86:AT:52:C:C4'	2.01	0.67
4:L5:387:G:HO2'	4:L5:412:G:H1	1.42	0.67
52:S2:690:G:H3'	52:S2:691:G:H21	1.58	0.67
52:S2:996:A:H2'	52:S2:997:A:C8	2.30	0.67
7:LA:114:CYS:HB3	7:LA:165:VAL:HB	1.76	0.67
72:ST:129:ARG:HH11	72:ST:133:ARG:HH21	1.41	0.67
76:SX:28:LYS:HD2	76:SX:32:LEU:HD22	1.77	0.67
4:L5:4594:U:H2'	4:L5:4595:G:H8	1.59	0.67
73:SU:49:LYS:HE3	73:SU:92:HIS:HB2	1.75	0.67
52:S2:508:A:H3'	52:S2:509:OMG:H8	1.58	0.67
54:SB:126:ASP:OD1	54:SB:136:ARG:HG2	1.94	0.67
70:SR:16:ILE:HD11	70:SR:54:VAL:HG21	1.76	0.66
74:SV:35:ASN:HB3	74:SV:50:PHE:HD2	1.60	0.66
50:Lt:19:GLY:HA2	50:Lt:48:LYS:HZ3	1.60	0.66
85:Sg:175:LYS:HB3	85:Sg:184:LEU:HD11	1.78	0.66
4:L5:1414:C:H2'	4:L5:1415:G:H8	1.61	0.66
18:LM:30:VAL:HG11	24:LS:150:ILE:HD13	1.78	0.66
52:S2:70:G:O6	59:SG:170:ARG:NH2	2.28	0.66
52:S2:165:G:OP2	52:S2:165:G:N2	2.27	0.66
54:SB:108:ASP:OD1	54:SB:109:LYS:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:SI:141:ARG:HD3	61:SI:145:ILE:HG21	1.78	0.66
4:L5:1188:C:H2'	4:L5:1189:G:H8	1.61	0.66
4:L5:2458:C:H5''	19:LN:67:ARG:HD2	1.77	0.66
4:L5:3910:C:H2'	4:L5:3911:C:C6	2.31	0.66
4:L5:4537:C:H2'	4:L5:4538:G:H8	1.59	0.66
4:L5:4910:G:N2	20:LO:106:ASP:O	2.28	0.66
59:SG:37:ALA:HA	59:SG:49:VAL:HA	1.77	0.66
64:SL:78:THR:HG22	64:SL:79:LYS:HG3	1.78	0.66
4:L5:4251:A:H5''	16:LJ:108:GLY:HA3	1.78	0.66
52:S2:380:G:N3	61:SI:5:ARG:NH1	2.43	0.66
52:S2:1424:G:H2'	52:S2:1425:G:C8	2.31	0.66
56:SD:164:VAL:O	56:SD:168:VAL:HG22	1.95	0.66
60:SH:69:LEU:HD12	60:SH:96:ALA:HB2	1.77	0.66
62:SJ:119:LEU:HD13	62:SJ:135:ILE:HD11	1.76	0.66
6:L8:96:C:H5''	39:Lh:66:LYS:HG2	1.78	0.66
49:Ls:159:GLN:NE2	49:Ls:161:ILE:O	2.27	0.66
58:SF:123:GLU:HG2	58:SF:140:ASP:HA	1.78	0.66
78:SZ:58:LEU:HD12	78:SZ:62:VAL:HG21	1.78	0.66
4:L5:1996:C:N4	4:L5:2000:G:H22	1.93	0.66
7:LA:147:ARG:HH21	7:LA:155:LYS:HG3	1.61	0.66
10:LD:120:GLU:O	10:LD:248:ARG:NH1	2.24	0.66
51:Pt:9:A:O2'	51:Pt:10:G:N7	2.28	0.66
52:S2:1756:C:OP2	52:S2:1757:G:N2	2.27	0.66
52:S2:1764:G:H5'	52:S2:1765:C:H5''	1.78	0.66
58:SF:49:LEU:HD12	58:SF:50:PRO:HD2	1.78	0.66
4:L5:663:G:H2'	4:L5:664:G:C8	2.31	0.66
39:Lh:43:LYS:HE2	87:CA:241:GLY:HA3	1.78	0.66
52:S2:1120:U:H5'	80:Sb:72:ARG:HH12	1.61	0.66
4:L5:1396:G:N7	32:La:110:LYS:NZ	2.41	0.65
8:LB:90:VAL:HG23	8:LB:163:ILE:HD11	1.77	0.65
10:LD:208:MET:HB2	10:LD:233:PRO:HG3	1.77	0.65
4:L5:3944:G:H1	4:L5:4069:U:H3	1.45	0.65
4:L5:4725:C:OP1	8:LB:103:LYS:NZ	2.29	0.65
52:S2:496:C:OP1	57:SE:49:ARG:NH2	2.29	0.65
53:SA:118:GLU:OE1	53:SA:118:GLU:N	2.29	0.65
4:L5:261:G:H2'	4:L5:262:G:C8	2.32	0.65
4:L5:665:C:H4'	4:L5:666:G:H5'	1.77	0.65
4:L5:2745:A:H2'	4:L5:2746:A:H8	1.61	0.65
23:LR:174:GLU:HA	23:LR:177:LEU:HB2	1.78	0.65
26:LU:18:VAL:HG13	26:LU:73:THR:HG23	1.78	0.65
26:LU:97:ARG:HH11	26:LU:97:ARG:HB3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:4525:C:OP1	8:LB:246:ARG:NH2	2.29	0.65
16:LJ:146:ARG:HG2	16:LJ:147:ARG:HG3	1.78	0.65
49:Ls:18:ILE:HG12	49:Ls:68:HIS:ND1	2.11	0.65
52:S2:851:C:H5''	52:S2:852:G:H5'	1.77	0.65
62:SJ:38:ARG:N	62:SJ:42:GLU:OE2	2.28	0.65
2:CI:49:ILE:HG13	2:CI:50:MET:H	1.61	0.65
4:L5:1435:G:N1	4:L5:1449:C:N3	2.30	0.65
52:S2:528:A:H2'	52:S2:529:A:C8	2.32	0.65
4:L5:4076:G:OP1	13:LG:73:ARG:NE	2.29	0.65
4:L5:4897:G:N2	4:L5:4924:C:O2	2.30	0.65
28:LW:105:ARG:NH2	59:SG:148:SER:OG	2.29	0.65
52:S2:837:A:H61	77:SY:9:THR:HG22	1.61	0.65
58:SF:123:GLU:OE2	81:Sc:63:ARG:NH1	2.29	0.65
82:Sd:38:MET:HE1	82:Sd:50:ILE:HD11	1.79	0.65
8:LB:17:LEU:O	8:LB:19:ARG:N	2.30	0.65
16:LJ:94:LEU:HD11	16:LJ:107:PHE:HB3	1.79	0.65
80:Sb:10:PRO:HG2	80:Sb:15:GLU:OE2	1.97	0.65
4:L5:3736:A:H2'	4:L5:3737:A:C8	2.31	0.65
52:S2:506:G:OP1	77:SY:108:LYS:NZ	2.29	0.65
52:S2:1757:G:O6	52:S2:1758:G:N2	2.29	0.65
23:LR:168:GLU:HA	23:LR:171:LYS:HE3	1.78	0.65
3:CF:7:HIS:ND1	3:CF:306:ASP:OD1	2.29	0.64
4:L5:2815:A2M:H2'	4:L5:2816:G:C8	2.32	0.64
7:LA:54:ARG:HG2	7:LA:56:ALA:H	1.62	0.64
52:S2:1228:A:H2'	52:S2:1229:G:H8	1.61	0.64
52:S2:1396:A:N7	52:S2:1449:G:O6	2.30	0.64
54:SB:107:ARG:NH1	67:SO:133:THR:O	2.30	0.64
58:SF:71:ARG:NH2	58:SF:148:ASN:OD1	2.28	0.64
59:SG:141:ILE:HD11	59:SG:153:VAL:HG13	1.79	0.64
4:L5:3664:G:H2'	4:L5:3665:G:H8	1.63	0.64
17:LL:178:ALA:N	32:La:134:GLU:OE2	2.29	0.64
21:LP:39:MET:HG2	21:LP:43:LYS:HD3	1.78	0.64
33:Lb:116:LEU:HG	33:Lb:117:ARG:HH21	1.61	0.64
57:SE:42:LEU:HD12	57:SE:101:LEU:HD21	1.77	0.64
4:L5:1187:G:OP2	4:L5:1187:G:N2	2.25	0.64
4:L5:4741:C:H3'	4:L5:4900:C:H42	1.62	0.64
52:S2:126:G:O6	59:SG:196:LYS:NZ	2.30	0.64
52:S2:981:A:H2'	52:S2:982:G:C8	2.31	0.64
52:S2:1801:A:H2'	52:S2:1802:C:C6	2.33	0.64
4:L5:109:G:OP2	17:LL:74:ARG:NH2	2.30	0.64
4:L5:2438:A:OP1	29:LX:106:LYS:NZ	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:2695:A:OP1	42:Lk:35:LYS:NZ	2.29	0.64
4:L5:4894:A:H5''	4:L5:4896:G:H5'	1.80	0.64
52:S2:379:C:H5''	61:SI:56:ARG:HH12	1.61	0.64
9:LC:134:PRO:HG3	9:LC:150:LEU:HD12	1.80	0.64
10:LD:111:ASN:ND2	10:LD:116:ASP:OD2	2.30	0.64
62:SJ:88:ASP:OD1	62:SJ:89:GLU:N	2.31	0.64
4:L5:1942:A:H2'	4:L5:1943:A:C8	2.32	0.64
4:L5:4220:6MZ:OP2	25:LT:2:THR:OG1	2.10	0.64
20:LO:61:ARG:HA	20:LO:70:PRO:HD2	1.79	0.64
26:LU:88:LYS:HD2	26:LU:97:ARG:HH21	1.62	0.64
55:SC:65:LYS:HD2	55:SC:273:LEU:HD13	1.78	0.64
55:SC:200:ARG:O	62:SJ:54:ARG:NH2	2.30	0.64
57:SE:125:LYS:HB2	57:SE:226:PHE:CD1	2.31	0.64
4:L5:2491:C:H2'	4:L5:2492:C:C6	2.33	0.64
34:Lc:22:MET:O	34:Lc:23:LYS:HG3	1.98	0.64
3:CF:427:ARG:HH21	3:CF:430:ARG:HA	1.61	0.64
29:LX:156:ILE:HG13	87:CA:291:MET:HA	1.79	0.64
50:Lt:106:PHE:HD2	50:Lt:109:ILE:HD11	1.62	0.64
52:S2:681:PSU:H4'	76:SX:9:THR:HG22	1.78	0.64
52:S2:1301:A:H4'	82:Sd:3:HIS:NE2	2.13	0.64
68:SP:20:VAL:HG11	68:SP:36:LEU:HD21	1.79	0.64
3:CF:353:ILE:HB	3:CF:394:LEU:HB3	1.80	0.64
4:L5:685:C:H5'	11:LE:101:ASN:ND2	2.12	0.64
52:S2:888:U:H4'	52:S2:889:U:H5'	1.79	0.64
52:S2:1467:C:H5''	70:SR:1:MET:HA	1.79	0.64
69:SQ:10:VAL:HG22	69:SQ:25:CYS:HB3	1.79	0.64
4:L5:137:G:H2'	4:L5:138:G:H8	1.62	0.63
4:L5:1961:G:N2	4:L5:2024:G:O2'	2.30	0.63
21:LP:128:ARG:NH2	94:LP:301:HOH:O	2.30	0.63
52:S2:201:C:H3'	52:S2:202:G:H21	1.63	0.63
69:SQ:58:LEU:HD22	69:SQ:108:ILE:HG13	1.80	0.63
85:Sg:191:HIS:ND1	85:Sg:213:ASP:OD2	2.20	0.63
4:L5:968:C:H5'	11:LE:110:ARG:HE	1.63	0.63
4:L5:4075:U:OP1	13:LG:249:ARG:NH1	2.31	0.63
52:S2:323:C:H2'	52:S2:327:G:H1	1.61	0.63
55:SC:196:ILE:HB	55:SC:223:TYR:HB2	1.78	0.63
82:Sd:6:LEU:HA	82:Sd:9:SER:HB3	1.80	0.63
53:SA:49:ILE:HD13	53:SA:163:CYS:HA	1.79	0.63
4:L5:4274:A:H2'	4:L5:4275:G:C8	2.33	0.63
52:S2:563:G:N7	62:SJ:172:ARG:NH2	2.46	0.63
66:SN:103:GLU:HA	66:SN:106:ARG:HH11	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:1591:U:OP2	4:L5:2856:C:O2'	2.16	0.63
4:L5:2017:A:O2'	4:L5:2018:C:O5'	2.16	0.63
7:LA:112:ILE:HD11	47:Lp:79:VAL:HG22	1.79	0.63
11:LE:225:PRO:O	11:LE:226:ARG:HD3	1.99	0.63
11:LE:225:PRO:HG2	11:LE:226:ARG:HH11	1.63	0.63
14:LH:106:GLN:HB2	14:LH:111:LEU:HB3	1.81	0.63
50:Lt:114:ARG:HH21	50:Lt:117:ARG:HH11	1.46	0.63
67:SO:101:GLY:HA3	67:SO:134:PRO:HD2	1.81	0.63
68:SP:18:ARG:NH1	71:SS:88:LYS:O	2.32	0.63
4:L5:1100:U:O3'	4:L5:1167:C:N4	2.32	0.63
4:L5:308:G:OP2	4:L5:308:G:N2	2.29	0.63
50:Lt:82:ILE:HD11	50:Lt:106:PHE:HE2	1.63	0.63
52:S2:1373:C:O2'	70:SR:10:LYS:NZ	2.31	0.63
64:SL:7:GLU:OE1	64:SL:7:GLU:N	2.32	0.63
4:L5:3954:A:H1'	4:L5:4058:U:H5'	1.79	0.63
52:S2:1550:G:O2'	52:S2:1558:C:O2	2.15	0.63
4:L5:1824:G:H5''	25:LT:35:LYS:HE2	1.81	0.63
4:L5:2773:G:H5'	42:Lk:17:ARG:HH21	1.64	0.63
4:L5:3680:U:H5''	7:LA:54:ARG:HH21	1.64	0.63
8:LB:219:VAL:HG11	8:LB:337:VAL:HG13	1.80	0.63
17:LL:63:THR:HG22	17:LL:64:VAL:H	1.63	0.63
52:S2:1550:G:H3'	52:S2:1579:A:H61	1.63	0.63
60:SH:87:PHE:HB3	60:SH:90:LYS:HG3	1.80	0.63
73:SU:66:ARG:HH22	73:SU:75:LYS:HD3	1.64	0.63
86:AT:16:C:O2'	86:AT:19:G:OP1	2.16	0.63
87:CA:18:VAL:HG12	87:CA:22:LYS:HE2	1.81	0.63
3:CF:267:VAL:O	3:CF:305:GLY:N	2.26	0.62
4:L5:1339:U:H2'	4:L5:1340:OMC:C6	2.33	0.62
11:LE:264:ILE:HD11	11:LE:267:LEU:HD22	1.81	0.62
37:Lf:71:TRP:HB2	37:Lf:89:ARG:HH11	1.64	0.62
68:SP:81:ARG:NH2	68:SP:117:GLY:O	2.32	0.62
4:L5:4279:A:H5'	4:L5:4281:A:H1'	1.80	0.62
14:LH:17:ASP:OD1	14:LH:28:LYS:HB3	1.99	0.62
52:S2:121:OMU:HM23	57:SE:144:ALA:HB3	1.81	0.62
52:S2:1850:MA6:H8	52:S2:1850:MA6:O5'	1.99	0.62
3:CF:198:GLY:HA2	3:CF:201:MET:HE1	1.81	0.62
3:CF:350:PRO:HB2	86:AT:55:U:P	2.40	0.62
4:L5:1095:A:C2	4:L5:1200:G:N1	2.62	0.62
31:LZ:46:ILE:HD11	31:LZ:49:TYR:CD1	2.34	0.62
52:S2:1261:C:O2	82:Sd:10:HIS:NE2	2.29	0.62
55:SC:94:ILE:O	55:SC:98:LEU:N	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CF:175:SER:OG	3:CF:179:LYS:NZ	2.32	0.62
4:L5:2092:G:O2'	4:L5:2262:G:N2	2.32	0.62
4:L5:3823:G:OP2	4:L5:3823:G:N2	2.26	0.62
4:L5:4088:C:OP1	7:LA:37:ARG:NH1	2.32	0.62
7:LA:116:LEU:HB3	7:LA:126:LEU:HB2	1.81	0.62
25:LT:102:ARG:HD3	25:LT:106:LEU:HD13	1.81	0.62
4:L5:4106:G:H3'	4:L5:4107:G:H8	1.62	0.62
4:L5:4113:U:H3'	4:L5:4114:C:H4'	1.81	0.62
59:SG:135:PRO:HG2	59:SG:141:ILE:HG22	1.81	0.62
4:L5:1973:G:HO2'	50:Lt:78:SER:HG	1.46	0.62
4:L5:4274:A:H2'	4:L5:4275:G:H8	1.65	0.62
52:S2:818:A:OP1	62:SJ:80:ARG:NH2	2.32	0.62
64:SL:22:ARG:HH21	64:SL:31:GLU:HG2	1.64	0.62
69:SQ:43:GLU:HG3	69:SQ:44:PRO:CD	2.26	0.62
4:L5:3732:A:H2'	4:L5:3733:A:H8	1.65	0.62
52:S2:1109:C:C4	70:SR:126:MET:HE2	2.35	0.62
87:CA:27:ILE:HG13	87:CA:30:ARG:HE	1.63	0.62
4:L5:1662:C:H2'	4:L5:1663:C:C6	2.35	0.62
17:LL:140:SER:HA	17:LL:143:GLU:HG2	1.81	0.62
52:S2:1752:C:N3	52:S2:1779:G:N1	2.34	0.62
62:SJ:108:ARG:HA	62:SJ:113:GLN:HE21	1.64	0.62
66:SN:29:THR:OG1	66:SN:31:ASP:OD1	2.17	0.62
8:LB:220:ILE:HG23	8:LB:278:THR:HG22	1.82	0.62
26:LU:63:ILE:HD13	26:LU:72:VAL:HG22	1.82	0.62
28:LW:105:ARG:NH1	59:SG:149:LYS:O	2.33	0.62
49:Ls:61:MET:HG2	49:Ls:88:PHE:HE2	1.65	0.62
52:S2:639:C:H2'	52:S2:640:A:H8	1.64	0.62
52:S2:1829:G:H1'	52:S2:1850:MA6:H2	1.82	0.62
81:Sc:20:ARG:HD3	81:Sc:28:THR:HG22	1.81	0.62
85:Sg:11:LEU:HB2	85:Sg:307:VAL:HG13	1.82	0.62
3:CF:371:LYS:NZ	86:AT:52:C:C5'	2.63	0.61
4:L5:184:U:O2'	4:L5:189:G:O4'	2.18	0.61
4:L5:2362:U:H2'	4:L5:2363:A2M:H8	1.82	0.61
8:LB:63:PRO:HD2	8:LB:357:ARG:HH21	1.64	0.61
52:S2:837:A:N6	77:SY:9:THR:HG22	2.15	0.61
52:S2:1673:U:H5''	69:SQ:78:VAL:HG12	1.82	0.61
60:SH:43:LEU:HD12	60:SH:72:PHE:CE2	2.35	0.61
4:L5:1976:G:H21	50:Lt:139:VAL:HG12	1.65	0.61
4:L5:2744:A:H2'	4:L5:2745:A:C8	2.35	0.61
4:L5:4281:A:H2'	4:L5:4282:A:H2'	1.80	0.61
54:SB:136:ARG:HH21	54:SB:218:LEU:HD11	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:SJ:131:ARG:NH1	62:SJ:143:ASN:O	2.32	0.61
71:SS:3:LEU:H	71:SS:3:LEU:HD23	1.64	0.61
14:LH:44:GLU:HG3	18:LM:2:VAL:HG23	1.80	0.61
35:Ld:33:ILE:HD11	35:Ld:45:ALA:HA	1.82	0.61
52:S2:495:U:OP1	57:SE:49:ARG:NH1	2.34	0.61
52:S2:889:U:OP2	52:S2:896:U:N3	2.33	0.61
65:SM:83:LYS:HE2	65:SM:103:VAL:HG13	1.83	0.61
69:SQ:58:LEU:HD11	69:SQ:112:LEU:HD11	1.81	0.61
77:SY:55:ILE:HD12	77:SY:75:ILE:HG22	1.81	0.61
4:L5:4260:U:H2'	4:L5:4261:C:C6	2.36	0.61
52:S2:103:A:H5'	61:SI:12:ARG:NH1	2.15	0.61
52:S2:885:U:O2	52:S2:901:G:O6	2.18	0.61
52:S2:1373:C:OP1	70:SR:7:LYS:HG3	1.99	0.61
57:SE:57:THR:OG1	57:SE:59:ASP:OD1	2.18	0.61
57:SE:64:ILE:HG13	57:SE:70:ILE:HD11	1.82	0.61
59:SG:85:ARG:NH2	77:SY:118:ARG:HG3	2.15	0.61
78:SZ:41:ARG:NH2	94:SZ:201:HOH:O	2.32	0.61
85:Sg:188:HIS:HD1	85:Sg:219:TRP:CG	2.18	0.61
87:CA:12:ILE:HG12	87:CA:324:LEU:HD11	1.82	0.61
3:CF:429:MET:SD	86:AT:54:G:H1'	2.41	0.61
3:CF:430:ARG:HG2	86:AT:64:G:O2'	2.01	0.61
4:L5:300:A:H2'	4:L5:301:G:H8	1.66	0.61
4:L5:730:G:C5	12:LF:73:ARG:HD3	2.36	0.61
4:L5:4431:PSU:OP2	15:LI:3:ARG:NH2	2.27	0.61
24:LS:27:LEU:HB3	25:LT:148:PRO:HB3	1.83	0.61
35:Ld:90:ARG:HD3	35:Ld:102:LEU:HD13	1.82	0.61
65:SM:96:ARG:NH2	65:SM:100:PRO:O	2.32	0.61
67:SO:59:GLY:HA2	67:SO:68:GLU:HG2	1.81	0.61
3:CF:69:ARG:HE	3:CF:71:ILE:HD12	1.65	0.61
4:L5:267:G:H2'	4:L5:268:G:H8	1.65	0.61
52:S2:640:A:H2'	52:S2:641:A:C8	2.36	0.61
57:SE:125:LYS:HB2	57:SE:226:PHE:CE1	2.35	0.61
62:SJ:103:GLU:OE1	62:SJ:103:GLU:N	2.30	0.61
3:CF:240:ARG:HB3	3:CF:304:PRO:HG2	1.82	0.61
4:L5:2484:A:H62	4:L5:2494:U:H3	1.48	0.61
52:S2:525:A:O3'	83:Se:31:ARG:NH2	2.33	0.61
77:SY:41:ARG:HG3	77:SY:55:ILE:HB	1.82	0.61
3:CF:429:MET:CE	86:AT:53:G:N3	2.64	0.61
4:L5:4069:U:H2'	4:L5:4070:U:C6	2.36	0.61
4:L5:4537:C:H2'	4:L5:4538:G:C8	2.35	0.61
13:LG:94:GLN:HG3	13:LG:218:LEU:HD21	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LX:87:MET:HB2	87:CA:259:MET:CE	2.29	0.61
61:SI:151:GLU:HA	61:SI:154:LYS:NZ	2.16	0.61
4:L5:3811:G:O2'	4:L5:3814:U:OP2	2.16	0.61
4:L5:3945:A:H2'	4:L5:3946:G:H8	1.66	0.61
6:L8:19:C:H2'	6:L8:20:A:C8	2.36	0.61
52:S2:1541:G:OP1	72:ST:56:ARG:HD2	2.01	0.61
59:SG:57:ASP:OD1	59:SG:58:LYS:N	2.34	0.61
59:SG:218:LYS:HA	59:SG:221:LYS:HE3	1.82	0.61
4:L5:4472:G:O2'	44:Lm:100:TYR:O	2.19	0.61
52:S2:1438:A:H2'	52:S2:1439:A:C8	2.36	0.61
4:L5:74:G:H5'	17:LL:59:VAL:HG13	1.82	0.60
4:L5:1857:C:H2'	4:L5:1858:A:H8	1.65	0.60
4:L5:4165:C:OP1	13:LG:53:ARG:NH2	2.34	0.60
7:LA:101:VAL:HG22	7:LA:165:VAL:HG22	1.82	0.60
52:S2:433:A:H5''	61:SI:22:HIS:HB3	1.81	0.60
52:S2:919:A:H4'	75:SW:57:ARG:HD2	1.83	0.60
54:SB:136:ARG:HG3	54:SB:218:LEU:HD21	1.83	0.60
72:ST:18:LEU:HD22	72:ST:58:ALA:HA	1.83	0.60
4:L5:4163:U:H5'	4:L5:4164:C:H5''	1.84	0.60
8:LB:47:LEU:HG	8:LB:181:MET:HE2	1.83	0.60
71:SS:48:ALA:O	71:SS:66:ARG:NH1	2.34	0.60
4:L5:1333:A:H2'	4:L5:1334:A:C8	2.36	0.60
4:L5:2745:A:H2'	4:L5:2746:A:C8	2.36	0.60
14:LH:93:ARG:HG2	14:LH:182:SER:HB3	1.83	0.60
52:S2:1285:G:N2	65:SM:58:GLU:HB2	2.16	0.60
58:SF:106:GLU:N	58:SF:106:GLU:OE1	2.34	0.60
58:SF:133:THR:HG22	58:SF:134:VAL:HG23	1.84	0.60
77:SY:12:PHE:HZ	77:SY:21:LYS:HD3	1.67	0.60
3:CF:349:HIS:NE2	86:AT:54:G:C5'	2.64	0.60
6:L8:90:C:H1'	30:LY:24:HIS:HB3	1.84	0.60
52:S2:1644:C:H4'	69:SQ:140:ARG:HB2	1.83	0.60
54:SB:127:VAL:HG23	54:SB:177:GLN:HG3	1.84	0.60
57:SE:233:LYS:HD2	57:SE:234:PRO:HD2	1.84	0.60
61:SI:31:ARG:NH1	94:SI:303:HOH:O	2.34	0.60
64:SL:57:ASP:OD1	64:SL:84:ARG:NH1	2.35	0.60
4:L5:4139:G:H21	4:L5:4140:C:H41	1.47	0.60
4:L5:4618:OMG:H5'	27:LV:15:ARG:HB2	1.83	0.60
52:S2:84:A:N3	52:S2:150:A:O2'	2.31	0.60
52:S2:921:G:OP2	80:Sb:26:GLN:NE2	2.32	0.60
54:SB:52:THR:HG23	54:SB:57:ILE:HA	1.84	0.60
54:SB:186:ASN:HA	54:SB:189:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SF:131:ALA:HA	58:SF:136:ARG:HG2	1.83	0.60
4:L5:1328:G:O2'	4:L5:2349:A:OP1	2.19	0.60
4:L5:2020:U:H2'	4:L5:2021:G:H8	1.67	0.60
52:S2:940:U:H3	52:S2:1002:U:H3	1.46	0.60
74:SV:15:ARG:HH21	74:SV:24:ILE:HG21	1.67	0.60
4:L5:71:C:H1'	17:LL:62:PRO:O	2.02	0.60
4:L5:1281:G:N1	11:LE:128:HIS:HB2	2.17	0.60
4:L5:1703:C:H2'	4:L5:1704:C:O4'	2.01	0.60
52:S2:120:U:H2'	52:S2:121:OMU:H6	1.83	0.60
52:S2:888:U:HO2'	52:S2:898:U:H3	1.50	0.60
54:SB:122:GLU:HG2	54:SB:140:VAL:HG12	1.84	0.60
4:L5:2613:C:OP1	38:Lg:24:ARG:NH2	2.34	0.60
4:L5:3910:C:H2'	4:L5:3911:C:H6	1.66	0.60
52:S2:448:A:H5''	61:SI:25:ARG:HA	1.84	0.60
53:SA:198:MET:HE1	53:SA:200:ASP:HB2	1.84	0.60
3:CF:256:ILE:HD12	86:AT:76:C:H1'	1.84	0.60
4:L5:1942:A:H2'	4:L5:1943:A:H8	1.67	0.60
19:LN:193:ARG:NH2	94:LN:401:HOH:O	2.35	0.60
4:L5:1258:G:H2'	4:L5:1259:G:C8	2.37	0.59
12:LF:59:LYS:HA	12:LF:62:ARG:HE	1.67	0.59
13:LG:209:SER:HA	13:LG:212:LYS:HG3	1.83	0.59
23:LR:31:GLU:OE1	23:LR:31:GLU:N	2.33	0.59
52:S2:145:G:H2'	52:S2:146:G:C8	2.37	0.59
52:S2:1091:C:HO2'	75:SW:2:VAL:N	2.00	0.59
56:SD:99:ILE:HG23	56:SD:173:ARG:HH21	1.66	0.59
59:SG:5:ILE:HD13	59:SG:16:ILE:HG12	1.83	0.59
4:L5:88:A:N7	22:LQ:173:LYS:NZ	2.49	0.59
4:L5:4967:A:H2'	4:L5:4968:A:H8	1.67	0.59
27:LV:60:MET:HE1	27:LV:108:ASN:HA	1.82	0.59
51:Pt:23:C:H2'	51:Pt:24:A:C8	2.37	0.59
52:S2:1476:A:H4'	52:S2:1477:U:H5''	1.84	0.59
52:S2:1536:G:H2'	52:S2:1537:A:C8	2.37	0.59
3:CF:141:TYR:O	3:CF:423:ARG:NH1	2.34	0.59
3:CF:178:ILE:HB	3:CF:183:TYR:HB2	1.84	0.59
4:L5:1982:G:N2	4:L5:2009:A:O2'	2.32	0.59
4:L5:4987:C:OP2	8:LB:116:ARG:NH2	2.35	0.59
35:Ld:22:THR:HG23	35:Ld:122:VAL:HG13	1.84	0.59
38:Lg:69:LYS:HG3	38:Lg:73:HIS:CD2	2.36	0.59
53:SA:22:GLY:O	53:SA:24:HIS:ND1	2.35	0.59
59:SG:157:VAL:HG11	59:SG:176:ILE:HG21	1.84	0.59
82:Sd:17:GLY:O	82:Sd:27:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:1307:A:H2'	4:L5:1308:C:C6	2.37	0.59
20:LO:34:VAL:HG22	20:LO:103:LYS:HB2	1.84	0.59
23:LR:44:LEU:HD22	23:LR:49:LEU:HD12	1.84	0.59
52:S2:332:G:O6	59:SG:186:GLN:NE2	2.35	0.59
52:S2:874:G:H2'	52:S2:875:A:H8	1.67	0.59
52:S2:1407:U:H2'	52:S2:1408:U:C6	2.38	0.59
54:SB:103:MET:HB3	54:SB:215:VAL:HG12	1.83	0.59
86:AT:18:G:O2'	86:AT:19:G:N7	2.35	0.59
8:LB:57:VAL:HG22	8:LB:73:VAL:HG12	1.83	0.59
52:S2:106:C:H2'	52:S2:107:A:H8	1.68	0.59
55:SC:191:VAL:HG11	55:SC:236:PHE:HA	1.84	0.59
60:SH:31:GLU:HA	60:SH:37:LYS:HD2	1.83	0.59
64:SL:103:GLU:HG3	76:SX:11:ARG:HB2	1.84	0.59
54:SB:84:PHE:HB3	54:SB:86:LEU:HD23	1.84	0.59
81:Sc:13:ARG:NH1	81:Sc:53:GLY:O	2.36	0.59
87:CA:11:THR:HG23	87:CA:13:ALA:H	1.68	0.59
4:L5:178:C:N4	4:L5:179:G:O6	2.35	0.59
4:L5:325:U:H2'	4:L5:326:C:C6	2.37	0.59
4:L5:4068:U:H2'	4:L5:4069:U:C6	2.37	0.59
4:L5:4162:C:H5	13:LG:73:ARG:HH12	1.50	0.59
4:L5:4591:U:H2'	4:L5:4592:C:C6	2.38	0.59
7:LA:229:ALA:HB3	7:LA:234:LYS:HB3	1.85	0.59
53:SA:164:ASN:OD1	53:SA:165:ASN:N	2.36	0.59
13:LG:38:ASN:ND2	13:LG:43:GLN:OE1	2.36	0.59
29:LX:87:MET:CB	87:CA:259:MET:HE1	2.29	0.59
32:La:30:GLY:O	32:La:40:HIS:NE2	2.34	0.59
52:S2:1277:C:H2'	52:S2:1278:A:H8	1.67	0.59
69:SQ:72:VAL:HG21	69:SQ:84:ILE:HG12	1.85	0.59
77:SY:11:LYS:HB2	77:SY:24:VAL:HG12	1.84	0.59
4:L5:4098:A:H62	4:L5:4099:G:H21	1.49	0.59
4:L5:4239:A:H2'	4:L5:4240:G:C8	2.37	0.59
52:S2:1115:U:O2'	52:S2:1117:C:OP2	2.19	0.59
4:L5:4934:A:H2'	4:L5:4935:C:H6	1.67	0.59
50:Lt:22:VAL:HA	50:Lt:48:LYS:HE3	1.83	0.59
52:S2:316:G:OP2	59:SG:183:ARG:NH2	2.34	0.59
52:S2:1629:C:H5''	71:SS:83:PHE:CE1	2.38	0.59
57:SE:250:GLU:OE1	57:SE:250:GLU:N	2.36	0.59
76:SX:123:VAL:HG12	76:SX:124:LYS:HG3	1.85	0.59
4:L5:711:A:H2'	4:L5:712:C:C6	2.38	0.58
4:L5:1503:A:H4'	4:L5:1504:G:H5'	1.85	0.58
31:LZ:46:ILE:HA	31:LZ:70:SER:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:383:G:H21	64:SL:133:PRO:HG2	1.68	0.58
52:S2:639:C:H2'	52:S2:640:A:C8	2.38	0.58
57:SE:7:LYS:NZ	94:SE:303:HOH:O	2.36	0.58
86:AT:51:U:O2	86:AT:65:G:N2	2.30	0.58
4:L5:1444:G:H22	4:L5:2104:G:H21	1.50	0.58
4:L5:4967:A:H2'	4:L5:4968:A:C8	2.38	0.58
4:L5:1695:U:O2'	4:L5:1719:A:N3	2.35	0.58
4:L5:1996:C:O3'	49:Ls:44:ARG:NH1	2.36	0.58
4:L5:2516:G:O2'	38:Lg:62:LYS:NZ	2.36	0.58
29:LX:151:ASN:HD22	87:CA:287:LYS:CD	2.14	0.58
31:LZ:9:LYS:NZ	31:LZ:83:THR:O	2.32	0.58
52:S2:616:A:OP1	76:SX:68:LYS:NZ	2.35	0.58
3:CF:43:GLU:HB3	3:CF:55:LYS:HG3	1.86	0.58
4:L5:4340:U:O2	90:L5:5261:SPD:N10	2.37	0.58
25:LT:14:MET:HE1	25:LT:55:LYS:HB2	1.84	0.58
28:LW:106:GLU:HA	28:LW:109:ILE:HD12	1.86	0.58
37:Lf:15:LYS:HB3	37:Lf:25:THR:HG23	1.85	0.58
46:Lo:53:LYS:NZ	94:Lo:303:HOH:O	2.36	0.58
52:S2:1010:G:H2'	52:S2:1011:A:H8	1.69	0.58
52:S2:1536:G:H2'	52:S2:1537:A:H8	1.69	0.58
53:SA:190:SER:OG	53:SA:192:GLU:OE1	2.19	0.58
54:SB:90:ASP:HB2	54:SB:223:PHE:HZ	1.68	0.58
60:SH:191:GLU:O	60:SH:193:GLN:NE2	2.32	0.58
64:SL:111:VAL:HG12	64:SL:140:PHE:HB2	1.85	0.58
4:L5:1686:C:O2'	33:Lb:18:ARG:NH2	2.35	0.58
4:L5:3908:A:N7	4:L5:4449:A:N6	2.52	0.58
4:L5:4934:A:H2'	4:L5:4935:C:C6	2.38	0.58
9:LC:156:ASP:OD2	9:LC:255:SER:OG	2.22	0.58
52:S2:51:U:H2'	52:S2:52:G:H8	1.66	0.58
54:SB:90:ASP:OD1	54:SB:91:VAL:N	2.36	0.58
56:SD:143:ARG:HG3	56:SD:144:GLY:H	1.68	0.58
65:SM:52:LEU:HD13	65:SM:65:VAL:HG21	1.85	0.58
65:SM:54:SER:HA	65:SM:78:LYS:HE3	1.84	0.58
3:CF:93:PRO:HD2	3:CF:102:MET:HG3	1.85	0.58
3:CF:259:ILE:HD13	86:AT:77:A:C6	2.38	0.58
4:L5:2000:G:O2'	4:L5:2001:G:N7	2.37	0.58
4:L5:2352:U:OP1	9:LC:78:ARG:NH2	2.36	0.58
4:L5:4620:OMU:OP2	4:L5:4670:C:N4	2.30	0.58
4:L5:4946:U:HO2'	37:Lf:2:SER:N	2.02	0.58
52:S2:84:A:H5''	77:SY:124:ASN:HD22	1.66	0.58
57:SE:18:TRP:HH2	57:SE:31:PRO:HD3	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:LZ:47:ASP:N	31:LZ:69:LYS:O	2.35	0.58
52:S2:17:C:O2'	52:S2:1194:A:N1	2.31	0.58
52:S2:420:G:OP1	75:SW:88:LYS:NZ	2.35	0.58
59:SG:22:ARG:N	59:SG:22:ARG:HD2	2.18	0.58
4:L5:455:C:O2'	4:L5:456:C:H5'	2.03	0.58
4:L5:4088:C:H2'	4:L5:4089:G:C8	2.39	0.58
4:L5:4098:A:N7	4:L5:4099:G:H1'	2.19	0.58
7:LA:133:TYR:HB3	7:LA:168:VAL:HG12	1.83	0.58
15:LI:152:LEU:HB3	15:LI:165:ILE:HD12	1.86	0.58
24:LS:83:ARG:HG3	24:LS:125:GLN:HB3	1.86	0.58
52:S2:159:A2M:O5'	52:S2:159:A2M:H8	2.04	0.58
52:S2:543:C:H3'	52:S2:544:G:H8	1.68	0.58
52:S2:798:G:H4'	60:SH:113:LYS:HE3	1.85	0.58
52:S2:1556:A:N3	52:S2:1556:A:H2'	2.18	0.58
52:S2:1845:A:H2'	52:S2:1846:G:C8	2.39	0.58
87:CA:21:TYR:HE1	87:CA:117:PHE:HB3	1.68	0.58
4:L5:982:U:H2'	4:L5:983:C:C6	2.38	0.58
13:LG:157:ILE:HA	13:LG:201:THR:HG22	1.86	0.58
52:S2:455:A:H2'	52:S2:456:C:H6	1.68	0.58
52:S2:1203:G:H2'	52:S2:1204:A:C8	2.39	0.58
52:S2:1588:A:H2'	52:S2:1589:A:C8	2.39	0.58
52:S2:1801:A:H2'	52:S2:1802:C:H6	1.68	0.58
57:SE:127:ARG:HD2	57:SE:142:HIS:HA	1.86	0.58
59:SG:85:ARG:HH21	77:SY:118:ARG:HG3	1.67	0.58
3:CF:85:TYR:OH	3:CF:232:LEU:O	2.14	0.58
4:L5:268:G:H2'	4:L5:269:G:H8	1.67	0.58
4:L5:3868:G:H22	4:L5:3900:G:H1'	1.68	0.58
52:S2:1217:A:H2'	52:S2:1218:C:C6	2.38	0.58
52:S2:1605:G:OP1	72:ST:84:ARG:NH2	2.37	0.58
53:SA:85:ARG:NH1	53:SA:203:PHE:O	2.37	0.58
73:SU:61:LEU:HB2	73:SU:82:MET:HB3	1.85	0.58
3:CF:176:THR:HA	3:CF:179:LYS:HD2	1.86	0.57
4:L5:1899:G:O2'	36:Le:57:ASN:OD1	2.22	0.57
4:L5:3917:A:H2'	4:L5:3918:G:H8	1.69	0.57
52:S2:115:U:H2'	52:S2:116:OMU:C6	2.33	0.57
52:S2:557:U:H2'	52:S2:558:G:C8	2.39	0.57
53:SA:5:LEU:O	53:SA:9:GLN:HG2	2.04	0.57
56:SD:106:ARG:HG3	56:SD:175:VAL:HG22	1.85	0.57
62:SJ:124:HIS:CD2	83:Se:35:ARG:HD2	2.39	0.57
73:SU:107:GLU:OE1	73:SU:107:GLU:N	2.37	0.57
4:L5:1095:A:N1	4:L5:1200:G:O6	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:4457:PSU:HI1'	8:LB:252:ALA:HB3	1.87	0.57
8:LB:122:TRP:O	8:LB:127:LYS:NZ	2.35	0.57
11:LE:203:ILE:O	11:LE:206:VAL:HG22	2.04	0.57
12:LF:105:VAL:HG13	12:LF:136:VAL:HG12	1.86	0.57
53:SA:198:MET:HG2	53:SA:199:PRO:HD2	1.87	0.57
60:SH:76:GLN:HG3	60:SH:94:PHE:HD2	1.69	0.57
4:L5:1933:G:H2'	4:L5:1934:A:C8	2.40	0.57
4:L5:4088:C:H2'	4:L5:4089:G:H8	1.69	0.57
8:LB:59:GLU:HB2	8:LB:366:LYS:HE3	1.85	0.57
31:LZ:12:LEU:HB2	31:LZ:81:MET:HB3	1.87	0.57
52:S2:496:C:H5'	57:SE:29:PRO:HA	1.86	0.57
52:S2:695:C:N4	52:S2:736:C:O2'	2.36	0.57
59:SG:44:GLU:HB2	59:SG:119:LYS:HZ1	1.69	0.57
69:SQ:58:LEU:HD21	69:SQ:112:LEU:HG	1.86	0.57
77:SY:27:VAL:HG22	77:SY:69:THR:HB	1.85	0.57
4:L5:454:U:H2'	4:L5:455:C:C6	2.38	0.57
4:L5:1241:C:H5'	11:LE:72:LYS:HZ1	1.69	0.57
4:L5:1645:C:H2'	4:L5:1646:A:C8	2.38	0.57
6:L8:75:OMG:OP2	30:LY:74:TYR:OH	2.21	0.57
6:L8:141:C:H2'	6:L8:142:U:C6	2.39	0.57
26:LU:97:ARG:HB3	26:LU:97:ARG:NH1	2.19	0.57
60:SH:31:GLU:HG3	60:SH:32:MET:SD	2.44	0.57
4:L5:1867:A:H2'	4:L5:1868:A:C8	2.40	0.57
4:L5:4069:U:H2'	4:L5:4070:U:H6	1.68	0.57
25:LT:115:LYS:HE2	25:LT:128:LEU:HD13	1.87	0.57
46:Lo:33:LEU:HA	46:Lo:38:LYS:HG2	1.86	0.57
52:S2:316:G:H5''	59:SG:183:ARG:HH12	1.69	0.57
52:S2:1372:U:OP1	52:S2:1385:G:N2	2.34	0.57
52:S2:1527:C:OP1	69:SQ:142:GLN:NE2	2.38	0.57
56:SD:68:GLU:O	56:SD:72:VAL:HG23	2.04	0.57
70:SR:93:GLN:HB2	70:SR:96:ILE:HD13	1.85	0.57
81:Sc:44:ARG:HH21	81:Sc:63:ARG:HH11	1.51	0.57
1:CD:2:PRO:HG2	1:CD:14:THR:HG22	1.85	0.57
4:L5:4978:G:OP1	8:LB:271:GLN:NE2	2.28	0.57
9:LC:266:THR:HG22	9:LC:267:TRP:H	1.68	0.57
52:S2:191:A:OP1	61:SI:141:ARG:NH2	2.38	0.57
52:S2:795:A:H2'	52:S2:796:G:C8	2.40	0.57
52:S2:1736:G:H2'	52:S2:1737:G:H8	1.70	0.57
54:SB:88:THR:HA	54:SB:98:THR:HA	1.87	0.57
64:SL:7:GLU:HG2	64:SL:9:ALA:H	1.68	0.57
65:SM:23:LYS:HZ3	65:SM:26:LEU:HB3	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:SS:61:GLU:OE1	71:SS:61:GLU:N	2.32	0.57
77:SY:106:GLN:OE1	77:SY:106:GLN:N	2.33	0.57
85:Sg:68:ASP:HB3	85:Sg:111:VAL:HG12	1.85	0.57
4:L5:62:A:N3	4:L5:77:U:O2'	2.31	0.57
4:L5:158:A:H5''	4:L5:159:C:H2'	1.86	0.57
4:L5:2539:C:H2'	4:L5:2540:C:C6	2.40	0.57
19:LN:5:LYS:HG3	40:Li:40:VAL:HG11	1.87	0.57
29:LX:156:ILE:HG13	87:CA:290:ARG:O	2.04	0.57
52:S2:1658:G:OP2	52:S2:1660:C:N4	2.37	0.57
85:Sg:178:ASN:HB2	85:Sg:185:LYS:HD3	1.85	0.57
85:Sg:207:CYS:HB3	85:Sg:221:LEU:HD21	1.85	0.57
4:L5:444:G:H22	4:L5:1303:A:H2	1.53	0.57
8:LB:161:ARG:HG2	8:LB:184:GLN:HA	1.87	0.57
23:LR:176:ARG:HH22	52:S2:910:G:P	2.28	0.57
49:Ls:127:ASN:HA	49:Ls:153:GLU:HG2	1.87	0.57
55:SC:94:ILE:HG13	55:SC:95:ASP:N	2.19	0.57
84:Sf:103:LEU:HB2	84:Sf:105:TYR:CD1	2.39	0.57
4:L5:1188:C:H2'	4:L5:1189:G:C8	2.40	0.57
4:L5:1509:C:H5''	32:La:2:PRO:HD3	1.87	0.57
4:L5:4220:6MZ:O5'	4:L5:4220:6MZ:H8	2.05	0.57
11:LE:87:LYS:HG3	11:LE:88:VAL:HG23	1.86	0.57
12:LF:171:ASP:OD1	12:LF:172:ASN:N	2.38	0.57
14:LH:93:ARG:HD2	14:LH:143:GLU:HG2	1.86	0.57
22:LQ:70:MET:HE1	22:LQ:137:VAL:HB	1.86	0.57
28:LW:96:GLN:HB2	28:LW:101:ARG:HE	1.69	0.57
52:S2:928:G:N2	80:Sb:68:GLY:O	2.34	0.57
70:SR:45:LYS:HA	70:SR:48:ASN:HD21	1.70	0.57
4:L5:1646:A:O2'	41:Lj:49:TRP:O	2.19	0.57
4:L5:4426:C:C2'	4:L5:4427:G:H5'	2.35	0.57
8:LB:90:VAL:HG22	8:LB:104:THR:HG23	1.86	0.57
11:LE:223:ARG:NH2	11:LE:238:GLU:HG3	2.19	0.57
16:LJ:166:PHE:HD2	16:LJ:174:ILE:HD11	1.69	0.57
18:LM:136:LEU:O	18:LM:137:LYS:HE2	2.04	0.57
21:LP:54:GLN:HA	21:LP:83:TRP:CD1	2.40	0.57
52:S2:453:C:O2'	59:SG:92:ARG:O	2.17	0.57
55:SC:70:VAL:HG11	55:SC:93:ILE:HG12	1.86	0.57
55:SC:176:LYS:O	55:SC:200:ARG:NH2	2.37	0.57
71:SS:25:LYS:HE2	71:SS:52:LEU:O	2.05	0.57
1:CD:32:LYS:HE2	31:LZ:128:LYS:HE3	1.86	0.56
4:L5:1179:U:H3'	4:L5:1180:C:H5''	1.86	0.56
4:L5:1270:A:O2'	4:L5:1439:C:O2'	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:3732:A:H2'	4:L5:3733:A:C8	2.40	0.56
8:LB:196:TRP:O	8:LB:200:ARG:HG2	2.05	0.56
11:LE:91:THR:HG22	11:LE:108:LYS:HB3	1.86	0.56
15:LI:73:ASN:HB2	15:LI:87:MET:HE1	1.86	0.56
20:LO:54:TYR:CD1	20:LO:145:VAL:HG21	2.39	0.56
45:Ln:15:ARG:HG3	45:Ln:18:ARG:NH2	2.15	0.56
52:S2:367:U:H4'	52:S2:371:A:C8	2.39	0.56
57:SE:159:THR:HB	57:SE:173:ILE:HB	1.85	0.56
60:SH:144:ILE:CD1	60:SH:154:ILE:HG13	2.32	0.56
69:SQ:98:LYS:HA	85:Sg:57:ARG:HH22	1.70	0.56
4:L5:4103:C:H2'	4:L5:4105:A:C4	2.40	0.56
4:L5:4188:U:H2'	4:L5:4189:U:C6	2.40	0.56
4:L5:4426:C:H2'	4:L5:4427:G:H5'	1.86	0.56
52:S2:390:C:H4'	64:SL:8:ARG:HH21	1.70	0.56
67:SO:97:LEU:HD12	79:Sa:44:ILE:HD11	1.87	0.56
3:CF:255:LYS:HE2	3:CF:317:VAL:HG23	1.88	0.56
4:L5:512:U:OP2	17:LL:165:LYS:NZ	2.29	0.56
4:L5:654:C:H2'	4:L5:655:C:C6	2.40	0.56
4:L5:730:G:C4	12:LF:73:ARG:HD3	2.40	0.56
4:L5:1332:C:H2'	4:L5:1333:A:H8	1.71	0.56
4:L5:1802:A:N3	25:LT:130:ARG:NH2	2.44	0.56
4:L5:2318:G:N2	4:L5:2321:G:OP2	2.36	0.56
4:L5:3611:A:H2	4:L5:5016:A:H8	1.52	0.56
27:LV:92:ASP:OD1	27:LV:94:VAL:HG22	2.05	0.56
27:LV:94:VAL:HG11	28:LW:20:ARG:NH2	2.19	0.56
32:La:63:LEU:HD21	32:La:65:ARG:HE	1.70	0.56
42:Lk:51:GLU:N	42:Lk:51:GLU:OE1	2.35	0.56
48:Lr:28:GLU:OE2	48:Lr:31:ASN:ND2	2.35	0.56
52:S2:455:A:H2'	52:S2:456:C:C6	2.39	0.56
52:S2:944:A:H5''	67:SO:134:PRO:HB3	1.87	0.56
52:S2:1010:G:H2'	52:S2:1011:A:C8	2.40	0.56
52:S2:1235:G:H21	68:SP:135:ALA:HB2	1.70	0.56
53:SA:77:ILE:HD13	53:SA:122:LEU:HD11	1.87	0.56
59:SG:162:LEU:HD12	59:SG:170:ARG:HH21	1.70	0.56
66:SN:99:ARG:HE	66:SN:115:LEU:HD21	1.70	0.56
66:SN:99:ARG:NE	66:SN:115:LEU:HD21	2.20	0.56
86:AT:18:G:H1	86:AT:56:U:H1'	1.70	0.56
87:CA:333:ILE:HG13	87:CA:334:THR:HG23	1.86	0.56
28:LW:90:ILE:HG13	28:LW:91:MET:N	2.21	0.56
51:Pt:23:C:H2'	51:Pt:24:A:H8	1.70	0.56
57:SE:246:LEU:HD11	57:SE:251:GLU:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:SP:57:LEU:HD11	68:SP:83:MET:HE2	1.87	0.56
4:L5:10:A:H2'	4:L5:11:G:C8	2.40	0.56
4:L5:4260:U:H2'	4:L5:4261:C:H6	1.70	0.56
16:LJ:48:PRO:HB2	16:LJ:70:VAL:HG22	1.88	0.56
16:LJ:95:ARG:N	16:LJ:95:ARG:HD2	2.20	0.56
29:LX:156:ILE:HD11	87:CA:291:MET:CA	2.35	0.56
52:S2:656:G:N2	52:S2:663:C:H5''	2.20	0.56
53:SA:42:LYS:HD3	53:SA:44:ASP:HB3	1.86	0.56
77:SY:6:THR:HG23	77:SY:28:LEU:HD13	1.87	0.56
85:Sg:173:LEU:HD11	85:Sg:187:ASN:HB3	1.86	0.56
4:L5:351:C:OP2	9:LC:197:ARG:NH1	2.31	0.56
4:L5:1700:G:H2'	4:L5:1703:C:H42	1.70	0.56
4:L5:2407:G:O6	43:LI:2:SER:N	2.38	0.56
4:L5:4717:A:OP2	8:LB:30:LYS:NZ	2.26	0.56
61:SI:81:VAL:HG22	61:SI:102:VAL:HG12	1.87	0.56
62:SJ:18:ARG:HB2	62:SJ:21:GLU:OE2	2.05	0.56
85:Sg:184:LEU:HD21	85:Sg:187:ASN:OD1	2.05	0.56
4:L5:2709:C:H5'	23:LR:43:LYS:HD2	1.88	0.56
4:L5:4913:G:H4'	4:L5:4914:C:O5'	2.05	0.56
27:LV:111:GLU:OE1	27:LV:111:GLU:N	2.38	0.56
39:Lh:19:LYS:NZ	39:Lh:23:ASP:OD1	2.39	0.56
44:Lm:109:ASN:ND2	44:Lm:117:HIS:O	2.37	0.56
56:SD:134:CYS:SG	56:SD:135:GLU:N	2.79	0.56
69:SQ:110:ASP:OD1	69:SQ:111:ILE:N	2.38	0.56
86:AT:63:C:H2'	86:AT:64:G:H8	1.71	0.56
8:LB:47:LEU:HB2	8:LB:84:MET:CE	2.36	0.56
32:La:72:THR:HG22	32:La:110:LYS:HB3	1.86	0.56
52:S2:327:G:H5''	52:S2:328:U:C2	2.40	0.56
52:S2:1305:C:H2'	52:S2:1306:U:C6	2.40	0.56
72:ST:143:LYS:O	72:ST:144:LYS:HE2	2.05	0.56
85:Sg:20:GLN:NE2	85:Sg:68:ASP:OD1	2.35	0.56
4:L5:138:G:H2'	4:L5:139:G:H8	1.70	0.56
4:L5:3641:U:H5	4:L5:3646:A:N7	2.03	0.56
7:LA:36:GLU:HG3	7:LA:91:GLY:HA2	1.88	0.56
11:LE:222:LEU:HB2	11:LE:237:LYS:HE2	1.88	0.56
57:SE:36:HIS:NE2	57:SE:143:ASP:OD1	2.39	0.56
59:SG:44:GLU:HB2	59:SG:119:LYS:NZ	2.21	0.56
4:L5:2580:U:O2'	31:LZ:79:HIS:ND1	2.36	0.56
4:L5:4927:G:H5''	4:L5:4928:C:C5	2.41	0.56
8:LB:288:GLY:HA3	8:LB:330:PHE:CE2	2.41	0.56
12:LF:50:ILE:HD12	12:LF:186:CYS:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LI:48:LEU:HD12	15:LI:142:LEU:HD12	1.87	0.56
20:LO:126:VAL:HG13	20:LO:127:VAL:HG13	1.88	0.56
52:S2:1740:C:OP1	61:SI:44:HIS:ND1	2.37	0.56
54:SB:30:TRP:CZ2	54:SB:48:LEU:HD23	2.41	0.56
57:SE:104:ASP:HB3	57:SE:110:ALA:HB2	1.88	0.56
62:SJ:169:ARG:HH12	62:SJ:175:ARG:NE	2.04	0.56
80:Sb:80:ARG:HH11	80:Sb:80:ARG:HG3	1.69	0.56
85:Sg:241:PHE:CE2	85:Sg:248:LEU:HD12	2.40	0.56
87:CA:205:PRO:HB2	87:CA:210:LYS:HG3	1.87	0.56
4:L5:1705:G:H2'	4:L5:1706:A:O4'	2.06	0.55
4:L5:1857:C:H2'	4:L5:1858:A:C8	2.40	0.55
4:L5:4093:G:H3'	4:L5:4094:G:H8	1.70	0.55
7:LA:115:CYS:SG	7:LA:124:GLY:HA3	2.46	0.55
23:LR:133:LYS:N	23:LR:137:ILE:HD11	2.19	0.55
33:Lb:55:LYS:HA	33:Lb:58:GLN:HE21	1.70	0.55
37:Lf:106:TYR:HB2	37:Lf:107:PRO:HD3	1.88	0.55
39:Lh:106:LYS:NZ	94:Lh:201:HOH:O	2.29	0.55
43:LI:12:PHE:CE2	43:LI:51:LEU:HD22	2.41	0.55
52:S2:116:OMU:O5'	52:S2:116:OMU:H6	2.06	0.55
52:S2:207:G:H3'	52:S2:208:G:H8	1.71	0.55
52:S2:1189:A:H2'	52:S2:1190:A:H8	1.71	0.55
52:S2:1419:C:H2'	52:S2:1420:G:H2'	1.88	0.55
52:S2:1542:C:OP1	72:ST:62:ARG:NE	2.36	0.55
52:S2:1705:C:H2'	52:S2:1706:G:C8	2.41	0.55
77:SY:7:ILE:HD12	77:SY:27:VAL:HG12	1.88	0.55
3:CF:178:ILE:HA	3:CF:181:ILE:HB	1.88	0.55
4:L5:1617:G:H1'	4:L5:2513:A:N6	2.21	0.55
4:L5:1683:PSU:H2'	4:L5:1684:A:C8	2.41	0.55
4:L5:3654:G:O2'	4:L5:3693:U:OP1	2.22	0.55
4:L5:4459:U:H2'	4:L5:4460:U:C6	2.40	0.55
23:LR:105:LEU:HD22	23:LR:135:LYS:HG3	1.87	0.55
49:Ls:61:MET:HG2	49:Ls:88:PHE:CE2	2.40	0.55
52:S2:334:C:OP2	59:SG:190:ARG:NH2	2.39	0.55
52:S2:674:C:H2'	52:S2:675:U:C6	2.41	0.55
77:SY:21:LYS:HB2	77:SY:75:ILE:HD11	1.88	0.55
85:Sg:77:PHE:HB3	85:Sg:89:LEU:HD21	1.89	0.55
4:L5:691:C:H2'	4:L5:692:A:C8	2.42	0.55
4:L5:3911:C:H2'	4:L5:3912:U:H6	1.70	0.55
4:L5:3932:U:H2'	4:L5:3933:G:H8	1.71	0.55
9:LC:317:ASN:HD22	9:LC:320:LYS:HD3	1.71	0.55
52:S2:1580:A:H5'	73:SU:56:MET:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:1679:A:H2'	58:SF:60:ARG:HD2	1.87	0.55
54:SB:171:ILE:HD11	54:SB:197:ILE:HA	1.88	0.55
56:SD:72:VAL:HG21	63:SK:70:TYR:HE1	1.72	0.55
3:CF:283:VAL:HG23	3:CF:285:VAL:HG22	1.88	0.55
4:L5:99:A:H2'	4:L5:100:C:O2	2.07	0.55
4:L5:2640:G:H2'	4:L5:2641:A:C8	2.42	0.55
4:L5:4100:C:OP2	4:L5:4101:C:N4	2.39	0.55
31:LZ:57:MET:HG2	31:LZ:61:LYS:HD3	1.87	0.55
52:S2:1101:U:OP1	54:SB:151:ARG:HG3	2.06	0.55
56:SD:141:LYS:HE2	56:SD:179:GLN:HB3	1.87	0.55
87:CA:181:PRO:HA	87:CA:230:VAL:HA	1.88	0.55
4:L5:1461:C:H2'	4:L5:1462:A:C8	2.41	0.55
52:S2:629:A:O2'	52:S2:631:U:OP1	2.24	0.55
52:S2:1307:U:O2'	84:Sf:135:HIS:ND1	2.34	0.55
52:S2:1581:C:H5'	52:S2:1582:C:H5	1.70	0.55
61:SI:133:GLU:HA	61:SI:136:ILE:HG12	1.89	0.55
4:L5:153:G:H2'	4:L5:154:G:H8	1.72	0.55
30:LY:60:GLY:O	30:LY:63:LYS:HG3	2.06	0.55
52:S2:17:C:H2'	52:S2:18:C:C6	2.42	0.55
57:SE:88:ASP:OD1	57:SE:122:LYS:NZ	2.38	0.55
60:SH:143:ARG:HB3	75:SW:51:GLU:OE2	2.06	0.55
4:L5:387:G:O2'	4:L5:412:G:N1	2.32	0.55
4:L5:2611:A:H2'	4:L5:2612:G:C8	2.42	0.55
4:L5:2899:C:OP1	23:LR:108:ARG:NH2	2.34	0.55
4:L5:3594:C:O2	4:L5:3597:G:N2	2.39	0.55
4:L5:3861:A:H2'	4:L5:3862:A:H8	1.71	0.55
89:L5:5292:SPM:N14	20:LO:91:LYS:O	2.40	0.55
9:LC:154:VAL:HG11	9:LC:174:LEU:HD11	1.88	0.55
14:LH:107:GLU:N	14:LH:107:GLU:OE1	2.38	0.55
19:LN:143:ARG:HD2	39:Lh:95:LEU:HD23	1.88	0.55
57:SE:89:VAL:HG11	57:SE:119:ALA:HB1	1.88	0.55
74:SV:7:GLU:OE1	74:SV:7:GLU:N	2.36	0.55
3:CF:259:ILE:HG21	86:AT:77:A:N6	2.21	0.55
4:L5:1283:G:N1	4:L5:2076:G:OP1	2.29	0.55
4:L5:1378:C:H4'	4:L5:1379:C:H5'	1.89	0.55
4:L5:2590:G:H2'	4:L5:2754:G:N2	2.22	0.55
18:LM:38:VAL:HG21	18:LM:50:MET:HB3	1.89	0.55
46:Lo:24:THR:HA	46:Lo:93:LEU:HD21	1.88	0.55
52:S2:672:A:C8	89:S2:1929:SPM:H82	2.42	0.55
52:S2:1238:U:O2	52:S2:1242:U:H5	1.90	0.55
71:SS:5:ILE:N	78:SZ:50:PHE:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:ST:129:ARG:HD2	72:ST:133:ARG:NH2	2.22	0.55
74:SV:17:CYS:HB2	74:SV:56:CYS:HB3	1.89	0.55
74:SV:43:THR:HG23	74:SV:45:ARG:HB2	1.89	0.55
76:SX:71:ARG:NH1	76:SX:82:THR:OG1	2.40	0.55
87:CA:142[A]:VAL:HG13	87:CA:143:ILE:HD12	1.87	0.55
4:L5:1351:G:P	9:LC:33:ARG:HH21	2.30	0.55
4:L5:3633:C:OP1	89:L5:5291:SPM:N10	2.40	0.55
4:L5:4600:G:H4'	4:L5:4601:U:O5'	2.06	0.55
9:LC:315:LYS:HD2	12:LF:168:ALA:HB1	1.89	0.55
41:Lj:2:THR:HG22	41:Lj:4:GLY:H	1.71	0.55
52:S2:16:G:H2'	52:S2:17:C:C6	2.41	0.55
52:S2:323:C:H4'	52:S2:324:C:H5	1.72	0.55
52:S2:853:C:N3	94:S2:2021:HOH:O	2.33	0.55
52:S2:1405:A:H2'	52:S2:1406:G:O4'	2.07	0.55
53:SA:77:ILE:HD11	53:SA:124:VAL:HG22	1.88	0.55
73:SU:33:GLU:OE2	73:SU:87:ARG:NE	2.39	0.55
4:L5:519:C:H1'	4:L5:643:C:C2	2.41	0.55
9:LC:73:VAL:HB	9:LC:78:ARG:HH12	1.72	0.55
20:LO:194:GLU:O	20:LO:198:THR:HG23	2.07	0.55
31:LZ:41:ALA:HB2	31:LZ:77:TYR:HE1	1.71	0.55
68:SP:28:MET:HG2	68:SP:32:GLN:HG2	1.89	0.55
1:CD:16:ARG:HB2	4:L5:4119:C:H41	1.71	0.54
4:L5:1279:A:OP1	11:LE:131:LYS:NZ	2.39	0.54
4:L5:1327:C:H2'	4:L5:1328:G:C8	2.42	0.54
4:L5:1461:C:H2'	4:L5:1462:A:H8	1.71	0.54
4:L5:2815:A2M:H2'	4:L5:2816:G:H8	1.72	0.54
4:L5:3736:A:H2'	4:L5:3737:A:H8	1.72	0.54
4:L5:4584:A:H2'	4:L5:4585:U:O4'	2.08	0.54
25:LT:43:LYS:O	25:LT:58:HIS:ND1	2.40	0.54
52:S2:115:U:H2'	52:S2:116:OMU:H6	1.88	0.54
60:SH:140:VAL:HG12	66:SN:19:ARG:HD3	1.87	0.54
82:Sd:3:HIS:CE1	82:Sd:5:GLN:HB2	2.42	0.54
3:CF:259:ILE:HD13	86:AT:77:A:H62	1.67	0.54
4:L5:3923:A:H2'	4:L5:3924:C:C6	2.43	0.54
4:L5:4095:G:H2'	4:L5:4096:C:C6	2.43	0.54
52:S2:1736:G:H2'	52:S2:1737:G:C8	2.41	0.54
60:SH:37:LYS:HE2	60:SH:40:LEU:HD13	1.89	0.54
70:SR:87:GLU:OE1	70:SR:87:GLU:N	2.41	0.54
3:CF:5:LYS:HB3	3:CF:86:TYR:N	2.22	0.54
4:L5:10:A:H2'	4:L5:11:G:H8	1.72	0.54
4:L5:1875:C:H2'	4:L5:1876:U:C6	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LC:10:VAL:O	9:LC:18:SER:OG	2.21	0.54
49:Ls:43:ILE:HD13	49:Ls:105:ASN:HD21	1.72	0.54
52:S2:1144:A:H2'	52:S2:1145:A:C8	2.42	0.54
53:SA:37:TYR:OH	53:SA:57:LYS:NZ	2.34	0.54
58:SF:195:GLU:OE1	58:SF:198:ARG:NH2	2.40	0.54
61:SI:12:ARG:HH21	61:SI:18:ARG:HG3	1.73	0.54
64:SL:13:GLN:HE22	64:SL:35:ARG:HE	1.55	0.54
70:SR:32:LYS:HE2	70:SR:47:ARG:NH1	2.19	0.54
71:SS:66:ARG:O	71:SS:70:ILE:HG12	2.08	0.54
79:Sa:36:ILE:HD11	79:Sa:75:VAL:HG12	1.90	0.54
80:Sb:34:ASP:O	80:Sb:79:PHE:HA	2.08	0.54
4:L5:1521:C:N4	94:L5:5596:HOH:O	2.41	0.54
6:L8:67:U:H2'	6:L8:68:G:H8	1.72	0.54
8:LB:122:TRP:CE2	8:LB:127:LYS:HE3	2.42	0.54
52:S2:107:A:H2'	52:S2:108:G:C8	2.43	0.54
52:S2:573:U:O2	52:S2:576:A2M:H8	2.07	0.54
52:S2:604:A:N3	52:S2:639:C:O2'	2.37	0.54
52:S2:1692:U:H2'	52:S2:1693:G:C8	2.42	0.54
52:S2:1777:G:H2'	52:S2:1778:C:H6	1.72	0.54
4:L5:2579:G:N2	4:L5:2582:A:OP2	2.34	0.54
6:L8:52:A:H4'	43:L1:19:GLN:HA	1.89	0.54
9:LC:352:ASP:OD1	9:LC:353:LYS:N	2.41	0.54
24:LS:90:THR:HB	25:LT:156:TYR:CD2	2.43	0.54
42:Lk:12:LEU:HB3	42:Lk:16:ARG:NH2	2.23	0.54
52:S2:327:G:H4'	52:S2:328:U:O5'	2.08	0.54
52:S2:1171:G:O2'	52:S2:1187:G:O6	2.22	0.54
52:S2:1593:C:O2	72:ST:12:GLN:NE2	2.26	0.54
52:S2:1656:G:H1	52:S2:1668:U:H3	1.54	0.54
54:SB:183:GLU:OE1	54:SB:183:GLU:N	2.35	0.54
71:SS:43:VAL:HG11	71:SS:83:PHE:CE2	2.43	0.54
75:SW:11:LEU:HD11	75:SW:37:PHE:CE2	2.43	0.54
3:CF:149:ILE:HD12	3:CF:189:ALA:HB3	1.90	0.54
4:L5:1084:C:H2'	4:L5:1085:C:H6	1.73	0.54
4:L5:1239:C:OP1	33:Lb:92:LYS:NZ	2.40	0.54
4:L5:1662:C:H2'	4:L5:1663:C:H6	1.73	0.54
4:L5:4563:U:H2'	4:L5:4564:A:H8	1.73	0.54
17:LL:100:PRO:O	40:Li:25:ARG:NH2	2.24	0.54
52:S2:656:G:H21	52:S2:663:C:H5''	1.72	0.54
52:S2:1533:A:N7	52:S2:1604:G:H1'	2.23	0.54
63:SK:80:ARG:HG3	63:SK:85:LEU:HB2	1.89	0.54
79:Sa:59:PHE:HB2	79:Sa:62:TYR:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CF:293:GLU:HB2	86:AT:77:A:C2	2.42	0.54
4:L5:3893:C:H2'	4:L5:3894:A:C8	2.43	0.54
10:LD:182:GLY:HA2	10:LD:194:VAL:HG23	1.90	0.54
12:LF:155:TYR:OH	12:LF:188:GLU:OE2	2.25	0.54
15:LI:53:VAL:HG11	25:LT:158:PHE:HZ	1.73	0.54
26:LU:23:LEU:HD13	26:LU:110:TYR:HB2	1.88	0.54
52:S2:600:G:H2'	52:S2:601:OMG:H8	1.73	0.54
52:S2:1745:A:H1'	59:SG:66:GLY:HA2	1.89	0.54
53:SA:80:ARG:O	53:SA:84:GLN:HG3	2.08	0.54
64:SL:16:ILE:HD11	64:SL:36:TYR:N	2.23	0.54
77:SY:37:LYS:HA	77:SY:40:ILE:HD12	1.89	0.54
80:Sb:67:THR:OG1	80:Sb:70:LYS:O	2.25	0.54
4:L5:468:U:C6	4:L5:469:C:H5	2.25	0.54
4:L5:2411:C:H2'	4:L5:2412:A:H8	1.73	0.54
4:L5:2568:C:H2'	4:L5:2569:G:H8	1.72	0.54
9:LC:144:ILE:HD12	9:LC:150:LEU:HD11	1.89	0.54
52:S2:380:G:OP2	61:SI:56:ARG:NH2	2.41	0.54
52:S2:1139:C:H2'	52:S2:1140:G:O4'	2.07	0.54
52:S2:1144:A:H5'	52:S2:1355:C:H41	1.73	0.54
52:S2:1651:A:O2'	58:SF:83:ASN:OD1	2.21	0.54
64:SL:61:PRO:HB3	64:SL:68:ILE:HD11	1.89	0.54
64:SL:151:THR:C	64:SL:152:LYS:HD2	2.33	0.54
70:SR:100:PRO:O	70:SR:104:GLU:HG2	2.08	0.54
76:SX:52:LEU:HD11	76:SX:73:GLN:HB2	1.90	0.54
3:CF:429:MET:SD	86:AT:54:G:C1'	2.96	0.54
4:L5:2630:U:O4	26:LU:89:LYS:NZ	2.41	0.54
4:L5:4473:A:H5''	44:Lm:95:ILE:HD12	1.90	0.54
8:LB:258:HIS:HA	8:LB:260:ALA:N	2.22	0.54
21:LP:27:LYS:NZ	94:LP:302:HOH:O	2.36	0.54
52:S2:153:G:N3	59:SG:13:GLN:NE2	2.56	0.54
52:S2:589:G:C8	52:S2:591:U:H2'	2.43	0.54
52:S2:1421:A:H3'	52:S2:1422:G:C8	2.43	0.54
52:S2:1854:U:H2'	52:S2:1855:G:H8	1.72	0.54
56:SD:222:PRO:HB3	85:Sg:190:GLY:HA3	1.90	0.54
4:L5:3893:C:O2'	4:L5:4979:A:N1	2.40	0.54
4:L5:4401:G:H2'	4:L5:4402:C:H6	1.73	0.54
12:LF:237:GLU:OE1	12:LF:237:GLU:N	2.41	0.54
21:LP:24:VAL:HG12	21:LP:86:LYS:HG2	1.89	0.54
23:LR:21:LYS:HE3	23:LR:55:VAL:HA	1.90	0.54
49:Ls:61:MET:CG	49:Ls:88:PHE:HE2	2.21	0.54
52:S2:118:C:H1'	52:S2:445:A:C5	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:919:A:OP2	66:SN:64:ARG:NH2	2.39	0.54
52:S2:1595:U:H2'	52:S2:1596:U:C6	2.43	0.54
65:SM:75:ASN:OD1	65:SM:76:LEU:N	2.41	0.54
82:Sd:39:CYS:HB3	82:Sd:42:CYS:HB2	1.90	0.54
85:Sg:42:MET:SD	85:Sg:57:ARG:HB2	2.47	0.54
86:AT:67:C:H2'	86:AT:68:G:C8	2.43	0.54
4:L5:406:C:O2'	4:L5:407:A:OP1	2.26	0.53
4:L5:2107:C:N4	4:L5:2108:G:O6	2.41	0.53
4:L5:2448:G:H2'	4:L5:2449:A:C8	2.43	0.53
8:LB:307:TYR:HD2	8:LB:366:LYS:HA	1.71	0.53
9:LC:106:LYS:HD3	9:LC:108:TRP:CZ2	2.43	0.53
10:LD:119:TYR:OH	10:LD:139:PRO:O	2.24	0.53
11:LE:149:ILE:HD12	11:LE:271:LEU:HD21	1.89	0.53
11:LE:190:HIS:HB3	11:LE:193:PHE:HD2	1.73	0.53
16:LJ:52:LYS:HG2	16:LJ:67:LYS:HD3	1.90	0.53
52:S2:126:G:N1	59:SG:192:ILE:HD11	2.23	0.53
52:S2:1628:C:H2'	52:S2:1629:C:H6	1.72	0.53
55:SC:248:TYR:O	74:SV:23:ILE:HG21	2.08	0.53
57:SE:50:ASN:OD1	94:SE:301:HOH:O	2.18	0.53
4:L5:264:C:H2'	4:L5:265:C:C4	2.43	0.53
4:L5:935:A:O2'	18:LM:44:GLN:O	2.21	0.53
4:L5:966:A:OP2	4:L5:2092:G:N2	2.39	0.53
4:L5:1855:G:OP1	33:Lb:4:SER:HB2	2.08	0.53
4:L5:2809:G:O2'	4:L5:4644:G:OP1	2.25	0.53
7:LA:225:ILE:HG12	7:LA:234:LYS:HA	1.91	0.53
50:Lt:12:VAL:HG11	50:Lt:65:GLN:HB2	1.90	0.53
50:Lt:47:ALA:HA	50:Lt:72:GLU:OE2	2.07	0.53
52:S2:102:A:H4'	52:S2:104:A:C8	2.44	0.53
52:S2:103:A:H5'	61:SI:12:ARG:HH12	1.70	0.53
52:S2:830:A:OP2	52:S2:846:G:N2	2.39	0.53
52:S2:1093:A:H5''	75:SW:28:ARG:HH22	1.74	0.53
52:S2:1533:A:H2	52:S2:1536:G:N3	2.07	0.53
4:L5:453:G:H2'	4:L5:453:G:N3	2.23	0.53
4:L5:965:G:N2	4:L5:2092:G:H1'	2.24	0.53
8:LB:71:GLU:HG3	28:LW:2:LYS:HG2	1.89	0.53
9:LC:11:TYR:CZ	9:LC:148:PRO:HB2	2.43	0.53
52:S2:659:G:O2'	52:S2:662:G:O2'	2.27	0.53
52:S2:733:C:C5	52:S2:734:C:H1'	2.43	0.53
61:SI:57:ALA:HB1	61:SI:60:LEU:CD2	2.38	0.53
81:Sc:35:MET:HE1	81:Sc:55:VAL:HG21	1.89	0.53
86:AT:21:U:C4	86:AT:47:G:H1'	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:CA:141:ASP:HB2	87:CA:177:PHE:HD2	1.73	0.53
87:CA:202:ILE:HD11	87:CA:209:GLN:HB3	1.89	0.53
3:CF:99:ILE:HG22	3:CF:430:ARG:HH21	1.72	0.53
4:L5:4389:C:H2'	4:L5:4390:A:C8	2.44	0.53
4:L5:4571:A2M:H2'	4:L5:4572:U:H6	1.72	0.53
4:L5:5057:C:H2'	4:L5:5058:A:C8	2.43	0.53
44:Lm:79:GLU:OE2	44:Lm:81:SER:OG	2.18	0.53
46:Lo:2:VAL:N	46:Lo:90:HIS:O	2.41	0.53
52:S2:1217:A:H2'	52:S2:1218:C:H6	1.73	0.53
52:S2:1239:U:H5''	68:SP:124:LYS:HD3	1.90	0.53
57:SE:112:HIS:NE2	57:SE:237:SER:O	2.41	0.53
57:SE:151:ASP:HB3	57:SE:154:ILE:CD1	2.39	0.53
71:SS:25:LYS:HZ1	71:SS:52:LEU:HD22	1.73	0.53
4:L5:173:C:H2'	4:L5:174:C:C6	2.43	0.53
4:L5:717:U:H2'	4:L5:718:C:C6	2.43	0.53
4:L5:1548:G:O2'	4:L5:2812:A:N3	2.38	0.53
4:L5:1741:G:O2'	4:L5:1781:PSU:OP2	2.26	0.53
18:LM:122:ILE:HB	20:LO:189:ILE:HD11	1.90	0.53
29:LX:156:ILE:OXT	87:CA:294:VAL:HG21	2.09	0.53
35:Ld:36:VAL:HG21	35:Ld:44:ARG:HG2	1.91	0.53
72:ST:56:ARG:NH2	72:ST:79:TYR:HB3	2.24	0.53
84:Sf:103:LEU:HB2	84:Sf:105:TYR:CE1	2.44	0.53
85:Sg:10:THR:HB	85:Sg:306:LEU:HD21	1.91	0.53
4:L5:327:U:O2'	40:Li:30:ARG:NH1	2.38	0.53
4:L5:425:U:H4'	21:LP:6:LEU:HD21	1.90	0.53
4:L5:3796:U:HO2'	52:S2:1720:U:HO2'	1.56	0.53
4:L5:4619:U:H2'	4:L5:4620:OMU:H6	1.90	0.53
4:L5:5024:C:H41	4:L5:5028:G:H21	1.56	0.53
8:LB:86:VAL:HG12	8:LB:201:LEU:HD23	1.90	0.53
11:LE:239:LYS:NZ	11:LE:240:TYR:O	2.41	0.53
20:LO:113:ASP:OD1	20:LO:114:LYS:HG2	2.08	0.53
30:LY:54:GLU:HG2	30:LY:108:ARG:HB3	1.91	0.53
34:Lc:51:ASN:HB2	34:Lc:77:ASN:HB2	1.90	0.53
52:S2:907:G:H2'	52:S2:908:A:C8	2.44	0.53
52:S2:1438:A:H2'	52:S2:1439:A:H8	1.73	0.53
58:SF:167:LYS:HD2	58:SF:172:CYS:SG	2.49	0.53
83:Se:39:ASN:HA	83:Se:43:VAL:HG22	1.90	0.53
4:L5:2057:A:N6	94:L5:5401:HOH:O	2.20	0.53
4:L5:2478:C:N3	4:L5:2591:A:O2'	2.42	0.53
4:L5:4239:A:H2'	4:L5:4240:G:H8	1.74	0.53
8:LB:47:LEU:HB2	8:LB:84:MET:HE1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LV:42:VAL:HB	27:LV:45:ILE:HG13	1.90	0.53
52:S2:1232:PSU:H2'	52:S2:1233:G:C8	2.43	0.53
52:S2:1679:A:OP1	81:Sc:20:ARG:NH2	2.41	0.53
59:SG:138:ALA:HB2	59:SG:179:LEU:HD12	1.91	0.53
73:SU:49:LYS:HZ3	73:SU:51:LYS:HG3	1.74	0.53
85:Sg:164:ILE:HD11	85:Sg:176:VAL:HB	1.91	0.53
3:CF:84:LYS:HZ2	3:CF:85:TYR:HD2	1.56	0.53
3:CF:427:ARG:HG2	3:CF:432:THR:HA	1.91	0.53
4:L5:1739:G:N3	4:L5:1742:A:N6	2.56	0.53
4:L5:1846:G:H2'	4:L5:1847:C:C6	2.43	0.53
4:L5:3659:G:OP1	7:LA:241:ARG:NH1	2.41	0.53
4:L5:3898:G:H5'	8:LB:254:ILE:HG13	1.91	0.53
4:L5:4364:G:H2'	4:L5:4365:C:H6	1.73	0.53
4:L5:4893:A:H4'	18:LM:125:ASN:ND2	2.23	0.53
4:L5:4966:A:H5''	8:LB:128:LYS:HG3	1.91	0.53
6:L8:89:U:H2'	6:L8:90:C:C6	2.43	0.53
10:LD:62:CYS:HB3	10:LD:105:LEU:HD22	1.91	0.53
25:LT:44:GLY:HA2	25:LT:95:HIS:HB3	1.90	0.53
27:LV:35:LYS:HD3	27:LV:68:GLY:HA2	1.89	0.53
28:LW:5:LEU:HD12	28:LW:30:GLN:NE2	2.23	0.53
52:S2:495:U:H2'	52:S2:496:C:O4'	2.09	0.53
52:S2:1845:A:H2'	52:S2:1846:G:H8	1.73	0.53
54:SB:48:LEU:HD12	67:SO:51:GLU:HG2	1.91	0.53
62:SJ:21:GLU:OE1	62:SJ:21:GLU:N	2.41	0.53
64:SL:121:GLN:N	64:SL:121:GLN:OE1	2.41	0.53
73:SU:24:LEU:HD22	73:SU:112:VAL:HG12	1.91	0.53
86:AT:18:G:H21	86:AT:59:A:H5'	1.74	0.53
87:CA:107:LYS:HZ2	87:CA:316:VAL:HG22	1.74	0.53
4:L5:1070:G:O2'	4:L5:1071:C:O5'	2.27	0.53
4:L5:2296:G:O2'	9:LC:242:PRO:O	2.25	0.53
4:L5:4174:U:H2'	4:L5:4175:G:H8	1.73	0.53
4:L5:4389:C:H2'	4:L5:4390:A:H8	1.74	0.53
4:L5:4612:C:C2	14:LH:120:GLU:HB2	2.43	0.53
4:L5:4699:U:H1'	4:L5:4700:A:H5''	1.90	0.53
6:L8:19:C:H2'	6:L8:20:A:H8	1.73	0.53
6:L8:67:U:H2'	6:L8:68:G:C8	2.44	0.53
7:LA:137:ILE:HD11	7:LA:149:LYS:HB2	1.90	0.53
28:LW:46:PRO:HB2	28:LW:52:THR:HG21	1.90	0.53
49:Ls:30:VAL:HG23	49:Ls:189:ILE:HA	1.91	0.53
52:S2:921:G:H2'	75:SW:28:ARG:HH12	1.74	0.53
52:S2:952:G:H4'	67:SO:51:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:1101:U:H2'	52:S2:1102:G:C8	2.44	0.53
53:SA:205:ARG:NH2	53:SA:210:ILE:HG13	2.24	0.53
59:SG:161:PRO:HA	59:SG:171:THR:HA	1.91	0.53
70:SR:58:MET:HA	70:SR:61:ILE:HG22	1.91	0.53
71:SS:86:ARG:HH21	71:SS:106:LYS:HB3	1.74	0.53
4:L5:1684:A:OP1	32:La:47:LYS:NZ	2.40	0.53
4:L5:1751:A:H2'	4:L5:1752:G:C8	2.44	0.53
6:L8:21:C:OP1	9:LC:195:LYS:NZ	2.40	0.53
52:S2:574:A:H4'	77:SY:89:HIS:HB3	1.91	0.53
52:S2:641:A:OP1	62:SJ:40:LYS:NZ	2.41	0.53
52:S2:1562:C:H2'	52:S2:1563:G:C8	2.41	0.53
3:CF:22:THR:HG23	3:CF:56:TYR:HB2	1.91	0.52
4:L5:1307:A:H2'	4:L5:1308:C:H6	1.74	0.52
4:L5:2696:A:OP1	42:Lk:26:LYS:NZ	2.38	0.52
4:L5:4935:C:H2'	4:L5:4936:G:C8	2.44	0.52
10:LD:258:LYS:C	10:LD:259:LYS:HD2	2.34	0.52
11:LE:225:PRO:C	11:LE:226:ARG:HD3	2.33	0.52
27:LV:46:LYS:NZ	94:LV:304:HOH:O	2.40	0.52
49:Ls:69:LEU:HD11	49:Ls:75:LEU:HB3	1.90	0.52
50:Lt:119:ARG:HG2	50:Lt:119:ARG:HH11	1.74	0.52
60:SH:157:HIS:HB3	60:SH:190:PRO:HG3	1.91	0.52
65:SM:30:GLY:HA3	65:SM:113:ASP:HB3	1.90	0.52
87:CA:105:LEU:HD23	87:CA:139:LYS:HD2	1.91	0.52
1:CD:27:PRO:HD3	31:LZ:85:TYR:CE1	2.45	0.52
4:L5:724:C:H1'	9:LC:343:GLN:HG2	1.91	0.52
4:L5:979:C:OP2	11:LE:66:LYS:HD3	2.09	0.52
4:L5:1683:PSU:OP1	32:La:44:ASN:ND2	2.40	0.52
4:L5:2094:G:H2'	4:L5:2094:G:N3	2.24	0.52
4:L5:2108:G:H2'	4:L5:2109:G:H8	1.75	0.52
4:L5:4251:A:H61	16:LJ:24:ILE:HG23	1.74	0.52
4:L5:4504:C:H2'	4:L5:4505:C:C6	2.44	0.52
48:Lr:65:LYS:O	48:Lr:102:TYR:OH	2.24	0.52
52:S2:1390:U:H2'	52:S2:1391:OMC:H6	1.74	0.52
53:SA:159:ILE:HD11	74:SV:34:MET:HE1	1.91	0.52
78:SZ:99:LEU:HD11	78:SZ:102:LYS:HB2	1.91	0.52
85:Sg:188:HIS:HD1	85:Sg:219:TRP:CD1	2.27	0.52
4:L5:2298:U:H5''	9:LC:204:ARG:HH12	1.75	0.52
45:Ln:11:ARG:NH2	52:S2:1844:U:OP1	2.42	0.52
52:S2:28:U:H2'	52:S2:29:G:H8	1.73	0.52
52:S2:649:PSU:H2'	52:S2:650:A:H8	1.74	0.52
52:S2:1093:A:H5''	75:SW:28:ARG:NH2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:SN:124:ARG:HG2	66:SN:127:ARG:HH21	1.74	0.52
68:SP:31:GLU:OE1	68:SP:31:GLU:N	2.42	0.52
69:SQ:15:ARG:HD3	69:SQ:126:ARG:HH12	1.74	0.52
69:SQ:19:ALA:HB2	69:SQ:75:GLY:HA3	1.91	0.52
69:SQ:40:GLU:OE1	69:SQ:40:GLU:N	2.40	0.52
74:SV:30:ALA:O	74:SV:60:ARG:HD3	2.09	0.52
87:CA:187:SER:HB2	87:CA:201:ILE:HB	1.91	0.52
3:CF:54:PHE:O	3:CF:58:TRP:HD1	1.91	0.52
4:L5:1243:C:H2'	4:L5:1244:G:H8	1.74	0.52
4:L5:1359:G:H4'	19:LN:203:TYR:HB2	1.91	0.52
4:L5:1785:C:OP1	15:LI:133:GLN:NE2	2.43	0.52
4:L5:3948:C:O2'	4:L5:3949:A:N7	2.38	0.52
13:LG:83:PHE:HA	13:LG:183:ILE:HD13	1.91	0.52
46:Lo:11:PHE:O	46:Lo:81:ARG:NH2	2.43	0.52
52:S2:952:G:H2'	52:S2:953:C:C6	2.45	0.52
53:SA:122:LEU:HB3	53:SA:144:THR:HG22	1.90	0.52
55:SC:95:ASP:HA	55:SC:98:LEU:O	2.09	0.52
57:SE:121:TYR:HA	57:SE:163:ASP:HA	1.90	0.52
72:ST:129:ARG:HD2	72:ST:133:ARG:HH21	1.74	0.52
3:CF:322:ARG:NH1	86:AT:1:G:O5'	2.42	0.52
4:L5:1538:U:H2'	4:L5:1539:G:H8	1.75	0.52
4:L5:1563:A:N6	52:S2:1028:A:N1	2.57	0.52
4:L5:4927:G:H5''	4:L5:4928:C:H5	1.73	0.52
27:LV:43:LYS:HG3	27:LV:60:MET:HG2	1.91	0.52
52:S2:15:U:H2'	52:S2:16:G:O4'	2.09	0.52
52:S2:1108:G:H21	70:SR:126:MET:HE1	1.75	0.52
53:SA:42:LYS:HD2	53:SA:46:ILE:HB	1.92	0.52
54:SB:30:TRP:CE2	67:SO:19:PRO:HD3	2.45	0.52
57:SE:180:LEU:HD21	57:SE:192:ILE:HG23	1.91	0.52
60:SH:91:HIS:ND1	60:SH:172:THR:HG21	2.24	0.52
70:SR:22:THR:O	85:Sg:212:LYS:NZ	2.42	0.52
4:L5:1095:A:H2	4:L5:1200:G:N1	2.03	0.52
4:L5:1345:A:H2'	4:L5:1346:C:C6	2.44	0.52
4:L5:1577:G:O2'	4:L5:1612:G:H4'	2.10	0.52
4:L5:1975:G:N2	4:L5:1983:A:OP1	2.42	0.52
4:L5:2638:G:H22	4:L5:2719:C:P	2.32	0.52
4:L5:2835:A:O2'	8:LB:228:TYR:O	2.20	0.52
4:L5:3861:A:H2'	4:L5:3862:A:C8	2.44	0.52
4:L5:4478:G:O2'	4:L5:4602:A:N1	2.41	0.52
8:LB:397:ILE:O	8:LB:401:GLU:HG2	2.09	0.52
52:S2:51:U:H2'	52:S2:52:G:C8	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:72:C:N4	59:SG:169:PRO:O	2.42	0.52
52:S2:1433:C:H42	73:SU:92:HIS:CD2	2.22	0.52
52:S2:1797:U:H2'	52:S2:1798:C:C6	2.44	0.52
57:SE:100:ARG:HB2	57:SE:114:ILE:HD13	1.92	0.52
61:SI:125:LYS:HB2	61:SI:128:LYS:NZ	2.24	0.52
67:SO:96:LYS:HD3	67:SO:132:VAL:HG11	1.92	0.52
72:ST:110:LEU:HD23	72:ST:112:MET:HE3	1.90	0.52
3:CF:350:PRO:HB3	86:AT:55:U:OP1	2.10	0.52
3:CF:360:VAL:HA	3:CF:369:ALA:HA	1.92	0.52
4:L5:171:U:OP2	4:L5:172:C:N4	2.42	0.52
4:L5:223:G:N7	9:LC:165:LYS:HE3	2.25	0.52
4:L5:1346:C:H2'	4:L5:1347:G:H8	1.74	0.52
4:L5:1998:A:H4'	49:Ls:9:TRP:HZ2	1.73	0.52
4:L5:3726:A:H2'	4:L5:3727:A:C8	2.44	0.52
12:LF:127:LYS:HB2	25:LT:133:ALA:HB3	1.91	0.52
52:S2:1711:U:H2'	52:S2:1712:A:H8	1.74	0.52
64:SL:126:VAL:HG12	64:SL:145:VAL:HG22	1.90	0.52
4:L5:457:G:H2'	4:L5:458:C:C6	2.45	0.52
16:LJ:57:VAL:HG12	16:LJ:60:PHE:H	1.74	0.52
27:LV:90:ARG:O	27:LV:90:ARG:HG2	2.09	0.52
52:S2:1391:OMC:H4'	82:Sd:55:LEU:HD13	1.92	0.52
59:SG:197:GLN:OE1	59:SG:197:GLN:N	2.41	0.52
66:SN:99:ARG:HH12	66:SN:143:SER:CB	2.19	0.52
71:SS:25:LYS:HD3	71:SS:27:ALA:N	2.24	0.52
4:L5:3599:A:H2'	4:L5:3600:G:C8	2.45	0.52
4:L5:3664:G:H2'	4:L5:3665:G:C8	2.43	0.52
8:LB:218:ASP:OD2	8:LB:348:ARG:NH2	2.34	0.52
16:LJ:113:ILE:HD11	16:LJ:125:ILE:HA	1.92	0.52
17:LL:103:ARG:H	17:LL:103:ARG:HD3	1.74	0.52
28:LW:97:LYS:HG3	28:LW:98:PRO:HD3	1.90	0.52
52:S2:1259:A:H1'	52:S2:1264:C:N4	2.25	0.52
54:SB:59:SER:OG	54:SB:63:LYS:NZ	2.42	0.52
55:SC:167:ARG:HB3	55:SC:177:PRO:HB2	1.92	0.52
57:SE:47:PHE:O	57:SE:51:ARG:HB2	2.09	0.52
59:SG:69:THR:O	59:SG:99:GLY:HA3	2.10	0.52
64:SL:73:LEU:HD11	64:SL:109:MET:HE1	1.91	0.52
71:SS:41:ALA:O	71:SS:45:LEU:HG	2.10	0.52
3:CF:153:ASN:OD1	3:CF:195:GLY:N	2.43	0.52
4:L5:1973:G:O2'	50:Lt:78:SER:OG	2.19	0.52
4:L5:3619:G:H22	4:L5:3624:A:H1'	1.75	0.52
4:L5:3932:U:H2'	4:L5:3933:G:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:4594:U:H2'	4:L5:4595:G:C8	2.41	0.52
7:LA:189:TYR:CD2	7:LA:196:TRP:HB2	2.44	0.52
9:LC:116:ASN:HB2	9:LC:119:GLN:HG2	1.92	0.52
11:LE:99:ASP:O	11:LE:100:LYS:HG2	2.10	0.52
15:LI:66:GLU:CD	15:LI:69:ARG:HH21	2.18	0.52
34:Lc:33:GLN:O	34:Lc:37:MET:HG2	2.10	0.52
52:S2:663:C:O2'	55:SC:227:ARG:NH2	2.43	0.52
52:S2:1292:C:N3	84:Sf:138:ARG:NH2	2.51	0.52
53:SA:76:VAL:HG12	53:SA:123:VAL:HB	1.90	0.52
54:SB:138:PHE:O	54:SB:213:ARG:N	2.43	0.52
4:L5:318:A:H2'	4:L5:319:A:C8	2.45	0.51
4:L5:1974:U:H4'	4:L5:1975:G:H3'	1.92	0.51
4:L5:1981:G:H2'	4:L5:1982:G:C8	2.45	0.51
4:L5:4068:U:H2'	4:L5:4069:U:C5	2.45	0.51
4:L5:4238:G:H2'	4:L5:4239:A:C8	2.45	0.51
4:L5:4238:G:H2'	4:L5:4239:A:H8	1.74	0.51
52:S2:1231:C:O2'	52:S2:1253:A:N6	2.43	0.51
52:S2:1373:C:OP1	70:SR:7:LYS:N	2.41	0.51
53:SA:22:GLY:C	53:SA:24:HIS:H	2.18	0.51
55:SC:104:ASP:HA	55:SC:130:ILE:HG22	1.92	0.51
64:SL:11:GLN:HB3	64:SL:56:ILE:HG21	1.91	0.51
68:SP:37:TYR:HB3	68:SP:41:GLN:HB2	1.92	0.51
87:CA:354:LEU:HD12	87:CA:357:LEU:HD21	1.92	0.51
2:CI:55:LEU:HB3	26:LU:99:TRP:NE1	2.25	0.51
4:L5:262:G:H2'	4:L5:263:G:C8	2.45	0.51
4:L5:1080:C:H2'	4:L5:1081:C:C6	2.45	0.51
5:L7:23:A:N3	5:L7:118:C:O2'	2.37	0.51
5:L7:119:U:C2	10:LD:261:VAL:HG21	2.45	0.51
9:LC:207:PRO:HB3	9:LC:249:PHE:CD2	2.45	0.51
11:LE:177:GLY:O	11:LE:178:PRO:C	2.53	0.51
20:LO:197:LYS:HG2	20:LO:202:LEU:O	2.11	0.51
29:LX:156:ILE:CD1	87:CA:291:MET:CB	2.75	0.51
52:S2:1528:G:O2'	52:S2:1666:C:OP1	2.24	0.51
54:SB:208:HIS:CD2	54:SB:209:ASP:HB2	2.44	0.51
59:SG:103:ASP:H	59:SG:106:LEU:HD13	1.74	0.51
63:SK:96:ARG:O	63:SK:98:ARG:N	2.43	0.51
64:SL:13:GLN:HE22	64:SL:35:ARG:NE	2.08	0.51
70:SR:98:VAL:HG13	70:SR:102:THR:OG1	2.10	0.51
77:SY:79:LEU:HG	77:SY:83:LYS:HE2	1.91	0.51
2:CI:66:GLY:O	2:CI:69:THR:OG1	2.26	0.51
4:L5:468:U:H6	4:L5:469:C:H5	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:1084:C:H2'	4:L5:1085:C:C6	2.45	0.51
4:L5:1495:G:N7	94:L5:5499:HOH:O	2.34	0.51
4:L5:1504:G:H2'	4:L5:1505:C:C6	2.45	0.51
7:LA:129:ALA:O	7:LA:169:VAL:HG11	2.10	0.51
13:LG:230:TYR:CZ	13:LG:234:ARG:HD2	2.45	0.51
14:LH:114:ILE:HB	14:LH:124:ARG:HB2	1.92	0.51
25:LT:27:LEU:HB3	25:LT:31:MET:HE3	1.92	0.51
26:LU:90:TYR:O	26:LU:94:ASN:ND2	2.40	0.51
52:S2:746:C:H2'	52:S2:747:U:C6	2.45	0.51
52:S2:941:C:H5''	54:SB:136:ARG:NH1	2.24	0.51
59:SG:46:LYS:HD2	59:SG:46:LYS:N	2.24	0.51
60:SH:144:ILE:CG2	75:SW:52:ILE:HB	2.41	0.51
64:SL:16:ILE:HD11	64:SL:36:TYR:H	1.75	0.51
65:SM:52:LEU:HD22	65:SM:65:VAL:HB	1.91	0.51
70:SR:29:HIS:O	70:SR:32:LYS:HG2	2.10	0.51
77:SY:3:ASP:N	77:SY:3:ASP:OD1	2.43	0.51
81:Sc:44:ARG:NH2	81:Sc:63:ARG:HH11	2.08	0.51
3:CF:294:MET:HB3	3:CF:308:VAL:HG23	1.93	0.51
4:L5:1675:C:H4'	94:L5:8119:HOH:O	2.11	0.51
4:L5:1732:C:H5''	25:LT:43:LYS:HE2	1.92	0.51
4:L5:2029:A:H2'	4:L5:2030:A:C8	2.44	0.51
4:L5:3709:U:H2'	4:L5:3710:G:O4'	2.11	0.51
7:LA:13:GLY:O	7:LA:17:ARG:HG3	2.11	0.51
23:LR:127:VAL:HG12	23:LR:132:PHE:HD2	1.76	0.51
52:S2:186:C:H2'	52:S2:187:G:H8	1.76	0.51
52:S2:544:G:H2'	52:S2:545:A:C8	2.45	0.51
59:SG:193:ALA:HA	59:SG:196:LYS:HG2	1.93	0.51
60:SH:86:LYS:C	60:SH:87:PHE:HD1	2.18	0.51
4:L5:126:C:H2'	4:L5:127:G:H8	1.75	0.51
4:L5:1195:G:H2'	4:L5:1196:G:C8	2.45	0.51
4:L5:1390:G:N2	4:L5:1393:G:OP2	2.37	0.51
4:L5:3707:U:H2'	4:L5:3708:C:C6	2.46	0.51
4:L5:4103:C:H1'	4:L5:4106:G:N1	2.22	0.51
4:L5:4524:G:C2	8:LB:252:ALA:HB1	2.45	0.51
4:L5:4536:OMC:HM22	4:L5:4537:C:O4'	2.11	0.51
15:LI:108:ALA:HA	15:LI:112:GLN:HG3	1.92	0.51
18:LM:119:ARG:HG3	20:LO:189:ILE:HG23	1.92	0.51
43:LI:43:HIS:HB3	43:LI:46:ARG:HD3	1.93	0.51
52:S2:349:A:H2'	52:S2:350:C:C6	2.44	0.51
52:S2:931:C:H2'	52:S2:932:G:C8	2.45	0.51
52:S2:1614:A:OP1	68:SP:42:ARG:NH2	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SM:52:LEU:HB2	65:SM:65:VAL:HG11	1.91	0.51
69:SQ:110:ASP:HA	69:SQ:113:ILE:HG22	1.92	0.51
85:Sg:191:HIS:CG	85:Sg:195:LEU:HD21	2.46	0.51
4:L5:187:U:H2'	4:L5:245:C:H1'	1.93	0.51
4:L5:1751:A:H2'	4:L5:1752:G:H8	1.75	0.51
4:L5:1985:G:N2	4:L5:2003:G:HO2'	2.08	0.51
4:L5:2083:C:OP2	22:LQ:14:ARG:NH2	2.44	0.51
33:Lb:99:ILE:O	33:Lb:109:ARG:NH1	2.44	0.51
52:S2:99:A2M:H8	52:S2:99:A2M:O5'	2.11	0.51
52:S2:120:U:H2'	52:S2:121:OMU:C6	2.41	0.51
52:S2:191:A:N6	52:S2:208:G:O2'	2.43	0.51
52:S2:1677:U:H2'	52:S2:1678:A:H8	1.75	0.51
52:S2:1749:G:H2'	52:S2:1750:C:C6	2.46	0.51
52:S2:1754:G:N7	52:S2:1779:G:N2	2.58	0.51
52:S2:1854:U:P	67:SO:147:ARG:HH22	2.33	0.51
57:SE:64:ILE:HD11	77:SY:17:LEU:HD12	1.91	0.51
4:L5:1241:C:H1'	33:Lb:120:ARG:H	1.75	0.51
4:L5:2520:C:H2'	4:L5:2521:G:H8	1.75	0.51
4:L5:2808:G:O3'	23:LR:60:ARG:NH1	2.44	0.51
4:L5:3597:G:H2'	4:L5:3598:C:H6	1.76	0.51
10:LD:37:VAL:HG12	10:LD:50:ARG:HH11	1.75	0.51
12:LF:136:VAL:HG23	12:LF:140:ILE:HD13	1.92	0.51
16:LJ:88:LYS:HE3	16:LJ:115:LEU:HD11	1.92	0.51
27:LV:112:MET:HE1	27:LV:117:ILE:HD11	1.92	0.51
44:Lm:79:GLU:OE2	44:Lm:82:LEU:HG	2.10	0.51
47:Lp:26:VAL:HG22	47:Lp:30:GLU:HG3	1.93	0.51
52:S2:466:G:O2'	59:SG:59:GLN:NE2	2.34	0.51
52:S2:561:A:O2'	62:SJ:134:HIS:NE2	2.33	0.51
52:S2:650:A:OP2	76:SX:108:LYS:HE3	2.11	0.51
52:S2:902:G:O2'	52:S2:903:A:O4'	2.29	0.51
56:SD:29:LEU:HB3	56:SD:34:TYR:HB2	1.92	0.51
86:AT:8:U:H5''	86:AT:50:C:H5'	1.93	0.51
3:CF:277:VAL:HA	3:CF:288:GLU:HA	1.93	0.51
4:L5:418:A:C2	6:L8:17:A:H1'	2.46	0.51
4:L5:2632:PSU:H2'	4:L5:2633:U:C6	2.46	0.51
4:L5:3873:G:H2'	4:L5:3874:G:C8	2.46	0.51
4:L5:4492:U:O2'	4:L5:4512:U:O2	2.27	0.51
4:L5:4685:U:H2'	4:L5:4686:G:C8	2.46	0.51
15:LI:38:ARG:NH1	15:LI:45:GLU:OE1	2.37	0.51
49:Ls:75:LEU:HD12	49:Ls:193:PHE:HE2	1.75	0.51
51:Pt:38:C:O2'	52:S2:1058:A:OP1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:65:C:H4'	59:SG:172:LYS:HE2	1.93	0.51
52:S2:563:G:O2'	52:S2:564:A:OP1	2.25	0.51
52:S2:1524:G:OP2	71:SS:141:ARG:NH1	2.44	0.51
52:S2:1597:C:H4'	52:S2:1603:G:O6	2.11	0.51
56:SD:42:THR:OG1	56:SD:45:ARG:O	2.27	0.51
75:SW:94:LEU:HD21	75:SW:102:ILE:HG13	1.93	0.51
3:CF:138:LEU:HD11	3:CF:435:VAL:HG21	1.93	0.51
3:CF:250:LEU:HB3	3:CF:322:ARG:HA	1.93	0.51
4:L5:3917:A:H2'	4:L5:3918:G:C8	2.46	0.51
4:L5:5004:C:H2'	4:L5:5005:G:O4'	2.10	0.51
12:LF:243:LEU:O	12:LF:247:MET:HB2	2.11	0.51
19:LN:116:LEU:HD22	19:LN:135:ILE:HD11	1.93	0.51
26:LU:65:ARG:HG2	26:LU:67:LYS:H	1.75	0.51
48:Lr:47:LYS:O	48:Lr:103:ARG:HD2	2.11	0.51
52:S2:72:C:N3	59:SG:170:ARG:HG3	2.26	0.51
52:S2:198:U:H2'	52:S2:199:C:H2'	1.92	0.51
52:S2:616:A:H1'	83:Se:12:VAL:HG23	1.93	0.51
52:S2:964:A:H2'	52:S2:965:U:H6	1.76	0.51
52:S2:1203:G:H2'	52:S2:1204:A:H8	1.76	0.51
65:SM:19:GLN:HB2	65:SM:88:TRP:CZ3	2.46	0.51
77:SY:39:GLU:OE1	77:SY:39:GLU:N	2.43	0.51
1:CD:26:ASP:O	1:CD:29:GLU:HG3	2.10	0.51
3:CF:132:GLN:O	3:CF:136:HIS:ND1	2.44	0.51
4:L5:1190:C:H2'	4:L5:1191:C:C6	2.46	0.51
4:L5:1613:A:H5''	7:LA:183:GLY:CA	2.41	0.51
4:L5:2079:G:H2'	4:L5:2080:U:C6	2.46	0.51
4:L5:3595:U:H5''	4:L5:3597:G:OP2	2.11	0.51
6:L8:40:A:H2'	6:L8:41:A:C8	2.46	0.51
9:LC:122:TYR:CD1	9:LC:280:PRO:HG3	2.46	0.51
10:LD:263:LYS:HA	10:LD:263:LYS:HE2	1.93	0.51
21:LP:118:GLN:NE2	21:LP:147:GLU:OE2	2.44	0.51
26:LU:22:THR:HA	26:LU:71:THR:HA	1.92	0.51
52:S2:122:G:H21	57:SE:146:THR:HG21	1.75	0.51
58:SF:59:LYS:HG3	58:SF:60:ARG:H	1.76	0.51
58:SF:79:HIS:O	58:SF:81:ARG:N	2.41	0.51
85:Sg:230:LEU:HD21	85:Sg:259:TRP:CE2	2.46	0.51
86:AT:68:G:H2'	86:AT:69:G:H8	1.76	0.51
3:CF:49:MET:SD	3:CF:51:LYS:N	2.77	0.50
3:CF:248:LEU:HD12	3:CF:267:VAL:HG22	1.94	0.50
4:L5:106:A:H2'	4:L5:107:G:O4'	2.10	0.50
4:L5:1437:C:H1'	4:L5:2098:G:H3'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:1669:A:H4'	4:L5:1685:G:N2	2.25	0.50
4:L5:1743:A:N1	4:L5:1789:C:O2'	2.40	0.50
14:LH:92:MET:HE2	14:LH:179:ILE:HG22	1.93	0.50
47:Lp:75:SER:O	47:Lp:79:VAL:HG23	2.11	0.50
52:S2:819:G:H5''	62:SJ:79:ARG:HH21	1.77	0.50
52:S2:1472:C:O3'	85:Sg:15:ASN:ND2	2.44	0.50
59:SG:227:GLN:HA	59:SG:230:LYS:HE2	1.93	0.50
62:SJ:179:LYS:O	62:SJ:182:GLN:NE2	2.41	0.50
78:SZ:58:LEU:HD21	78:SZ:87:ALA:HB1	1.92	0.50
85:Sg:217:MET:HG3	85:Sg:229:THR:HG23	1.92	0.50
1:CD:27:PRO:HA	1:CD:30:VAL:HG22	1.93	0.50
3:CF:175:SER:HA	3:CF:178:ILE:HG12	1.92	0.50
4:L5:1352:C:O2'	4:L5:1356:U:OP1	2.27	0.50
4:L5:1672:U:H2'	4:L5:1673:U:C6	2.46	0.50
4:L5:3953:G:N2	4:L5:4059:C:O2'	2.43	0.50
8:LB:50:LYS:NZ	8:LB:337:VAL:O	2.41	0.50
8:LB:337:VAL:HG11	8:LB:345:LEU:HD13	1.93	0.50
11:LE:91:THR:HA	11:LE:108:LYS:HA	1.94	0.50
19:LN:143:ARG:CD	39:Lh:95:LEU:HD23	2.40	0.50
40:Li:85:ARG:NH1	94:Li:201:HOH:O	2.33	0.50
52:S2:166:A2M:HM'1	59:SG:11:GLY:HA2	1.93	0.50
59:SG:22:ARG:HA	59:SG:25:ARG:HG2	1.92	0.50
3:CF:379:ILE:HD12	3:CF:384:GLY:HA2	1.92	0.50
4:L5:652:G:H2'	4:L5:653:U:C6	2.46	0.50
4:L5:982:U:C4	11:LE:71:ARG:HD2	2.47	0.50
4:L5:1308:C:H2'	4:L5:1309:C:C6	2.46	0.50
4:L5:4893:A:H4'	18:LM:125:ASN:HD21	1.76	0.50
7:LA:28:ARG:HD2	7:LA:123:ARG:HG3	1.93	0.50
8:LB:228:TYR:CE1	8:LB:270:GLY:HA2	2.46	0.50
49:Ls:78:LEU:O	49:Ls:82:ILE:HG12	2.12	0.50
51:Pt:47:U:O2'	51:Pt:50:U:OP1	2.20	0.50
52:S2:1227:G:C2	52:S2:1228:A:C8	3.00	0.50
52:S2:1370:A:O2'	52:S2:1372:U:OP1	2.28	0.50
52:S2:1407:U:O2'	69:SQ:11:GLN:OE1	2.29	0.50
52:S2:1770:G:O3'	52:S2:1771:G:N2	2.39	0.50
57:SE:124:CYS:HB3	57:SE:141:THR:OG1	2.11	0.50
57:SE:125:LYS:O	57:SE:142:HIS:N	2.44	0.50
58:SF:127:ARG:HB3	58:SF:136:ARG:HB2	1.92	0.50
63:SK:81:ASP:OD1	63:SK:82:TYR:N	2.44	0.50
66:SN:89:TYR:CE1	66:SN:150:VAL:HG23	2.47	0.50
81:Sc:10:LYS:HE3	81:Sc:61:SER:OG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Sg:233:GLY:H	85:Sg:257:LYS:HZ1	1.60	0.50
85:Sg:289:LEU:HD11	85:Sg:298:LEU:HD21	1.93	0.50
87:CA:246:ILE:HB	87:CA:305:PHE:HB2	1.93	0.50
4:L5:137:G:H2'	4:L5:138:G:C8	2.46	0.50
4:L5:432:U:H1'	89:L5:5292:SPM:H82	1.94	0.50
4:L5:2876:OMG:HM22	4:L5:2877:G:H5'	1.92	0.50
4:L5:4694:G:H4'	14:LH:71:ARG:HH12	1.76	0.50
9:LC:293:LEU:O	9:LC:299:GLN:NE2	2.41	0.50
17:LL:101:ARG:HA	40:Li:25:ARG:NH2	2.26	0.50
22:LQ:115:ARG:HB3	22:LQ:115:ARG:HH11	1.76	0.50
26:LU:100:LEU:HD13	26:LU:112:LEU:HD12	1.93	0.50
27:LV:73:ARG:NH1	94:LV:307:HOH:O	2.43	0.50
52:S2:1417:C:H42	52:S2:1422:G:H22	1.58	0.50
52:S2:1556:A:C8	82:Sd:13:LYS:HG3	2.46	0.50
52:S2:1611:G:H4'	71:SS:86:ARG:HH11	1.76	0.50
63:SK:80:ARG:NH1	63:SK:87:PRO:HA	2.27	0.50
66:SN:54:LEU:HB3	66:SN:60:VAL:CG2	2.41	0.50
74:SV:35:ASN:HB3	74:SV:50:PHE:CD2	2.44	0.50
3:CF:5:LYS:HB3	3:CF:86:TYR:H	1.77	0.50
4:L5:67:C:OP2	4:L5:312:G:N2	2.44	0.50
4:L5:1725:U:H2'	4:L5:1726:U:H6	1.77	0.50
4:L5:1979:A:H2	4:L5:1987:C:H42	1.57	0.50
4:L5:2108:G:H2'	4:L5:2109:G:C8	2.46	0.50
4:L5:4071:U:H2'	4:L5:4072:C:C6	2.47	0.50
8:LB:77:THR:OG1	8:LB:335:GLY:O	2.29	0.50
11:LE:223:ARG:HH22	11:LE:238:GLU:HG3	1.77	0.50
16:LJ:94:LEU:O	16:LJ:174:ILE:HA	2.12	0.50
19:LN:126:THR:HG23	19:LN:127:TYR:CD2	2.47	0.50
52:S2:1115:U:H3	52:S2:1118:C:H41	1.60	0.50
52:S2:1498:A:P	56:SD:27:ARG:HH22	2.35	0.50
52:S2:1755:C:H2'	52:S2:1756:C:C6	2.47	0.50
55:SC:84:PHE:HA	74:SV:15:ARG:NH1	2.27	0.50
57:SE:180:LEU:HD23	57:SE:181:CYS:N	2.26	0.50
59:SG:227:GLN:HB3	59:SG:231:ARG:HH21	1.75	0.50
63:SK:26:ASP:O	63:SK:42:ASN:ND2	2.42	0.50
68:SP:48:GLY:HA3	68:SP:50:ARG:HH12	1.77	0.50
73:SU:40:ILE:O	73:SU:44:LYS:HG2	2.11	0.50
73:SU:66:ARG:HH12	73:SU:75:LYS:HD3	1.76	0.50
78:SZ:91:LEU:HD22	78:SZ:96:LEU:HD21	1.93	0.50
86:AT:29:U:H2'	86:AT:30:C:O4'	2.11	0.50
4:L5:7:C:H2'	4:L5:8:U:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:93:G:H2'	4:L5:94:A:C8	2.47	0.50
4:L5:162:A:H2'	4:L5:163:A:H8	1.76	0.50
4:L5:372:A:OP1	41:Lj:36:LYS:HE2	2.11	0.50
4:L5:2708:U:H2'	4:L5:2709:C:C5	2.46	0.50
4:L5:4077:A:N1	4:L5:4171:C:N4	2.58	0.50
4:L5:4611:A:H2'	4:L5:4612:C:H6	1.77	0.50
8:LB:291:TYR:OH	8:LB:315:ASN:ND2	2.44	0.50
14:LH:113:GLU:OE1	14:LH:125:ARG:HG2	2.12	0.50
15:LI:162:ARG:HH21	15:LI:164:LYS:HE3	1.77	0.50
24:LS:5:GLY:O	24:LS:111:ARG:NH2	2.45	0.50
24:LS:68:PHE:O	24:LS:70:LYS:NZ	2.44	0.50
34:Lc:77:ASN:OD1	34:Lc:80:GLU:HG2	2.12	0.50
52:S2:543:C:H3'	52:S2:544:G:C8	2.47	0.50
52:S2:698:G:H2'	52:S2:733:C:C4	2.46	0.50
52:S2:932:G:O2'	52:S2:934:G:OP2	2.22	0.50
52:S2:1464:C:H4'	70:SR:60:ARG:HH11	1.77	0.50
52:S2:1692:U:H2'	52:S2:1693:G:H8	1.77	0.50
53:SA:38:ILE:HD12	53:SA:49:ILE:HA	1.93	0.50
58:SF:162:ALA:HB2	58:SF:172:CYS:SG	2.52	0.50
73:SU:20:ILE:HD13	73:SU:97:ILE:HB	1.94	0.50
3:CF:200:ASN:ND2	3:CF:200:ASN:O	2.45	0.50
4:L5:667:A:H5''	4:L5:668:C:H5''	1.93	0.50
4:L5:1243:C:H2'	4:L5:1244:G:C8	2.46	0.50
4:L5:1426:G:N1	4:L5:1458:C:OP2	2.34	0.50
4:L5:2096:G:H2'	4:L5:2096:G:N3	2.27	0.50
4:L5:2583:C:OP2	38:Lg:76:ARG:NH1	2.43	0.50
4:L5:4220:6MZ:H2'	4:L5:4222:G:H5''	1.94	0.50
12:LF:69:ILE:O	12:LF:73:ARG:HB2	2.12	0.50
16:LJ:20:LEU:HD21	16:LJ:130:PHE:CD1	2.47	0.50
30:LY:4:ASN:HB3	30:LY:7:VAL:HG12	1.94	0.50
52:S2:568:C:H42	52:S2:582:U:H3	1.60	0.50
52:S2:1017:U:H5'	66:SN:55:ARG:HD3	1.93	0.50
55:SC:98:LEU:HB3	55:SC:102:LEU:HD11	1.94	0.50
60:SH:159:ASP:C	60:SH:161:ALA:H	2.19	0.50
63:SK:96:ARG:C	63:SK:98:ARG:H	2.20	0.50
71:SS:80:PRO:HG2	72:ST:36:THR:HG21	1.92	0.50
76:SX:91:LEU:HD21	83:Se:6:LEU:HD23	1.92	0.50
4:L5:433:A:C2	4:L5:3867:A2M:H4'	2.47	0.50
4:L5:3825:A2M:H2'	4:L5:3826:C:O4'	2.12	0.50
16:LJ:114:ASP:OD1	16:LJ:115:LEU:N	2.44	0.50
17:LL:63:THR:HG22	17:LL:64:VAL:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:186:C:H2'	52:S2:187:G:C8	2.47	0.50
52:S2:1284:A:C2	65:SM:104:VAL:HG21	2.47	0.50
70:SR:5:ARG:HD3	70:SR:53:TYR:HB2	1.93	0.50
73:SU:100:GLN:N	73:SU:100:GLN:OE1	2.44	0.50
4:L5:267:G:H2'	4:L5:268:G:C8	2.46	0.50
4:L5:2497:C:H2'	4:L5:2498:C:H6	1.77	0.50
4:L5:2568:C:H2'	4:L5:2569:G:C8	2.47	0.50
4:L5:3748:A:H5''	7:LA:243:THR:HB	1.93	0.50
4:L5:4174:U:H2'	4:L5:4175:G:C8	2.46	0.50
4:L5:4346:U:O2'	46:Lo:80:LYS:O	2.29	0.50
6:L8:8:U:H2'	6:L8:9:A:C8	2.47	0.50
15:LI:36:LEU:HD21	15:LI:69:ARG:NH1	2.25	0.50
28:LW:87:LEU:HD12	28:LW:90:ILE:HD11	1.93	0.50
46:Lo:70:LEU:HD11	46:Lo:83:LEU:HD12	1.94	0.50
52:S2:616:A:N3	83:Se:12:VAL:HG21	2.27	0.50
52:S2:1101:U:H2'	52:S2:1102:G:H8	1.77	0.50
52:S2:1406:G:H2'	52:S2:1407:U:C6	2.46	0.50
54:SB:192:SER:HA	54:SB:195:LYS:HD2	1.94	0.50
58:SF:101:HIS:HB2	58:SF:108:PRO:HG3	1.94	0.50
61:SI:151:GLU:HA	61:SI:154:LYS:HZ3	1.76	0.50
61:SI:153:LYS:O	61:SI:153:LYS:NZ	2.34	0.50
64:SL:125:ILE:HB	64:SL:146:THR:OG1	2.12	0.50
68:SP:76:VAL:O	68:SP:95:GLY:N	2.32	0.50
4:L5:162:A:H2'	4:L5:163:A:C8	2.47	0.49
4:L5:1186:U:H2'	4:L5:1187:G:N3	2.27	0.49
4:L5:2846:G:O2'	27:LV:19:GLY:O	2.22	0.49
4:L5:2870:A:H2'	4:L5:2871:A:C8	2.47	0.49
4:L5:4071:U:H2'	4:L5:4072:C:H6	1.76	0.49
4:L5:4859:C:H2'	4:L5:4860:G:C8	2.47	0.49
6:L8:26:C:O2'	9:LC:53:ALA:O	2.27	0.49
9:LC:325:MET:HE1	12:LF:155:TYR:CZ	2.47	0.49
17:LL:91:ALA:HB1	17:LL:96:ILE:HB	1.94	0.49
52:S2:562:U:H2'	52:S2:563:G:C8	2.47	0.49
52:S2:1310:U:H2'	52:S2:1311:C:C6	2.47	0.49
52:S2:1337:4AC:H2'	52:S2:1338:G:H8	1.77	0.49
52:S2:1628:C:H2'	52:S2:1629:C:C6	2.47	0.49
52:S2:1643:U:H2'	52:S2:1644:C:C6	2.46	0.49
58:SF:183:GLY:HA2	58:SF:190:ILE:HD13	1.93	0.49
60:SH:17:ASP:OD1	60:SH:17:ASP:N	2.43	0.49
73:SU:21:ARG:N	73:SU:115:THR:O	2.37	0.49
3:CF:16:VAL:HG13	3:CF:95:HIS:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:239:C:OP1	30:LY:46:SER:OG	2.30	0.49
4:L5:1514:U:H2'	4:L5:1515:A:C8	2.47	0.49
4:L5:2730:U:H2'	4:L5:2731:C:C6	2.48	0.49
4:L5:3607:U:H2'	4:L5:3608:A:C8	2.48	0.49
4:L5:4080:C:H2'	4:L5:4081:G:H8	1.78	0.49
4:L5:4347:G:H2'	4:L5:4348:A:C8	2.46	0.49
8:LB:122:TRP:CH2	8:LB:127:LYS:HG3	2.47	0.49
10:LD:223:PHE:HB3	10:LD:226:TYR:HB2	1.93	0.49
13:LG:250:ILE:O	13:LG:254:GLU:HG2	2.12	0.49
17:LL:142:GLU:O	17:LL:146:LEU:HB2	2.12	0.49
21:LP:5:SER:OG	21:LP:118:GLN:NE2	2.45	0.49
52:S2:290:U:H5'	52:S2:291:G:OP2	2.11	0.49
52:S2:837:A:H62	77:SY:8:ARG:HD3	1.76	0.49
52:S2:1665:G:C5	72:ST:88:MET:HE1	2.47	0.49
53:SA:104:THR:O	53:SA:107:THR:OG1	2.27	0.49
59:SG:10:THR:HA	59:SG:128:THR:HG23	1.93	0.49
61:SI:162:LEU:HD11	61:SI:191:GLU:HG3	1.92	0.49
84:Sf:139:HIS:O	84:Sf:147:THR:HA	2.12	0.49
85:Sg:259:TRP:CD1	85:Sg:266:ILE:HG12	2.48	0.49
4:L5:500:G:N2	4:L5:504:G:O2'	2.41	0.49
4:L5:3880:G:H2'	4:L5:3881:G:C8	2.47	0.49
4:L5:4066:U:H2'	4:L5:4067:U:C6	2.47	0.49
4:L5:4543:G:H2'	4:L5:4544:A:C8	2.47	0.49
4:L5:4966:A:OP2	8:LB:126:LYS:HE3	2.12	0.49
7:LA:206:PRO:HG3	7:LA:213:GLY:HA3	1.93	0.49
24:LS:154:LEU:HB3	24:LS:157:ARG:HD3	1.94	0.49
32:La:63:LEU:CD2	32:La:65:ARG:HE	2.26	0.49
49:Ls:17:ILE:HD13	49:Ls:54:LEU:HD23	1.94	0.49
49:Ls:125:ALA:N	49:Ls:157:ASP:OD1	2.45	0.49
51:Pt:58:A:O2'	51:Pt:60:A:OP2	2.26	0.49
52:S2:344:U:H2'	52:S2:345:U:C6	2.47	0.49
52:S2:553:U:O4	52:S2:554:A:N6	2.38	0.49
52:S2:1317:C:H2'	52:S2:1318:G:H8	1.78	0.49
52:S2:1454:A:C8	70:SR:3:ARG:HD2	2.47	0.49
52:S2:1568:C:H2'	52:S2:1569:A:C8	2.47	0.49
52:S2:1600:G:O2'	52:S2:1601:A:H4'	2.11	0.49
56:SD:74:GLN:NE2	56:SD:81:GLU:HA	2.27	0.49
58:SF:134:VAL:HG12	58:SF:135:ARG:HG2	1.95	0.49
69:SQ:130:LYS:NZ	69:SQ:131:LYS:O	2.45	0.49
76:SX:107:ARG:HG3	76:SX:110:HIS:HB3	1.93	0.49
78:SZ:58:LEU:O	78:SZ:62:VAL:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:Sc:7:GLN:NE2	81:Sc:61:SER:OG	2.45	0.49
81:Sc:61:SER:HB2	81:Sc:62:GLU:OE1	2.12	0.49
4:L5:293:G:OP1	89:L5:5264:SPM:N1	2.31	0.49
4:L5:737:C:C5	4:L5:739:G:H5'	2.47	0.49
4:L5:1338:G:H4'	4:L5:1339:U:H6	1.77	0.49
4:L5:1907:A:H2'	4:L5:1908:A:C8	2.48	0.49
4:L5:2823:G:N7	23:LR:20:LYS:HD3	2.27	0.49
4:L5:4873:G:C8	20:LO:179:LYS:HE3	2.48	0.49
6:L8:36:G:C5	39:Lh:89:ARG:HD3	2.47	0.49
10:LD:265:ARG:NH1	10:LD:267:ASN:O	2.37	0.49
26:LU:23:LEU:N	26:LU:70:ILE:O	2.34	0.49
29:LX:147:LEU:HD13	87:CA:291:MET:SD	2.52	0.49
37:Lf:106:TYR:O	37:Lf:108:SER:N	2.45	0.49
52:S2:155:G:H4'	59:SG:15:LEU:HD22	1.94	0.49
52:S2:1277:C:H2'	52:S2:1278:A:C8	2.45	0.49
53:SA:142:LEU:HD12	53:SA:143:PRO:HD2	1.93	0.49
54:SB:123:ALA:HB2	54:SB:165:ARG:HG2	1.95	0.49
61:SI:47:ARG:HE	61:SI:51:GLY:HA2	1.75	0.49
65:SM:35:ILE:CG1	65:SM:61:TYR:HE1	2.25	0.49
70:SR:57:LEU:O	70:SR:61:ILE:N	2.41	0.49
78:SZ:101:SER:OG	78:SZ:108:ILE:N	2.43	0.49
85:Sg:18:VAL:O	85:Sg:287:THR:OG1	2.31	0.49
4:L5:37:U:H2'	4:L5:38:A:O4'	2.12	0.49
4:L5:92:C:C2	32:La:55:LYS:HE2	2.47	0.49
4:L5:1444:G:N2	4:L5:2104:G:H21	2.10	0.49
4:L5:3785:A2M:H2	4:L5:4551:U:O2	2.11	0.49
4:L5:3911:C:H2'	4:L5:3912:U:C6	2.47	0.49
8:LB:307:TYR:CD2	8:LB:366:LYS:HA	2.47	0.49
10:LD:211:LEU:HB3	10:LD:219:TYR:HB2	1.95	0.49
14:LH:41:ILE:HG22	14:LH:43:VAL:HG13	1.93	0.49
20:LO:119:VAL:N	24:LS:168:THR:O	2.45	0.49
29:LX:156:ILE:OXT	87:CA:294:VAL:HG11	2.12	0.49
30:LY:112:ASP:OD1	30:LY:115:ARG:HG2	2.12	0.49
44:Lm:126:LYS:HB3	44:Lm:128:LYS:HG2	1.94	0.49
49:Ls:81:HIS:CG	49:Ls:191:GLN:HE22	2.29	0.49
52:S2:388:U:H2'	52:S2:389:A:C8	2.48	0.49
52:S2:942:G:H2'	52:S2:943:U:C6	2.47	0.49
60:SH:23:ILE:HD13	60:SH:87:PHE:HE2	1.77	0.49
60:SH:133:LEU:HD11	60:SH:176:VAL:HG13	1.94	0.49
72:ST:33:TRP:CZ2	72:ST:102:ARG:HD2	2.47	0.49
84:Sf:112:GLY:O	84:Sf:113:LYS:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CI:59:GLN:HG2	26:LU:98:ASP:OD2	2.12	0.49
4:L5:92:C:OP2	4:L5:4341:C:O2'	2.26	0.49
4:L5:444:G:H2'	4:L5:445:U:C6	2.48	0.49
4:L5:494:U:H2'	4:L5:495:C:C6	2.48	0.49
4:L5:716:C:OP1	9:LC:317:ASN:HB2	2.12	0.49
4:L5:729:G:H5''	12:LF:76:ARG:HD2	1.94	0.49
4:L5:1537:A:H2'	4:L5:1538:U:C6	2.48	0.49
4:L5:4625:C:O2'	4:L5:4626:A:H5'	2.13	0.49
4:L5:4910:G:H4'	8:LB:95:THR:HG22	1.93	0.49
15:LI:61:SER:HA	15:LI:126:VAL:HG12	1.93	0.49
27:LV:37:LEU:HD23	27:LV:65:VAL:HG12	1.94	0.49
51:Pt:18:G:H21	51:Pt:58:A:H5'	1.77	0.49
52:S2:656:G:H5'	52:S2:662:G:N2	2.26	0.49
65:SM:18:LEU:HA	65:SM:21:VAL:HB	1.94	0.49
66:SN:52:VAL:HG23	66:SN:55:ARG:NH2	2.27	0.49
77:SY:27:VAL:CG2	77:SY:69:THR:HB	2.43	0.49
4:L5:462:G:H2'	4:L5:463:A:C8	2.48	0.49
4:L5:1080:C:H2'	4:L5:1081:C:H6	1.78	0.49
4:L5:2284:G:OP1	32:La:7:LYS:NZ	2.42	0.49
4:L5:2400:G:H21	38:Lg:6:THR:HG22	1.78	0.49
4:L5:2415:U:H2'	4:L5:2416:G:C8	2.48	0.49
4:L5:2671:C:H2'	4:L5:2672:C:C6	2.48	0.49
4:L5:2844:A:O2'	4:L5:4631:G:H4'	2.13	0.49
4:L5:4327:C:OP1	25:LT:70:HIS:NE2	2.45	0.49
8:LB:133:TYR:O	8:LB:136:LYS:HG2	2.12	0.49
13:LG:51:LEU:O	13:LG:55:VAL:HG23	2.13	0.49
13:LG:218:LEU:O	13:LG:222:ILE:HG12	2.12	0.49
21:LP:16:LYS:HG2	21:LP:149:ILE:HG12	1.95	0.49
23:LR:93:VAL:HA	23:LR:96:MET:HE3	1.95	0.49
25:LT:75:VAL:HG22	25:LT:88:ARG:HG2	1.95	0.49
47:Lp:64:VAL:HG11	47:Lp:71:TYR:HE1	1.77	0.49
52:S2:114:G:H5'	64:SL:132:ARG:HD3	1.94	0.49
52:S2:223:C:H2'	52:S2:224:A:C8	2.46	0.49
52:S2:1093:A:H2'	52:S2:1094:C:H6	1.76	0.49
52:S2:1199:A:H2'	52:S2:1200:A:C8	2.47	0.49
52:S2:1215:C:N4	94:S2:2056:HOH:O	2.43	0.49
52:S2:1589:A:N3	52:S2:1653:U:O2'	2.44	0.49
68:SP:24:GLN:OE1	68:SP:24:GLN:N	2.45	0.49
71:SS:51:ASP:HB3	71:SS:54:LYS:HE3	1.95	0.49
75:SW:111:MET:HE1	75:SW:119:LYS:HD2	1.95	0.49
4:L5:206:U:O2'	4:L5:208:A:N7	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:286:U:H2'	4:L5:287:U:C6	2.48	0.49
4:L5:497:G:N2	4:L5:498:C:H41	2.10	0.49
4:L5:1333:A:H2'	4:L5:1334:A:H8	1.77	0.49
4:L5:1733:G:N3	4:L5:4214:A:H2'	2.27	0.49
4:L5:1920:C:H3'	4:L5:1921:C:H5''	1.95	0.49
4:L5:1992:U:H4'	4:L5:1993:C:H5''	1.93	0.49
6:L8:5:U:H2'	6:L8:6:C:H6	1.78	0.49
10:LD:84:PRO:HG3	10:LD:89:LYS:HA	1.95	0.49
28:LW:7:SER:OG	28:LW:8:PHE:N	2.45	0.49
35:Ld:63:ARG:HD3	35:Ld:103:TYR:CD2	2.48	0.49
52:S2:834:C:N4	52:S2:839:C:H42	2.11	0.49
52:S2:1386:A:OP2	56:SD:160:SER:OG	2.22	0.49
52:S2:1409:A:H2'	52:S2:1410:C:C6	2.48	0.49
52:S2:1533:A:C8	52:S2:1604:G:H1'	2.47	0.49
55:SC:168:GLY:N	55:SC:179:THR:O	2.36	0.49
57:SE:94:LYS:NZ	77:SY:19:GLN:HE21	2.10	0.49
85:Sg:52:TYR:CE2	85:Sg:309:VAL:HG21	2.47	0.49
85:Sg:259:TRP:HE1	85:Sg:266:ILE:HG12	1.78	0.49
87:CA:162:GLN:HB3	87:CA:215[A]:LYS:HE2	1.95	0.49
3:CF:15:HIS:CE1	3:CF:132:GLN:H	2.31	0.49
3:CF:99:ILE:HG23	3:CF:100:LYS:HD2	1.95	0.49
4:L5:424:U:H2'	4:L5:425:U:C6	2.47	0.49
4:L5:4322:G:N2	4:L5:4325:A:OP2	2.39	0.49
15:LI:54:SER:HB3	15:LI:135:ILE:HD11	1.94	0.49
31:LZ:46:ILE:HD11	31:LZ:49:TYR:CE1	2.48	0.49
43:Ll:23:ILE:HG23	43:Ll:38:ASN:HB2	1.95	0.49
52:S2:295:C:H2'	52:S2:296:U:H6	1.78	0.49
56:SD:163:PRO:HG3	56:SD:205:PRO:HG2	1.94	0.49
69:SQ:21:ALA:O	69:SQ:87:SER:OG	2.25	0.49
71:SS:121:ARG:HG3	71:SS:131:VAL:HB	1.95	0.49
74:SV:38:GLU:OE1	74:SV:38:GLU:N	2.40	0.49
82:Sd:4:GLN:OE1	82:Sd:4:GLN:N	2.38	0.49
85:Sg:206:LEU:HD12	85:Sg:218:LEU:HD12	1.94	0.49
4:L5:457:G:H2'	4:L5:458:C:H6	1.77	0.49
4:L5:498:C:C2	4:L5:499:G:H1'	2.48	0.49
4:L5:4541:G:N2	4:L5:4544:A:OP2	2.37	0.49
4:L5:5006:U:H4'	4:L5:5007:A:H5'	1.94	0.49
14:LH:57:VAL:HG23	14:LH:70:VAL:HG13	1.94	0.49
15:LI:52:MET:HE1	15:LI:155:ALA:HB3	1.95	0.49
52:S2:219:U:H1'	61:SI:184:ARG:HD2	1.93	0.49
52:S2:1402:A:H5'	73:SU:51:LYS:NZ	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SG:194:LEU:HD13	59:SG:197:GLN:HE22	1.78	0.49
69:SQ:102:GLU:O	69:SQ:106:LYS:N	2.42	0.49
75:SW:11:LEU:HD21	75:SW:37:PHE:CE2	2.47	0.49
3:CF:250:LEU:HD11	3:CF:263:PRO:HB3	1.95	0.48
4:L5:381:U:H4'	4:L5:415:G:H5'	1.94	0.48
4:L5:2109:G:H2'	4:L5:2110:C:C6	2.48	0.48
4:L5:2306:G:H1'	4:L5:2332:A:N6	2.28	0.48
4:L5:3690:U:H2'	4:L5:3691:G:O4'	2.13	0.48
4:L5:3856:A:H5''	21:LP:83:TRP:O	2.13	0.48
7:LA:105:GLY:HA3	7:LA:160:SER:HB3	1.95	0.48
8:LB:397:ILE:HG13	8:LB:398:ALA:N	2.26	0.48
10:LD:238:GLU:HG3	10:LD:242:LYS:HZ2	1.78	0.48
15:LI:51:HIS:CD2	15:LI:168:SER:HB3	2.48	0.48
52:S2:1189:A:H2'	52:S2:1190:A:C8	2.47	0.48
52:S2:1201:U:H2'	52:S2:1202:U:C6	2.48	0.48
52:S2:1337:4AC:O5'	52:S2:1337:4AC:H6	2.13	0.48
59:SG:138:ALA:O	59:SG:142:ARG:HG3	2.13	0.48
64:SL:13:GLN:NE2	64:SL:35:ARG:HE	2.11	0.48
64:SL:75:GLY:HA3	64:SL:88:ILE:HD12	1.95	0.48
65:SM:58:GLU:OE1	65:SM:61:TYR:N	2.46	0.48
71:SS:5:ILE:HD11	71:SS:9:PHE:CD1	2.48	0.48
71:SS:25:LYS:HD2	71:SS:28:PHE:HD2	1.77	0.48
85:Sg:176:VAL:HG23	85:Sg:185:LYS:HB2	1.95	0.48
85:Sg:259:TRP:NE1	85:Sg:266:ILE:HG12	2.28	0.48
4:L5:2481:G:H2'	4:L5:2482:C:C6	2.48	0.48
4:L5:2543:A:H2	4:L5:2773:G:H22	1.62	0.48
4:L5:4919:G:H2'	4:L5:4920:C:C6	2.48	0.48
8:LB:57:VAL:HB	8:LB:367:PHE:HB3	1.95	0.48
21:LP:42:ARG:HH11	21:LP:42:ARG:HG2	1.78	0.48
50:Lt:117:ARG:HE	50:Lt:119:ARG:H	1.61	0.48
52:S2:65:C:C4	59:SG:133:LEU:HD12	2.48	0.48
52:S2:751:G:H1'	52:S2:793:G:H21	1.78	0.48
52:S2:1500:G:H2'	52:S2:1501:C:C6	2.47	0.48
52:S2:1738:C:OP1	59:SG:92:ARG:NH1	2.37	0.48
56:SD:116:ARG:HD3	56:SD:152:PHE:CZ	2.49	0.48
61:SI:44:HIS:N	94:SI:301:HOH:O	2.36	0.48
70:SR:29:HIS:HA	70:SR:32:LYS:HD2	1.95	0.48
72:ST:104:LEU:HD13	72:ST:121:ARG:HD2	1.96	0.48
3:CF:296:HIS:N	86:AT:77:A:O2'	2.41	0.48
3:CF:398:ASP:OD1	3:CF:398:ASP:N	2.47	0.48
4:L5:1081:C:O2'	4:L5:1082:C:H5'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:1269:G:O2'	4:L5:1440:U:O2'	2.18	0.48
4:L5:2008:U:H1'	4:L5:2011:C:H5	1.79	0.48
4:L5:2059:C:O2	24:LS:118:ARG:NH2	2.46	0.48
4:L5:2517:A:H5'	38:Lg:62:LYS:HD3	1.95	0.48
4:L5:3867:A2M:H2'	4:L5:3868:G:O4'	2.12	0.48
4:L5:4458:C:H2'	4:L5:4459:U:C6	2.47	0.48
4:L5:4481:U:H2'	4:L5:4482:U:C6	2.48	0.48
4:L5:4991:U:H2'	4:L5:4992:G:H8	1.79	0.48
19:LN:178:HIS:HA	19:LN:181:HIS:NE2	2.28	0.48
32:La:125:LYS:HG2	32:La:145:VAL:CG2	2.44	0.48
35:Ld:37:GLY:O	35:Ld:41:ARG:HG3	2.12	0.48
52:S2:300:U:H2'	52:S2:301:A:C8	2.49	0.48
52:S2:496:C:H2'	52:S2:497:C:H6	1.78	0.48
52:S2:511:U:H2'	52:S2:512:A:C8	2.49	0.48
52:S2:1511:U:H2'	52:S2:1512:C:C6	2.48	0.48
52:S2:1748:G:H1	52:S2:1786:U:H3	1.60	0.48
52:S2:1825:A:H61	86:AT:37:C:H42	1.61	0.48
59:SG:194:LEU:HA	59:SG:197:GLN:HE22	1.78	0.48
67:SO:56:VAL:HG23	67:SO:60:MET:SD	2.54	0.48
70:SR:59:LYS:O	70:SR:62:GLN:HG2	2.14	0.48
4:L5:1588:U:H2'	4:L5:1589:C:C6	2.48	0.48
4:L5:1977:C:O2'	4:L5:1978:C:OP1	2.27	0.48
4:L5:1997:U:H4'	49:Ls:44:ARG:HH12	1.78	0.48
4:L5:4921:C:O2'	4:L5:4922:C:H5'	2.13	0.48
8:LB:291:TYR:CE1	8:LB:299:ILE:HG23	2.48	0.48
20:LO:53:LYS:NZ	94:LO:302:HOH:O	2.45	0.48
43:Ll:25:GLN:OE1	43:Ll:28:ARG:NH2	2.46	0.48
52:S2:441:C:H2'	52:S2:442:C:C6	2.48	0.48
52:S2:1017:U:H2'	52:S2:1018:U:H6	1.78	0.48
52:S2:1020:A:OP2	66:SN:70:LYS:NZ	2.40	0.48
52:S2:1252:C:H42	69:SQ:146:ARG:C	2.21	0.48
52:S2:1289:U:OP2	84:Sf:97:LYS:NZ	2.41	0.48
52:S2:1671:G:H2'	52:S2:1672:U:H6	1.77	0.48
52:S2:1825:A:N6	86:AT:37:C:H42	2.12	0.48
53:SA:22:GLY:O	53:SA:24:HIS:N	2.43	0.48
55:SC:64:THR:HG22	55:SC:66:LEU:H	1.78	0.48
57:SE:252:ARG:O	57:SE:256:LEU:HG	2.13	0.48
68:SP:74:GLU:OE1	68:SP:74:GLU:N	2.42	0.48
72:ST:57:ALA:HA	72:ST:60:THR:HG22	1.95	0.48
85:Sg:249:CYS:HB3	85:Sg:258:ILE:HD13	1.95	0.48
4:L5:148:C:OP2	13:LG:197:LYS:NZ	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:1273:G:C8	33:Lb:117:ARG:NH1	2.82	0.48
4:L5:1366:G:OP2	17:LL:36:ARG:NH2	2.45	0.48
4:L5:1378:C:N4	17:LL:159:ASN:O	2.42	0.48
4:L5:1961:G:O2'	4:L5:2025:A:N6	2.46	0.48
6:L8:47:C:H1'	6:L8:61:A:H2'	1.94	0.48
6:L8:144:U:H2'	6:L8:145:C:C6	2.48	0.48
48:Lr:38:PHE:O	48:Lr:45:HIS:NE2	2.38	0.48
52:S2:508:A:H3'	52:S2:509:OMG:C8	2.44	0.48
52:S2:731:G:H5'	52:S2:732:U:OP1	2.14	0.48
52:S2:1206:G:O2'	52:S2:1208:A:OP1	2.27	0.48
57:SE:79:ASP:HB3	57:SE:82:TYR:HB2	1.95	0.48
71:SS:20:ILE:HG22	71:SS:32:ALA:HB3	1.95	0.48
72:ST:135:ALA:HA	72:ST:138:VAL:HG12	1.94	0.48
85:Sg:44:LYS:HG2	85:Sg:46:THR:HG23	1.95	0.48
86:AT:15:G:H2'	86:AT:60:A:H61	1.79	0.48
4:L5:1241:C:O2'	33:Lb:120:ARG:O	2.31	0.48
4:L5:1298:C:H2'	4:L5:1299:G:C8	2.47	0.48
4:L5:1601:A:OP1	41:Lj:5:THR:OG1	2.21	0.48
4:L5:1847:C:H2'	4:L5:1848:C:C6	2.48	0.48
4:L5:3718:A2M:H2	4:L5:3934:G:O4'	2.14	0.48
4:L5:4098:A:N6	4:L5:4099:G:H21	2.11	0.48
4:L5:4363:A:H5''	46:Lo:36:GLN:HG2	1.94	0.48
4:L5:4425:G:OP1	44:Lm:100:TYR:OH	2.21	0.48
7:LA:53:GLY:O	7:LA:192:LYS:NZ	2.45	0.48
11:LE:223:ARG:NE	11:LE:234:ASP:O	2.47	0.48
14:LH:104:VAL:HB	14:LH:113:GLU:HB2	1.94	0.48
52:S2:325:C:H3'	52:S2:326:C:H4'	1.96	0.48
52:S2:595:U:H2'	52:S2:596:U:C6	2.49	0.48
52:S2:929:G:H2'	52:S2:930:C:O4'	2.13	0.48
52:S2:1390:U:H2'	52:S2:1391:OMC:C6	2.48	0.48
85:Sg:166:VAL:HG12	85:Sg:176:VAL:HG12	1.96	0.48
3:CF:430:ARG:HD3	86:AT:65:G:C5'	2.37	0.48
4:L5:308:G:O6	19:LN:12:ARG:NH1	2.47	0.48
4:L5:702:U:H2'	4:L5:703:G:O4'	2.14	0.48
4:L5:1214:C:N3	33:Lb:90:SER:OG	2.47	0.48
4:L5:4954:G:H2'	4:L5:4955:A:C8	2.49	0.48
11:LE:227:HIS:HE1	11:LE:230:GLY:HA2	1.79	0.48
31:LZ:57:MET:CG	31:LZ:61:LYS:HD3	2.43	0.48
52:S2:1422:G:C4	52:S2:1424:G:C8	3.01	0.48
52:S2:1447:G:H1'	73:SU:55:ARG:HH12	1.79	0.48
59:SG:38:ALA:O	59:SG:45:TRP:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SH:10:LYS:HE2	60:SH:20:GLU:OE1	2.13	0.48
72:ST:34:VAL:HA	72:ST:52:TRP:HZ2	1.78	0.48
3:CF:294:MET:HG2	3:CF:299:LEU:HD11	1.95	0.48
4:L5:1806:G:H2'	4:L5:1807:C:H6	1.78	0.48
4:L5:2749:C:H2'	4:L5:2750:G:C8	2.49	0.48
4:L5:4122:G:H4'	38:Lg:90:ARG:HG2	1.96	0.48
4:L5:5015:G:H2'	4:L5:5016:A:C2	2.48	0.48
20:LO:54:TYR:OH	20:LO:73:PHE:O	2.30	0.48
37:Lf:41:PHE:HE1	37:Lf:110:ILE:HD13	1.78	0.48
57:SE:131:VAL:HA	57:SE:137:PRO:HA	1.94	0.48
57:SE:204:SER:OG	57:SE:205:PHE:N	2.47	0.48
58:SF:30:ILE:HG13	58:SF:113:VAL:HG11	1.95	0.48
61:SI:141:ARG:HA	61:SI:141:ARG:CZ	2.44	0.48
65:SM:56:CYS:HB3	65:SM:62:VAL:HG13	1.95	0.48
67:SO:33:ILE:HG22	67:SO:42:VAL:HA	1.95	0.48
69:SQ:93:VAL:O	69:SQ:97:GLN:HB2	2.13	0.48
77:SY:45:ALA:HB1	77:SY:50:THR:O	2.14	0.48
4:L5:465:G:H2'	4:L5:466:A:C8	2.49	0.48
4:L5:1348:U:H2'	4:L5:1349:G:H8	1.79	0.48
4:L5:2520:C:H2'	4:L5:2521:G:C8	2.49	0.48
4:L5:3697:U:H5''	4:L5:3698:G:H5'	1.96	0.48
4:L5:4742:G:H2'	4:L5:4743:G:H8	1.78	0.48
89:L5:5259:SPM:H32	25:LT:13:TYR:CD1	2.49	0.48
14:LH:51:LYS:HG3	14:LH:52:LYS:N	2.28	0.48
19:LN:176:LYS:NZ	94:LN:411:HOH:O	2.47	0.48
42:Lk:12:LEU:HB3	42:Lk:16:ARG:HH21	1.79	0.48
49:Ls:29:ILE:HG13	49:Ls:29:ILE:O	2.13	0.48
50:Lt:150:ASP:OD1	50:Lt:151:ILE:N	2.47	0.48
52:S2:815:U:C2	52:S2:816:A:C8	3.02	0.48
53:SA:42:LYS:HG2	53:SA:46:ILE:O	2.14	0.48
56:SD:116:ARG:HD3	56:SD:152:PHE:HZ	1.79	0.48
56:SD:163:PRO:HA	56:SD:166:TYR:CE1	2.48	0.48
57:SE:122:LYS:N	57:SE:162:ILE:O	2.39	0.48
87:CA:23:MET:HE2	87:CA:63:ILE:HG13	1.96	0.48
3:CF:272:LEU:HB3	3:CF:302:ALA:HB3	1.95	0.48
4:L5:423:G:H2'	4:L5:424:U:C6	2.49	0.48
4:L5:705:G:H2'	4:L5:706:C:C6	2.49	0.48
4:L5:712:C:OP1	11:LE:139:LYS:HE3	2.14	0.48
4:L5:3661:G:N7	7:LA:152:SER:OG	2.43	0.48
4:L5:3954:A:O2'	4:L5:4058:U:OP1	2.27	0.48
5:L7:4:U:H2'	5:L7:5:A:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L7:110:G:H2'	5:L7:111:C:C6	2.48	0.48
6:L8:66:A:H2'	6:L8:67:U:C6	2.48	0.48
15:LI:102:MET:HB3	15:LI:112:GLN:HE22	1.79	0.48
31:LZ:68:ILE:HD12	31:LZ:119:GLU:HG2	1.96	0.48
52:S2:5:U:H2'	52:S2:6:G:H8	1.79	0.48
52:S2:138:C:OP2	52:S2:1774:C:O2'	2.29	0.48
52:S2:690:G:OP2	52:S2:690:G:N2	2.45	0.48
52:S2:989:C:OP2	54:SB:155:TYR:OH	2.27	0.48
52:S2:1617:G:N1	52:S2:1620:A:OP2	2.46	0.48
52:S2:1673:U:O2'	58:SF:84:GLY:O	2.18	0.48
56:SD:5:ILE:HD11	56:SD:9:ARG:HD3	1.95	0.48
57:SE:61:VAL:HA	57:SE:64:ILE:HG22	1.95	0.48
58:SF:30:ILE:HB	58:SF:36:GLN:HG2	1.95	0.48
65:SM:20:GLU:OE2	65:SM:119:GLN:HB2	2.14	0.48
66:SN:66:VAL:HG13	66:SN:67:THR:HG23	1.96	0.48
70:SR:98:VAL:O	70:SR:120:THR:N	2.47	0.48
71:SS:43:VAL:HG11	71:SS:83:PHE:HE2	1.79	0.48
71:SS:60:THR:O	71:SS:64:VAL:HG23	2.14	0.48
3:CF:35:ASP:OD1	3:CF:35:ASP:N	2.43	0.47
3:CF:184:ASN:HB2	3:CF:187:THR:OG1	2.14	0.47
4:L5:318:A:H2'	4:L5:319:A:H8	1.78	0.47
4:L5:1558:A:H2'	4:L5:1559:G:H8	1.79	0.47
4:L5:2749:C:H2'	4:L5:2750:G:H8	1.78	0.47
4:L5:3799:A:N3	4:L5:4506:C:O2'	2.39	0.47
4:L5:4636:PSU:N1	35:Ld:79:ASN:OD1	2.45	0.47
6:L8:70:G:H5''	30:LY:27:ARG:CZ	2.44	0.47
6:L8:148:A:H2'	6:L8:149:G:C8	2.49	0.47
33:Lb:116:LEU:HG	33:Lb:117:ARG:NH2	2.29	0.47
50:Lt:114:ARG:HD3	50:Lt:133:LEU:HD22	1.95	0.47
52:S2:291:G:H2'	52:S2:292:A:C8	2.48	0.47
52:S2:484:A2M:H8	52:S2:484:A2M:O5'	2.13	0.47
52:S2:1733:U:H2'	52:S2:1734:G:O4'	2.14	0.47
56:SD:195:THR:HG22	56:SD:197:LYS:HG2	1.94	0.47
60:SH:37:LYS:HB3	60:SH:41:ARG:HH21	1.79	0.47
67:SO:33:ILE:HG13	67:SO:97:LEU:HD23	1.96	0.47
4:L5:85:G:O2'	4:L5:97:G:O6	2.25	0.47
4:L5:1357:C:H2'	4:L5:1358:G:H5''	1.96	0.47
4:L5:1669:A:OP1	33:Lb:18:ARG:NH2	2.36	0.47
4:L5:2279:A:O2'	36:Le:48:ARG:NH2	2.47	0.47
4:L5:3610:A:H2'	4:L5:3611:A:H8	1.79	0.47
4:L5:3684:G:H2'	4:L5:3685:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:4318:C:O2'	46:Lo:18:HIS:ND1	2.40	0.47
8:LB:117:ARG:HG2	8:LB:180:LEU:HD12	1.95	0.47
9:LC:150:LEU:O	9:LC:152:LEU:N	2.47	0.47
13:LG:162:ASP:HB3	13:LG:163:PRO:HD3	1.96	0.47
49:Ls:114:GLY:HA2	49:Ls:166:LYS:HD2	1.95	0.47
52:S2:985:G:H1'	67:SO:138:ASP:OD1	2.14	0.47
52:S2:1711:U:H2'	52:S2:1712:A:C8	2.49	0.47
53:SA:120:ARG:HD2	55:SC:266:TYR:HB3	1.97	0.47
60:SH:18:GLU:C	60:SH:20:GLU:H	2.22	0.47
60:SH:145:ARG:HD2	60:SH:155:LYS:NZ	2.28	0.47
62:SJ:104:ASP:HA	62:SJ:107:GLU:HG3	1.96	0.47
86:AT:7:G:O2'	86:AT:50:C:OP2	2.29	0.47
4:L5:159:C:H5''	40:Li:25:ARG:NH2	2.29	0.47
4:L5:179:G:H2'	4:L5:180:C:C6	2.49	0.47
4:L5:1332:C:H2'	4:L5:1333:A:C8	2.50	0.47
4:L5:1340:OMC:HM23	4:L5:1340:OMC:H1'	1.69	0.47
4:L5:1734:G:N2	4:L5:1735:U:O4	2.33	0.47
4:L5:2743:A:H2'	4:L5:2744:A:C8	2.49	0.47
4:L5:3848:U:H2'	4:L5:3849:A:H8	1.79	0.47
4:L5:4339:A:H2'	4:L5:4340:U:H6	1.79	0.47
4:L5:4578:G:H2'	4:L5:4579:PSU:H6	1.80	0.47
4:L5:5062:G:H2'	4:L5:5063:G:H8	1.79	0.47
7:LA:117:GLU:O	7:LA:162:ASN:ND2	2.39	0.47
25:LT:122:LYS:HZ3	25:LT:124:THR:HG22	1.79	0.47
28:LW:35:LYS:HE3	28:LW:51:TRP:CZ2	2.49	0.47
28:LW:89:ASP:O	28:LW:93:LYS:HG2	2.15	0.47
31:LZ:50:PRO:HD3	31:LZ:68:ILE:HG12	1.96	0.47
52:S2:1264:C:P	82:Sd:28:HIS:HE2	2.38	0.47
55:SC:92:GLU:OE1	55:SC:92:GLU:N	2.39	0.47
59:SG:67:VAL:HG12	59:SG:69:THR:HG22	1.96	0.47
65:SM:44:LYS:HE3	84:Sf:129:GLY:HA3	1.96	0.47
68:SP:81:ARG:HH12	68:SP:122:THR:HG22	1.80	0.47
69:SQ:9:SER:OG	69:SQ:25:CYS:O	2.22	0.47
70:SR:53:TYR:CZ	70:SR:57:LEU:HD21	2.50	0.47
71:SS:42:HIS:CE1	72:ST:45:LEU:HD21	2.48	0.47
75:SW:45:GLY:O	75:SW:68:ARG:HD2	2.15	0.47
87:CA:49:CYS:HB3	87:CA:281:ARG:NH2	2.29	0.47
4:L5:257:C:H2'	4:L5:258:G:C8	2.48	0.47
4:L5:268:G:H2'	4:L5:269:G:C8	2.46	0.47
4:L5:485:C:O2	4:L5:485:C:H2'	2.13	0.47
4:L5:2481:G:H2'	4:L5:2482:C:H6	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:3666:C:OP1	7:LA:234:LYS:NZ	2.47	0.47
7:LA:131:GLY:H	7:LA:169:VAL:HG13	1.78	0.47
7:LA:140:ASN:ND2	7:LA:142:GLU:OE2	2.48	0.47
22:LQ:43:PHE:CD2	22:LQ:133:GLY:HA3	2.49	0.47
46:Lo:74:GLU:OE1	46:Lo:76:ASN:HB2	2.14	0.47
52:S2:84:A:H5''	77:SY:124:ASN:ND2	2.29	0.47
52:S2:909:G:H2'	52:S2:910:G:C8	2.48	0.47
52:S2:1037:G:H4'	52:S2:1845:A:H4'	1.95	0.47
52:S2:1235:G:N2	68:SP:135:ALA:HB2	2.29	0.47
69:SQ:44:PRO:HG2	69:SQ:81:ILE:HD11	1.96	0.47
73:SU:35:VAL:O	73:SU:39:LEU:HD23	2.14	0.47
84:Sf:90:LYS:HD2	84:Sf:90:LYS:HA	1.69	0.47
2:CI:55:LEU:HB3	26:LU:99:TRP:CE2	2.49	0.47
4:L5:4742:G:H2'	4:L5:4743:G:C8	2.49	0.47
17:LL:80:GLU:HG3	17:LL:110:LEU:HD12	1.97	0.47
27:LV:73:ARG:NH2	94:LV:308:HOH:O	2.48	0.47
49:Ls:134:LYS:HD2	49:Ls:137:PHE:HE2	1.79	0.47
52:S2:300:U:H2'	52:S2:301:A:H8	1.77	0.47
52:S2:352:U:H2'	52:S2:353:C:C6	2.49	0.47
52:S2:550:C:H2'	52:S2:551:U:C6	2.48	0.47
52:S2:659:G:H21	76:SX:17:ARG:HH22	1.62	0.47
52:S2:661:U:OP2	76:SX:3:LYS:NZ	2.46	0.47
52:S2:1215:C:O2'	52:S2:1645:C:OP2	2.30	0.47
52:S2:1713:C:H2'	52:S2:1714:U:C6	2.50	0.47
64:SL:6:THR:N	64:SL:7:GLU:OE1	2.47	0.47
73:SU:68:THR:O	82:Sd:40:ARG:NH1	2.46	0.47
85:Sg:191:HIS:ND1	85:Sg:195:LEU:HD21	2.30	0.47
87:CA:191:LYS:HE3	87:CA:194:VAL:HG21	1.96	0.47
4:L5:1199:G:H2'	4:L5:1200:G:C8	2.50	0.47
4:L5:1998:A:H4'	49:Ls:9:TRP:CZ2	2.49	0.47
4:L5:2417:A:H2'	4:L5:2418:A:H8	1.78	0.47
4:L5:2676:A:OP2	4:L5:2676:A:H8	1.98	0.47
4:L5:4291:G:H4'	4:L5:4292:A:H5''	1.96	0.47
4:L5:4653:C:H2'	4:L5:4654:C:C6	2.49	0.47
13:LG:52:THR:HG22	29:LX:41:ARG:HG3	1.97	0.47
28:LW:52:THR:HG22	28:LW:54:LEU:H	1.79	0.47
34:Lc:49:ALA:HB1	34:Lc:77:ASN:HA	1.97	0.47
51:Pt:74:C:O2'	51:Pt:75:C:H5'	2.14	0.47
52:S2:77:A:O2'	59:SG:174:PRO:O	2.32	0.47
52:S2:454:U:H2'	52:S2:455:A:H8	1.79	0.47
52:S2:1270:G:O2'	52:S2:1301:A:N7	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:1305:C:H2'	52:S2:1306:U:C5	2.49	0.47
52:S2:1864:U:H5'	79:Sa:79:ILE:HD11	1.97	0.47
53:SA:24:HIS:HA	53:SA:49:ILE:HG12	1.97	0.47
58:SF:22:LYS:HD2	58:SF:23:TRP:CE2	2.50	0.47
60:SH:143:ARG:HB2	60:SH:155:LYS:HB2	1.95	0.47
68:SP:60:LEU:HD23	68:SP:89:MET:HG2	1.97	0.47
70:SR:128:PHE:O	70:SR:129:LYS:HB2	2.14	0.47
71:SS:43:VAL:CG1	71:SS:83:PHE:HE2	2.28	0.47
1:CD:31:LEU:HD21	38:Lg:105:LYS:HD3	1.95	0.47
3:CF:162:TYR:HE2	3:CF:208:MET:HE2	1.80	0.47
3:CF:231:ALA:O	3:CF:235:ILE:HG23	2.14	0.47
3:CF:250:LEU:N	3:CF:324:ASN:O	2.43	0.47
4:L5:369:G:N2	4:L5:372:A:OP2	2.41	0.47
4:L5:685:C:H5'	11:LE:101:ASN:HD22	1.79	0.47
4:L5:3928:A:H2'	4:L5:3929:G:O4'	2.13	0.47
4:L5:4345:C:H2'	4:L5:4346:U:C6	2.50	0.47
4:L5:4508:C:N3	4:L5:4512:U:H5	2.12	0.47
4:L5:4638:U:H2'	4:L5:4639:G:N3	2.30	0.47
4:L5:4769:G:H5''	20:LO:176:ARG:HD3	1.97	0.47
4:L5:4769:G:OP1	20:LO:176:ARG:NH1	2.44	0.47
4:L5:4940:C:H5'	4:L5:4941:G:H5''	1.95	0.47
9:LC:109:ARG:O	9:LC:109:ARG:HG2	2.14	0.47
9:LC:110:ARG:O	9:LC:113:ARG:NH1	2.44	0.47
10:LD:33:ARG:NH1	10:LD:50:ARG:HH12	2.12	0.47
14:LH:45:LEU:CD2	14:LH:57:VAL:HG12	2.45	0.47
17:LL:81:LEU:HD11	17:LL:98:VAL:CG1	2.44	0.47
18:LM:24:LEU:HD11	18:LM:86:TRP:CG	2.49	0.47
21:LP:114:ILE:HG12	21:LP:150:LEU:HD22	1.95	0.47
26:LU:18:VAL:HG12	26:LU:20:LYS:HB2	1.95	0.47
26:LU:62:THR:OG1	26:LU:73:THR:HB	2.15	0.47
28:LW:78:PHE:CE2	59:SG:9:ALA:HA	2.49	0.47
46:Lo:32:SER:C	46:Lo:34:TYR:H	2.23	0.47
52:S2:65:C:N4	59:SG:136:LYS:HB2	2.29	0.47
52:S2:1058:A:H2'	52:S2:1059:G:C8	2.50	0.47
52:S2:1088:U:H4'	52:S2:1089:G:OP2	2.12	0.47
52:S2:1220:A:N3	52:S2:1677:U:O2'	2.41	0.47
52:S2:1452:A:OP2	70:SR:32:LYS:NZ	2.48	0.47
52:S2:1597:C:OP2	78:SZ:85:ARG:NH2	2.36	0.47
52:S2:1648:G:O2'	52:S2:1674:G:O6	2.28	0.47
53:SA:38:ILE:HD11	53:SA:47:TYR:HB3	1.95	0.47
55:SC:183:LYS:HA	55:SC:195:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SF:22:LYS:HG3	58:SF:23:TRP:CD2	2.49	0.47
58:SF:39:ILE:HD12	58:SF:68:ILE:HD12	1.95	0.47
59:SG:152:ASP:OD2	59:SG:155:GLN:HB2	2.14	0.47
59:SG:218:LYS:O	59:SG:222:GLU:HG2	2.15	0.47
60:SH:51:ILE:HG21	60:SH:179:LYS:HG2	1.95	0.47
61:SI:66:SER:HA	61:SI:73:THR:HA	1.97	0.47
62:SJ:93:LYS:HB2	62:SJ:96:TYR:CD2	2.49	0.47
66:SN:87:ASP:OD1	66:SN:88:LEU:N	2.48	0.47
71:SS:129:LEU:HD23	71:SS:144:ARG:HH21	1.78	0.47
73:SU:20:ILE:HG13	73:SU:116:ILE:HG22	1.96	0.47
79:Sa:38:LYS:HB2	79:Sa:71:LEU:HB2	1.97	0.47
4:L5:683:C:H2'	4:L5:684:G:O4'	2.14	0.47
4:L5:1097:C:H2'	4:L5:1098:G:C8	2.49	0.47
4:L5:1503:A:N6	22:LQ:87:THR:HG21	2.26	0.47
4:L5:1998:A:H2'	4:L5:1999:A:C8	2.49	0.47
13:LG:161:VAL:HG21	13:LG:200:THR:HG23	1.97	0.47
15:LI:179:ASP:OD1	15:LI:180:GLU:HG3	2.15	0.47
52:S2:1093:A:H2'	52:S2:1094:C:C6	2.49	0.47
52:S2:1648:G:C8	69:SQ:125:ARG:HG3	2.50	0.47
52:S2:1754:G:OP1	52:S2:1780:G:N2	2.48	0.47
56:SD:32:ASP:OD2	56:SD:65:ARG:NH1	2.48	0.47
56:SD:45:ARG:HB2	56:SD:83:SER:O	2.14	0.47
57:SE:246:LEU:HB2	57:SE:250:GLU:CG	2.45	0.47
63:SK:3:MET:HE1	63:SK:48:ALA:HB2	1.96	0.47
63:SK:15:LEU:HD22	63:SK:49:MET:HE1	1.97	0.47
64:SL:13:GLN:HB2	64:SL:16:ILE:HD12	1.96	0.47
68:SP:29:SER:OG	68:SP:30:TYR:N	2.47	0.47
84:Sf:105:TYR:CD2	84:Sf:118:ARG:HG2	2.48	0.47
85:Sg:201:SER:HB3	85:Sg:206:LEU:HB2	1.96	0.47
85:Sg:270:LEU:HD13	85:Sg:310:TRP:CD2	2.49	0.47
86:AT:9:A:O2'	86:AT:10:G:N7	2.44	0.47
87:CA:17:VAL:HA	87:CA:20:LYS:HZ2	1.78	0.47
3:CF:268:GLU:OE1	3:CF:268:GLU:N	2.47	0.47
4:L5:423:G:H5'	21:LP:26:PHE:HZ	1.79	0.47
4:L5:490:C:H2'	4:L5:491:G:C8	2.50	0.47
4:L5:1589:C:H2'	4:L5:1590:C:C6	2.50	0.47
4:L5:4401:G:H2'	4:L5:4402:C:C6	2.50	0.47
4:L5:4749:C:H2'	4:L5:4750:G:O4'	2.14	0.47
8:LB:163:ILE:HG22	8:LB:180:LEU:HD22	1.97	0.47
9:LC:266:THR:HG22	9:LC:267:TRP:N	2.30	0.47
20:LO:3:GLU:OE2	20:LO:5:GLN:NE2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LO:166:ILE:HG22	20:LO:170:LYS:HE2	1.96	0.47
41:Lj:27:TYR:HA	41:Lj:34:CYS:HA	1.97	0.47
49:Ls:29:ILE:HD11	49:Ls:191:GLN:HG2	1.96	0.47
50:Lt:19:GLY:CA	50:Lt:48:LYS:HZ3	2.27	0.47
52:S2:38:A:OP1	62:SJ:5:ARG:HG3	2.14	0.47
52:S2:808:A:H2	52:S2:855:G:H22	1.63	0.47
52:S2:1788:A:H2'	52:S2:1789:G:O4'	2.15	0.47
55:SC:138:GLY:HA3	55:SC:162:ILE:HD13	1.95	0.47
62:SJ:110:LEU:O	62:SJ:114:VAL:HG22	2.14	0.47
66:SN:31:ASP:OD1	66:SN:31:ASP:N	2.48	0.47
72:ST:114:GLU:HB3	72:ST:124:THR:HG22	1.97	0.47
77:SY:36:PRO:HB2	77:SY:39:GLU:OE1	2.15	0.47
85:Sg:199:THR:HG21	85:Sg:239:LEU:O	2.15	0.47
4:L5:2570:U:H2'	4:L5:2571:C:C6	2.50	0.47
4:L5:3690:U:H5''	4:L5:3819:G:OP2	2.14	0.47
4:L5:4587:G:O2'	8:LB:17:LEU:HD12	2.15	0.47
4:L5:4896:G:H2'	4:L5:4897:G:H8	1.80	0.47
7:LA:171:GLY:O	47:Lp:68:ALA:HB2	2.14	0.47
10:LD:64:ILE:HD13	10:LD:109:LEU:HD22	1.97	0.47
13:LG:205:THR:HG22	13:LG:206:GLN:N	2.24	0.47
16:LJ:90:ARG:NH2	16:LJ:108:GLY:O	2.48	0.47
52:S2:1019:C:H2'	52:S2:1020:A:O4'	2.15	0.47
52:S2:1120:U:H5'	80:Sb:72:ARG:NH1	2.28	0.47
52:S2:1232:PSU:H2'	52:S2:1233:G:H8	1.80	0.47
52:S2:1337:4AC:H2'	52:S2:1338:G:C8	2.50	0.47
52:S2:1832:6MZ:H9C2	52:S2:1833:C:H41	1.79	0.47
53:SA:157:VAL:O	74:SV:65:SER:OG	2.32	0.47
58:SF:73:THR:O	58:SF:89:THR:HG21	2.15	0.47
60:SH:134:VAL:HG23	60:SH:173:PHE:CE2	2.49	0.47
68:SP:130:ARG:HD3	68:SP:131:PRO:HD2	1.96	0.47
75:SW:11:LEU:HD12	75:SW:74:VAL:HB	1.96	0.47
3:CF:95:HIS:HB2	3:CF:98:PHE:HD2	1.79	0.46
3:CF:342:ALA:HB2	3:CF:438:ILE:HG12	1.96	0.46
4:L5:734:G:C2	4:L5:735:G:C8	3.03	0.46
4:L5:919:C:OP1	18:LM:69:HIS:ND1	2.46	0.46
4:L5:2411:C:H2'	4:L5:2412:A:C8	2.50	0.46
4:L5:3720:G:H22	4:L5:3733:A:H2	1.62	0.46
4:L5:4101:C:H4'	4:L5:4109:G:H1	1.80	0.46
4:L5:4928:C:H2'	4:L5:4929:C:C6	2.50	0.46
9:LC:195:LYS:HB3	9:LC:200:ARG:HE	1.80	0.46
25:LT:48:VAL:HG21	25:LT:94:GLU:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LU:112:LEU:HD23	26:LU:112:LEU:H	1.80	0.46
42:Lk:26:LYS:HD3	42:Lk:69:LEU:HD22	1.97	0.46
52:S2:149:A:H3'	52:S2:150:A:H8	1.79	0.46
52:S2:512:A:C2	52:S2:513:G:C8	3.03	0.46
52:S2:730:C:OP2	52:S2:734:C:N4	2.47	0.46
52:S2:1433:C:N4	73:SU:49:LYS:HZ1	2.14	0.46
55:SC:212:LYS:O	55:SC:216:MET:HG2	2.14	0.46
57:SE:39:ARG:HB2	57:SE:40:GLU:OE1	2.16	0.46
60:SH:159:ASP:O	60:SH:160:LYS:HB3	2.15	0.46
64:SL:152:LYS:HD2	64:SL:152:LYS:N	2.29	0.46
65:SM:89:VAL:HG13	65:SM:91:LEU:HG	1.96	0.46
4:L5:458:C:OP2	11:LE:114:ARG:NH1	2.48	0.46
4:L5:1076:C:H2'	4:L5:1077:C:C6	2.50	0.46
4:L5:1095:A:N1	4:L5:1200:G:C6	2.84	0.46
4:L5:1462:A:H4'	33:Lb:27:GLN:NE2	2.31	0.46
4:L5:1870:C:H2'	4:L5:1871:A2M:H8	1.97	0.46
4:L5:2521:G:H5'	4:L5:2640:G:H1'	1.97	0.46
4:L5:3607:U:H2'	4:L5:3608:A:H8	1.79	0.46
4:L5:3610:A:H2'	4:L5:3611:A:C8	2.50	0.46
4:L5:4364:G:H2'	4:L5:4365:C:C6	2.50	0.46
4:L5:4723:A:H2'	4:L5:4724:A:C8	2.50	0.46
4:L5:4954:G:H2'	4:L5:4955:A:H8	1.79	0.46
4:L5:4991:U:H2'	4:L5:4992:G:C8	2.50	0.46
22:LQ:35:LEU:O	22:LQ:39:THR:OG1	2.21	0.46
43:Ll:9:ILE:HD12	43:Ll:51:LEU:HD12	1.97	0.46
52:S2:804:U:H2'	52:S2:805:U:C6	2.51	0.46
52:S2:862:A:C8	75:SW:107:SER:HA	2.50	0.46
52:S2:880:G:H2'	52:S2:881:G:O4'	2.14	0.46
64:SL:28:THR:OG1	64:SL:31:GLU:OE2	2.21	0.46
72:ST:127:GLY:O	72:ST:131:LEU:HD23	2.16	0.46
3:CF:186:ASP:OD2	3:CF:217:THR:HB	2.15	0.46
3:CF:377:GLU:OE1	3:CF:378:LYS:N	2.47	0.46
4:L5:116:G:H2'	4:L5:117:C:C6	2.50	0.46
4:L5:138:G:H2'	4:L5:139:G:C8	2.49	0.46
4:L5:1100:U:H1'	4:L5:1167:C:H42	1.80	0.46
4:L5:1613:A:H5''	7:LA:183:GLY:HA3	1.97	0.46
4:L5:3727:A:H2'	4:L5:3728:A:C8	2.50	0.46
4:L5:3871:A:H2'	4:L5:3872:A:C8	2.49	0.46
4:L5:3922[A]:G:H4'	4:L5:3923:A:OP2	2.14	0.46
4:L5:4688:C:H2'	4:L5:4689:PSU:C6	2.50	0.46
8:LB:71:GLU:OE2	8:LB:366:LYS:NZ	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LC:334:THR:HG21	12:LF:51:TYR:OH	2.13	0.46
10:LD:152:ARG:HG3	10:LD:154:THR:HG23	1.97	0.46
11:LE:150:LEU:HD11	11:LE:164:PHE:HB2	1.97	0.46
19:LN:140:LYS:HD3	19:LN:140:LYS:HA	1.66	0.46
21:LP:112:LEU:HD23	21:LP:150:LEU:HD12	1.97	0.46
32:La:93:ASN:ND2	32:La:97:ALA:HB3	2.30	0.46
38:Lg:69:LYS:HG3	38:Lg:73:HIS:HD2	1.80	0.46
52:S2:126:G:OP2	59:SG:198:ARG:NH2	2.48	0.46
52:S2:162:C:H2'	52:S2:163:U:O4'	2.16	0.46
52:S2:388:U:H2'	52:S2:389:A:H8	1.79	0.46
52:S2:672:A:OP2	89:S2:1929:SPM:N1	2.48	0.46
52:S2:945:U:H2'	52:S2:946:U:C6	2.51	0.46
54:SB:71:LEU:HD21	54:SB:189:ILE:HG23	1.98	0.46
59:SG:181:THR:HB	59:SG:184:VAL:HG23	1.97	0.46
59:SG:231:ARG:O	59:SG:235:SER:OG	2.34	0.46
65:SM:20:GLU:HA	65:SM:23:LYS:HB3	1.97	0.46
65:SM:35:ILE:HG13	65:SM:61:TYR:HE1	1.81	0.46
73:SU:80:PHE:HB3	82:Sd:52:PHE:HB3	1.98	0.46
87:CA:64:PHE:HB2	87:CA:72:LYS:HE3	1.97	0.46
4:L5:2864:A:H2'	4:L5:2865:U:C6	2.50	0.46
4:L5:4070:U:H2'	4:L5:4071:U:H6	1.79	0.46
4:L5:4258:C:H2'	4:L5:4259:C:H6	1.81	0.46
4:L5:4507:A:H2'	4:L5:4508:C:C6	2.50	0.46
4:L5:4873:G:N2	20:LO:172:LYS:HG2	2.31	0.46
6:L8:6:C:H2'	6:L8:7:U:H6	1.81	0.46
8:LB:50:LYS:HB2	8:LB:345:LEU:HD11	1.96	0.46
10:LD:181:PRO:HD2	10:LD:195:HIS:CD2	2.51	0.46
14:LH:43:VAL:HG21	14:LH:73:ILE:HD13	1.98	0.46
15:LI:103:LEU:N	15:LI:112:GLN:OE1	2.48	0.46
16:LJ:16:ARG:NH1	16:LJ:18:ARG:HG2	2.30	0.46
22:LQ:12:LYS:HB2	22:LQ:14:ARG:NH1	2.31	0.46
29:LX:82:THR:HG21	39:Lh:37:THR:HG22	1.96	0.46
38:Lg:41:ALA:O	38:Lg:52:ARG:HD3	2.15	0.46
52:S2:323:C:O2	52:S2:327:G:N2	2.49	0.46
52:S2:370:G:O2'	61:SI:10:LYS:NZ	2.48	0.46
52:S2:943:U:OP1	54:SB:214:LYS:NZ	2.40	0.46
52:S2:1408:U:C2	52:S2:1409:A:C8	3.04	0.46
52:S2:1464:C:O3'	70:SR:60:ARG:NH1	2.48	0.46
72:ST:129:ARG:O	72:ST:133:ARG:HG3	2.15	0.46
80:Sb:11:SER:OG	80:Sb:14:GLU:OE1	2.24	0.46
85:Sg:251:ALA:HB1	85:Sg:286:CYS:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CF:108:GLN:HE22	3:CF:249:PRO:HG2	1.80	0.46
4:L5:448:G:H2'	4:L5:450:G:H5'	1.98	0.46
4:L5:1866:U:H2'	4:L5:1867:A:O4'	2.16	0.46
4:L5:2292:C:H2'	4:L5:2293:U:C6	2.50	0.46
4:L5:2376:A:H2'	4:L5:2377:C:C6	2.51	0.46
4:L5:2421:G:OP2	4:L5:2828:U:H1'	2.15	0.46
4:L5:2517:A:N3	4:L5:2539:C:O2'	2.46	0.46
4:L5:5004:C:OP1	28:LW:35:LYS:HD3	2.15	0.46
6:L8:8:U:H2'	6:L8:9:A:H8	1.80	0.46
8:LB:80:GLU:OE1	8:LB:323:TYR:OH	2.19	0.46
12:LF:182:TYR:CZ	12:LF:203:GLU:HG2	2.51	0.46
43:LL:12:PHE:HE2	43:LL:51:LEU:HD22	1.79	0.46
52:S2:929:G:N2	52:S2:1104:G:H4'	2.31	0.46
52:S2:1374:C:O2'	52:S2:1464:C:O2	2.30	0.46
52:S2:1404:U:C5	73:SU:88:LEU:HD21	2.51	0.46
52:S2:1478:U:H2'	52:S2:1479:G:C8	2.50	0.46
52:S2:1605:G:N2	52:S2:1633:A:OP2	2.43	0.46
73:SU:93:SER:OG	73:SU:97:ILE:HG12	2.14	0.46
81:Sc:7:GLN:HE22	81:Sc:10:LYS:NZ	2.13	0.46
84:Sf:110:GLU:O	84:Sf:113:LYS:NZ	2.36	0.46
4:L5:458:C:H2'	4:L5:459:C:H6	1.81	0.46
4:L5:674:G:H2'	4:L5:675:C:C6	2.50	0.46
4:L5:2610:G:H2'	4:L5:2611:A:C8	2.51	0.46
4:L5:4062:A:H2'	4:L5:4063:U:C6	2.51	0.46
4:L5:4633:G:N2	4:L5:4664:A:N7	2.64	0.46
4:L5:4642:U:H2'	4:L5:4643:G:H8	1.81	0.46
4:L5:4859:C:H2'	4:L5:4860:G:H8	1.80	0.46
4:L5:4957:C:H2'	4:L5:4958:C:C6	2.51	0.46
17:LL:110:LEU:O	17:LL:114:VAL:HG13	2.15	0.46
28:LW:113:LYS:HD2	28:LW:117:LYS:HE3	1.97	0.46
48:Lr:54:ALA:HA	48:Lr:61:VAL:HG23	1.98	0.46
52:S2:85:A:H2'	52:S2:86:C:H6	1.81	0.46
52:S2:291:G:HO2'	52:S2:292:A:P	2.38	0.46
52:S2:511:U:H2'	52:S2:512:A:H8	1.80	0.46
52:S2:1745:A:H2'	52:S2:1746:U:O4'	2.16	0.46
63:SK:63:ALA:HB2	63:SK:68:TYR:HE2	1.81	0.46
70:SR:9:VAL:HG23	70:SR:50:ILE:HA	1.98	0.46
75:SW:3:ARG:NH2	75:SW:28:ARG:HH21	2.12	0.46
81:Sc:10:LYS:HD2	81:Sc:34:PHE:HE1	1.81	0.46
87:CA:209:GLN:O	87:CA:213:HIS:HB2	2.16	0.46
4:L5:123:C:H2'	4:L5:124:C:H6	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:1534:A2M:H8	41:Lj:15:THR:OG1	2.15	0.46
4:L5:1846:G:H2'	4:L5:1847:C:H6	1.79	0.46
4:L5:2399:G:O2'	4:L5:2822:G:O2'	2.32	0.46
4:L5:3663:A:N6	4:L5:4168:G:O2'	2.48	0.46
4:L5:3916:G:H2'	4:L5:3917:A:C8	2.50	0.46
4:L5:4345:C:H2'	4:L5:4346:U:H6	1.79	0.46
4:L5:4524:G:N3	8:LB:252:ALA:HB1	2.31	0.46
4:L5:4896:G:H2'	4:L5:4897:G:C8	2.51	0.46
4:L5:5023:C:H5''	61:SI:124:LYS:NZ	2.31	0.46
6:L8:12:G:OP1	21:LP:3:ARG:NH1	2.49	0.46
13:LG:254:GLU:HA	13:LG:257:LYS:NZ	2.31	0.46
19:LN:24:ARG:CB	19:LN:24:ARG:HH11	2.29	0.46
23:LR:112:SER:OG	23:LR:114:LYS:HG3	2.16	0.46
52:S2:12:U:H2'	52:S2:13:C:C6	2.50	0.46
52:S2:116:OMU:HM23	52:S2:116:OMU:H1'	1.75	0.46
52:S2:1292:C:H1'	84:Sf:147:THR:HG21	1.97	0.46
52:S2:1457:U:H2'	52:S2:1458:G:H8	1.81	0.46
52:S2:1681:U:H2'	52:S2:1682:C:C6	2.50	0.46
59:SG:189:ARG:HA	59:SG:192:ILE:HG22	1.98	0.46
65:SM:12:MET:SD	65:SM:13:ASP:N	2.89	0.46
65:SM:31:LEU:O	65:SM:109:VAL:HG13	2.15	0.46
69:SQ:10:VAL:HG12	69:SQ:98:LYS:HD3	1.98	0.46
69:SQ:42:ILE:HG13	69:SQ:43:GLU:H	1.80	0.46
72:ST:39:LEU:HD23	72:ST:56:ARG:NH1	2.30	0.46
86:AT:51:U:H2'	86:AT:52:C:C6	2.51	0.46
4:L5:139:G:H2'	4:L5:140:G:C8	2.51	0.46
4:L5:937:U:C6	18:LM:46:ARG:HD2	2.51	0.46
4:L5:1633:G:H5'	4:L5:1634:A:OP1	2.16	0.46
4:L5:2521:G:H4'	38:Lg:26:PRO:HD2	1.98	0.46
4:L5:4383:U:H2'	4:L5:4384:U:C6	2.51	0.46
6:L8:123:U:H2'	6:L8:126:C:H41	1.81	0.46
7:LA:109:GLU:OE1	7:LA:138:SER:HA	2.16	0.46
16:LJ:81:GLU:O	16:LJ:84:GLU:HG3	2.16	0.46
28:LW:79:GLN:HE21	28:LW:94:ARG:NH1	2.14	0.46
52:S2:648:A:H4'	76:SX:104:GLY:O	2.16	0.46
52:S2:1839:U:H2'	52:S2:1840:U:C6	2.50	0.46
58:SF:42:LYS:HB3	58:SF:43:GLU:OE1	2.16	0.46
60:SH:19:PHE:CZ	60:SH:50:GLU:HB2	2.50	0.46
61:SI:144:LYS:O	61:SI:148:LYS:N	2.48	0.46
87:CA:113:HIS:HA	87:CA:117:PHE:O	2.16	0.46
4:L5:2864:A:H2'	4:L5:2865:U:H6	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:3722:G:H2'	4:L5:3723:A:H8	1.80	0.46
4:L5:4413:C:O2	15:LI:158:LYS:NZ	2.49	0.46
8:LB:307:TYR:CE2	8:LB:366:LYS:HG2	2.51	0.46
10:LD:37:VAL:CG1	10:LD:50:ARG:HH11	2.29	0.46
12:LF:60:GLU:O	12:LF:64:MET:HG3	2.16	0.46
15:LI:206:LEU:O	15:LI:210:ARG:HG2	2.15	0.46
23:LR:172:ARG:HH12	52:S2:909:G:P	2.39	0.46
30:LY:55:VAL:HG12	30:LY:106:ILE:HA	1.98	0.46
32:La:110:LYS:HG3	32:La:128:PHE:HB2	1.97	0.46
52:S2:420:G:O2'	52:S2:660:C:N3	2.46	0.46
52:S2:907:G:H2'	52:S2:908:A:H8	1.81	0.46
52:S2:1328:OMG:HM23	52:S2:1328:OMG:H1'	1.75	0.46
63:SK:77:GLN:OE1	63:SK:77:GLN:N	2.43	0.46
65:SM:128:PHE:O	65:SM:132:LYS:HG2	2.16	0.46
66:SN:46:THR:HB	66:SN:86:GLU:HG3	1.97	0.46
70:SR:7:LYS:HE2	70:SR:7:LYS:HB2	1.70	0.46
4:L5:1664:U:H2'	4:L5:1665:C:C6	2.51	0.46
4:L5:1806:G:H2'	4:L5:1807:C:C6	2.51	0.46
4:L5:3848:U:H2'	4:L5:3849:A:C8	2.51	0.46
4:L5:4342:C:O3'	46:Lc:37:GLY:HA3	2.16	0.46
4:L5:4708:A:N3	4:L5:4709:U:H5'	2.31	0.46
4:L5:5003:U:H2'	4:L5:5004:C:C6	2.51	0.46
4:L5:5066:U:OP1	21:LP:43:LYS:NZ	2.42	0.46
8:LB:37:PRO:HA	8:LB:188:GLY:N	2.31	0.46
12:LF:157:ARG:HE	12:LF:248:ASN:HB2	1.81	0.46
16:LJ:26:VAL:HG22	16:LJ:33:LEU:HD13	1.98	0.46
16:LJ:39:VAL:HA	16:LJ:42:GLN:NE2	2.31	0.46
16:LJ:113:ILE:HG21	16:LJ:119:TYR:HB2	1.98	0.46
21:LP:85:LYS:O	21:LP:89:GLU:HG2	2.16	0.46
30:LY:31:SER:HA	30:LY:48:PRO:HA	1.97	0.46
34:Lc:20:LEU:O	34:Lc:24:SER:HB3	2.15	0.46
52:S2:140:C:H42	52:S2:313:A:H61	1.64	0.46
52:S2:736:C:H2'	52:S2:737:G:C4	2.51	0.46
52:S2:1164:G:O2'	52:S2:1165:G:H5'	2.16	0.46
52:S2:1623:A:C6	71:SS:132:ARG:HD3	2.51	0.46
53:SA:69:GLU:OE1	53:SA:69:GLU:N	2.40	0.46
53:SA:213:GLU:HB3	70:SR:84:TYR:OH	2.16	0.46
57:SE:45:ILE:HG13	57:SE:61:VAL:HG11	1.97	0.46
57:SE:104:ASP:N	57:SE:108:ARG:O	2.33	0.46
58:SF:167:LYS:HA	78:SZ:71:ALA:HB1	1.98	0.46
65:SM:50:CYS:SG	65:SM:110:VAL:HG22	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:SU:49:LYS:NZ	73:SU:51:LYS:HG3	2.31	0.46
77:SY:12:PHE:CZ	77:SY:21:LYS:HD3	2.50	0.46
86:AT:23:U:H2'	86:AT:24:C:O4'	2.16	0.46
87:CA:12:ILE:HD13	87:CA:21:TYR:CE2	2.50	0.46
3:CF:95:HIS:HB2	3:CF:98:PHE:CD2	2.51	0.45
4:L5:1338:G:H4'	4:L5:1339:U:C6	2.51	0.45
4:L5:1673:U:H2'	4:L5:1674:C:C6	2.51	0.45
4:L5:1872:G:O2'	4:L5:4219:A:N3	2.39	0.45
4:L5:1972:G:N1	4:L5:1994:C:N3	2.36	0.45
4:L5:2335:C:H2'	4:L5:2336:G:H8	1.80	0.45
4:L5:2654:C:H2'	4:L5:2655:C:H6	1.81	0.45
4:L5:5002:U:H2'	4:L5:5003:U:C6	2.51	0.45
5:L7:54:A:C8	16:LJ:10:ASN:ND2	2.84	0.45
8:LB:29:VAL:HA	8:LB:220:ILE:HD13	1.97	0.45
10:LD:83:LEU:HB3	10:LD:88:VAL:HG13	1.99	0.45
15:LI:205:PRO:HD2	15:LI:208:LYS:HE2	1.98	0.45
16:LJ:40:LEU:HD12	16:LJ:70:VAL:HG13	1.98	0.45
17:LL:59:VAL:HG21	17:LL:73:GLY:HA3	1.97	0.45
18:LM:71:LYS:O	18:LM:75:GLN:HG3	2.16	0.45
29:LX:88:LYS:HE2	87:CA:258:LYS:O	2.15	0.45
39:Lh:5:LYS:HE2	39:Lh:7:ARG:HH12	1.80	0.45
40:Li:29:ARG:HD3	40:Li:29:ARG:C	2.42	0.45
43:Ll:41:ARG:HA	43:Ll:41:ARG:HD2	1.75	0.45
52:S2:568:C:H2'	52:S2:569:A:O4'	2.16	0.45
54:SB:136:ARG:O	54:SB:215:VAL:HA	2.16	0.45
57:SE:11:ARG:HH11	57:SE:20:LEU:HB3	1.81	0.45
57:SE:40:GLU:OE1	57:SE:40:GLU:N	2.49	0.45
57:SE:182:MET:HE3	57:SE:190:GLY:HA2	1.98	0.45
58:SF:168:THR:OG1	78:SZ:106:GLN:OE1	2.30	0.45
59:SG:163:ASN:O	59:SG:164:LYS:HE2	2.15	0.45
68:SP:50:ARG:HB2	68:SP:53:GLN:OE1	2.16	0.45
73:SU:34:LYS:C	73:SU:34:LYS:HD3	2.41	0.45
73:SU:48:LEU:HD22	73:SU:101:ILE:HD11	1.98	0.45
4:L5:500:G:H1'	4:L5:504:G:H3'	1.98	0.45
4:L5:502:C:H3'	4:L5:503:C:H3'	1.98	0.45
4:L5:1504:G:H2'	4:L5:1505:C:H6	1.80	0.45
4:L5:1895:G:OP1	12:LF:96:ARG:NH2	2.50	0.45
4:L5:1962:A:H2	4:L5:2024:G:H21	1.64	0.45
4:L5:3721:U:H2'	4:L5:3722:G:H8	1.81	0.45
4:L5:4563:U:H2'	4:L5:4564:A:C8	2.50	0.45
4:L5:4941:G:OP2	11:LE:188:ARG:NH2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L8:92:U:H2'	6:L8:93:C:O4'	2.16	0.45
16:LJ:113:ILE:H	16:LJ:113:ILE:HD12	1.81	0.45
52:S2:937:C:OP1	66:SN:107:LYS:HE2	2.17	0.45
52:S2:1614:A:N6	94:S2:2037:HOH:O	2.38	0.45
52:S2:1667:U:H2'	52:S2:1668:U:C6	2.51	0.45
63:SK:41:PRO:HG2	63:SK:44:HIS:CD2	2.52	0.45
76:SX:68:LYS:HB3	76:SX:91:LEU:HD13	1.97	0.45
80:Sb:54:VAL:HG22	80:Sb:64:CYS:SG	2.56	0.45
85:Sg:104:HIS:NE2	85:Sg:122:SER:OG	2.46	0.45
3:CF:430:ARG:CG	86:AT:64:G:O2'	2.64	0.45
4:L5:99:A:H5''	19:LN:184:ILE:HD12	1.97	0.45
4:L5:1392:A:H2'	4:L5:1393:G:C8	2.51	0.45
4:L5:1431:C:H2'	4:L5:1432:G:O4'	2.16	0.45
4:L5:2418:A:C5	4:L5:2419:C:C5	3.04	0.45
4:L5:2467:U:H4'	4:L5:2468:U:H5'	1.99	0.45
4:L5:2726:G:H2'	4:L5:2727:C:C6	2.52	0.45
4:L5:3770:U:O2'	51:Pt:12:G:H1'	2.17	0.45
4:L5:3870:C:H2'	4:L5:3871:A:H8	1.81	0.45
4:L5:4184:G:H5'	7:LA:233:ARG:HB2	1.98	0.45
4:L5:4523:A2M:HM'3	4:L5:4523:A2M:H1'	1.76	0.45
4:L5:4578:G:H2'	4:L5:4579:PSU:C6	2.51	0.45
6:L8:81:C:H5'	39:Lh:3:LYS:NZ	2.30	0.45
14:LH:51:LYS:HG3	14:LH:52:LYS:HG2	1.98	0.45
16:LJ:17:ILE:HG23	16:LJ:132:VAL:HG23	1.98	0.45
19:LN:189:ARG:HB3	19:LN:193:ARG:NH1	2.30	0.45
31:LZ:99:ASP:HA	31:LZ:102:ARG:HH21	1.80	0.45
36:Le:92:ASN:ND2	36:Le:118:LEU:O	2.48	0.45
52:S2:171:A:OP2	59:SG:137:ARG:NH2	2.46	0.45
52:S2:368:U:OP1	52:S2:369:C:O2'	2.29	0.45
52:S2:1310:U:H2'	52:S2:1311:C:H6	1.81	0.45
52:S2:1566:G:N7	72:ST:101:ARG:NH2	2.60	0.45
56:SD:8:LYS:HG2	73:SU:61:LEU:HD11	1.99	0.45
62:SJ:124:HIS:HD2	83:Se:31:ARG:HD2	1.82	0.45
71:SS:7:GLU:OE1	71:SS:7:GLU:N	2.50	0.45
77:SY:88:LYS:N	77:SY:88:LYS:HD2	2.30	0.45
87:CA:27:ILE:O	87:CA:31:VAL:HG23	2.16	0.45
87:CA:86:VAL:HG13	87:CA:229:LEU:HD21	1.98	0.45
4:L5:121:A:OP1	13:LG:110:LYS:NZ	2.32	0.45
4:L5:679:C:H2'	4:L5:680:G:H8	1.81	0.45
4:L5:754:U:H2'	4:L5:755:C:C6	2.51	0.45
4:L5:919:C:H2'	4:L5:920:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:1697:G:H22	4:L5:2084:C:P	2.39	0.45
4:L5:1745:G:N7	94:L5:5519:HOH:O	2.36	0.45
4:L5:1802:A:H5''	4:L5:1803:G:H5'	1.97	0.45
4:L5:2539:C:H2'	4:L5:2540:C:H6	1.79	0.45
4:L5:2861:OMC:HM23	4:L5:2861:OMC:H1'	1.66	0.45
4:L5:4601:U:OP2	4:L5:4609:G:N1	2.46	0.45
4:L5:4901:G:OP1	4:L5:4901:G:H3'	2.16	0.45
10:LD:271:MET:HE2	10:LD:276:LYS:HG2	1.98	0.45
13:LG:182:CYS:HB3	13:LG:222:ILE:HD12	1.97	0.45
20:LO:37:ARG:HD3	20:LO:108:ILE:HD11	1.98	0.45
22:LQ:115:ARG:HH11	22:LQ:115:ARG:CB	2.30	0.45
23:LR:76:MET:O	23:LR:80:LYS:HB2	2.16	0.45
34:Lc:82:GLY:HA2	34:Lc:91:VAL:HG12	1.98	0.45
35:Ld:64:ILE:HG23	35:Ld:68:LEU:HD23	1.98	0.45
51:Pt:51:C:H2'	51:Pt:52:G:H8	1.82	0.45
52:S2:324:C:H2'	52:S2:325:C:C2	2.51	0.45
52:S2:528:A:H5'	62:SJ:121:LYS:NZ	2.31	0.45
52:S2:695:C:H5''	52:S2:696:G:C4	2.51	0.45
52:S2:1671:G:H2'	52:S2:1672:U:C6	2.51	0.45
52:S2:1714:U:H2'	52:S2:1715:A:C8	2.51	0.45
65:SM:35:ILE:HA	65:SM:38:ALA:HB3	1.99	0.45
65:SM:61:TYR:O	65:SM:65:VAL:HG23	2.17	0.45
87:CA:16:LEU:O	87:CA:20:LYS:HG2	2.16	0.45
3:CF:49:MET:SD	3:CF:50:GLY:N	2.89	0.45
4:L5:1346:C:H2'	4:L5:1347:G:C8	2.51	0.45
4:L5:1628:C:OP2	7:LA:9:ARG:HD2	2.17	0.45
4:L5:2878:G:OP2	4:L5:2879:A:O2'	2.32	0.45
4:L5:4920:C:H2'	4:L5:4921:C:C6	2.52	0.45
4:L5:5002:U:OP2	8:LB:385:LYS:NZ	2.49	0.45
10:LD:152:ARG:O	10:LD:157:ASN:ND2	2.49	0.45
22:LQ:3:VAL:HG23	22:LQ:5:ILE:HG12	1.99	0.45
22:LQ:175:GLU:HA	32:La:51:GLY:C	2.42	0.45
24:LS:19:THR:C	24:LS:21:LYS:H	2.25	0.45
28:LW:104:GLN:O	28:LW:107:GLN:NE2	2.49	0.45
36:Le:35:TRP:CH2	36:Le:55:MET:HG2	2.51	0.45
42:Lk:13:LEU:HD23	42:Lk:13:LEU:H	1.81	0.45
52:S2:106:C:OP1	52:S2:431:G:O2'	2.33	0.45
52:S2:391:C:H2'	52:S2:392:A:H8	1.81	0.45
52:S2:1030:A:H2'	52:S2:1031:A2M:H8	1.99	0.45
53:SA:10:MET:HG3	53:SA:55:TRP:CG	2.52	0.45
53:SA:70:ASN:HB3	53:SA:73:ASP:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:SD:123:LEU:O	56:SD:127:MET:HG2	2.16	0.45
64:SL:150:GLY:O	64:SL:151:THR:OG1	2.30	0.45
85:Sg:248:LEU:HD23	85:Sg:249:CYS:N	2.32	0.45
4:L5:73:A:OP1	17:LL:106:SER:HB3	2.17	0.45
4:L5:1244:G:H2'	4:L5:1245:C:H6	1.81	0.45
4:L5:2634:C:H2'	4:L5:2635:U:H6	1.82	0.45
4:L5:4481:U:H2'	4:L5:4482:U:H6	1.82	0.45
6:L8:74:U:C4	30:LY:74:TYR:CD1	3.04	0.45
14:LH:4:ILE:HG12	14:LH:61:TRP:CH2	2.51	0.45
25:LT:4:THR:OG1	25:LT:9:ARG:HD3	2.16	0.45
52:S2:159:A2M:H1'	52:S2:159:A2M:HM'3	1.61	0.45
52:S2:445:A:H2'	52:S2:446:G:C8	2.52	0.45
52:S2:1093:A:H1'	75:SW:9:ASP:OD1	2.16	0.45
52:S2:1388:A:H61	56:SD:161:GLY:HA3	1.82	0.45
52:S2:1600:G:N3	52:S2:1600:G:H2'	2.30	0.45
61:SI:191:GLU:HB2	64:SL:19:ASN:ND2	2.32	0.45
71:SS:25:LYS:NZ	71:SS:52:LEU:HD22	2.32	0.45
79:Sa:89:ARG:HG3	79:Sa:92:ARG:HH21	1.82	0.45
86:AT:28:U:H2'	86:AT:29:U:C6	2.52	0.45
3:CF:258:GLY:HA3	52:S2:50:A:C4	2.51	0.45
4:L5:748:G:O6	24:LS:98:ARG:NH2	2.40	0.45
4:L5:1403:G:N7	4:L5:1408:G:N2	2.65	0.45
4:L5:1631:A:C8	7:LA:199:VAL:HG21	2.52	0.45
4:L5:2610:G:H2'	4:L5:2611:A:H8	1.82	0.45
4:L5:2885:A:N3	94:L5:5521:HOH:O	2.36	0.45
4:L5:3909:C:O2	4:L5:4396:A:N1	2.50	0.45
4:L5:4273:A:H2'	4:L5:4274:A:C8	2.52	0.45
4:L5:4291:G:H5'	4:L5:4293:PSU:C6	2.52	0.45
4:L5:4344:U:H2'	4:L5:4345:C:C6	2.52	0.45
4:L5:4459:U:H2'	4:L5:4460:U:H6	1.82	0.45
4:L5:4754:G:N7	11:LE:278:THR:HG23	2.31	0.45
13:LG:187:LYS:HB2	13:LG:198:THR:HG23	1.99	0.45
16:LJ:113:ILE:HD13	16:LJ:125:ILE:HD12	1.98	0.45
16:LJ:120:ASP:HB3	16:LJ:123:ILE:HG12	1.98	0.45
23:LR:4:LEU:HD11	23:LR:29:THR:HG23	1.98	0.45
28:LW:9:SER:HA	28:LW:52:THR:HG23	1.99	0.45
49:Ls:61:MET:O	49:Ls:65:ILE:HG12	2.16	0.45
52:S2:380:G:H1'	61:SI:5:ARG:HH11	1.82	0.45
52:S2:496:C:P	57:SE:49:ARG:HH22	2.39	0.45
52:S2:917:U:H2'	52:S2:918:U:C6	2.52	0.45
52:S2:1156:U:OP1	75:SW:71:LYS:NZ	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:1562:C:H4'	72:ST:120:GLY:N	2.32	0.45
52:S2:1713:C:H2'	52:S2:1714:U:H6	1.81	0.45
52:S2:1731:A:H2'	52:S2:1732:G:C8	2.52	0.45
52:S2:1784:G:H2'	52:S2:1785:C:C6	2.51	0.45
57:SE:26:VAL:HG21	62:SJ:2:PRO:O	2.17	0.45
57:SE:246:LEU:CD1	57:SE:251:GLU:HB3	2.47	0.45
58:SF:43:GLU:HG2	58:SF:44:LYS:N	2.31	0.45
58:SF:109:LEU:O	58:SF:113:VAL:HG23	2.17	0.45
58:SF:204:ARG:HG2	81:Sc:63:ARG:HE	1.81	0.45
59:SG:142:ARG:HA	59:SG:147:LEU:HB2	1.98	0.45
68:SP:24:GLN:O	68:SP:28:MET:HB2	2.17	0.45
86:AT:24:C:N3	86:AT:25:A:N6	2.65	0.45
4:L5:170:C:H42	4:L5:266:C:N4	2.15	0.45
4:L5:256:G:H2'	4:L5:257:C:C6	2.52	0.45
4:L5:302:C:H2'	4:L5:303:C:C6	2.51	0.45
4:L5:481:G:H2'	4:L5:482:G:C8	2.52	0.45
4:L5:1696:C:H5'	4:L5:1719:A:H1'	1.99	0.45
4:L5:2018:C:H2'	4:L5:2019:C:H6	1.82	0.45
4:L5:2496:G:H2'	4:L5:2497:C:C6	2.51	0.45
4:L5:2602:G:H2'	4:L5:2603:C:C6	2.52	0.45
4:L5:2614:C:O2'	4:L5:2808:G:OP1	2.35	0.45
4:L5:3951:G:H8	4:L5:3951:G:OP2	2.00	0.45
4:L5:4590:A2M:HM'3	4:L5:4590:A2M:H1'	1.71	0.45
6:L8:90:C:H2'	6:L8:91:A:C8	2.52	0.45
9:LC:13:GLU:OE1	9:LC:161:TYR:OH	2.29	0.45
9:LC:33:ARG:HH12	22:LQ:22:ASP:CG	2.24	0.45
10:LD:264:LYS:HG2	10:LD:266:TRP:CZ2	2.51	0.45
11:LE:141:ARG:NH1	37:Lf:108:SER:O	2.49	0.45
12:LF:114:LEU:HD21	12:LF:121:THR:HG22	1.99	0.45
13:LG:255:LYS:C	13:LG:255:LYS:HD3	2.42	0.45
15:LI:183:ASP:O	15:LI:187:LYS:HG2	2.17	0.45
23:LR:167:LYS:HB3	23:LR:167:LYS:HE2	1.68	0.45
25:LT:102:ARG:HD3	25:LT:106:LEU:CD1	2.46	0.45
36:Le:35:TRP:CZ2	36:Le:56:PRO:HD2	2.52	0.45
46:Lo:33:LEU:O	46:Lo:33:LEU:HD23	2.16	0.45
52:S2:295:C:H2'	52:S2:296:U:C6	2.51	0.45
52:S2:554:A:O2'	52:S2:555:A:H8	2.00	0.45
52:S2:913:A:N6	60:SH:98:ARG:O	2.38	0.45
52:S2:1409:A:H2'	52:S2:1410:C:H6	1.81	0.45
52:S2:1620:A:H1'	52:S2:1624:U:OP2	2.17	0.45
56:SD:70:THR:HA	56:SD:86:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:SF:35:LEU:O	58:SF:39:ILE:HG12	2.17	0.45
60:SH:73:GLN:HA	60:SH:76:GLN:HB2	1.97	0.45
63:SK:76:ILE:CG2	63:SK:80:ARG:HH21	2.30	0.45
84:Sf:103:LEU:HG	84:Sf:104:LYS:H	1.82	0.45
4:L5:260:C:H2'	4:L5:261:G:C8	2.52	0.45
4:L5:347:A:H2'	4:L5:348:G:C8	2.51	0.45
4:L5:1558:A:H2'	4:L5:1559:G:C8	2.52	0.45
4:L5:1971:C:O2	49:Ls:41:GLN:NE2	2.49	0.45
4:L5:2079:G:H2'	4:L5:2080:U:H6	1.82	0.45
4:L5:2382:A:N1	4:L5:2829:U:O2'	2.46	0.45
4:L5:2495:U:H2'	4:L5:2496:G:C8	2.52	0.45
4:L5:2709:C:H4'	4:L5:2710:C:OP1	2.17	0.45
4:L5:4616:A:H2'	4:L5:4617:G:O4'	2.17	0.45
4:L5:4667:C:OP1	8:LB:224:LYS:NZ	2.45	0.45
4:L5:4761:G:H2'	4:L5:4762:A:C8	2.52	0.45
7:LA:20:VAL:HA	7:LA:23:ARG:HG3	1.98	0.45
8:LB:217:ILE:HD12	8:LB:347:LEU:HB3	1.98	0.45
52:S2:72:C:H5'	52:S2:73:C:C5	2.52	0.45
52:S2:298:G:OP1	57:SE:134:LYS:N	2.40	0.45
52:S2:484:A2M:HM'3	52:S2:484:A2M:HI'	1.82	0.45
52:S2:878:G:H22	52:S2:908:A:H2	1.65	0.45
52:S2:1158:G:O3'	75:SW:76:SER:OG	2.28	0.45
52:S2:1777:G:H2'	52:S2:1778:C:C6	2.52	0.45
55:SC:144:SER:OG	55:SC:145:LYS:N	2.50	0.45
60:SH:64:VAL:O	60:SH:96:ALA:HA	2.17	0.45
72:ST:126:GLN:HG2	72:ST:129:ARG:NH2	2.32	0.45
77:SY:35:VAL:HG13	77:SY:40:ILE:HD11	1.98	0.45
87:CA:70:MET:HE2	87:CA:115:ASP:HA	1.99	0.45
3:CF:251:GLN:HB3	3:CF:264:VAL:O	2.17	0.45
4:L5:113:A:H2'	4:L5:114:G:O4'	2.17	0.45
4:L5:491:G:H2'	4:L5:492:U:C6	2.52	0.45
4:L5:715:G:H5''	9:LC:316:LYS:HG2	1.99	0.45
4:L5:1195:G:H2'	4:L5:1196:G:H8	1.80	0.45
4:L5:1625:OMG:HM23	19:LN:81:TYR:HE2	1.82	0.45
4:L5:1739:G:H2'	4:L5:1740:C:C6	2.52	0.45
4:L5:4236:G:H4'	4:L5:4328:G:O2'	2.17	0.45
10:LD:238:GLU:HG3	10:LD:242:LYS:NZ	2.32	0.45
15:LI:43:VAL:HG11	15:LI:197:VAL:HG13	1.99	0.45
16:LJ:144:LYS:O	16:LJ:148:THR:HB	2.16	0.45
18:LM:96:GLU:O	18:LM:100:ARG:HG2	2.17	0.45
23:LR:149:LYS:O	23:LR:152:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LT:122:LYS:NZ	25:LT:124:THR:HG22	2.31	0.45
28:LW:2:LYS:HE2	28:LW:15:PRO:HB3	1.99	0.45
28:LW:7:SER:HB2	28:LW:13:ILE:HD11	1.99	0.45
51:Pt:27:U:H2'	51:Pt:28:U:H6	1.82	0.45
51:Pt:43:A:H2'	51:Pt:44:A:C8	2.52	0.45
52:S2:323:C:O2'	52:S2:325:C:N4	2.45	0.45
52:S2:1588:A:H2'	52:S2:1589:A:H8	1.82	0.45
69:SQ:8:GLN:HG3	69:SQ:99:TYR:CZ	2.52	0.45
78:SZ:88:LEU:HD23	78:SZ:88:LEU:HA	1.82	0.45
86:AT:68:G:H2'	86:AT:69:G:C8	2.51	0.45
3:CF:15:HIS:HE1	3:CF:131:GLY:HA2	1.82	0.44
3:CF:16:VAL:HG22	3:CF:95:HIS:HA	1.99	0.44
3:CF:26:HIS:CE1	3:CF:30:LYS:HE2	2.52	0.44
4:L5:1326:A2M:OP2	4:L5:4445:U:O2'	2.33	0.44
4:L5:1369:C:OP2	4:L5:1370:G:O2'	2.32	0.44
4:L5:2611:A:H2'	4:L5:2612:G:H8	1.81	0.44
4:L5:2708:U:C5'	87:CA:263:ARG:HG2	2.42	0.44
4:L5:2720:C:H2'	4:L5:2721:G:O4'	2.18	0.44
7:LA:96:LEU:O	47:Lp:87:LYS:HD2	2.17	0.44
15:LI:183:ASP:OD1	15:LI:184:MET:N	2.50	0.44
41:Lj:67:LEU:HD23	41:Lj:67:LEU:HA	1.85	0.44
49:Ls:100:ASP:OD1	49:Ls:101:MET:N	2.50	0.44
52:S2:191:A:H5''	61:SI:141:ARG:NH2	2.32	0.44
52:S2:508:A:H5'	52:S2:509:OMG:OP2	2.17	0.44
52:S2:520:A:O2'	52:S2:825:A:N3	2.48	0.44
52:S2:1158:G:H5''	75:SW:76:SER:HB2	1.97	0.44
52:S2:1221:G:H2'	52:S2:1222:G:C8	2.53	0.44
52:S2:1533:A:N3	52:S2:1533:A:H2'	2.32	0.44
52:S2:1786:U:H2'	52:S2:1787:G:H8	1.82	0.44
53:SA:85:ARG:NH1	53:SA:205:ARG:HG3	2.32	0.44
53:SA:122:LEU:HD21	53:SA:133:PRO:HB2	1.99	0.44
53:SA:209:GLU:HA	53:SA:212:LYS:HZ3	1.81	0.44
62:SJ:91:LYS:HG2	62:SJ:96:TYR:CD2	2.53	0.44
85:Sg:300:ALA:O	85:Sg:307:VAL:HG23	2.18	0.44
87:CA:123:HIS:NE2	87:CA:125:PHE:HB3	2.32	0.44
4:L5:108:A:N1	4:L5:333:U:O2'	2.47	0.44
4:L5:467:U:H2'	4:L5:468:U:C4'	2.48	0.44
4:L5:1096:C:H2'	4:L5:1097:C:C6	2.52	0.44
4:L5:1190:C:H2'	4:L5:1191:C:H6	1.82	0.44
4:L5:1414:C:H2'	4:L5:1415:G:C8	2.48	0.44
4:L5:1444:G:O2'	4:L5:1445:U:O4'	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:1998:A:O2'	4:L5:1999:A:H5'	2.17	0.44
4:L5:2663:G:H4'	23:LR:117:ARG:HH11	1.82	0.44
4:L5:2683:C:H2'	4:L5:2684:C:C6	2.53	0.44
4:L5:2732:G:H2'	4:L5:2733:C:C6	2.51	0.44
4:L5:4139:G:N2	4:L5:4140:C:H41	2.14	0.44
4:L5:4605:A:H2'	4:L5:4606:G:O4'	2.16	0.44
4:L5:4970:C:C2	4:L5:4971:A:C8	3.05	0.44
4:L5:4987:C:P	8:LB:116:ARG:HH22	2.40	0.44
5:L7:112:U:H2'	5:L7:113:G:H8	1.82	0.44
7:LA:27:ALA:HB1	7:LA:77:ILE:HG13	1.98	0.44
8:LB:81:THR:O	8:LB:329:ASP:HB2	2.17	0.44
20:LO:110:PRO:N	20:LO:111:PRO:HD2	2.33	0.44
21:LP:23:ARG:HD3	21:LP:125:MET:CE	2.44	0.44
26:LU:48:LYS:HG2	26:LU:53:ALA:HB2	1.99	0.44
26:LU:63:ILE:HD11	26:LU:70:ILE:HG22	1.98	0.44
52:S2:169:U:H5''	59:SG:135:PRO:HA	1.99	0.44
52:S2:179:C:H3'	52:S2:180:G:H8	1.82	0.44
52:S2:752:G:OP2	52:S2:752:G:N2	2.50	0.44
52:S2:857:U:H2'	52:S2:858:A:C8	2.51	0.44
52:S2:1060:A:H1'	52:S2:1062:A:N7	2.32	0.44
52:S2:1223:A:H2'	52:S2:1224:G:O4'	2.18	0.44
52:S2:1378:A:OP2	53:SA:102:ARG:NH1	2.49	0.44
52:S2:1398:G:H1'	85:Sg:63:SER:HB2	2.00	0.44
52:S2:1678:A:O2'	52:S2:1679:A:H5'	2.17	0.44
61:SI:36:THR:OG1	61:SI:57:ALA:O	2.20	0.44
70:SR:6:THR:HG22	70:SR:7:LYS:N	2.32	0.44
87:CA:173:VAL:HB	87:CA:354:LEU:HD21	1.98	0.44
3:CF:358:ALA:HB2	3:CF:371:LYS:HD3	1.99	0.44
4:L5:6:C:H2'	4:L5:7:C:H6	1.83	0.44
4:L5:1086:C:H2'	4:L5:1087:A:H8	1.82	0.44
4:L5:1178:G:H2'	4:L5:1178:G:N3	2.33	0.44
4:L5:1877:G:O6	33:Lb:10:HIS:NE2	2.48	0.44
4:L5:2368:A:N6	4:L5:2827:G:O2'	2.50	0.44
4:L5:2431:A:OP1	43:Ll:22:PRO:HG3	2.17	0.44
4:L5:4348:A:H5''	4:L5:4349:C:OP2	2.17	0.44
12:LF:226:HIS:NE2	12:LF:234:GLY:HA3	2.32	0.44
19:LN:68:ARG:HG2	19:LN:128:LYS:HG3	1.98	0.44
22:LQ:178:ARG:HA	22:LQ:184:ARG:O	2.17	0.44
24:LS:86:SER:N	24:LS:89:GLY:O	2.44	0.44
41:Lj:14:LYS:NZ	43:Ll:51:LEU:OXT	2.44	0.44
49:Ls:62:ARG:HB3	49:Ls:66:ARG:HH22	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:27:A2M:H2'	52:S2:28:U:O4'	2.17	0.44
52:S2:99:A2M:H2'	52:S2:100:U:O4'	2.18	0.44
52:S2:867:OMG:H8	52:S2:867:OMG:H5''	1.83	0.44
52:S2:1490:OMG:HM23	52:S2:1490:OMG:H1'	1.71	0.44
60:SH:76:GLN:NE2	60:SH:94:PHE:HB2	2.33	0.44
67:SO:62:VAL:HG21	67:SO:67:ASP:HB2	2.00	0.44
73:SU:21:ARG:HE	73:SU:90:ASP:CG	2.26	0.44
76:SX:68:LYS:HG2	76:SX:91:LEU:HD22	1.98	0.44
77:SY:28:LEU:O	77:SY:30:PRO:HD3	2.16	0.44
81:Sc:37:ASP:OD1	81:Sc:39:SER:OG	2.36	0.44
84:Sf:105:TYR:HD2	84:Sf:118:ARG:HG2	1.82	0.44
4:L5:135:G:H5''	4:L5:136:C:O4'	2.18	0.44
4:L5:263:G:H2'	4:L5:263:G:N3	2.32	0.44
4:L5:432:U:O2	89:L5:5292:SPM:H61	2.18	0.44
4:L5:1664:U:H2'	4:L5:1665:C:H6	1.83	0.44
4:L5:1760:G:N2	4:L5:1761:G:O6	2.50	0.44
4:L5:2264:C:H2'	4:L5:2265:G:O4'	2.17	0.44
4:L5:2293:U:H2'	4:L5:2294:G:C8	2.53	0.44
4:L5:2815:A2M:HM'3	4:L5:2815:A2M:H1'	1.73	0.44
4:L5:4244:A:H2'	4:L5:4245:G:O4'	2.17	0.44
4:L5:4685:U:H2'	4:L5:4686:G:H8	1.82	0.44
5:L7:63:C:H3'	15:LI:204:GLY:O	2.17	0.44
6:L8:5:U:H2'	6:L8:6:C:C6	2.52	0.44
29:LX:156:ILE:HG13	87:CA:290:ARG:C	2.42	0.44
31:LZ:14:LEU:O	38:Lg:88:ARG:HG2	2.17	0.44
35:Ld:59:THR:OG1	35:Ld:104:THR:OG1	2.23	0.44
49:Ls:50:LYS:O	49:Ls:92:LYS:NZ	2.50	0.44
50:Lt:127:GLY:O	50:Lt:131:GLU:HG2	2.18	0.44
52:S2:85:A:H5''	77:SY:118:ARG:NH1	2.33	0.44
52:S2:329:G:H2'	52:S2:330:G:C8	2.53	0.44
52:S2:837:A:H61	77:SY:9:THR:H	1.65	0.44
52:S2:958:G:H2'	52:S2:959:G:C8	2.53	0.44
52:S2:1330:G:N7	52:S2:1492:U:H3'	2.33	0.44
59:SG:192:ILE:HD12	59:SG:195:LYS:HD2	1.99	0.44
62:SJ:22:LYS:HA	62:SJ:22:LYS:HD2	1.63	0.44
64:SL:7:GLU:OE2	64:SL:11:GLN:NE2	2.50	0.44
70:SR:18:GLU:OE2	70:SR:19:LYS:HE3	2.17	0.44
71:SS:12:ILE:HD12	71:SS:19:ASN:HB2	2.00	0.44
84:Sf:119:ARG:HB3	84:Sf:132:MET:HB2	1.99	0.44
86:AT:4:U:H2'	86:AT:5:C:C6	2.53	0.44
86:AT:63:C:H2'	86:AT:64:G:C8	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:CA:81:SER:HB2	87:CA:107:LYS:HB2	1.99	0.44
3:CF:272:LEU:HD23	3:CF:273:LYS:N	2.31	0.44
3:CF:358:ALA:CB	86:AT:52:C:O4'	2.32	0.44
4:L5:1241:C:H5'	11:LE:72:LYS:NZ	2.32	0.44
4:L5:1910:G:O2'	4:L5:1917:A:N1	2.49	0.44
4:L5:2323:C:H2'	4:L5:2324:C:C6	2.53	0.44
4:L5:3859:G:OP2	21:LP:25:HIS:NE2	2.46	0.44
4:L5:4113:U:C3'	4:L5:4114:C:H4'	2.46	0.44
4:L5:4563:U:C2	4:L5:4564:A:C8	3.05	0.44
4:L5:4775:C:H41	4:L5:4859:C:H42	1.66	0.44
4:L5:5053:U:H3'	4:L5:5054:C:C6	2.52	0.44
7:LA:102:LEU:HD11	7:LA:107:MET:HG2	1.99	0.44
12:LF:241:ASN:O	12:LF:245:ARG:HG2	2.17	0.44
13:LG:70:LEU:HD23	13:LG:70:LEU:HA	1.86	0.44
14:LH:95:VAL:HG12	44:Lm:82:LEU:HB3	1.99	0.44
16:LJ:95:ARG:HB3	16:LJ:177:GLY:C	2.42	0.44
28:LW:45:ASN:ND2	28:LW:47:ARG:HB2	2.33	0.44
31:LZ:100:VAL:HG22	31:LZ:107:LYS:HA	1.99	0.44
36:Le:92:ASN:OD1	36:Le:120:ILE:HG12	2.17	0.44
52:S2:181:A:OP2	52:S2:182:C:O2'	2.31	0.44
52:S2:496:C:H2'	52:S2:497:C:C6	2.53	0.44
52:S2:659:G:H21	76:SX:17:ARG:NH2	2.16	0.44
52:S2:1391:OMC:HM23	52:S2:1391:OMC:H1'	1.75	0.44
57:SE:101:LEU:HD12	57:SE:101:LEU:HA	1.81	0.44
57:SE:246:LEU:HB2	57:SE:250:GLU:HG2	1.99	0.44
59:SG:141:ILE:HG13	59:SG:142:ARG:N	2.30	0.44
61:SI:138:ASN:C	61:SI:140:LYS:H	2.26	0.44
65:SM:52:LEU:O	65:SM:78:LYS:HA	2.18	0.44
71:SS:89:ASP:HB3	71:SS:93:GLY:H	1.82	0.44
71:SS:137:LYS:HG3	71:SS:138:THR:HG23	1.98	0.44
84:Sf:89:LYS:HE2	84:Sf:89:LYS:HB3	1.81	0.44
3:CF:40:GLU:O	3:CF:43:GLU:HG3	2.17	0.44
4:L5:31:U:H2'	4:L5:32:G:O4'	2.18	0.44
4:L5:280:G:H5''	19:LN:14:LYS:HE2	2.00	0.44
4:L5:1091:C:H2'	4:L5:1092:G:H8	1.81	0.44
4:L5:1270:A:HO2'	4:L5:1439:C:HO2'	1.62	0.44
4:L5:1732:C:H5''	25:LT:43:LYS:CE	2.48	0.44
4:L5:2358:G:H2'	4:L5:2359:U:O4'	2.16	0.44
4:L5:4097:G:O6	4:L5:4098:A:N6	2.51	0.44
4:L5:4300:U:H2'	4:L5:4301:U:C6	2.52	0.44
5:L7:39:C:O2'	16:LJ:46:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LA:118:GLU:OE2	7:LA:156:LYS:NZ	2.51	0.44
12:LF:48:LYS:HE3	33:Lb:96:LEU:HD21	1.98	0.44
18:LM:62:LEU:HD21	18:LM:82:ILE:HD11	1.99	0.44
23:LR:171:LYS:O	23:LR:175:GLU:HG2	2.18	0.44
49:Ls:37:SER:HA	49:Ls:40:MET:HE2	2.00	0.44
52:S2:1162:C:H2'	52:S2:1163:C:O4'	2.18	0.44
52:S2:1284:A:N6	52:S2:1313:A:O2'	2.50	0.44
53:SA:174:MET:HA	53:SA:177:MET:HB2	2.00	0.44
57:SE:46:ILE:HG13	57:SE:47:PHE:N	2.32	0.44
59:SG:3:LEU:HD22	59:SG:109:LEU:HB3	1.99	0.44
59:SG:147:LEU:CD1	59:SG:151:ASP:HB2	2.48	0.44
66:SN:83:ASP:OD1	66:SN:83:ASP:N	2.50	0.44
68:SP:45:LEU:HD23	68:SP:45:LEU:HA	1.86	0.44
70:SR:98:VAL:HG21	70:SR:117:LEU:HB3	1.99	0.44
71:SS:51:ASP:OD1	71:SS:53:THR:N	2.40	0.44
71:SS:76:GLN:OE1	71:SS:76:GLN:N	2.39	0.44
78:SZ:56:ASP:OD1	78:SZ:56:ASP:N	2.51	0.44
81:Sc:12:ALA:O	81:Sc:55:VAL:HG23	2.17	0.44
84:Sf:133:ALA:N	84:Sf:140:TYR:O	2.36	0.44
86:AT:67:C:H2'	86:AT:68:G:H8	1.83	0.44
3:CF:246:LEU:HD11	3:CF:272:LEU:HB2	1.99	0.44
4:L5:135:G:H22	39:Lh:94:ARG:HG2	1.83	0.44
4:L5:224:U:O2	9:LC:219:LYS:NZ	2.35	0.44
4:L5:253:G:H2'	4:L5:254:G:C8	2.53	0.44
4:L5:302:C:H2'	4:L5:303:C:H6	1.83	0.44
4:L5:1460:C:H2'	4:L5:1461:C:H6	1.83	0.44
4:L5:1475:G:H2'	4:L5:1476:C:C6	2.53	0.44
4:L5:1534:A2M:N3	41:Lj:11:ARG:HB2	2.32	0.44
4:L5:1552:G:O2'	4:L5:1574:G:N2	2.36	0.44
4:L5:1591:U:OP1	8:LB:243:LYS:HG2	2.18	0.44
4:L5:2303:C:H5''	36:Le:104:SER:HB3	1.98	0.44
4:L5:2461:G:H2'	4:L5:2462:C:C6	2.52	0.44
4:L5:2475:G:H5''	4:L5:2476:G:C8	2.53	0.44
4:L5:2732:G:H2'	4:L5:2733:C:H6	1.83	0.44
4:L5:3919:C:OP1	7:LA:2:GLY:HA3	2.18	0.44
4:L5:4111:U:H2'	4:L5:4112:C:C5	2.52	0.44
4:L5:4390:A:H2'	4:L5:4391:G:O4'	2.18	0.44
4:L5:4538:G:H2'	4:L5:4539:U:C6	2.52	0.44
5:L7:111:C:H2'	5:L7:112:U:O4'	2.17	0.44
8:LB:196:TRP:HE1	8:LB:200:ARG:HH21	1.66	0.44
12:LF:46:ARG:O	12:LF:50:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:LL:61:CYS:HB2	17:LL:66:TYR:O	2.18	0.44
50:Lt:104:ILE:HG13	50:Lt:106:PHE:HB3	1.99	0.44
52:S2:380:G:N1	52:S2:383:G:OP2	2.40	0.44
52:S2:1433:C:H41	73:SU:51:LYS:HD2	1.82	0.44
52:S2:1500:G:H2'	52:S2:1501:C:H6	1.80	0.44
52:S2:1540:G:H2'	52:S2:1541:G:H8	1.83	0.44
52:S2:1606:G:N1	52:S2:1632:G:O2'	2.44	0.44
52:S2:1856:C:H2'	52:S2:1857:G:C8	2.53	0.44
53:SA:63:ARG:HG2	74:SV:37:ALA:O	2.17	0.44
61:SI:21:TYR:N	94:SI:304:HOH:O	2.50	0.44
61:SI:125:LYS:HB2	61:SI:128:LYS:HZ1	1.83	0.44
62:SJ:2:PRO:HB2	62:SJ:3:VAL:H	1.69	0.44
85:Sg:257:LYS:HE3	85:Sg:259:TRP:HZ2	1.83	0.44
3:CF:15:HIS:CE1	3:CF:126:GLY:HA2	2.52	0.44
4:L5:473:C:H2'	4:L5:474:C:C6	2.53	0.44
4:L5:677:G:H2'	4:L5:678:C:C6	2.53	0.44
4:L5:1194:G:H2'	4:L5:1195:G:H8	1.82	0.44
4:L5:1742:A:OP2	10:LD:10:LYS:HD2	2.18	0.44
4:L5:2111:G:N2	4:L5:2251:G:O2'	2.51	0.44
4:L5:3718:A2M:H2'	4:L5:3719:A:O4'	2.18	0.44
5:L7:23:A:H2'	5:L7:24:C:C6	2.53	0.44
13:LG:144:THR:HG21	19:LN:3:ALA:N	2.33	0.44
16:LJ:115:LEU:HA	16:LJ:115:LEU:HD13	1.77	0.44
19:LN:60:VAL:HG23	19:LN:134:LEU:HB2	2.00	0.44
19:LN:90:ASN:O	46:Lo:48:TYR:OH	2.34	0.44
36:Le:11:LYS:H	36:Le:11:LYS:HD2	1.81	0.44
48:Lr:47:LYS:HB2	48:Lr:102:TYR:CZ	2.52	0.44
52:S2:1674:G:P	69:SQ:78:VAL:HG11	2.58	0.44
52:S2:1757:G:C8	52:S2:1758:G:H1'	2.53	0.44
60:SH:30:LEU:HG	60:SH:33:ASN:HD22	1.82	0.44
64:SL:150:GLY:C	64:SL:152:LYS:H	2.25	0.44
67:SO:45:THR:OG1	67:SO:49:GLY:HA2	2.18	0.44
71:SS:10:GLN:N	71:SS:10:GLN:OE1	2.51	0.44
75:SW:53:ILE:N	75:SW:60:LYS:O	2.50	0.44
82:Sd:21:CYS:SG	82:Sd:39:CYS:N	2.91	0.44
86:AT:18:G:N1	86:AT:56:U:H1'	2.32	0.44
87:CA:248:LYS:HB2	87:CA:248:LYS:HE2	1.79	0.44
3:CF:177:TYR:HA	3:CF:180:LYS:NZ	2.33	0.44
4:L5:25:A:H2'	4:L5:26:C:H6	1.82	0.44
4:L5:467:U:H2'	4:L5:468:U:H4'	2.00	0.44
4:L5:919:C:H2'	4:L5:920:C:H6	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:1278:C:H2'	4:L5:1279:A:O4'	2.18	0.44
4:L5:1314:C:C2	4:L5:1315:C:C5	3.06	0.44
4:L5:1354:A:OP2	22:LQ:87:THR:HG23	2.18	0.44
4:L5:1647:U:OP1	90:L5:5290:SPD:H51	2.18	0.44
4:L5:1704:C:O3'	12:LF:46:ARG:NH1	2.51	0.44
4:L5:1741:G:O6	5:L7:103:A:O2'	2.27	0.44
4:L5:2569:G:H2'	4:L5:2570:U:C6	2.52	0.44
4:L5:2811:G:N1	4:L5:2814:C:OP2	2.46	0.44
4:L5:3597:G:H2'	4:L5:3598:C:C6	2.53	0.44
4:L5:3758:U:H2'	4:L5:3765:G:N2	2.33	0.44
4:L5:4070:U:H2'	4:L5:4071:U:C6	2.52	0.44
4:L5:5024:C:N4	4:L5:5028:G:H21	2.16	0.44
7:LA:145:LYS:HD3	7:LA:145:LYS:HA	1.80	0.44
11:LE:223:ARG:HA	11:LE:224:LYS:HA	1.74	0.44
15:LI:87:MET:HB2	15:LI:87:MET:HE3	1.81	0.44
29:LX:112:ALA:O	29:LX:116:LEU:HG	2.18	0.44
39:Lh:95:LEU:HB2	39:Lh:100:GLU:OE1	2.17	0.44
42:Lk:10:ASP:HA	42:Lk:13:LEU:CD2	2.48	0.44
52:S2:29:G:H2'	52:S2:30:C:C6	2.53	0.44
52:S2:833:C:H2'	52:S2:834:C:C6	2.53	0.44
52:S2:1016:U:H5'	66:SN:15:ALA:O	2.18	0.44
52:S2:1272:OMC:HM23	52:S2:1272:OMC:H1'	1.71	0.44
52:S2:1278:A:H2'	52:S2:1279:C:C6	2.53	0.44
52:S2:1417:C:H3'	52:S2:1418:C:O4'	2.17	0.44
52:S2:1724:A:H2'	52:S2:1725:U:C6	2.53	0.44
60:SH:130:LEU:HD23	60:SH:130:LEU:O	2.18	0.44
69:SQ:15:ARG:HA	69:SQ:19:ALA:O	2.18	0.44
69:SQ:90:LYS:HB3	69:SQ:90:LYS:HE2	1.82	0.44
86:AT:61:A:OP2	86:AT:62:C:N4	2.40	0.44
87:CA:143:ILE:HD13	87:CA:343:TYR:OH	2.18	0.44
3:CF:318:LYS:HD3	3:CF:318:LYS:HA	1.75	0.43
4:L5:62:A:OP1	19:LN:172:ARG:NH1	2.43	0.43
4:L5:239:C:H5'	30:LY:33:PRO:HD3	2.00	0.43
4:L5:750:U:H1'	4:L5:917:A:C8	2.53	0.43
4:L5:1087:A:H2'	4:L5:1088:C:C6	2.53	0.43
4:L5:1318:C:N4	94:L5:5691:HOH:O	2.45	0.43
4:L5:1786:A:H2'	4:L5:1789:C:C5	2.52	0.43
4:L5:2276:A:H2'	4:L5:2277:C:O4'	2.18	0.43
4:L5:3939:G:O2'	4:L5:4076:G:N1	2.39	0.43
4:L5:4254:G:H2'	4:L5:4254:G:N3	2.32	0.43
4:L5:4743:G:H2'	4:L5:4744:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LO:173:GLN:HG2	20:LO:176:ARG:HH21	1.81	0.43
52:S2:49:C:H2'	52:S2:472:C:H41	1.83	0.43
57:SE:153:LEU:HD12	59:SG:216:ARG:HH11	1.82	0.43
59:SG:56:ASN:HB2	59:SG:108:VAL:HG22	2.00	0.43
60:SH:142:LYS:HB3	75:SW:54:ASP:HB3	1.99	0.43
67:SO:34:PHE:HB3	67:SO:41:PHE:HB2	2.00	0.43
70:SR:134:PRO:O	70:SR:135:VAL:HB	2.18	0.43
76:SX:46:HIS:CD2	76:SX:103:ALA:HB2	2.53	0.43
87:CA:234:GLU:HG2	87:CA:236:LYS:NZ	2.33	0.43
3:CF:371:LYS:HZ3	86:AT:52:C:H5'	1.83	0.43
4:L5:1341:U:H2'	4:L5:1342:A:H8	1.83	0.43
4:L5:2666:U:O2'	4:L5:2668:G:N7	2.47	0.43
4:L5:3652:A:H2'	4:L5:3653:A:C5	2.53	0.43
6:L8:74:U:C4	30:LY:74:TYR:HD1	2.36	0.43
15:LI:112:GLN:C	15:LI:114:GLY:H	2.26	0.43
15:LI:208:LYS:HB2	15:LI:208:LYS:HE3	1.85	0.43
19:LN:148:THR:O	19:LN:151:ILE:HG22	2.18	0.43
42:Lk:13:LEU:O	42:Lk:17:ARG:HG3	2.17	0.43
47:Lp:19:GLY:O	47:Lp:23:ARG:HG3	2.18	0.43
50:Lt:66:ASN:O	50:Lt:68:GLN:N	2.51	0.43
52:S2:380:G:P	61:SI:56:ARG:NH2	2.92	0.43
52:S2:468:A2M:HM'3	52:S2:468:A2M:H1'	1.59	0.43
52:S2:551:U:H2'	52:S2:552:G:C8	2.52	0.43
52:S2:864:A:H2'	52:S2:865:A:H8	1.83	0.43
52:S2:1060:A:H4'	52:S2:1061:U:O5'	2.18	0.43
52:S2:1152:U:O2'	75:SW:16:ASN:OD1	2.26	0.43
52:S2:1155:U:OP1	55:SC:185:THR:OG1	2.19	0.43
52:S2:1204:A:O2'	52:S2:1700:C:OP2	2.30	0.43
52:S2:1425:G:H2'	52:S2:1426:U:C6	2.53	0.43
52:S2:1614:A:OP2	68:SP:42:ARG:NH1	2.51	0.43
52:S2:1629:C:C2	52:S2:1630:A:C8	3.06	0.43
53:SA:124:VAL:HG13	53:SA:130:ASP:HB2	2.00	0.43
53:SA:158:ASP:OD2	74:SV:32:ILE:HD13	2.18	0.43
54:SB:144:LYS:CD	54:SB:208:HIS:HB3	2.40	0.43
54:SB:217:MET:HE3	54:SB:217:MET:HB2	1.89	0.43
61:SI:23:LYS:HE2	61:SI:23:LYS:HB3	1.69	0.43
64:SL:153:LYS:HA	64:SL:153:LYS:HD3	1.88	0.43
69:SQ:39:LEU:HD11	69:SQ:51:LEU:HB3	1.99	0.43
69:SQ:41:MET:HE2	72:ST:10:ASN:HA	2.00	0.43
75:SW:32:LYS:O	75:SW:36:ARG:HG2	2.18	0.43
86:AT:65:G:H2'	86:AT:66:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:CA:19:THR:HA	87:CA:22:LYS:HE3	1.99	0.43
3:CF:77:LEU:HD21	3:CF:307:ASN:ND2	2.33	0.43
3:CF:103:ILE:HG21	3:CF:362:ASP:HB3	2.01	0.43
3:CF:115:ILE:O	3:CF:115:ILE:HG13	2.17	0.43
4:L5:287:U:H2'	4:L5:288:G:C8	2.53	0.43
4:L5:1365:C:H2'	4:L5:1366:G:H3'	2.00	0.43
4:L5:1507:C:H5''	9:LC:114:ARG:HG3	1.99	0.43
4:L5:1770:A:N7	4:L5:1771:U:N3	2.67	0.43
4:L5:2496:G:H2'	4:L5:2497:C:H6	1.84	0.43
4:L5:3719:A:C4	4:L5:3720:G:C8	3.06	0.43
4:L5:4750:G:H2'	4:L5:4751:G:H8	1.83	0.43
4:L5:4935:C:H2'	4:L5:4936:G:H8	1.81	0.43
4:L5:5000:G:O2'	8:LB:382:MET:HE1	2.19	0.43
6:L8:12:G:N2	21:LP:120:ASN:OD1	2.41	0.43
15:LI:113:THR:HG22	15:LI:116:ARG:HB3	2.00	0.43
21:LP:14:SER:OG	21:LP:151:THR:HG22	2.18	0.43
27:LV:57:VAL:HG13	27:LV:84:GLN:HB3	2.00	0.43
36:Le:89:LEU:HD13	36:Le:118:LEU:HD22	2.01	0.43
49:Ls:53:VAL:HA	49:Ls:89:VAL:HA	2.00	0.43
52:S2:1317:C:H2'	52:S2:1318:G:C8	2.54	0.43
52:S2:1421:A:H5''	52:S2:1422:G:C4	2.53	0.43
52:S2:1464:C:H4'	70:SR:60:ARG:NH1	2.33	0.43
54:SB:30:TRP:CH2	54:SB:48:LEU:HD23	2.53	0.43
54:SB:145:LYS:HB2	54:SB:145:LYS:HE3	1.68	0.43
55:SC:72:ASP:OD2	55:SC:272:HIS:NE2	2.51	0.43
58:SF:100:ILE:HD11	58:SF:108:PRO:HB3	2.01	0.43
3:CF:11:VAL:HG22	3:CF:13:ILE:HG23	2.00	0.43
4:L5:35:U:H4'	4:L5:1525:A:C2	2.52	0.43
4:L5:468:U:H3'	4:L5:684:G:H1	1.82	0.43
4:L5:1415:G:H2'	4:L5:1416:G:C8	2.54	0.43
4:L5:1631:A:C2	7:LA:204:MET:HG2	2.53	0.43
4:L5:2072:C:OP1	22:LQ:2:GLY:N	2.52	0.43
4:L5:2351:OMC:HM23	4:L5:2351:OMC:H1'	1.64	0.43
4:L5:2389:A:H5'	35:Ld:70:LYS:HE2	1.99	0.43
4:L5:2464:C:HO2'	4:L5:2465:C:H6	1.62	0.43
4:L5:3855:C:H2'	4:L5:3856:A:H8	1.83	0.43
4:L5:4460:U:H2'	4:L5:4461:C:C6	2.53	0.43
5:L7:64:G:OP1	15:LI:203:HIS:HB2	2.18	0.43
6:L8:66:A:H2'	6:L8:67:U:H6	1.83	0.43
8:LB:165:HIS:HB3	8:LB:180:LEU:HD23	2.00	0.43
14:LH:14:GLU:H	14:LH:14:GLU:CD	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:LQ:86:ILE:HD12	22:LQ:102:ALA:HB2	2.00	0.43
23:LR:148:ASP:OD1	23:LR:148:ASP:N	2.51	0.43
23:LR:176:ARG:NH2	52:S2:910:G:OP1	2.49	0.43
32:La:103:VAL:HG22	32:La:125:LYS:O	2.19	0.43
49:Ls:30:VAL:HG21	49:Ls:187:LEU:HG	2.01	0.43
52:S2:96:C:H2'	52:S2:97:U:C6	2.53	0.43
52:S2:374:G:H2'	52:S2:375:U:H6	1.83	0.43
52:S2:592:C:H5'	52:S2:592:C:H6	1.83	0.43
52:S2:677:G:N1	52:S2:1027:A:OP2	2.33	0.43
52:S2:921:G:C4	75:SW:28:ARG:NH1	2.87	0.43
52:S2:1286:G:N1	65:SM:37:GLU:OE2	2.52	0.43
52:S2:1661:A:OP1	82:Sd:19:ARG:NH2	2.50	0.43
54:SB:131:ASP:HB2	54:SB:180:ASP:OD1	2.18	0.43
57:SE:107:GLY:HA2	57:SE:189:LEU:HG	2.01	0.43
59:SG:14:LYS:HE2	59:SG:16:ILE:HD11	2.01	0.43
59:SG:67:VAL:HB	59:SG:99:GLY:HA2	2.01	0.43
61:SI:58:LEU:HG	94:SI:301:HOH:O	2.17	0.43
66:SN:47:PRO:HA	66:SN:50:ILE:HD12	1.99	0.43
72:ST:30:VAL:HG13	72:ST:34:VAL:HG11	1.99	0.43
75:SW:11:LEU:HD23	75:SW:11:LEU:HA	1.83	0.43
85:Sg:194:TYR:CZ	85:Sg:212:LYS:HD3	2.53	0.43
3:CF:77:LEU:HD11	3:CF:251:GLN:HE22	1.83	0.43
4:L5:163:A:H2'	4:L5:164:G:H8	1.83	0.43
4:L5:1563:A:H2'	4:L5:1564:A:C8	2.53	0.43
4:L5:1725:U:H2'	4:L5:1726:U:C6	2.53	0.43
4:L5:1878:G:H2'	4:L5:1879:C:C6	2.53	0.43
4:L5:2323:C:H2'	4:L5:2324:C:H6	1.84	0.43
4:L5:2372:U:H2'	4:L5:2373:C:C6	2.53	0.43
4:L5:2630:U:OP1	26:LU:48:LYS:NZ	2.47	0.43
4:L5:3689:G:O2'	4:L5:3818:UY1:OP2	2.35	0.43
4:L5:3707:U:H2'	4:L5:3708:C:H6	1.84	0.43
4:L5:3718:A2M:HM'3	4:L5:3718:A2M:H1'	1.80	0.43
4:L5:4066:U:H2'	4:L5:4067:U:H6	1.81	0.43
4:L5:4127:A:C2	13:LG:37:LYS:HG2	2.53	0.43
4:L5:4637:OMG:H2'	4:L5:4638:U:C6	2.54	0.43
6:L8:150:C:N4	13:LG:52:THR:O	2.50	0.43
14:LH:12:ILE:HG12	14:LH:18:ILE:HD12	1.99	0.43
16:LJ:22:LEU:HD11	16:LJ:82:ILE:HG21	2.00	0.43
19:LN:146:PRO:HB2	39:Lh:104:THR:HG23	2.00	0.43
33:Lb:111:ARG:O	33:Lb:114:LYS:HG2	2.18	0.43
52:S2:57:U:OP1	52:S2:504:G:O2'	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:601:OMG:HM23	52:S2:601:OMG:H1'	1.69	0.43
52:S2:1547:C:H1'	52:S2:1670:C:H4'	2.01	0.43
52:S2:1629:C:H5''	71:SS:83:PHE:HE1	1.83	0.43
54:SB:164:ILE:HD13	54:SB:207:LEU:HD11	1.99	0.43
57:SE:126:VAL:HG23	57:SE:139:LEU:HG	2.00	0.43
59:SG:147:LEU:HD13	59:SG:151:ASP:HB2	2.00	0.43
64:SL:68:ILE:HG12	64:SL:143:LEU:HD11	2.01	0.43
64:SL:97:ARG:N	64:SL:97:ARG:HD3	2.34	0.43
74:SV:15:ARG:HE	74:SV:15:ARG:HB2	1.59	0.43
4:L5:123:C:H2'	4:L5:124:C:C6	2.53	0.43
4:L5:1194:G:H2'	4:L5:1195:G:C8	2.53	0.43
4:L5:1282:G:OP2	11:LE:128:HIS:NE2	2.52	0.43
4:L5:2465:C:H2'	4:L5:2466:G:O4'	2.18	0.43
4:L5:2640:G:H2'	4:L5:2641:A:H8	1.82	0.43
4:L5:3685:C:H5'	7:LA:193:ARG:CZ	2.49	0.43
4:L5:4571:A2M:H2'	4:L5:4572:U:C6	2.51	0.43
6:L8:83:C:H42	30:LY:50:ARG:NH2	2.17	0.43
7:LA:27:ALA:HB3	7:LA:54:ARG:HH12	1.84	0.43
8:LB:18:PRO:O	8:LB:20:LYS:N	2.51	0.43
9:LC:76:ILE:HG12	9:LC:96:CYS:SG	2.59	0.43
16:LJ:159:LYS:HE2	16:LJ:163:MET:HE1	2.00	0.43
18:LM:100:ARG:HD3	20:LO:198:THR:O	2.18	0.43
35:Ld:123:ASP:OD1	35:Ld:123:ASP:N	2.51	0.43
52:S2:43:U:OP2	52:S2:485:A:N6	2.48	0.43
52:S2:99:A2M:HM'3	52:S2:99:A2M:H1'	1.72	0.43
52:S2:509:OMG:HM23	52:S2:509:OMG:H1'	1.78	0.43
52:S2:963:A:H2'	52:S2:964:A:C8	2.54	0.43
52:S2:1025:U:H2'	52:S2:1026:C:O4'	2.17	0.43
52:S2:1120:U:H5'	80:Sb:72:ARG:HH22	1.83	0.43
58:SF:55:ARG:HE	58:SF:55:ARG:HB3	1.71	0.43
60:SH:63:PHE:HA	60:SH:95:ILE:O	2.18	0.43
60:SH:145:ARG:HD2	60:SH:155:LYS:HZ1	1.83	0.43
61:SI:110:ARG:HH21	61:SI:123:ARG:NH1	2.17	0.43
65:SM:23:LYS:O	65:SM:27:ILE:HG12	2.19	0.43
84:Sf:105:TYR:HB2	84:Sf:117:LEU:HD11	2.01	0.43
86:AT:24:C:H2'	86:AT:25:A:C8	2.52	0.43
86:AT:30:C:H2'	86:AT:31:G:C8	2.54	0.43
87:CA:108:ILE:O	87:CA:122:ALA:HA	2.19	0.43
4:L5:50:C:C2	4:L5:51:A:C8	3.07	0.43
4:L5:60:G:H2'	4:L5:61:A:C8	2.54	0.43
4:L5:128:C:H2'	4:L5:129:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:347:A:OP2	30:LY:8:THR:OG1	2.27	0.43
4:L5:400:A2M:HM'3	4:L5:400:A2M:H1'	1.60	0.43
4:L5:426:A:H2'	4:L5:427:A:C8	2.53	0.43
4:L5:746:A:H61	4:L5:918:G:H1	1.67	0.43
4:L5:1344:C:H1'	17:LL:10:LEU:HD11	2.01	0.43
4:L5:1578:U:H2'	4:L5:1579:C:H6	1.83	0.43
4:L5:1893:C:H1'	4:L5:1937:C:O2	2.19	0.43
4:L5:2424:OMG:H1'	4:L5:2424:OMG:HM23	1.79	0.43
4:L5:3841:OMC:H1'	4:L5:3841:OMC:HM23	1.71	0.43
4:L5:3896:C:H1'	8:LB:268:ARG:NH2	2.32	0.43
4:L5:4119:C:H42	38:Lg:100:GLN:CD	2.27	0.43
4:L5:4710:C:H2'	4:L5:4711:C:C6	2.54	0.43
4:L5:4741:C:H4'	4:L5:4742:G:H5'	1.99	0.43
4:L5:4759:C:H2'	4:L5:4760:G:C8	2.53	0.43
4:L5:4860:G:H5'	20:LO:169:ARG:HD2	1.99	0.43
94:L5:6618:HOH:O	21:LP:6:LEU:HD13	2.17	0.43
8:LB:144:LYS:HB3	8:LB:144:LYS:HE2	1.88	0.43
13:LG:50:ASP:OD1	13:LG:52:THR:HG23	2.18	0.43
27:LV:91:LYS:HA	27:LV:91:LYS:HD3	1.77	0.43
28:LW:77:LYS:C	28:LW:77:LYS:HD3	2.43	0.43
29:LX:129:ARG:NH2	29:LX:131:ASP:OD2	2.52	0.43
49:Ls:173:THR:O	49:Ls:177:MET:HG2	2.19	0.43
52:S2:17:C:H2'	52:S2:18:C:H6	1.82	0.43
52:S2:609:U:H2'	52:S2:610:G:H8	1.82	0.43
58:SF:87:LEU:HD11	69:SQ:47:LEU:HD11	2.01	0.43
59:SG:23:LYS:HZ2	59:SG:41:LEU:HA	1.83	0.43
62:SJ:131:ARG:HD2	62:SJ:131:ARG:HA	1.75	0.43
65:SM:52:LEU:HB3	65:SM:76:LEU:HD11	1.99	0.43
69:SQ:31:LEU:O	69:SQ:68:ILE:N	2.48	0.43
79:Sa:12:LYS:HE3	79:Sa:12:LYS:HB3	1.85	0.43
85:Sg:258:ILE:HG23	85:Sg:267:VAL:HB	2.01	0.43
2:CI:53:GLU:CD	2:CI:53:GLU:H	2.26	0.43
4:L5:978:G:H2'	4:L5:979:C:C6	2.53	0.43
4:L5:1779:U:H2'	4:L5:1780:A:C8	2.53	0.43
4:L5:1788:A:H2'	15:LI:22:PHE:CZ	2.53	0.43
4:L5:2487:G:C4	4:L5:2489:C:H5''	2.53	0.43
4:L5:2638:G:N1	4:L5:2718:U:H2'	2.34	0.43
4:L5:2902:G:N2	4:L5:3597:G:O6	2.51	0.43
4:L5:4173:G:H2'	4:L5:4174:U:C6	2.54	0.43
5:L7:26:C:OP1	10:LD:56:THR:HG21	2.19	0.43
6:L8:6:C:H2'	6:L8:7:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:LE:176:THR:HB	11:LE:186:LEU:HD23	2.00	0.43
18:LM:37:LEU:HD12	18:LM:37:LEU:HA	1.86	0.43
24:LS:28:TYR:CZ	24:LS:52:LYS:HE2	2.53	0.43
24:LS:76:LYS:NZ	24:LS:100:LEU:O	2.52	0.43
29:LX:156:ILE:CG1	87:CA:291:MET:HA	2.47	0.43
48:Lr:82:ILE:HD11	48:Lr:96:MET:HE1	1.99	0.43
52:S2:461:U:H2'	52:S2:462:OMC:C6	2.54	0.43
52:S2:1221:G:O2'	52:S2:1676:U:O2	2.31	0.43
52:S2:1365:G:H2'	52:S2:1366:G:H8	1.84	0.43
63:SK:14:LEU:HD22	63:SK:35:LEU:CD1	2.45	0.43
65:SM:24:THR:O	65:SM:28:HIS:ND1	2.43	0.43
84:Sf:103:LEU:HG	84:Sf:104:LYS:N	2.34	0.43
87:CA:89:PHE:HE1	87:CA:242:GLN:HE22	1.66	0.43
87:CA:354:LEU:HA	87:CA:357:LEU:HG	2.01	0.43
3:CF:63:LEU:HB3	3:CF:66:GLU:HB2	2.00	0.43
3:CF:168:GLU:O	3:CF:172:LYS:HG2	2.19	0.43
4:L5:935:A:O2'	4:L5:936:C:OP1	2.37	0.43
4:L5:1507:C:H4'	9:LC:114:ARG:O	2.17	0.43
4:L5:2045:G:O6	4:L5:3870:C:O2'	2.37	0.43
4:L5:3807:A:OP1	45:Ln:23:ARG:HD3	2.19	0.43
4:L5:3893:C:H2'	4:L5:3894:A:H8	1.81	0.43
4:L5:4208:U:OP1	4:L5:4334:U:O2'	2.33	0.43
4:L5:4920:C:H2'	4:L5:4921:C:H6	1.84	0.43
6:L8:152:U:H2'	6:L8:153:C:O4'	2.19	0.43
8:LB:17:LEU:HA	8:LB:17:LEU:HD23	1.80	0.43
8:LB:56:ILE:O	8:LB:73:VAL:HA	2.19	0.43
8:LB:61:ASP:O	8:LB:63:PRO:HD3	2.19	0.43
9:LC:279:LEU:HD23	9:LC:279:LEU:HA	1.85	0.43
14:LH:103:VAL:HA	14:LH:113:GLU:O	2.19	0.43
16:LJ:22:LEU:HD22	16:LJ:128:LEU:HD12	2.01	0.43
17:LL:46:ILE:HB	17:LL:49:ARG:HB2	2.01	0.43
17:LL:111:GLN:HE21	17:LL:115:GLN:NE2	2.17	0.43
24:LS:90:THR:HB	25:LT:156:TYR:CE2	2.54	0.43
50:Lt:116:MET:HG3	50:Lt:117:ARG:N	2.34	0.43
52:S2:5:U:H2'	52:S2:6:G:C8	2.54	0.43
52:S2:696:G:O6	52:S2:730:C:H3'	2.19	0.43
52:S2:1276:A:C5	52:S2:1322:G:H1'	2.54	0.43
52:S2:1779:G:H2'	52:S2:1780:G:C8	2.54	0.43
52:S2:1849:G:H2'	52:S2:1850:MA6:C8	2.48	0.43
57:SE:86:PHE:HE2	57:SE:226:PHE:CD2	2.36	0.43
57:SE:118:GLU:HG2	57:SE:121:TYR:HE1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:SE:153:LEU:HD12	59:SG:216:ARG:NH1	2.34	0.43
60:SH:20:GLU:CD	60:SH:48:ALA:H	2.27	0.43
60:SH:81:ARG:O	60:SH:85:LYS:HG3	2.18	0.43
62:SJ:137:VAL:HG12	62:SJ:138:ARG:HG2	2.00	0.43
71:SS:36:VAL:HG23	71:SS:99:LEU:HD22	2.01	0.43
77:SY:122:LYS:HD2	77:SY:123:ALA:N	2.34	0.43
4:L5:470:A:H61	4:L5:684:G:H1'	1.83	0.43
4:L5:4303:C:O2'	4:L5:4304:A:H2'	2.19	0.43
89:L5:5292:SPM:H31	89:L5:5292:SPM:H62	1.82	0.43
17:LL:179:PHE:CD2	32:La:131:ARG:HG3	2.54	0.43
18:LM:29:ASP:O	18:LM:37:LEU:N	2.47	0.43
19:LN:24:ARG:HH11	19:LN:24:ARG:HB3	1.84	0.43
29:LX:156:ILE:HD12	29:LX:156:ILE:HA	1.91	0.43
31:LZ:135:ARG:HA	31:LZ:135:ARG:HD2	1.73	0.43
35:Ld:75:LYS:HB2	35:Ld:79:ASN:O	2.19	0.43
44:Lm:93:LYS:HD3	44:Lm:102:ARG:HG2	1.99	0.43
49:Ls:175:LEU:HD21	49:Ls:182:PRO:HG3	1.99	0.43
52:S2:65:C:C2	59:SG:133:LEU:HD12	2.54	0.43
52:S2:194:C:H2'	52:S2:195:C:H6	1.84	0.43
52:S2:608:C:H2'	52:S2:609:U:C6	2.53	0.43
52:S2:1005:G:H2'	52:S2:1006:C:C6	2.53	0.43
52:S2:1286:G:HO2'	52:S2:1312:G:H22	1.67	0.43
52:S2:1740:C:H2'	52:S2:1741:U:C6	2.54	0.43
53:SA:26:GLY:O	53:SA:46:ILE:HG23	2.19	0.43
54:SB:30:TRP:CZ2	67:SO:19:PRO:HD3	2.54	0.43
54:SB:75:GLN:HB2	54:SB:78:GLU:HB2	2.00	0.43
55:SC:248:TYR:OH	74:SV:11:LEU:HD23	2.18	0.43
75:SW:30:CYS:SG	75:SW:31:SER:N	2.91	0.43
87:CA:88:HIS:CG	87:CA:305:PHE:HB3	2.53	0.43
3:CF:429:MET:SD	86:AT:54:G:O4'	2.77	0.42
4:L5:6:C:H2'	4:L5:7:C:C6	2.54	0.42
4:L5:21:G:H1'	6:L8:103:A:N3	2.34	0.42
4:L5:1081:C:C2'	4:L5:1082:C:H5'	2.49	0.42
4:L5:1367:C:O2'	4:L5:1369:C:OP2	2.35	0.42
4:L5:1553:A:O2'	47:Lp:9:GLY:O	2.34	0.42
4:L5:2870:A:H2'	4:L5:2871:A:H8	1.82	0.42
4:L5:2895:A:H2'	4:L5:2896:G:C8	2.53	0.42
4:L5:4196:OMG:HM23	4:L5:4196:OMG:H1'	1.68	0.42
4:L5:4250:G:O2'	16:LJ:129:ASP:OD1	2.31	0.42
4:L5:4737:G:H2'	4:L5:4738:C:C6	2.54	0.42
4:L5:4757:C:H4'	20:LO:114:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
90:L5:5284:SPD:H51	90:L5:5284:SPD:H82	1.76	0.42
5:L7:58:A:H2'	5:L7:59:G:C8	2.54	0.42
6:L8:97:A:OP2	39:Lh:66:LYS:NZ	2.44	0.42
9:LC:150:LEU:HD23	9:LC:150:LEU:HA	1.72	0.42
13:LG:111:LYS:HB3	13:LG:111:LYS:HE3	1.86	0.42
26:LU:63:ILE:HD11	26:LU:70:ILE:CG2	2.49	0.42
26:LU:80:LYS:HG2	26:LU:110:TYR:CE2	2.54	0.42
30:LY:100:HIS:ND1	30:LY:102:SER:OG	2.38	0.42
33:Lb:93:LEU:HD12	33:Lb:93:LEU:HA	1.92	0.42
34:Lc:48:LEU:HD23	34:Lc:57:LYS:HG2	2.01	0.42
34:Lc:50:ASN:OD1	34:Lc:50:ASN:N	2.49	0.42
39:Lh:15:GLU:OE1	39:Lh:15:GLU:N	2.47	0.42
45:Ln:17:ARG:NH1	52:S2:1173:A:OP1	2.52	0.42
52:S2:986:G:C8	67:SO:137:SER:O	2.72	0.42
52:S2:1102:G:H2'	52:S2:1103:C:C6	2.54	0.42
61:SI:136:ILE:HG13	61:SI:137:LEU:N	2.33	0.42
63:SK:97:SER:O	63:SK:98:ARG:HD2	2.19	0.42
65:SM:97:GLU:H	65:SM:97:GLU:CD	2.27	0.42
67:SO:15:ILE:HG12	67:SO:16:SER:H	1.83	0.42
85:Sg:124:SER:HG	85:Sg:125:ARG:H	1.65	0.42
3:CF:364:HIS:NE2	3:CF:411:CYS:O	2.52	0.42
4:L5:100:C:H2'	4:L5:101:A:O4'	2.18	0.42
4:L5:170:C:H42	4:L5:266:C:H42	1.66	0.42
4:L5:223:G:H4'	4:L5:225:G:C8	2.53	0.42
4:L5:2457:G:O2'	4:L5:3672:G:H1'	2.19	0.42
4:L5:2634:C:H2'	4:L5:2635:U:C6	2.55	0.42
4:L5:2683:C:H2'	4:L5:2684:C:H6	1.84	0.42
4:L5:4334:U:H5''	25:LT:7:LYS:HD2	2.01	0.42
4:L5:4460:U:H2'	4:L5:4461:C:H6	1.83	0.42
4:L5:4565:C:O2'	8:LB:268:ARG:HD3	2.18	0.42
4:L5:4770:U:H2'	4:L5:4771:C:C6	2.53	0.42
4:L5:4872:G:OP2	18:LM:94:LYS:NZ	2.46	0.42
5:L7:4:U:H2'	5:L7:5:A:C8	2.53	0.42
9:LC:33:ARG:HH12	22:LQ:22:ASP:CB	2.32	0.42
13:LG:175:ARG:HG3	13:LG:230:TYR:CG	2.54	0.42
18:LM:38:VAL:O	18:LM:47:ARG:HA	2.18	0.42
24:LS:30:MET:HE2	24:LS:30:MET:HB3	1.96	0.42
34:Lc:34:THR:HG23	34:Lc:95:ALA:HB2	2.01	0.42
50:Lt:32:ILE:HG13	50:Lt:35:LEU:HD13	2.01	0.42
50:Lt:123:ARG:HD2	50:Lt:129:ILE:HD11	2.00	0.42
52:S2:14:C:H2'	52:S2:15:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:575:A:H2'	52:S2:576:A2M:O4'	2.19	0.42
52:S2:1466:G:H2'	52:S2:1467:C:C6	2.55	0.42
52:S2:1665:G:N7	72:ST:88:MET:HE1	2.34	0.42
54:SB:36:PRO:HB2	54:SB:38:MET:HG2	2.00	0.42
54:SB:152:LYS:HD3	70:SR:133:GLY:HA3	1.99	0.42
57:SE:36:HIS:ND1	57:SE:85:GLY:HA3	2.34	0.42
57:SE:43:PRO:HB2	57:SE:45:ILE:HG22	2.01	0.42
58:SF:81:ARG:O	58:SF:85:LYS:NZ	2.49	0.42
61:SI:76:THR:HG21	61:SI:104:ILE:HD12	2.01	0.42
61:SI:83:TYR:HB3	61:SI:101:ILE:HG12	2.01	0.42
62:SJ:101:LYS:HA	62:SJ:101:LYS:HD2	1.93	0.42
69:SQ:96:TYR:HD1	69:SQ:100:VAL:HG21	1.83	0.42
75:SW:57:ARG:HH21	80:Sb:26:GLN:CD	2.27	0.42
81:Sc:10:LYS:HD2	81:Sc:34:PHE:CE1	2.54	0.42
81:Sc:35:MET:HE3	81:Sc:35:MET:HB2	1.92	0.42
86:AT:14:A:H2'	86:AT:15:G:O4'	2.19	0.42
3:CF:13:ILE:HG13	3:CF:114:LEU:HD23	2.01	0.42
4:L5:270:U:H2'	4:L5:271:C:C6	2.54	0.42
4:L5:408:A:O2'	4:L5:411:G:OP2	2.22	0.42
4:L5:1298:C:H2'	4:L5:1299:G:H8	1.83	0.42
4:L5:1366:G:H1'	4:L5:1367:C:C6	2.55	0.42
4:L5:1557:C:H2'	4:L5:1558:A:C8	2.54	0.42
4:L5:1693:U:H2'	4:L5:1694:C:O4'	2.19	0.42
4:L5:2283:G:H5''	32:La:18:GLY:O	2.19	0.42
4:L5:4098:A:C8	4:L5:4099:G:H1'	2.55	0.42
4:L5:4126:C:OP1	13:LG:37:LYS:NZ	2.52	0.42
4:L5:4258:C:H2'	4:L5:4259:C:C6	2.54	0.42
4:L5:4393:G:O4'	4:L5:4447:5MC:HM53	2.18	0.42
4:L5:4604:G:N2	4:L5:4607:A:OP2	2.43	0.42
4:L5:4899:G:H3'	4:L5:4901:G:OP2	2.19	0.42
4:L5:4911:A:OP2	8:LB:100:ARG:HD3	2.19	0.42
5:L7:38:U:N3	5:L7:41:G:OP2	2.29	0.42
6:L8:93:C:HO2'	6:L8:94:G:H8	1.67	0.42
8:LB:28:LYS:HG3	8:LB:30:LYS:HG3	2.00	0.42
13:LG:30:PRO:HG2	31:LZ:124:THR:HA	2.00	0.42
14:LH:34:LEU:HD23	14:LH:34:LEU:HA	1.87	0.42
14:LH:60:TRP:CE3	24:LS:153:PRO:HD2	2.53	0.42
20:LO:189:ILE:HD13	20:LO:189:ILE:HA	1.90	0.42
23:LR:177:LEU:O	23:LR:181:LYS:HG2	2.19	0.42
31:LZ:95:VAL:HG12	31:LZ:110:ALA:HA	2.01	0.42
32:La:125:LYS:HG2	32:La:145:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:Lr:28:GLU:CD	48:Lr:31:ASN:HD22	2.26	0.42
52:S2:380:G:P	61:SI:56:ARG:HH22	2.42	0.42
52:S2:472:C:O2	52:S2:475:C:N4	2.49	0.42
52:S2:1540:G:H2'	52:S2:1541:G:C8	2.55	0.42
52:S2:1679:A:P	58:SF:60:ARG:HE	2.41	0.42
53:SA:55:TRP:HZ3	53:SA:177:MET:HE2	1.84	0.42
53:SA:121:LEU:HD11	53:SA:145:ILE:CD1	2.49	0.42
54:SB:139:CYS:HB2	54:SB:172:MET:SD	2.59	0.42
60:SH:160:LYS:HE3	60:SH:189:PHE:HB3	2.01	0.42
63:SK:64:TRP:CD1	82:Sd:23:VAL:HG13	2.54	0.42
63:SK:96:ARG:O	63:SK:96:ARG:HD2	2.19	0.42
72:ST:18:LEU:HD23	72:ST:22:LEU:HG	2.02	0.42
72:ST:24:LYS:HD2	72:ST:24:LYS:C	2.44	0.42
78:SZ:86:ALA:O	78:SZ:89:GLN:HG2	2.19	0.42
3:CF:296:HIS:HA	86:AT:77:A:O2'	2.19	0.42
4:L5:23:C:H2'	4:L5:24:G:O4'	2.19	0.42
4:L5:962:C:O3'	12:LF:32:ARG:NH1	2.53	0.42
4:L5:1079:C:O2	4:L5:1221:G:N2	2.53	0.42
4:L5:1837:A:OP2	25:LT:130:ARG:NE	2.52	0.42
4:L5:2890:C:H2'	4:L5:2891:U:C6	2.54	0.42
4:L5:3760:A:H4'	4:L5:3761:C:H5''	2.01	0.42
4:L5:3869:OMC:OP2	94:L5:5403:HOH:O	2.22	0.42
4:L5:4458:C:H2'	4:L5:4459:U:H6	1.84	0.42
13:LG:182:CYS:HB3	13:LG:222:ILE:HG23	2.01	0.42
35:Ld:29:ILE:O	35:Ld:33:ILE:HG12	2.19	0.42
35:Ld:117:LEU:HD23	35:Ld:117:LEU:HA	1.90	0.42
39:Lh:89:ARG:O	39:Lh:93:ARG:HG2	2.19	0.42
52:S2:1035:A:H2'	52:S2:1036:A:O4'	2.18	0.42
52:S2:1089:G:H2'	52:S2:1090:C:C6	2.54	0.42
57:SE:11:ARG:NH2	57:SE:24:THR:OG1	2.51	0.42
58:SF:99:ILE:HG23	78:SZ:67:LEU:HD13	2.00	0.42
59:SG:2:LYS:O	59:SG:3:LEU:HD23	2.20	0.42
59:SG:42:GLY:O	59:SG:46:LYS:NZ	2.38	0.42
59:SG:194:LEU:HD13	59:SG:197:GLN:NE2	2.34	0.42
60:SH:79:LEU:HD23	60:SH:79:LEU:H	1.84	0.42
62:SJ:136:ARG:NH1	62:SJ:159:PHE:O	2.50	0.42
63:SK:80:ARG:O	63:SK:85:LEU:N	2.48	0.42
64:SL:30:LYS:HE3	64:SL:32:LYS:HA	2.01	0.42
71:SS:111:LEU:HD11	71:SS:125:HIS:CG	2.54	0.42
72:ST:39:LEU:HD13	72:ST:47:PRO:HG3	2.02	0.42
76:SX:41:PHE:CZ	76:SX:102:VAL:HG23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:Sf:107:LYS:NZ	84:Sf:108:VAL:HG22	2.35	0.42
85:Sg:248:LEU:O	85:Sg:258:ILE:HD12	2.20	0.42
3:CF:363:CYS:HB3	3:CF:424:PHE:HB2	2.02	0.42
4:L5:72:C:C5	17:LL:67:HIS:ND1	2.81	0.42
4:L5:262:G:H2'	4:L5:263:G:H8	1.84	0.42
4:L5:705:G:H2'	4:L5:706:C:H6	1.85	0.42
4:L5:1184:A:H2'	4:L5:1185:G:C8	2.54	0.42
4:L5:1881:C:H5'	4:L5:2281:U:H1'	2.01	0.42
4:L5:1995:G:H2'	4:L5:1996:C:C6	2.54	0.42
4:L5:2497:C:H2'	4:L5:2498:C:C6	2.54	0.42
4:L5:2506:G:H4'	4:L5:2507:A:OP1	2.20	0.42
4:L5:2858:A:H2'	4:L5:2859:G:H8	1.84	0.42
4:L5:3668:C:H5'	7:LA:8:GLN:O	2.19	0.42
4:L5:4589:A:N1	4:L5:4621:C:O2'	2.42	0.42
8:LB:84:MET:O	8:LB:204:GLN:HA	2.20	0.42
11:LE:72:LYS:NZ	33:Lb:115:GLY:O	2.52	0.42
11:LE:99:ASP:OD1	11:LE:99:ASP:N	2.49	0.42
49:Ls:83:ARG:HD3	49:Ls:83:ARG:HA	1.70	0.42
52:S2:2:A:C2	55:SC:196:ILE:HD13	2.54	0.42
52:S2:24:C:O2'	52:S2:25:A:H8	2.02	0.42
52:S2:1436:C:H4'	52:S2:1437:C:H2'	2.01	0.42
52:S2:1719:A:N6	52:S2:1814:G:O2'	2.53	0.42
52:S2:1798:C:H2'	52:S2:1799:G:O4'	2.19	0.42
54:SB:98:THR:O	54:SB:232:HIS:NE2	2.50	0.42
55:SC:234:GLY:O	55:SC:238:LYS:HB2	2.20	0.42
60:SH:133:LEU:HD23	60:SH:133:LEU:O	2.20	0.42
62:SJ:81:LEU:HD23	62:SJ:81:LEU:HA	1.88	0.42
63:SK:45:VAL:O	63:SK:49:MET:HG2	2.19	0.42
68:SP:81:ARG:HH12	68:SP:122:THR:CG2	2.32	0.42
71:SS:62:ASP:O	71:SS:65:GLU:HG3	2.20	0.42
86:AT:26:C:H2'	86:AT:27:G:H8	1.84	0.42
86:AT:60:A:H2'	86:AT:61:A:O4'	2.19	0.42
87:CA:36:VAL:HG12	87:CA:125:PHE:CE1	2.54	0.42
3:CF:99:ILE:HG21	3:CF:427:ARG:NH2	2.33	0.42
3:CF:106:THR:OG1	3:CF:143:LEU:HD12	2.19	0.42
4:L5:1555:G:O6	47:Lp:4:ARG:NH1	2.52	0.42
4:L5:1631:A:H2	7:LA:208:GLU:HG3	1.85	0.42
4:L5:2326:G:H5''	36:Le:127:ALA:HB1	2.01	0.42
4:L5:2417:A:C4	4:L5:2418:A:C8	3.08	0.42
4:L5:2519:U:H1'	4:L5:2520:C:C6	2.54	0.42
4:L5:2804:OMC:HM21	38:Lg:32:TYR:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:2891:U:H2'	4:L5:2892:C:O4'	2.20	0.42
4:L5:4088:C:C5	13:LG:54:PHE:HZ	2.36	0.42
4:L5:4456:OMC:HM21	8:LB:241:PRO:HD3	2.02	0.42
4:L5:4593:C:H2'	4:L5:4594:U:H6	1.84	0.42
4:L5:4771:C:H2'	4:L5:4772:C:C6	2.53	0.42
6:L8:78:G:H2'	6:L8:79:G:C8	2.55	0.42
6:L8:79:G:H2'	6:L8:80:A:O4'	2.20	0.42
7:LA:131:GLY:N	7:LA:169:VAL:HG13	2.35	0.42
12:LF:110:GLN:HG2	12:LF:115:ARG:NH1	2.35	0.42
15:LI:101:LYS:NZ	15:LI:102:MET:O	2.52	0.42
17:LL:7:GLY:O	32:La:49:HIS:NE2	2.42	0.42
28:LW:115:ALA:O	28:LW:119:LYS:N	2.48	0.42
30:LY:112:ASP:OD1	30:LY:112:ASP:N	2.50	0.42
30:LY:116:LYS:O	30:LY:120:GLU:HG3	2.19	0.42
33:Lb:55:LYS:O	33:Lb:58:GLN:NE2	2.53	0.42
42:Lk:10:ASP:HA	42:Lk:13:LEU:HD21	2.02	0.42
50:Lt:79:ALA:HA	50:Lt:82:ILE:HG22	2.01	0.42
50:Lt:106:PHE:CD2	50:Lt:109:ILE:HD11	2.48	0.42
52:S2:461:U:H2'	52:S2:462:OMC:H6	1.83	0.42
52:S2:1005:G:H2'	52:S2:1006:C:H6	1.83	0.42
52:S2:1670:C:H2'	52:S2:1671:G:C8	2.53	0.42
53:SA:144:THR:OG1	53:SA:156:TYR:O	2.37	0.42
53:SA:158:ASP:O	74:SV:66:ASP:HA	2.20	0.42
55:SC:255:LEU:O	74:SV:16:LYS:NZ	2.42	0.42
56:SD:72:VAL:HG21	63:SK:70:TYR:CE1	2.54	0.42
56:SD:167:TYR:CE2	56:SD:204:LEU:HG	2.55	0.42
58:SF:18:LYS:HE2	58:SF:22:LYS:HA	2.02	0.42
61:SI:42:ARG:HH21	61:SI:59:ARG:CZ	2.33	0.42
65:SM:95:ASP:O	65:SM:99:LYS:N	2.51	0.42
75:SW:26:LEU:HB2	80:Sb:7:LEU:HD23	2.02	0.42
76:SX:140:ARG:HH22	76:SX:142:ARG:HH21	1.67	0.42
86:AT:22:A:H2'	86:AT:23:U:C6	2.54	0.42
4:L5:1683:PSU:H2'	4:L5:1684:A:H8	1.84	0.42
4:L5:1701:A:C2'	4:L5:1702:C:H5'	2.50	0.42
4:L5:2409:U:H5	4:L5:2783:A:N1	2.17	0.42
4:L5:2656:U:OP1	31:LZ:78:ASN:ND2	2.52	0.42
4:L5:2693:G:H2'	4:L5:2694:G:N2	2.34	0.42
4:L5:2858:A:H2'	4:L5:2859:G:C8	2.54	0.42
4:L5:3920:PSU:H2'	4:L5:3921:U:C6	2.54	0.42
4:L5:4305:G:O5'	25:LT:83:LYS:NZ	2.53	0.42
4:L5:4344:U:H2'	4:L5:4345:C:H6	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LA:196:TRP:HB3	7:LA:197:PRO:HD3	2.02	0.42
8:LB:348:ARG:HG2	8:LB:349:LYS:O	2.20	0.42
13:LG:180:PRO:HG3	13:LG:219:VAL:HG13	2.01	0.42
23:LR:154:LEU:HD12	23:LR:155:LEU:N	2.35	0.42
24:LS:11:LYS:HE3	24:LS:29:ARG:HD3	2.01	0.42
49:Ls:25:PRO:HB2	49:Ls:195:ASN:OD1	2.20	0.42
52:S2:52:G:H2'	52:S2:53:C:H6	1.85	0.42
52:S2:375:U:H2'	52:S2:376:A:C8	2.55	0.42
52:S2:483:C:OP2	76:SX:75:ILE:HD11	2.20	0.42
52:S2:1270:G:OP1	84:Sf:89:LYS:HD3	2.19	0.42
58:SF:112:LEU:HD13	58:SF:177:LEU:HD21	2.01	0.42
62:SJ:176:LYS:HA	62:SJ:179:LYS:HG2	2.00	0.42
63:SK:97:SER:C	63:SK:98:ARG:HD2	2.44	0.42
65:SM:99:LYS:HG2	65:SM:100:PRO:HD2	2.00	0.42
84:Sf:107:LYS:HG3	84:Sf:108:VAL:N	2.34	0.42
85:Sg:112:ALA:HB3	85:Sg:121:VAL:HG12	2.01	0.42
85:Sg:201:SER:N	85:Sg:206:LEU:O	2.53	0.42
85:Sg:239:LEU:HD11	85:Sg:248:LEU:HD21	2.02	0.42
1:CD:9:PHE:CD2	34:Lc:104:ILE:HG22	2.54	0.42
3:CF:138:LEU:CD2	3:CF:347:LEU:HD22	2.50	0.42
4:L5:106:A:H1'	4:L5:336:A:N3	2.34	0.42
4:L5:458:C:H2'	4:L5:459:C:C6	2.55	0.42
4:L5:956:A:H1'	4:L5:2076:G:H5''	2.01	0.42
4:L5:1326:A2M:H2'	4:L5:1327:C:H6	1.81	0.42
4:L5:2041:A:N7	4:L5:4434:C:O2'	2.53	0.42
4:L5:2521:G:H2'	4:L5:2522:G:C8	2.55	0.42
4:L5:3867:A2M:HM'3	4:L5:3867:A2M:H1'	1.61	0.42
4:L5:4371:G:O2'	4:L5:4372:U:OP2	2.31	0.42
4:L5:4376:A:H5''	4:L5:4377:G:O5'	2.20	0.42
8:LB:14:LEU:HD22	8:LB:17:LEU:HD21	2.02	0.42
8:LB:168:MET:HG3	8:LB:176:LYS:C	2.44	0.42
9:LC:233:SER:HA	9:LC:263:LEU:HD21	2.02	0.42
9:LC:367:GLU:OE1	9:LC:367:GLU:N	2.38	0.42
13:LG:99:ALA:HB1	13:LG:193:LEU:HD21	2.01	0.42
15:LI:36:LEU:HD13	15:LI:87:MET:HE3	2.02	0.42
21:LP:55:LYS:HD2	21:LP:55:LYS:HA	1.86	0.42
32:La:93:ASN:OD1	32:La:95:THR:N	2.49	0.42
48:Lr:45:HIS:HB2	48:Lr:48:THR:HG22	2.02	0.42
52:S2:433:A:H2'	52:S2:434:G:C8	2.55	0.42
52:S2:1149:A:N3	52:S2:1149:A:H2'	2.34	0.42
52:S2:1190:A:N3	52:S2:1714:U:O2'	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:1300:U:O2'	68:SP:51:ARG:HD3	2.19	0.42
52:S2:1417:C:N4	52:S2:1422:G:H22	2.16	0.42
52:S2:1447:G:P	73:SU:87:ARG:HH22	2.43	0.42
55:SC:83:LEU:HD11	74:SV:15:ARG:HG3	2.02	0.42
59:SG:63:MET:HE1	59:SG:102:VAL:HG12	2.01	0.42
60:SH:74:LYS:HG3	60:SH:75:ILE:HG23	2.02	0.42
64:SL:28:THR:HA	64:SL:29:GLY:HA2	1.63	0.42
73:SU:38:ASP:OD1	73:SU:38:ASP:N	2.53	0.42
74:SV:70:LEU:HD12	74:SV:79:VAL:HG21	2.02	0.42
85:Sg:99:ARG:NH1	85:Sg:135:LEU:HA	2.35	0.42
85:Sg:260:ASP:OD2	85:Sg:263:GLY:N	2.45	0.42
86:AT:4:U:H2'	86:AT:5:C:H6	1.84	0.42
4:L5:153:G:H2'	4:L5:154:G:C8	2.52	0.42
4:L5:1093:C:H2'	4:L5:1094:G:O4'	2.20	0.42
4:L5:1096:C:H2'	4:L5:1097:C:H6	1.85	0.42
4:L5:1317:U:H2'	4:L5:1318:C:C6	2.55	0.42
4:L5:1468:C:H2'	4:L5:1469:C:C6	2.55	0.42
4:L5:2463:G:O2'	4:L5:2464:C:H5'	2.20	0.42
4:L5:2474:G:H2'	4:L5:2502:G:N2	2.34	0.42
4:L5:4112:C:H2'	4:L5:4113:U:O4'	2.19	0.42
4:L5:4195:G:O2'	4:L5:4442:PSU:OP1	2.33	0.42
4:L5:4642:U:H2'	4:L5:4643:G:C8	2.55	0.42
4:L5:5027:C:O2'	4:L5:5028:G:H5''	2.19	0.42
8:LB:196:TRP:NE1	8:LB:200:ARG:HH21	2.18	0.42
16:LJ:89:VAL:HG22	16:LJ:115:LEU:CD2	2.50	0.42
23:LR:172:ARG:HA	23:LR:175:GLU:HG2	2.00	0.42
28:LW:94:ARG:HH21	59:SG:146:ASN:HD21	1.68	0.42
28:LW:100:VAL:O	28:LW:104:GLN:HG2	2.18	0.42
37:Lf:36:ARG:HD2	37:Lf:79:GLY:O	2.20	0.42
49:Ls:60:MET:HE2	49:Ls:60:MET:HA	2.02	0.42
52:S2:12:U:H2'	52:S2:13:C:H6	1.84	0.42
52:S2:462:OMC:HM23	52:S2:462:OMC:H1'	1.81	0.42
52:S2:528:A:H5'	62:SJ:121:LYS:HZ1	1.85	0.42
52:S2:834:C:N3	52:S2:839:C:N3	2.68	0.42
53:SA:42:LYS:CD	53:SA:44:ASP:HB3	2.50	0.42
55:SC:169:TYR:OH	55:SC:175:GLY:O	2.28	0.42
56:SD:41:VAL:HG23	56:SD:46:THR:HB	2.00	0.42
57:SE:212:ASP:OD1	57:SE:216:ASN:N	2.52	0.42
57:SE:233:LYS:HD2	57:SE:233:LYS:HA	1.70	0.42
58:SF:121:PRO:HA	58:SF:193:LYS:HG3	2.02	0.42
58:SF:162:ALA:HB3	58:SF:169:ILE:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:SG:2:LYS:O	59:SG:108:VAL:HA	2.19	0.42
75:SW:3:ARG:NH2	75:SW:28:ARG:NH2	2.67	0.42
75:SW:6:VAL:HG12	75:SW:34:ILE:HD11	2.00	0.42
75:SW:11:LEU:HD21	75:SW:37:PHE:HE2	1.84	0.42
77:SY:89:HIS:CE1	77:SY:90:ARG:HG3	2.55	0.42
79:Sa:64:LEU:HA	79:Sa:65:PRO:HD3	1.95	0.42
3:CF:371:LYS:HZ3	86:AT:52:C:C5'	2.32	0.42
4:L5:45:U:OP2	89:L5:5264:SPM:H112	2.20	0.42
4:L5:66:A:N1	4:L5:311:G:O2'	2.49	0.42
4:L5:499:G:O6	4:L5:657:C:N4	2.53	0.42
4:L5:907:C:H2'	4:L5:908:G:H8	1.85	0.42
4:L5:1468:C:H2'	4:L5:1469:C:H6	1.85	0.42
4:L5:1554:A:OP1	47:Lp:5:THR:OG1	2.32	0.42
4:L5:2608:G:H2'	4:L5:2609:G:H8	1.85	0.42
4:L5:3765:G:O2'	4:L5:3767:C:N4	2.52	0.42
4:L5:3877:A:N3	4:L5:4401:G:O2'	2.40	0.42
4:L5:4500:PSU:H2'	4:L5:4501:U:C6	2.55	0.42
4:L5:4620:OMU:H1'	4:L5:4620:OMU:HM23	1.76	0.42
7:LA:112:ILE:HG22	7:LA:135:THR:HG23	2.02	0.42
7:LA:114:CYS:N	7:LA:165:VAL:O	2.47	0.42
8:LB:59:GLU:OE2	8:LB:60:VAL:N	2.53	0.42
8:LB:300:LYS:HZ1	8:LB:309:LEU:C	2.28	0.42
11:LE:178:PRO:O	11:LE:181:LEU:N	2.43	0.42
21:LP:42:ARG:HD3	21:LP:42:ARG:HA	1.74	0.42
52:S2:59:U:H5''	52:S2:503:C:N4	2.34	0.42
52:S2:1208:A:H2'	52:S2:1209:A:H8	1.85	0.42
52:S2:1311:C:OP1	65:SM:40:LYS:NZ	2.42	0.42
52:S2:1862:G:N2	79:Sa:76:SER:OG	2.47	0.42
75:SW:11:LEU:HB3	75:SW:72:CYS:O	2.20	0.42
79:Sa:51:ARG:NH1	81:Sc:39:SER:HB2	2.35	0.42
85:Sg:208:ALA:HB2	85:Sg:218:LEU:HD13	2.01	0.42
3:CF:55:LYS:HE3	3:CF:55:LYS:HB3	1.92	0.41
3:CF:357:TYR:CD1	86:AT:53:G:H4'	2.55	0.41
4:L5:25:A:C8	4:L5:341:G:C8	3.08	0.41
4:L5:264:C:H2'	4:L5:265:C:C5	2.55	0.41
4:L5:324:A:H2'	4:L5:325:U:C6	2.55	0.41
4:L5:513:U:H3'	4:L5:514:U:H4'	2.02	0.41
4:L5:980:U:H2'	4:L5:981:C:C6	2.55	0.41
4:L5:1178:G:H2'	10:LD:286:SER:HB3	2.02	0.41
4:L5:1304:C:H2'	4:L5:1305:C:C6	2.55	0.41
4:L5:3668:C:OP1	7:LA:8:GLN:NE2	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L7:16:A:H2'	5:L7:17:C:C6	2.54	0.41
6:L8:43:A:H4'	41:Lj:22:CYS:O	2.20	0.41
8:LB:117:ARG:NH2	8:LB:177:LYS:HG2	2.35	0.41
8:LB:213:GLN:HE22	8:LB:285:TYR:C	2.28	0.41
11:LE:222:LEU:HB2	11:LE:237:LYS:CE	2.50	0.41
13:LG:57:TRP:O	13:LG:62:ARG:NH1	2.53	0.41
21:LP:40:HIS:NE2	21:LP:110:ASP:O	2.49	0.41
22:LQ:82:VAL:HG11	22:LQ:86:ILE:HG13	2.02	0.41
27:LV:65:VAL:HG23	27:LV:73:ARG:HA	2.02	0.41
47:Lp:48:LYS:HE3	47:Lp:48:LYS:HB2	1.87	0.41
52:S2:77:A:H2	59:SG:175:LYS:HD2	1.85	0.41
52:S2:323:C:H4'	52:S2:324:C:C5	2.53	0.41
52:S2:374:G:H2'	52:S2:375:U:C6	2.54	0.41
52:S2:432:G:H2'	52:S2:433:A:C8	2.55	0.41
52:S2:509:OMG:OP1	62:SJ:2:PRO:HA	2.19	0.41
52:S2:1221:G:H2'	52:S2:1222:G:H8	1.85	0.41
52:S2:1265:A:O2'	52:S2:1327:G:OP2	2.24	0.41
52:S2:1433:C:N4	73:SU:51:LYS:HD2	2.35	0.41
52:S2:1703:OMC:H2'	52:S2:1704:C:O4'	2.20	0.41
52:S2:1758:G:N2	52:S2:1773:C:O4'	2.53	0.41
55:SC:142:LYS:HG2	55:SC:153:GLY:HA3	2.02	0.41
58:SF:59:LYS:HA	58:SF:59:LYS:HD2	1.81	0.41
60:SH:58:LYS:HB3	60:SH:90:LYS:HD3	2.02	0.41
61:SI:140:LYS:HD2	61:SI:140:LYS:O	2.19	0.41
72:ST:105:GLN:HA	72:ST:108:GLU:OE1	2.20	0.41
77:SY:26:ASP:OD1	77:SY:26:ASP:N	2.54	0.41
79:Sa:19:GLN:OE1	79:Sa:19:GLN:N	2.33	0.41
85:Sg:158:PRO:HD3	85:Sg:200:VAL:HG21	2.02	0.41
85:Sg:165:ILE:HB	85:Sg:179:LEU:HD21	2.01	0.41
85:Sg:172:LYS:HG2	85:Sg:193:GLY:O	2.20	0.41
3:CF:43:GLU:CB	3:CF:55:LYS:HG3	2.49	0.41
3:CF:147:GLN:OE1	3:CF:235:ILE:HB	2.20	0.41
3:CF:217:THR:C	3:CF:218:ARG:HD3	2.44	0.41
4:L5:261:G:C6	4:L5:262:G:C6	3.08	0.41
4:L5:460:C:H2'	4:L5:461:G:H8	1.85	0.41
4:L5:1773:U:H2'	4:L5:1774:C:C6	2.55	0.41
4:L5:2095:A:H1'	4:L5:2096:G:C2	2.54	0.41
4:L5:4232:U:H5''	46:Lo:3:ASN:O	2.20	0.41
4:L5:4678:G:N2	4:L5:4713:G:H1'	2.35	0.41
6:L8:41:A:H4'	41:Lj:59:THR:HG23	2.02	0.41
7:LA:108:PRO:HG2	47:Lp:86:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LC:187:GLN:NE2	9:LC:203:GLN:OE1	2.48	0.41
13:LG:100:HIS:O	13:LG:103:ARG:HG3	2.19	0.41
15:LI:208:LYS:O	15:LI:211:VAL:HG22	2.21	0.41
22:LQ:172:ARG:HA	22:LQ:176:ARG:HD2	2.01	0.41
23:LR:103:ARG:HG2	23:LR:124:TYR:CE2	2.55	0.41
34:Lc:103:ASP:OD1	34:Lc:103:ASP:N	2.53	0.41
37:Lf:102:ARG:HB2	37:Lf:104:MET:HE2	2.01	0.41
39:Lh:8:ASP:OD1	39:Lh:8:ASP:N	2.52	0.41
39:Lh:57:VAL:O	39:Lh:61:ILE:HG13	2.21	0.41
49:Ls:29:ILE:HG22	49:Ls:88:PHE:CD1	2.54	0.41
52:S2:434:G:H5'	61:SI:23:LYS:HE3	2.01	0.41
52:S2:834:C:H42	52:S2:839:C:H42	1.68	0.41
52:S2:1677:U:H2'	52:S2:1678:A:C8	2.54	0.41
53:SA:54:THR:HA	53:SA:162:PRO:HD2	2.02	0.41
55:SC:257:LYS:O	74:SV:16:LYS:NZ	2.42	0.41
57:SE:208:VAL:HG21	57:SE:225:ILE:HG13	2.01	0.41
59:SG:23:LYS:HA	59:SG:40:ALA:HB1	2.02	0.41
64:SL:80:MET:HE2	64:SL:122:ILE:HG13	2.02	0.41
74:SV:15:ARG:NH2	74:SV:24:ILE:HG21	2.34	0.41
78:SZ:101:SER:OG	78:SZ:102:LYS:N	2.52	0.41
80:Sb:38:PRO:HD3	80:Sb:76:GLY:O	2.20	0.41
80:Sb:45:THR:HG23	80:Sb:82:LYS:HZ1	1.85	0.41
3:CF:378:LYS:HE3	3:CF:391:PRO:HB3	2.02	0.41
4:L5:231:U:H4'	30:LY:100:HIS:CD2	2.55	0.41
4:L5:426:A:H2'	4:L5:427:A:H8	1.84	0.41
4:L5:481:G:H2'	4:L5:482:G:H8	1.85	0.41
4:L5:699:C:O2'	4:L5:968:C:O2	2.38	0.41
4:L5:959:G:C8	11:LE:123:ARG:HG2	2.56	0.41
4:L5:1197:C:H2'	4:L5:1198:G:C8	2.56	0.41
4:L5:1562:G:H5'	4:L5:1563:A:OP2	2.20	0.41
4:L5:1567:U:H2'	4:L5:1568:C:C6	2.55	0.41
4:L5:1604:G:H2'	4:L5:1605:G:C8	2.55	0.41
4:L5:1631:A:N1	94:L5:5528:HOH:O	2.37	0.41
4:L5:1687:U:H2'	4:L5:1688:G:C8	2.56	0.41
4:L5:1824:G:H2'	4:L5:1825:A:C8	2.55	0.41
4:L5:2696:A:H62	42:Lk:35:LYS:HZ2	1.69	0.41
4:L5:2838:G:H5'	8:LB:247:GLY:HA2	2.02	0.41
4:L5:3651:A:N6	94:L5:5898:HOH:O	2.53	0.41
4:L5:4306:OMU:H1'	4:L5:4306:OMU:HM23	1.81	0.41
4:L5:4521:PSU:H1'	8:LB:253:CYS:SG	2.61	0.41
4:L5:5048:A:OP1	35:Ld:31:LYS:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LC:195:LYS:HB3	9:LC:200:ARG:NE	2.35	0.41
13:LG:257:LYS:O	13:LG:261:LEU:HG	2.19	0.41
17:LL:31:ARG:O	17:LL:35:ARG:HG3	2.20	0.41
20:LO:174:LEU:HD23	20:LO:174:LEU:HA	1.93	0.41
50:Lt:38:SER:N	50:Lt:39:PRO:HD2	2.34	0.41
51:Pt:4:U:H2'	51:Pt:5:C:H6	1.84	0.41
52:S2:29:G:H2'	52:S2:30:C:H6	1.84	0.41
52:S2:60:A:N3	52:S2:316:G:O2'	2.42	0.41
52:S2:456:C:H2'	52:S2:457:C:H6	1.85	0.41
52:S2:1457:U:H2'	52:S2:1458:G:C8	2.54	0.41
53:SA:180:ARG:HD2	53:SA:184:ARG:CZ	2.50	0.41
54:SB:224:GLU:O	54:SB:227:LYS:HG2	2.19	0.41
57:SE:141:THR:HG23	57:SE:143:ASP:N	2.36	0.41
59:SG:31:ARG:HG2	59:SG:101:ILE:HG13	2.03	0.41
59:SG:59:GLN:OE1	59:SG:59:GLN:N	2.53	0.41
70:SR:112:GLY:O	70:SR:113:SER:OG	2.31	0.41
85:Sg:49:GLU:HG2	85:Sg:50:THR:N	2.36	0.41
85:Sg:101:PHE:CD2	85:Sg:136:GLY:HA2	2.54	0.41
87:CA:208:GLN:HA	87:CA:211:LYS:HE3	2.01	0.41
3:CF:357:TYR:CD2	3:CF:372:PHE:HE2	2.38	0.41
4:L5:105:A:O2'	17:LL:35:ARG:NH1	2.51	0.41
4:L5:386:A:O2'	30:LY:87:ARG:NH1	2.53	0.41
4:L5:972:C:C6	11:LE:126:LEU:HD13	2.55	0.41
4:L5:1172:C:O2'	4:L5:1173:G:O5'	2.37	0.41
4:L5:1339:U:OP1	32:La:8:THR:OG1	2.33	0.41
4:L5:1512:G:H2'	4:L5:1513:U:H6	1.86	0.41
4:L5:1701:A:H2'	4:L5:1702:C:H5'	2.02	0.41
4:L5:1921:C:C4	24:LS:161:ARG:HD2	2.55	0.41
4:L5:2573:A:H2'	4:L5:2574:G:O4'	2.19	0.41
4:L5:3793:U:H2'	4:L5:3794:C:C6	2.55	0.41
4:L5:4173:G:H2'	4:L5:4174:U:H6	1.85	0.41
4:L5:4928:C:H2'	4:L5:4929:C:H6	1.85	0.41
5:L7:7:G:OP1	10:LD:33:ARG:HD2	2.20	0.41
16:LJ:164:ARG:HA	16:LJ:164:ARG:HD3	1.94	0.41
18:LM:123:ILE:HD13	20:LO:182:GLU:HG2	2.01	0.41
34:Lc:48:LEU:HD11	34:Lc:60:ILE:HG21	2.02	0.41
40:Li:76:ARG:HA	40:Li:76:ARG:HD3	1.79	0.41
52:S2:218:U:H2'	52:S2:219:U:C6	2.56	0.41
52:S2:697:G:H8	52:S2:733:C:O2	2.02	0.41
52:S2:985:G:H2'	52:S2:1002:U:OP2	2.21	0.41
52:S2:1017:U:H2'	52:S2:1018:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:S2:1098:C:H2'	52:S2:1099:G:C8	2.56	0.41
52:S2:1418:C:H4'	52:S2:1419:C:C5	2.55	0.41
52:S2:1433:C:N4	73:SU:92:HIS:HD2	2.10	0.41
52:S2:1539:U:H2'	52:S2:1540:G:C8	2.56	0.41
65:SM:84:LYS:HE2	65:SM:88:TRP:CE2	2.56	0.41
65:SM:126:GLU:O	65:SM:130:CYS:N	2.47	0.41
69:SQ:98:LYS:HE2	69:SQ:98:LYS:HB2	1.91	0.41
73:SU:66:ARG:HH12	73:SU:75:LYS:CD	2.31	0.41
84:Sf:126:CYS:SG	84:Sf:144:CYS:N	2.89	0.41
86:AT:25:A:H2'	86:AT:26:C:O4'	2.20	0.41
87:CA:158:LYS:HA	87:CA:325:LEU:HD11	2.02	0.41
4:L5:1341:U:H2'	4:L5:1342:A:C8	2.55	0.41
4:L5:1883:G:O6	4:L5:1896:A:H2	2.03	0.41
4:L5:1994:C:H1'	50:Lt:132:ILE:HA	2.02	0.41
4:L5:2658:G:N2	4:L5:2676:A:OP2	2.53	0.41
4:L5:2835:A:N3	8:LB:228:TYR:HD2	2.18	0.41
4:L5:3925:OMU:HM23	4:L5:3925:OMU:H1'	1.86	0.41
4:L5:4080:C:H2'	4:L5:4081:G:C8	2.55	0.41
94:L5:8119:HOH:O	32:La:39:HIS:HA	2.19	0.41
6:L8:130:C:H2'	6:L8:131:G:H8	1.85	0.41
8:LB:37:PRO:HA	8:LB:188:GLY:H	1.85	0.41
12:LF:147:LEU:O	12:LF:151:ASN:ND2	2.44	0.41
28:LW:96:GLN:O	28:LW:101:ARG:N	2.49	0.41
42:Lk:7:GLU:OE1	42:Lk:8:ILE:N	2.53	0.41
45:Ln:11:ARG:HD3	52:S2:1183:A:H5'	2.03	0.41
51:Pt:50:U:H2'	51:Pt:51:C:H6	1.86	0.41
52:S2:835:C:H4'	52:S2:836:G:C8	2.55	0.41
60:SH:76:GLN:HG3	60:SH:94:PHE:CD2	2.53	0.41
69:SQ:13:PHE:HB3	69:SQ:22:VAL:HG22	2.02	0.41
69:SQ:89:SER:HB2	69:SQ:112:LEU:HD13	2.03	0.41
74:SV:51:LYS:HB3	74:SV:51:LYS:HE2	1.68	0.41
3:CF:97:ASP:OD2	86:AT:3:C:OP1	2.38	0.41
3:CF:273:LYS:HG2	3:CF:301:GLU:HG2	2.01	0.41
4:L5:271:C:H2'	4:L5:272:U:C6	2.55	0.41
4:L5:319:A:H1'	4:L5:3726:A:N3	2.35	0.41
4:L5:351:C:H2'	4:L5:352:G:O4'	2.20	0.41
4:L5:1565:A:C5	4:L5:1566:C:H1'	2.55	0.41
4:L5:1727:U:H2'	4:L5:1728:U:C6	2.55	0.41
4:L5:2273:G:H2'	4:L5:2274:C:C6	2.55	0.41
4:L5:3934:G:H2'	4:L5:3935:C:C6	2.55	0.41
4:L5:4152:G:H2'	4:L5:4153:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:4261:C:H2'	4:L5:4262:C:H6	1.85	0.41
4:L5:4615:C:H5''	8:LB:357:ARG:HD3	2.02	0.41
4:L5:4619:U:H2'	4:L5:4620:OMU:C6	2.49	0.41
4:L5:4897:G:N2	4:L5:4924:C:C2	2.88	0.41
4:L5:4968:A:H2'	4:L5:4969:C:H6	1.85	0.41
10:LD:59:ASP:OD1	10:LD:60:ILE:N	2.54	0.41
11:LE:161:ARG:O	11:LE:182:ASN:ND2	2.54	0.41
12:LF:157:ARG:HH21	12:LF:248:ASN:HA	1.85	0.41
14:LH:27:VAL:HG12	14:LH:84:VAL:HG21	2.02	0.41
15:LI:193:ASP:O	15:LI:193:ASP:OD1	2.39	0.41
30:LY:67:ILE:HD12	30:LY:107:THR:HG21	2.03	0.41
33:Lb:54:LEU:O	33:Lb:58:GLN:HG3	2.21	0.41
39:Lh:3:LYS:HB3	39:Lh:3:LYS:HE2	1.88	0.41
46:Lo:6:LYS:HG3	46:Lo:94:GLY:HA3	2.03	0.41
49:Ls:102:LEU:HD23	49:Ls:189:ILE:HD11	2.03	0.41
52:S2:525:A:H2'	52:S2:526:A:C8	2.56	0.41
52:S2:1531:A:H2'	52:S2:1532:C:C6	2.56	0.41
52:S2:1720:U:H5''	52:S2:1721:U:H5''	2.02	0.41
53:SA:85:ARG:HB2	70:SR:81:ARG:NH1	2.35	0.41
53:SA:180:ARG:HH11	53:SA:184:ARG:NH1	2.17	0.41
58:SF:17:ILE:HG21	58:SF:46:ALA:HB1	2.02	0.41
58:SF:187:SER:HB3	58:SF:190:ILE:HG12	2.03	0.41
59:SG:154:ARG:O	59:SG:157:VAL:HG22	2.20	0.41
61:SI:130:THR:N	61:SI:131:PRO:HD2	2.36	0.41
70:SR:5:ARG:HB3	70:SR:9:VAL:CG1	2.51	0.41
72:ST:99:VAL:O	72:ST:103:VAL:HG23	2.20	0.41
77:SY:5:VAL:HG23	77:SY:32:LYS:NZ	2.36	0.41
85:Sg:244:ASN:OD1	85:Sg:244:ASN:N	2.53	0.41
1:CD:27:PRO:O	1:CD:30:VAL:HG22	2.20	0.41
4:L5:1251:C:H2'	4:L5:1252:C:C6	2.55	0.41
4:L5:1942:A:N3	4:L5:4432:C:O2'	2.47	0.41
4:L5:2267:U:OP1	48:Lr:37:SER:HB2	2.20	0.41
4:L5:2297:G:H4'	9:LC:242:PRO:HB2	2.02	0.41
4:L5:2375:A:H2'	4:L5:2376:A:H8	1.86	0.41
4:L5:2521:G:H2'	4:L5:2522:G:H8	1.85	0.41
4:L5:2693:G:OP2	42:Lk:33:LYS:NZ	2.49	0.41
4:L5:2849:A:O2'	4:L5:2855:G:N7	2.54	0.41
4:L5:3723:A:H2'	4:L5:3724:A:C8	2.56	0.41
4:L5:4152:G:H2'	4:L5:4153:C:H6	1.86	0.41
4:L5:4192:A:H2'	4:L5:4193:C:H6	1.84	0.41
4:L5:4219:A:H2'	4:L5:4220:6MZ:C8	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L8:18:U:H2'	6:L8:19:C:C6	2.56	0.41
6:L8:67:U:P	41:Lj:87:LYS:HE3	2.60	0.41
8:LB:216:MET:HG3	8:LB:354:GLN:HE21	1.85	0.41
9:LC:325:MET:HE2	9:LC:329:ASN:HB3	2.02	0.41
14:LH:61:TRP:CZ3	18:LM:33:GLN:HG3	2.56	0.41
16:LJ:48:PRO:HB2	16:LJ:70:VAL:CG2	2.49	0.41
17:LL:47:ALA:HB3	17:LL:48:PRO:HD3	2.03	0.41
27:LV:70:PRO:HA	27:LV:73:ARG:HG3	2.01	0.41
27:LV:90:ARG:C	27:LV:92:ASP:H	2.29	0.41
30:LY:37:GLU:H	30:LY:37:GLU:CD	2.28	0.41
34:Lc:48:LEU:HD13	34:Lc:71:VAL:HG13	2.03	0.41
34:Lc:52:CYS:HB3	34:Lc:57:LYS:HE2	2.01	0.41
36:Le:97:ALA:O	36:Le:122:VAL:HA	2.21	0.41
43:Ll:28:ARG:HA	43:Ll:33:ASN:ND2	2.35	0.41
49:Ls:58:ASN:HA	49:Ls:61:MET:HE2	2.02	0.41
50:Lt:119:ARG:HG3	50:Lt:129:ILE:HG12	2.02	0.41
51:Pt:3:C:H42	51:Pt:70:A:H61	1.69	0.41
52:S2:326:C:C3'	52:S2:327:G:H5'	2.50	0.41
52:S2:1047:C:H2'	52:S2:1048:G:O4'	2.21	0.41
52:S2:1373:C:P	70:SR:7:LYS:HG3	2.60	0.41
52:S2:1621:U:O2'	52:S2:1622:U:H2'	2.21	0.41
52:S2:1712:A:H2'	52:S2:1713:C:C6	2.55	0.41
52:S2:1731:A:H2'	52:S2:1732:G:H8	1.85	0.41
53:SA:158:ASP:HB2	53:SA:159:ILE:HD12	2.02	0.41
58:SF:42:LYS:HD3	58:SF:42:LYS:HA	1.84	0.41
58:SF:82:ASN:ND2	94:SF:303:HOH:O	2.53	0.41
59:SG:144:LEU:HG	59:SG:145:PHE:CD1	2.56	0.41
61:SI:11:ARG:O	64:SL:136:LYS:NZ	2.29	0.41
63:SK:73:ASN:HA	63:SK:76:ILE:HG12	2.03	0.41
63:SK:96:ARG:C	63:SK:96:ARG:HD2	2.45	0.41
69:SQ:93:VAL:HG12	69:SQ:108:ILE:HG12	2.01	0.41
75:SW:28:ARG:HB3	75:SW:29:PRO:HD3	2.03	0.41
87:CA:27:ILE:HA	87:CA:30:ARG:HG2	2.03	0.41
87:CA:202:ILE:HG12	87:CA:205:PRO:HG3	2.01	0.41
4:L5:1351:G:H2'	4:L5:1352:C:C6	2.55	0.41
4:L5:1352:C:H2'	4:L5:1353:G:O4'	2.21	0.41
4:L5:2439:G:H5'	4:L5:2778:G:OP2	2.21	0.41
4:L5:2480:G:H2'	4:L5:2481:G:H8	1.86	0.41
4:L5:3637:PSU:O2	4:L5:3651:A:H2	2.03	0.41
4:L5:4688:C:O2'	14:LH:155:SER:OG	2.38	0.41
4:L5:4776:G:N2	4:L5:4859:C:O2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:LB:122:TRP:CZ2	8:LB:127:LYS:HE3	2.56	0.41
10:LD:204:VAL:O	10:LD:208:MET:HG3	2.20	0.41
11:LE:95:PRO:HA	11:LE:104:THR:HG22	2.02	0.41
17:LL:154:VAL:HG12	17:LL:155:MET:HG3	2.02	0.41
21:LP:107:LEU:HB2	21:LP:152:GLU:OE2	2.20	0.41
21:LP:131:ARG:HG3	21:LP:137:ASN:OD1	2.21	0.41
23:LR:80:LYS:HA	23:LR:80:LYS:HD2	1.83	0.41
42:Lk:66:VAL:O	42:Lk:66:VAL:HG12	2.21	0.41
50:Lt:10:ILE:HD12	50:Lt:10:ILE:HA	1.95	0.41
50:Lt:105:THR:C	50:Lt:106:PHE:CD1	2.99	0.41
52:S2:106:C:H2'	52:S2:107:A:C8	2.52	0.41
52:S2:121:OMU:HM23	52:S2:121:OMU:H1'	1.91	0.41
52:S2:507:G:OP2	77:SY:104:ARG:NH1	2.47	0.41
52:S2:549:C:H2'	52:S2:550:C:C6	2.56	0.41
52:S2:921:G:C2	80:Sb:22:LYS:HG2	2.55	0.41
52:S2:1018:U:H2'	52:S2:1019:C:H6	1.85	0.41
52:S2:1367:PSU:N1	94:S2:2031:HOH:O	2.36	0.41
52:S2:1750:C:H2'	52:S2:1751:C:C6	2.56	0.41
52:S2:1840:U:H2'	52:S2:1841:C:C6	2.56	0.41
52:S2:1840:U:H2'	52:S2:1841:C:H6	1.85	0.41
52:S2:1867:U:O2'	79:Sa:38:LYS:HD2	2.21	0.41
53:SA:77:ILE:HD12	53:SA:133:PRO:HG3	2.03	0.41
53:SA:84:GLN:O	53:SA:88:LEU:HD23	2.21	0.41
57:SE:137:PRO:HG2	57:SE:150:PRO:HD2	2.02	0.41
60:SH:131:GLU:HG2	60:SH:139:ILE:HD13	2.01	0.41
63:SK:42:ASN:O	63:SK:46:MET:HG3	2.21	0.41
65:SM:53:ALA:HA	65:SM:79:VAL:HG12	2.01	0.41
76:SX:95:GLU:HG2	76:SX:98:ASP:OD2	2.21	0.41
82:Sd:38:MET:HG2	82:Sd:39:CYS:H	1.85	0.41
84:Sf:108:VAL:HB	84:Sf:112:GLY:HA2	2.02	0.41
85:Sg:74:ASP:OD1	85:Sg:75:GLY:N	2.54	0.41
85:Sg:164:ILE:HD12	85:Sg:177:TRP:O	2.21	0.41
86:AT:43:A:H2'	86:AT:44:A:O4'	2.20	0.41
2:CI:62:VAL:HG22	2:CI:71:ARG:HB3	2.03	0.41
3:CF:76:SER:HB2	3:CF:91:ASP:HB3	2.03	0.41
3:CF:250:LEU:CD1	3:CF:263:PRO:HB3	2.51	0.41
4:L5:223:G:H4'	4:L5:225:G:N7	2.36	0.41
4:L5:270:U:H2'	4:L5:271:C:H6	1.86	0.41
4:L5:429:A:H2'	4:L5:430:G:C8	2.56	0.41
4:L5:444:G:H2'	4:L5:445:U:H6	1.84	0.41
4:L5:679:C:H2'	4:L5:680:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:690:C:H2'	4:L5:691:C:C6	2.56	0.41
4:L5:730:G:C6	12:LF:73:ARG:HD3	2.56	0.41
4:L5:754:U:H2'	4:L5:755:C:H6	1.85	0.41
4:L5:1071:C:C5	11:LE:67:ALA:HB2	2.56	0.41
4:L5:1076:C:H2'	4:L5:1077:C:H6	1.85	0.41
4:L5:1400:G:H2'	4:L5:1401:C:C6	2.56	0.41
4:L5:1544:G:H5''	38:Lg:14:ASN:O	2.21	0.41
4:L5:1578:U:H2'	4:L5:1579:C:C6	2.55	0.41
4:L5:1590:C:H5''	4:L5:1591:U:O5'	2.20	0.41
4:L5:1858:A:H2'	4:L5:1859:C:H6	1.86	0.41
4:L5:1940:G:N2	94:L5:5931:HOH:O	2.54	0.41
4:L5:1961:G:C8	49:Ls:59:THR:HG21	2.56	0.41
4:L5:2046:G:O2'	4:L5:2047:A:N7	2.52	0.41
4:L5:2374:A:H5'	35:Ld:64:ILE:O	2.20	0.41
4:L5:2385:U:H2'	4:L5:2386:U:C6	2.55	0.41
4:L5:2621:A:H2'	4:L5:2622:G:C8	2.56	0.41
4:L5:3614:G:N7	94:L5:5535:HOH:O	2.37	0.41
4:L5:3619:G:H4'	23:LR:79:GLY:O	2.20	0.41
4:L5:3753:G:OP1	94:L5:5405:HOH:O	2.22	0.41
4:L5:4253:A:H5'	4:L5:4254:G:C8	2.55	0.41
4:L5:4287:G:H2'	4:L5:4288:C:C6	2.56	0.41
4:L5:4739:C:H2'	4:L5:4740:G:H5'	2.03	0.41
4:L5:5001:PSU:H2'	4:L5:5002:U:O4'	2.20	0.41
89:L5:5288:SPM:HN5	89:L5:5288:SPM:H22	1.78	0.41
94:L5:5700:HOH:O	9:LC:80:ARG:NH1	2.53	0.41
5:L7:3:C:H2'	5:L7:4:U:H6	1.86	0.41
8:LB:14:LEU:HA	8:LB:17:LEU:HG	2.01	0.41
8:LB:33:PRO:HG2	8:LB:349:LYS:HB2	2.03	0.41
8:LB:299:ILE:HG22	8:LB:313:SER:HB3	2.02	0.41
10:LD:53:VAL:HG11	10:LD:159:VAL:HA	2.03	0.41
11:LE:202:ASP:OD1	11:LE:204:SER:OG	2.31	0.41
13:LG:93:THR:O	13:LG:97:LYS:HB2	2.20	0.41
16:LJ:42:GLN:CD	16:LJ:117:ILE:HG12	2.46	0.41
17:LL:63:THR:HG21	32:La:66:ASN:HB3	2.02	0.41
18:LM:96:GLU:OE2	18:LM:100:ARG:NH2	2.50	0.41
20:LO:81:TRP:HB2	20:LO:104:VAL:HG21	2.03	0.41
23:LR:169:ALA:O	23:LR:173:ARG:HB2	2.21	0.41
25:LT:85:LEU:CD1	25:LT:87:LYS:HD3	2.51	0.41
28:LW:102:LYS:HD2	28:LW:102:LYS:C	2.46	0.41
39:Lh:52:LYS:HA	39:Lh:52:LYS:HD3	1.88	0.41
47:Lp:64:VAL:HG11	47:Lp:71:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Pt:37:A:N1	94:Pt:101:HOH:O	2.37	0.41
52:S2:52:G:H2'	52:S2:53:C:C6	2.56	0.41
52:S2:77:A:C8	59:SG:154:ARG:HG2	2.55	0.41
52:S2:85:A:H2'	52:S2:86:C:C6	2.56	0.41
52:S2:96:C:O2	52:S2:473:A:O2'	2.36	0.41
52:S2:161:U:O3'	59:SG:87:ARG:NH2	2.54	0.41
52:S2:301:A:H2'	52:S2:302:A:O4'	2.20	0.41
52:S2:399:C:H5	52:S2:680:G:H5''	1.85	0.41
52:S2:483:C:H4'	76:SX:101:LEU:HD11	2.02	0.41
52:S2:536:A:H3'	52:S2:537:C:H5''	2.03	0.41
52:S2:737:G:H8	52:S2:738:C:H4'	1.86	0.41
52:S2:816:A:H2'	52:S2:817:G:O4'	2.21	0.41
52:S2:962:A:N1	52:S2:1055:A:O2'	2.53	0.41
52:S2:1025:U:OP1	52:S2:1090:C:O2'	2.38	0.41
52:S2:1231:C:OP1	71:SS:134:GLN:HB2	2.21	0.41
52:S2:1383:A2M:HM'3	52:S2:1383:A2M:H1'	1.53	0.41
52:S2:1513:C:OP1	82:Sd:10:HIS:HB3	2.21	0.41
52:S2:1528:G:H2'	52:S2:1529:C:C6	2.56	0.41
52:S2:1676:U:H2'	52:S2:1677:U:O4'	2.21	0.41
52:S2:1863:A:H1'	79:Sa:79:ILE:HD13	2.03	0.41
53:SA:118:GLU:HG2	53:SA:118:GLU:O	2.21	0.41
53:SA:149:ASN:HB2	53:SA:165:ASN:OD1	2.21	0.41
53:SA:213:GLU:HB3	70:SR:84:TYR:CZ	2.56	0.41
55:SC:275:LYS:HB2	55:SC:275:LYS:HE2	1.93	0.41
56:SD:143:ARG:HD2	56:SD:148:LYS:HE3	2.03	0.41
57:SE:71:LYS:HE2	57:SE:74:GLY:O	2.21	0.41
57:SE:153:LEU:HD23	57:SE:153:LEU:HA	1.89	0.41
57:SE:250:GLU:HA	57:SE:253:ASP:OD2	2.21	0.41
59:SG:59:GLN:NE2	59:SG:72:ARG:HH22	2.18	0.41
62:SJ:17:ARG:NH1	62:SJ:18:ARG:NH1	2.69	0.41
65:SM:33:ARG:H	65:SM:33:ARG:HG2	1.70	0.41
67:SO:47:LEU:HD23	67:SO:47:LEU:HA	1.88	0.41
68:SP:28:MET:HE1	68:SP:36:LEU:HD22	2.03	0.41
69:SQ:44:PRO:HG2	69:SQ:81:ILE:CD1	2.51	0.41
69:SQ:63:PHE:CE2	69:SQ:92:LEU:HD22	2.56	0.41
72:ST:26:GLY:C	72:ST:27:LYS:HD3	2.45	0.41
72:ST:31:PRO:HG2	72:ST:34:VAL:HG13	2.02	0.41
74:SV:35:ASN:ND2	74:SV:50:PHE:HE2	2.19	0.41
76:SX:85:VAL:HA	76:SX:122:VAL:HG12	2.03	0.41
77:SY:20:ARG:NH1	77:SY:74:MET:SD	2.94	0.41
78:SZ:86:ALA:O	78:SZ:90:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:Sg:21:ILE:N	85:Sg:288:SER:OG	2.54	0.41
85:Sg:195:LEU:HD23	85:Sg:195:LEU:HA	1.81	0.41
85:Sg:300:ALA:C	85:Sg:307:VAL:HG23	2.46	0.41
4:L5:313:U:H5''	19:LN:179:LYS:HE3	2.03	0.41
4:L5:385:A:N3	4:L5:387:G:H5''	2.36	0.41
4:L5:917:A:H2'	4:L5:918:G:O4'	2.21	0.41
4:L5:1097:C:H2'	4:L5:1098:G:H8	1.85	0.41
4:L5:1273:G:O2'	4:L5:1274:A:H5'	2.21	0.41
4:L5:1915:C:OP2	20:LO:94:ARG:NH2	2.53	0.41
4:L5:3923:A:H2'	4:L5:3924:C:H6	1.82	0.41
4:L5:4691:A:OP1	14:LH:75:SER:OG	2.31	0.41
4:L5:4862:G:H2'	4:L5:4863:G:C8	2.56	0.41
5:L7:7:G:OP1	10:LD:33:ARG:NH1	2.52	0.41
5:L7:37:G:H2'	5:L7:38:U:O4'	2.21	0.41
5:L7:58:A:H2'	5:L7:59:G:H8	1.86	0.41
6:L8:154:G:H2'	6:L8:155:C:C6	2.55	0.41
8:LB:28:LYS:HE2	8:LB:28:LYS:HB2	1.84	0.41
9:LC:116:ASN:O	9:LC:119:GLN:HB2	2.20	0.41
9:LC:230:LEU:HD21	9:LC:236:ASN:H	1.86	0.41
23:LR:3:MET:CE	23:LR:5:ARG:HH21	2.34	0.41
23:LR:155:LEU:HD23	23:LR:158:GLN:HE21	1.85	0.41
37:Lf:48:ALA:HB2	37:Lf:71:TRP:CZ3	2.55	0.41
42:Lk:30:ASP:OD1	42:Lk:30:ASP:N	2.54	0.41
52:S2:644:OMG:HM23	52:S2:644:OMG:H1'	1.78	0.41
52:S2:793:G:H2'	52:S2:794:A:H8	1.86	0.41
52:S2:1031:A2M:HM'3	52:S2:1031:A2M:H1'	1.94	0.41
52:S2:1177:PSU:H2'	52:S2:1178:U:C6	2.56	0.41
52:S2:1376:A:H8	52:S2:1376:A:OP2	2.04	0.41
52:S2:1627:C:H5''	72:ST:41:LYS:HD2	2.02	0.41
52:S2:1802:C:H2'	52:S2:1803:U:C6	2.56	0.41
54:SB:97:LEU:HD23	54:SB:232:HIS:CG	2.56	0.41
57:SE:141:THR:HG22	57:SE:145:ARG:O	2.21	0.41
61:SI:37:LYS:NZ	61:SI:93:THR:HB	2.35	0.41
64:SL:48:LYS:O	64:SL:52:GLU:HG3	2.21	0.41
77:SY:77:ASP:N	77:SY:77:ASP:OD1	2.53	0.41
85:Sg:176:VAL:O	85:Sg:184:LEU:HD12	2.21	0.41
87:CA:291:MET:O	87:CA:294:VAL:HG22	2.20	0.41
1:CD:5:LEU:O	1:CD:9:PHE:HD1	2.04	0.40
3:CF:410:MET:HE2	3:CF:410:MET:HB2	1.91	0.40
4:L5:1199:G:H2'	4:L5:1200:G:H8	1.87	0.40
4:L5:1280:C:O2'	9:LC:321:ASN:OD1	2.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:1309:C:H2'	4:L5:1310:C:C6	2.56	0.40
4:L5:1577:G:H5'	4:L5:1578:U:H5''	2.02	0.40
4:L5:1717:C:H2'	4:L5:1718:C:C4	2.56	0.40
4:L5:1743:A:O4'	10:LD:15:ARG:HD2	2.20	0.40
4:L5:1834:U:C2	25:LT:128:LEU:HD23	2.56	0.40
4:L5:1999:A:H8	4:L5:1999:A:OP2	2.04	0.40
4:L5:2656:U:H5''	31:LZ:38:TYR:HB3	2.02	0.40
4:L5:3762:U:C2	4:L5:3763:A:C8	3.09	0.40
4:L5:3870:C:H2'	4:L5:3871:A:C8	2.55	0.40
4:L5:3951:G:N2	4:L5:4062:A:N6	2.69	0.40
4:L5:4227:OMU:H1'	4:L5:4227:OMU:HM23	1.89	0.40
4:L5:4680:G:H2'	4:L5:4681:A:C8	2.55	0.40
5:L7:35:U:O2	5:L7:45:U:O2'	2.37	0.40
8:LB:279:GLU:HB3	8:LB:282:LYS:HZ3	1.84	0.40
8:LB:302:ASN:HB2	8:LB:313:SER:HA	2.02	0.40
11:LE:183:ARG:HA	11:LE:183:ARG:HD2	1.89	0.40
13:LG:50:ASP:HB2	29:LX:40:ILE:HD11	2.03	0.40
17:LL:194:ILE:HD12	17:LL:194:ILE:HA	1.93	0.40
20:LO:74:ARG:HG2	20:LO:146:GLY:HA3	2.03	0.40
24:LS:16:CYS:SG	24:LS:54:MET:HG2	2.62	0.40
25:LT:85:LEU:HD11	25:LT:87:LYS:HD3	2.03	0.40
25:LT:107:LYS:HD2	25:LT:107:LYS:C	2.46	0.40
28:LW:2:LYS:HZ3	28:LW:2:LYS:HG3	1.75	0.40
30:LY:32:SER:OG	30:LY:101:PRO:O	2.30	0.40
49:Ls:13:TYR:O	49:Ls:17:ILE:HG22	2.21	0.40
52:S2:446:G:OP1	94:S2:2001:HOH:O	2.21	0.40
52:S2:888:U:O2'	52:S2:898:U:N3	2.41	0.40
52:S2:1375:G:H5''	70:SR:67:ARG:HH12	1.85	0.40
52:S2:1417:C:H42	52:S2:1422:G:N2	2.19	0.40
52:S2:1695:A:N1	52:S2:1832:6MZ:O2'	2.52	0.40
52:S2:1737:G:H2'	52:S2:1738:C:H6	1.86	0.40
55:SC:205:VAL:O	55:SC:205:VAL:HG13	2.21	0.40
56:SD:31:GLU:O	56:SD:54:ARG:NH2	2.51	0.40
64:SL:57:ASP:HB3	64:SL:60:CYS:HB2	2.03	0.40
68:SP:33:LEU:HD21	68:SP:87:PRO:HG3	2.03	0.40
73:SU:46:LYS:HB2	73:SU:46:LYS:HE3	1.77	0.40
73:SU:46:LYS:NZ	73:SU:101:ILE:HG12	2.37	0.40
73:SU:107:GLU:O	73:SU:110:VAL:HG12	2.21	0.40
74:SV:50:PHE:N	74:SV:50:PHE:CD1	2.89	0.40
85:Sg:101:PHE:CE2	85:Sg:136:GLY:HA2	2.56	0.40
3:CF:28:ILE:HG23	3:CF:33:GLY:HA3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:422:C:H2'	4:L5:423:G:H8	1.87	0.40
4:L5:424:U:H2'	4:L5:425:U:H6	1.86	0.40
4:L5:688:U:OP1	11:LE:94:LYS:NZ	2.39	0.40
4:L5:1613:A:H5''	7:LA:183:GLY:HA2	2.03	0.40
4:L5:1700:G:H2'	4:L5:1703:C:N4	2.36	0.40
4:L5:1726:U:H5'	12:LF:135:ILE:HD11	2.02	0.40
4:L5:1727:U:OP1	12:LF:131:ASN:ND2	2.51	0.40
4:L5:1989:G:H2'	4:L5:1990:A:C8	2.56	0.40
4:L5:2078:C:H2'	4:L5:2079:G:C8	2.56	0.40
4:L5:2095:A:H1'	4:L5:2096:G:N2	2.36	0.40
4:L5:3723:A:H2'	4:L5:3724:A:H8	1.86	0.40
4:L5:3866:C:H2'	4:L5:3867:A2M:O4'	2.22	0.40
4:L5:4940:C:O2'	11:LE:246:ARG:NH2	2.53	0.40
10:LD:179:ARG:HD3	10:LD:179:ARG:HA	1.78	0.40
16:LJ:78:LYS:O	16:LJ:81:GLU:HG2	2.21	0.40
16:LJ:85:LYS:O	16:LJ:89:VAL:HG23	2.21	0.40
21:LP:47:TYR:OH	21:LP:58:VAL:HG12	2.20	0.40
31:LZ:7:PRO:HA	31:LZ:25:ILE:HG22	2.04	0.40
31:LZ:35:ASP:OD1	31:LZ:35:ASP:N	2.55	0.40
35:Ld:114:PHE:HA	35:Ld:117:LEU:HD12	2.02	0.40
51:Pt:51:C:H2'	51:Pt:52:G:C8	2.56	0.40
52:S2:919:A:OP2	52:S2:919:A:H8	2.04	0.40
52:S2:1288:OMU:OP2	84:Sf:99:LYS:HE3	2.21	0.40
52:S2:1608:U:H4'	71:SS:130:ARG:NH1	2.36	0.40
52:S2:1859:A:P	79:Sa:10:ARG:HH12	2.45	0.40
54:SB:82:ARG:NH1	54:SB:189:ILE:O	2.54	0.40
55:SC:272:HIS:HA	55:SC:275:LYS:NZ	2.37	0.40
58:SF:193:LYS:O	58:SF:197:GLU:HG2	2.21	0.40
59:SG:98:ARG:NH2	59:SG:101:ILE:O	2.38	0.40
67:SO:58:GLY:O	67:SO:62:VAL:HG12	2.21	0.40
69:SQ:57:LEU:HD11	69:SQ:115:TYR:CD2	2.56	0.40
71:SS:46:ARG:HG2	72:ST:35:ASP:HB2	2.03	0.40
74:SV:42:VAL:HG23	74:SV:43:THR:N	2.36	0.40
77:SY:18:LEU:HD12	77:SY:20:ARG:CZ	2.51	0.40
3:CF:73:ILE:HG21	86:AT:2:U:H4'	2.01	0.40
4:L5:429:A:N7	94:L5:5542:HOH:O	2.37	0.40
4:L5:660:A:H2'	4:L5:661:C:C6	2.56	0.40
4:L5:1180:C:H5''	4:L5:1180:C:H6	1.87	0.40
4:L5:1494:U:H2'	4:L5:1495:G:H8	1.86	0.40
4:L5:1510:G:H2'	4:L5:1511:U:C6	2.56	0.40
4:L5:1930:U:OP2	20:LO:49:ARG:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:3823:G:H2'	4:L5:3824:A:H8	1.85	0.40
4:L5:3842:C:H3'	4:L5:3843:C:H2'	2.02	0.40
4:L5:3933:G:H2'	4:L5:3934:G:H8	1.86	0.40
4:L5:4140:C:N3	4:L5:4145:C:O2'	2.48	0.40
4:L5:4585:U:H2'	4:L5:4586:G:C8	2.57	0.40
4:L5:4762:A:H2'	4:L5:4763:U:O4'	2.22	0.40
8:LB:165:HIS:HA	8:LB:179:HIS:O	2.21	0.40
13:LG:121:LYS:HE3	13:LG:121:LYS:HB3	1.82	0.40
14:LH:105:ILE:CG2	14:LH:109:GLY:HA2	2.52	0.40
29:LX:80:PRO:CG	29:LX:155:ILE:HG21	2.45	0.40
30:LY:111:LEU:HD23	30:LY:111:LEU:HA	1.91	0.40
49:Ls:33:ASP:O	49:Ls:35:VAL:HG22	2.22	0.40
52:S2:27:A2M:H1'	52:S2:27:A2M:HM'3	1.56	0.40
52:S2:107:A:H2'	52:S2:108:G:H8	1.83	0.40
52:S2:353:C:H2'	52:S2:354:OMU:H6	2.04	0.40
52:S2:454:U:H2'	52:S2:455:A:C8	2.56	0.40
52:S2:689:U:H3'	52:S2:690:G:H21	1.86	0.40
52:S2:1378:A:H4'	52:S2:1379:A:O5'	2.20	0.40
52:S2:1525:C:H2'	52:S2:1526:G:H8	1.86	0.40
52:S2:1614:A:P	68:SP:42:ARG:HH22	2.41	0.40
52:S2:1693:G:O2'	52:S2:1694:U:H5'	2.21	0.40
55:SC:186:GLY:HA3	55:SC:239:ALA:O	2.22	0.40
55:SC:213:LEU:HD12	55:SC:213:LEU:HA	1.91	0.40
65:SM:17:ALA:O	65:SM:20:GLU:HG3	2.20	0.40
70:SR:17:ILE:HD11	70:SR:54:VAL:HA	2.03	0.40
71:SS:15:VAL:HB	71:SS:68:ILE:HD11	2.04	0.40
76:SX:70:VAL:HG11	76:SX:94:ILE:HG21	2.03	0.40
77:SY:7:ILE:CD1	77:SY:27:VAL:HG12	2.50	0.40
87:CA:273:PHE:CG	87:CA:278:PHE:HB3	2.56	0.40
2:CI:54:LYS:HA	2:CI:57:LYS:HG2	2.02	0.40
3:CF:357:TYR:OH	3:CF:359:PRO:HB3	2.21	0.40
3:CF:362:ASP:HA	3:CF:366:ALA:O	2.22	0.40
4:L5:97:G:OP1	17:LL:16:LYS:NZ	2.37	0.40
4:L5:374:G:OP2	41:Lj:56:ARG:NH1	2.36	0.40
4:L5:493:G:O2'	4:L5:494:U:OP1	2.37	0.40
4:L5:1405:C:N4	4:L5:1408:G:N3	2.46	0.40
4:L5:2372:U:O2'	35:Ld:46:LEU:HD13	2.21	0.40
4:L5:2639:U:O2'	4:L5:2694:G:O6	2.40	0.40
4:L5:2848:G:O2'	4:L5:3838:U:O4	2.31	0.40
4:L5:2871:A:H2'	4:L5:2872:C:O4'	2.22	0.40
4:L5:3599:A:H2'	4:L5:3600:G:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L5:3661:G:H4'	4:L5:3662:A:H5'	2.02	0.40
4:L5:4926:C:H3'	4:L5:4927:G:N3	2.36	0.40
4:L5:5002:U:H2'	4:L5:5003:U:H6	1.87	0.40
8:LB:19:ARG:HD2	94:LB:521:HOH:O	2.21	0.40
23:LR:172:ARG:NH1	52:S2:909:G:OP1	2.46	0.40
27:LV:107:ASN:OD1	27:LV:111:GLU:N	2.49	0.40
31:LZ:5:MET:O	31:LZ:28:ASN:ND2	2.54	0.40
41:Lj:20:ARG:HD2	41:Lj:39:TYR:CZ	2.55	0.40
43:Ll:36:ARG:HH11	43:Ll:36:ARG:HG3	1.87	0.40
52:S2:28:U:H2'	52:S2:29:G:C8	2.55	0.40
52:S2:617:G:H4'	76:SX:88:ASP:HA	2.03	0.40
52:S2:634:A:H2'	52:S2:635:G:C8	2.56	0.40
52:S2:837:A:N6	77:SY:9:THR:H	2.19	0.40
52:S2:941:C:H5''	54:SB:136:ARG:HH11	1.86	0.40
52:S2:1513:C:OP1	82:Sd:12:ARG:NH2	2.44	0.40
53:SA:141:ASN:ND2	74:SV:29:HIS:O	2.55	0.40
56:SD:12:VAL:HG21	82:Sd:34:TYR:HB3	2.04	0.40
58:SF:190:ILE:HG13	58:SF:191:LYS:N	2.36	0.40
59:SG:218:LYS:HA	59:SG:218:LYS:HD2	1.87	0.40
63:SK:9:ILE:HG13	63:SK:10:ALA:N	2.36	0.40
64:SL:13:GLN:OE1	64:SL:36:TYR:HB3	2.21	0.40
72:ST:103:VAL:O	72:ST:107:LEU:HD13	2.21	0.40
73:SU:66:ARG:NH1	73:SU:75:LYS:HA	2.37	0.40
76:SX:119:ARG:HG3	76:SX:120:PHE:CE2	2.56	0.40
85:Sg:54:ILE:HG13	85:Sg:55:PRO:HD2	2.03	0.40
85:Sg:242:SER:HA	85:Sg:291:TRP:CD1	2.56	0.40
87:CA:101:LYS:HE2	87:CA:101:LYS:HB2	1.97	0.40
3:CF:291:SER:H	3:CF:311:ASN:HB3	1.86	0.40
3:CF:377:GLU:HB3	3:CF:401:ILE:HG22	2.03	0.40
4:L5:19:G:P	39:Lh:93:ARG:HE	2.44	0.40
4:L5:21:G:H5''	41:Lj:43:ARG:HG2	2.04	0.40
4:L5:24:G:N7	41:Lj:46:LYS:NZ	2.70	0.40
4:L5:300:A:H2'	4:L5:301:G:C8	2.51	0.40
4:L5:375:G:OP2	41:Lj:52:LYS:NZ	2.39	0.40
4:L5:1735:U:OP2	89:L5:5259:SPM:N10	2.55	0.40
4:L5:2550:G:O2'	4:L5:2587:A:N1	2.52	0.40
4:L5:3606:U:H2'	4:L5:3607:U:C6	2.57	0.40
4:L5:4350:C:C2	4:L5:4351:U:C5	3.09	0.40
4:L5:4412:C:C2	4:L5:4413:C:C5	3.09	0.40
4:L5:4572:U:H2'	4:L5:4573:G:C8	2.57	0.40
5:L7:117:G:OP1	10:LD:253:TYR:OH	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LC:4:ALA:O	9:LC:29:LYS:NZ	2.54	0.40
23:LR:77:GLY:O	23:LR:81:ARG:NE	2.55	0.40
24:LS:69:GLU:HG3	24:LS:71:SER:H	1.87	0.40
51:Pt:29:C:H2'	51:Pt:30:G:H8	1.87	0.40
51:Pt:50:U:H2'	51:Pt:51:C:C6	2.56	0.40
52:S2:509:OMG:H2'	52:S2:510:G:H8	1.86	0.40
52:S2:1114:U:O2'	52:S2:1115:U:H2'	2.22	0.40
52:S2:1340:U:OP2	52:S2:1341:C:O2'	2.29	0.40
52:S2:1395:C:H1'	52:S2:1474:A:C5	2.56	0.40
52:S2:1567:G:H2'	52:S2:1568:C:C6	2.57	0.40
52:S2:1672:U:O3'	69:SQ:76:GLY:HA3	2.21	0.40
52:S2:1716:C:H2'	52:S2:1717:C:H6	1.86	0.40
53:SA:81:ASN:OD1	53:SA:81:ASN:N	2.54	0.40
56:SD:55:THR:HA	56:SD:58:VAL:HG22	2.04	0.40
58:SF:33:ILE:HA	58:SF:36:GLN:HG3	2.03	0.40
58:SF:144:LEU:HD23	81:Sc:49:PRO:HB2	2.04	0.40
60:SH:86:LYS:C	60:SH:87:PHE:CD1	2.99	0.40
63:SK:22:VAL:HG22	63:SK:68:TYR:HD1	1.86	0.40
67:SO:31:CYS:HA	67:SO:44:VAL:HA	2.03	0.40
70:SR:34:VAL:O	70:SR:38:ILE:HG12	2.22	0.40
72:ST:39:LEU:HB3	72:ST:56:ARG:HH12	1.86	0.40
73:SU:49:LYS:CE	73:SU:92:HIS:HB2	2.48	0.40
74:SV:69:ILE:HD13	74:SV:69:ILE:HA	1.98	0.40
84:Sf:124:ASP:OD1	84:Sf:124:ASP:N	2.54	0.40
85:Sg:234:ASP:OD1	85:Sg:234:ASP:N	2.55	0.40
85:Sg:272:GLN:OE1	85:Sg:284:PRO:HB2	2.21	0.40
86:AT:21:U:OP1	86:AT:49:C:N4	2.55	0.40
86:AT:62:C:H2'	86:AT:63:C:C6	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CD	34/36 (94%)	34 (100%)	0	0	100	100
2	CI	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
3	CF	438/441 (99%)	410 (94%)	28 (6%)	0	100	100
7	LA	246/248 (99%)	223 (91%)	23 (9%)	0	100	100
8	LB	400/402 (100%)	383 (96%)	17 (4%)	0	100	100
9	LC	366/368 (100%)	347 (95%)	19 (5%)	0	100	100
10	LD	291/293 (99%)	279 (96%)	12 (4%)	0	100	100
11	LE	236/250 (94%)	216 (92%)	20 (8%)	0	100	100
12	LF	223/225 (99%)	216 (97%)	6 (3%)	1 (0%)	30	51
13	LG	239/241 (99%)	227 (95%)	12 (5%)	0	100	100
14	LH	188/190 (99%)	178 (95%)	10 (5%)	0	100	100
15	LI	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
16	LJ	168/176 (96%)	164 (98%)	4 (2%)	0	100	100
17	LL	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
18	LM	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
19	LN	201/203 (99%)	196 (98%)	5 (2%)	0	100	100
20	LO	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
21	LP	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
22	LQ	185/187 (99%)	179 (97%)	6 (3%)	0	100	100
23	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
24	LS	173/175 (99%)	167 (96%)	6 (4%)	0	100	100
25	LT	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
26	LU	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
27	LV	129/131 (98%)	122 (95%)	7 (5%)	0	100	100
28	LW	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
29	LX	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
30	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
31	LZ	133/135 (98%)	124 (93%)	9 (7%)	0	100	100
32	La	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
33	Lb	105/109 (96%)	99 (94%)	6 (6%)	0	100	100
34	Lc	96/98 (98%)	89 (93%)	6 (6%)	1 (1%)	12	28
35	Ld	105/107 (98%)	100 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Le	126/128 (98%)	123 (98%)	3 (2%)	0	100	100
37	Lf	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
38	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
39	Lh	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
40	Li	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
41	Lj	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
42	Lk	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
43	Ll	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
44	Lm	50/52 (96%)	50 (100%)	0	0	100	100
45	Ln	22/24 (92%)	22 (100%)	0	0	100	100
46	Lo	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
47	Lp	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
48	Lr	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
49	Ls	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
50	Lt	128/141 (91%)	107 (84%)	21 (16%)	0	100	100
53	SA	219/221 (99%)	207 (94%)	12 (6%)	0	100	100
54	SB	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
55	SC	218/222 (98%)	204 (94%)	14 (6%)	0	100	100
56	SD	225/227 (99%)	213 (95%)	12 (5%)	0	100	100
57	SE	260/262 (99%)	244 (94%)	16 (6%)	0	100	100
58	SF	187/189 (99%)	173 (92%)	14 (8%)	0	100	100
59	SG	235/237 (99%)	220 (94%)	15 (6%)	0	100	100
60	SH	182/186 (98%)	166 (91%)	15 (8%)	1 (0%)	24	45
61	SI	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
62	SJ	183/185 (99%)	169 (92%)	14 (8%)	0	100	100
63	SK	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
64	SL	151/153 (99%)	140 (93%)	11 (7%)	0	100	100
65	SM	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
66	SN	148/150 (99%)	146 (99%)	2 (1%)	0	100	100
67	SO	135/140 (96%)	129 (96%)	6 (4%)	0	100	100
68	SP	119/121 (98%)	115 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	SQ	142/144 (99%)	130 (92%)	11 (8%)	1 (1%)	18	37
70	SR	133/135 (98%)	121 (91%)	12 (9%)	0	100	100
71	SS	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
72	ST	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
73	SU	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
74	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
75	SW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
76	SX	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
77	SY	129/131 (98%)	118 (92%)	11 (8%)	0	100	100
78	SZ	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
79	Sa	100/102 (98%)	94 (94%)	6 (6%)	0	100	100
80	Sb	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
81	Sc	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
82	Sd	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
83	Se	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
84	Sf	65/67 (97%)	54 (83%)	11 (17%)	0	100	100
85	Sg	311/313 (99%)	286 (92%)	25 (8%)	0	100	100
87	CA	350/354 (99%)	334 (95%)	16 (5%)	0	100	100
All	All	12494/12701 (98%)	11820 (95%)	670 (5%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	LF	197	VAL
34	Lc	99	PRO
69	SQ	44	PRO
60	SH	15	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CD	31/31 (100%)	31 (100%)	0	100	100
2	CI	25/25 (100%)	25 (100%)	0	100	100
3	CF	365/366 (100%)	365 (100%)	0	100	100
7	LA	190/190 (100%)	190 (100%)	0	100	100
8	LB	348/348 (100%)	348 (100%)	0	100	100
9	LC	306/306 (100%)	306 (100%)	0	100	100
10	LD	246/247 (100%)	246 (100%)	0	100	100
11	LE	212/222 (96%)	212 (100%)	0	100	100
12	LF	194/194 (100%)	194 (100%)	0	100	100
13	LG	203/205 (99%)	203 (100%)	0	100	100
14	LH	169/169 (100%)	169 (100%)	0	100	100
15	LI	180/180 (100%)	180 (100%)	0	100	100
16	LJ	143/148 (97%)	143 (100%)	0	100	100
17	LL	176/176 (100%)	176 (100%)	0	100	100
18	LM	118/118 (100%)	118 (100%)	0	100	100
19	LN	171/171 (100%)	171 (100%)	0	100	100
20	LO	173/173 (100%)	173 (100%)	0	100	100
21	LP	134/134 (100%)	134 (100%)	0	100	100
22	LQ	164/164 (100%)	164 (100%)	0	100	100
23	LR	166/166 (100%)	166 (100%)	0	100	100
24	LS	156/156 (100%)	156 (100%)	0	100	100
25	LT	139/139 (100%)	139 (100%)	0	100	100
26	LU	91/91 (100%)	91 (100%)	0	100	100
27	LV	101/101 (100%)	101 (100%)	0	100	100
28	LW	95/97 (98%)	95 (100%)	0	100	100
29	LX	108/108 (100%)	108 (100%)	0	100	100
30	LY	124/124 (100%)	124 (100%)	0	100	100
31	LZ	117/117 (100%)	117 (100%)	0	100	100
32	La	120/120 (100%)	120 (100%)	0	100	100
33	Lb	88/90 (98%)	88 (100%)	0	100	100
34	Lc	83/83 (100%)	83 (100%)	0	100	100
35	Ld	98/98 (100%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	Le	114/114 (100%)	114 (100%)	0	100	100
37	Lf	88/88 (100%)	88 (100%)	0	100	100
38	Lg	98/98 (100%)	98 (100%)	0	100	100
39	Lh	109/109 (100%)	109 (100%)	0	100	100
40	Li	86/86 (100%)	86 (100%)	0	100	100
41	Lj	73/73 (100%)	73 (100%)	0	100	100
42	Lk	64/64 (100%)	64 (100%)	0	100	100
43	Ll	47/47 (100%)	47 (100%)	0	100	100
44	Lm	48/48 (100%)	48 (100%)	0	100	100
45	Ln	23/23 (100%)	23 (100%)	0	100	100
46	Lo	93/93 (100%)	93 (100%)	0	100	100
47	Lp	74/74 (100%)	74 (100%)	0	100	100
48	Lr	109/109 (100%)	109 (100%)	0	100	100
49	Ls	162/164 (99%)	162 (100%)	0	100	100
50	Lt	107/115 (93%)	107 (100%)	0	100	100
53	SA	183/183 (100%)	183 (100%)	0	100	100
54	SB	195/195 (100%)	195 (100%)	0	100	100
55	SC	186/188 (99%)	186 (100%)	0	100	100
56	SD	190/190 (100%)	190 (100%)	0	100	100
57	SE	224/224 (100%)	224 (100%)	0	100	100
58	SF	159/159 (100%)	159 (100%)	0	100	100
59	SG	207/207 (100%)	207 (100%)	0	100	100
60	SH	166/166 (100%)	166 (100%)	0	100	100
61	SI	178/178 (100%)	178 (100%)	0	100	100
62	SJ	161/161 (100%)	161 (100%)	0	100	100
63	SK	89/89 (100%)	89 (100%)	0	100	100
64	SL	137/137 (100%)	137 (100%)	0	100	100
65	SM	102/104 (98%)	102 (100%)	0	100	100
66	SN	130/130 (100%)	130 (100%)	0	100	100
67	SO	107/110 (97%)	107 (100%)	0	100	100
68	SP	107/107 (100%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	SQ	119/119 (100%)	119 (100%)	0	100	100
70	SR	122/122 (100%)	122 (100%)	0	100	100
71	SS	126/126 (100%)	126 (100%)	0	100	100
72	ST	113/113 (100%)	113 (100%)	0	100	100
73	SU	94/94 (100%)	94 (100%)	0	100	100
74	SV	67/67 (100%)	67 (100%)	0	100	100
75	SW	112/112 (100%)	112 (100%)	0	100	100
76	SX	113/113 (100%)	113 (100%)	0	100	100
77	SY	113/113 (100%)	113 (100%)	0	100	100
78	SZ	66/66 (100%)	66 (100%)	0	100	100
79	Sa	89/89 (100%)	89 (100%)	0	100	100
80	Sb	75/75 (100%)	75 (100%)	0	100	100
81	Sc	57/57 (100%)	57 (100%)	0	100	100
82	Sd	48/48 (100%)	48 (100%)	0	100	100
83	Se	47/47 (100%)	47 (100%)	0	100	100
84	Sf	60/60 (100%)	60 (100%)	0	100	100
85	Sg	272/272 (100%)	272 (100%)	0	100	100
87	CA	303/303 (100%)	303 (100%)	0	100	100
All	All	10846/10886 (100%)	10846 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
3	CF	15	HIS
3	CF	26	HIS
3	CF	95	HIS
3	CF	251	GLN
7	LA	50	HIS
8	LB	68	ASN
8	LB	354	GLN
9	LC	38	ASN
10	LD	202	GLN
13	LG	90	GLN

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Mol	Chain	Res	Type
13	LG	94	GLN
13	LG	100	HIS
13	LG	141	ASN
14	LH	39	ASN
15	LI	59	GLN
15	LI	73	ASN
16	LJ	65	ASN
17	LL	111	GLN
17	LL	149	GLN
19	LN	201	HIS
20	LO	72	HIS
21	LP	10	ASN
21	LP	133	HIS
21	LP	137	ASN
22	LQ	21	GLN
22	LQ	45	GLN
23	LR	134	ASN
23	LR	143	HIS
24	LS	108	GLN
28	LW	79	GLN
28	LW	104	GLN
28	LW	107	GLN
30	LY	40	GLN
30	LY	61	HIS
30	LY	65	GLN
30	LY	72	GLN
32	La	34	ASN
32	La	89	ASN
33	Lb	11	ASN
33	Lb	27	GLN
33	Lb	58	GLN
35	Ld	100	ASN
36	Le	52	GLN
37	Lf	24	HIS
39	Lh	65	GLN
41	Lj	57	ASN
46	Lo	105	GLN
49	Ls	105	ASN
49	Ls	190	GLN
49	Ls	191	GLN
53	SA	132	GLN
54	SB	76	ASN

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Mol	Chain	Res	Type
54	SB	158	HIS
55	SC	113	GLN
56	SD	101	GLN
56	SD	145	GLN
59	SG	4	ASN
59	SG	105	ASN
59	SG	163	ASN
60	SH	68	GLN
61	SI	9	HIS
62	SJ	124	HIS
62	SJ	156	HIS
64	SL	106	HIS
65	SM	119	GLN
68	SP	79	HIS
69	SQ	77	HIS
72	ST	51	ASN
72	ST	63	HIS
72	ST	85	ASN
73	SU	92	HIS
74	SV	33	GLN
74	SV	35	ASN
76	SX	16	HIS
77	SY	19	GLN
80	Sb	65	GLN
81	Sc	7	GLN
82	Sd	37	ASN
85	Sg	76	GLN
85	Sg	226	HIS
85	Sg	285	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	L5	3643/5070 (71%)	707 (19%)	24 (0%)
5	L7	119/120 (99%)	9 (7%)	0
51	Pt	72/74 (97%)	16 (22%)	0
52	S2	1715/1740 (98%)	379 (22%)	9 (0%)
6	L8	155/156 (99%)	24 (15%)	0
86	AT	74/76 (97%)	25 (33%)	1 (1%)
All	All	5778/7236 (79%)	1160 (20%)	34 (0%)

All (1160) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	L5	25	A
4	L5	30	C
4	L5	39	A
4	L5	42	A
4	L5	48	G
4	L5	56	A
4	L5	59	A
4	L5	64	A
4	L5	65	A
4	L5	73	A
4	L5	91	G
4	L5	104	G
4	L5	108	A
4	L5	109	G
4	L5	110	C
4	L5	119	G
4	L5	120	A
4	L5	132	G
4	L5	133	C
4	L5	134	G
4	L5	135	G
4	L5	159	C
4	L5	165	A
4	L5	172	C
4	L5	175	C
4	L5	182	G
4	L5	183	C
4	L5	184	U
4	L5	185	C
4	L5	186	G
4	L5	188	G
4	L5	189	G
4	L5	200	U
4	L5	209	U
4	L5	216	C
4	L5	218	A
4	L5	220	C
4	L5	234	G
4	L5	237	G
4	L5	255	C
4	L5	256	G
4	L5	261	G
4	L5	263	G

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Mol	Chain	Res	Type
4	L5	264	C
4	L5	265	C
4	L5	266	C
4	L5	267	G
4	L5	276	C
4	L5	280	G
4	L5	297	U
4	L5	306	A
4	L5	315	G
4	L5	316	U
4	L5	340	C
4	L5	387	G
4	L5	388	A
4	L5	396	A
4	L5	407	A
4	L5	409	G
4	L5	410	A
4	L5	411	G
4	L5	412	G
4	L5	431	G
4	L5	432	U
4	L5	449	C
4	L5	452	A
4	L5	453	G
4	L5	456	C
4	L5	457	G
4	L5	467	U
4	L5	468	U
4	L5	485	C
4	L5	486	C
4	L5	489	C
4	L5	493	G
4	L5	494	U
4	L5	497	G
4	L5	498	C
4	L5	499	G
4	L5	500	G
4	L5	501	C
4	L5	502	C
4	L5	503	C
4	L5	504	G
4	L5	509	A

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Mol	Chain	Res	Type
4	L5	510	U
4	L5	512	U
4	L5	513	U
4	L5	514	U
4	L5	515	C
4	L5	518	G
4	L5	643	C
4	L5	644	G
4	L5	646	G
4	L5	654	C
4	L5	655	C
4	L5	656	C
4	L5	657	C
4	L5	659	G
4	L5	666	G
4	L5	667	A
4	L5	668	C
4	L5	669	C
4	L5	673	C
4	L5	686	A
4	L5	700	G
4	L5	704	C
4	L5	730	G
4	L5	731	G
4	L5	738	C
4	L5	739	G
4	L5	742	G
4	L5	746	A
4	L5	759	G
4	L5	904	C
4	L5	905	C
4	L5	906	C
4	L5	913	U
4	L5	914	U
4	L5	915	A
4	L5	917	A
4	L5	923	C
4	L5	924	C
4	L5	926	G
4	L5	932	A
4	L5	933	G
4	L5	936	C

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Mol	Chain	Res	Type
4	L5	943	A
4	L5	944	A
4	L5	945	U
4	L5	946	C
4	L5	956	A
4	L5	959	G
4	L5	960	A
4	L5	961	G
4	L5	962	C
4	L5	965	G
4	L5	966	A
4	L5	967	C
4	L5	969	C
4	L5	970	G
4	L5	977	C
4	L5	982	U
4	L5	985	C
4	L5	989	U
4	L5	1066	G
4	L5	1070	G
4	L5	1071	C
4	L5	1072	C
4	L5	1075	G
4	L5	1082	C
4	L5	1083	U
4	L5	1095	A
4	L5	1168	G
4	L5	1171	G
4	L5	1172	C
4	L5	1173	G
4	L5	1179	U
4	L5	1180	C
4	L5	1181	C
4	L5	1182	C
4	L5	1183	C
4	L5	1184	A
4	L5	1202	C
4	L5	1203	G
4	L5	1210	C
4	L5	1211	G
4	L5	1214	C
4	L5	1215	C

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Mol	Chain	Res	Type
4	L5	1216	C
4	L5	1218	G
4	L5	1219	G
4	L5	1222	A
4	L5	1235	G
4	L5	1245	C
4	L5	1246	G
4	L5	1253	G
4	L5	1254	A
4	L5	1257	A
4	L5	1258	G
4	L5	1266	G
4	L5	1267	C
4	L5	1269	G
4	L5	1270	A
4	L5	1271	G
4	L5	1272	C
4	L5	1273	G
4	L5	1275	G
4	L5	1280	C
4	L5	1284	G
4	L5	1285	U
4	L5	1287	G
4	L5	1293	G
4	L5	1294	A
4	L5	1295	C
4	L5	1296	G
4	L5	1301	C
4	L5	1326	A2M
4	L5	1337	A
4	L5	1354	A
4	L5	1359	G
4	L5	1365	C
4	L5	1366	G
4	L5	1367	C
4	L5	1387	A
4	L5	1394	G
4	L5	1397	A
4	L5	1398	A
4	L5	1404	G
4	L5	1407	C
4	L5	1409	C

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Mol	Chain	Res	Type
4	L5	1410	U
4	L5	1415	G
4	L5	1417	C
4	L5	1420	A
4	L5	1437	C
4	L5	1439	C
4	L5	1442	C
4	L5	1443	A
4	L5	1444	G
4	L5	1446	C
4	L5	1447	C
4	L5	1482	G
4	L5	1483	C
4	L5	1497	A
4	L5	1498	G
4	L5	1502	G
4	L5	1517	G
4	L5	1534	A2M
4	L5	1535	C
4	L5	1537	A
4	L5	1547	A
4	L5	1564	A
4	L5	1566	C
4	L5	1578	U
4	L5	1591	U
4	L5	1596	U
4	L5	1624	G
4	L5	1625	OMG
4	L5	1631	A
4	L5	1633	G
4	L5	1634	A
4	L5	1638	A
4	L5	1640	C
4	L5	1641	G
4	L5	1642	A
4	L5	1654	G
4	L5	1661	C
4	L5	1676	C
4	L5	1677	PSU
4	L5	1694	C
4	L5	1697	G
4	L5	1699	A

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Mol	Chain	Res	Type
4	L5	1700	G
4	L5	1702	C
4	L5	1704	C
4	L5	1705	G
4	L5	1717	C
4	L5	1718	C
4	L5	1719	A
4	L5	1721	G
4	L5	1731	C
4	L5	1734	G
4	L5	1741	G
4	L5	1742	A
4	L5	1750	G
4	L5	1757	U
4	L5	1758	G
4	L5	1760	G
4	L5	1761	G
4	L5	1762	C
4	L5	1763	C
4	L5	1764	G
4	L5	1765	A
4	L5	1766	A
4	L5	1767	A
4	L5	1768	C
4	L5	1770	A
4	L5	1787	A
4	L5	1804	A
4	L5	1806	G
4	L5	1810	G
4	L5	1820	C
4	L5	1821	G
4	L5	1822	U
4	L5	1834	U
4	L5	1836	G
4	L5	1837	A
4	L5	1842	G
4	L5	1855	G
4	L5	1869	G
4	L5	1882	U
4	L5	1892	A
4	L5	1897	A
4	L5	1918	U

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Mol	Chain	Res	Type
4	L5	1919	G
4	L5	1920	C
4	L5	1921	C
4	L5	1922	G
4	L5	1925	G
4	L5	1931	C
4	L5	1932	A
4	L5	1936	C
4	L5	1940	G
4	L5	1948	G
4	L5	1961	G
4	L5	1962	A
4	L5	1974	U
4	L5	1975	G
4	L5	1978	C
4	L5	1980	U
4	L5	1981	G
4	L5	1982	G
4	L5	1983	A
4	L5	1984	A
4	L5	1985	G
4	L5	1991	A
4	L5	1992	U
4	L5	1993	C
4	L5	1997	U
4	L5	1998	A
4	L5	1999	A
4	L5	2001	G
4	L5	2002	A
4	L5	2011	C
4	L5	2017	A
4	L5	2018	C
4	L5	2024	G
4	L5	2026	A
4	L5	2046	G
4	L5	2048	U
4	L5	2055	G
4	L5	2056	G
4	L5	2069	A
4	L5	2084	C
4	L5	2085	G
4	L5	2092	G

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Mol	Chain	Res	Type
4	L5	2093	A
4	L5	2094	G
4	L5	2095	A
4	L5	2096	G
4	L5	2097	U
4	L5	2098	G
4	L5	2100	A
4	L5	2101	C
4	L5	2102	G
4	L5	2103	G
4	L5	2107	C
4	L5	2108	G
4	L5	2110	C
4	L5	2111	G
4	L5	2112	G
4	L5	2250	C
4	L5	2252	G
4	L5	2253	A
4	L5	2256	C
4	L5	2258	C
4	L5	2269	C
4	L5	2289	C
4	L5	2300	A
4	L5	2301	G
4	L5	2313	A
4	L5	2332	A
4	L5	2333	G
4	L5	2348	G
4	L5	2351	OMC
4	L5	2360	A
4	L5	2364	OMG
4	L5	2395	A
4	L5	2397	G
4	L5	2411	C
4	L5	2412	A
4	L5	2416	G
4	L5	2417	A
4	L5	2425	U
4	L5	2450	G
4	L5	2453	A
4	L5	2464	C
4	L5	2465	C

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Mol	Chain	Res	Type
4	L5	2471	G
4	L5	2474	G
4	L5	2475	G
4	L5	2478	C
4	L5	2479	G
4	L5	2483	G
4	L5	2484	A
4	L5	2485	U
4	L5	2486	G
4	L5	2487	G
4	L5	2488	C
4	L5	2489	C
4	L5	2490	U
4	L5	2494	U
4	L5	2504	C
4	L5	2506	G
4	L5	2513	A
4	L5	2519	U
4	L5	2520	C
4	L5	2529	A
4	L5	2537	A
4	L5	2544	G
4	L5	2546	G
4	L5	2547	G
4	L5	2554	U
4	L5	2555	G
4	L5	2560	C
4	L5	2565	A
4	L5	2573	A
4	L5	2583	C
4	L5	2587	A
4	L5	2589	C
4	L5	2601	A
4	L5	2602	G
4	L5	2618	G
4	L5	2627	C
4	L5	2653	C
4	L5	2662	G
4	L5	2664	G
4	L5	2669	C
4	L5	2676	A
4	L5	2687	U

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Mol	Chain	Res	Type
4	L5	2694	G
4	L5	2695	A
4	L5	2696	A
4	L5	2706	G
4	L5	2707	U
4	L5	2708	U
4	L5	2709	C
4	L5	2710	C
4	L5	2711	G
4	L5	2721	G
4	L5	2724	G
4	L5	2726	G
4	L5	2739	C
4	L5	2742	G
4	L5	2743	A
4	L5	2746	A
4	L5	2761	U
4	L5	2763	U
4	L5	2769	U
4	L5	2770	C
4	L5	2788	U
4	L5	2790	U
4	L5	2826	U
4	L5	2827	G
4	L5	2829	U
4	L5	2838	G
4	L5	2855	G
4	L5	2877	G
4	L5	2894	A
4	L5	2900	U
4	L5	2902	G
4	L5	2903	G
4	L5	2904	U
4	L5	2905	C
4	L5	2906	G
4	L5	2908	U
4	L5	3588	C
4	L5	3590	G
4	L5	3591	C
4	L5	3594	C
4	L5	3595	U
4	L5	3596	A

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Mol	Chain	Res	Type
4	L5	3597	G
4	L5	3599	A
4	L5	3605	C
4	L5	3626	G
4	L5	3630	A
4	L5	3635	A
4	L5	3644	U
4	L5	3646	A
4	L5	3648	A
4	L5	3662	A
4	L5	3664	G
4	L5	3670	C
4	L5	3673	C
4	L5	3674	G
4	L5	3685	C
4	L5	3701	OMC
4	L5	3710	G
4	L5	3711	A
4	L5	3713	U
4	L5	3714	G
4	L5	3727	A
4	L5	3748	A
4	L5	3753	G
4	L5	3760	A
4	L5	3770	U
4	L5	3774	A
4	L5	3775	A
4	L5	3776	G
4	L5	3777	G
4	L5	3785	A2M
4	L5	3786	U
4	L5	3792	OMG
4	L5	3811	G
4	L5	3814	U
4	L5	3817	A
4	L5	3819	G
4	L5	3824	A
4	L5	3838	U
4	L5	3839	G
4	L5	3840	U
4	L5	3867	A2M
4	L5	3877	A

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Mol	Chain	Res	Type
4	L5	3878	C
4	L5	3879	G
4	L5	3885	G
4	L5	3890	A
4	L5	3892	U
4	L5	3897	G
4	L5	3901	A
4	L5	3906	A
4	L5	3907	G
4	L5	3908	A
4	L5	3915	U
4	L5	3923	A
4	L5	3938	G
4	L5	3942	A
4	L5	3943	A
4	L5	3944	G
4	L5	3947	A
4	L5	3949	A
4	L5	3950	U
4	L5	3953	G
4	L5	4057	C
4	L5	4058	U
4	L5	4059	C
4	L5	4060	U
4	L5	4061	G
4	L5	4062	A
4	L5	4064	C
4	L5	4068	U
4	L5	4069	U
4	L5	4076	G
4	L5	4084	G
4	L5	4095	G
4	L5	4097	G
4	L5	4099	G
4	L5	4101	C
4	L5	4104	G
4	L5	4105	A
4	L5	4108	G
4	L5	4111	U
4	L5	4112	C
4	L5	4114	C
4	L5	4115	G

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Mol	Chain	Res	Type
4	L5	4116	C
4	L5	4122	G
4	L5	4127	A
4	L5	4133	C
4	L5	4140	C
4	L5	4141	G
4	L5	4142	C
4	L5	4143	G
4	L5	4144	C
4	L5	4146	G
4	L5	4150	G
4	L5	4163	U
4	L5	4170	A
4	L5	4183	G
4	L5	4184	G
4	L5	4191	G
4	L5	4201	G
4	L5	4203	A
4	L5	4222	G
4	L5	4225	G
4	L5	4229	U
4	L5	4233	A
4	L5	4234	A
4	L5	4251	A
4	L5	4254	G
4	L5	4256	A
4	L5	4257	A
4	L5	4258	C
4	L5	4265	U
4	L5	4268	A
4	L5	4273	A
4	L5	4281	A
4	L5	4291	G
4	L5	4305	G
4	L5	4306	OMU
4	L5	4314	C
4	L5	4319	C
4	L5	4329	G
4	L5	4330	G
4	L5	4332	C
4	L5	4349	C
4	L5	4350	C

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Mol	Chain	Res	Type
4	L5	4354	U
4	L5	4373	G
4	L5	4376	A
4	L5	4377	G
4	L5	4378	A
4	L5	4380	A
4	L5	4387	C
4	L5	4391	G
4	L5	4394	A
4	L5	4421	C
4	L5	4422	A
4	L5	4427	G
4	L5	4438	U
4	L5	4444	C
4	L5	4448	G
4	L5	4449	A
4	L5	4464	A
4	L5	4466	C
4	L5	4488	A
4	L5	4500	PSU
4	L5	4512	U
4	L5	4513	A
4	L5	4519	C
4	L5	4524	G
4	L5	4525	C
4	L5	4545	G
4	L5	4548	A
4	L5	4549	G
4	L5	4557	U
4	L5	4560	C
4	L5	4567	G
4	L5	4573	G
4	L5	4575	G
4	L5	4584	A
4	L5	4589	A
4	L5	4590	A2M
4	L5	4600	G
4	L5	4601	U
4	L5	4617	G
4	L5	4636	PSU
4	L5	4637	OMG
4	L5	4648	A

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Mol	Chain	Res	Type
4	L5	4656	A
4	L5	4670	C
4	L5	4672	A
4	L5	4694	G
4	L5	4695	C
4	L5	4700	A
4	L5	4708	A
4	L5	4709	U
4	L5	4719	G
4	L5	4734	A
4	L5	4740	G
4	L5	4741	C
4	L5	4742	G
4	L5	4745	G
4	L5	4754	G
4	L5	4757	C
4	L5	4759	C
4	L5	4761	G
4	L5	4765	G
4	L5	4771	C
4	L5	4772	C
4	L5	4775	C
4	L5	4859	C
4	L5	4870	G
4	L5	4871	C
4	L5	4875	G
4	L5	4881	U
4	L5	4882	U
4	L5	4883	C
4	L5	4889	G
4	L5	4895	C
4	L5	4896	G
4	L5	4898	G
4	L5	4899	G
4	L5	4900	C
4	L5	4901	G
4	L5	4910	G
4	L5	4912	G
4	L5	4914	C
4	L5	4922	C
4	L5	4925	U
4	L5	4926	C

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Mol	Chain	Res	Type
4	L5	4927	G
4	L5	4928	C
4	L5	4934	A
4	L5	4940	C
4	L5	4941	G
4	L5	4943	A
4	L5	4951	G
4	L5	4960	G
4	L5	4963	G
4	L5	4976	U
4	L5	4985	U
4	L5	4988	U
4	L5	4989	U
4	L5	4990	C
4	L5	4991	U
4	L5	4995	U
4	L5	5007	A
4	L5	5013	C
4	L5	5014	A
4	L5	5017	G
4	L5	5020	G
4	L5	5022	U
4	L5	5023	C
4	L5	5024	C
4	L5	5027	C
4	L5	5028	G
4	L5	5030	U
4	L5	5034	A
4	L5	5041	G
4	L5	5050	C
4	L5	5054	C
4	L5	5055	G
4	L5	5061	A
4	L5	5069	U
5	L7	24	C
5	L7	33	U
5	L7	38	U
5	L7	53	U
5	L7	54	A
5	L7	64	G
5	L7	100	A
5	L7	110	G

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Mol	Chain	Res	Type
5	L7	111	C
6	L8	25	G
6	L8	34	U
6	L8	35	C
6	L8	59	A
6	L8	62	A
6	L8	63	U
6	L8	80	A
6	L8	82	A
6	L8	84	A
6	L8	85	U
6	L8	86	U
6	L8	87	G
6	L8	94	G
6	L8	103	A
6	L8	105	C
6	L8	111	U
6	L8	114	G
6	L8	123	U
6	L8	124	U
6	L8	125	C
6	L8	126	C
6	L8	127	U
6	L8	147	G
6	L8	153	C
51	Pt	2	U
51	Pt	9	A
51	Pt	13	U
51	Pt	19	G
51	Pt	20(A)	U
51	Pt	21	A
51	Pt	46	G
51	Pt	47	U
51	Pt	48	C
51	Pt	49	C
51	Pt	58	A
51	Pt	64	G
51	Pt	67	G
51	Pt	70	A
51	Pt	75	C
51	Pt	76	A
52	S2	4	C

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Mol	Chain	Res	Type
52	S2	13	C
52	S2	14	C
52	S2	24	C
52	S2	25	A
52	S2	33	G
52	S2	41	G
52	S2	44	U
52	S2	45	A
52	S2	46	A
52	S2	56	G
52	S2	58	C
52	S2	67	C
52	S2	68	A
52	S2	72	C
52	S2	73	C
52	S2	74	G
52	S2	76	U
52	S2	92	A
52	S2	99	A2M
52	S2	103	A
52	S2	113	G
52	S2	115	U
52	S2	126	G
52	S2	130	G
52	S2	143	U
52	S2	149	A
52	S2	158	A
52	S2	160	U
52	S2	170	A
52	S2	179	C
52	S2	190	G
52	S2	196	C
52	S2	197	U
52	S2	198	U
52	S2	200	G
52	S2	203	G
52	S2	204	G
52	S2	207	G
52	S2	208	G
52	S2	209	A
52	S2	214	U
52	S2	291	G

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Mol	Chain	Res	Type
52	S2	292	A
52	S2	295	C
52	S2	302	A
52	S2	306	C
52	S2	307	G
52	S2	308	G
52	S2	309	G
52	S2	312	G
52	S2	318	A
52	S2	319	C
52	S2	323	C
52	S2	324	C
52	S2	325	C
52	S2	326	C
52	S2	327	G
52	S2	328	U
52	S2	329	G
52	S2	332	G
52	S2	339	A
52	S2	340	C
52	S2	347	G
52	S2	360	A
52	S2	361	U
52	S2	362	C
52	S2	364	A
52	S2	368	U
52	S2	369	C
52	S2	370	G
52	S2	385	G
52	S2	386	C
52	S2	398	A
52	S2	407	G
52	S2	408	A
52	S2	409	C
52	S2	427	U
52	S2	438	G
52	S2	448	A
52	S2	449	A
52	S2	450	C
52	S2	452	G
52	S2	464	A
52	S2	465	A

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Mol	Chain	Res	Type
52	S2	471	G
52	S2	472	C
52	S2	473	A
52	S2	474	G
52	S2	476	A
52	S2	482	G
52	S2	487	U
52	S2	488	U
52	S2	492	C
52	S2	493	A
52	S2	502	C
52	S2	516	A
52	S2	531	A
52	S2	532	C
52	S2	536	A
52	S2	537	C
52	S2	540	U
52	S2	542	U
52	S2	544	G
52	S2	546	G
52	S2	547	G
52	S2	555	A
52	S2	557	U
52	S2	558	G
52	S2	559	G
52	S2	563	G
52	S2	564	A
52	S2	566	U
52	S2	576	A2M
52	S2	581	U
52	S2	587	A
52	S2	589	G
52	S2	590	A
52	S2	591	U
52	S2	592	C
52	S2	593	C
52	S2	594	A
52	S2	604	A
52	S2	614	C
52	S2	617	G
52	S2	623	G
52	S2	627	OMU

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Mol	Chain	Res	Type
52	S2	628	A
52	S2	631	U
52	S2	643	A
52	S2	644	OMG
52	S2	655	A
52	S2	660	C
52	S2	664	A
52	S2	668	A2M
52	S2	669	A
52	S2	671	A
52	S2	672	A
52	S2	673	G
52	S2	688	U
52	S2	689	U
52	S2	692	G
52	S2	693	A
52	S2	695	C
52	S2	696	G
52	S2	697	G
52	S2	698	G
52	S2	732	U
52	S2	733	C
52	S2	736	C
52	S2	737	G
52	S2	738	C
52	S2	749	U
52	S2	751	G
52	S2	752	G
52	S2	753	C
52	S2	788	G
52	S2	791	C
52	S2	792	C
52	S2	798	G
52	S2	799	OMU
52	S2	821	G
52	S2	822	U
52	S2	823	U
52	S2	824	C
52	S2	827	A
52	S2	830	A
52	S2	834	C
52	S2	835	C

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Mol	Chain	Res	Type
52	S2	836	G
52	S2	837	A
52	S2	838	G
52	S2	839	C
52	S2	842	C
52	S2	844	U
52	S2	847	A
52	S2	863	PSU
52	S2	867	OMG
52	S2	870	A
52	S2	874	G
52	S2	877	C
52	S2	878	G
52	S2	880	G
52	S2	888	U
52	S2	889	U
52	S2	891	G
52	S2	894	G
52	S2	896	U
52	S2	897	U
52	S2	898	U
52	S2	899	U
52	S2	900	C
52	S2	901	G
52	S2	903	A
52	S2	913	A
52	S2	920	A
52	S2	922	A
52	S2	933	G
52	S2	934	G
52	S2	963	A
52	S2	970	G
52	S2	971	G
52	S2	972	A
52	S2	990	A
52	S2	992	A
52	S2	997	A
52	S2	999	G
52	S2	1001	A
52	S2	1008	A
52	S2	1017	U
52	S2	1023	A

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Mol	Chain	Res	Type
52	S2	1027	A
52	S2	1033	G
52	S2	1044	G
52	S2	1045	PSU
52	S2	1061	U
52	S2	1062	A
52	S2	1067	C
52	S2	1083	A
52	S2	1085	C
52	S2	1107	G
52	S2	1108	G
52	S2	1109	C
52	S2	1113	A
52	S2	1114	U
52	S2	1116	C
52	S2	1118	C
52	S2	1119	A
52	S2	1121	G
52	S2	1123	C
52	S2	1133	A
52	S2	1138	C
52	S2	1148	A
52	S2	1149	A
52	S2	1153	C
52	S2	1154	U
52	S2	1195	A
52	S2	1207	G
52	S2	1208	A
52	S2	1215	C
52	S2	1216	C
52	S2	1217	A
52	S2	1220	A
52	S2	1224	G
52	S2	1227	G
52	S2	1242	U
52	S2	1243	U
52	S2	1248	B8N
52	S2	1251	A
52	S2	1253	A
52	S2	1256	G
52	S2	1257	G
52	S2	1259	A

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Mol	Chain	Res	Type
52	S2	1269	G
52	S2	1271	C
52	S2	1272	OMC
52	S2	1274	G
52	S2	1275	G
52	S2	1283	C
52	S2	1288	OMU
52	S2	1290	G
52	S2	1293	A
52	S2	1294	G
52	S2	1295	A
52	S2	1301	A
52	S2	1302	G
52	S2	1308	U
52	S2	1342	U
52	S2	1357	A
52	S2	1358	U
52	S2	1371	U
52	S2	1372	U
52	S2	1373	C
52	S2	1376	A
52	S2	1378	A
52	S2	1382	A
52	S2	1401	A
52	S2	1402	A
52	S2	1408	U
52	S2	1413	G
52	S2	1414	A
52	S2	1415	C
52	S2	1417	C
52	S2	1418	C
52	S2	1419	C
52	S2	1420	G
52	S2	1421	A
52	S2	1422	G
52	S2	1423	C
52	S2	1424	G
52	S2	1431	G
52	S2	1433	C
52	S2	1435	C
52	S2	1438	A
52	S2	1439	A

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Mol	Chain	Res	Type
52	S2	1442	OMU
52	S2	1449	G
52	S2	1454	A
52	S2	1463	U
52	S2	1478	U
52	S2	1480	A
52	S2	1489	A
52	S2	1490	OMG
52	S2	1492	U
52	S2	1494	U
52	S2	1495	G
52	S2	1497	G
52	S2	1498	A
52	S2	1521	C
52	S2	1522	A
52	S2	1531	A
52	S2	1533	A
52	S2	1544	C
52	S2	1552	G
52	S2	1556	A
52	S2	1557	C
52	S2	1574	C
52	S2	1578	U
52	S2	1580	A
52	S2	1581	C
52	S2	1582	C
52	S2	1585	U
52	S2	1587	G
52	S2	1588	A
52	S2	1600	G
52	S2	1604	G
52	S2	1621	U
52	S2	1623	A
52	S2	1633	A
52	S2	1634	A
52	S2	1637	A
52	S2	1646	C
52	S2	1648	G
52	S2	1654	G
52	S2	1663	A
52	S2	1665	G
52	S2	1683	C

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Mol	Chain	Res	Type
52	S2	1694	U
52	S2	1695	A
52	S2	1698	C
52	S2	1699	A
52	S2	1703	OMC
52	S2	1712	A
52	S2	1715	A
52	S2	1721	U
52	S2	1722	G
52	S2	1744	G
52	S2	1745	A
52	S2	1752	C
52	S2	1753	C
52	S2	1754	G
52	S2	1755	C
52	S2	1757	G
52	S2	1758	G
52	S2	1759	G
52	S2	1761	U
52	S2	1772	C
52	S2	1773	C
52	S2	1774	C
52	S2	1777	G
52	S2	1782	G
52	S2	1783	C
52	S2	1784	G
52	S2	1786	U
52	S2	1798	C
52	S2	1810	U
52	S2	1825	A
52	S2	1826	G
52	S2	1829	G
52	S2	1831	A
52	S2	1832	6MZ
52	S2	1835	A
52	S2	1838	U
52	S2	1849	G
52	S2	1851	MA6
52	S2	1861	G
52	S2	1862	G
52	S2	1863	A
52	S2	1865	C

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Mol	Chain	Res	Type
86	AT	4	U
86	AT	8	U
86	AT	9	A
86	AT	10	G
86	AT	12	G
86	AT	14	A
86	AT	16	C
86	AT	19	G
86	AT	20	U
86	AT	21	U
86	AT	22	A
86	AT	27	G
86	AT	31	G
86	AT	33	C
86	AT	37	C
86	AT	44	A
86	AT	47	G
86	AT	49	C
86	AT	50	C
86	AT	59	A
86	AT	60	A
86	AT	62	C
86	AT	72	A
86	AT	76	C
86	AT	77	A

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L5	406	C
4	L5	493	G
4	L5	914	U
4	L5	1082	C
4	L5	1366	G
4	L5	1590	C
4	L5	1633	G
4	L5	1703	C
4	L5	1977	C
4	L5	2094	G
4	L5	2416	G
4	L5	2485	U
4	L5	2587	A

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Mol	Chain	Res	Type
4	L5	2675	G
4	L5	2709	C
4	L5	2760	G
4	L5	3673	C
4	L5	4061	G
4	L5	4104	G
4	L5	4447	5MC
4	L5	4600	G
4	L5	4699	U
4	L5	4899	G
4	L5	4913	G
52	S2	291	G
52	S2	531	A
52	S2	563	G
52	S2	593	C
52	S2	688	U
52	S2	1418	C
52	S2	1434	C
52	S2	1477	U
52	S2	1556	A
86	AT	11	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PSU	L5	4673	4,88	18,21,22	1.12	1 (5%)	21,30,33	1.88	5 (23%)
52	OMU	S2	1288	52	19,22,23	3.34	7 (36%)	25,31,34	1.74	5 (20%)
4	OMG	L5	3744	4	23,26,27	0.45	0	32,38,41	0.50	0
52	PSU	S2	1367	52	18,21,22	1.13	1 (5%)	21,30,33	1.88	5 (23%)
4	OMG	L5	4370	4	23,26,27	0.47	0	32,38,41	0.52	0
52	PSU	S2	406	52	18,21,22	1.14	1 (5%)	21,30,33	1.94	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OMU	L5	4498	91,4	19,22,23	3.32	7 (36%)	25,31,34	1.77	5 (20%)
4	OMG	L5	3627	4	23,26,27	0.45	0	32,38,41	0.56	0
52	PSU	S2	93	52	18,21,22	1.13	1 (5%)	21,30,33	1.82	4 (19%)
52	PSU	S2	105	52	18,21,22	1.15	1 (5%)	21,30,33	1.79	4 (19%)
4	PSU	L5	4361	4	18,21,22	1.09	1 (5%)	21,30,33	1.87	4 (19%)
52	OMU	S2	627	52	19,22,23	3.40	7 (36%)	25,31,34	1.79	5 (20%)
52	A2M	S2	1383	52	22,25,26	1.24	1 (4%)	30,36,39	1.60	6 (20%)
4	OMC	L5	2422	4,88	19,22,23	0.50	0	25,31,34	0.64	0
4	PSU	L5	4353	4	18,21,22	1.14	1 (5%)	21,30,33	1.93	6 (28%)
52	A2M	S2	576	52	22,25,26	1.25	2 (9%)	30,36,39	1.53	5 (16%)
4	A2M	L5	398	4	22,25,26	1.26	2 (9%)	30,36,39	1.60	5 (16%)
52	A2M	S2	468	52	22,25,26	1.25	1 (4%)	30,36,39	1.57	6 (20%)
4	A2M	L5	2363	4,88	22,25,26	1.18	1 (4%)	30,36,39	1.48	6 (20%)
52	A2M	S2	166	52	22,25,26	1.27	2 (9%)	30,36,39	1.48	4 (13%)
4	1MA	L5	1322	4,88	21,25,26	0.50	0	30,37,40	0.77	1 (3%)
4	PSU	L5	4973	4	18,21,22	1.11	1 (5%)	21,30,33	1.92	5 (23%)
4	OMC	L5	1340	4	19,22,23	0.52	0	25,31,34	0.76	0
52	A2M	S2	99	52,88	22,25,26	1.25	2 (9%)	30,36,39	1.41	4 (13%)
4	PSU	L5	3920	4,88	18,21,22	1.11	1 (5%)	21,30,33	1.91	5 (23%)
52	PSU	S2	801	52	18,21,22	1.12	1 (5%)	21,30,33	1.85	4 (19%)
6	PSU	L8	55	6	18,21,22	1.16	1 (5%)	21,30,33	1.84	4 (19%)
4	5MC	L5	4447	91,4	19,22,23	0.68	0	26,32,35	0.62	0
4	PSU	L5	4532	4	18,21,22	1.13	1 (5%)	21,30,33	1.88	4 (19%)
4	A2M	L5	1534	4,88	22,25,26	1.24	2 (9%)	30,36,39	1.46	6 (20%)
4	OMU	L5	2837	4	19,22,23	3.39	7 (36%)	25,31,34	1.83	5 (20%)
4	OMU	L5	4620	4	19,22,23	3.34	7 (36%)	25,31,34	1.66	4 (16%)
52	OMC	S2	462	52	19,22,23	0.49	0	25,31,34	0.68	0
4	6MZ	L5	4220	4	26,26,26	2.78	5 (19%)	36,39,39	2.83	17 (47%)
4	A2M	L5	400	4	22,25,26	1.27	1 (4%)	30,36,39	1.57	7 (23%)
4	OMC	L5	3869	4	19,22,23	0.50	0	25,31,34	0.70	0
4	PSU	L5	4628	4	18,21,22	1.09	1 (5%)	21,30,33	1.87	4 (19%)
52	B8N	S2	1248	52	25,29,30	3.27	6 (24%)	28,42,45	1.99	8 (28%)
4	OMG	L5	1625	91,4	23,26,27	0.47	0	32,38,41	0.48	0
4	OMG	L5	2424	4	23,26,27	0.46	0	32,38,41	0.45	0
52	OMG	S2	683	52	23,26,27	0.48	0	32,38,41	0.49	0
4	A2M	L5	3718	4	22,25,26	1.20	2 (9%)	30,36,39	1.48	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	PSU	S2	866	52	18,21,22	1.14	1 (5%)	21,30,33	1.92	5 (23%)
4	PSU	L5	3844	4	18,21,22	1.18	1 (5%)	21,30,33	1.87	4 (19%)
4	PSU	L5	1677	4	18,21,22	1.21	2 (11%)	21,30,33	1.98	6 (28%)
4	A2M	L5	1871	4,88	22,25,26	1.23	1 (4%)	30,36,39	1.48	6 (20%)
52	A2M	S2	159	52	22,25,26	1.21	1 (4%)	30,36,39	1.52	5 (16%)
3	SEP	CF	163	3	8,9,10	1.61	1 (12%)	7,12,14	1.28	1 (14%)
4	5MC	L5	3782	4,88	19,22,23	0.51	0	26,32,35	0.67	0
4	PSU	L5	4442	4	18,21,22	1.13	1 (5%)	21,30,33	1.94	6 (28%)
4	OMG	L5	3792	4	23,26,27	0.45	0	32,38,41	0.51	0
4	A2M	L5	1323	4	22,25,26	1.24	2 (9%)	30,36,39	1.45	5 (16%)
52	PSU	S2	1244	52	18,21,22	1.12	1 (5%)	21,30,33	1.87	5 (23%)
4	PSU	L5	1862	4	18,21,22	1.10	1 (5%)	21,30,33	1.87	4 (19%)
52	4AC	S2	1842	52	21,24,25	0.35	0	28,34,37	0.40	0
4	PSU	L5	4972	4	18,21,22	1.15	1 (5%)	21,30,33	1.89	5 (23%)
4	PSU	L5	3822	4	18,21,22	1.14	1 (5%)	21,30,33	1.89	6 (28%)
4	PSU	L5	3851	4	18,21,22	1.12	1 (5%)	21,30,33	1.87	4 (19%)
52	OMG	S2	601	52	23,26,27	0.45	0	32,38,41	0.46	0
4	OMC	L5	3808	4	19,22,23	0.53	0	25,31,34	0.79	1 (4%)
4	PSU	L5	1792	4	18,21,22	1.10	1 (5%)	21,30,33	1.86	4 (19%)
52	OMU	S2	1326	52	19,22,23	3.36	7 (36%)	25,31,34	1.82	5 (20%)
4	PSU	L5	3637	91,4	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
4	OMG	L5	4228	4	23,26,27	0.48	0	32,38,41	0.62	0
52	4AC	S2	1337	52	21,24,25	0.37	0	28,34,37	0.56	0
4	PSU	L5	4403	91,4	18,21,22	1.15	1 (5%)	21,30,33	1.95	6 (28%)
4	OMG	L5	2364	4,88	23,26,27	0.47	0	32,38,41	0.46	0
52	PSU	S2	863	52	18,21,22	1.11	1 (5%)	21,30,33	1.80	4 (19%)
4	OMG	L5	4392	4	23,26,27	0.44	0	32,38,41	0.51	0
4	OMC	L5	4536	4	19,22,23	0.53	0	25,31,34	0.70	0
4	PSU	L5	4500	4	18,21,22	1.18	1 (5%)	21,30,33	1.87	4 (19%)
4	PSU	L5	4521	91,4,88	18,21,22	1.14	1 (5%)	21,30,33	1.91	5 (23%)
52	MA6	S2	1850	52	23,26,27	1.28	2 (8%)	33,38,41	3.13	11 (33%)
4	OMC	L5	3701	91,4	19,22,23	0.57	0	25,31,34	1.51	4 (16%)
6	OMG	L8	75	6	23,26,27	0.45	0	32,38,41	0.47	0
52	PSU	S2	686	52	18,21,22	1.11	1 (5%)	21,30,33	1.84	4 (19%)
52	PSU	S2	1177	52	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
52	PSU	S2	1056	52	18,21,22	1.13	1 (5%)	21,30,33	1.93	6 (28%)
4	PSU	L5	3639	4	18,21,22	1.13	1 (5%)	21,30,33	1.94	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	L5	4689	4	18,21,22	1.13	1 (5%)	21,30,33	1.99	4 (19%)
4	PSU	L5	4299	4	18,21,22	1.12	1 (5%)	21,30,33	1.86	5 (23%)
52	OMU	S2	1442	52	19,22,23	3.40	7 (36%)	25,31,34	1.78	4 (16%)
4	OMG	L5	1522	4	23,26,27	0.48	0	32,38,41	0.62	0
4	PSU	L5	1782	4	18,21,22	1.12	1 (5%)	21,30,33	1.87	4 (19%)
4	PSU	L5	4576	4	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
52	OMU	S2	428	52	19,22,23	3.33	7 (36%)	25,31,34	1.76	5 (20%)
52	PSU	S2	651	52	18,21,22	1.13	1 (5%)	21,30,33	1.90	5 (23%)
4	A2M	L5	4523	4,88	22,25,26	1.26	1 (4%)	30,36,39	1.54	6 (20%)
52	OMU	S2	116	52	19,22,23	3.32	7 (36%)	25,31,34	1.67	5 (20%)
4	PSU	L5	1582	4	18,21,22	1.12	1 (5%)	21,30,33	1.79	4 (19%)
4	PSU	L5	4293	4	18,21,22	1.16	1 (5%)	21,30,33	1.95	5 (23%)
52	PSU	S2	1046	52	18,21,22	1.13	1 (5%)	21,30,33	1.80	5 (23%)
52	A2M	S2	484	52	22,25,26	1.25	2 (9%)	30,36,39	1.51	7 (23%)
4	PSU	L5	4296	4	18,21,22	1.12	1 (5%)	21,30,33	1.90	5 (23%)
4	A2M	L5	3867	4	22,25,26	1.24	1 (4%)	30,36,39	1.50	8 (26%)
52	OMC	S2	174	52	19,22,23	0.49	0	25,31,34	0.65	0
4	PSU	L5	4636	4	18,21,22	1.12	1 (5%)	21,30,33	2.02	6 (28%)
52	PSU	S2	1081	52	18,21,22	1.14	1 (5%)	21,30,33	1.74	5 (23%)
52	PSU	S2	681	52	18,21,22	1.11	1 (5%)	21,30,33	1.87	4 (19%)
4	PSU	L5	4552	4	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
52	OMU	S2	354	52	19,22,23	3.33	7 (36%)	25,31,34	1.79	5 (20%)
4	A2M	L5	1326	4	22,25,26	1.22	2 (9%)	30,36,39	1.36	5 (16%)
4	PSU	L5	1860	4	18,21,22	1.13	1 (5%)	21,30,33	1.83	4 (19%)
4	A2M	L5	4571	4	22,25,26	1.28	2 (9%)	30,36,39	1.59	7 (23%)
52	OMG	S2	644	52	23,26,27	0.45	0	32,38,41	0.51	0
52	OMU	S2	799	52	19,22,23	3.44	7 (36%)	25,31,34	1.79	5 (20%)
4	PSU	L5	2632	4	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
4	OMC	L5	3887	4	19,22,23	0.51	0	25,31,34	0.67	0
4	OMC	L5	2861	4	19,22,23	0.51	0	25,31,34	0.82	1 (4%)
52	PSU	S2	1174	52	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)
52	OMC	S2	1391	52	19,22,23	0.51	0	25,31,34	0.71	0
4	A2M	L5	2787	4	22,25,26	1.25	1 (4%)	30,36,39	1.52	7 (23%)
4	OMG	L5	2876	4	23,26,27	0.47	0	32,38,41	0.51	0
52	G7M	S2	1639	52,51	23,26,27	2.68	8 (34%)	34,39,42	2.61	11 (32%)
4	PSU	L5	3695	91,4	18,21,22	1.13	1 (5%)	21,30,33	1.87	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	L5	5001	4	18,21,22	1.16	1 (5%)	21,30,33	1.79	4 (19%)
52	MA6	S2	1851	52	23,26,27	1.26	2 (8%)	33,38,41	3.23	12 (36%)
4	OMC	L5	3841	4	19,22,23	0.49	0	25,31,34	0.60	0
4	UY1	L5	3818	91,4	19,22,23	4.92	10 (52%)	21,31,34	2.01	5 (23%)
52	OMG	S2	1328	52	23,26,27	0.46	0	32,38,41	0.46	0
52	OMC	S2	517	52	19,22,23	0.50	0	25,31,34	0.71	0
4	PSU	L5	4431	4	18,21,22	1.14	1 (5%)	21,30,33	1.88	4 (19%)
4	A2M	L5	3785	4,88	22,25,26	1.18	1 (4%)	30,36,39	1.63	10 (33%)
4	A2M	L5	4590	4	22,25,26	1.22	1 (4%)	30,36,39	1.53	6 (20%)
4	OMG	L5	3899	4	23,26,27	0.51	0	32,38,41	0.54	0
52	A2M	S2	668	52,88	22,25,26	1.34	2 (9%)	30,36,39	1.59	6 (20%)
4	A2M	L5	1524	4	22,25,26	1.30	2 (9%)	30,36,39	1.53	5 (16%)
4	PSU	L5	4457	4	18,21,22	1.12	1 (5%)	21,30,33	1.84	5 (23%)
52	PSU	S2	649	52	18,21,22	1.14	1 (5%)	21,30,33	1.92	5 (23%)
4	PSU	L5	4493	91,4	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
4	OMG	L5	1316	4	23,26,27	0.49	0	32,38,41	0.56	0
4	OMG	L5	4499	4	23,26,27	0.44	0	32,38,41	0.47	0
4	A2M	L5	2815	4	22,25,26	1.24	2 (9%)	30,36,39	1.41	7 (23%)
4	OMG	L5	4637	91,4	23,26,27	0.47	0	32,38,41	0.49	0
4	PSU	L5	4579	4	18,21,22	1.10	1 (5%)	21,30,33	1.90	5 (23%)
4	OMC	L5	2365	4,88	19,22,23	0.49	0	25,31,34	0.59	0
52	PSU	S2	109	52	18,21,22	1.15	1 (5%)	21,30,33	1.90	6 (28%)
4	UR3	L5	4530	4	19,22,23	2.78	7 (36%)	26,32,35	1.56	3 (11%)
4	OMU	L5	4227	4	19,22,23	3.39	7 (36%)	25,31,34	1.79	4 (16%)
52	A2M	S2	27	52	22,25,26	1.25	2 (9%)	30,36,39	1.40	4 (13%)
4	OMG	L5	4494	4	23,26,27	0.47	0	32,38,41	0.50	0
4	OMC	L5	2824	4	19,22,23	0.50	0	25,31,34	0.68	0
4	A2M	L5	3825	4	22,25,26	1.24	1 (4%)	30,36,39	1.57	7 (23%)
4	OMC	L5	4456	4	19,22,23	0.55	0	25,31,34	0.63	0
52	A2M	S2	1031	52	22,25,26	1.21	2 (9%)	30,36,39	1.46	5 (16%)
52	OMC	S2	1703	52	19,22,23	0.50	0	25,31,34	0.51	0
4	PSU	L5	1744	4,88	18,21,22	1.14	1 (5%)	21,30,33	1.91	5 (23%)
52	PSU	S2	1004	52	18,21,22	1.13	1 (5%)	21,30,33	1.91	5 (23%)
52	OMG	S2	509	52	23,26,27	0.47	0	32,38,41	0.51	0
4	A2M	L5	2401	4	22,25,26	1.25	1 (4%)	30,36,39	1.61	6 (20%)
4	OMG	L5	4623	4	23,26,27	0.48	0	32,38,41	0.61	0
6	PSU	L8	69	6	18,21,22	1.14	1 (5%)	21,30,33	1.89	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PSU	L5	2839	4	18,21,22	1.13	1 (5%)	21,30,33	1.93	5 (23%)
4	PSU	L5	3884	4	18,21,22	1.15	1 (5%)	21,30,33	1.93	5 (23%)
4	PSU	L5	4312	4	18,21,22	1.14	1 (5%)	21,30,33	1.89	4 (19%)
52	OMG	S2	436	52	23,26,27	0.47	0	32,38,41	0.54	0
52	PSU	S2	1045	52	18,21,22	1.10	1 (5%)	21,30,33	1.80	4 (19%)
52	OMC	S2	1272	52	19,22,23	0.55	0	25,31,34	0.91	2 (8%)
4	OMC	L5	2351	4	19,22,23	0.53	0	25,31,34	0.88	1 (4%)
4	OMU	L5	3925	4	19,22,23	3.38	7 (36%)	25,31,34	1.80	4 (16%)
52	6MZ	S2	1832	52,88	26,26,26	2.81	5 (19%)	36,39,39	2.47	13 (36%)
4	OMG	L5	4196	4,51	23,26,27	0.46	0	32,38,41	0.47	0
4	OMC	L5	2804	4	19,22,23	0.50	0	25,31,34	0.72	0
52	OMU	S2	121	52	19,22,23	3.33	7 (36%)	25,31,34	1.68	4 (16%)
4	A2M	L5	3830	4	22,25,26	1.25	1 (4%)	30,36,39	1.59	6 (20%)
4	PSU	L5	1781	4	18,21,22	1.09	1 (5%)	21,30,33	1.85	4 (19%)
4	PSU	L5	5010	4	18,21,22	1.13	1 (5%)	21,30,33	1.88	5 (23%)
52	PSU	S2	1232	52	18,21,22	1.15	1 (5%)	21,30,33	1.90	5 (23%)
4	PSU	L5	4471	4	18,21,22	1.10	1 (5%)	21,30,33	1.84	4 (19%)
4	OMG	L5	4618	4	23,26,27	0.48	0	32,38,41	0.53	0
52	PSU	S2	814	52	18,21,22	1.09	1 (5%)	21,30,33	1.76	4 (19%)
52	OMG	S2	867	52	23,26,27	0.51	0	32,38,41	0.48	0
52	PSU	S2	966	52,88	18,21,22	1.12	1 (5%)	21,30,33	1.85	4 (19%)
4	PSU	L5	1683	91,4	18,21,22	1.15	1 (5%)	21,30,33	1.83	4 (19%)
52	OMG	S2	1490	52	23,26,27	0.50	0	32,38,41	0.53	0
52	OMU	S2	172	52	19,22,23	3.40	7 (36%)	25,31,34	1.85	5 (20%)
4	PSU	L5	3853	91,4,88	18,21,22	1.09	1 (5%)	21,30,33	1.79	4 (19%)
4	PSU	L5	1536	4	18,21,22	1.12	1 (5%)	21,30,33	1.90	4 (19%)
4	OMU	L5	4306	4	19,22,23	3.33	7 (36%)	25,31,34	1.79	4 (16%)

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
4	PSU	L5	4673	4,88	-	0/7/25/26	0/2/2/2
52	OMU	S2	1288	52	-	2/9/27/28	0/2/2/2
4	OMG	L5	3744	4	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	S2	1367	52	-	0/7/25/26	0/2/2/2
4	OMG	L5	4370	4	-	0/9/27/28	0/3/3/3
52	PSU	S2	406	52	-	0/7/25/26	0/2/2/2
4	OMU	L5	4498	91,4	-	0/9/27/28	0/2/2/2
4	OMG	L5	3627	4	-	1/9/27/28	0/3/3/3
52	PSU	S2	93	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	105	52	-	0/7/25/26	0/2/2/2
4	PSU	L5	4361	4	-	0/7/25/26	0/2/2/2
52	OMU	S2	627	52	-	6/9/27/28	0/2/2/2
52	A2M	S2	1383	52	-	3/9/27/28	0/3/3/3
4	OMC	L5	2422	4,88	-	2/9/27/28	0/2/2/2
4	PSU	L5	4353	4	-	0/7/25/26	0/2/2/2
52	A2M	S2	576	52	-	3/9/27/28	0/3/3/3
4	A2M	L5	398	4	-	0/9/27/28	0/3/3/3
52	A2M	S2	468	52	-	1/9/27/28	0/3/3/3
4	A2M	L5	2363	4,88	-	0/9/27/28	0/3/3/3
52	A2M	S2	166	52	-	0/9/27/28	0/3/3/3
4	1MA	L5	1322	4,88	-	0/7/25/26	0/3/3/3
4	PSU	L5	4973	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	1340	4	-	1/9/27/28	0/2/2/2
52	A2M	S2	99	52,88	-	1/9/27/28	0/3/3/3
4	PSU	L5	3920	4,88	-	0/7/25/26	0/2/2/2
52	PSU	S2	801	52	-	1/7/25/26	0/2/2/2
6	PSU	L8	55	6	-	0/7/25/26	0/2/2/2
4	5MC	L5	4447	91,4	-	4/7/25/26	0/2/2/2
4	PSU	L5	4532	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	1534	4,88	-	1/9/27/28	0/3/3/3
4	OMU	L5	2837	4	-	0/9/27/28	0/2/2/2
4	OMU	L5	4620	4	-	1/9/27/28	0/2/2/2
52	OMC	S2	462	52	-	0/9/27/28	0/2/2/2
4	6MZ	L5	4220	4	-	1/12/28/28	0/3/3/3
4	A2M	L5	400	4	-	1/9/27/28	0/3/3/3
4	OMC	L5	3869	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	4628	4	-	0/7/25/26	0/2/2/2
52	B8N	S2	1248	52	-	4/16/34/35	0/2/2/2
4	OMG	L5	1625	91,4	-	2/9/27/28	0/3/3/3
4	OMG	L5	2424	4	-	1/9/27/28	0/3/3/3
52	OMG	S2	683	52	-	0/9/27/28	0/3/3/3
4	A2M	L5	3718	4	-	0/9/27/28	0/3/3/3
52	PSU	S2	866	52	-	0/7/25/26	0/2/2/2
4	PSU	L5	3844	4	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	L5	1677	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	1871	4,88	-	0/9/27/28	0/3/3/3
52	A2M	S2	159	52	-	1/9/27/28	0/3/3/3
3	SEP	CF	163	3	-	3/6/8/10	-
4	5MC	L5	3782	4,88	-	0/7/25/26	0/2/2/2
4	PSU	L5	4442	4	-	0/7/25/26	0/2/2/2
4	OMG	L5	3792	4	-	2/9/27/28	0/3/3/3
4	A2M	L5	1323	4	-	1/9/27/28	0/3/3/3
52	PSU	S2	1244	52	-	0/7/25/26	0/2/2/2
4	PSU	L5	1862	4	-	0/7/25/26	0/2/2/2
52	4AC	S2	1842	52	-	0/11/29/30	0/2/2/2
4	PSU	L5	4972	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	3822	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	3851	4	-	1/7/25/26	0/2/2/2
52	OMG	S2	601	52	-	1/9/27/28	0/3/3/3
4	OMC	L5	3808	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	1792	4	-	0/7/25/26	0/2/2/2
52	OMU	S2	1326	52	-	0/9/27/28	0/2/2/2
4	PSU	L5	3637	91,4	-	0/7/25/26	0/2/2/2
4	OMG	L5	4228	4	-	0/9/27/28	0/3/3/3
52	4AC	S2	1337	52	-	1/11/29/30	0/2/2/2
4	PSU	L5	4403	91,4	-	0/7/25/26	0/2/2/2
4	OMG	L5	2364	4,88	-	3/9/27/28	0/3/3/3
52	PSU	S2	863	52	-	2/7/25/26	0/2/2/2
4	OMG	L5	4392	4	-	0/9/27/28	0/3/3/3
4	OMC	L5	4536	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	4500	4	-	4/7/25/26	0/2/2/2
4	PSU	L5	4521	91,4,88	-	0/7/25/26	0/2/2/2
52	MA6	S2	1850	52	-	1/11/29/30	0/3/3/3
4	OMC	L5	3701	91,4	-	6/9/27/28	0/2/2/2
6	OMG	L8	75	6	-	1/9/27/28	0/3/3/3
52	PSU	S2	686	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	1177	52	-	0/7/25/26	0/2/2/2
52	PSU	S2	1056	52	-	0/7/25/26	0/2/2/2
4	PSU	L5	3639	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4689	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4299	4	-	0/7/25/26	0/2/2/2
52	OMU	S2	1442	52	-	2/9/27/28	0/2/2/2
4	OMG	L5	1522	4	-	0/9/27/28	0/3/3/3
4	PSU	L5	1782	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4576	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	OMU	S2	428	52	-	4/9/27/28	0/2/2/2
52	PSU	S2	651	52	-	0/7/25/26	0/2/2/2
4	A2M	L5	4523	4,88	-	0/9/27/28	0/3/3/3
52	OMU	S2	116	52	-	1/9/27/28	0/2/2/2
4	PSU	L5	1582	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4293	4	-	0/7/25/26	0/2/2/2
52	PSU	S2	1046	52	-	0/7/25/26	0/2/2/2
52	A2M	S2	484	52	-	0/9/27/28	0/3/3/3
4	PSU	L5	4296	4	-	1/7/25/26	0/2/2/2
4	A2M	L5	3867	4	-	3/9/27/28	0/3/3/3
52	OMC	S2	174	52	-	0/9/27/28	0/2/2/2
4	PSU	L5	4636	4	-	2/7/25/26	0/2/2/2
52	PSU	S2	1081	52	-	1/7/25/26	0/2/2/2
52	PSU	S2	681	52	-	0/7/25/26	0/2/2/2
4	PSU	L5	4552	4	-	0/7/25/26	0/2/2/2
52	OMU	S2	354	52	-	1/9/27/28	0/2/2/2
4	A2M	L5	1326	4	-	3/9/27/28	0/3/3/3
4	PSU	L5	1860	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	4571	4	-	0/9/27/28	0/3/3/3
52	OMG	S2	644	52	-	4/9/27/28	0/3/3/3
52	OMU	S2	799	52	-	0/9/27/28	0/2/2/2
4	PSU	L5	2632	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	3887	4	-	1/9/27/28	0/2/2/2
4	OMC	L5	2861	4	-	1/9/27/28	0/2/2/2
52	PSU	S2	1174	52	-	0/7/25/26	0/2/2/2
52	OMC	S2	1391	52	-	1/9/27/28	0/2/2/2
4	A2M	L5	2787	4	-	5/9/27/28	0/3/3/3
4	OMG	L5	2876	4	-	0/9/27/28	0/3/3/3
52	G7M	S2	1639	52,51	-	2/7/25/26	0/3/3/3
4	PSU	L5	3695	91,4	-	0/7/25/26	0/2/2/2
4	PSU	L5	5001	4	-	0/7/25/26	0/2/2/2
52	MA6	S2	1851	52	-	1/11/29/30	0/3/3/3
4	OMC	L5	3841	4	-	1/9/27/28	0/2/2/2
4	UY1	L5	3818	91,4	-	3/9/27/28	0/2/2/2
52	OMG	S2	1328	52	-	1/9/27/28	0/3/3/3
52	OMC	S2	517	52	-	0/9/27/28	0/2/2/2
4	PSU	L5	4431	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	3785	4,88	-	0/9/27/28	0/3/3/3
4	A2M	L5	4590	4	-	3/9/27/28	0/3/3/3
4	OMG	L5	3899	4	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	A2M	S2	668	52,88	-	4/9/27/28	0/3/3/3
4	A2M	L5	1524	4	-	2/9/27/28	0/3/3/3
4	PSU	L5	4457	4	-	0/7/25/26	0/2/2/2
52	PSU	S2	649	52	-	0/7/25/26	0/2/2/2
4	PSU	L5	4493	91,4	-	0/7/25/26	0/2/2/2
4	OMG	L5	1316	4	-	0/9/27/28	0/3/3/3
4	OMG	L5	4499	4	-	0/9/27/28	0/3/3/3
4	A2M	L5	2815	4	-	1/9/27/28	0/3/3/3
4	OMG	L5	4637	91,4	-	2/9/27/28	0/3/3/3
4	PSU	L5	4579	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	2365	4,88	-	0/9/27/28	0/2/2/2
52	PSU	S2	109	52	-	0/7/25/26	0/2/2/2
4	UR3	L5	4530	4	-	0/7/25/26	0/2/2/2
4	OMU	L5	4227	4	-	0/9/27/28	0/2/2/2
52	A2M	S2	27	52	-	1/9/27/28	0/3/3/3
4	OMG	L5	4494	4	-	0/9/27/28	0/3/3/3
4	OMC	L5	2824	4	-	1/9/27/28	0/2/2/2
4	A2M	L5	3825	4	-	0/9/27/28	0/3/3/3
4	OMC	L5	4456	4	-	0/9/27/28	0/2/2/2
52	A2M	S2	1031	52	-	0/9/27/28	0/3/3/3
52	OMC	S2	1703	52	-	2/9/27/28	0/2/2/2
4	PSU	L5	1744	4,88	-	0/7/25/26	0/2/2/2
52	PSU	S2	1004	52	-	0/7/25/26	0/2/2/2
52	OMG	S2	509	52	-	0/9/27/28	0/3/3/3
4	A2M	L5	2401	4	-	0/9/27/28	0/3/3/3
4	OMG	L5	4623	4	-	0/9/27/28	0/3/3/3
6	PSU	L8	69	6	-	0/7/25/26	0/2/2/2
4	PSU	L5	2839	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	3884	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4312	4	-	0/7/25/26	0/2/2/2
52	OMG	S2	436	52	-	0/9/27/28	0/3/3/3
52	PSU	S2	1045	52	-	0/7/25/26	0/2/2/2
52	OMC	S2	1272	52	-	4/9/27/28	0/2/2/2
4	OMC	L5	2351	4	-	3/9/27/28	0/2/2/2
4	OMU	L5	3925	4	-	0/9/27/28	0/2/2/2
52	6MZ	S2	1832	52,88	-	5/12/28/28	0/3/3/3
4	OMG	L5	4196	4,51	-	1/9/27/28	0/3/3/3
4	OMC	L5	2804	4	-	0/9/27/28	0/2/2/2
52	OMU	S2	121	52	-	0/9/27/28	0/2/2/2
4	A2M	L5	3830	4	-	0/9/27/28	0/3/3/3
4	PSU	L5	1781	4	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	L5	5010	4	-	0/7/25/26	0/2/2/2
52	PSU	S2	1232	52	-	0/7/25/26	0/2/2/2
4	PSU	L5	4471	4	-	0/7/25/26	0/2/2/2
4	OMG	L5	4618	4	-	2/9/27/28	0/3/3/3
52	PSU	S2	814	52	-	0/7/25/26	0/2/2/2
52	OMG	S2	867	52	-	3/9/27/28	0/3/3/3
52	PSU	S2	966	52,88	-	0/7/25/26	0/2/2/2
4	PSU	L5	1683	91,4	-	0/7/25/26	0/2/2/2
52	OMG	S2	1490	52	-	2/9/27/28	0/3/3/3
52	OMU	S2	172	52	-	0/9/27/28	0/2/2/2
4	PSU	L5	3853	91,4,88	-	0/7/25/26	0/2/2/2
4	PSU	L5	1536	4	-	2/7/25/26	0/2/2/2
4	OMU	L5	4306	4	-	0/9/27/28	0/2/2/2

All (275) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L5	3818	UY1	C6-C5	12.94	1.49	1.35
52	S2	1832	6MZ	C6-N6	12.64	1.48	1.34
4	L5	4220	6MZ	C6-N6	12.44	1.48	1.34
4	L5	3818	UY1	C2-N1	11.69	1.51	1.36
52	S2	799	OMU	C2-N1	8.66	1.52	1.38
4	L5	3925	OMU	C2-N1	8.44	1.51	1.38
52	S2	172	OMU	C2-N1	8.39	1.51	1.38
52	S2	1442	OMU	C2-N1	8.38	1.51	1.38
4	L5	2837	OMU	C2-N1	8.34	1.51	1.38
52	S2	627	OMU	C2-N1	8.33	1.51	1.38
4	L5	4227	OMU	C2-N1	8.32	1.51	1.38
52	S2	1326	OMU	C2-N1	8.18	1.51	1.38
52	S2	1288	OMU	C2-N1	8.14	1.51	1.38
4	L5	4306	OMU	C2-N1	8.13	1.51	1.38
52	S2	116	OMU	C2-N1	8.13	1.51	1.38
4	L5	4620	OMU	C2-N1	8.12	1.51	1.38
52	S2	354	OMU	C2-N1	8.07	1.51	1.38
52	S2	121	OMU	C2-N1	8.07	1.51	1.38
52	S2	428	OMU	C2-N1	7.98	1.51	1.38
4	L5	4498	OMU	C2-N1	7.98	1.51	1.38
52	S2	1248	B8N	C6-N1	7.94	1.55	1.36
4	L5	3818	UY1	C2-N3	7.88	1.50	1.37
52	S2	1248	B8N	C4-N3	-7.74	1.26	1.40
52	S2	1248	B8N	C4-C5	7.12	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	799	OMU	C2-N3	7.02	1.50	1.38
52	S2	1442	OMU	C2-N3	6.99	1.50	1.38
52	S2	172	OMU	C2-N3	6.98	1.50	1.38
4	L5	2837	OMU	C2-N3	6.97	1.50	1.38
52	S2	627	OMU	C2-N3	6.95	1.50	1.38
4	L5	4227	OMU	C2-N3	6.93	1.50	1.38
52	S2	1288	OMU	C2-N3	6.91	1.50	1.38
52	S2	1326	OMU	C2-N3	6.90	1.50	1.38
52	S2	116	OMU	C2-N3	6.89	1.50	1.38
4	L5	3925	OMU	C2-N3	6.86	1.49	1.38
52	S2	121	OMU	C2-N3	6.85	1.49	1.38
4	L5	4620	OMU	C2-N3	6.83	1.49	1.38
52	S2	428	OMU	C2-N3	6.83	1.49	1.38
52	S2	354	OMU	C2-N3	6.80	1.49	1.38
4	L5	4498	OMU	C2-N3	6.74	1.49	1.38
4	L5	4306	OMU	C2-N3	6.69	1.49	1.38
52	S2	1639	G7M	C4-N3	6.68	1.49	1.34
4	L5	4530	UR3	C2-N1	6.59	1.47	1.38
4	L5	4530	UR3	C6-C5	6.27	1.49	1.35
52	S2	172	OMU	C6-C5	5.94	1.48	1.35
52	S2	1248	B8N	C2-N1	5.94	1.56	1.39
4	L5	4227	OMU	C6-C5	5.92	1.48	1.35
52	S2	799	OMU	C6-C5	5.92	1.48	1.35
52	S2	627	OMU	C6-C5	5.91	1.48	1.35
4	L5	4530	UR3	C2-N3	5.91	1.50	1.39
4	L5	2837	OMU	C6-C5	5.87	1.48	1.35
52	S2	1326	OMU	C6-C5	5.87	1.48	1.35
52	S2	121	OMU	C6-C5	5.86	1.48	1.35
4	L5	3925	OMU	C6-C5	5.86	1.48	1.35
52	S2	1288	OMU	C6-C5	5.84	1.48	1.35
52	S2	428	OMU	C6-C5	5.83	1.48	1.35
4	L5	4498	OMU	C6-C5	5.82	1.48	1.35
4	L5	4620	OMU	C6-C5	5.82	1.48	1.35
52	S2	354	OMU	C6-C5	5.81	1.48	1.35
52	S2	1442	OMU	C6-C5	5.81	1.48	1.35
4	L5	4306	OMU	C6-C5	5.79	1.48	1.35
52	S2	116	OMU	C6-C5	5.71	1.48	1.35
4	L5	4620	OMU	O4-C4	-5.53	1.13	1.24
52	S2	1639	G7M	C2-N3	5.51	1.46	1.33
4	L5	4306	OMU	O4-C4	-5.46	1.13	1.24
52	S2	121	OMU	O4-C4	-5.45	1.13	1.24
52	S2	428	OMU	O4-C4	-5.45	1.13	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	1248	B8N	C6-C5	5.45	1.42	1.35
52	S2	354	OMU	O4-C4	-5.44	1.13	1.24
52	S2	799	OMU	O4-C4	-5.43	1.13	1.24
4	L5	2837	OMU	O4-C4	-5.42	1.13	1.24
52	S2	172	OMU	O4-C4	-5.42	1.13	1.24
4	L5	4498	OMU	O4-C4	-5.40	1.14	1.24
52	S2	1326	OMU	O4-C4	-5.40	1.14	1.24
52	S2	627	OMU	O4-C4	-5.40	1.14	1.24
4	L5	4227	OMU	O4-C4	-5.40	1.14	1.24
52	S2	1442	OMU	O4-C4	-5.39	1.14	1.24
4	L5	3925	OMU	O4-C4	-5.39	1.14	1.24
4	L5	3818	UY1	C6-N1	5.38	1.45	1.36
52	S2	116	OMU	O4-C4	-5.38	1.14	1.24
52	S2	1288	OMU	O4-C4	-5.33	1.14	1.24
52	S2	1639	G7M	C2-N2	4.95	1.45	1.34
52	S2	1639	G7M	C5-N7	-4.76	1.33	1.39
52	S2	627	OMU	C4-N3	4.57	1.46	1.38
52	S2	1442	OMU	C4-N3	4.52	1.46	1.38
52	S2	172	OMU	C4-N3	4.49	1.46	1.38
4	L5	3818	UY1	C4-N3	4.47	1.47	1.38
52	S2	354	OMU	C4-N3	4.44	1.46	1.38
52	S2	1326	OMU	C4-N3	4.44	1.46	1.38
52	S2	428	OMU	C4-N3	4.44	1.46	1.38
52	S2	116	OMU	C4-N3	4.43	1.46	1.38
4	L5	4498	OMU	C4-N3	4.41	1.46	1.38
52	S2	799	OMU	C4-N3	4.40	1.46	1.38
4	L5	4227	OMU	C4-N3	4.39	1.46	1.38
4	L5	4306	OMU	C4-N3	4.38	1.46	1.38
52	S2	1288	OMU	C4-N3	4.37	1.46	1.38
4	L5	2837	OMU	C4-N3	4.34	1.46	1.38
4	L5	3925	OMU	C4-N3	4.31	1.46	1.38
4	L5	4620	OMU	C4-N3	4.30	1.46	1.38
52	S2	121	OMU	C4-N3	4.28	1.45	1.38
4	L5	3844	PSU	C6-C5	3.98	1.39	1.35
6	L8	55	PSU	C6-C5	3.95	1.39	1.35
4	L5	5001	PSU	C6-C5	3.89	1.39	1.35
52	S2	1081	PSU	C6-C5	3.88	1.39	1.35
52	S2	1639	G7M	C5-C6	3.87	1.54	1.43
4	L5	1683	PSU	C6-C5	3.87	1.39	1.35
4	L5	4972	PSU	C6-C5	3.86	1.39	1.35
4	L5	4500	PSU	C6-C5	3.83	1.39	1.35
4	L5	4293	PSU	C6-C5	3.82	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	105	PSU	C6-C5	3.82	1.39	1.35
52	S2	966	PSU	C6-C5	3.82	1.39	1.35
4	L5	2632	PSU	C6-C5	3.80	1.39	1.35
52	S2	109	PSU	C6-C5	3.80	1.39	1.35
4	L5	3637	PSU	C6-C5	3.80	1.39	1.35
4	L5	4312	PSU	C6-C5	3.80	1.39	1.35
52	S2	1232	PSU	C6-C5	3.79	1.39	1.35
4	L5	3695	PSU	C6-C5	3.79	1.39	1.35
4	L5	4431	PSU	C6-C5	3.79	1.39	1.35
4	L5	1860	PSU	C6-C5	3.78	1.39	1.35
52	S2	93	PSU	C6-C5	3.78	1.39	1.35
52	S2	801	PSU	C6-C5	3.78	1.39	1.35
4	L5	1744	PSU	C6-C5	3.77	1.39	1.35
4	L5	4296	PSU	C6-C5	3.77	1.39	1.35
52	S2	863	PSU	C6-C5	3.76	1.39	1.35
4	L5	1536	PSU	C6-C5	3.75	1.39	1.35
4	L5	1782	PSU	C6-C5	3.75	1.39	1.35
52	S2	1004	PSU	C6-C5	3.75	1.39	1.35
4	L5	4521	PSU	C6-C5	3.74	1.39	1.35
52	S2	866	PSU	C6-C5	3.74	1.39	1.35
52	S2	1056	PSU	C6-C5	3.74	1.39	1.35
4	L5	3884	PSU	C6-C5	3.74	1.39	1.35
52	S2	406	PSU	C6-C5	3.74	1.39	1.35
52	S2	651	PSU	C6-C5	3.74	1.39	1.35
4	L5	5010	PSU	C6-C5	3.74	1.39	1.35
52	S2	1244	PSU	C6-C5	3.74	1.39	1.35
4	L5	1582	PSU	C6-C5	3.73	1.39	1.35
52	S2	686	PSU	C6-C5	3.73	1.39	1.35
4	L5	1792	PSU	C6-C5	3.73	1.39	1.35
4	L5	4532	PSU	C6-C5	3.73	1.39	1.35
4	L5	4576	PSU	C6-C5	3.73	1.39	1.35
52	S2	814	PSU	C6-C5	3.73	1.39	1.35
4	L5	4403	PSU	C6-C5	3.73	1.39	1.35
4	L5	4552	PSU	C6-C5	3.73	1.39	1.35
52	S2	649	PSU	C6-C5	3.73	1.39	1.35
52	S2	1046	PSU	C6-C5	3.72	1.39	1.35
52	S2	1045	PSU	C6-C5	3.72	1.39	1.35
52	S2	1177	PSU	C6-C5	3.72	1.39	1.35
52	S2	1367	PSU	C6-C5	3.72	1.39	1.35
52	S2	1174	PSU	C6-C5	3.72	1.39	1.35
4	L5	3851	PSU	C6-C5	3.71	1.39	1.35
4	L5	3853	PSU	C6-C5	3.70	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L5	3639	PSU	C6-C5	3.70	1.39	1.35
4	L5	4689	PSU	C6-C5	3.70	1.39	1.35
52	S2	681	PSU	C6-C5	3.70	1.39	1.35
4	L5	4299	PSU	C6-C5	3.69	1.39	1.35
4	L5	4353	PSU	C6-C5	3.69	1.39	1.35
4	L5	2839	PSU	C6-C5	3.69	1.39	1.35
4	L5	4493	PSU	C6-C5	3.68	1.39	1.35
4	L5	3822	PSU	C6-C5	3.68	1.39	1.35
4	L5	4579	PSU	C6-C5	3.67	1.39	1.35
4	L5	1862	PSU	C6-C5	3.67	1.39	1.35
4	L5	4471	PSU	C6-C5	3.67	1.39	1.35
4	L5	1781	PSU	C6-C5	3.67	1.39	1.35
4	L5	4457	PSU	C6-C5	3.67	1.39	1.35
6	L8	69	PSU	C6-C5	3.67	1.39	1.35
4	L5	4442	PSU	C6-C5	3.64	1.39	1.35
4	L5	4673	PSU	C6-C5	3.64	1.39	1.35
4	L5	3920	PSU	C6-C5	3.64	1.39	1.35
4	L5	4973	PSU	C6-C5	3.61	1.39	1.35
52	S2	1248	B8N	C1'-C5	3.60	1.58	1.50
4	L5	4361	PSU	C6-C5	3.58	1.39	1.35
4	L5	4636	PSU	C6-C5	3.57	1.39	1.35
4	L5	4628	PSU	C6-C5	3.57	1.39	1.35
3	CF	163	SEP	P-O1P	3.55	1.61	1.50
4	L5	3818	UY1	O4-C4	-3.53	1.16	1.23
4	L5	1677	PSU	C6-C5	3.47	1.39	1.35
4	L5	2401	A2M	O5'-C5'	-3.46	1.34	1.44
52	S2	99	A2M	O5'-C5'	-3.44	1.34	1.44
52	S2	576	A2M	O5'-C5'	-3.40	1.34	1.44
52	S2	668	A2M	O5'-C5'	-3.38	1.34	1.44
4	L5	2815	A2M	O5'-C5'	-3.32	1.34	1.44
4	L5	3785	A2M	O5'-C5'	-3.32	1.34	1.44
4	L5	2787	A2M	O5'-C5'	-3.32	1.34	1.44
4	L5	1323	A2M	O5'-C5'	-3.31	1.34	1.44
4	L5	1524	A2M	O5'-C5'	-3.31	1.34	1.44
4	L5	3830	A2M	O5'-C5'	-3.31	1.34	1.44
4	L5	400	A2M	O5'-C5'	-3.31	1.34	1.44
4	L5	3825	A2M	O5'-C5'	-3.30	1.34	1.44
52	S2	166	A2M	O5'-C5'	-3.30	1.34	1.44
4	L5	3867	A2M	O5'-C5'	-3.28	1.34	1.44
4	L5	1871	A2M	O5'-C5'	-3.28	1.34	1.44
4	L5	3718	A2M	O5'-C5'	-3.28	1.34	1.44
52	S2	1383	A2M	O5'-C5'	-3.27	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L5	4571	A2M	O5'-C5'	-3.27	1.34	1.44
4	L5	3818	UY1	O2-C2	-3.27	1.16	1.23
52	S2	1031	A2M	O5'-C5'	-3.26	1.34	1.44
4	L5	3818	UY1	C1'-C5	3.25	1.57	1.50
52	S2	27	A2M	O5'-C5'	-3.25	1.34	1.44
4	L5	398	A2M	O5'-C5'	-3.23	1.34	1.44
52	S2	484	A2M	O5'-C5'	-3.23	1.34	1.44
52	S2	468	A2M	O5'-C5'	-3.22	1.34	1.44
4	L5	4523	A2M	O5'-C5'	-3.19	1.34	1.44
4	L5	2363	A2M	O5'-C5'	-3.18	1.34	1.44
52	S2	159	A2M	O5'-C5'	-3.15	1.35	1.44
4	L5	4590	A2M	O5'-C5'	-3.14	1.35	1.44
52	S2	1851	MA6	C6-N6	3.12	1.45	1.36
4	L5	1326	A2M	O5'-C5'	-3.11	1.35	1.44
52	S2	1850	MA6	C6-N6	3.09	1.45	1.36
4	L5	4220	6MZ	C5-N7	-3.06	1.33	1.39
4	L5	1534	A2M	O5'-C5'	-3.04	1.35	1.44
4	L5	4220	6MZ	C5-C4	-3.03	1.33	1.39
52	S2	1832	6MZ	C5-N7	-2.97	1.33	1.39
52	S2	1832	6MZ	C5-C4	-2.96	1.33	1.39
4	L5	4498	OMU	C5-C4	2.91	1.50	1.43
4	L5	3925	OMU	C5-C4	2.90	1.50	1.43
52	S2	1639	G7M	C2-N1	2.89	1.44	1.37
4	L5	2837	OMU	C5-C4	2.88	1.50	1.43
4	L5	4227	OMU	C5-C4	2.87	1.49	1.43
52	S2	799	OMU	C5-C4	2.87	1.49	1.43
52	S2	428	OMU	C5-C4	2.87	1.49	1.43
52	S2	172	OMU	C5-C4	2.84	1.49	1.43
52	S2	1326	OMU	C5-C4	2.83	1.49	1.43
52	S2	1442	OMU	C5-C4	2.83	1.49	1.43
52	S2	627	OMU	C5-C4	2.83	1.49	1.43
4	L5	4306	OMU	C5-C4	2.82	1.49	1.43
52	S2	1288	OMU	C5-C4	2.80	1.49	1.43
52	S2	354	OMU	C5-C4	2.80	1.49	1.43
4	L5	4620	OMU	C5-C4	2.79	1.49	1.43
4	L5	2837	OMU	C6-N1	2.79	1.44	1.38
4	L5	4620	OMU	C6-N1	2.76	1.44	1.38
52	S2	121	OMU	C5-C4	2.75	1.49	1.43
4	L5	4306	OMU	C6-N1	2.73	1.44	1.38
4	L5	4498	OMU	C6-N1	2.73	1.44	1.38
52	S2	799	OMU	C6-N1	2.73	1.44	1.38
52	S2	354	OMU	C6-N1	2.73	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	S2	116	OMU	C5-C4	2.71	1.49	1.43
52	S2	121	OMU	C6-N1	2.71	1.44	1.38
4	L5	3925	OMU	C6-N1	2.71	1.44	1.38
52	S2	1442	OMU	C6-N1	2.71	1.44	1.38
4	L5	4530	UR3	C6-N1	2.70	1.44	1.38
4	L5	4227	OMU	C6-N1	2.69	1.44	1.38
4	L5	1677	PSU	O4'-C1'	-2.68	1.40	1.43
52	S2	1326	OMU	C6-N1	2.68	1.44	1.38
52	S2	428	OMU	C6-N1	2.67	1.44	1.38
52	S2	627	OMU	C6-N1	2.67	1.44	1.38
52	S2	1288	OMU	C6-N1	2.66	1.44	1.38
52	S2	172	OMU	C6-N1	2.62	1.44	1.38
52	S2	1832	6MZ	C8-N9	-2.59	1.33	1.37
4	L5	4220	6MZ	C8-N9	-2.58	1.33	1.37
52	S2	116	OMU	C6-N1	2.57	1.44	1.38
4	L5	4530	UR3	O2-C2	-2.56	1.17	1.22
52	S2	1639	G7M	C6-N1	2.50	1.43	1.38
52	S2	1639	G7M	O6-C6	-2.45	1.18	1.23
52	S2	1851	MA6	C5-C4	-2.44	1.34	1.39
52	S2	668	A2M	O4'-C4'	-2.44	1.39	1.45
52	S2	1850	MA6	C5-C4	-2.34	1.34	1.39
4	L5	4530	UR3	C5-C4	2.32	1.49	1.43
4	L5	4530	UR3	C3U-N3	2.24	1.51	1.47
4	L5	1326	A2M	C5-C4	2.19	1.43	1.39
4	L5	3818	UY1	C4-C5	2.18	1.50	1.44
4	L5	2815	A2M	C5-C4	2.16	1.42	1.39
52	S2	166	A2M	C5-C4	2.16	1.42	1.39
4	L5	3818	UY1	O4'-C1'	-2.14	1.40	1.43
4	L5	3718	A2M	C5-C4	2.13	1.42	1.39
52	S2	484	A2M	C5-C4	2.12	1.42	1.39
4	L5	1524	A2M	O4'-C4'	-2.10	1.40	1.45
52	S2	99	A2M	C5-C4	2.09	1.42	1.39
4	L5	1323	A2M	C5-C4	2.08	1.42	1.39
4	L5	4220	6MZ	C6-N1	-2.07	1.31	1.35
52	S2	1832	6MZ	C6-N1	-2.06	1.31	1.35
52	S2	27	A2M	C5-C4	2.04	1.42	1.39
4	L5	4571	A2M	C5-C4	2.04	1.42	1.39
4	L5	398	A2M	C5-C4	2.04	1.42	1.39
52	S2	1031	A2M	C5-C4	2.04	1.42	1.39
52	S2	576	A2M	C5-C4	2.03	1.42	1.39
4	L5	1534	A2M	C5-C4	2.03	1.42	1.39

All (671) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	1851	MA6	N1-C6-N6	-11.20	103.22	116.86
52	S2	1850	MA6	N1-C6-N6	-10.69	103.83	116.86
52	S2	1832	6MZ	OP3-P-O5'	7.78	126.94	106.67
52	S2	1639	G7M	C1'-N9-C4	7.71	149.28	126.49
52	S2	1639	G7M	C1'-N9-C8	-7.66	100.89	126.74
52	S2	1851	MA6	C5-C6-N6	7.23	136.78	125.33
52	S2	1850	MA6	C5-C6-N6	7.00	136.41	125.33
4	L5	4220	6MZ	OP3-P-OP1	-5.88	87.91	110.83
4	L5	4220	6MZ	OP3-P-O5'	-5.80	91.55	106.67
4	L5	4220	6MZ	N1-C2-N3	-5.74	119.90	128.58
52	S2	172	OMU	C4-N3-C2	-5.73	119.50	126.61
52	S2	1326	OMU	C4-N3-C2	-5.69	119.54	126.61
4	L5	2837	OMU	C4-N3-C2	-5.63	119.62	126.61
4	L5	3925	OMU	C4-N3-C2	-5.62	119.63	126.61
4	L5	4227	OMU	C4-N3-C2	-5.61	119.65	126.61
52	S2	627	OMU	C4-N3-C2	-5.59	119.67	126.61
52	S2	1832	6MZ	N1-C2-N3	-5.58	120.13	128.58
4	L5	4306	OMU	C4-N3-C2	-5.58	119.69	126.61
52	S2	428	OMU	C4-N3-C2	-5.58	119.69	126.61
52	S2	354	OMU	C4-N3-C2	-5.57	119.69	126.61
4	L5	4498	OMU	C4-N3-C2	-5.51	119.77	126.61
52	S2	1442	OMU	C4-N3-C2	-5.51	119.78	126.61
52	S2	1288	OMU	C4-N3-C2	-5.45	119.85	126.61
52	S2	1851	MA6	N1-C2-N3	-5.43	120.36	128.58
52	S2	799	OMU	C4-N3-C2	-5.42	119.88	126.61
52	S2	1850	MA6	N1-C2-N3	-5.38	120.44	128.58
4	L5	4530	UR3	C4-N3-C2	-5.36	120.27	124.58
52	S2	1851	MA6	N9-C8-N7	-5.32	106.39	113.94
52	S2	1248	B8N	C5-C4-N3	5.19	125.57	116.15
52	S2	1850	MA6	N9-C8-N7	-5.15	106.63	113.94
4	L5	4689	PSU	N1-C2-N3	5.09	120.53	115.17
4	L5	4220	6MZ	OP3-P-OP2	-4.98	89.14	107.80
4	L5	4220	6MZ	OP2-P-OP1	4.97	130.20	110.83
52	S2	116	OMU	C4-N3-C2	-4.96	120.45	126.61
4	L5	3637	PSU	N1-C2-N3	4.94	120.38	115.17
52	S2	121	OMU	C4-N3-C2	-4.93	120.50	126.61
4	L5	4636	PSU	N1-C2-N3	4.91	120.34	115.17
4	L5	4636	PSU	C4-N3-C2	-4.90	119.62	126.37
4	L5	4620	OMU	C4-N3-C2	-4.90	120.53	126.61
4	L5	4293	PSU	N1-C2-N3	4.88	120.32	115.17
4	L5	3639	PSU	N1-C2-N3	4.86	120.30	115.17
4	L5	2839	PSU	N1-C2-N3	4.86	120.29	115.17
4	L5	1677	PSU	C4-N3-C2	-4.84	119.70	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L5	3920	PSU	N1-C2-N3	4.84	120.27	115.17
4	L5	1536	PSU	N1-C2-N3	4.83	120.27	115.17
52	S2	406	PSU	N1-C2-N3	4.83	120.26	115.17
4	L5	4689	PSU	C4-N3-C2	-4.82	119.73	126.37
4	L5	4493	PSU	N1-C2-N3	4.81	120.24	115.17
52	S2	1056	PSU	N1-C2-N3	4.81	120.24	115.17
4	L5	4293	PSU	C4-N3-C2	-4.80	119.75	126.37
4	L5	3818	UY1	C4-N3-C2	-4.80	119.76	126.37
4	L5	4353	PSU	C4-N3-C2	-4.80	119.76	126.37
4	L5	4403	PSU	N1-C2-N3	4.79	120.22	115.17
4	L5	3884	PSU	N1-C2-N3	4.79	120.22	115.17
4	L5	4442	PSU	N1-C2-N3	4.79	120.22	115.17
4	L5	4973	PSU	N1-C2-N3	4.79	120.22	115.17
52	S2	649	PSU	C4-N3-C2	-4.79	119.78	126.37
4	L5	1744	PSU	N1-C2-N3	4.79	120.22	115.17
52	S2	1177	PSU	C4-N3-C2	-4.78	119.78	126.37
4	L5	4296	PSU	C4-N3-C2	-4.78	119.78	126.37
4	L5	3884	PSU	C4-N3-C2	-4.78	119.79	126.37
52	S2	406	PSU	C4-N3-C2	-4.78	119.79	126.37
4	L5	4552	PSU	N1-C2-N3	4.77	120.20	115.17
4	L5	4353	PSU	N1-C2-N3	4.77	120.20	115.17
4	L5	4972	PSU	N1-C2-N3	4.77	120.20	115.17
52	S2	866	PSU	C4-N3-C2	-4.77	119.80	126.37
4	L5	3844	PSU	N1-C2-N3	4.77	120.20	115.17
52	S2	1004	PSU	N1-C2-N3	4.77	120.20	115.17
4	L5	2839	PSU	C4-N3-C2	-4.77	119.81	126.37
52	S2	651	PSU	N1-C2-N3	4.76	120.19	115.17
4	L5	1781	PSU	N1-C2-N3	4.76	120.19	115.17
52	S2	1177	PSU	N1-C2-N3	4.76	120.19	115.17
4	L5	4973	PSU	C4-N3-C2	-4.76	119.81	126.37
52	S2	866	PSU	N1-C2-N3	4.76	120.19	115.17
4	L5	4576	PSU	N1-C2-N3	4.76	120.19	115.17
52	S2	649	PSU	N1-C2-N3	4.76	120.18	115.17
52	S2	1004	PSU	C4-N3-C2	-4.75	119.82	126.37
4	L5	4312	PSU	N1-C2-N3	4.75	120.18	115.17
4	L5	4532	PSU	N1-C2-N3	4.75	120.18	115.17
4	L5	4579	PSU	N1-C2-N3	4.75	120.18	115.17
4	L5	4296	PSU	N1-C2-N3	4.75	120.18	115.17
4	L5	4673	PSU	N1-C2-N3	4.75	120.18	115.17
4	L5	2632	PSU	N1-C2-N3	4.74	120.17	115.17
4	L5	4521	PSU	N1-C2-N3	4.74	120.17	115.17
4	L5	3851	PSU	N1-C2-N3	4.74	120.16	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L5	3639	PSU	C4-N3-C2	-4.74	119.85	126.37
52	S2	1232	PSU	N1-C2-N3	4.73	120.16	115.17
52	S2	651	PSU	C4-N3-C2	-4.73	119.85	126.37
4	L5	4628	PSU	N1-C2-N3	4.73	120.16	115.17
4	L5	4431	PSU	N1-C2-N3	4.73	120.15	115.17
52	S2	681	PSU	N1-C2-N3	4.73	120.15	115.17
4	L5	4403	PSU	C4-N3-C2	-4.73	119.86	126.37
4	L5	4552	PSU	C4-N3-C2	-4.72	119.87	126.37
4	L5	1862	PSU	N1-C2-N3	4.72	120.14	115.17
4	L5	1792	PSU	N1-C2-N3	4.71	120.14	115.17
4	L5	4220	6MZ	N9-C8-N7	-4.71	107.25	113.94
52	S2	801	PSU	N1-C2-N3	4.71	120.14	115.17
4	L5	3920	PSU	C4-N3-C2	-4.71	119.88	126.37
4	L5	1677	PSU	N1-C2-N3	4.71	120.13	115.17
4	L5	4521	PSU	C4-N3-C2	-4.71	119.89	126.37
4	L5	4493	PSU	C4-N3-C2	-4.71	119.89	126.37
4	L5	4972	PSU	C4-N3-C2	-4.71	119.89	126.37
52	S2	966	PSU	N1-C2-N3	4.70	120.13	115.17
52	S2	109	PSU	C4-N3-C2	-4.70	119.89	126.37
52	S2	1056	PSU	C4-N3-C2	-4.70	119.90	126.37
4	L5	4299	PSU	N1-C2-N3	4.70	120.12	115.17
4	L5	4442	PSU	C4-N3-C2	-4.70	119.90	126.37
4	L5	4361	PSU	N1-C2-N3	4.70	120.12	115.17
4	L5	4471	PSU	N1-C2-N3	4.69	120.12	115.17
52	S2	109	PSU	N1-C2-N3	4.69	120.12	115.17
4	L5	4500	PSU	N1-C2-N3	4.69	120.12	115.17
4	L5	4431	PSU	C4-N3-C2	-4.69	119.91	126.37
4	L5	1744	PSU	C4-N3-C2	-4.69	119.91	126.37
4	L5	4361	PSU	C4-N3-C2	-4.69	119.91	126.37
4	L5	4312	PSU	C4-N3-C2	-4.69	119.91	126.37
4	L5	3695	PSU	C4-N3-C2	-4.69	119.91	126.37
4	L5	3637	PSU	C4-N3-C2	-4.68	119.92	126.37
52	S2	1232	PSU	C4-N3-C2	-4.68	119.92	126.37
4	L5	3851	PSU	C4-N3-C2	-4.68	119.93	126.37
4	L5	1792	PSU	C4-N3-C2	-4.68	119.93	126.37
52	S2	1832	6MZ	N9-C8-N7	-4.68	107.30	113.94
4	L5	1782	PSU	C4-N3-C2	-4.68	119.93	126.37
4	L5	4576	PSU	C4-N3-C2	-4.67	119.93	126.37
4	L5	4532	PSU	C4-N3-C2	-4.67	119.93	126.37
52	S2	1174	PSU	C4-N3-C2	-4.67	119.94	126.37
4	L5	1782	PSU	N1-C2-N3	4.67	120.09	115.17
4	L5	5010	PSU	N1-C2-N3	4.67	120.09	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L5	5010	PSU	C4-N3-C2	-4.66	119.95	126.37
4	L5	3822	PSU	N1-C2-N3	4.66	120.09	115.17
4	L5	1683	PSU	N1-C2-N3	4.66	120.08	115.17
4	L5	4579	PSU	C4-N3-C2	-4.66	119.95	126.37
52	S2	1367	PSU	C4-N3-C2	-4.66	119.95	126.37
4	L5	3695	PSU	N1-C2-N3	4.65	120.08	115.17
52	S2	1367	PSU	N1-C2-N3	4.65	120.08	115.17
4	L5	1862	PSU	C4-N3-C2	-4.65	119.96	126.37
52	S2	1244	PSU	N1-C2-N3	4.65	120.07	115.17
52	S2	966	PSU	C4-N3-C2	-4.65	119.97	126.37
52	S2	1174	PSU	N1-C2-N3	4.65	120.07	115.17
6	L8	55	PSU	N1-C2-N3	4.65	120.07	115.17
52	S2	93	PSU	N1-C2-N3	4.65	120.07	115.17
6	L8	55	PSU	C4-N3-C2	-4.64	119.97	126.37
4	L5	4673	PSU	C4-N3-C2	-4.64	119.97	126.37
4	L5	1536	PSU	C4-N3-C2	-4.64	119.98	126.37
52	S2	801	PSU	C4-N3-C2	-4.63	119.99	126.37
4	L5	4457	PSU	C4-N3-C2	-4.63	119.99	126.37
52	S2	863	PSU	N1-C2-N3	4.63	120.05	115.17
52	S2	681	PSU	C4-N3-C2	-4.62	120.00	126.37
4	L5	4299	PSU	C4-N3-C2	-4.62	120.01	126.37
52	S2	93	PSU	C4-N3-C2	-4.62	120.01	126.37
52	S2	1851	MA6	C5-C4-N3	-4.62	120.36	126.72
6	L8	69	PSU	C4-N3-C2	-4.62	120.01	126.37
52	S2	1244	PSU	C4-N3-C2	-4.61	120.02	126.37
6	L8	69	PSU	N1-C2-N3	4.61	120.03	115.17
4	L5	1860	PSU	C4-N3-C2	-4.61	120.03	126.37
52	S2	686	PSU	C4-N3-C2	-4.61	120.03	126.37
4	L5	1860	PSU	N1-C2-N3	4.60	120.02	115.17
4	L5	3701	OMC	C1'-N1-C2	4.59	128.59	118.44
4	L5	1582	PSU	N1-C2-N3	4.59	120.01	115.17
4	L5	3853	PSU	N1-C2-N3	4.59	120.01	115.17
52	S2	686	PSU	N1-C2-N3	4.59	120.01	115.17
4	L5	3844	PSU	C4-N3-C2	-4.59	120.05	126.37
4	L5	2632	PSU	C4-N3-C2	-4.59	120.05	126.37
52	S2	1045	PSU	C4-N3-C2	-4.57	120.07	126.37
4	L5	4628	PSU	C4-N3-C2	-4.56	120.08	126.37
4	L5	3822	PSU	C4-N3-C2	-4.55	120.11	126.37
4	L5	1781	PSU	C4-N3-C2	-4.54	120.11	126.37
4	L5	4471	PSU	C4-N3-C2	-4.54	120.12	126.37
4	L5	1683	PSU	C4-N3-C2	-4.53	120.12	126.37
52	S2	1045	PSU	N1-C2-N3	4.53	119.95	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L5	4457	PSU	N1-C2-N3	4.52	119.94	115.17
4	L5	5001	PSU	C4-N3-C2	-4.51	120.15	126.37
52	S2	105	PSU	N1-C2-N3	4.51	119.93	115.17
52	S2	1850	MA6	C5-C4-N3	-4.51	120.51	126.72
52	S2	814	PSU	N1-C2-N3	4.50	119.92	115.17
52	S2	1046	PSU	C4-N3-C2	-4.50	120.17	126.37
52	S2	1248	B8N	C4-N3-C2	-4.50	120.08	125.62
52	S2	863	PSU	C4-N3-C2	-4.49	120.18	126.37
4	L5	5001	PSU	N1-C2-N3	4.47	119.89	115.17
4	L5	3818	UY1	N1-C2-N3	4.47	119.88	115.17
52	S2	105	PSU	C4-N3-C2	-4.47	120.22	126.37
4	L5	4500	PSU	C4-N3-C2	-4.46	120.23	126.37
52	S2	1046	PSU	N1-C2-N3	4.45	119.86	115.17
52	S2	1639	G7M	C2-N3-C4	4.43	119.94	112.30
52	S2	1832	6MZ	C5-C4-N3	-4.41	120.64	126.72
4	L5	3853	PSU	C4-N3-C2	-4.40	120.31	126.37
4	L5	4220	6MZ	C5-C4-N3	-4.38	120.69	126.72
52	S2	1081	PSU	N1-C2-N3	4.37	119.78	115.17
52	S2	1081	PSU	C4-N3-C2	-4.36	120.36	126.37
4	L5	1582	PSU	C4-N3-C2	-4.36	120.37	126.37
52	S2	814	PSU	C4-N3-C2	-4.34	120.39	126.37
4	L5	3830	A2M	C3'-C2'-C1'	-4.30	94.57	102.81
52	S2	1851	MA6	C4-N9-C8	4.02	109.96	105.74
52	S2	1639	G7M	C5-C4-N3	-4.01	120.56	128.15
4	L5	4220	6MZ	C9-N6-C6	-3.98	119.16	122.85
52	S2	1850	MA6	C4-N9-C8	3.95	109.89	105.74
4	L5	4220	6MZ	O5'-P-OP1	3.94	117.09	106.44
52	S2	1639	G7M	C5-C6-N1	3.93	119.97	111.84
52	S2	1832	6MZ	OP3-P-OP1	-3.90	95.63	110.83
52	S2	1850	MA6	C4-C5-C6	3.89	119.94	115.91
52	S2	1383	A2M	C3'-C2'-C1'	-3.88	95.38	102.81
52	S2	1248	B8N	C1'-C5-C4	3.85	123.45	117.61
4	L5	2837	OMU	N3-C2-N1	3.82	119.87	114.89
4	L5	398	A2M	C3'-C2'-C1'	-3.82	95.49	102.81
52	S2	172	OMU	N3-C2-N1	3.80	119.84	114.89
4	L5	4227	OMU	N3-C2-N1	3.79	119.82	114.89
4	L5	4523	A2M	C3'-C2'-C1'	-3.78	95.57	102.81
52	S2	1326	OMU	N3-C2-N1	3.78	119.81	114.89
4	L5	4306	OMU	C5-C4-N3	3.77	120.09	114.80
4	L5	3925	OMU	N3-C2-N1	3.77	119.80	114.89
4	L5	3701	OMC	C1'-N1-C6	-3.77	112.73	120.78
52	S2	799	OMU	N3-C2-N1	3.75	119.77	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L5	4498	OMU	N3-C2-N1	3.73	119.74	114.89
52	S2	121	OMU	N3-C2-N1	3.72	119.73	114.89
52	S2	354	OMU	N3-C2-N1	3.72	119.73	114.89
52	S2	354	OMU	C5-C4-N3	3.71	120.00	114.80
52	S2	627	OMU	C5-C4-N3	3.71	120.00	114.80
52	S2	1326	OMU	C5-C4-N3	3.69	119.97	114.80
4	L5	3925	OMU	C5-C4-N3	3.69	119.96	114.80
52	S2	428	OMU	C5-C4-N3	3.68	119.95	114.80
4	L5	4306	OMU	N3-C2-N1	3.67	119.67	114.89
52	S2	1851	MA6	C4-C5-C6	3.66	119.69	115.91
4	L5	1871	A2M	C3'-C2'-C1'	-3.66	95.80	102.81
52	S2	1288	OMU	N3-C2-N1	3.66	119.65	114.89
52	S2	172	OMU	C5-C4-N3	3.65	119.92	114.80
4	L5	4227	OMU	C5-C4-N3	3.65	119.91	114.80
4	L5	4498	OMU	C5-C4-N3	3.65	119.91	114.80
52	S2	1442	OMU	N3-C2-N1	3.65	119.64	114.89
4	L5	4530	UR3	C5-C4-N3	3.64	119.84	115.04
52	S2	1442	OMU	C5-C4-N3	3.64	119.89	114.80
4	L5	2837	OMU	C5-C4-N3	3.63	119.89	114.80
52	S2	428	OMU	N3-C2-N1	3.59	119.57	114.89
52	S2	799	OMU	C5-C4-N3	3.59	119.83	114.80
4	L5	2401	A2M	O3'-C3'-C2'	3.58	121.21	111.19
4	L5	398	A2M	O3'-C3'-C2'	3.57	121.19	111.19
52	S2	627	OMU	N3-C2-N1	3.57	119.54	114.89
52	S2	468	A2M	C3'-C2'-C1'	-3.57	95.97	102.81
4	L5	2787	A2M	O3'-C3'-C2'	3.56	121.14	111.19
4	L5	3818	UY1	C6-C5-C4	3.54	120.56	118.17
52	S2	1288	OMU	C5-C4-N3	3.54	119.75	114.80
4	L5	4590	A2M	C3'-C2'-C1'	-3.52	96.07	102.81
4	L5	3825	A2M	C3'-C2'-C1'	-3.50	96.10	102.81
4	L5	4620	OMU	N3-C2-N1	3.47	119.42	114.89
52	S2	576	A2M	O3'-C3'-C2'	3.45	120.85	111.19
52	S2	116	OMU	C5-C4-N3	3.44	119.62	114.80
52	S2	116	OMU	N3-C2-N1	3.43	119.36	114.89
52	S2	1031	A2M	C3'-C2'-C1'	-3.41	96.28	102.81
52	S2	1639	G7M	O6-C6-C5	-3.39	120.44	128.01
52	S2	1248	B8N	N3-C2-N1	3.39	120.86	116.72
52	S2	1850	MA6	C2-N1-C6	3.38	120.09	111.83
4	L5	4571	A2M	O3'-C3'-C2'	3.36	120.60	111.19
4	L5	4620	OMU	C5-C4-N3	3.35	119.50	114.80
4	L5	2401	A2M	C3'-C2'-C1'	-3.35	96.40	102.81
4	L5	3718	A2M	C3'-C2'-C1'	-3.34	96.41	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	1851	MA6	N3-C4-N9	3.34	132.85	127.17
52	S2	1639	G7M	N9-C4-N3	3.34	132.63	125.95
52	S2	1850	MA6	N3-C4-N9	3.32	132.82	127.17
4	L5	4220	6MZ	C2-N3-C4	3.32	119.94	111.83
52	S2	1832	6MZ	C2-N3-C4	3.30	119.90	111.83
52	S2	159	A2M	C3'-C2'-C1'	-3.28	96.53	102.81
52	S2	1851	MA6	C2-N1-C6	3.27	119.82	111.83
52	S2	99	A2M	C3'-C2'-C1'	-3.26	96.57	102.81
52	S2	1383	A2M	O3'-C3'-C2'	3.25	120.30	111.19
52	S2	121	OMU	C5-C4-N3	3.25	119.36	114.80
52	S2	468	A2M	O3'-C3'-C2'	3.25	120.28	111.19
52	S2	1851	MA6	C2-N3-C4	3.25	119.76	111.83
52	S2	166	A2M	O3'-C3'-C2'	3.24	120.27	111.19
4	L5	3830	A2M	O3'-C3'-C2'	3.23	120.22	111.19
4	L5	1524	A2M	O3'-C3'-C2'	3.22	120.19	111.19
52	S2	159	A2M	O3'-C3'-C2'	3.21	120.17	111.19
4	L5	3718	A2M	O3'-C3'-C2'	3.19	120.10	111.19
4	L5	400	A2M	O3'-C3'-C2'	3.18	120.10	111.19
52	S2	166	A2M	C3'-C2'-C1'	-3.15	96.78	102.81
4	L5	1534	A2M	C3'-C2'-C1'	-3.15	96.78	102.81
52	S2	576	A2M	C3'-C2'-C1'	-3.14	96.80	102.81
52	S2	668	A2M	C4-N9-C1'	-3.13	119.31	126.63
52	S2	1851	MA6	C5-N7-C8	3.10	108.32	103.45
4	L5	3825	A2M	O3'-C3'-C2'	3.10	119.86	111.19
4	L5	4220	6MZ	C5-N7-C8	3.05	108.25	103.45
52	S2	1850	MA6	C2-N3-C4	3.05	119.28	111.83
52	S2	1442	OMU	O4-C4-C5	-3.05	119.91	125.16
52	S2	1639	G7M	CN7-N7-C5	3.04	130.59	126.80
52	S2	484	A2M	O3'-C3'-C2'	3.03	119.68	111.19
52	S2	1832	6MZ	C5-N7-C8	3.02	108.20	103.45
52	S2	627	OMU	O4-C4-C5	-3.02	119.95	125.16
52	S2	1850	MA6	C5-N7-C8	3.02	108.20	103.45
4	L5	3785	A2M	C4'-O4'-C1'	-3.02	102.80	109.47
4	L5	2401	A2M	C4-N9-C1'	-3.01	119.58	126.63
4	L5	4571	A2M	C3'-C2'-C1'	-3.01	97.04	102.81
4	L5	3785	A2M	O3'-C3'-C2'	3.00	119.60	111.19
4	L5	3818	UY1	C6-N1-C2	-3.00	119.90	122.69
4	L5	4500	PSU	O2-C2-N1	-2.98	119.71	122.79
52	S2	27	A2M	C3'-C2'-C1'	-2.97	97.12	102.81
4	L5	1871	A2M	O3'-C3'-C2'	2.96	119.48	111.19
52	S2	1383	A2M	C4-N9-C1'	-2.96	119.72	126.63
4	L5	400	A2M	C3'-C2'-C1'	-2.95	97.15	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	1326	OMU	O4-C4-C5	-2.95	120.07	125.16
52	S2	1031	A2M	O3'-C3'-C2'	2.95	119.44	111.19
4	L5	3867	A2M	C2'-C1'-N9	2.95	118.60	113.75
52	S2	172	OMU	O4-C4-C5	-2.94	120.09	125.16
4	L5	4220	6MZ	C4-N9-C8	2.94	108.82	105.74
4	L5	4523	A2M	O3'-C3'-C2'	2.94	119.41	111.19
52	S2	1832	6MZ	C4-N9-C8	2.94	108.82	105.74
4	L5	3925	OMU	O4-C4-C5	-2.93	120.12	125.16
4	L5	4628	PSU	O2-C2-N1	-2.92	119.77	122.79
52	S2	1639	G7M	C2-N1-C6	-2.92	119.81	125.11
4	L5	4636	PSU	C6-C5-C4	2.92	120.15	118.17
4	L5	2363	A2M	O3'-C3'-C2'	2.92	119.36	111.19
4	L5	4590	A2M	C4-N9-C1'	-2.92	119.81	126.63
52	S2	1288	OMU	O4-C4-C5	-2.91	120.14	125.16
52	S2	116	OMU	O4-C4-C5	-2.91	120.14	125.16
4	L5	4689	PSU	O2-C2-N1	-2.90	119.79	122.79
4	L5	4579	PSU	O2-C2-N1	-2.90	119.80	122.79
52	S2	668	A2M	C1'-N9-C8	2.90	133.53	127.09
4	L5	4306	OMU	O4-C4-C5	-2.89	120.17	125.16
52	S2	468	A2M	C4-N9-C1'	-2.89	119.87	126.63
4	L5	4689	PSU	C6-N1-C2	-2.89	120.01	122.69
4	L5	1536	PSU	O2-C2-N1	-2.88	119.81	122.79
52	S2	668	A2M	O3'-C3'-C2'	2.88	119.25	111.19
52	S2	799	OMU	O4-C4-C5	-2.88	120.20	125.16
52	S2	428	OMU	O4-C4-C5	-2.88	120.20	125.16
4	L5	2837	OMU	O4-C4-C5	-2.87	120.20	125.16
52	S2	354	OMU	O4-C4-C5	-2.87	120.22	125.16
4	L5	4293	PSU	O2-C2-N1	-2.86	119.84	122.79
52	S2	668	A2M	O4'-C1'-C2'	2.85	111.49	106.59
4	L5	4227	OMU	O4-C4-C5	-2.84	120.26	125.16
4	L5	4498	OMU	O4-C4-C5	-2.84	120.26	125.16
4	L5	2839	PSU	O2-C2-N1	-2.84	119.86	122.79
4	L5	3785	A2M	C4-N9-C1'	-2.84	120.00	126.63
4	L5	3844	PSU	O2-C2-N1	-2.83	119.87	122.79
4	L5	4403	PSU	O2-C2-N1	-2.82	119.88	122.79
52	S2	99	A2M	O3'-C3'-C2'	2.82	119.08	111.19
4	L5	3825	A2M	C4-N9-C1'	-2.81	120.05	126.63
4	L5	4500	PSU	C6-N1-C2	-2.81	120.08	122.69
4	L5	2632	PSU	O2-C2-N1	-2.81	119.89	122.79
4	L5	2363	A2M	C3'-C2'-C1'	-2.80	97.44	102.81
52	S2	1056	PSU	O2-C2-N1	-2.80	119.90	122.79
4	L5	1323	A2M	C2'-C1'-N9	2.80	118.36	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L5	4590	A2M	O3'-C3'-C2'	2.80	119.01	111.19
52	S2	1232	PSU	O2-C2-N1	-2.79	119.91	122.79
52	S2	1244	PSU	O2-C2-N1	-2.79	119.91	122.79
4	L5	398	A2M	C4-N9-C1'	-2.78	120.13	126.63
4	L5	4576	PSU	O2-C2-N1	-2.77	119.93	122.79
4	L5	1781	PSU	O2-C2-N1	-2.77	119.93	122.79
4	L5	3822	PSU	O2-C2-N1	-2.77	119.93	122.79
4	L5	1744	PSU	O2-C2-N1	-2.77	119.94	122.79
4	L5	4442	PSU	O2-C2-N1	-2.75	119.95	122.79
4	L5	4523	A2M	C4-N9-C1'	-2.75	120.21	126.63
4	L5	4532	PSU	O2-C2-N1	-2.74	119.96	122.79
52	S2	406	PSU	O2-C2-N1	-2.74	119.96	122.79
52	S2	1367	PSU	O2-C2-N1	-2.74	119.97	122.79
52	S2	159	A2M	C4-N9-C1'	-2.73	120.24	126.63
52	S2	649	PSU	O2-C2-N1	-2.73	119.97	122.79
52	S2	576	A2M	C4-N9-C1'	-2.72	120.26	126.63
52	S2	109	PSU	O2-C2-N1	-2.72	119.98	122.79
52	S2	651	PSU	O2-C2-N1	-2.72	119.98	122.79
4	L5	3830	A2M	C4-N9-C1'	-2.72	120.27	126.63
4	L5	4620	OMU	O4-C4-C5	-2.72	120.48	125.16
4	L5	2401	A2M	C1'-N9-C8	2.72	133.12	127.09
4	L5	4552	PSU	O2-C2-N1	-2.72	119.99	122.79
4	L5	4628	PSU	C6-N1-C2	-2.71	120.18	122.69
52	S2	866	PSU	O2-C2-N1	-2.71	120.00	122.79
52	S2	1272	OMC	C1'-N1-C2	2.71	124.42	118.44
4	L5	4220	6MZ	N3-C4-N9	2.71	131.77	127.17
4	L5	1323	A2M	O3'-C3'-C2'	2.70	118.75	111.19
4	L5	4296	PSU	O2-C2-N1	-2.70	120.00	122.79
52	S2	801	PSU	O2-C2-N1	-2.70	120.01	122.79
52	S2	1383	A2M	C1'-N9-C8	2.70	133.08	127.09
4	L5	5010	PSU	O2-C2-N1	-2.69	120.01	122.79
4	L5	1862	PSU	O2-C2-N1	-2.69	120.02	122.79
52	S2	1832	6MZ	C4-C5-C6	2.69	119.01	116.78
52	S2	121	OMU	O4-C4-C5	-2.69	120.53	125.16
6	L8	69	PSU	O2-C2-N1	-2.68	120.02	122.79
52	S2	1832	6MZ	N3-C4-N9	2.68	131.73	127.17
52	S2	1004	PSU	O2-C2-N1	-2.68	120.02	122.79
52	S2	468	A2M	C1'-N9-C8	2.68	133.04	127.09
4	L5	4571	A2M	C4-N9-C1'	-2.68	120.37	126.63
4	L5	3920	PSU	O2-C2-N1	-2.68	120.03	122.79
4	L5	1524	A2M	O4'-C1'-C2'	2.68	111.20	106.59
4	L5	3851	PSU	O2-C2-N1	-2.68	120.03	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L5	4673	PSU	O2-C2-N1	-2.67	120.03	122.79
4	L5	4590	A2M	C1'-N9-C8	2.67	133.02	127.09
52	S2	1248	B8N	O4-C4-N3	-2.67	115.66	119.99
52	S2	863	PSU	O2-C2-N1	-2.67	120.04	122.79
52	S2	681	PSU	O2-C2-N1	-2.67	120.04	122.79
4	L5	3853	PSU	O2-C2-N1	-2.66	120.04	122.79
4	L5	3639	PSU	O2-C2-N1	-2.66	120.05	122.79
4	L5	2787	A2M	O4'-C1'-C2'	2.66	111.16	106.59
52	S2	686	PSU	O2-C2-N1	-2.65	120.05	122.79
52	S2	1174	PSU	O2-C2-N1	-2.65	120.05	122.79
4	L5	400	A2M	C4-N9-C1'	-2.65	120.43	126.63
4	L5	2815	A2M	O3'-C3'-C2'	2.65	118.60	111.19
4	L5	1792	PSU	O2-C2-N1	-2.65	120.06	122.79
4	L5	4521	PSU	O2-C2-N1	-2.64	120.07	122.79
52	S2	1177	PSU	O2-C2-N1	-2.64	120.07	122.79
4	L5	4493	PSU	O2-C2-N1	-2.64	120.07	122.79
4	L5	1677	PSU	O2-C2-N1	-2.63	120.07	122.79
4	L5	1683	PSU	O2-C2-N1	-2.63	120.08	122.79
4	L5	1582	PSU	O2-C2-N1	-2.62	120.08	122.79
52	S2	966	PSU	O2-C2-N1	-2.62	120.09	122.79
52	S2	484	A2M	C4-N9-C1'	-2.61	120.52	126.63
4	L5	4973	PSU	O2-C2-N1	-2.61	120.09	122.79
4	L5	3695	PSU	O2-C2-N1	-2.61	120.10	122.79
4	L5	4361	PSU	O2-C2-N1	-2.61	120.10	122.79
4	L5	1782	PSU	O2-C2-N1	-2.61	120.10	122.79
4	L5	1536	PSU	C6-N1-C2	-2.61	120.27	122.69
4	L5	4220	6MZ	C4-C5-C6	2.60	118.94	116.78
4	L5	1871	A2M	C4-N9-C1'	-2.60	120.55	126.63
4	L5	1582	PSU	C6-N1-C2	-2.60	120.28	122.69
4	L5	398	A2M	C1'-N9-C8	2.60	132.86	127.09
4	L5	3844	PSU	C6-N1-C2	-2.60	120.28	122.69
4	L5	4636	PSU	O2-C2-N1	-2.59	120.11	122.79
4	L5	4972	PSU	O2-C2-N1	-2.59	120.12	122.79
4	L5	4293	PSU	C6-N1-C2	-2.58	120.29	122.69
52	S2	105	PSU	O2-C2-N1	-2.58	120.12	122.79
4	L5	4312	PSU	O2-C2-N1	-2.58	120.12	122.79
4	L5	3785	A2M	C3'-C2'-C1'	-2.58	97.86	102.81
4	L5	4431	PSU	O2-C2-N1	-2.58	120.13	122.79
4	L5	2839	PSU	C6-N1-C2	-2.58	120.30	122.69
6	L8	55	PSU	O2-C2-N1	-2.58	120.13	122.79
4	L5	3825	A2M	C1'-N9-C8	2.57	132.81	127.09
4	L5	1781	PSU	C6-N1-C2	-2.57	120.30	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	S2	863	PSU	C6-N1-C2	-2.57	120.30	122.69
4	L5	3822	PSU	C6-N1-C2	-2.57	120.30	122.69
4	L5	4673	PSU	C6-N1-C2	-2.57	120.31	122.69
4	L5	4457	PSU	O2-C2-N1	-2.57	120.14	122.79
4	L5	3639	PSU	C6-N1-C2	-2.55	120.32	122.69
4	L5	3920	PSU	C6-N1-C2	-2.55	120.32	122.69
52	S2	814	PSU	C6-N1-C2	-2.55	120.32	122.69
4	L5	1524	A2M	C4-N9-C1'	-2.55	120.67	126.63
4	L5	1860	PSU	O2-C2-N1	-2.55	120.16	122.79
4	L5	3884	PSU	O2-C2-N1	-2.55	120.16	122.79
4	L5	3830	A2M	C1'-N9-C8	2.55	132.74	127.09
4	L5	3785	A2M	C1'-N9-C8	2.54	132.74	127.09
52	S2	576	A2M	C1'-N9-C8	2.54	132.74	127.09
4	L5	2632	PSU	C6-N1-C2	-2.54	120.33	122.69
52	S2	1639	G7M	CN7-N7-C8	-2.54	120.95	124.79
4	L5	3818	UY1	O2-C2-N1	-2.54	120.17	122.79
4	L5	1326	A2M	C2'-C1'-N9	2.54	117.92	113.75
4	L5	3867	A2M	C4-N9-C1'	-2.53	120.70	126.63
52	S2	484	A2M	C1'-N9-C8	2.53	132.71	127.09
4	L5	2363	A2M	C2'-C1'-N9	2.53	117.91	113.75
4	L5	4532	PSU	C6-N1-C2	-2.53	120.35	122.69
4	L5	4353	PSU	O2-C2-N1	-2.53	120.18	122.79
4	L5	3884	PSU	C6-N1-C2	-2.52	120.35	122.69
4	L5	4442	PSU	C6-N1-C2	-2.52	120.35	122.69
52	S2	159	A2M	C1'-N9-C8	2.52	132.70	127.09
4	L5	1524	A2M	C4'-O4'-C1'	-2.52	103.90	109.47
52	S2	93	PSU	O2-C2-N1	-2.52	120.19	122.79
4	L5	4471	PSU	O2-C2-N1	-2.52	120.19	122.79
52	S2	1046	PSU	O2-C2-N1	-2.51	120.19	122.79
4	L5	3867	A2M	O3'-C3'-C2'	2.51	118.22	111.19
4	L5	1683	PSU	C6-N1-C2	-2.51	120.36	122.69
4	L5	3853	PSU	C6-N1-C2	-2.51	120.36	122.69
4	L5	4312	PSU	C6-N1-C2	-2.51	120.36	122.69
52	S2	681	PSU	C6-N1-C2	-2.50	120.37	122.69
3	CF	163	SEP	OG-CB-CA	2.50	110.58	108.14
4	L5	4471	PSU	C6-N1-C2	-2.50	120.37	122.69
4	L5	4493	PSU	C6-N1-C2	-2.50	120.37	122.69
52	S2	1232	PSU	C6-N1-C2	-2.50	120.38	122.69
4	L5	2787	A2M	C4-N9-C1'	-2.49	120.81	126.63
52	S2	484	A2M	O4'-C1'-C2'	2.49	110.87	106.59
4	L5	4523	A2M	C1'-N9-C8	2.49	132.62	127.09
52	S2	1004	PSU	C6-N1-C2	-2.49	120.39	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L5	5001	PSU	O2-C2-N1	-2.48	120.23	122.79
52	S2	814	PSU	O2-C2-N1	-2.48	120.23	122.79
4	L5	4576	PSU	C6-N1-C2	-2.48	120.39	122.69
4	L5	4299	PSU	O2-C2-N1	-2.47	120.24	122.79
4	L5	2351	OMC	C1'-N1-C2	2.47	123.89	118.44
4	L5	4571	A2M	C1'-N9-C8	2.46	132.56	127.09
4	L5	1744	PSU	C6-N1-C2	-2.46	120.41	122.69
52	S2	1045	PSU	O2-C2-N1	-2.46	120.25	122.79
52	S2	801	PSU	C6-N1-C2	-2.45	120.41	122.69
52	S2	166	A2M	C4-N9-C1'	-2.45	120.89	126.63
4	L5	1677	PSU	C6-C5-C4	2.45	119.83	118.17
4	L5	3718	A2M	C1'-N9-C8	2.45	132.53	127.09
52	S2	105	PSU	C6-N1-C2	-2.45	120.42	122.69
52	S2	1056	PSU	C6-N1-C2	-2.45	120.42	122.69
4	L5	2815	A2M	C2'-C1'-N9	2.45	117.78	113.75
4	L5	4973	PSU	C6-N1-C2	-2.45	120.42	122.69
4	L5	400	A2M	C1'-N9-C8	2.45	132.52	127.09
52	S2	93	PSU	C6-N1-C2	-2.45	120.42	122.69
4	L5	1534	A2M	C4-N9-C1'	-2.44	120.92	126.63
4	L5	2861	OMC	C1'-N1-C2	2.44	123.83	118.44
4	L5	4521	PSU	C6-C5-C4	2.44	119.82	118.17
4	L5	4353	PSU	C6-C5-C4	2.43	119.82	118.17
4	L5	1862	PSU	C6-N1-C2	-2.43	120.44	122.69
4	L5	2363	A2M	C4-N9-C1'	-2.43	120.95	126.63
4	L5	4431	PSU	C6-N1-C2	-2.43	120.44	122.69
52	S2	27	A2M	O3'-C3'-C2'	2.42	117.97	111.19
4	L5	3695	PSU	C6-N1-C2	-2.42	120.44	122.69
6	L8	55	PSU	C6-N1-C2	-2.42	120.44	122.69
52	S2	1174	PSU	C6-N1-C2	-2.42	120.44	122.69
4	L5	4579	PSU	C6-N1-C2	-2.42	120.45	122.69
6	L8	69	PSU	C6-N1-C2	-2.42	120.45	122.69
52	S2	406	PSU	C6-N1-C2	-2.42	120.45	122.69
52	S2	966	PSU	C6-N1-C2	-2.42	120.45	122.69
52	S2	649	PSU	C6-N1-C2	-2.41	120.45	122.69
4	L5	4403	PSU	C6-N1-C2	-2.41	120.45	122.69
4	L5	3851	PSU	C6-N1-C2	-2.41	120.45	122.69
4	L5	1323	A2M	C3'-C2'-C1'	-2.41	98.20	102.81
52	S2	799	OMU	C1'-N1-C2	2.41	121.91	117.59
4	L5	4299	PSU	C6-N1-C2	-2.41	120.46	122.69
4	L5	4530	UR3	C6-N1-C2	-2.40	119.84	121.80
6	L8	69	PSU	O4'-C1'-C2'	2.40	108.47	105.15
52	S2	866	PSU	C6-N1-C2	-2.40	120.47	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L5	1871	A2M	C1'-N9-C8	2.40	132.42	127.09
4	L5	4361	PSU	C6-N1-C2	-2.40	120.47	122.69
52	S2	1031	A2M	C4-N9-C1'	-2.39	121.04	126.63
4	L5	5010	PSU	C6-N1-C2	-2.39	120.48	122.69
4	L5	4972	PSU	C6-N1-C2	-2.39	120.48	122.69
4	L5	4552	PSU	C6-N1-C2	-2.38	120.48	122.69
52	S2	1177	PSU	C6-N1-C2	-2.38	120.48	122.69
52	S2	668	A2M	C2'-C1'-N9	2.38	117.67	113.75
4	L5	3637	PSU	C6-N1-C2	-2.38	120.48	122.69
4	L5	1524	A2M	C1'-N9-C8	2.38	132.38	127.09
52	S2	406	PSU	C6-C5-C4	2.38	119.78	118.17
4	L5	4636	PSU	C6-N1-C2	-2.37	120.49	122.69
52	S2	1081	PSU	O2-C2-N1	-2.37	120.34	122.79
52	S2	686	PSU	C6-N1-C2	-2.37	120.49	122.69
4	L5	1782	PSU	C6-N1-C2	-2.37	120.49	122.69
4	L5	1792	PSU	C6-N1-C2	-2.37	120.49	122.69
52	S2	109	PSU	C6-N1-C2	-2.37	120.50	122.69
52	S2	1367	PSU	C6-N1-C2	-2.37	120.50	122.69
4	L5	3639	PSU	C6-C5-C4	2.36	119.77	118.17
52	S2	1046	PSU	C6-N1-C2	-2.36	120.50	122.69
4	L5	3701	OMC	O2-C2-N1	2.36	123.52	118.90
4	L5	3808	OMC	C1'-N1-C2	2.36	123.65	118.44
4	L5	1323	A2M	O4'-C1'-C2'	2.35	110.64	106.59
4	L5	3867	A2M	C1'-N9-C8	2.35	132.32	127.09
4	L5	4403	PSU	O4'-C1'-C2'	2.35	108.40	105.15
4	L5	1860	PSU	C6-N1-C2	-2.35	120.51	122.69
4	L5	3718	A2M	C4-N9-C1'	-2.35	121.14	126.63
52	S2	1639	G7M	N9-C8-N7	-2.34	106.79	112.48
4	L5	4353	PSU	C6-N1-C2	-2.34	120.52	122.69
4	L5	5001	PSU	C6-N1-C2	-2.34	120.52	122.69
4	L5	3822	PSU	O4'-C1'-C2'	2.33	108.38	105.15
52	S2	484	A2M	O4'-C4'-C3'	2.33	109.77	105.15
52	S2	1244	PSU	C6-N1-C2	-2.32	120.53	122.69
4	L5	4403	PSU	C6-C5-C4	2.32	119.74	118.17
4	L5	4521	PSU	C6-N1-C2	-2.32	120.54	122.69
52	S2	166	A2M	C1'-N9-C8	2.32	132.24	127.09
4	L5	1534	A2M	C1'-N9-C8	2.31	132.23	127.09
4	L5	4296	PSU	C6-N1-C2	-2.31	120.55	122.69
4	L5	4220	6MZ	OP2-P-O5'	2.30	112.67	106.67
52	S2	651	PSU	C6-N1-C2	-2.30	120.56	122.69
52	S2	1832	6MZ	C9-N6-C6	-2.30	120.72	122.85
52	S2	1248	B8N	C31-N3-C4	2.29	120.43	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L5	4571	A2M	C2'-C1'-N9	2.29	117.52	113.75
4	L5	2363	A2M	C1'-N9-C8	2.28	132.16	127.09
52	S2	866	PSU	C6-C5-C4	2.28	119.71	118.17
4	L5	400	A2M	O4'-C1'-C2'	2.27	110.50	106.59
4	L5	2787	A2M	C1'-N9-C8	2.27	132.14	127.09
4	L5	3637	PSU	C6-C5-C4	2.27	119.70	118.17
52	S2	1288	OMU	O2-C2-N1	-2.27	119.85	122.80
52	S2	1851	MA6	C1'-N9-C8	-2.26	122.08	127.09
52	S2	1045	PSU	C6-N1-C2	-2.26	120.59	122.69
52	S2	27	A2M	C4-N9-C1'	-2.26	121.35	126.63
52	S2	1056	PSU	C6-C5-C4	2.25	119.69	118.17
4	L5	4442	PSU	O4'-C1'-C2'	2.25	108.26	105.15
4	L5	1677	PSU	C6-N1-C2	-2.25	120.61	122.69
4	L5	1322	1MA	N1-C6-N6	2.24	125.35	119.71
4	L5	4442	PSU	C6-C5-C4	2.24	119.69	118.17
52	S2	668	A2M	C6-C5-C4	-2.23	114.13	117.18
52	S2	1031	A2M	C1'-N9-C8	2.23	132.05	127.09
52	S2	1081	PSU	C6-N1-C2	-2.23	120.62	122.69
4	L5	4457	PSU	C6-N1-C2	-2.23	120.63	122.69
4	L5	3884	PSU	C6-C5-C4	2.22	119.67	118.17
4	L5	4973	PSU	C6-C5-C4	2.22	119.67	118.17
4	L5	3701	OMC	O2-C2-N3	-2.22	118.83	122.33
52	S2	1326	OMU	O2-C2-N1	-2.22	119.91	122.80
52	S2	1832	6MZ	C4-C5-N7	-2.22	108.05	110.58
4	L5	3867	A2M	C3'-C2'-C1'	-2.21	98.58	102.81
52	S2	1248	B8N	O4'-C1'-C2'	2.21	108.20	105.15
52	S2	1248	B8N	O4-C4-C5	-2.20	118.77	122.58
4	L5	4590	A2M	C6-C5-C4	-2.20	114.18	117.18
4	L5	2363	A2M	O4'-C1'-C2'	2.19	110.36	106.59
4	L5	1534	A2M	O4'-C1'-C2'	2.19	110.36	106.59
52	S2	1367	PSU	C6-C5-C4	2.19	119.65	118.17
4	L5	4552	PSU	C6-C5-C4	2.18	119.65	118.17
4	L5	398	A2M	C6-C5-C4	-2.18	114.20	117.18
4	L5	2401	A2M	C6-C5-C4	-2.18	114.20	117.18
4	L5	4636	PSU	O4'-C1'-C2'	2.18	108.17	105.15
52	S2	428	OMU	O2-C2-N1	-2.18	119.96	122.80
4	L5	4220	6MZ	C5-C6-N1	2.18	120.49	118.15
52	S2	468	A2M	O4'-C1'-C2'	2.17	110.33	106.59
52	S2	99	A2M	C4-N9-C1'	-2.17	121.56	126.63
52	S2	651	PSU	C6-C5-C4	2.17	119.64	118.17
52	S2	1383	A2M	C6-C5-C4	-2.16	114.22	117.18
4	L5	1871	A2M	C4'-O4'-C1'	-2.16	104.70	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L5	4571	A2M	O4'-C1'-C2'	2.16	110.30	106.59
52	S2	27	A2M	C1'-N9-C8	2.16	131.88	127.09
4	L5	2787	A2M	O4'-C4'-C3'	2.16	109.43	105.15
52	S2	576	A2M	C6-C5-C4	-2.15	114.24	117.18
4	L5	3785	A2M	C6-C5-C4	-2.15	114.24	117.18
4	L5	4493	PSU	C6-C5-C4	2.15	119.62	118.17
4	L5	4523	A2M	C6-C5-C4	-2.15	114.25	117.18
4	L5	400	A2M	C2'-C1'-N9	2.14	117.27	113.75
4	L5	3785	A2M	O4'-C4'-C3'	2.14	109.39	105.15
4	L5	5010	PSU	C6-C5-C4	2.14	119.61	118.17
4	L5	4220	6MZ	C4-C5-N7	-2.13	108.14	110.58
4	L5	3785	A2M	O4'-C1'-N9	2.13	112.18	108.09
4	L5	4579	PSU	C6-C5-C4	2.13	119.61	118.17
52	S2	99	A2M	C1'-N9-C8	2.13	131.82	127.09
4	L5	4457	PSU	O4'-C1'-C2'	2.13	108.09	105.15
4	L5	1326	A2M	O3'-C3'-C2'	2.12	117.12	111.19
4	L5	4498	OMU	O2-C2-N1	-2.12	120.04	122.80
4	L5	4590	A2M	O4'-C1'-C2'	2.12	110.23	106.59
52	S2	1081	PSU	O4'-C1'-C2'	2.11	108.08	105.15
4	L5	4571	A2M	C6-C5-C4	-2.11	114.29	117.18
4	L5	2815	A2M	C3'-C2'-C1'	-2.11	98.76	102.81
4	L5	400	A2M	C6-C5-C4	-2.11	114.30	117.18
52	S2	649	PSU	C6-C5-C4	2.11	119.60	118.17
4	L5	1326	A2M	C3'-C2'-C1'	-2.11	98.77	102.81
4	L5	3867	A2M	O4'-C1'-C2'	2.11	110.22	106.59
4	L5	3825	A2M	C6-C5-C4	-2.10	114.31	117.18
4	L5	2401	A2M	O4'-C1'-C2'	2.10	110.21	106.59
4	L5	2787	A2M	C6-C5-C4	-2.10	114.31	117.18
4	L5	3830	A2M	C6-C5-C4	-2.10	114.31	117.18
52	S2	468	A2M	C6-C5-C4	-2.10	114.31	117.18
4	L5	4293	PSU	C6-C5-C4	2.10	119.59	118.17
52	S2	1177	PSU	C6-C5-C4	2.10	119.59	118.17
4	L5	2787	A2M	C3'-C2'-C1'	-2.09	98.80	102.81
4	L5	2839	PSU	C6-C5-C4	2.09	119.59	118.17
4	L5	3920	PSU	C6-C5-C4	2.09	119.59	118.17
4	L5	3785	A2M	C2-N1-C6	-2.09	115.29	118.73
4	L5	4299	PSU	C6-C5-C4	2.09	119.58	118.17
4	L5	4576	PSU	C6-C5-C4	2.09	119.58	118.17
52	S2	172	OMU	O2-C2-N1	-2.08	120.08	122.80
52	S2	109	PSU	C6-C5-C4	2.08	119.58	118.17
4	L5	2815	A2M	O4'-C1'-C2'	2.08	110.17	106.59
4	L5	2815	A2M	C4-N9-C1'	-2.08	121.76	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L5	3785	A2M	C5-C6-N1	2.08	122.79	117.51
4	L5	3867	A2M	C6-C5-C4	-2.08	114.34	117.18
4	L5	1744	PSU	C6-C5-C4	2.08	119.58	118.17
4	L5	3830	A2M	C4'-O4'-C1'	-2.08	104.88	109.47
4	L5	1323	A2M	C4-N9-C1'	-2.07	121.78	126.63
4	L5	1534	A2M	O3'-C3'-C2'	2.07	116.98	111.19
4	L5	4972	PSU	C6-C5-C4	2.07	119.57	118.17
52	S2	1272	OMC	C1'-N1-C6	-2.07	116.36	120.78
4	L5	4523	A2M	C4'-O4'-C1'	-2.06	104.91	109.47
4	L5	1871	A2M	C6-C5-C4	-2.06	114.36	117.18
4	L5	1677	PSU	O4'-C1'-C2'	2.06	108.01	105.15
4	L5	3637	PSU	O2-C2-N1	-2.06	120.66	122.79
52	S2	484	A2M	C2'-C1'-N9	2.06	117.14	113.75
4	L5	4296	PSU	C6-C5-C4	2.06	119.56	118.17
52	S2	1046	PSU	O4'-C1'-C2'	2.05	107.99	105.15
4	L5	3822	PSU	C6-C5-C4	2.05	119.56	118.17
52	S2	354	OMU	O2-C2-N1	-2.05	120.13	122.80
52	S2	484	A2M	C6-C5-C4	-2.05	114.38	117.18
52	S2	1056	PSU	O4'-C1'-C2'	2.05	107.98	105.15
52	S2	159	A2M	C6-C5-C4	-2.05	114.39	117.18
52	S2	1232	PSU	C6-C5-C4	2.05	119.55	118.17
52	S2	1832	6MZ	C5-C6-N1	2.04	120.34	118.15
4	L5	2815	A2M	C1'-N9-C8	2.04	131.63	127.09
52	S2	1244	PSU	C6-C5-C4	2.04	119.55	118.17
52	S2	1004	PSU	C6-C5-C4	2.03	119.55	118.17
4	L5	4673	PSU	C6-C5-C4	2.03	119.55	118.17
4	L5	1534	A2M	C6-C5-C4	-2.03	114.41	117.18
52	S2	116	OMU	O2-C2-N1	-2.03	120.16	122.80
4	L5	4353	PSU	O4'-C1'-C2'	2.03	107.96	105.15
52	S2	1031	A2M	C6-C5-C4	-2.02	114.41	117.18
4	L5	1326	A2M	C4-N9-C1'	-2.02	121.91	126.63
52	S2	109	PSU	O4'-C1'-C2'	2.01	107.94	105.15
4	L5	3825	A2M	O4'-C1'-C2'	2.01	110.06	106.59
4	L5	1326	A2M	O4'-C1'-C2'	2.01	110.06	106.59
52	S2	627	OMU	O2-C2-N1	-2.01	120.18	122.80
4	L5	3867	A2M	C2-N1-C6	-2.01	115.42	118.73
52	S2	1383	A2M	O4'-C1'-C2'	2.01	110.05	106.59
4	L5	3825	A2M	C2-N1-C6	-2.01	115.43	118.73
4	L5	2815	A2M	C2-N1-C6	-2.01	115.43	118.73
4	L5	2837	OMU	O2-C2-N1	-2.00	120.19	122.80

There are no chirality outliers.

All (143) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	CF	163	SEP	N-CA-CB-OG
3	CF	163	SEP	C-CA-CB-OG
3	CF	163	SEP	CA-CB-OG-P
6	L8	75	OMG	C1'-C2'-O2'-CM2
4	L5	400	A2M	C1'-C2'-O2'-CM'
4	L5	1326	A2M	O4'-C4'-C5'-O5'
4	L5	1340	OMC	C1'-C2'-O2'-CM2
4	L5	1625	OMG	O4'-C4'-C5'-O5'
4	L5	2351	OMC	C1'-C2'-O2'-CM2
4	L5	2787	A2M	C1'-C2'-O2'-CM'
4	L5	2824	OMC	C1'-C2'-O2'-CM2
4	L5	2861	OMC	C1'-C2'-O2'-CM2
4	L5	3627	OMG	C1'-C2'-O2'-CM2
4	L5	3701	OMC	O4'-C4'-C5'-O5'
4	L5	3792	OMG	O4'-C4'-C5'-O5'
4	L5	3841	OMC	C1'-C2'-O2'-CM2
4	L5	3867	A2M	C1'-C2'-O2'-CM'
4	L5	4196	OMG	C1'-C2'-O2'-CM2
4	L5	4220	6MZ	C5'-O5'-P-OP1
4	L5	4590	A2M	O4'-C4'-C5'-O5'
4	L5	4620	OMU	C1'-C2'-O2'-CM2
4	L5	4637	OMG	C1'-C2'-O2'-CM2
52	S2	27	A2M	C1'-C2'-O2'-CM'
52	S2	116	OMU	C1'-C2'-O2'-CM2
52	S2	159	A2M	C1'-C2'-O2'-CM'
52	S2	354	OMU	C1'-C2'-O2'-CM2
52	S2	468	A2M	C1'-C2'-O2'-CM'
52	S2	601	OMG	C1'-C2'-O2'-CM2
52	S2	644	OMG	O4'-C4'-C5'-O5'
52	S2	644	OMG	C1'-C2'-O2'-CM2
52	S2	863	PSU	C3'-C4'-C5'-O5'
52	S2	863	PSU	O4'-C4'-C5'-O5'
52	S2	1248	B8N	O4'-C4'-C5'-O5'
52	S2	1272	OMC	C1'-C2'-O2'-CM2
52	S2	1272	OMC	O4'-C4'-C5'-O5'
52	S2	1288	OMU	O4'-C4'-C5'-O5'
52	S2	1328	OMG	C1'-C2'-O2'-CM2
52	S2	1337	4AC	N3-C4-N4-C7
52	S2	1383	A2M	C1'-C2'-O2'-CM'
52	S2	1391	OMC	C1'-C2'-O2'-CM2
52	S2	1490	OMG	C1'-C2'-O2'-CM2
52	S2	1832	6MZ	C5-C6-N6-C9

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Mol	Chain	Res	Type	Atoms
52	S2	1832	6MZ	N1-C6-N6-C9
52	S2	1832	6MZ	C5'-O5'-P-OP2
52	S2	1832	6MZ	C5'-O5'-P-OP1
52	S2	1832	6MZ	C5'-O5'-P-OP3
4	L5	3701	OMC	C2'-C1'-N1-C2
4	L5	1536	PSU	C3'-C4'-C5'-O5'
4	L5	1536	PSU	O4'-C4'-C5'-O5'
4	L5	2364	OMG	O4'-C4'-C5'-O5'
4	L5	3867	A2M	C3'-C4'-C5'-O5'
4	L5	3899	OMG	C3'-C4'-C5'-O5'
4	L5	4590	A2M	C3'-C4'-C5'-O5'
52	S2	576	A2M	O4'-C4'-C5'-O5'
52	S2	867	OMG	C3'-C4'-C5'-O5'
52	S2	1272	OMC	C3'-C4'-C5'-O5'
52	S2	1288	OMU	C3'-C4'-C5'-O5'
52	S2	1442	OMU	O4'-C4'-C5'-O5'
52	S2	1703	OMC	O4'-C4'-C5'-O5'
52	S2	1248	B8N	N34-C33-C34-O36
4	L5	3701	OMC	C3'-C4'-C5'-O5'
4	L5	3899	OMG	O4'-C4'-C5'-O5'
4	L5	4500	PSU	O4'-C4'-C5'-O5'
52	S2	576	A2M	C3'-C4'-C5'-O5'
52	S2	627	OMU	O4'-C4'-C5'-O5'
52	S2	867	OMG	O4'-C4'-C5'-O5'
52	S2	1442	OMU	C3'-C4'-C5'-O5'
4	L5	3701	OMC	C2'-C1'-N1-C6
4	L5	4447	5MC	C2'-C1'-N1-C6
4	L5	1625	OMG	C3'-C4'-C5'-O5'
4	L5	3792	OMG	C3'-C4'-C5'-O5'
4	L5	4500	PSU	C3'-C4'-C5'-O5'
52	S2	644	OMG	C3'-C4'-C5'-O5'
52	S2	1248	B8N	C3'-C4'-C5'-O5'
52	S2	428	OMU	C2'-C1'-N1-C6
4	L5	1326	A2M	C3'-C4'-C5'-O5'
52	S2	627	OMU	C3'-C4'-C5'-O5'
4	L5	4447	5MC	C2'-C1'-N1-C2
4	L5	2364	OMG	C3'-C4'-C5'-O5'
4	L5	2422	OMC	O4'-C4'-C5'-O5'
4	L5	2787	A2M	C3'-C4'-C5'-O5'
4	L5	3867	A2M	O4'-C4'-C5'-O5'
4	L5	4618	OMG	C3'-C4'-C5'-O5'
52	S2	1703	OMC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	L5	2422	OMC	C3'-C4'-C5'-O5'
4	L5	1524	A2M	O4'-C4'-C5'-O5'
52	S2	668	A2M	O4'-C4'-C5'-O5'
52	S2	1639	G7M	O4'-C4'-C5'-O5'
4	L5	2787	A2M	C2'-C1'-N9-C8
4	L5	1524	A2M	C3'-C4'-C5'-O5'
52	S2	1639	G7M	C3'-C4'-C5'-O5'
52	S2	1850	MA6	O4'-C4'-C5'-O5'
4	L5	4590	A2M	C4'-C5'-O5'-P
4	L5	2364	OMG	C1'-C2'-O2'-CM2
4	L5	4618	OMG	O4'-C4'-C5'-O5'
4	L5	1781	PSU	C3'-C4'-C5'-O5'
52	S2	428	OMU	O4'-C1'-N1-C6
52	S2	627	OMU	C2'-C1'-N1-C6
4	L5	4447	5MC	O4'-C1'-N1-C2
52	S2	428	OMU	C2'-C1'-N1-C2
4	L5	3701	OMC	O4'-C1'-N1-C6
52	S2	428	OMU	O4'-C1'-N1-C2
4	L5	4447	5MC	O4'-C1'-N1-C6
4	L5	3818	UY1	C4'-C5'-O5'-P
52	S2	576	A2M	C4'-C5'-O5'-P
52	S2	1851	MA6	C4'-C5'-O5'-P
4	L5	3818	UY1	O4'-C1'-C5-C4
4	L5	4500	PSU	O4'-C1'-C5-C4
4	L5	2787	A2M	C2'-C1'-N9-C4
52	S2	668	A2M	C3'-C4'-C5'-O5'
4	L5	1326	A2M	C4'-C5'-O5'-P
4	L5	1534	A2M	C4'-C5'-O5'-P
4	L5	4500	PSU	C4'-C5'-O5'-P
4	L5	3851	PSU	C3'-C4'-C5'-O5'
52	S2	627	OMU	O4'-C1'-N1-C6
52	S2	99	A2M	O4'-C4'-C5'-O5'
4	L5	3844	PSU	C4'-C5'-O5'-P
4	L5	3887	OMC	C4'-C5'-O5'-P
52	S2	644	OMG	C4'-C5'-O5'-P
52	S2	1490	OMG	C4'-C5'-O5'-P
4	L5	2424	OMG	C1'-C2'-O2'-CM2
52	S2	867	OMG	C1'-C2'-O2'-CM2
4	L5	4296	PSU	C3'-C4'-C5'-O5'
4	L5	3818	UY1	O4'-C1'-C5-C6
4	L5	4636	PSU	O4'-C1'-C5-C6
4	L5	3701	OMC	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
4	L5	2815	A2M	O4'-C4'-C5'-O5'
52	S2	668	A2M	O4'-C1'-N9-C8
4	L5	1323	A2M	O4'-C4'-C5'-O5'
4	L5	2351	OMC	O4'-C4'-C5'-O5'
4	L5	4637	OMG	O4'-C4'-C5'-O5'
52	S2	801	PSU	C3'-C4'-C5'-O5'
52	S2	1272	OMC	C2'-C1'-N1-C2
52	S2	1081	PSU	C4'-C5'-O5'-P
52	S2	1383	A2M	O4'-C4'-C5'-O5'
52	S2	1383	A2M	C3'-C4'-C5'-O5'
4	L5	4636	PSU	C4'-C5'-O5'-P
52	S2	627	OMU	O4'-C1'-N1-C2
4	L5	2787	A2M	O4'-C1'-N9-C8
52	S2	668	A2M	C2'-C1'-N9-C8
4	L5	2351	OMC	C2'-C1'-N1-C2
52	S2	627	OMU	C2'-C1'-N1-C2
52	S2	1248	B8N	N34-C33-C34-O35

There are no ring outliers.

82 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	S2	1288	OMU	1	0
52	S2	1367	PSU	1	0
52	S2	1383	A2M	1	0
52	S2	576	A2M	2	0
52	S2	468	A2M	1	0
4	L5	2363	A2M	1	0
52	S2	166	A2M	1	0
4	L5	1340	OMC	2	0
52	S2	99	A2M	3	0
4	L5	3920	PSU	1	0
4	L5	4447	5MC	1	0
4	L5	1534	A2M	2	0
4	L5	4620	OMU	4	0
52	S2	462	OMC	3	0
4	L5	4220	6MZ	4	0
4	L5	400	A2M	1	0
4	L5	3869	OMC	1	0
4	L5	1625	OMG	1	0
4	L5	2424	OMG	1	0
4	L5	3718	A2M	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L5	1871	A2M	1	0
52	S2	159	A2M	2	0
4	L5	4442	PSU	1	0
52	S2	601	OMG	2	0
4	L5	3637	PSU	1	0
52	S2	1337	4AC	3	0
4	L5	4536	OMC	1	0
4	L5	4500	PSU	1	0
4	L5	4521	PSU	1	0
52	S2	1850	MA6	3	0
4	L5	3701	OMC	1	0
6	L8	75	OMG	1	0
52	S2	1177	PSU	1	0
4	L5	4689	PSU	1	0
4	L5	4523	A2M	1	0
52	S2	116	OMU	4	0
4	L5	4293	PSU	1	0
52	S2	484	A2M	2	0
4	L5	3867	A2M	4	0
4	L5	4636	PSU	1	0
52	S2	681	PSU	1	0
52	S2	354	OMU	1	0
4	L5	1326	A2M	3	0
4	L5	4571	A2M	2	0
52	S2	644	OMG	1	0
4	L5	2632	PSU	1	0
4	L5	2861	OMC	1	0
52	S2	1391	OMC	4	0
4	L5	2876	OMG	1	0
4	L5	5001	PSU	1	0
4	L5	3841	OMC	1	0
4	L5	3818	UY1	1	0
52	S2	1328	OMG	1	0
4	L5	4431	PSU	1	0
4	L5	3785	A2M	1	0
4	L5	4590	A2M	1	0
4	L5	4457	PSU	1	0
52	S2	649	PSU	1	0
4	L5	2815	A2M	3	0
4	L5	4637	OMG	1	0
4	L5	4579	PSU	2	0
4	L5	4227	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	S2	27	A2M	2	0
4	L5	3825	A2M	1	0
4	L5	4456	OMC	1	0
52	S2	1031	A2M	2	0
52	S2	1703	OMC	1	0
52	S2	509	OMG	6	0
52	S2	1272	OMC	1	0
4	L5	2351	OMC	2	0
4	L5	3925	OMU	1	0
52	S2	1832	6MZ	2	0
4	L5	4196	OMG	1	0
4	L5	2804	OMC	1	0
52	S2	121	OMU	4	0
4	L5	1781	PSU	1	0
52	S2	1232	PSU	2	0
4	L5	4618	OMG	1	0
52	S2	867	OMG	1	0
4	L5	1683	PSU	3	0
52	S2	1490	OMG	1	0
4	L5	4306	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 328 ligands modelled in this entry, 307 are monoatomic - leaving 21 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	$\# Z > 2$
89	SPM	L5	5264	-	13,13,13	0.34	0	12,12,12	0.98	0
89	SPM	L5	5292	-	13,13,13	0.35	0	12,12,12	0.83	0
90	SPD	S2	1931	-	9,9,9	0.32	0	8,8,8	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
89	SPM	L5	5263	-	13,13,13	0.34	0	12,12,12	0.95	0
89	SPM	L5	5259	-	13,13,13	0.35	0	12,12,12	0.95	0
89	SPM	S2	1929	-	13,13,13	0.36	0	12,12,12	1.01	0
90	SPD	S2	1930	-	9,9,9	0.31	0	8,8,8	0.83	0
89	SPM	L5	5291	-	13,13,13	0.35	0	12,12,12	0.74	0
90	SPD	L8	202	-	9,9,9	0.33	0	8,8,8	0.86	0
89	SPM	L5	5288	-	13,13,13	0.35	0	12,12,12	1.02	0
90	SPD	L5	5290	-	9,9,9	0.32	0	8,8,8	0.68	0
90	SPD	L5	5289	-	9,9,9	0.32	0	8,8,8	0.85	0
93	PUT	S2	1932	-	5,5,5	0.24	0	4,4,4	0.52	0
90	SPD	L5	5285	-	9,9,9	0.33	0	8,8,8	0.91	0
89	SPM	L5	5267	-	13,13,13	0.34	0	12,12,12	0.97	0
90	SPD	L5	5283	88	9,9,9	0.33	0	8,8,8	0.84	0
90	SPD	L5	5261	-	9,9,9	0.32	0	8,8,8	0.94	0
90	SPD	LN	301	-	9,9,9	0.32	0	8,8,8	0.75	0
90	SPD	L5	5287	-	9,9,9	0.32	0	8,8,8	0.85	0
90	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.85	0
90	SPD	L5	5284	-	9,9,9	0.32	0	8,8,8	0.77	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
89	SPM	L5	5264	-	-	3/11/11/11	-
89	SPM	L5	5292	-	-	3/11/11/11	-
90	SPD	S2	1931	-	-	4/7/7/7	-
89	SPM	L5	5263	-	-	4/11/11/11	-
89	SPM	L5	5259	-	-	1/11/11/11	-
89	SPM	S2	1929	-	-	5/11/11/11	-
90	SPD	S2	1930	-	-	2/7/7/7	-
89	SPM	L5	5291	-	-	2/11/11/11	-
90	SPD	L8	202	-	-	2/7/7/7	-
89	SPM	L5	5288	-	-	6/11/11/11	-
90	SPD	L5	5290	-	-	3/7/7/7	-
90	SPD	L5	5289	-	-	1/7/7/7	-
93	PUT	S2	1932	-	-	0/3/3/3	-
90	SPD	L5	5285	-	-	4/7/7/7	-
89	SPM	L5	5267	-	-	4/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	SPD	L5	5283	88	-	1/7/7/7	-
90	SPD	L5	5261	-	-	0/7/7/7	-
90	SPD	LN	301	-	-	1/7/7/7	-
90	SPD	L5	5287	-	-	1/7/7/7	-
90	SPD	L5	5286	-	-	2/7/7/7	-
90	SPD	L5	5284	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
89	L5	5263	SPM	N10-C11-C12-C13
89	L5	5267	SPM	C7-C8-C9-N10
89	S2	1929	SPM	C7-C8-C9-N10
90	L5	5285	SPD	C3-C4-C5-N6
90	L8	202	SPD	C3-C4-C5-N6
90	S2	1931	SPD	N6-C7-C8-C9
89	L5	5263	SPM	N5-C6-C7-C8
89	L5	5264	SPM	N5-C6-C7-C8
89	L5	5263	SPM	C7-C6-N5-C4
90	L5	5284	SPD	C3-C4-C5-N6
89	L5	5288	SPM	C7-C6-N5-C4
89	L5	5288	SPM	C12-C11-N10-C9
90	L5	5285	SPD	C2-C3-C4-C5
89	L5	5291	SPM	C8-C9-N10-C11
89	L5	5292	SPM	C8-C9-N10-C11
90	L5	5290	SPD	C8-C7-N6-C5
90	S2	1930	SPD	C8-C7-N6-C5
90	L8	202	SPD	N6-C7-C8-C9
89	S2	1929	SPM	C2-C3-C4-N5
89	L5	5292	SPM	C3-C4-N5-C6
89	L5	5288	SPM	C8-C9-N10-C11
89	L5	5267	SPM	C6-C7-C8-C9
90	L5	5285	SPD	N6-C7-C8-C9
90	L5	5286	SPD	C2-C3-C4-C5
89	L5	5267	SPM	C11-C12-C13-N14
90	L5	5285	SPD	C7-C8-C9-N10
89	L5	5292	SPM	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
89	L5	5288	SPM	C2-C3-C4-N5
90	L5	5289	SPD	C2-C3-C4-C5
90	L5	5283	SPD	C2-C3-C4-C5
89	L5	5264	SPM	C2-C3-C4-N5
89	S2	1929	SPM	C8-C9-N10-C11
90	S2	1931	SPD	C3-C4-C5-N6
90	S2	1931	SPD	N1-C2-C3-C4
89	S2	1929	SPM	C3-C4-N5-C6
90	S2	1930	SPD	C4-C5-N6-C7
89	L5	5264	SPM	C6-C7-C8-C9
90	L5	5286	SPD	N6-C7-C8-C9
89	L5	5259	SPM	C7-C6-N5-C4
90	L5	5290	SPD	C4-C5-N6-C7
89	L5	5263	SPM	C11-C12-C13-N14
90	L5	5284	SPD	N6-C7-C8-C9
90	S2	1931	SPD	C4-C5-N6-C7
89	S2	1929	SPM	C6-C7-C8-C9
90	L5	5287	SPD	C8-C7-N6-C5
89	L5	5288	SPM	C3-C4-N5-C6
89	L5	5288	SPM	N1-C2-C3-C4
90	L5	5290	SPD	C7-C8-C9-N10
90	LN	301	SPD	C8-C7-N6-C5
89	L5	5291	SPM	C7-C8-C9-N10
89	L5	5267	SPM	C12-C11-N10-C9

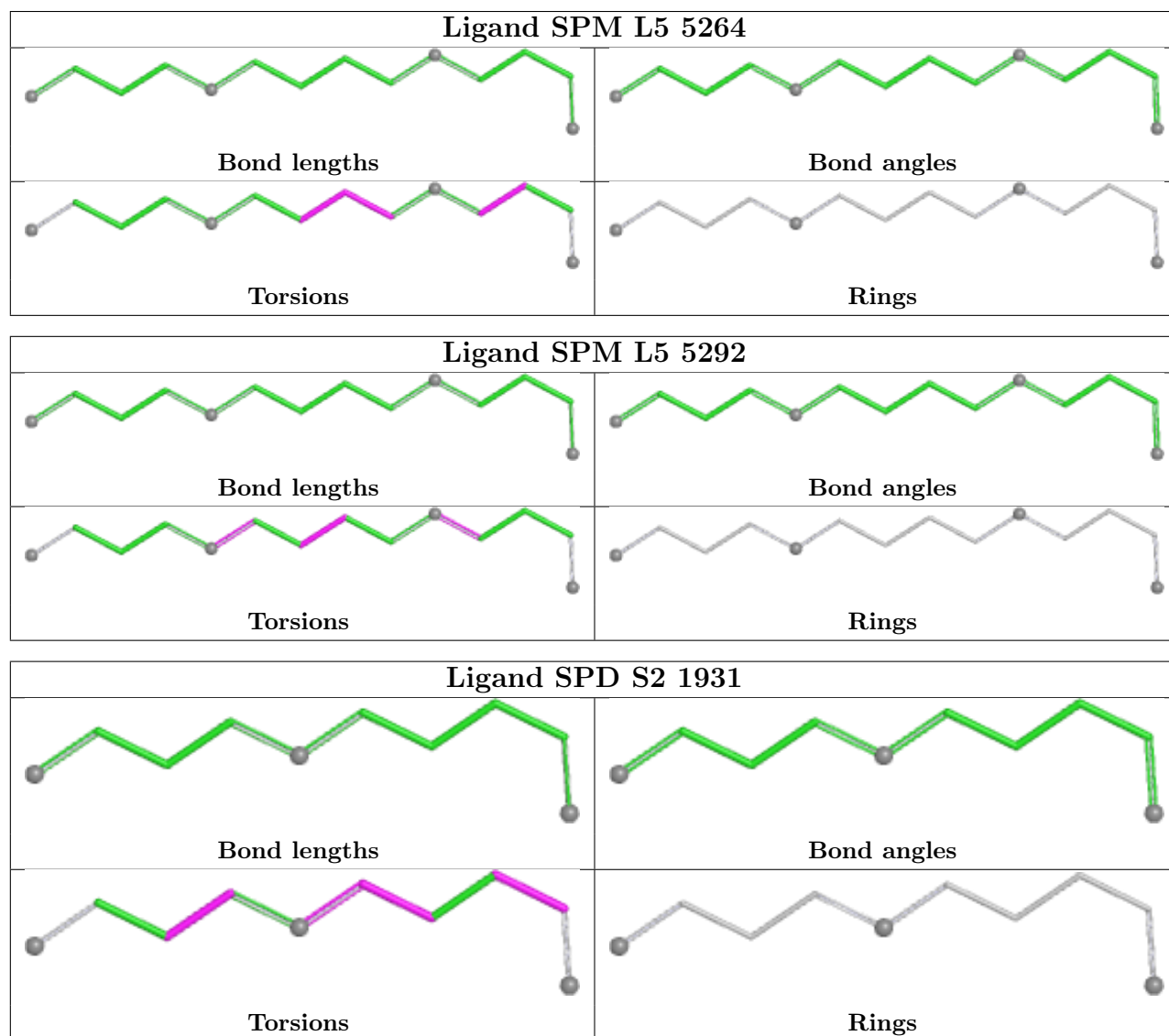
There are no ring outliers.

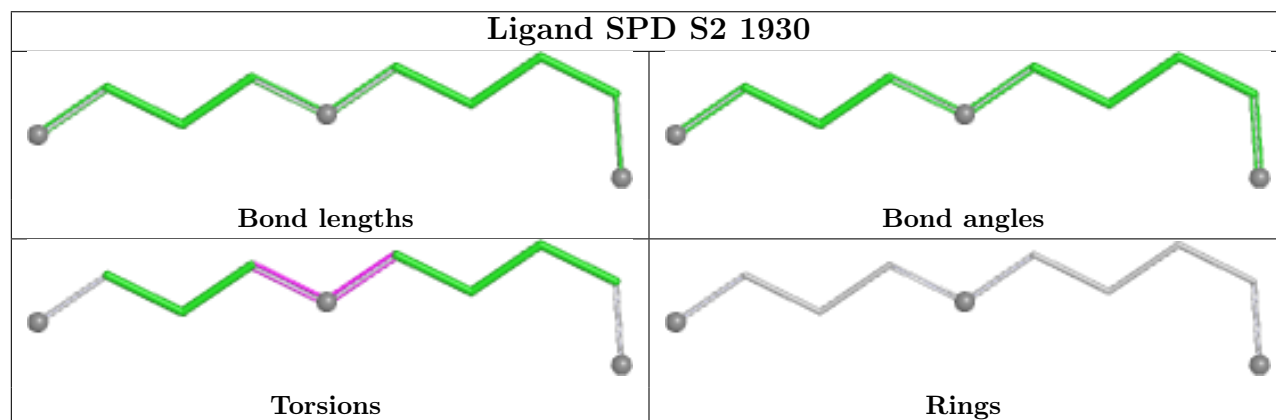
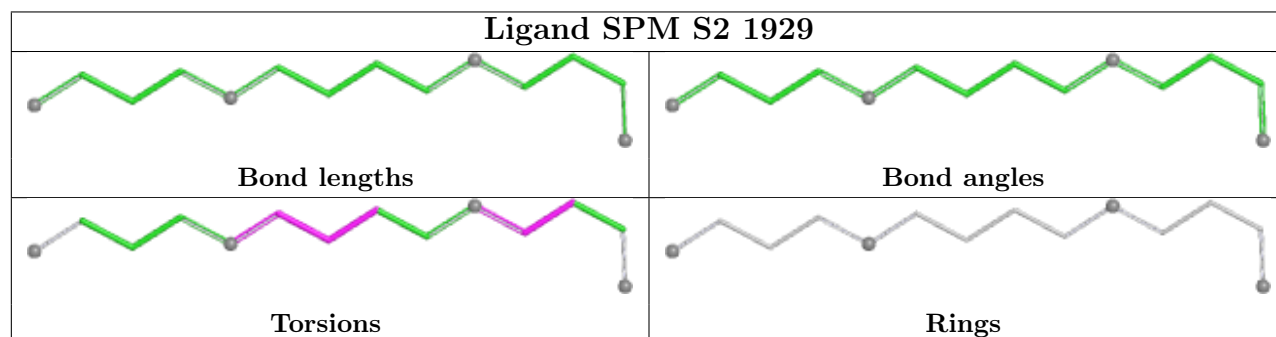
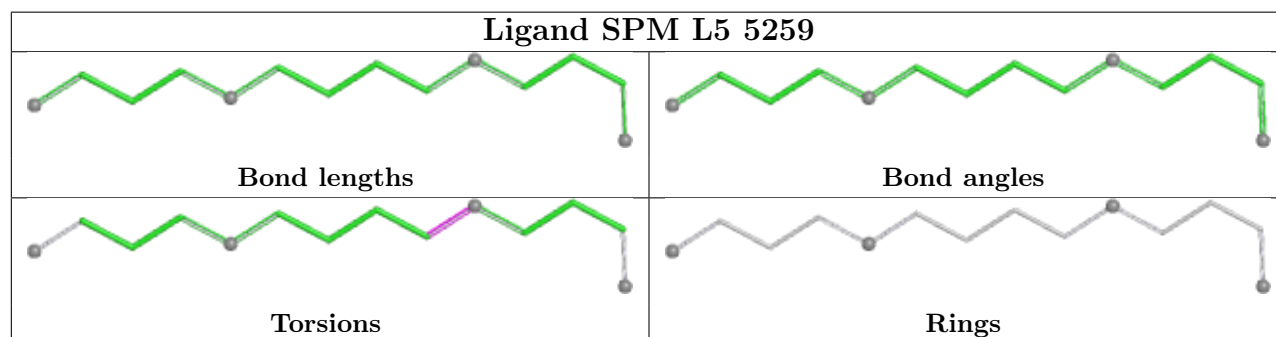
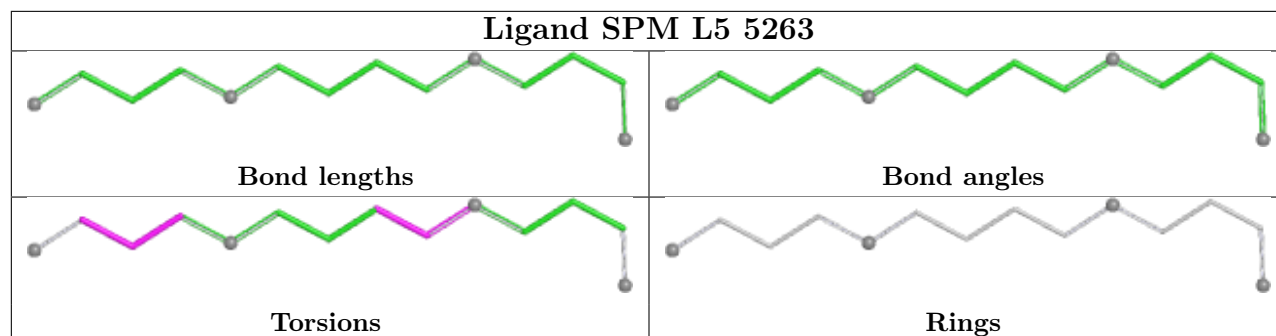
9 monomers are involved in 15 short contacts:

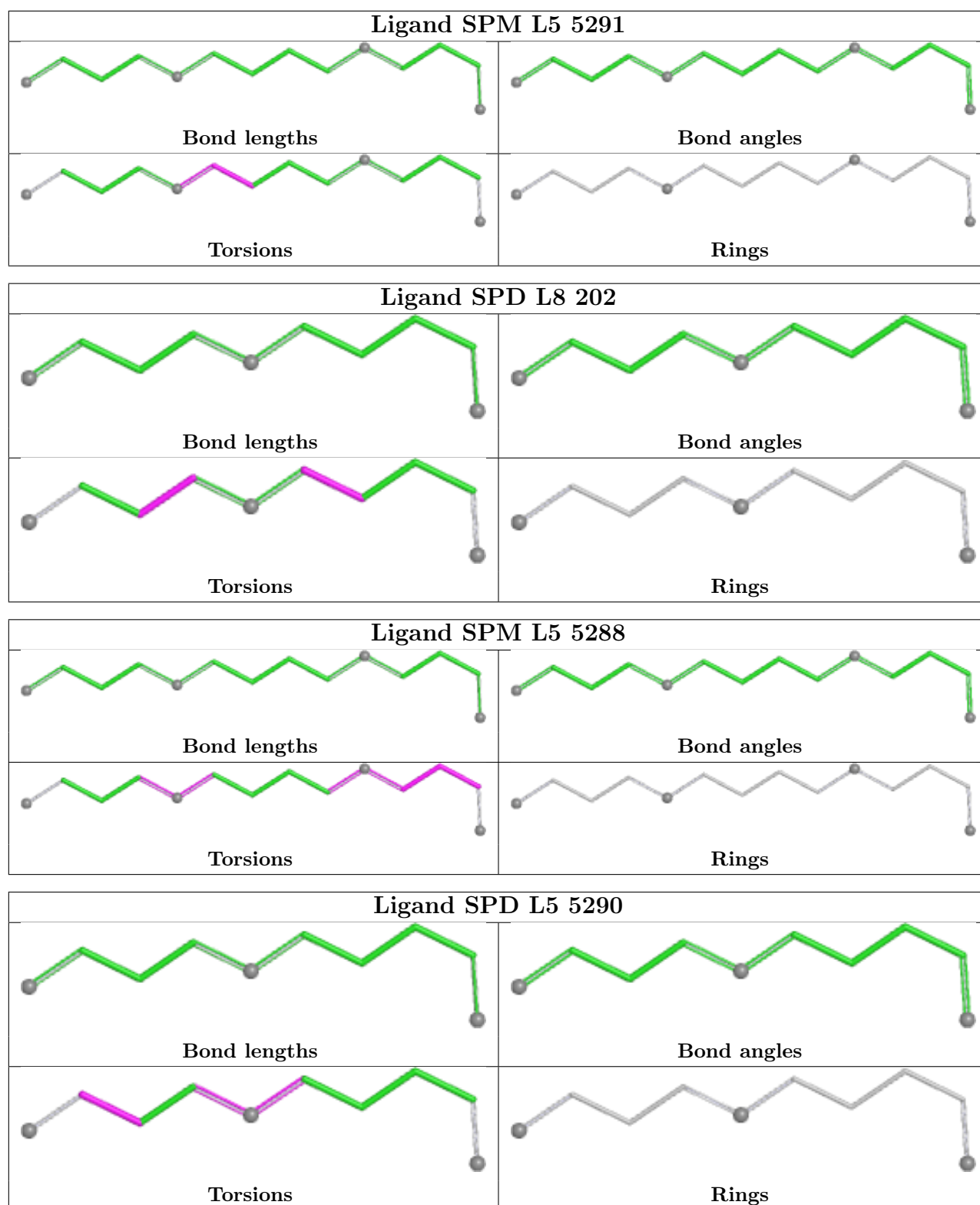
Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	L5	5264	SPM	2	0
89	L5	5292	SPM	4	0
89	L5	5259	SPM	2	0
89	S2	1929	SPM	2	0
89	L5	5291	SPM	1	0
89	L5	5288	SPM	1	0
90	L5	5290	SPD	1	0
90	L5	5261	SPD	1	0
90	L5	5284	SPD	1	0

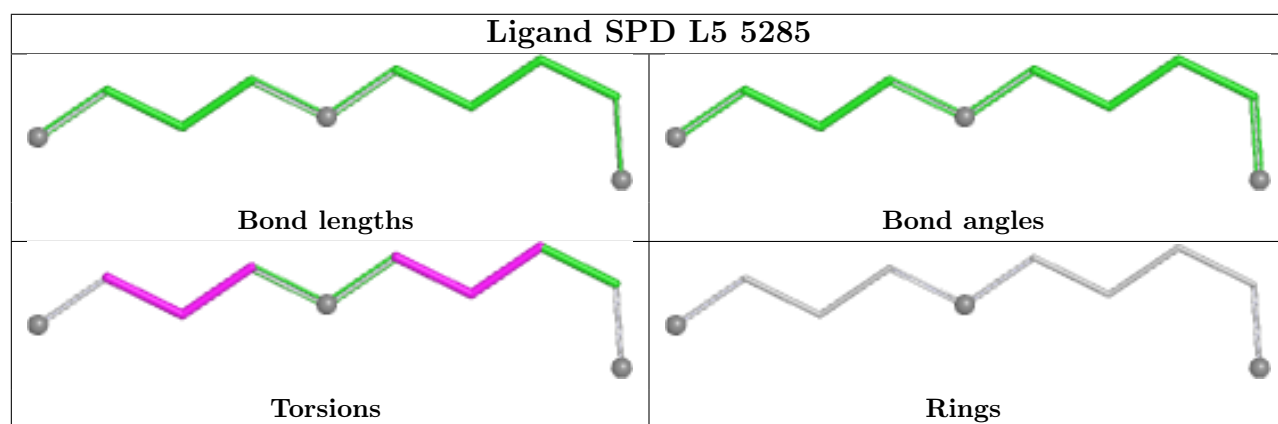
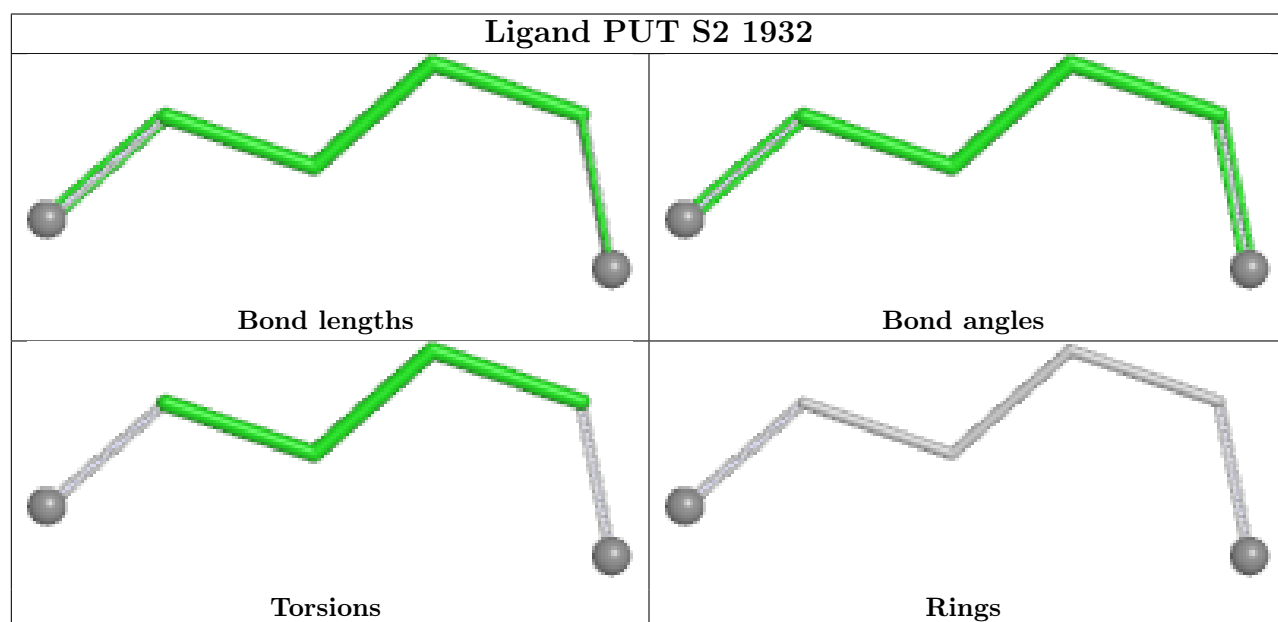
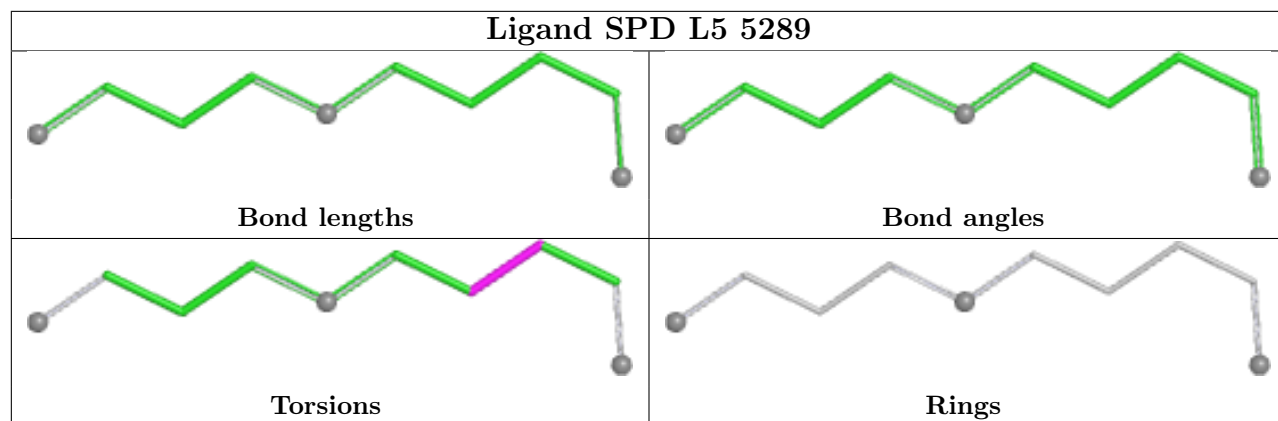
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

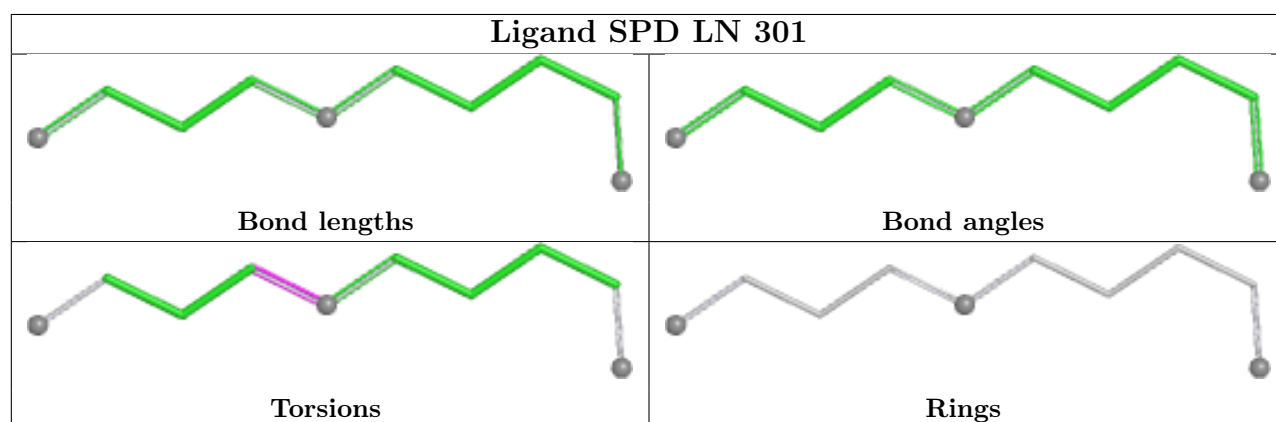
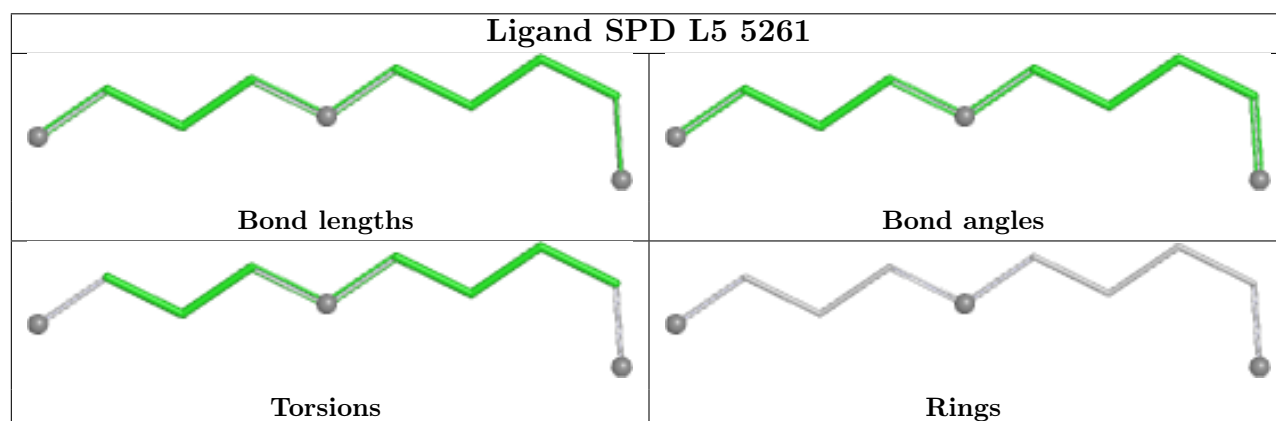
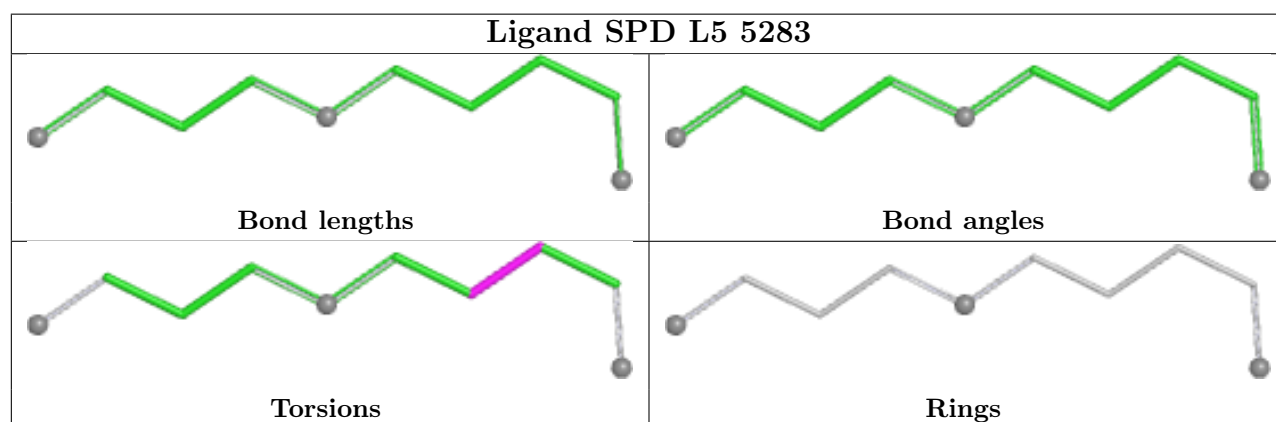
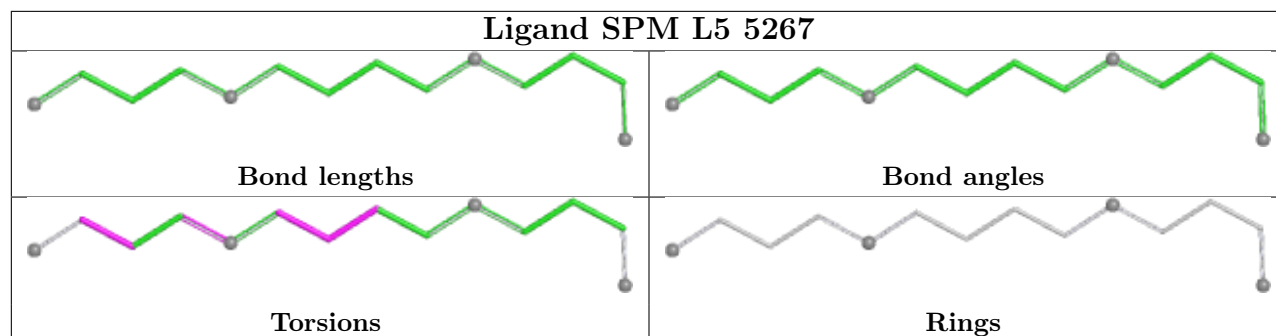
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

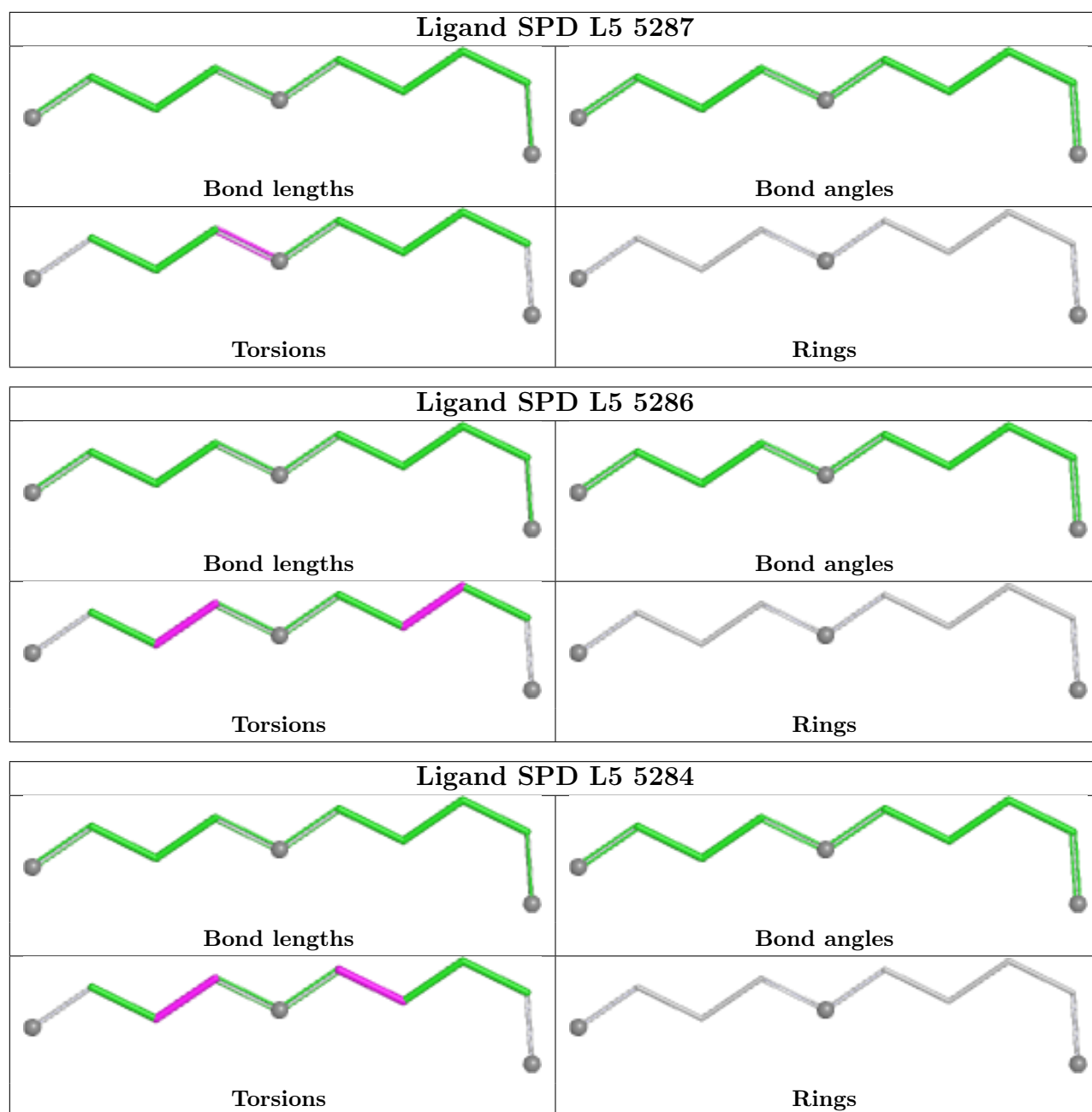












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
52	S2	5

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Mol	Chain	Number of breaks
33	Lb	1
50	Lt	1
60	SH	1
51	Pt	1
86	AT	1
87	CA	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	35.22
1	S2	753:C	O3'	785:C	P	28.37
1	S2	739:C	O3'	746:C	P	13.09
1	S2	698:G	O3'	730:C	P	12.71
1	Lt	87:GLU	C	104:ILE	N	12.55
1	SH	107:LYS	C	111:LYS	N	11.54
1	Pt	15:G	O3'	18:G	P	10.59
1	S2	225:G	O3'	287:U	P	6.98
1	AT	16:C	O3'	18:G	P	4.99
1	CA	283:PHE	C	286:GLU	N	3.31
1	S2	1210:G	O3'	1211:G	P	3.16

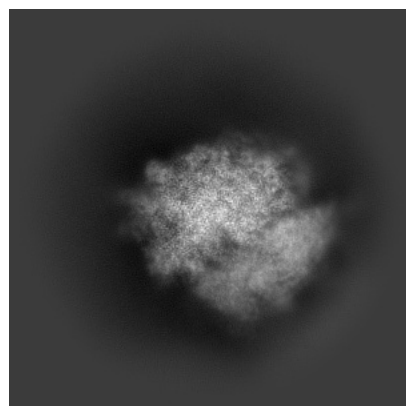
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71435. These allow visual inspection of the internal detail of the map and identification of artifacts.

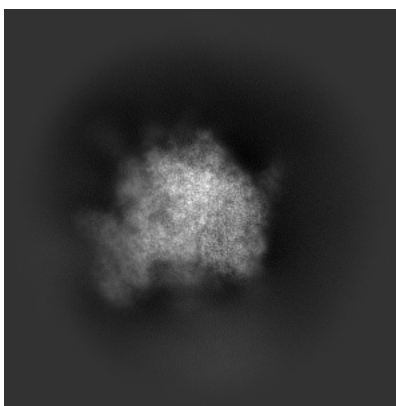
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

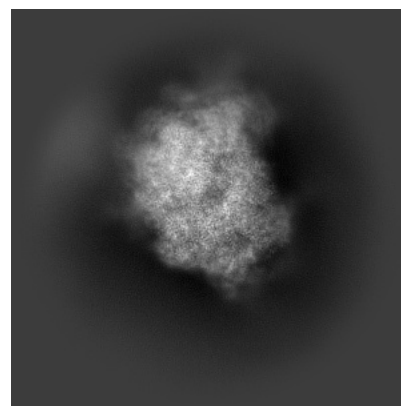
6.1.1 Primary map



X

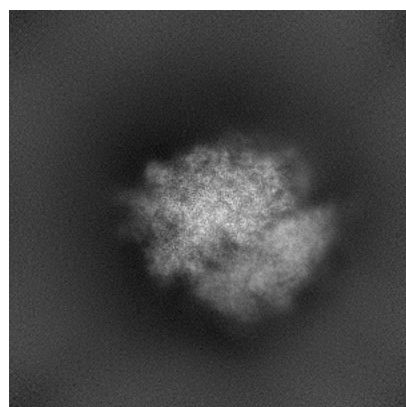


Y

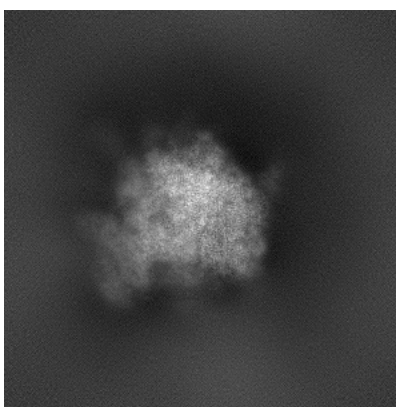


Z

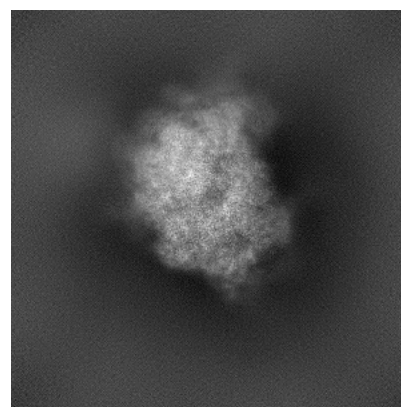
6.1.2 Raw map



X



Y

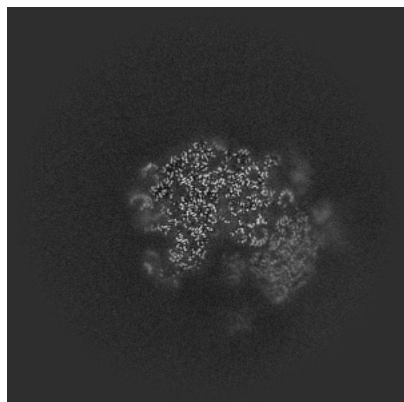


Z

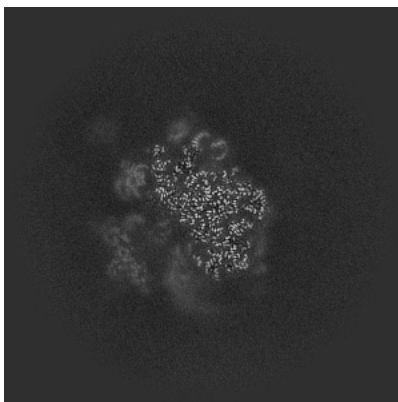
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

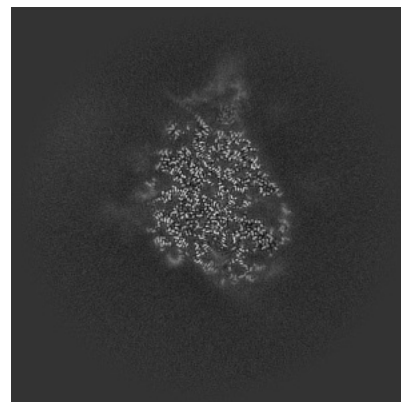
6.2.1 Primary map



X Index: 256

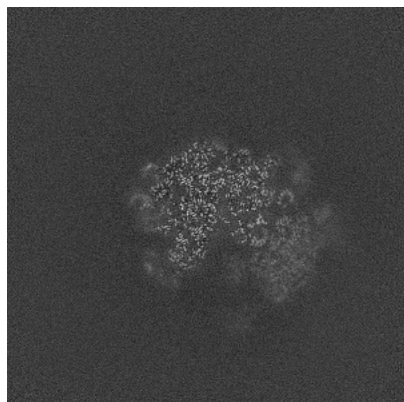


Y Index: 256

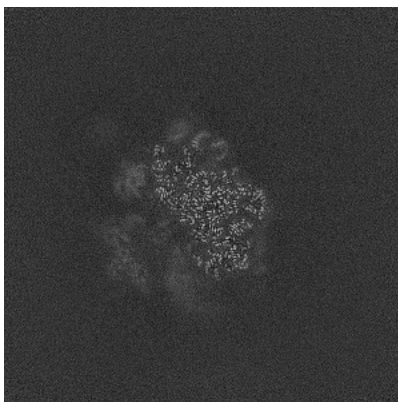


Z Index: 256

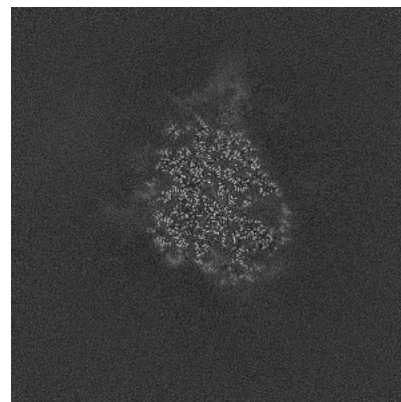
6.2.2 Raw map



X Index: 256



Y Index: 256

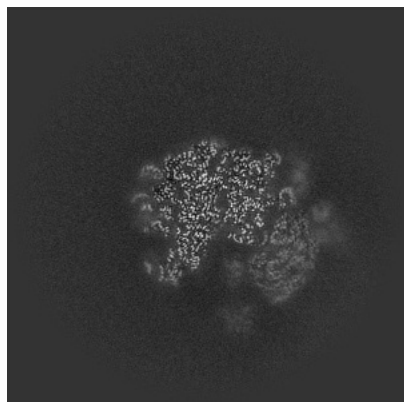


Z Index: 256

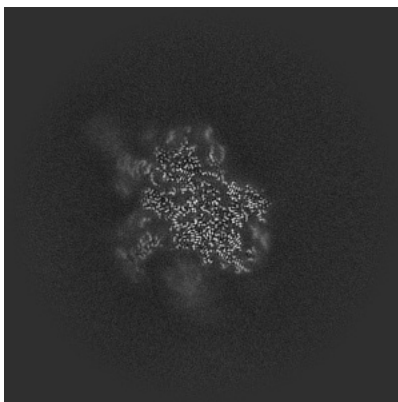
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

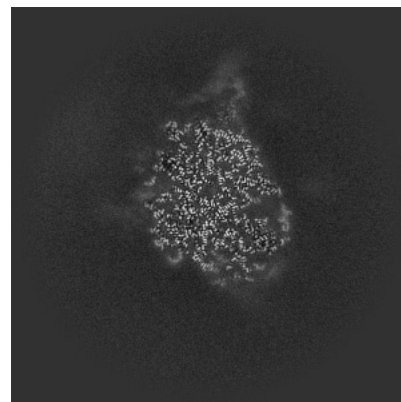
6.3.1 Primary map



X Index: 253

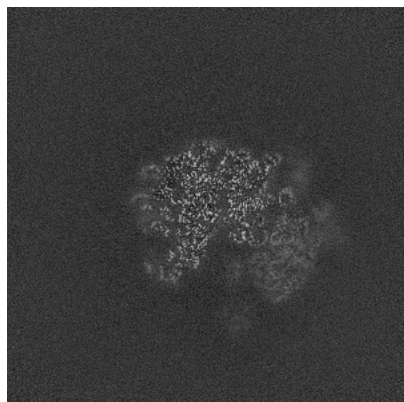


Y Index: 243

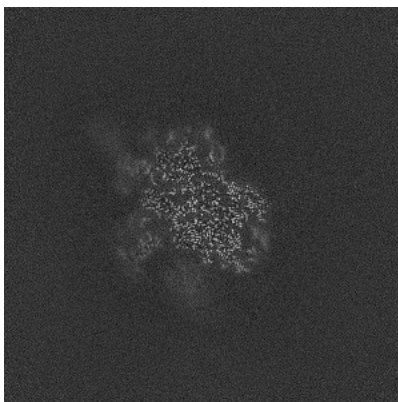


Z Index: 258

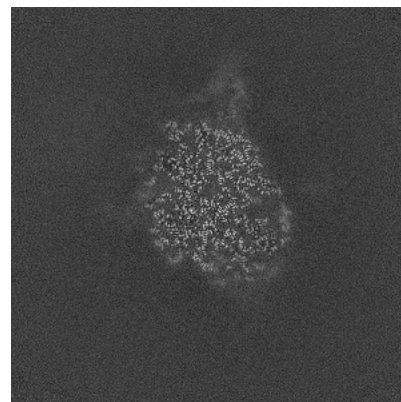
6.3.2 Raw map



X Index: 254



Y Index: 243

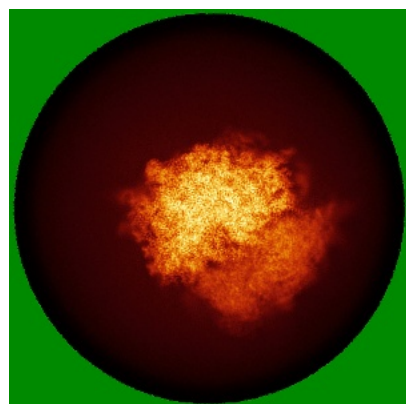


Z Index: 258

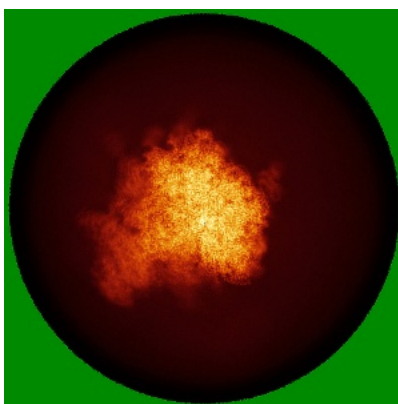
The images above show the largest variance slices of the map in three orthogonal directions.

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

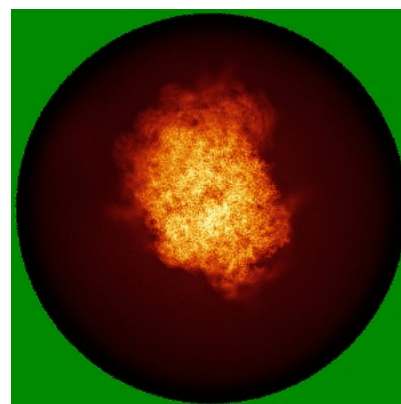
6.4.1 Primary map



X

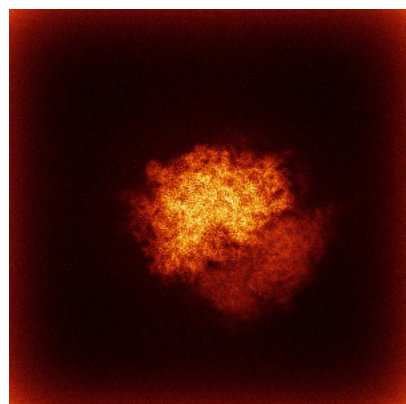


Y

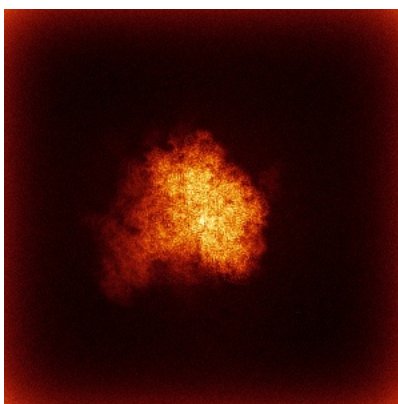


Z

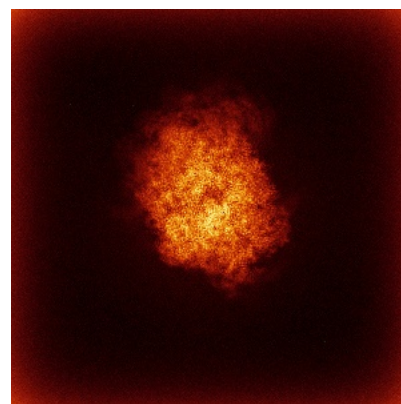
6.4.2 Raw map



X



Y

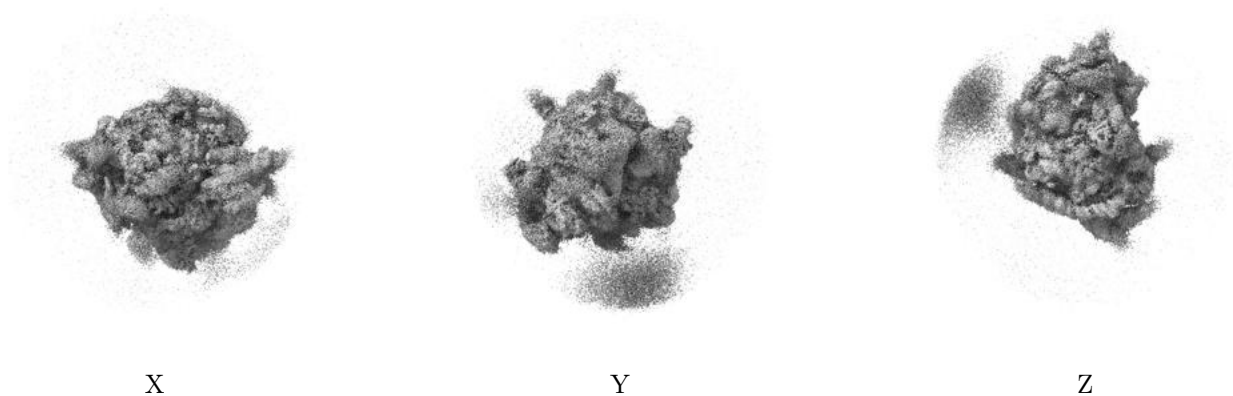


Z

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

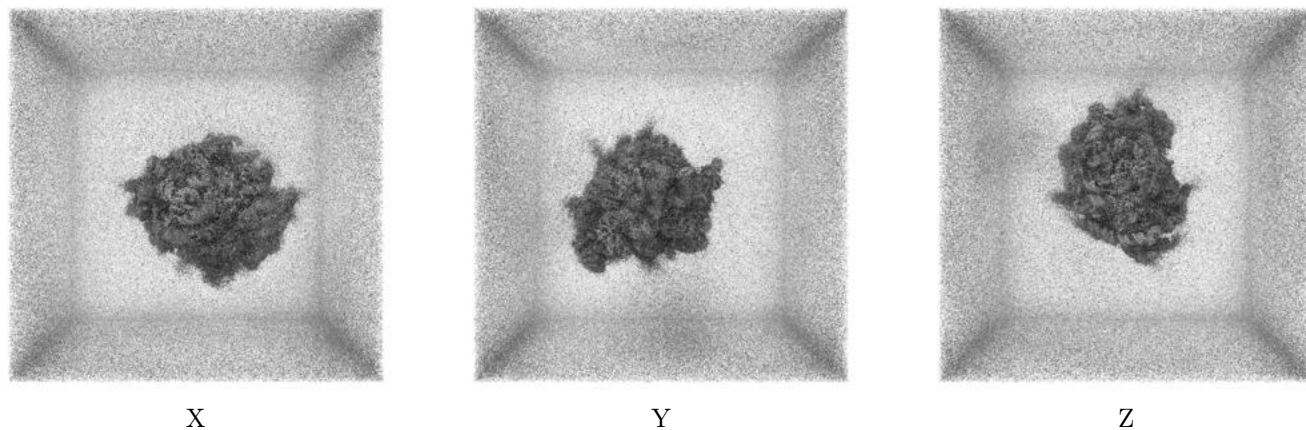
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0575. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

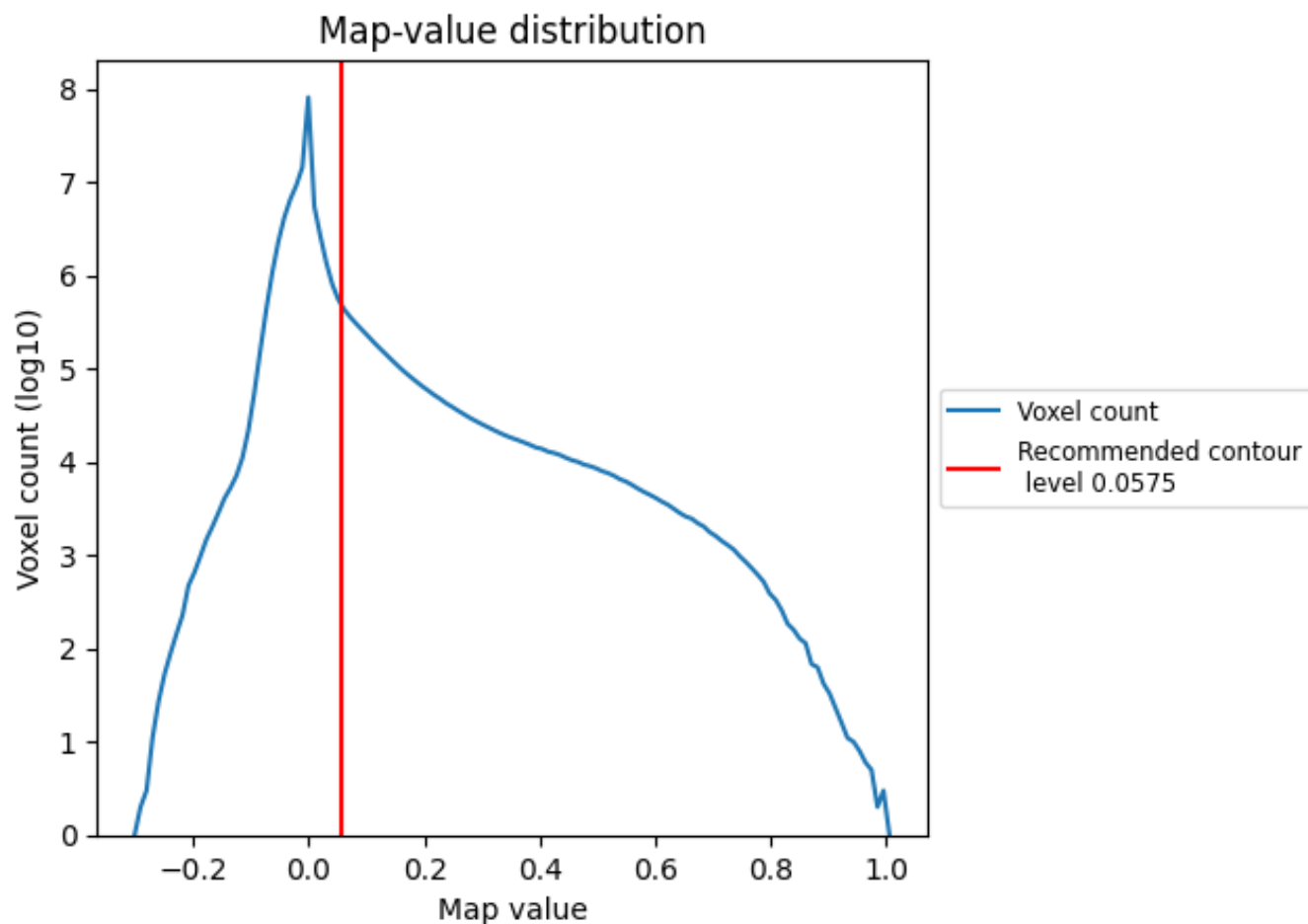
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

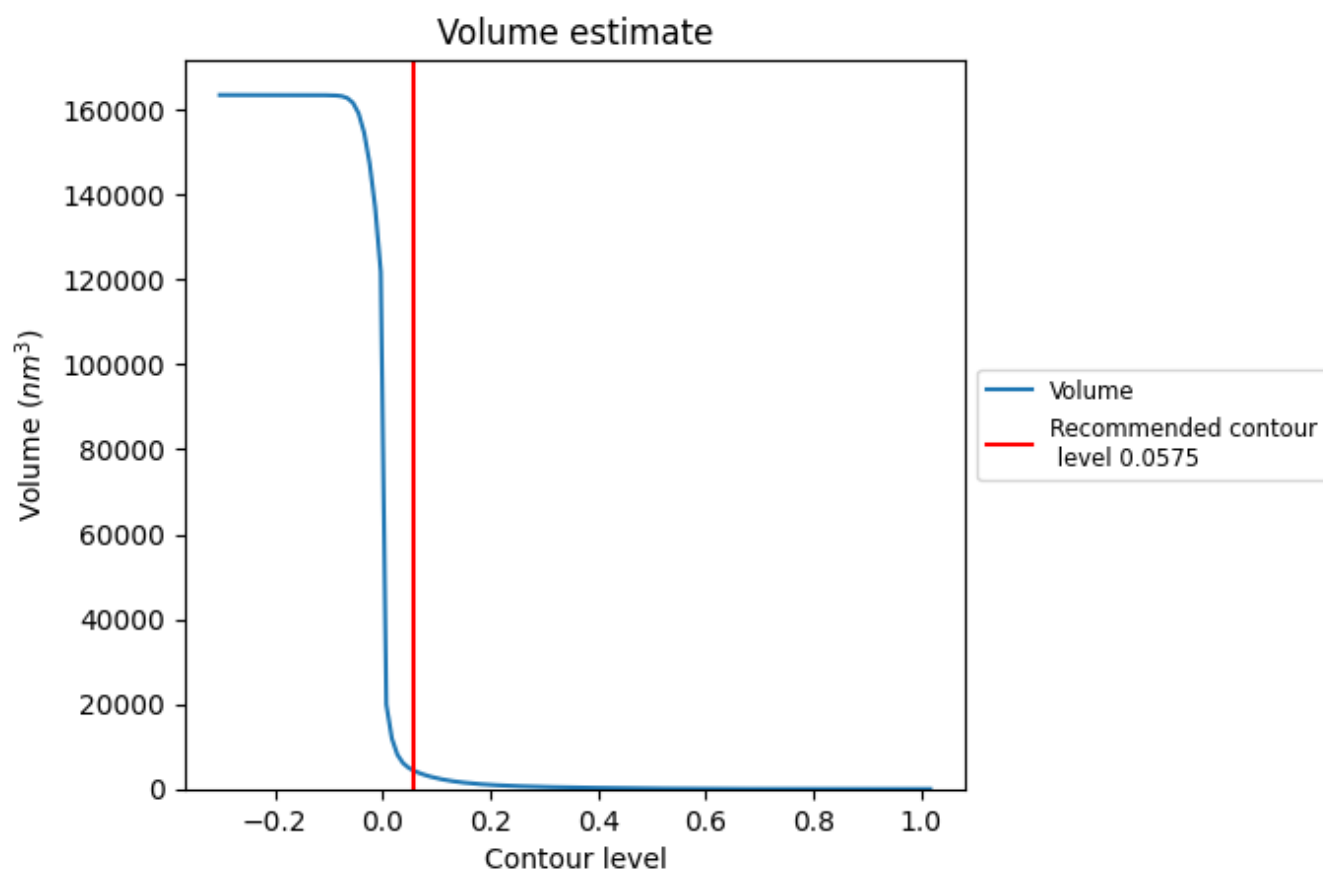
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

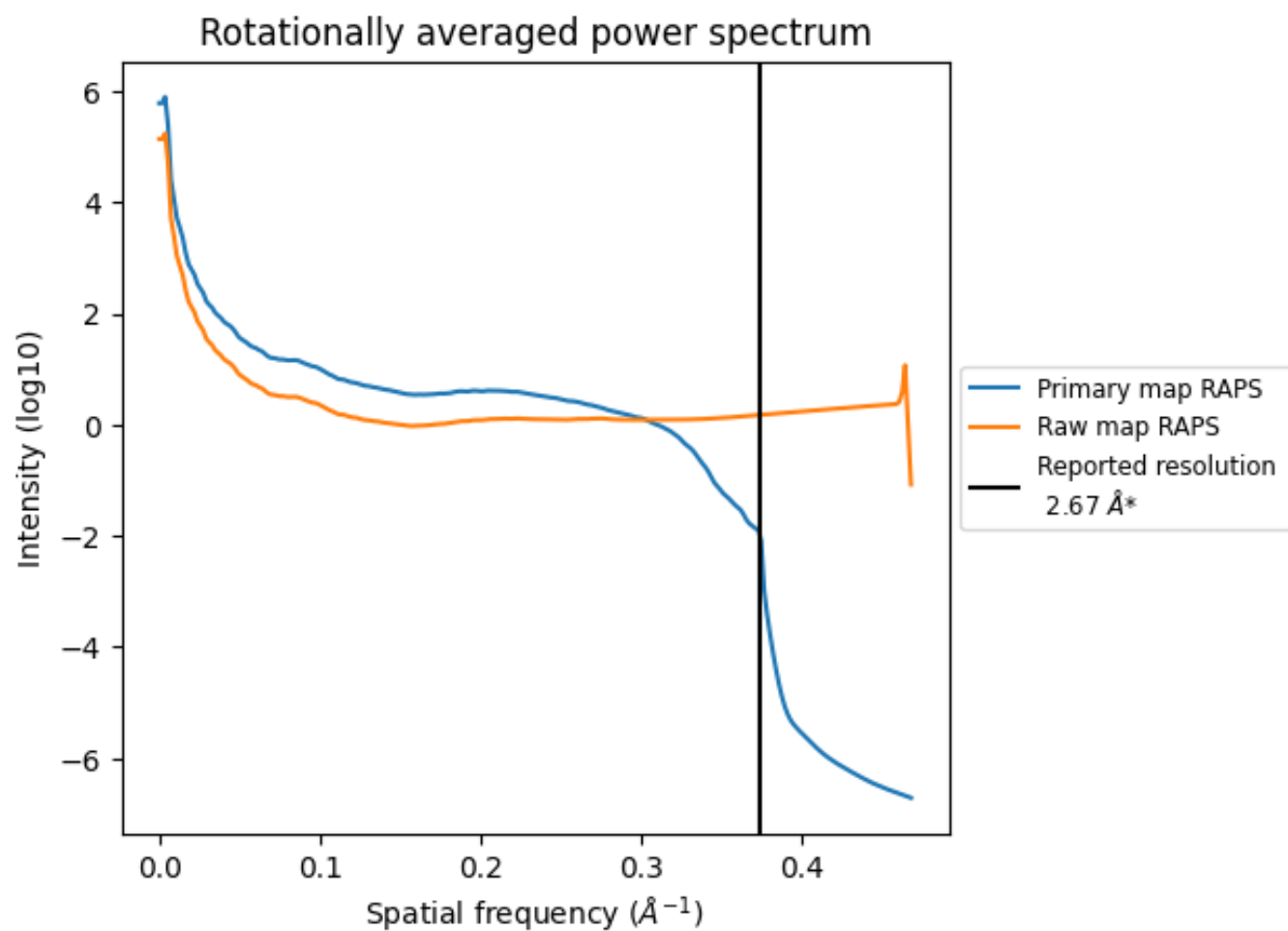
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4349 nm^3 ; this corresponds to an approximate mass of 3929 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 ⓘ

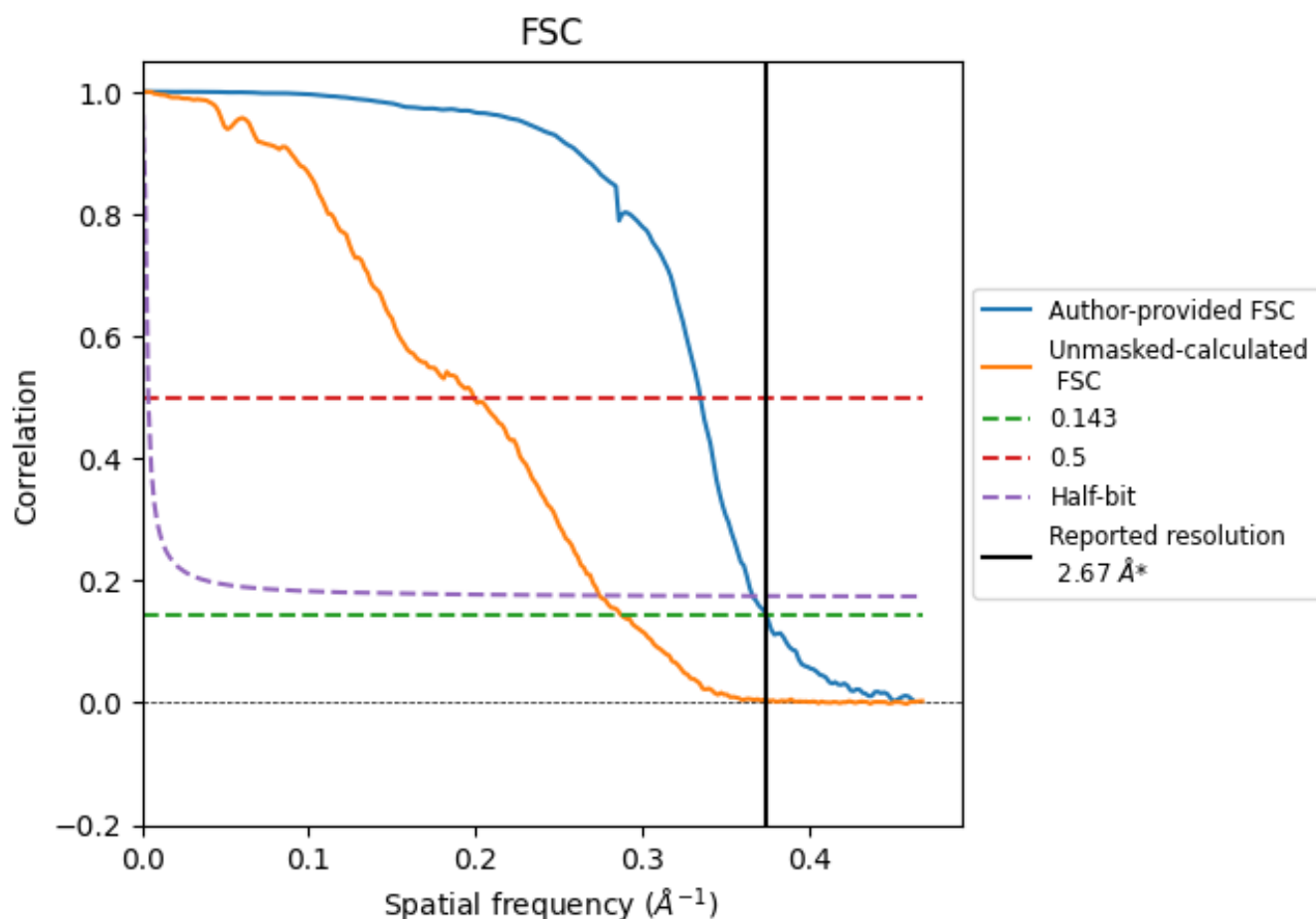


*Reported resolution corresponds to spatial frequency of 0.375 Å⁻¹

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 0.375 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

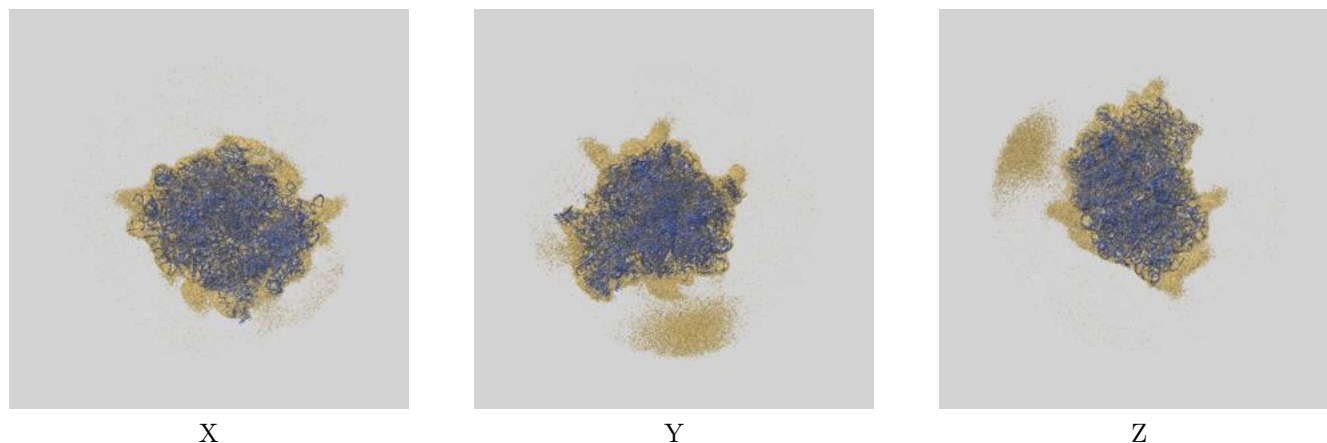
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.67	-	-
Author-provided FSC curve	2.67	2.99	2.73
Unmasked-calculated*	3.48	5.03	3.65

*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 3.48 differs from the reported value 2.67 by more than 10 %

9 Map-model fit [i](#)

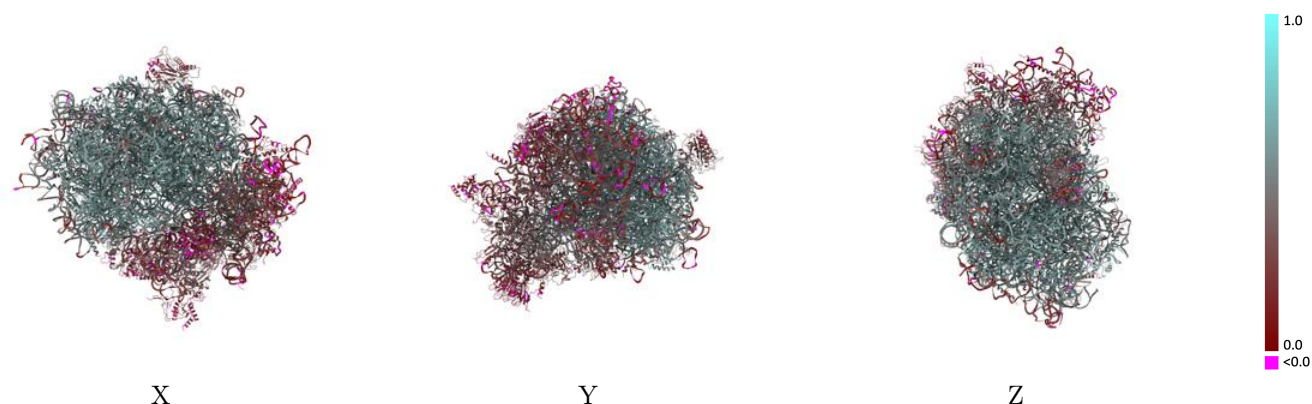
This section contains information regarding the fit between EMDB map EMD-71435 and PDB model 9PA7. Per-residue inclusion information can be found in [section 3](#) on [page 28](#).

9.1 Map-model overlay [i](#)



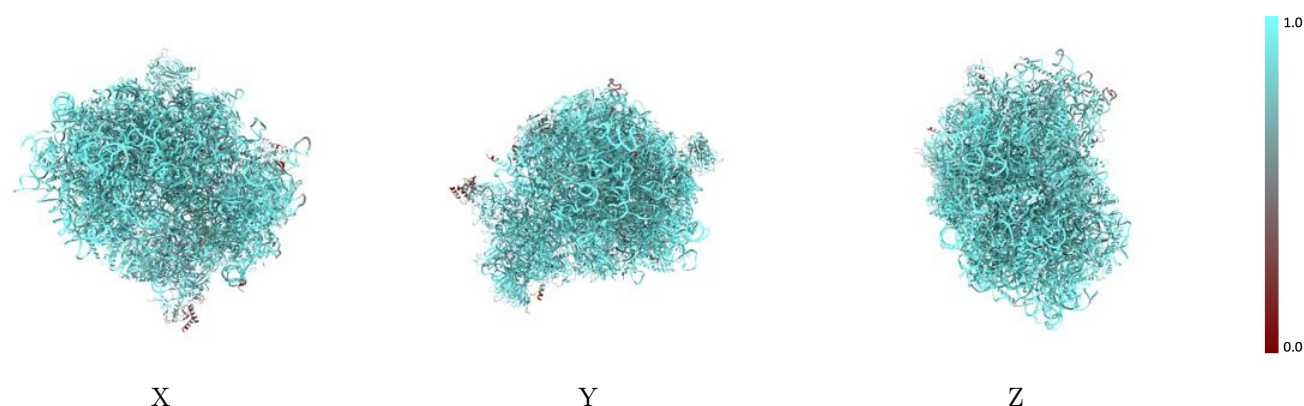
The images above show the 3D surface view of the map at the recommended contour level 0.0575 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



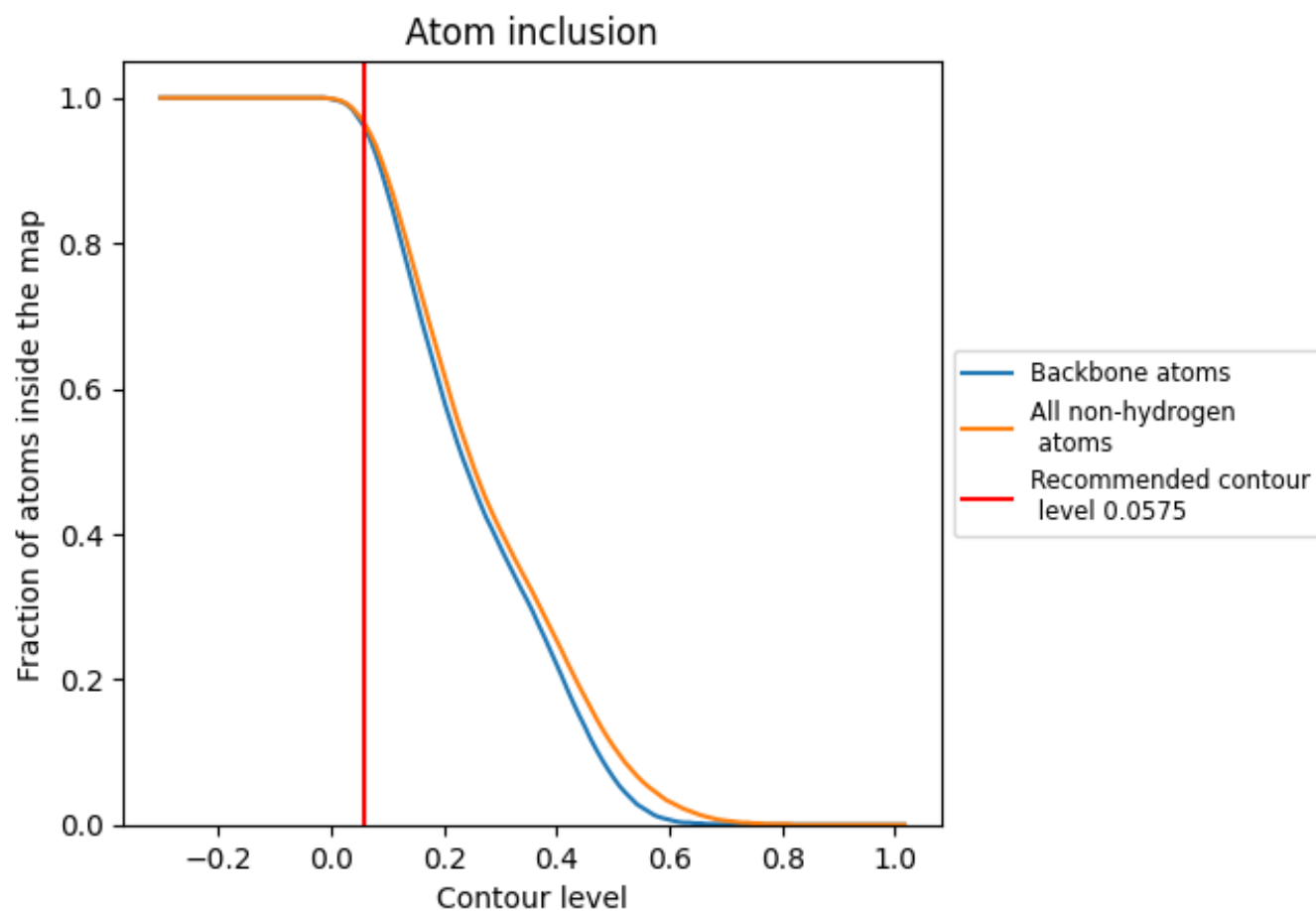
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0575).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 97% 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 (0.0575) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9680	 0.4530
AT	 0.9150	 0.1400
CA	 0.8400	 0.2860
CD	 0.8660	 0.4180
CF	 0.7510	 0.1490
CI	 0.8790	 0.4240
L5	 0.9950	 0.5320
L7	 1.0000	 0.5760
L8	 0.9960	 0.5550
LA	 0.9980	 0.5920
LB	 0.9830	 0.5790
LC	 0.9850	 0.5750
LD	 0.9830	 0.5410
LE	 0.9800	 0.5170
LF	 0.9920	 0.5790
LG	 0.9620	 0.5210
LH	 0.9910	 0.5700
LI	 0.9900	 0.5780
LJ	 0.9600	 0.4900
LL	 0.9680	 0.5510
LM	 0.9890	 0.5640
LN	 1.0000	 0.6050
LO	 0.9910	 0.5840
LP	 0.9950	 0.5920
LQ	 0.9980	 0.6020
LR	 0.9230	 0.5160
LS	 0.9990	 0.6020
LT	 0.9830	 0.5630
LU	 0.9700	 0.4910
LV	 0.9950	 0.5790
LW	 0.9310	 0.3790
LX	 0.9850	 0.5650
LY	 0.9900	 0.5690
LZ	 0.9960	 0.5640
La	 0.9960	 0.6030



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Chain	Atom inclusion	Q-score
Lb	 0.9590	 0.5150
Lc	 0.9720	 0.5320
Ld	 0.9840	 0.5640
Le	 0.9920	 0.5970
Lf	 0.9960	 0.6040
Lg	 0.9870	 0.5670
Lh	 0.9850	 0.5620
Li	 0.9900	 0.5590
Lj	 0.9960	 0.5980
Lk	 0.9700	 0.5080
Ll	 0.9950	 0.5790
Lm	 0.9830	 0.5860
Ln	 0.9860	 0.5510
Lo	 0.9870	 0.5770
Lp	 0.9860	 0.5690
Lr	 0.9900	 0.5850
Ls	 0.9040	 0.2910
Lt	 0.8120	 0.1510
Pt	 0.9400	 0.3930
S2	 0.9840	 0.3550
SA	 0.9290	 0.3820
SB	 0.9480	 0.3720
SC	 0.9810	 0.4300
SD	 0.9440	 0.3210
SE	 0.9450	 0.2820
SF	 0.9340	 0.2290
SG	 0.9190	 0.2510
SH	 0.8670	 0.2620
SI	 0.8580	 0.3570
SJ	 0.9350	 0.3140
SK	 0.8830	 0.2750
SL	 0.8590	 0.3580
SM	 0.4280	 0.1080
SN	 0.9660	 0.4090
SO	 0.9290	 0.4010
SP	 0.8800	 0.1820
SQ	 0.9610	 0.2370
SR	 0.9020	 0.2720
SS	 0.8660	 0.1650
ST	 0.9140	 0.2040
SU	 0.9150	 0.2810
SV	 0.9730	 0.3960

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Chain	Atom inclusion	Q-score
SW	 0.9800	 0.4060
SX	 0.9600	 0.3740
SY	 0.9290	 0.2080
SZ	 0.8410	 0.1190
Sa	 0.9630	 0.4210
Sb	 0.9300	 0.3390
Sc	 0.9220	 0.2370
Sd	 0.9910	 0.3520
Se	 0.9300	 0.2630
Sf	 0.7950	 0.1290
Sg	 0.8980	 0.1680