



Full wwPDB EM Validation Report ⓘ

Jul 6, 2026 – 04:15 pm BST

PDB ID : 9RU7 / pdb_00009ru7
EMDB ID : EMD-54265
Title : WT-HEK 80S ribosome bound to Kozak mRNA (WT-Kozak)
Authors : Hiregange, D.G.; Fraticelli, D.; Bashan, A.; Yonath, A.; Dikstein, R.
Deposited on : 2025-07-03
Resolution : 3.00 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:

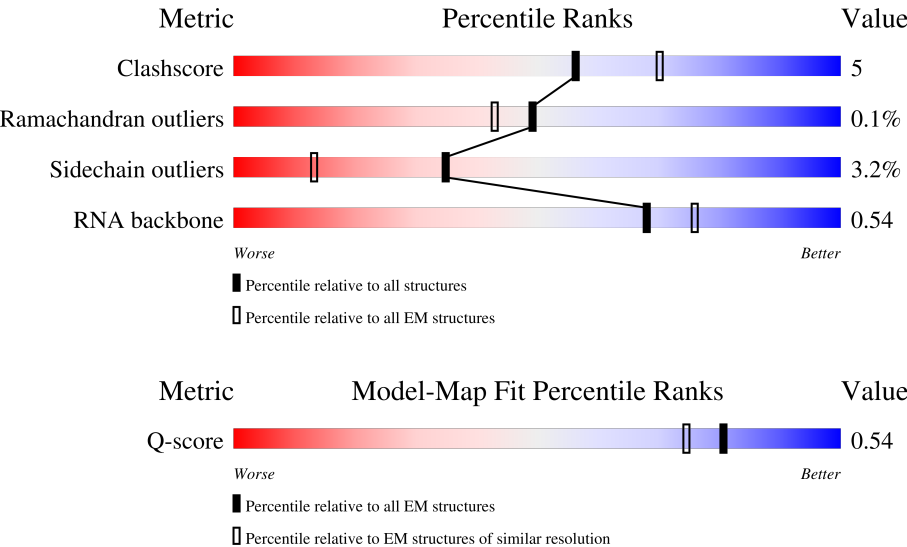
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.00 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.



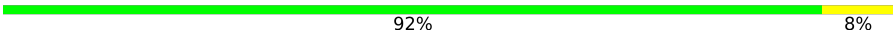
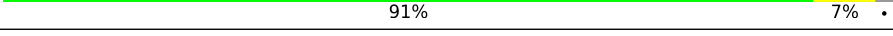
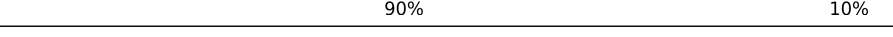
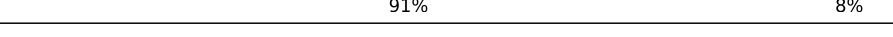
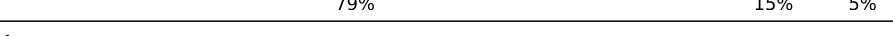
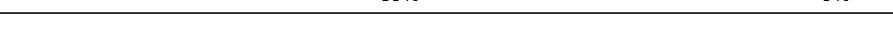
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	SP	145	
2	L8	156	
3	L5	5069	

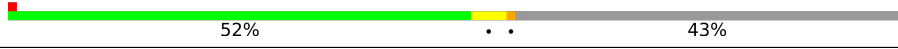
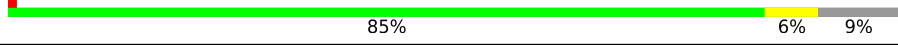
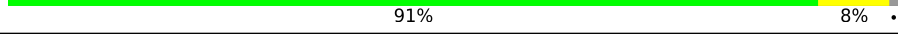
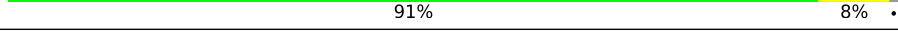
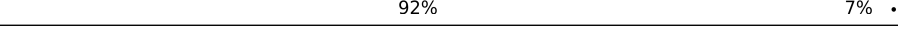
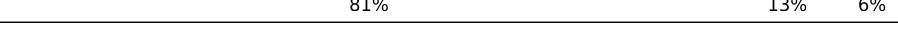
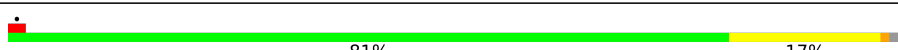
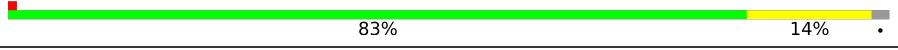
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Mol	Chain	Length	Quality of chain
4	LA	252	
5	LB	396	
6	LC	427	
7	LJ	178	
8	LH	192	
9	LE	288	
10	LG	266	
11	LO	203	
12	LL	211	
13	LV	140	
14	LM	136	
15	La	148	
16	LN	204	
17	LI	214	
18	LD	297	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LP	154	
24	LU	128	
25	LX	156	
26	LY	145	
27	LW	157	
28	LZ	136	

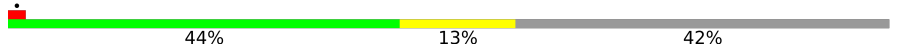
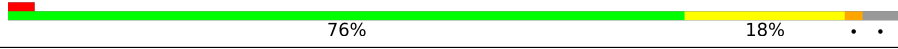
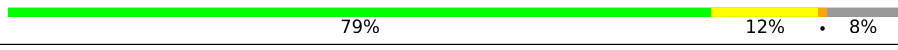
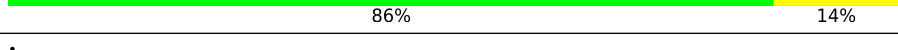
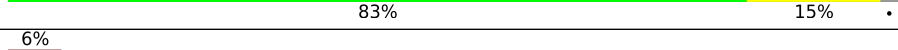
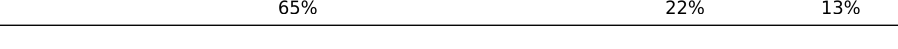
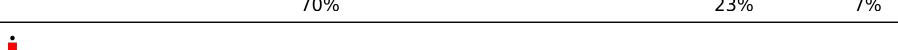
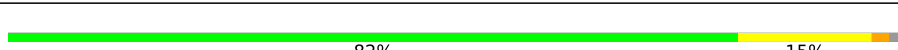
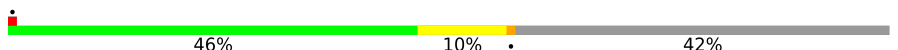
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Mol	Chain	Length	Quality of chain
29	Lr	137	
30	Lh	123	
31	Lb	159	
32	LF	248	
33	Lc	115	
34	Ld	125	
35	Le	129	
36	Lf	110	
37	Lg	109	
38	Li	105	
39	Lj	87	
40	Lk	70	
41	Ll	51	
42	Lm	128	
43	Ln	25	
44	Lo	106	
45	Lp	89	
46	Pt	77	
47	L7	120	
48	SA	295	
49	SB	264	
50	SE	263	
51	SF	204	
52	SH	194	
53	SI	208	

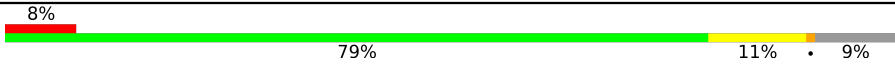
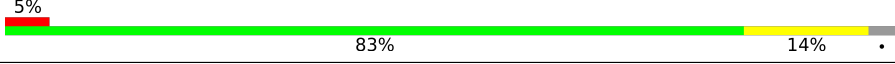
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Mol	Chain	Length	Quality of chain
54	SK	165	
55	SL	158	
56	SQ	146	
57	SS	152	
58	ST	145	
59	SU	119	
60	SV	83	
61	SX	143	
62	Sc	69	
63	Sd	56	
64	SC	293	
65	SG	249	
66	SJ	194	
67	SN	151	
68	SO	151	
69	SW	130	
70	SY	133	
71	SZ	125	
72	Sb	84	
73	Se	133	
74	Sa	115	
75	S2	1868	
76	mR	27	
77	S6	74	
78	Sg	317	

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Mol	Chain	Length	Quality of chain
79	SD	243	
80	SM	132	
81	SR	135	
82	Sf	156	

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 199163 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 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	SP	129	Total	C	N	O	S	0	0
			814	505	163	144	2		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L8	151	Total	C	N	O	P	0	0
			3215	1434	570	1060	151		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3376	Total	C	N	O	P	1	0
			72477	32309	13259	23532	3377		

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LA	251	Total	C	N	O	S	0	0
			1895	1188	391	310	6		

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB	395	Total	C	N	O	S	0	0
			2719	1725	544	442	8		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	365	Total	C	N	O	S	0	0
			2836	1786	570	467	13		

- Molecule 7 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LJ	168	Total	C	N	O	S	0	0
			1207	773	230	199	5		

- Molecule 8 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LH	190	Total	C	N	O	S	0	0
			1435	911	275	243	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LE	208	Total	C	N	O	S	0	0
			1584	1018	302	260	4		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	230	Total	C	N	O	S	1	0
			1696	1082	326	285	3		

- Molecule 11 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LO	199	Total	C	N	O	S	0	0
			1605	1036	317	248	4		

- Molecule 12 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LL	206	Total	C	N	O	S	0	0
			1583	992	335	252	4		

- Molecule 13 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LV	132	Total	C	N	O	S	0	0
			943	596	178	164	5		

- Molecule 14 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LM	136	Total	C	N	O	S	0	0
			1089	700	212	170	7		

- Molecule 15 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	La	147	Total	C	N	O	S	1	0
			1157	731	239	184	3		

- Molecule 16 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LN	203	Total	C	N	O	S	0	0
			1694	1069	356	265	4		

- Molecule 17 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LI	203	Total	C	N	O	S	0	0
			1610	1024	313	261	12		

- Molecule 18 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LD	293	Total	C	N	O	S	0	0
			2232	1417	416	387	12		

- Molecule 19 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	187	Total	C	N	O	S	0	0
			1497	936	312	244	5		

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	175	Total	C	N	O	S	0	0
			1391	864	298	220	9		

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	176	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 22 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LT	159	Total	C	N	O	S	0	0
			1221	773	241	202	5		

- Molecule 23 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 24 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LU	99	Total	C	N	O	S	0	0
			781	504	139	136	2		

- Molecule 25 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LX	118	Total	C	N	O	S	0	0
			955	612	180	162	1		

- Molecule 26 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LY	130	Total	C	N	O	S	0	0
			1057	665	215	174	3		

- Molecule 27 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LW	61	Total	C	N	O	S	0	0
			515	330	100	82	3		

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LZ	135	Total	C	N	O	S	0	0
			1088	703	205	177	3		

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lr	122	Total	C	N	O	S	0	0
			973	603	202	164	4		

- Molecule 30 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lh	122	Total	C	N	O	S	0	0
			954	604	197	152	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lb	91	Total	C	N	O	S	0	0
			700	437	150	111	2		

- Molecule 32 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LF	225	Total	C	N	O	S	0	0
			1756	1123	337	289	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lc	98	Total	C	N	O	S	0	0
			740	469	132	134	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ld	107	Total	C	N	O	S	0	0
			877	554	170	151	2		

- Molecule 35 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Le	128	Total	C	N	O	S	0	0
			1045	661	214	165	5		

- Molecule 36 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lf	109	Total	C	N	O	S	0	0
			860	546	174	137	3		

- Molecule 37 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lg	108	Total	C	N	O	S	0	0
			838	522	175	135	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Li	99	Total	C	N	O	S	0	0
			756	474	159	119	4		

- Molecule 39 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lj	86	Total	C	N	O	S	0	0
			695	427	153	110	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lk	68	Total	C	N	O	S	0	0
			545	350	98	96	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ll	50	Total	C	N	O	S	0	0
			433	275	94	63	1		

- Molecule 42 is a protein called Ubiquitin-ribosomal protein eL40 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lm	51	Total	C	N	O	S	0	0
			408	253	87	63	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ln	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 44 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lo	105	Total	C	N	O	S	1	0
			849	535	170	138	6		

- Molecule 45 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lp	88	Total	C	N	O	S	1	0
			682	429	133	113	7		

- Molecule 46 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	Pt	76	Total	C	N	O	P	S	0	0
			1624	724	296	527	76	1		

- Molecule 47 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	L7	119	Total	C	N	O	P	0	0
			2542	1132	454	837	119		

- Molecule 48 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SA	217	Total	C	N	O	S	0	0
			1624	1035	290	292	7		

- Molecule 49 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SB	214	Total	C	N	O	S	0	0
			1708	1086	307	301	14		

- Molecule 50 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SE	258	Total	C	N	O	S	0	0
			1914	1220	363	324	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SF	182	Total	C	N	O	S	0	0
			1350	843	261	240	6		

- Molecule 52 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	SH	178	Total	C	N	O	S	0	0
			1173	743	221	209			

- Molecule 53 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SI	186	Total	C	N	O	S	0	0
			1446	906	287	248	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SK	95	Total	C	N	O	S	0	0
			690	451	125	111	3		

- Molecule 55 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SL	138	Total	C	N	O	S	0	0
			1071	687	201	177	6		

- Molecule 56 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SQ	140	Total	C	N	O	S	0	0
			1019	639	197	181	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SS	140	Total	C	N	O		1	0
			956	594	202	160			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	ST	141	Total	C	N	O	S	0	0
			1000	626	193	179	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SU	97	Total	C	N	O		0	0
			487	291	97	99			

- Molecule 60 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SV	83	Total	C	N	O	S	1	0
			587	362	110	110	5		

- Molecule 61 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SX	140	Total	C	N	O	S	0	0
			1065	675	214	173	3		

- Molecule 62 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Sc	60	Total	C	N	O	S	0	0
			447	274	90	81	2		

- Molecule 63 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Sd	52	Total	C	N	O	S	0	0
			425	266	87	67	5		

- Molecule 64 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SC	216	Total	C	N	O	S	0	0
			1608	1044	274	280	10		

- Molecule 65 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SG	224	Total	C	N	O	S	0	0
			1325	806	271	247	1		

- Molecule 66 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SJ	178	Total	C	N	O	S	0	0
			1427	912	286	227	2		

- Molecule 67 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SN	150	Total	C	N	O	S	0	0
			1163	748	219	195	1		

- Molecule 68 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SO	136	Total	C	N	O	S	0	0
			995	610	195	184	6		

- Molecule 69 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SW	129	Total	C	N	O	S	0	0
			1021	654	193	168	6		

- Molecule 70 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SY	124	Total	C	N	O	S	0	0
			966	612	187	163	4		

- Molecule 71 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms				AltConf	Trace
71	SZ	72	Total	C	N	O	0	0
			474	293	95	86		

- Molecule 72 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Sb	81	Total	C	N	O	S	0	0
			542	337	108	96	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Sb	82	ARG	LYS	conflict	UNP P42677

- Molecule 73 is a protein called Ubiquitin-like FUBI-ribosomal protein eS30 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Se	49	Total	C	N	O	S	0	0
			386	236	87	62	1		

- Molecule 74 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sa	106	Total	C	N	O	S	0	0
			811	503	168	135	5		

- Molecule 75 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	S2	1563	Total	C	N	O	P	0	0
			33366	14900	6003	10901	1562		

- Molecule 76 is a RNA chain called Kozak mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	mR	14	Total	C	N	O	P	0	0
			304	135	58	97	14		

- Molecule 77 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	S6	72	Total	C	N	O	P	S	0	0
			1542	687	282	500	72	1		

- Molecule 78 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sg	309	Total	C	N	O	S	0	0
			2064	1297	379	381	7		

- Molecule 79 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	SD	221	Total	C	N	O	S	0	0
			1457	932	268	253	4		

- Molecule 80 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	SM	106	Total	C	N	O	S	0	0
			534	318	106	107	3		

- Molecule 81 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	SR	131	Total	C	N	O	S	0	0
			858	538	165	153	2		

- Molecule 82 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	Sf	45	Total	C	N	O	0	0
			224	134	45	45		

- Molecule 83 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
83	SP	1	Total 1	K 1	0
83	L5	9	Total 9	K 9	0
83	Lf	1	Total 1	K 1	0
83	SQ	1	Total 1	K 1	0
83	S2	5	Total 5	K 5	0

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

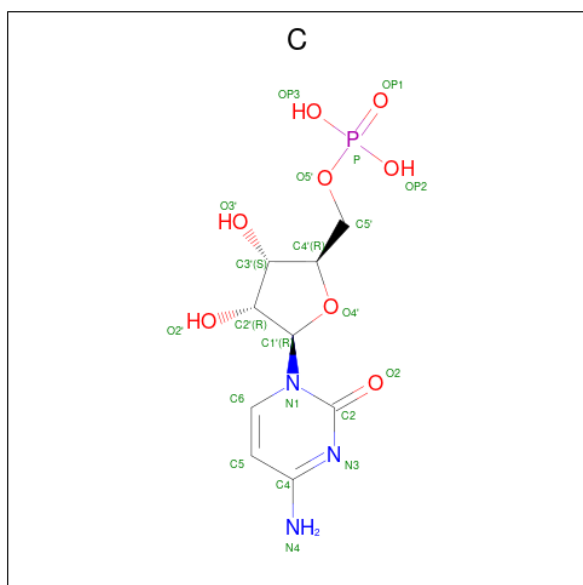
Mol	Chain	Residues	Atoms		AltConf
84	L8	4	Total 4	Mg 4	0
84	L5	43	Total 43	Mg 43	0
84	LA	1	Total 1	Mg 1	0
84	LB	1	Total 1	Mg 1	0
84	LH	1	Total 1	Mg 1	0
84	LV	1	Total 1	Mg 1	0
84	LN	1	Total 1	Mg 1	0
84	LI	2	Total 2	Mg 2	0
84	LQ	1	Total 1	Mg 1	0
84	LS	1	Total 1	Mg 1	0
84	LP	1	Total 1	Mg 1	0
84	Le	1	Total 1	Mg 1	0
84	Lg	1	Total 1	Mg 1	0
84	Lj	1	Total 1	Mg 1	0
84	Pt	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
84	L7	3	Total	Mg	0
			3	3	
84	S2	10	Total	Mg	0
			10	10	

- Molecule 85 is CYTIDINE-5'-MONOPHOSPHATE (CCD ID: C) (formula: $C_9H_{14}N_3O_8P$).



Mol	Chain	Residues	Atoms					AltConf
85	L5	1	Total	C	N	O	P	0
			20	9	3	7	1	
85	Lo	1	Total	C	N	O	P	0
			20	9	3	7	1	

- Molecule 86 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
86	L5	3	Total	Na	0
			3	3	
86	S2	4	Total	Na	0
			4	4	

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

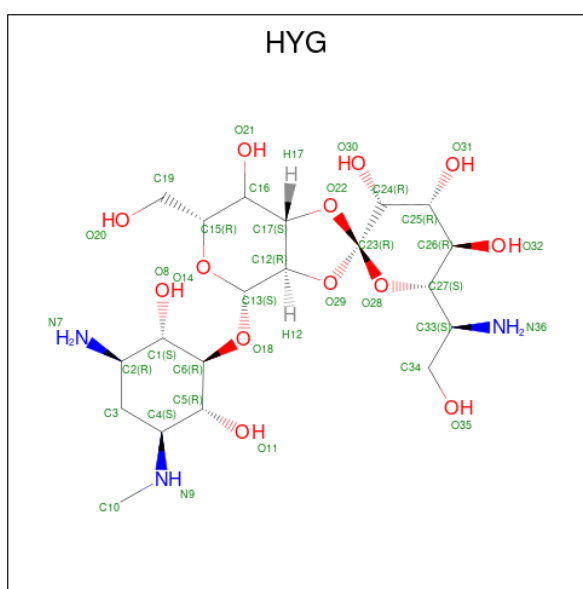
Mol	Chain	Residues	Atoms		AltConf
87	Lg	1	Total	Zn	0
			1	1	

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

- Molecule 88 is HYGROMYCIN B (CCD ID: HYG) (formula: $C_{20}H_{37}N_3O_{13}$).



Mol	Chain	Residues	Atoms				AltConf
88	S2	1	Total	C	N	O	0
			36	20	3	13	

- Molecule 89 is water.

Mol	Chain	Residues	Atoms		AltConf
89	L8	8	Total	O	0
			8	8	
89	L5	273	Total	O	0
			273	273	
89	LA	6	Total	O	0
			6	6	
89	LB	3	Total	O	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
89	LC	2	Total 2	O 2	0
89	LJ	1	Total 1	O 1	0
89	LH	2	Total 2	O 2	0
89	LO	1	Total 1	O 1	0
89	LV	1	Total 1	O 1	0
89	La	2	Total 2	O 2	0
89	LI	2	Total 2	O 2	0
89	LQ	1	Total 1	O 1	0
89	LR	5	Total 5	O 5	0
89	LW	2	Total 2	O 2	0
89	Lr	2	Total 2	O 2	0
89	LF	1	Total 1	O 1	0
89	Lc	4	Total 4	O 4	0
89	Lg	1	Total 1	O 1	0
89	Li	1	Total 1	O 1	0
89	Lm	1	Total 1	O 1	0
89	Ln	1	Total 1	O 1	0
89	Lp	3	Total 3	O 3	0
89	Pt	9	Total 9	O 9	0
89	L7	9	Total 9	O 9	0
89	SB	1	Total 1	O 1	0

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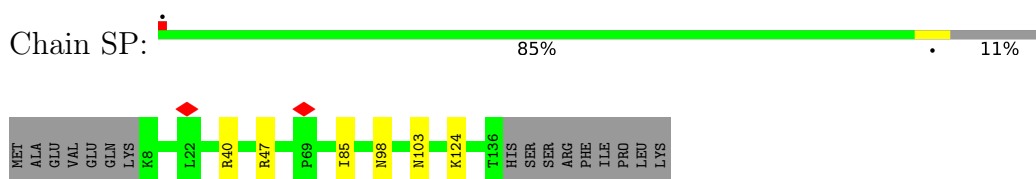
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Mol	Chain	Residues	Atoms		AltConf
89	SF	1	Total 1	O 1	0
89	SS	1	Total 1	O 1	0
89	Sd	2	Total 2	O 2	0
89	SC	1	Total 1	O 1	0
89	SG	2	Total 2	O 2	0
89	SJ	2	Total 2	O 2	0
89	SO	2	Total 2	O 2	0
89	Sa	1	Total 1	O 1	0
89	S2	92	Total 92	O 92	0
89	S6	1	Total 1	O 1	0
89	Sg	1	Total 1	O 1	0

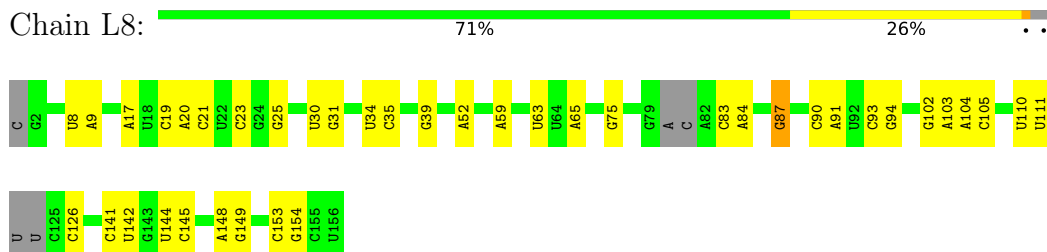
3 Residue-property plots [i](#)

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

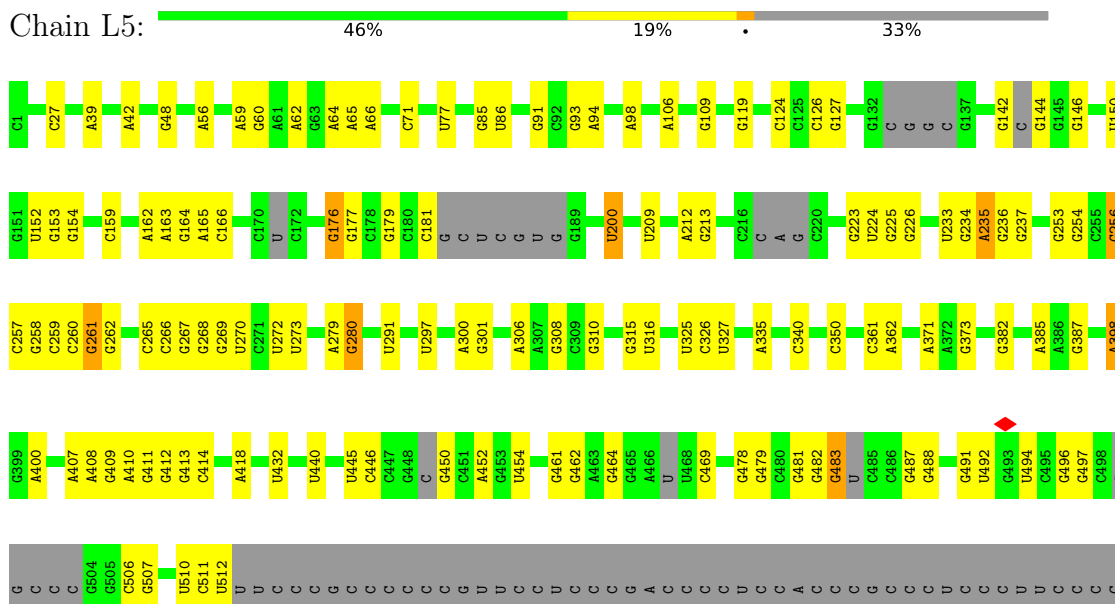
- Molecule 1: 40S ribosomal protein S15

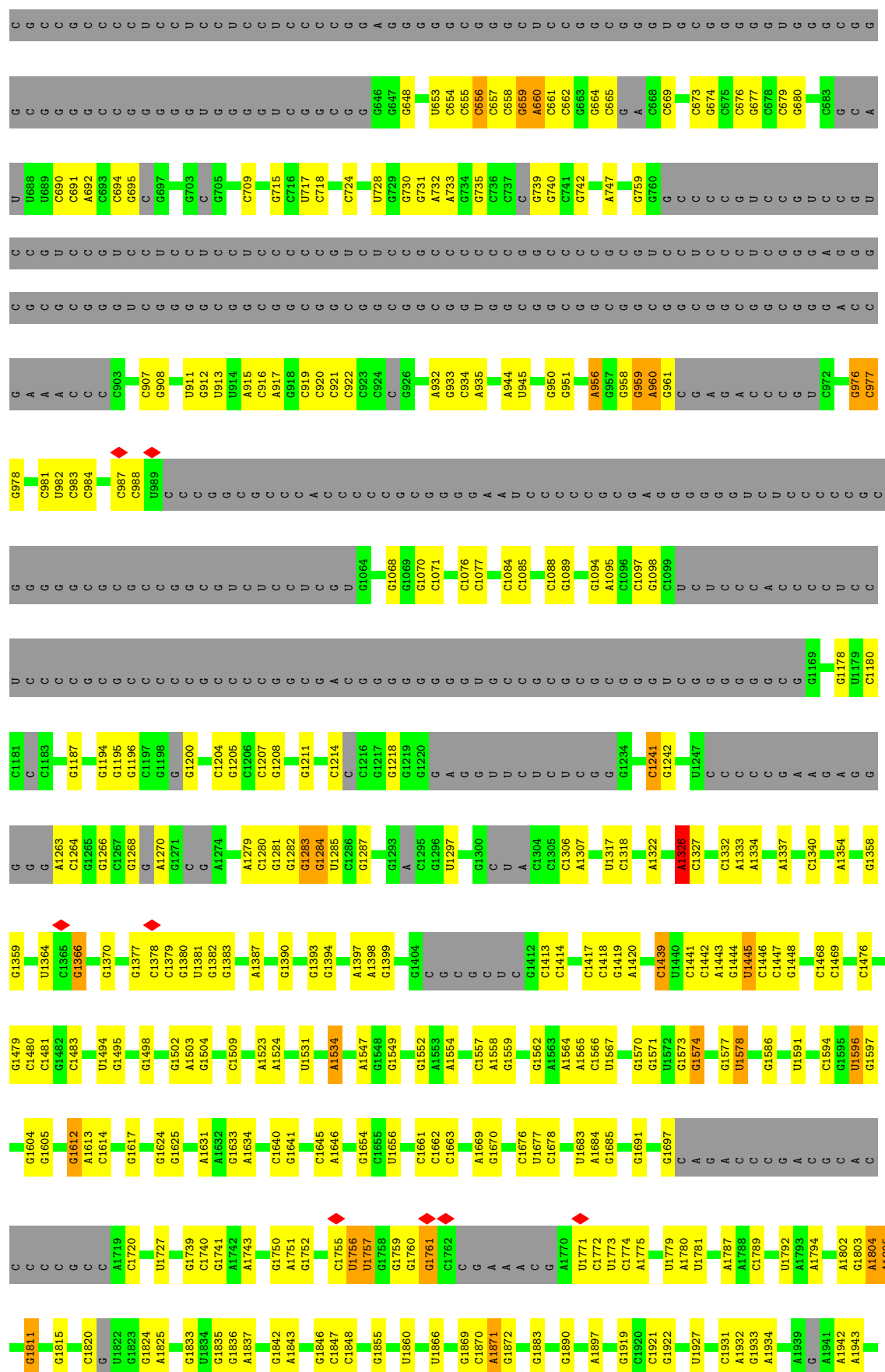


- Molecule 2: 5.8S rRNA



- Molecule 3: 28S rRNA





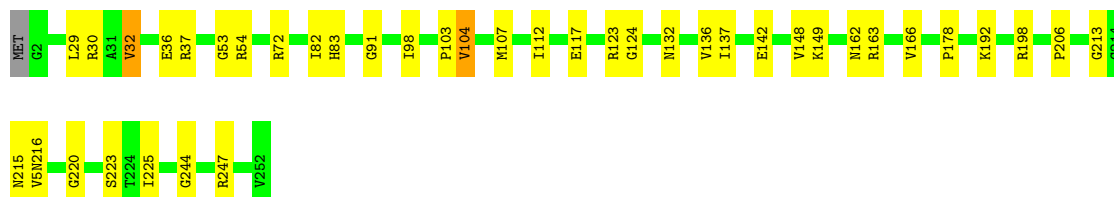


G4870	C4741	G4509	G4254	G4136	U	C3924	A3825	U3721	C	G
C4871	A4610	U4512	C4258	C	A	U3925	A3826	G3722	U	C
G4872	G4618	A4513	C4259	C	C	C3926	A3830	A3723	A	C
A4873	U4619	G4519	C4263	C	U	G3934	U3838	A3724	G3597	C
A4874	U4620	G4520	U4264	C	U	G3938	G3839	A3727	C3602	C
G4877	C4749	U4521	U4265	C	U	G3939	U3840	A3728	G3603	C
U4882	U4627	G4522	G4266	C	A	G	C3841	U3729	A3610	C
C4883	U4628	A4523	G4267	C	U	G3944	C3842	A3732	A3611	C
G4884	U4636	G4524	A4268	C	A	G3945	C3843	A3733	G3615	C
C	U4637	A4525	A4269	C	U	G3946	U3844	U3734	U3616	C
C4895	G4637	U4530	A4273	C	G4065	G3947	U3848	G3735	G3617	C
G4896	U4642	U4531	A4274	G	U4067	C3948	A3849	A3736	C3618	C
G4897	G4643	U4532	G4275	G	U4068	U	C3850	A3737	G3626	C
G4898	G4644	C4537	A4280	C	U4070	G	U3851	A3746	G3626	C
G4899	C4645	G4538	A4281	C	U4071	G	U3852	A3747	A3630	C
C	U4646	U4539	A4282	C	G4076	G	U3853	A3748	A3630	C
G4901	U4656	G4540	G4291	C	C4080	G	C3854	G3749	A3635	C
C4906	U4657	C4541	U4295	C	G4081	G	A3856	C3750	A3635	C
G4907	C4670	A4544	U4296	C	G	G	U3861	G3753	U3641	C
G4908	A4671	G4545	G4297	C	G4084	G	A3862	U3758	A3646	C
A4909	U4672	A4546	U4298	C	C4088	G	A3867	A3759	A3647	C
G4910	U4673	C4547	U4299	C	G4089	G	A3870	A3760	A3648	C
G4913	C4771	A4548	G4305	C	G4090	G	C3871	C3761	A3661	C
C4914	C4772	G4549	U4306	C	G4091	G	C3870	U3762	A3662	C
G4915	C4773	A4550	U4307	C	G4092	G	A3871	A3763	A3663	C
C	C4774	U4551	U4308	C	G4093	G	A3872	U3764	G3664	C
C4921	G4775	U4552	U4309	C	G4094	G	A3873	G3765	G3664	C
C4922	G4776	C4553	U4310	C	G4095	G	A3874	A3766	G3665	C
C	C	U4554	U4311	C	C4096	G	A3875	G3767	G3666	C
C4928	C	C4555	U4312	C	G4097	G	A3876	U3768	G3669	C
C4929	U	G4556	U4313	C	A4098	G	C3877	C3769	G3672	C
C4930	U	U4557	A4314	C	G4099	G	A3894	U3770	C3673	C
A4934	C	C4558	C4318	C	C	G	G3895	G3776	U3680	C
G4935	C	U4559	C4319	C	C	G	C3896	G3777	U3680	C
G4936	C	G4560	G4320	C	C	G	C3897	G3778	U3680	C
C4937	C	G4561	U4321	C	C	G	C3898	A3783	A3687	C
A4943	C	U4562	G4322	C	C	G	C3899	A3784	U3688	C
G4954	C	G4563	A4324	C	A	C	G3900	A3785	G3689	C
A4955	C	U4564	G4325	C	G	C	A3901	U3786	U3690	C
G4956	C	G4565	U4326	C	G	C	A3906	C3787	G3691	C
U4959	C	U4566	U4227	C	G4109	C	A3907	C3788	A3692	C
G4960	C	G4567	G4228	C	U4111	C	A3908	A3807	U3707	C
U4965	C	U4568	U4229	C	C4112	C	C3909	C3808	C3708	C
A4966	C	A4569	A4233	C	G4115	C	C3910	U3709	U3709	C
A4967	C	C4570	C4346	C	G4119	C	C3911	G3710	G3710	C
A4968	C	U4571	U4343	C	C4122	C	U3912	A3711	A3711	C
G4969	C	G4572	U4361	C	G4126	C	U3915	U3715	U3715	C
U4972	C	U4573	U4362	C	A4127	C	A3916	G3716	G3716	C
U4976	C	G4574	A4363	C	A4128	C	A3917	A3717	A3717	C
C	C	G4575	C4568	C	C	C	C3918	A3718	A3718	C
C	C	U4576	G4600	C	C	C	U3920	U3818	A3719	C
C	C	U4577	C4608	C	C	C	G	G3819	G3720	C



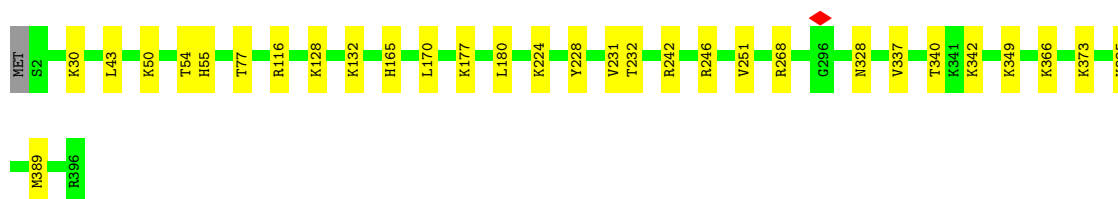
- Molecule 4: Large ribosomal subunit protein uL2

Chain LA: 84% 15% .



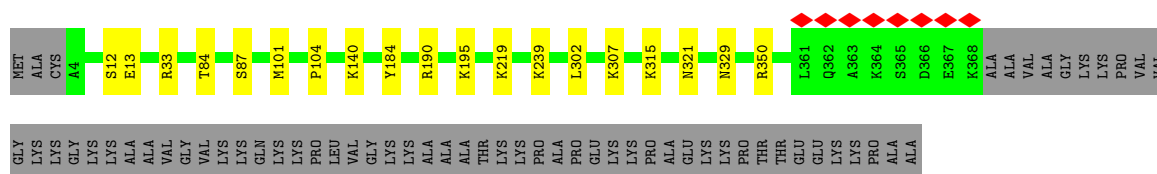
- Molecule 5: Large ribosomal subunit protein uL3

Chain LB: 92% 8%



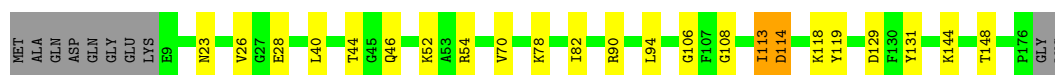
- Molecule 6: 60S ribosomal protein L4

Chain LC: 81% 15%



- Molecule 7: 60S ribosomal protein L11

Chain LJ: 81% 12% 6%



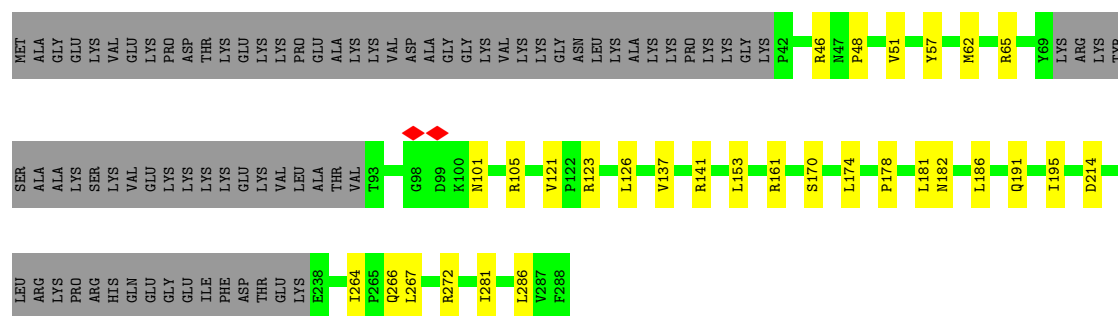
- Molecule 8: 60S ribosomal protein L9

Chain LH: 87% 12%



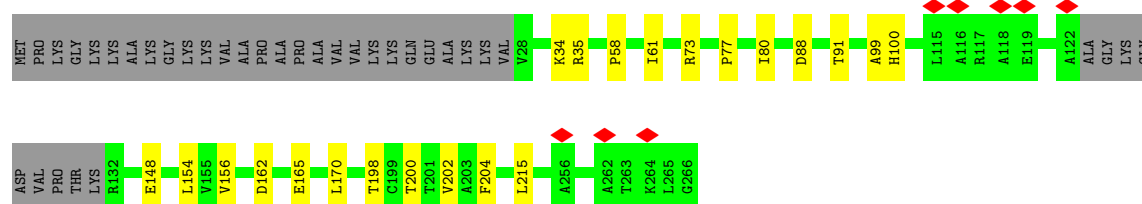
- Molecule 9: Large ribosomal subunit protein eL6

Chain LE:  62% 10% 28%



- Molecule 10: 60S ribosomal protein L7a

Chain LG:  78% 8% 14%



- Molecule 11: 60S ribosomal protein L13a

Chain LO:  85% 13% .



- Molecule 12: 60S ribosomal protein L13

Chain LL:  91% 7% .



- Molecule 13: 60S ribosomal protein L23

Chain LV:  86% 8% . 6%

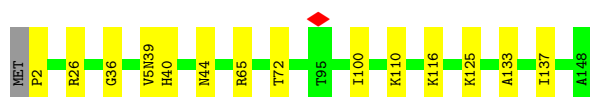


- Molecule 14: Large ribosomal subunit protein eL14

Chain LM:  90% 10%



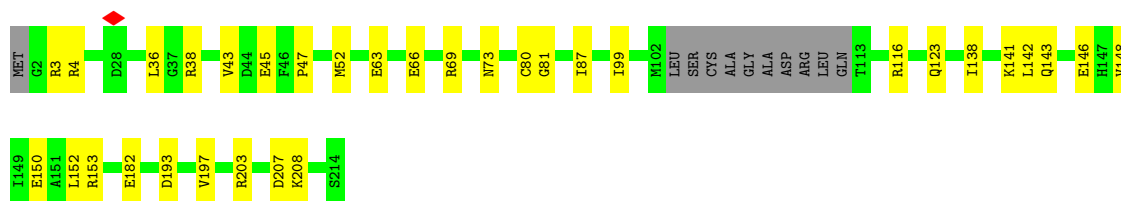
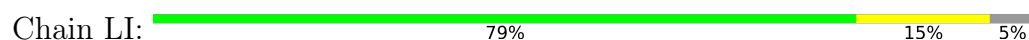
- Molecule 15: Large ribosomal subunit protein uL15



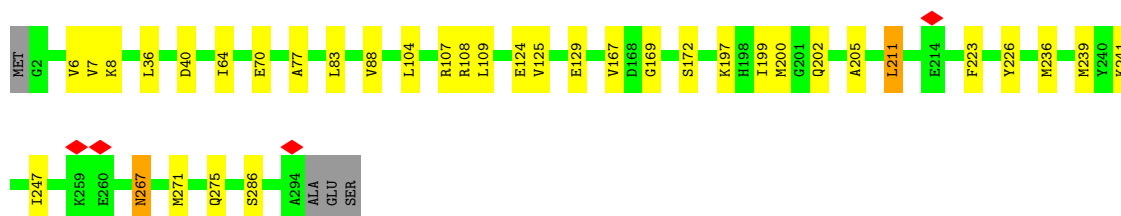
- Molecule 16: 60S ribosomal protein L15



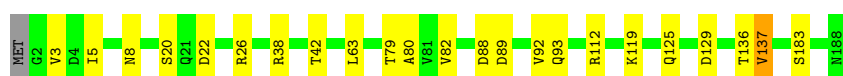
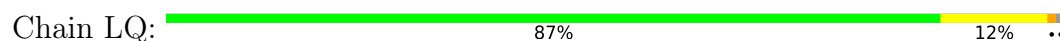
- Molecule 17: 60S ribosomal protein L10



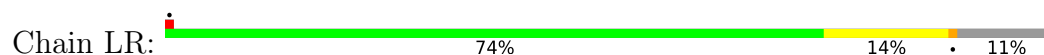
- Molecule 18: 60S ribosomal protein L5

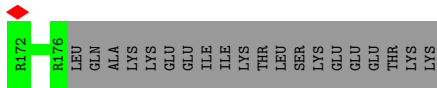


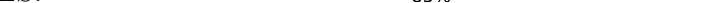
- Molecule 19: 60S ribosomal protein L18

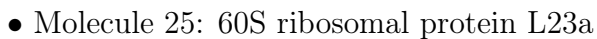
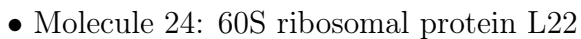
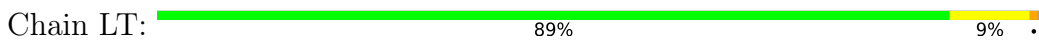
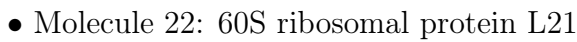


- Molecule 20: 60S ribosomal protein L19





- Chain LS:  85% 14%



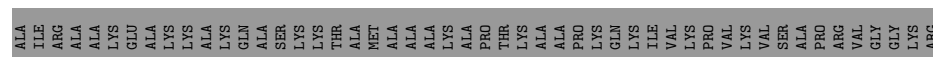
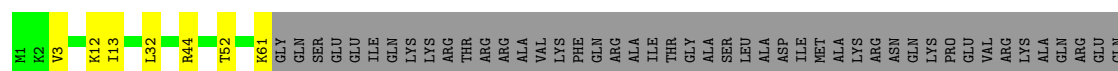
- 

Chain LY:  73% 17% 10%



- Molecule 27: 60S ribosomal protein L24

Chain LW:  34% 61%



- Molecule 28: 60S ribosomal protein L27

Chain LZ:  76% 21% ..



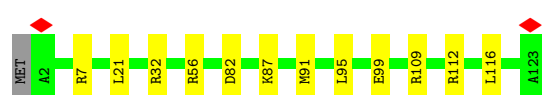
- Molecule 29: 60S ribosomal protein L28

Chain Lr:  75% 14% 11%



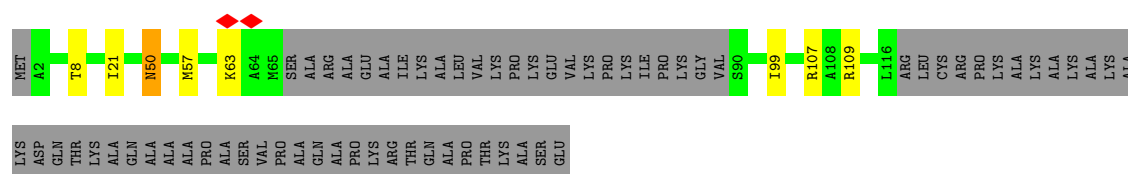
- Molecule 30: 60S ribosomal protein L35

Chain Lh:  89% 10% .



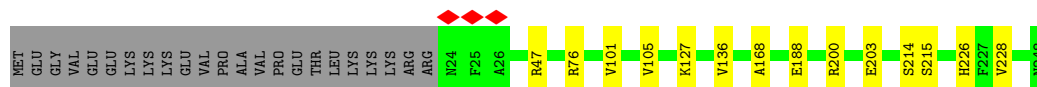
- Molecule 31: Large ribosomal subunit protein eL29

Chain Lb:  52% 43%



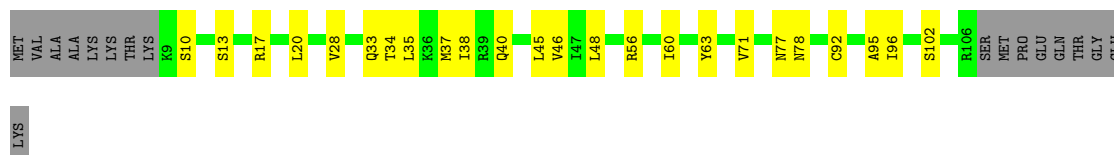
- Molecule 32: Large ribosomal subunit protein uL30

Chain LF:  85% 6% 9%



- Molecule 33: 60S ribosomal protein L30

Chain Lc:  64% 21% 15%

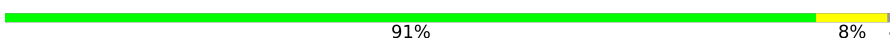


- Molecule 34: 60S ribosomal protein L31

Chain Ld:  68% 18% 14%



- Molecule 35: Large ribosomal subunit protein eL32

Chain Le:  91% 8% 1%

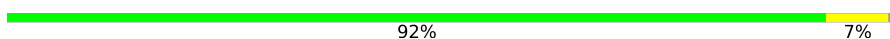


- Molecule 36: Large ribosomal subunit protein eL33

Chain Lf:  91% 8% 1%



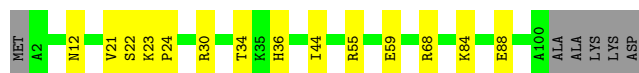
- Molecule 37: Large ribosomal subunit protein eL34

Chain Lg:  92% 7% 1%



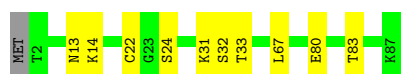
- Molecule 38: 60S ribosomal protein L36

Chain Li:  81% 13% 6%



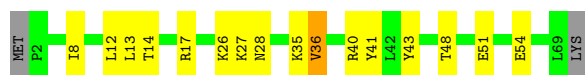
- Molecule 39: Large ribosomal subunit protein eL37

Chain Lj:  87% 11% .



- Molecule 40: 60S ribosomal protein L38

Chain Lk:  74% 21% ..



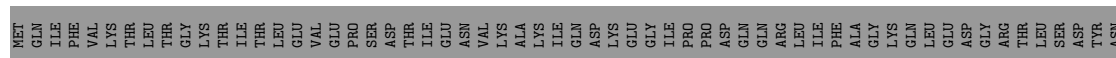
- Molecule 41: 60S ribosomal protein L39

Chain Ll:  86% 12% .



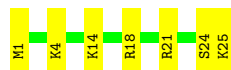
- Molecule 42: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Lm:  31% 9% 60%



- Molecule 43: 60S ribosomal protein L41

Chain Ln:  72% 28%



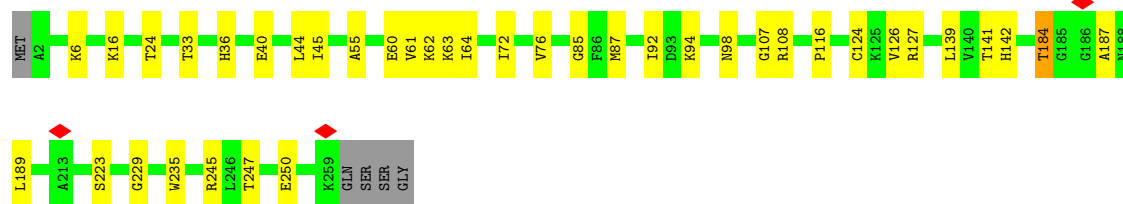
- Molecule 44: Large ribosomal subunit protein eL42

Chain Lo:  81% 17% ..



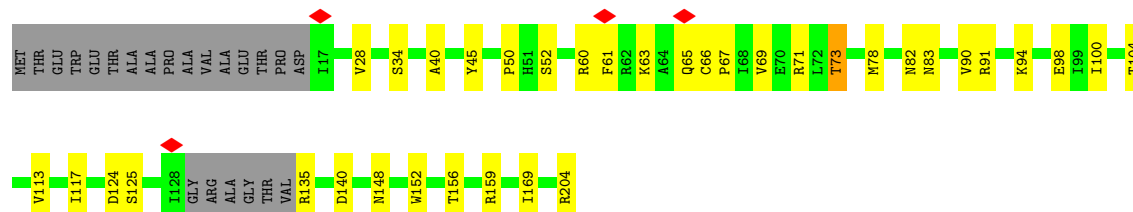
- Molecule 50: Small ribosomal subunit protein eS4, X isoform

Chain SE:  83% 14%



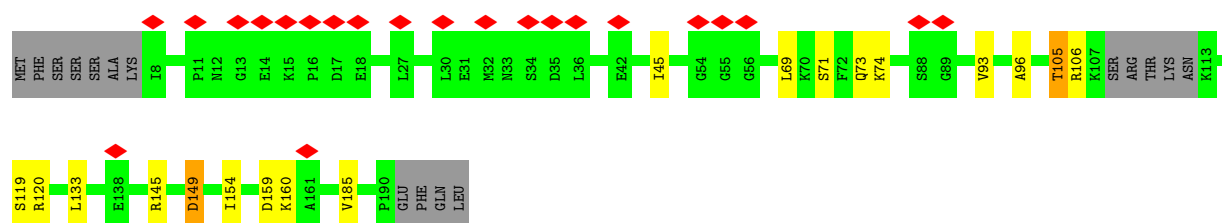
- Molecule 51: 40S ribosomal protein S5

Chain SF:  72% 17% 11%



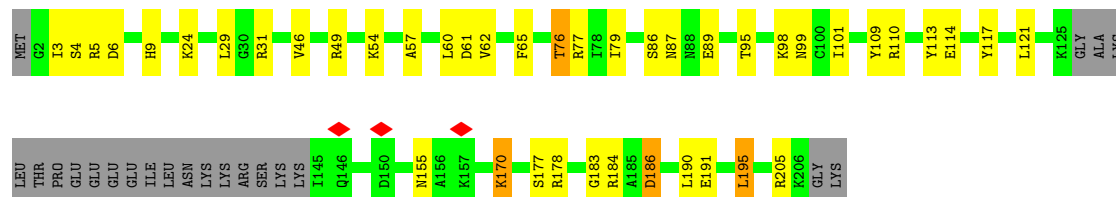
- Molecule 52: 40S ribosomal protein S7

Chain SH:  11% 82% 8% 8%

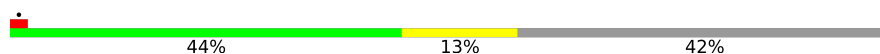


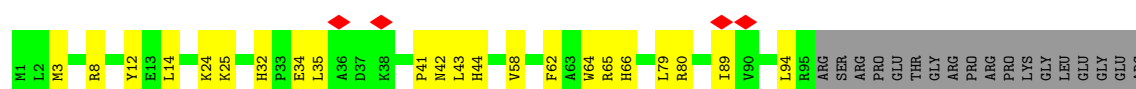
- Molecule 53: 40S ribosomal protein S8

Chain SI:  69% 19% 11%



- Molecule 54: 40S ribosomal protein S10

Chain SK:  44% 13% 42%



PRO ALA ARG LEU THR ARG GLY GLU
ALA ASP ARG ASP THR ARG
SER ARG SER ALA VAL
PRO PRO GLY ALA ASP LYS
LYS LYS ALA ALA ALA
GLY GLY ALA ALA
GLY SER
THR THR
PHE PHE
GLN GLN
PHE ARG
GLY GLY
ARG ARG
GLY GLN
GLN PRO
PRO GLN

- Molecule 55: 40S ribosomal protein S11

Chain SL:  76% 10% 13%

MET R2 Q13 I16 R22 VAL LEU ARG GLY THR LYS LYS GLU K32 I40 T54 F62 S67 I72 M90 K81 M82 T85 K104 S114 F115 C116 D119 T127 E130 C131 S135 K136 A148 ALA GLY THR LYS LYS GLN PHE GLN
LYS PHE

- Molecule 56: 40S ribosomal protein S16

Chain SQ:  76% 18% 6%

MET PRO SER LYS PRO GLY L7 Q8 S9 V10 Q11 V12 F13 G14 T20 H24 R27 R37 L51 R69 V72 Q75 I81 R85 Q86 S87 I88 A91 Y95 Y96 Q97 D101 K105 K106 E107 I108 K109 D110 I111 I112 I113 Q114 R117 L120
C127 Q142 R146

- Molecule 57: 40S ribosomal protein S18

Chain SS:  79% 12% 8%

MET SER L3 Q10 L13 R14 V15 L16 N17 G22 K25 V34 I26 A27 F28 T31 A32 I33 R38 A56 H125 R130 V131 R132 G133 T136 R142 GLY ARG THR VAL GLY VAL SER LYS LYS
L3 Q10 L13 R14 V15 L16 N17 G22 K25 V34 I26 A27 F28 T31 A32 I33 R38 A56 H125 R130 V131 R132 G133 T136 R142 GLY ARG THR VAL GLY VAL SER LYS LYS

- Molecule 58: 40S ribosomal protein S19

Chain ST:  80% 16% 4%

MET P2 V6 Q11 F14 S25 L28 K29 W33 V34 D35 T36 V37 K38 L39 A40 K43 R62 H63 L64 S74 I78 Q83 R84 N85 M88 G95 S96 K97 D118 R121 V138 A141 A142 LYS LYS HIS
P2 V6 Q11 F14 S25 L28 K29 W33 V34 D35 T36 V37 K38 L39 A40 K43 R62 H63 L64 S74 I78 Q83 R84 N85 M88 G95 S96 K97 D118 R121 V138 A141 A142 LYS LYS HIS

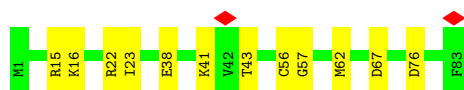
- Molecule 59: 40S ribosomal protein S20

Chain SU:  6% 78% 18%

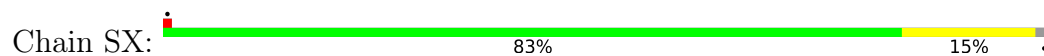
MET ALA PHE LYS ASP THR GLY LYS THR PRO VAL GLU PRO GLU VAL I17 R41 W47 E72 G73 P94 K99 G99 ILE THR SER ILE S105 P108 I116 A117 D118 ALA
I17 R41 W47 E72 G73 P94 K99 G99 ILE THR SER ILE S105 P108 I116 A117 D118 ALA

- Molecule 60: 40S ribosomal protein S21

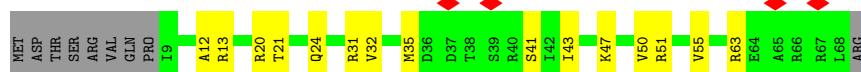
Chain SV:  86% 14%



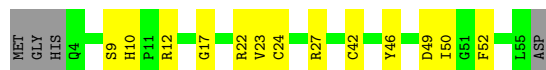
- Molecule 61: 40S ribosomal protein S23



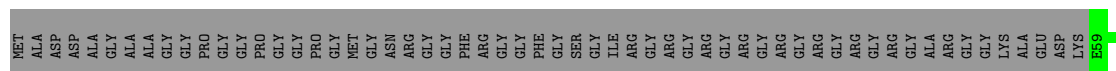
- Molecule 62: 40S ribosomal protein S28



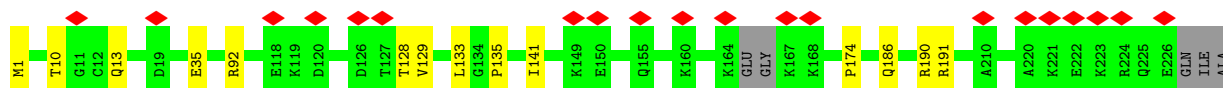
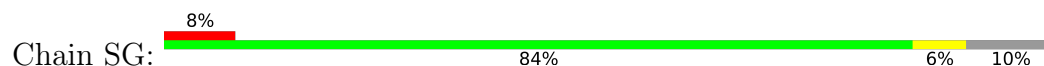
- Molecule 63: 40S ribosomal protein S29



- Molecule 64: 40S ribosomal protein S2

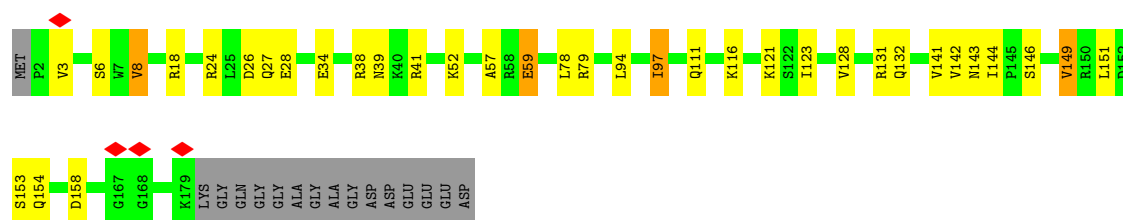


- Molecule 65: 40S ribosomal protein S6



- Molecule 66: 40S ribosomal protein S9

Chain SJ:  73% 16% 8%



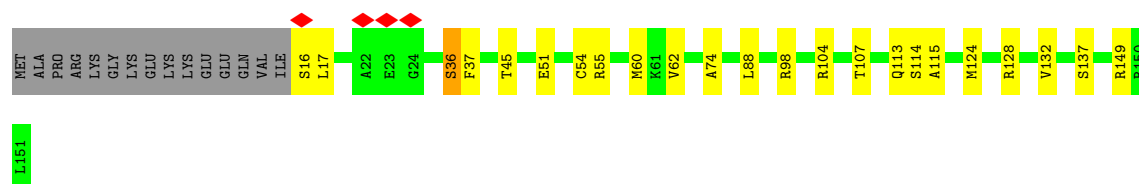
- Molecule 67: 40S ribosomal protein S13

Chain SN:  86% 11% ..



- Molecule 68: 40S ribosomal protein S14

Chain SO:  75% 15% 10%



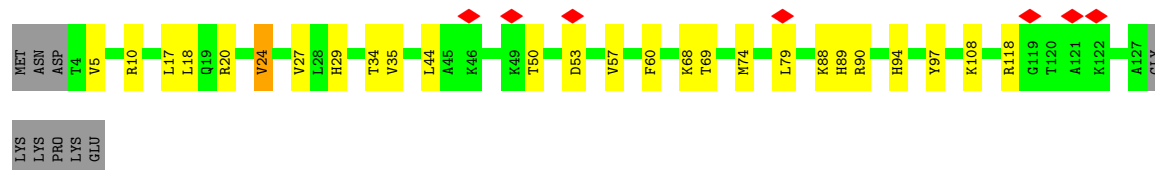
- Molecule 69: 40S ribosomal protein S15a

Chain SW:  82% 15% ..

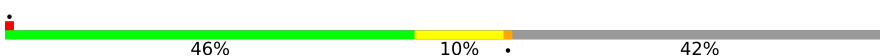


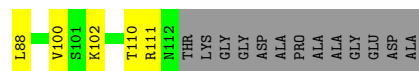
- Molecule 70: 40S ribosomal protein S24

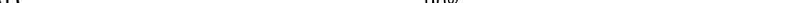
Chain SY:  5% 74% 19% 7%



- Molecule 71: 40S ribosomal protein S25

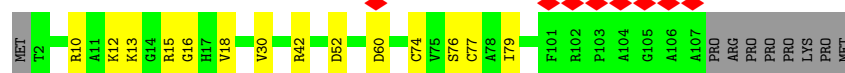
Chain SZ:  46% 10% 42%



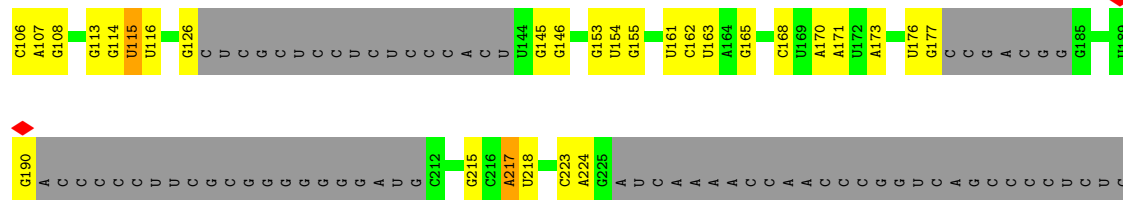
- Chain Sb:  90% 6%



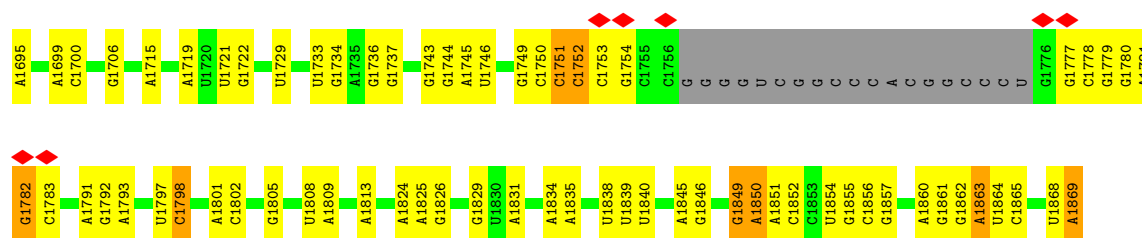
- Chain Sa: 



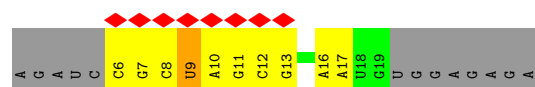
- Chain S2:



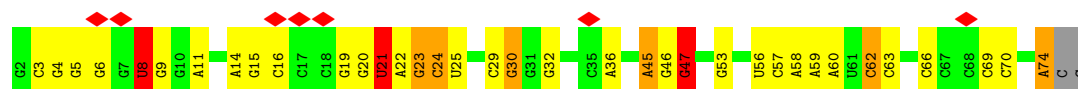




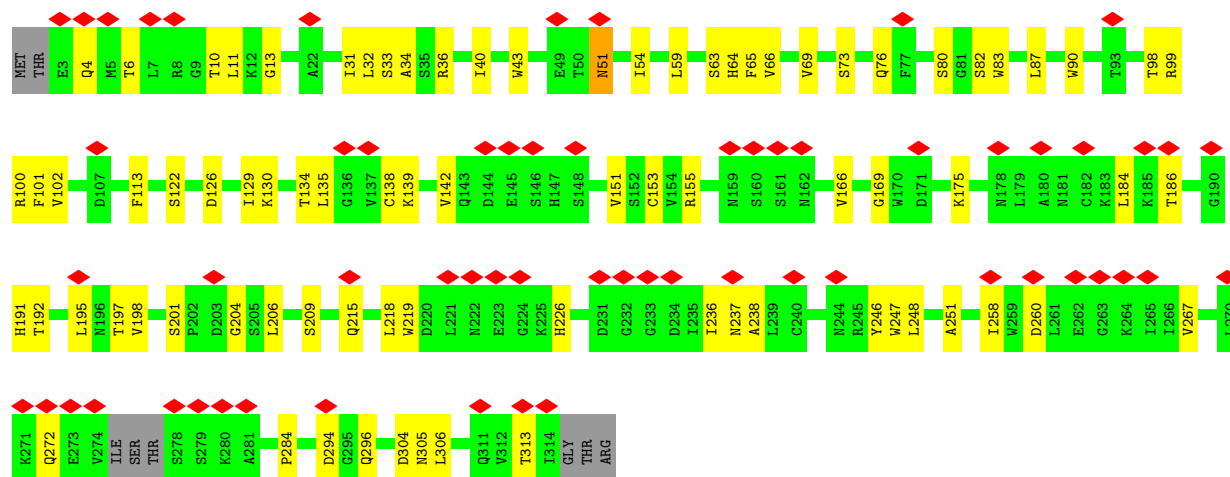
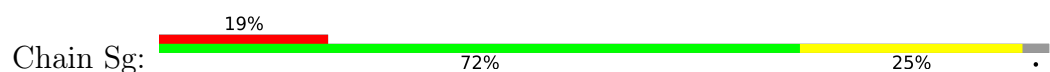
• Molecule 76: Kozak mRNA



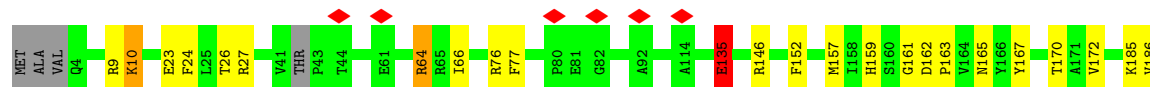
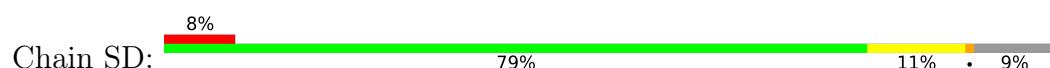
• Molecule 77: E-site tRNA



• Molecule 78: Receptor of activated protein C kinase 1



• Molecule 79: 40S ribosomal protein S3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55958	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	404.16, 404.16, 404.16	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.842, 0.842, 0.842	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: M3L, ZN, MG, HYG, 6MZ, A2M, OMC, MLZ, NA, HIC, OMG, K, PSU, UR3, 5MC, H2U, G7M, V5N, OMU, 1MA, 4SU

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	SP	0.08	0/824	0.24	0/1121
2	L8	0.14	0/3589	0.28	0/5587
3	L5	0.16	1/78615 (0.0%)	0.28	0/122538
4	LA	0.14	0/1920	0.29	0/2576
5	LB	0.12	0/2768	0.27	0/3754
6	LC	0.12	0/2890	0.25	0/3891
7	LJ	0.11	0/1227	0.29	0/1655
8	LH	0.11	0/1454	0.26	0/1964
9	LE	0.11	0/1616	0.26	0/2180
10	LG	0.12	0/1727	0.26	0/2353
11	LO	0.13	0/1637	0.28	0/2193
12	LL	0.30	0/1614	0.44	0/2177
13	LV	0.13	0/957	0.28	0/1293
14	LM	0.13	0/1111	0.25	0/1491
15	La	0.13	0/1173	0.28	0/1566
16	LN	0.14	0/1739	0.28	0/2331
17	LI	0.15	0/1648	0.33	0/2206
18	LD	0.11	0/2276	0.27	0/3072
19	LQ	0.13	0/1521	0.29	0/2034
20	LR	0.13	0/1407	0.28	0/1871
21	LS	0.13	0/1492	0.29	0/2003
22	LT	0.13	0/1246	0.28	0/1674
23	LP	0.13	0/1268	0.31	0/1701
24	LU	0.11	0/795	0.26	0/1071
25	LX	0.12	0/972	0.28	0/1307
26	LY	0.12	0/1074	0.28	0/1434
27	LW	0.11	0/528	0.23	0/703
28	LZ	0.12	0/1111	0.30	0/1487
29	Lr	0.12	0/988	0.28	0/1328
30	Lh	0.10	0/962	0.23	0/1282
31	Lb	0.12	0/701	0.28	0/929

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LF	0.13	0/1789	0.26	0/2402
33	Lc	0.12	0/750	0.25	0/1011
34	Ld	0.13	0/892	0.28	0/1203
35	Le	0.13	0/1063	0.28	0/1421
36	Lf	0.14	0/879	0.28	0/1179
37	Lg	0.13	0/848	0.29	0/1132
38	Li	0.10	0/767	0.24	0/1025
39	Lj	0.13	0/710	0.30	0/941
40	Lk	0.14	0/549	0.32	0/728
41	Ll	0.13	0/443	0.38	0/588
42	Lm	0.11	0/402	0.28	0/536
43	Ln	0.11	0/240	0.18	0/305
44	Lo	0.15	0/856	0.32	0/1133
45	Lp	0.17	0/695	0.31	0/925
46	Pt	0.17	0/1720	0.27	0/2675
47	L7	0.15	0/2840	0.28	0/4425
48	SA	0.13	0/1660	0.33	0/2266
49	SB	0.15	0/1735	0.40	0/2327
50	SE	0.12	0/1956	0.31	0/2654
51	SF	0.12	0/1369	0.36	0/1851
52	SH	0.12	0/1189	0.28	0/1622
53	SI	0.14	0/1472	0.34	0/1977
54	SK	0.18	0/711	0.43	0/973
55	SL	0.12	0/1091	0.29	0/1471
56	SQ	0.13	0/1034	0.38	0/1395
57	SS	0.10	0/970	0.29	0/1312
58	ST	0.12	0/1017	0.36	0/1374
59	SU	0.07	0/485	0.26	0/672
60	SV	0.12	0/592	0.33	0/797
61	SX	0.13	0/1083	0.34	0/1450
62	Sc	0.11	0/448	0.29	0/601
63	Sd	0.12	0/435	0.31	0/579
64	SC	0.14	0/1644	0.36	0/2232
65	SG	0.10	0/1332	0.27	0/1823
66	SJ	0.13	0/1452	0.34	0/1952
67	SN	0.12	0/1187	0.27	0/1604
68	SO	0.14	0/1008	0.39	0/1355
69	SW	0.13	0/1038	0.29	0/1389
70	SY	0.12	0/983	0.34	0/1316
71	SZ	0.10	0/477	0.33	0/652
72	Sb	0.11	0/550	0.33	0/742
73	Se	0.10	0/388	0.28	0/508
74	Sa	0.11	0/823	0.27	0/1106

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	S2	0.14	0/37306	0.29	0/58113
76	mR	0.13	0/340	0.30	0/529
77	S6	0.25	0/1629	0.44	0/2537
78	Sg	0.27	0/2110	0.71	0/2905
79	SD	0.31	0/1474	0.87	3/2003 (0.1%)
80	SM	0.19	0/532	0.54	0/737
81	SR	0.25	0/869	0.71	0/1187
82	Sf	0.13	0/220	0.32	0/301
All	All	0.15	1/210902 (0.0%)	0.31	3/310713 (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
12	LL	0	1
79	SD	0	5
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4523	A2M	O3'-P	5.05	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
79	SD	189	MET	CA-C-N	8.87	132.72	120.39
79	SD	189	MET	C-N-CA	8.87	132.72	120.39
79	SD	135	GLU	CB-CG-CD	5.99	122.78	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	LL	49	ARG	Sidechain
79	SD	135	GLU	Sidechain
79	SD	146	ARG	Sidechain
79	SD	152	PHE	Sidechain
79	SD	24	PHE	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
79	SD	64	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	SP	814	0	628	5	0
2	L8	3215	0	1631	20	0
3	L5	72477	0	36733	490	0
4	LA	1895	0	1967	29	0
5	LB	2719	0	2344	22	0
6	LC	2836	0	2954	16	0
7	LJ	1207	0	1138	15	0
8	LH	1435	0	1457	15	0
9	LE	1584	0	1620	21	0
10	LG	1696	0	1649	15	0
11	LO	1605	0	1726	19	0
12	LL	1583	0	1613	9	0
13	LV	943	0	959	8	0
14	LM	1089	0	1128	18	0
15	La	1157	0	1177	10	0
16	LN	1694	0	1738	12	0
17	LI	1610	0	1629	26	0
18	LD	2232	0	2145	23	0
19	LQ	1497	0	1605	14	0
20	LR	1391	0	1469	23	0
21	LS	1453	0	1482	18	0
22	LT	1221	0	1222	11	0
23	LP	1242	0	1269	6	0
24	LU	781	0	790	11	0
25	LX	955	0	1023	12	0
26	LY	1057	0	1119	18	0
27	LW	515	0	530	4	0
28	LZ	1088	0	1145	22	0
29	Lr	973	0	1023	11	0
30	Lh	954	0	1034	8	0
31	Lb	700	0	710	6	0
32	LF	1756	0	1765	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	Lc	740	0	751	15	0
34	Ld	877	0	913	11	0
35	Le	1045	0	1125	9	0
36	Lf	860	0	890	6	0
37	Lg	838	0	895	7	0
38	Li	756	0	772	10	0
39	Lj	695	0	710	6	0
40	Lk	545	0	589	7	0
41	Ll	433	0	461	5	0
42	Lm	408	0	423	8	0
43	Ln	239	0	289	4	0
44	Lo	849	0	888	12	0
45	Lp	682	0	724	9	0
46	Pt	1624	0	833	13	0
47	L7	2542	0	1285	7	0
48	SA	1624	0	1568	17	0
49	SB	1708	0	1760	53	0
50	SE	1914	0	1860	32	0
51	SF	1350	0	1291	25	0
52	SH	1173	0	998	10	0
53	SI	1446	0	1426	28	0
54	SK	690	0	603	19	0
55	SL	1071	0	1073	9	0
56	SQ	1019	0	976	20	0
57	SS	956	0	826	16	0
58	ST	1000	0	931	18	0
59	SU	487	0	214	2	0
60	SV	587	0	553	8	0
61	SX	1065	0	1112	10	0
62	Sc	447	0	448	11	0
63	Sd	425	0	412	9	0
64	SC	1608	0	1628	28	0
65	SG	1325	0	977	10	0
66	SJ	1427	0	1490	27	0
67	SN	1163	0	1208	13	0
68	SO	995	0	1007	15	0
69	SW	1021	0	1070	16	0
70	SY	966	0	986	18	0
71	SZ	474	0	407	11	0
72	Sb	542	0	433	4	0
73	Se	386	0	422	6	0
74	Sa	811	0	835	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	S2	33366	0	16861	309	0
76	mR	304	0	153	3	0
77	S6	1542	0	789	19	0
78	Sg	2064	0	1698	40	0
79	SD	1457	0	1310	24	0
80	SM	534	0	281	2	0
81	SR	858	0	703	13	0
82	Sf	224	0	92	3	0
83	L5	9	0	0	0	0
83	Lf	1	0	0	0	0
83	S2	5	0	0	0	0
83	SP	1	0	0	0	0
83	SQ	1	0	0	0	0
84	L5	43	0	0	0	0
84	L7	3	0	0	0	0
84	L8	4	0	0	0	0
84	LA	1	0	0	0	0
84	LB	1	0	0	0	0
84	LH	1	0	0	0	0
84	LI	2	0	0	0	0
84	LN	1	0	0	0	0
84	LP	1	0	0	0	0
84	LQ	1	0	0	0	0
84	LS	1	0	0	0	0
84	LV	1	0	0	0	0
84	Le	1	0	0	0	0
84	Lg	1	0	0	0	0
84	Lj	1	0	0	0	0
84	Pt	1	0	0	0	0
84	S2	10	0	0	0	0
85	L5	20	0	12	0	0
85	Lo	20	0	11	1	0
86	L5	3	0	0	0	0
86	S2	4	0	0	0	0
87	Lg	1	0	0	0	0
87	Lj	1	0	0	0	0
87	Lm	1	0	0	0	0
87	Lo	1	0	0	0	0
87	Lp	1	0	0	0	0
88	S2	36	0	37	0	0
89	L5	273	0	0	1	0
89	L7	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	L8	8	0	0	0	0
89	LA	6	0	0	0	0
89	LB	3	0	0	0	0
89	LC	2	0	0	0	0
89	LF	1	0	0	0	0
89	LH	2	0	0	0	0
89	LI	2	0	0	1	0
89	LJ	1	0	0	0	0
89	LO	1	0	0	0	0
89	LQ	1	0	0	0	0
89	LR	5	0	0	0	0
89	LV	1	0	0	0	0
89	LW	2	0	0	0	0
89	La	2	0	0	0	0
89	Lc	4	0	0	1	0
89	Lg	1	0	0	0	0
89	Li	1	0	0	0	0
89	Lm	1	0	0	0	0
89	Ln	1	0	0	0	0
89	Lp	3	0	0	0	0
89	Lr	2	0	0	0	0
89	Pt	9	0	0	0	0
89	S2	92	0	0	3	0
89	S6	1	0	0	0	0
89	SB	1	0	0	0	0
89	SC	1	0	0	0	0
89	SF	1	0	0	0	0
89	SG	2	0	0	0	0
89	SJ	2	0	0	0	0
89	SO	2	0	0	0	0
89	SS	1	0	0	0	0
89	Sa	1	0	0	0	0
89	Sd	2	0	0	1	0
89	Sg	1	0	0	0	0
All	All	199163	0	140431	1625	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 5.

All (1625) 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)
50:SE:16:LYS:CE	75:S2:812:A:H5'	1.51	1.38
50:SE:16:LYS:NZ	75:S2:812:A:H5'	1.55	1.21
50:SE:16:LYS:NZ	75:S2:812:A:C5'	2.13	1.11
50:SE:16:LYS:HE2	75:S2:812:A:H5'	1.12	1.09
40:Lk:54:GLU:OE1	40:Lk:54:GLU:N	1.86	1.08
50:SE:16:LYS:HE2	75:S2:812:A:C5'	2.01	0.90
66:SJ:121:LYS:HZ3	66:SJ:121:LYS:HB2	1.35	0.90
50:SE:16:LYS:CE	75:S2:812:A:C5'	2.47	0.89
50:SE:229:GLY:HA2	50:SE:235:TRP:HE3	1.35	0.88
3:L5:2557:G:H1	3:L5:2570:U:H3	1.20	0.85
61:SX:52:LEU:HD11	61:SX:73:GLN:HB2	1.60	0.84
65:SG:1:MET:HE2	65:SG:1:MET:HA	1.61	0.83
54:SK:64:TRP:CD1	79:SD:23:GLU:OE2	2.31	0.83
46:Pt:51:U:H3	46:Pt:65:G:H1	1.28	0.81
3:L5:735:G:OP1	14:LM:70:GLN:NE2	2.15	0.79
75:S2:1348:G:H1	75:S2:1381:G:H22	1.31	0.79
3:L5:3717:A:H2'	3:L5:3718:A2M:H8	1.66	0.78
3:L5:3946:G:H1	3:L5:4067:U:H3	1.29	0.77
6:LC:101:MET:HE3	6:LC:104:PRO:HA	1.66	0.77
3:L5:2520:C:O2	3:L5:2640:G:N2	2.19	0.76
17:LI:63:GLU:N	17:LI:63:GLU:OE2	2.17	0.76
75:S2:1550:G:H3'	75:S2:1579:A:H61	1.52	0.75
39:Lj:80:GLU:N	39:Lj:80:GLU:OE2	2.19	0.75
61:SX:52:LEU:CD1	61:SX:73:GLN:HB2	2.16	0.75
3:L5:1804:A:H4'	3:L5:1805:A:H5''	1.69	0.74
4:LA:142:GLU:OE2	4:LA:142:GLU:N	2.19	0.74
3:L5:1656:U:OP2	15:La:26:ARG:NH2	2.22	0.73
64:SC:227:ARG:NH2	75:S2:656:G:O2'	2.21	0.73
36:Lf:63:LYS:HD3	36:Lf:63:LYS:N	2.04	0.73
4:LA:104:VAL:HA	4:LA:107:MET:HE3	1.71	0.72
78:Sg:175:LYS:HD3	78:Sg:184:LEU:HD11	1.71	0.72
78:Sg:201:SER:HB2	78:Sg:206:LEU:HD23	1.71	0.72
49:SB:142:PHE:HB2	49:SB:208:HIS:HE1	1.53	0.72
60:SV:38:GLU:OE2	60:SV:38:GLU:N	2.21	0.72
81:SR:5:ARG:HG2	81:SR:9:VAL:HG11	1.71	0.71
53:SI:29:LEU:C	53:SI:29:LEU:HD12	2.15	0.71
49:SB:144:LYS:HD3	49:SB:208:HIS:HB3	1.71	0.71
8:LH:48:LEU:HD11	8:LH:56:ARG:HE	1.56	0.70
66:SJ:121:LYS:HB2	66:SJ:121:LYS:NZ	2.00	0.70
3:L5:450:G:H1	3:L5:1297:U:H3	1.40	0.70
3:L5:907:C:H2'	3:L5:908:G:H8	1.57	0.69
75:S2:1729:U:H3	75:S2:1805:G:H1	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LY:120:GLU:N	26:LY:120:GLU:OE2	2.26	0.69
49:SB:68:GLU:OE2	49:SB:68:GLU:N	2.26	0.69
75:S2:1658:G:OP2	75:S2:1660:C:N4	2.25	0.69
78:Sg:198:VAL:HG12	78:Sg:209:SER:HB3	1.74	0.69
3:L5:730:G:OP2	32:LF:76:ARG:NH1	2.26	0.68
3:L5:1364:U:OP2	12:LL:36:ARG:NH1	2.25	0.68
21:LS:82:LEU:HA	21:LS:127:MET:HG2	1.75	0.68
75:S2:1488:C:O2'	75:S2:1490:G:OP2	2.10	0.68
50:SE:229:GLY:HA2	50:SE:235:TRP:CE3	2.25	0.68
75:S2:1459:G:H1	75:S2:1466:G:H22	1.39	0.68
78:Sg:272:GLN:NE2	78:Sg:284:PRO:O	2.25	0.68
3:L5:4076:G:OP1	10:LG:73:ARG:NH1	2.27	0.68
49:SB:152:LYS:HB2	81:SR:132:ARG:HG3	1.76	0.68
17:LI:87:ILE:HG12	17:LI:138:ILE:HG12	1.76	0.67
42:Lm:83:ARG:NH1	42:Lm:87:GLN:OE1	2.27	0.67
75:S2:1451:G:H21	75:S2:1473:G:H1	1.43	0.67
20:LR:148:ASP:OD2	20:LR:149:LYS:N	2.27	0.67
78:Sg:191:HIS:CD2	78:Sg:195:LEU:HD11	2.29	0.67
3:L5:4212:A:N1	22:LT:3:ASN:ND2	2.42	0.67
20:LR:116:ASP:OD1	20:LR:116:ASP:N	2.28	0.67
3:L5:3641:U:OP2	3:L5:3646:A:N6	2.28	0.67
56:SQ:107:GLU:OE2	56:SQ:107:GLU:C	2.38	0.67
75:S2:30:C:O2'	75:S2:596:U:OP1	2.12	0.67
14:LM:70:GLN:CD	14:LM:70:GLN:H	2.03	0.66
28:LZ:84:ARG:HH22	37:Lg:102:ILE:HD11	1.59	0.66
16:LN:160:GLU:OE2	16:LN:161:MET:HE3	1.94	0.66
67:SN:142:GLU:N	67:SN:142:GLU:OE2	2.28	0.66
81:SR:53:TYR:O	81:SR:57:LEU:HD13	1.95	0.66
49:SB:38:MET:HE2	49:SB:231:LEU:HD11	1.77	0.66
75:S2:805:U:H3	75:S2:858:A:H62	1.44	0.66
3:L5:1870:C:H2'	3:L5:1871:A2M:H8	1.78	0.66
35:Le:113:GLU:OE2	35:Le:113:GLU:N	2.28	0.66
3:L5:4646:U:OP2	20:LR:62:ARG:NH2	2.27	0.66
3:L5:4763:U:HO2'	21:LS:174:THR:HG1	1.41	0.66
75:S2:848:U:H2'	75:S2:849:A:H8	1.61	0.66
74:Sa:74:CYS:SG	74:Sa:77:CYS:N	2.63	0.66
58:ST:88:MET:HE1	75:S2:1665:G:C5	2.30	0.66
78:Sg:260:ASP:HB2	78:Sg:267:VAL:HG23	1.76	0.65
3:L5:1366:G:N7	12:LL:37:LYS:NZ	2.40	0.65
4:LA:30:ARG:O	4:LA:163:ARG:NH2	2.29	0.65
49:SB:65:ARG:NH2	68:SO:51:GLU:OE2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:La:133:ALA:O	15:La:137:ILE:HD12	1.97	0.65
55:SL:104:LYS:O	61:SX:11:ARG:NH2	2.29	0.65
3:L5:2578:G:N7	28:LZ:17:ARG:NH2	2.45	0.65
65:SG:186:GLN:NE2	75:S2:332:G:N7	2.45	0.65
49:SB:142:PHE:HB2	49:SB:208:HIS:CE1	2.31	0.64
3:L5:4508:C:OP1	13:LV:43:LYS:NZ	2.30	0.64
75:S2:89:C:N3	89:S2:2004:HOH:O	2.29	0.64
75:S2:1115:U:O2'	75:S2:1118:C:N4	2.29	0.64
75:S2:1276:A:H62	75:S2:1321:G:H8	1.43	0.64
3:L5:4088:C:OP1	4:LA:37:ARG:NH2	2.31	0.64
75:S2:1498:A:OP2	79:SD:27:ARG:NH2	2.30	0.64
3:L5:1377:G:H21	3:L5:1380:G:H5'	1.61	0.64
49:SB:25:PHE:HB3	68:SO:17:LEU:HD11	1.78	0.64
56:SQ:75:GLY:HA2	75:S2:1545:A:H4'	1.78	0.64
3:L5:4929:C:C1'	14:LM:118:MET:HE2	2.28	0.64
48:SA:196:GLU:OE2	48:SA:196:GLU:N	2.31	0.64
51:SF:60:ARG:O	62:Sc:51:ARG:NH2	2.31	0.64
3:L5:1596:U:O2'	23:LP:135:ARG:NH2	2.31	0.64
50:SE:40:GLU:N	50:SE:40:GLU:OE2	2.30	0.64
3:L5:3748:A:HO2'	4:LA:223:SER:HG	1.44	0.63
70:SY:34:THR:O	75:S2:570:C:O2'	2.16	0.63
49:SB:47:THR:OG1	49:SB:65:ARG:NH1	2.31	0.63
5:LB:43:LEU:O	5:LB:349:LYS:NZ	2.31	0.63
58:ST:64:LEU:HD21	58:ST:121:ARG:HB2	1.80	0.63
60:SV:16:LYS:HG2	60:SV:23:ILE:HG22	1.80	0.63
44:Lo:34:TYR:O	44:Lo:39:ARG:NH1	2.31	0.63
79:SD:66:ILE:HD12	79:SD:66:ILE:H	1.62	0.63
26:LY:1:MET:HE3	26:LY:2:LYS:N	2.12	0.62
7:LJ:90:ARG:NH2	7:LJ:108:GLY:O	2.31	0.62
67:SN:64:ARG:NH2	75:S2:919:A:OP2	2.29	0.62
75:S2:928:G:H1	75:S2:1013:U:H3	1.47	0.62
3:L5:469:C:N3	9:LE:105:ARG:NH2	2.42	0.62
71:SZ:80:ARG:O	75:S2:1598:G:O2'	2.14	0.62
3:L5:3689:G:O2'	3:L5:3818:U:OP2	2.16	0.62
18:LD:129:GLU:C	18:LD:129:GLU:OE2	2.42	0.62
48:SA:128:ARG:NH2	48:SA:151:ASP:O	2.33	0.62
3:L5:4472:G:O2'	42:Lm:100:TYR:O	2.18	0.62
49:SB:197:ILE:HB	49:SB:210:VAL:HG11	1.80	0.62
52:SH:159:ASP:OD1	52:SH:160:LYS:N	2.33	0.62
75:S2:1459:G:H22	75:S2:1466:G:H22	1.47	0.62
18:LD:70:GLU:N	18:LD:70:GLU:OE2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4525:C:OP1	5:LB:246:ARG:NH1	2.33	0.62
22:LT:11:THR:HG22	22:LT:14:MET:HE3	1.82	0.62
28:LZ:36:ARG:NH1	28:LZ:38:TYR:OH	2.32	0.62
3:L5:4258:C:OP2	7:LJ:54:ARG:NH1	2.33	0.61
3:L5:1241:C:H2'	3:L5:1242:G:H8	1.64	0.61
3:L5:4572:U:H3'	3:L5:4573:G:H21	1.65	0.61
17:LI:148:VAL:O	17:LI:152:LEU:HD12	1.99	0.61
3:L5:690:C:OP1	29:Lr:87:ARG:NH1	2.33	0.61
11:LO:32:LYS:HD3	11:LO:101:ARG:HG2	1.83	0.61
33:Lc:38:ILE:HD11	33:Lc:46:VAL:HG21	1.81	0.61
34:Ld:64:ILE:HG23	34:Ld:68:LEU:HD23	1.82	0.61
49:SB:44:ILE:HD12	49:SB:44:ILE:C	2.26	0.61
3:L5:308:G:OP2	3:L5:308:G:N2	2.31	0.61
39:Lj:14:LYS:HE3	41:Ll:51:LEU:HD12	1.81	0.61
51:SF:60:ARG:NH1	75:S2:1680:G:OP1	2.34	0.61
60:SV:62:MET:SD	69:SW:20:ARG:NH2	2.73	0.61
3:L5:2263:A:OP1	29:Lr:107:ARG:NH2	2.29	0.61
49:SB:41:ILE:HD11	49:SB:76:ASN:HB3	1.81	0.61
78:Sg:151:VAL:HA	78:Sg:169:GLY:HA2	1.82	0.61
3:L5:2267:U:OP1	29:Lr:37:SER:OG	2.19	0.61
3:L5:2631:U:OP2	24:LU:48:LYS:NZ	2.34	0.61
24:LU:105:ASN:HB2	24:LU:111:GLU:HG2	1.82	0.61
33:Lc:28:VAL:HG21	33:Lc:37:MET:HE3	1.82	0.60
2:L8:52:A:OP1	41:Ll:21:ARG:NH1	2.33	0.60
4:LA:36:GLU:HB2	4:LA:91:GLY:HA2	1.83	0.60
24:LU:48:LYS:HG3	24:LU:53:ALA:HB2	1.83	0.60
26:LY:1:MET:HE3	26:LY:2:LYS:H	1.66	0.60
3:L5:4922:C:N4	3:L5:4923:C:N4	2.49	0.60
75:S2:1547:C:N4	75:S2:1586:U:O4	2.28	0.60
29:Lr:20:ARG:NH1	35:Le:78:LEU:O	2.33	0.60
49:SB:129:THR:OG1	49:SB:130:THR:N	2.34	0.60
66:SJ:59:GLU:C	66:SJ:59:GLU:OE2	2.44	0.60
16:LN:44:ARG:NH1	16:LN:120:TRP:O	2.33	0.60
69:SW:106:THR:HG23	69:SW:108:ALA:H	1.66	0.60
3:L5:1802:A:H5''	3:L5:1803:G:H5'	1.83	0.60
81:SR:46:LEU:O	81:SR:50:ILE:HG12	2.01	0.60
3:L5:2351:OMC:HM22	3:L5:2352:U:H5'	1.84	0.60
11:LO:113:ASP:OD2	11:LO:113:ASP:C	2.45	0.60
63:Sd:46:TYR:OH	79:SD:23:GLU:OE1	2.06	0.60
34:Ld:57:MET:HG2	34:Ld:88:LEU:HD23	1.84	0.60
3:L5:4126:C:H5''	3:L5:4127:A:H5''	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LE:46:ARG:O	9:LE:65:ARG:NH2	2.34	0.59
22:LT:111:GLU:OE2	22:LT:111:GLU:N	2.34	0.59
70:SY:29:HIS:NE2	70:SY:69:THR:OG1	2.29	0.59
33:Lc:48:LEU:HD21	33:Lc:60:ILE:HG21	1.84	0.59
58:ST:97:LYS:NZ	75:S2:1570:G:N7	2.49	0.59
66:SJ:18:ARG:NH1	75:S2:3:C:O2	2.34	0.59
2:L8:65:A:OP1	30:Lh:56:ARG:NH1	2.35	0.59
3:L5:1326:A2M:OP2	3:L5:4445:U:O2'	2.19	0.59
3:L5:4967:A:H2'	3:L5:4968:A:H8	1.67	0.59
72:Sb:20:LYS:NZ	75:S2:1015:U:OP2	2.34	0.59
3:L5:2579:G:N2	3:L5:2582:A:OP2	2.32	0.59
56:SQ:37:ARG:NH2	75:S2:1543:U:OP1	2.36	0.59
32:LF:105:VAL:HG13	32:LF:136:VAL:HG12	1.84	0.59
71:SZ:66:LYS:HG3	71:SZ:111:ARG:HH22	1.67	0.59
74:Sa:13:LYS:O	74:Sa:15:ARG:NH1	2.35	0.59
3:L5:494:U:N3	3:L5:661:C:O2	2.36	0.59
28:LZ:89:ILE:HD11	28:LZ:121:ARG:HE	1.68	0.59
66:SJ:158:ASP:OD2	66:SJ:158:ASP:C	2.46	0.59
3:L5:235:A:O2'	3:L5:237:G:OP2	2.21	0.59
3:L5:4546:A:N7	4:LA:215:ASN:ND2	2.51	0.59
3:L5:4594:U:H2'	3:L5:4595:G:H8	1.66	0.59
3:L5:4930:C:OP1	9:LE:266:GLN:NE2	2.35	0.59
29:Lr:47:LYS:O	29:Lr:103:ARG:NH1	2.35	0.59
75:S2:94:G:HO2'	75:S2:508:A:HO2'	1.41	0.59
75:S2:981:A:H2'	75:S2:982:G:C8	2.37	0.59
3:L5:1279:A:O2'	3:L5:1281:G:N7	2.33	0.59
14:LM:39:ASP:O	14:LM:39:ASP:OD1	2.20	0.59
37:Lg:49:CYS:SG	37:Lg:85:LYS:NZ	2.73	0.59
57:SS:131:VAL:HG22	75:S2:1609:C:H5''	1.85	0.59
3:L5:1750:G:N2	17:LI:193:ASP:OD2	2.35	0.59
3:L5:4274:A:H2'	3:L5:4275:G:C8	2.37	0.59
3:L5:4537:C:H2'	3:L5:4538:G:H8	1.66	0.59
11:LO:166:ILE:HD13	11:LO:169:ARG:HH21	1.68	0.59
66:SJ:79:ARG:NH2	75:S2:819:G:OP1	2.36	0.59
66:SJ:132:GLN:OE1	75:S2:562:U:O2'	2.15	0.59
5:LB:170:LEU:O	5:LB:328:ASN:ND2	2.35	0.58
17:LI:36:LEU:HD11	17:LI:69:ARG:HE	1.67	0.58
64:SC:84:PHE:HB2	64:SC:86:LEU:HD11	1.85	0.58
64:SC:132:ASP:OD2	64:SC:132:ASP:C	2.46	0.58
75:S2:920:A:O2'	75:S2:922:A:OP1	2.21	0.58
50:SE:187:ALA:O	50:SE:245:ARG:NH1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SF:204:ARG:HG2	62:Sc:63:ARG:HH22	1.67	0.58
70:SY:20:ARG:NH1	70:SY:74:MET:SD	2.76	0.58
75:S2:535:G:N2	75:S2:551:U:O2	2.34	0.58
75:S2:1532:C:O2'	75:S2:1601:A:N1	2.36	0.58
18:LD:70:GLU:CD	18:LD:70:GLU:H	2.11	0.58
78:Sg:87:LEU:HB2	78:Sg:101:PHE:HB2	1.85	0.58
3:L5:3687:A:OP2	4:LA:198:ARG:NH2	2.36	0.58
3:L5:4618:OMG:H5''	13:LV:15:ARG:HB2	1.84	0.58
51:SF:50:PRO:HG2	51:SF:90:VAL:HG22	1.84	0.58
51:SF:71:ARG:NH2	51:SF:148:ASN:OD1	2.36	0.58
75:S2:1228:A:H2'	75:S2:1229:G:C8	2.39	0.58
3:L5:3615:G:O2'	27:LW:44:ARG:NH1	2.37	0.58
33:Lc:56:ARG:NH2	89:Lc:203:HOH:O	2.37	0.58
3:L5:4991:U:H2'	3:L5:4992:G:C8	2.38	0.58
8:LH:136:VAL:O	8:LH:138:GLN:NE2	2.36	0.58
25:LX:87:MET:HA	25:LX:90:ILE:HD12	1.86	0.58
58:ST:83:GLN:NE2	58:ST:85:ASN:OD1	2.35	0.58
3:L5:1332:C:H2'	3:L5:1333:A:H8	1.68	0.58
3:L5:1594:C:O2'	3:L5:1597:G:O2'	2.21	0.58
3:L5:1761:G:O6	3:L5:1772:C:N4	2.36	0.58
3:L5:4274:A:H2'	3:L5:4275:G:H8	1.69	0.58
7:LJ:114:ASP:OD1	7:LJ:114:ASP:N	2.37	0.58
70:SY:108:LYS:NZ	75:S2:506:G:OP1	2.36	0.58
75:S2:980:A:H2'	75:S2:981:A:C8	2.39	0.58
2:L8:102:G:OP2	2:L8:104:A:O2'	2.22	0.58
9:LE:141:ARG:NH2	9:LE:191:GLN:O	2.37	0.58
52:SH:69:LEU:HD23	52:SH:96:ALA:HB2	1.85	0.58
65:SG:191:ARG:NH2	75:S2:312:G:O2'	2.37	0.58
75:S2:1402:A:H2'	75:S2:1405:A:H61	1.68	0.58
75:S2:1562:C:H2'	75:S2:1563:G:H8	1.68	0.58
78:Sg:238:ALA:H	78:Sg:251:ALA:HB3	1.69	0.58
1:SP:40:ARG:NH2	75:S2:1616:U:O4	2.37	0.57
3:L5:4237:C:O2	3:L5:4321:U:O2'	2.21	0.57
10:LG:58:PRO:HD2	10:LG:61:ILE:HD12	1.86	0.57
40:Lk:26:LYS:NZ	40:Lk:28:ASN:OD1	2.35	0.57
63:Sd:24:CYS:SG	89:Sd:102:HOH:O	2.57	0.57
49:SB:25:PHE:HA	49:SB:28:LYS:HG3	1.85	0.57
64:SC:205:VAL:HG13	64:SC:223:TYR:HA	1.87	0.57
3:L5:4084:G:O6	4:LA:72:ARG:NH2	2.38	0.57
21:LS:53:LYS:NZ	47:L7:74:A:O2'	2.35	0.57
31:Lb:99:ILE:O	31:Lb:109:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:S2:1226:G:N1	75:S2:1639:G:OP2	2.35	0.57
3:L5:1194:G:H2'	3:L5:1195:G:H8	1.69	0.57
3:L5:4473:A:OP1	42:Lm:124:LYS:NZ	2.35	0.57
8:LH:115:ARG:HB3	8:LH:123:ILE:HG12	1.86	0.57
34:Ld:61:ASP:OD1	34:Ld:100:ASN:ND2	2.29	0.57
3:L5:150:U:OP2	10:LG:200:THR:OG1	2.22	0.57
3:L5:2279:A:O2'	35:Le:48:ARG:NH2	2.38	0.57
18:LD:267:ASN:N	18:LD:267:ASN:OD1	2.36	0.57
56:SQ:69:ARG:NH1	75:S2:1429:G:OP1	2.37	0.57
52:SH:105:THR:OG1	52:SH:106:ARG:N	2.35	0.57
71:SZ:85:ARG:NH2	75:S2:1598:G:O6	2.38	0.57
70:SY:5:VAL:HG13	70:SY:29:HIS:HB3	1.86	0.57
5:LB:231:VAL:HG11	5:LB:251:VAL:HG23	1.87	0.57
67:SN:124:ARG:NH2	75:S2:1024:A:OP2	2.37	0.57
68:SO:74:ALA:HB1	68:SO:115:ALA:HB2	1.87	0.57
3:L5:735:G:H5''	14:LM:70:GLN:HE21	1.70	0.57
3:L5:1683:U:OP1	15:La:44:ASN:ND2	2.37	0.57
3:L5:1947:U:H2'	42:Lm:109:ASN:HD22	1.70	0.57
10:LG:77:PRO:HG2	10:LG:80:ILE:HD12	1.85	0.57
10:LG:148:GLU:OE2	38:Li:36:HIS:NE2	2.38	0.57
34:Ld:57:MET:HE3	34:Ld:90:ARG:HB2	1.85	0.57
62:Sc:20:ARG:HD3	75:S2:1680:G:H4'	1.87	0.57
75:S2:56:G:N1	89:S2:2004:HOH:O	2.33	0.57
3:L5:715:G:OP1	6:LC:321:ASN:ND2	2.36	0.57
3:L5:327:U:O2'	38:Li:30:ARG:NH1	2.38	0.56
3:L5:4485:C:O2'	42:Lm:114:LYS:NZ	2.38	0.56
6:LC:329:ASN:ND2	32:LF:188:GLU:OE2	2.38	0.56
73:Se:22:GLN:O	73:Se:24:LYS:NZ	2.37	0.56
78:Sg:80:SER:HB2	78:Sg:90:TRP:HE1	1.70	0.56
3:L5:3610:A:O2'	53:SI:89:GLU:OE2	2.22	0.56
3:L5:4431:PSU:OP2	17:LI:3:ARG:NH2	2.38	0.56
4:LA:117:GLU:HG2	4:LA:124:GLY:H	1.69	0.56
39:Lj:32:SER:O	39:Lj:32:SER:OG	2.22	0.56
49:SB:115:LYS:HD2	75:S2:1869:A:H1'	1.88	0.56
61:SX:73:GLN:HG3	61:SX:80:LYS:HD2	1.87	0.56
68:SO:113:GLN:OE1	68:SO:113:GLN:HA	2.04	0.56
75:S2:17:C:O2'	75:S2:1194:A:N1	2.36	0.56
75:S2:96:C:H1'	75:S2:474:G:H5'	1.87	0.56
75:S2:1144:A:H5'	75:S2:1355:C:H41	1.70	0.56
3:L5:382:G:O2'	3:L5:407:A:N6	2.38	0.56
3:L5:2408:U:OP1	41:Ll:42:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4095:G:H2'	3:L5:4096:C:C2	2.40	0.56
3:L5:4620:U:OP2	3:L5:4670:C:N4	2.34	0.56
3:L5:4736:C:H2'	3:L5:4737:G:H8	1.69	0.56
17:LI:38:ARG:NH2	17:LI:45:GLU:OE2	2.31	0.56
56:SQ:11:GLN:OE1	75:S2:1408:U:O2'	2.24	0.56
65:SG:92:ARG:O	75:S2:453:C:O2'	2.24	0.56
75:S2:1354:G:N2	75:S2:1357:A:OP2	2.30	0.56
34:Ld:32:ARG:HB3	34:Ld:48:GLU:HG2	1.86	0.56
1:SP:47:ARG:NH1	75:S2:1619:A:OP2	2.39	0.56
3:L5:4922:C:C4	3:L5:4923:C:N4	2.74	0.56
3:L5:4312:U:H2'	3:L5:4313:A:C8	2.40	0.56
1:SP:124:LYS:HE3	75:S2:1239:U:H5''	1.88	0.56
28:LZ:96:VAL:HG13	28:LZ:110:ALA:HB1	1.87	0.56
53:SI:101:ILE:HD12	53:SI:190:LEU:HD11	1.88	0.56
58:ST:35:ASP:N	58:ST:35:ASP:OD1	2.35	0.56
33:Lc:38:ILE:HG21	33:Lc:63:TYR:HB3	1.87	0.56
57:SS:26:ILE:HD12	57:SS:26:ILE:H	1.70	0.56
75:S2:1010:G:H2'	75:S2:1011:A:H8	1.70	0.56
75:S2:1098:C:H2'	75:S2:1099:G:C8	2.41	0.56
1:SP:98:ASN:ND2	1:SP:103:ASN:OD1	2.38	0.56
5:LB:165:HIS:HB3	5:LB:180:LEU:HD12	1.87	0.56
79:SD:157:MET:HA	79:SD:189:MET:SD	2.46	0.56
17:LI:141:LYS:HD2	17:LI:143:GLN:HE22	1.71	0.55
51:SF:82:ASN:HD21	75:S2:1535:U:H1'	1.72	0.55
75:S2:1552:G:H1'	79:SD:9:ARG:HH22	1.71	0.55
75:S2:1553:C:H4'	75:S2:1554:C:H5'	1.87	0.55
78:Sg:197:THR:OG1	78:Sg:237:ASN:O	2.24	0.55
3:L5:1872:G:O2'	3:L5:4219:A:N3	2.36	0.55
4:LA:32:VAL:HG22	4:LA:163:ARG:HH12	1.72	0.55
3:L5:2745:A:H2'	3:L5:2746:A:H8	1.71	0.55
3:L5:3749:C:O2'	4:LA:220:GLY:O	2.24	0.55
3:L5:4162:C:O2	10:LG:73:ARG:NH2	2.39	0.55
3:L5:4264:G:OP1	18:LD:8:LYS:NZ	2.39	0.55
3:L5:5027:C:H41	53:SI:170:LYS:HD3	1.70	0.55
24:LU:106:SER:OG	24:LU:107:LYS:N	2.39	0.55
25:LX:78:LYS:O	30:Lh:32:ARG:NH1	2.39	0.55
3:L5:1204:C:H2'	3:L5:1205:G:H8	1.72	0.55
11:LO:118:MET:HE3	21:LS:169:THR:HG23	1.88	0.55
21:LS:80:ILE:HG12	21:LS:129:VAL:HG13	1.89	0.55
52:SH:154:ILE:HB	52:SH:185:VAL:HG12	1.88	0.55
64:SC:168:GLY:N	64:SC:179:THR:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:SO:104:ARG:NH2	75:S2:959:G:OP1	2.40	0.55
75:S2:1228:A:H2'	75:S2:1229:G:H8	1.71	0.55
78:Sg:87:LEU:HD21	78:Sg:122:SER:HB3	1.89	0.55
79:SD:192:TRP:NE1	79:SD:201:LYS:O	2.40	0.55
3:L5:62:A:N3	3:L5:77:U:O2'	2.34	0.55
3:L5:1263:A:H2'	3:L5:1264:C:H6	1.71	0.55
11:LO:54:TYR:OH	11:LO:73:PHE:O	2.25	0.55
75:S2:640:A:H2'	75:S2:641:A:C8	2.42	0.55
3:L5:1933:G:H2'	3:L5:1934:A:C8	2.42	0.55
10:LG:88:ASP:OD1	10:LG:88:ASP:N	2.40	0.55
15:La:72:THR:HG22	15:La:110:LYS:HB3	1.89	0.55
68:SO:149:ARG:NH1	75:S2:1064:C:O3'	2.40	0.55
3:L5:907:C:H2'	3:L5:908:G:C8	2.39	0.55
3:L5:1950:U:O2'	21:LS:116:ARG:NH1	2.40	0.55
3:L5:4537:C:H2'	3:L5:4538:G:C8	2.41	0.55
49:SB:70:SER:OG	68:SO:128:ARG:NH1	2.39	0.55
64:SC:166:ARG:HG3	64:SC:248:TYR:CE1	2.41	0.55
67:SN:40:LEU:HB3	67:SN:50:ILE:HD12	1.88	0.55
75:S2:1264:C:H4'	75:S2:1265:A:H5'	1.89	0.55
75:S2:1693:G:N2	75:S2:1834:A:H8	2.05	0.55
75:S2:1854:U:H2'	75:S2:1855:G:H8	1.71	0.55
3:L5:1774:C:H2'	3:L5:1775:A:C8	2.41	0.55
21:LS:95:ARG:NH1	21:LS:112:ASP:OD2	2.39	0.55
33:Lc:13:SER:OG	33:Lc:17:ARG:NH2	2.39	0.55
51:SF:69:VAL:O	51:SF:73:THR:OG1	2.25	0.55
54:SK:80:ARG:HH22	54:SK:89:ILE:HA	1.70	0.55
75:S2:928:G:H2'	75:S2:929:G:C8	2.42	0.55
3:L5:2089:G:O2'	6:LC:307:LYS:NZ	2.35	0.54
6:LC:315:LYS:HD2	32:LF:168:ALA:HB1	1.88	0.54
3:L5:4670:C:O2'	3:L5:4672:A:OP2	2.22	0.54
28:LZ:21:ARG:NH1	28:LZ:47:ASP:O	2.40	0.54
57:SS:136:THR:OG1	75:S2:1521:C:OP2	2.23	0.54
69:SW:3:ARG:NH2	75:S2:922:A:OP2	2.39	0.54
3:L5:1771:U:H2'	3:L5:1772:C:C6	2.42	0.54
3:L5:4227:OMU:HM21	3:L5:4336:A:H1'	1.90	0.54
52:SH:145:ARG:NH1	69:SW:51:GLU:OE1	2.39	0.54
3:L5:2894:A:OP2	53:SI:205:ARG:NH1	2.40	0.54
17:LI:150:GLU:OE2	17:LI:153:ARG:NH1	2.40	0.54
71:SZ:66:LYS:H	71:SZ:66:LYS:HZ3	1.55	0.54
3:L5:86:U:O2'	15:La:65:ARG:NH1	2.40	0.54
3:L5:4717:A:OP2	5:LB:30:LYS:NZ	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LP:117:ILE:HD12	23:LP:148:MET:HE2	1.88	0.54
21:LS:85:ASP:C	21:LS:85:ASP:OD2	2.50	0.54
3:L5:1811:G:H21	31:Lb:57:MET:HE2	1.72	0.54
3:L5:3848:U:H2'	3:L5:3849:A:H8	1.73	0.54
74:Sa:76:SER:OG	75:S2:1863:A:N6	2.41	0.54
3:L5:1270:A:O2'	3:L5:1439:C:O2	2.26	0.54
3:L5:2611:A:H5'	3:L5:2688:G:H4'	1.90	0.54
7:LJ:44:THR:HG23	7:LJ:46:GLN:H	1.73	0.54
26:LY:109:LEU:O	26:LY:111:LEU:HD22	2.08	0.54
54:SK:12:TYR:HB3	54:SK:79:LEU:HD11	1.90	0.54
64:SC:108:LYS:HE2	64:SC:110:MET:HG3	1.90	0.54
77:S6:29:C:H2'	77:S6:30:G:H8	1.73	0.54
3:L5:1509:C:H5''	15:La:2:PRO:HD2	1.90	0.54
44:Lo:11:PHE:O	44:Lo:81:ARG:NH2	2.34	0.54
48:SA:31:ASP:OD1	48:SA:32:PHE:N	2.41	0.54
48:SA:42:LYS:HD3	48:SA:46:ILE:HB	1.89	0.54
51:SF:45:TYR:OH	51:SF:65:GLN:HG3	2.08	0.54
3:L5:1774:C:H2'	3:L5:1775:A:H8	1.73	0.53
6:LC:33:ARG:NH2	19:LQ:22:ASP:OD1	2.41	0.53
49:SB:91:VAL:HG12	49:SB:96:CYS:HA	1.90	0.53
40:Lk:51:GLU:O	40:Lk:54:GLU:OE2	2.27	0.53
54:SK:25:LYS:NZ	75:S2:1497:G:N7	2.56	0.53
75:S2:1292:C:N4	89:S2:2018:HOH:O	2.40	0.53
75:S2:1373:C:OP1	81:SR:7:LYS:N	2.41	0.53
75:S2:1599:U:H4'	75:S2:1600:G:H5'	1.88	0.53
30:Lh:95:LEU:HB3	30:Lh:99:GLU:HB3	1.91	0.53
40:Lk:40:ARG:NH2	40:Lk:41:TYR:OH	2.41	0.53
71:SZ:50:PHE:O	71:SZ:54:THR:OG1	2.20	0.53
75:S2:389:A:H2'	75:S2:390:C:H6	1.73	0.53
18:LD:271:MET:HG3	18:LD:275:GLN:HB2	1.89	0.53
53:SI:31:ARG:NH1	75:S2:380:G:OP1	2.35	0.53
58:ST:11:GLN:OE1	58:ST:62:ARG:NE	2.32	0.53
66:SJ:57:ALA:HB2	66:SJ:97:ILE:HD11	1.90	0.53
78:Sg:11:LEU:HD21	78:Sg:43:TRP:CG	2.44	0.53
64:SC:77:SER:OG	64:SC:78:LEU:N	2.41	0.53
64:SC:86:LEU:HD12	64:SC:86:LEU:H	1.74	0.53
3:L5:1942:A:H2'	3:L5:1943:A:C8	2.44	0.53
3:L5:2459:G:N2	3:L5:2462:C:OP2	2.41	0.53
3:L5:260:C:N4	3:L5:261:G:O6	2.42	0.53
3:L5:2556:G:H2'	3:L5:2557:G:H8	1.73	0.53
3:L5:4363:A:H5''	44:Lo:36:GLN:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:LX:143:ASP:OD1	25:LX:143:ASP:N	2.35	0.53
75:S2:1536:G:H2'	75:S2:1537:A:C8	2.43	0.53
3:L5:200:U:O2'	26:LY:59:ARG:NH2	2.41	0.53
3:L5:1942:A:H2'	3:L5:1943:A:H8	1.73	0.53
3:L5:2568:C:H2'	3:L5:2569:G:C8	2.43	0.53
51:SF:63:LYS:NZ	75:S2:1678:A:OP2	2.35	0.53
75:S2:527:C:H2'	75:S2:528:A:C8	2.44	0.53
75:S2:996:A:H2'	75:S2:997:A:C8	2.44	0.53
3:L5:728:U:OP1	32:LF:76:ARG:NH2	2.42	0.53
36:Lf:62:GLY:C	36:Lf:63:LYS:HD3	2.34	0.53
66:SJ:39:ASN:N	66:SJ:39:ASN:OD1	2.42	0.53
75:S2:1174:U:H2'	75:S2:1175:G:H8	1.74	0.53
75:S2:1459:G:H22	75:S2:1466:G:N2	2.07	0.53
3:L5:2478:C:H2'	3:L5:2479:G:H8	1.74	0.53
17:LI:116:ARG:NH1	89:LI:401:HOH:O	2.40	0.53
38:Li:23:LYS:HD3	38:Li:24:PRO:HD2	1.90	0.53
75:S2:1752:C:OP1	75:S2:1782:G:N1	2.39	0.53
3:L5:2520:C:H2'	3:L5:2521:G:H8	1.73	0.52
2:L8:75:G:OP2	26:LY:74:TYR:OH	2.26	0.52
3:L5:4991:U:H2'	3:L5:4992:G:H8	1.73	0.52
7:LJ:144:LYS:O	7:LJ:148:THR:OG1	2.25	0.52
64:SC:220:ASP:OD1	64:SC:220:ASP:N	2.42	0.52
66:SJ:34:GLU:OE1	66:SJ:34:GLU:N	2.31	0.52
75:S2:335:G:O2'	75:S2:336:A:O5'	2.28	0.52
3:L5:267:G:OP1	30:Lh:109:ARG:NH1	2.42	0.52
3:L5:956:A:H1'	3:L5:2076:G:H5''	1.91	0.52
3:L5:1743:A:N1	3:L5:1789:C:O2'	2.41	0.52
3:L5:1890:G:N2	3:L5:1890:G:OP2	2.42	0.52
18:LD:271:MET:HG3	18:LD:275:GLN:CB	2.40	0.52
20:LR:4:LEU:HD23	20:LR:24:LEU:HD13	1.92	0.52
48:SA:119:PRO:HG2	48:SA:142:LEU:HD11	1.91	0.52
51:SF:98:GLU:OE1	51:SF:98:GLU:N	2.34	0.52
63:Sd:17:GLY:HA2	63:Sd:27:ARG:HH11	1.75	0.52
77:S6:3:C:H2'	77:S6:4:G:C8	2.44	0.52
40:Lk:36:VAL:HG13	40:Lk:43:TYR:HB2	1.90	0.52
49:SB:151:ARG:NH2	75:S2:1123:C:OP1	2.43	0.52
50:SE:184:THR:O	50:SE:184:THR:OG1	2.21	0.52
75:S2:1010:G:H2'	75:S2:1011:A:C8	2.44	0.52
14:LM:39:ASP:OD1	14:LM:39:ASP:C	2.52	0.52
20:LR:7:GLN:NE2	20:LR:35:ALA:O	2.38	0.52
34:Ld:90:ARG:HD2	34:Ld:102:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:SF:34:SER:HA	62:Sc:55:VAL:HB	1.91	0.52
64:SC:72:ASP:OD2	64:SC:272:HIS:NE2	2.41	0.52
75:S2:145:G:H2'	75:S2:146:G:C8	2.45	0.52
3:L5:2621:A:OP1	24:LU:80:LYS:NZ	2.36	0.52
3:L5:4768:G:OP1	11:LO:168:TYR:OH	2.27	0.52
3:L5:4908:G:N2	3:L5:4913:G:OP1	2.40	0.52
9:LE:161:ARG:O	9:LE:182:ASN:ND2	2.42	0.52
35:Le:109:LYS:O	35:Le:113:GLU:OE2	2.28	0.52
49:SB:188:LEU:HD21	49:SB:215:VAL:HG11	1.92	0.52
49:SB:214:LYS:NZ	75:S2:943:U:OP1	2.35	0.52
67:SN:16:LEU:O	69:SW:57:ARG:NH2	2.43	0.52
21:LS:82:LEU:HA	21:LS:127:MET:CG	2.40	0.52
22:LT:39:ILE:HG13	22:LT:102:ARG:HG3	1.90	0.52
3:L5:1333:A:H2'	3:L5:1334:A:C8	2.45	0.52
3:L5:3946:G:N2	3:L5:4067:U:O2	2.33	0.52
17:LI:47:PRO:CG	17:LI:142:LEU:HD11	2.40	0.52
19:LQ:89:ASP:HB3	19:LQ:92:VAL:HG22	1.92	0.52
19:LQ:93:GLN:N	19:LQ:93:GLN:OE1	2.43	0.52
49:SB:175:GLU:HG3	49:SB:187:LYS:HZ2	1.74	0.52
75:S2:1555:U:O4	75:S2:1556:A:N6	2.42	0.52
75:S2:1597:C:H4'	75:S2:1603:G:C6	2.44	0.52
78:Sg:13:GLY:HA3	78:Sg:43:TRP:HH2	1.74	0.52
3:L5:4541:G:N2	3:L5:4544:A:OP2	2.36	0.52
3:L5:4868:G:O2'	3:L5:4872:G:OP1	2.27	0.52
3:L5:4967:A:H2'	3:L5:4968:A:C8	2.45	0.52
49:SB:139:CYS:HB2	49:SB:172:MET:HE2	1.92	0.52
54:SK:64:TRP:NE1	79:SD:23:GLU:OE2	2.42	0.52
3:L5:3718:A2M:H2	3:L5:3934:G:O4'	2.10	0.52
17:LI:47:PRO:HG3	17:LI:142:LEU:HD11	1.90	0.52
68:SO:36:SER:OG	68:SO:37:PHE:N	2.39	0.52
75:S2:527:C:H2'	75:S2:528:A:H8	1.74	0.52
75:S2:1459:G:H1	75:S2:1466:G:H1	1.58	0.52
75:S2:1778:C:H2'	75:S2:1779:G:C4	2.45	0.52
1:SP:40:ARG:HD3	75:S2:1620:A:H3'	1.92	0.51
3:L5:106:A:O2'	3:L5:335:A:N3	2.41	0.51
3:L5:956:A:N6	3:L5:1284:G:OP1	2.43	0.51
4:LA:178:PRO:HD2	45:Lp:26:VAL:HG22	1.92	0.51
19:LQ:89:ASP:O	19:LQ:112:ARG:NH1	2.38	0.51
21:LS:19:THR:HG23	21:LS:22:CYS:H	1.75	0.51
55:SL:130:GLU:OE1	55:SL:131:CYS:N	2.43	0.51
66:SJ:24:ARG:NH1	66:SJ:28:GLU:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2667:C:OP2	20:LR:103:ARG:NH1	2.43	0.51
28:LZ:88:ASP:OD1	28:LZ:88:ASP:N	2.44	0.51
43:Ln:18:ARG:NH1	75:S2:1182:A:OP1	2.44	0.51
49:SB:169:MET:O	49:SB:173:THR:OG1	2.28	0.51
73:Se:44:ASN:OD1	75:S2:552:G:O2'	2.28	0.51
3:L5:300:A:H2'	3:L5:301:G:H8	1.75	0.51
3:L5:491:G:H2'	3:L5:492:U:C6	2.45	0.51
3:L5:4420:PSU:H5'	3:L5:4421:C:H5	1.75	0.51
68:SO:55:ARG:NH2	75:S2:954:U:O2	2.43	0.51
75:S2:562:U:H2'	75:S2:563:G:C8	2.46	0.51
49:SB:103:MET:HB3	49:SB:215:VAL:HG13	1.92	0.51
50:SE:44:LEU:HD21	50:SE:72:ILE:HD11	1.92	0.51
75:S2:528:A:H2'	75:S2:529:A:H8	1.75	0.51
75:S2:1693:G:H21	75:S2:1834:A:H8	1.57	0.51
28:LZ:54:THR:HG23	28:LZ:57:MET:HE3	1.92	0.51
43:Ln:21:ARG:O	43:Ln:25:LYS:NZ	2.43	0.51
49:SB:120:MET:HG3	49:SB:142:PHE:CE2	2.46	0.51
50:SE:45:ILE:HA	50:SE:61:VAL:HG11	1.92	0.51
66:SJ:128:VAL:O	66:SJ:132:GLN:HG2	2.11	0.51
67:SN:132:LYS:NZ	75:S2:1021:U:OP1	2.42	0.51
75:S2:1347:U:H2'	75:S2:1348:G:C8	2.45	0.51
75:S2:1459:G:H1	75:S2:1466:G:N2	2.07	0.51
3:L5:2735:G:H2'	3:L5:2736:G:H8	1.74	0.51
50:SE:107:GLY:HA3	50:SE:189:LEU:HD13	1.92	0.51
68:SO:113:GLN:OE1	68:SO:113:GLN:CA	2.58	0.51
75:S2:16:G:H2'	75:S2:17:C:C6	2.45	0.51
75:S2:639:C:H2'	75:S2:640:A:C8	2.46	0.51
5:LB:50:LYS:NZ	5:LB:337:VAL:O	2.44	0.51
13:LV:30:ASP:OD1	13:LV:31:ASN:N	2.43	0.51
75:S2:416:U:O4	75:S2:417:C:N4	2.44	0.51
75:S2:656:G:N2	75:S2:663:C:H5''	2.26	0.51
77:S6:29:C:H2'	77:S6:30:G:C8	2.46	0.51
78:Sg:126:ASP:N	78:Sg:126:ASP:OD1	2.43	0.51
3:L5:2296:G:OP2	6:LC:190:ARG:NH2	2.43	0.51
3:L5:2856:C:O2	5:LB:242:ARG:NH2	2.44	0.51
3:L5:4896:G:H2'	3:L5:4897:G:H8	1.76	0.51
17:LI:80:CYS:SG	17:LI:81:GLY:N	2.83	0.51
50:SE:64:ILE:HG13	70:SY:17:LEU:HD12	1.93	0.51
51:SF:125:SER:HB2	51:SF:135:ARG:HB3	1.91	0.51
75:S2:639:C:H2'	75:S2:640:A:H8	1.75	0.51
3:L5:1332:C:H2'	3:L5:1333:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:2672:C:OP1	45:Lp:44:LYS:NZ	2.38	0.51
3:L5:3746:A:H5'	4:LA:244:GLY:HA3	1.91	0.51
20:LR:13:SER:OG	20:LR:38:ARG:NH1	2.41	0.51
3:L5:93:G:H2'	3:L5:94:A:C8	2.46	0.51
3:L5:960:A:N6	3:L5:1283:G:OP1	2.41	0.51
3:L5:2029:A:H2'	3:L5:2030:A:C8	2.45	0.51
3:L5:2557:G:O6	3:L5:2570:U:O4	2.29	0.51
6:LC:12:SER:OG	6:LC:13:GLU:N	2.44	0.51
58:ST:78:ILE:HD11	75:S2:1587:G:C5	2.46	0.51
79:SD:76:ARG:HG3	79:SD:77:PHE:CD2	2.46	0.51
3:L5:2539:C:H2'	3:L5:2540:C:C6	2.46	0.50
3:L5:2754:G:O2'	28:LZ:51:ARG:NH2	2.44	0.50
3:L5:3717:A:H2'	3:L5:3718:A2M:C8	2.39	0.50
3:L5:4954:G:H2'	3:L5:4955:A:C8	2.45	0.50
50:SE:107:GLY:HA3	50:SE:189:LEU:HB3	1.93	0.50
74:Sa:10:ARG:NH2	75:S2:1860:A:OP2	2.40	0.50
3:L5:481:G:H2'	3:L5:482:G:C8	2.47	0.50
3:L5:1187:G:H1'	18:LD:275:GLN:HE21	1.76	0.50
71:SZ:79:ILE:HG23	71:SZ:83:LEU:HD23	1.93	0.50
3:L5:2411:C:H2'	3:L5:2412:A:H8	1.76	0.50
7:LJ:26:VAL:HG12	7:LJ:28:GLU:H	1.75	0.50
9:LE:101:ASN:O	9:LE:105:ARG:NH1	2.44	0.50
74:Sa:12:LYS:HD3	74:Sa:16:GLY:H	1.76	0.50
75:S2:17:C:H2'	75:S2:18:C:C6	2.46	0.50
75:S2:1033:G:N1	75:S2:1080:A:O2'	2.36	0.50
3:L5:4594:U:H2'	3:L5:4595:G:C8	2.46	0.50
20:LR:148:ASP:OD2	20:LR:148:ASP:C	2.53	0.50
37:Lg:93:ARG:O	37:Lg:97:ILE:HG13	2.12	0.50
28:LZ:50:PRO:HD3	28:LZ:68:ILE:HG12	1.94	0.50
63:Sd:22:ARG:NH2	75:S2:1554:C:OP1	2.45	0.50
77:S6:45:A:H3'	77:S6:46:G:H8	1.77	0.50
80:SM:47:ALA:HA	80:SM:112:LYS:HA	1.92	0.50
3:L5:4115:G:OP2	3:L5:4115:G:N2	2.28	0.50
17:LI:203:ARG:NH2	47:L7:105:C:OP2	2.38	0.50
19:LQ:92:VAL:O	19:LQ:112:ARG:NH2	2.44	0.50
46:Pt:16:C:H5'	46:Pt:60:A:N1	2.27	0.50
57:SS:13:LEU:HB3	57:SS:15:VAL:HG23	1.93	0.50
2:L8:148:A:H2'	2:L8:149:G:C8	2.47	0.50
3:L5:1503:A:H4'	3:L5:1504:G:H5'	1.94	0.50
3:L5:4959:U:H2'	3:L5:4960:G:H8	1.76	0.50
49:SB:134:LEU:HB3	49:SB:218:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SI:191:GLU:HA	53:SI:195:LEU:HD12	1.93	0.50
66:SJ:41:ARG:HH22	75:S2:522:A:H62	1.60	0.50
75:S2:165:G:OP2	75:S2:165:G:N2	2.44	0.50
3:L5:226:G:OP2	26:LY:1:MET:N	2.37	0.50
3:L5:1370:G:O6	6:LC:239:LYS:NZ	2.44	0.50
3:L5:1866:U:OP1	17:LI:4:ARG:NH1	2.39	0.50
3:L5:2745:A:H2'	3:L5:2746:A:C8	2.46	0.50
3:L5:3732:A:H2'	3:L5:3733:A:C8	2.47	0.50
19:LQ:8:ASN:OD1	19:LQ:8:ASN:N	2.45	0.50
19:LQ:80:ALA:HA	19:LQ:137:VAL:HG22	1.94	0.50
21:LS:80:ILE:HG23	21:LS:129:VAL:HG22	1.93	0.50
35:Le:124:ASN:OD1	35:Le:124:ASN:N	2.45	0.50
53:SI:5:ARG:NE	75:S2:379:C:O2	2.45	0.50
63:Sd:12:ARG:NH2	75:S2:1513:C:OP2	2.41	0.50
75:S2:64:A:H2	75:S2:83:A:H62	1.60	0.50
3:L5:2478:C:H2'	3:L5:2479:G:C8	2.47	0.50
3:L5:4899:G:H2'	3:L5:4901:G:H8	1.77	0.50
28:LZ:78:ASN:N	28:LZ:78:ASN:OD1	2.45	0.50
54:SK:94:LEU:HD21	79:SD:64:ARG:HH11	1.76	0.50
55:SL:67:SER:OG	75:S2:114:G:OP2	2.29	0.50
74:Sa:60:ASP:OD1	74:Sa:60:ASP:N	2.44	0.50
77:S6:5:G:N1	77:S6:69:C:O2	2.45	0.50
3:L5:253:G:H2'	3:L5:254:G:C8	2.47	0.49
3:L5:2695:A:OP1	40:Lk:35:LYS:NZ	2.41	0.49
3:L5:4680:G:H2'	3:L5:4681:A:C8	2.47	0.49
49:SB:139:CYS:HB2	49:SB:172:MET:CE	2.42	0.49
69:SW:90:GLN:HB2	69:SW:94:LEU:HD12	1.93	0.49
3:L5:1178:G:O2'	18:LD:286:SER:OG	2.26	0.49
75:S2:389:A:H2'	75:S2:390:C:C6	2.48	0.49
77:S6:8:4SU:H2'	77:S6:47:G7M:H22	1.77	0.49
8:LH:86:LEU:HB3	8:LH:186:THR:HG23	1.94	0.49
10:LG:88:ASP:OD1	10:LG:91:THR:OG1	2.26	0.49
56:SQ:112:LEU:HB3	56:SQ:120:LEU:HD11	1.93	0.49
63:Sd:10:HIS:NE2	75:S2:1261:C:O2	2.34	0.49
75:S2:88:G:H21	75:S2:500:A:H5'	1.77	0.49
75:S2:419:G:N2	75:S2:661:U:O2	2.45	0.49
75:S2:498:C:H2'	75:S2:499:G:C8	2.47	0.49
75:S2:1458:G:H2'	75:S2:1459:G:C8	2.47	0.49
78:Sg:36:ARG:HA	78:Sg:65:PHE:HB3	1.93	0.49
3:L5:478:G:H2'	3:L5:479:G:H8	1.77	0.49
3:L5:4238:G:H2'	3:L5:4239:A:H8	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4734:A:H2'	3:L5:4735:G:C8	2.47	0.49
26:LY:54:GLU:HB2	26:LY:108:ARG:HB3	1.94	0.49
55:SL:82:MET:SD	55:SL:85:THR:OG1	2.71	0.49
77:S6:15:G:H21	77:S6:21:H2U:HN3	1.61	0.49
79:SD:157:MET:HE2	79:SD:159:HIS:CD2	2.47	0.49
3:L5:163:A:H2'	3:L5:164:G:H8	1.78	0.49
3:L5:256:G:H2'	3:L5:257:C:C6	2.47	0.49
3:L5:4906:C:H2'	3:L5:4907:G:C8	2.48	0.49
3:L5:4992:G:H2'	3:L5:4993:G:C8	2.47	0.49
11:LO:149:TYR:O	11:LO:153:THR:OG1	2.24	0.49
59:SU:17:ILE:HA	59:SU:94:PRO:HA	1.93	0.49
75:S2:882:U:H3	75:S2:904:A:H2	1.59	0.49
2:L8:21:C:OP1	6:LC:195:LYS:NZ	2.45	0.49
3:L5:2667:C:OP1	20:LR:100:ARG:NH1	2.44	0.49
3:L5:3680:U:OP1	4:LA:54:ARG:NH2	2.33	0.49
3:L5:4314:C:H4'	22:LT:68:THR:HG21	1.94	0.49
75:S2:495:U:HO2'	75:S2:496:C:H6	1.59	0.49
3:L5:4929:C:O4'	14:LM:118:MET:HE2	2.13	0.49
53:SI:49:ARG:NH1	75:S2:447:A:OP1	2.45	0.49
61:SX:140:ARG:HD2	61:SX:141:PRO:HD2	1.94	0.49
78:Sg:64:HIS:HB3	78:Sg:83:TRP:HB2	1.94	0.49
3:L5:679:C:H2'	3:L5:680:G:H8	1.77	0.49
3:L5:2583:C:OP2	37:Lg:76:ARG:NH1	2.43	0.49
7:LJ:118:LYS:NZ	7:LJ:119:TYR:O	2.41	0.49
20:LR:105:LEU:HD23	20:LR:138:LEU:HD23	1.93	0.49
69:SW:16:ASN:ND2	75:S2:1094:C:O2	2.45	0.49
75:S2:1599:U:O2	75:S2:1600:G:N1	2.45	0.49
78:Sg:33:SER:HG	78:Sg:43:TRP:CD1	2.30	0.49
3:L5:1194:G:H2'	3:L5:1195:G:C8	2.47	0.49
3:L5:1333:A:H2'	3:L5:1334:A:H8	1.78	0.49
3:L5:2611:A:H2'	3:L5:2612:G:C8	2.48	0.49
4:LA:32:VAL:HA	4:LA:36:GLU:OE2	2.13	0.49
17:LI:207:ASP:OD1	17:LI:208:LYS:N	2.46	0.49
18:LD:223:PHE:HB3	18:LD:226:TYR:HB2	1.94	0.49
49:SB:196:ASP:OD2	49:SB:196:ASP:C	2.56	0.49
58:ST:40:ALA:HB2	58:ST:95:GLY:HA2	1.95	0.49
78:Sg:98:THR:OG1	78:Sg:99:ARG:N	2.45	0.49
11:LO:128:ARG:NH1	21:LS:162:GLN:OE1	2.46	0.49
36:Lf:63:LYS:N	36:Lf:63:LYS:CD	2.73	0.49
70:SY:10:ARG:HG2	70:SY:24:VAL:HG13	1.95	0.49
71:SZ:102:LYS:NZ	75:S2:1595:U:OP1	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:S2:17:C:H2'	75:S2:18:C:H6	1.78	0.49
75:S2:1348:G:H22	75:S2:1381:G:N2	2.10	0.49
67:SN:145:THR:O	67:SN:145:THR:OG1	2.28	0.48
75:S2:1849:G:HO2'	75:S2:1850:A:H8	1.60	0.48
3:L5:1927:U:OP1	3:L5:1949:U:O2'	2.28	0.48
3:L5:4896:G:H2'	3:L5:4897:G:C8	2.47	0.48
3:L5:5002:U:OP2	5:LB:385:LYS:NZ	2.42	0.48
8:LH:120:GLU:OE1	8:LH:124:ARG:NH2	2.46	0.48
12:LL:77:SER:N	12:LL:80:GLU:OE1	2.42	0.48
15:La:137:ILE:HD12	15:La:137:ILE:H	1.77	0.48
27:LW:13:ILE:HG12	27:LW:32:LEU:HD13	1.95	0.48
75:S2:1808:U:H2'	75:S2:1809:A:C8	2.48	0.48
76:mR:6:C:H2'	76:mR:7:G:H8	1.78	0.48
3:L5:958:G:O2'	9:LE:123:ARG:O	2.27	0.48
3:L5:1554:A:OP1	45:Lp:5:THR:OG1	2.30	0.48
3:L5:2580:U:O2'	28:LZ:79:HIS:ND1	2.46	0.48
3:L5:3669:G:H21	3:L5:3672:G:N2	2.11	0.48
3:L5:3786:U:OP1	3:L5:4550:G:O2'	2.31	0.48
43:Ln:14:LYS:HD2	75:S2:1172:U:H5'	1.95	0.48
75:S2:106:C:H2'	75:S2:107:A:H8	1.77	0.48
75:S2:388:U:H2'	75:S2:389:A:C8	2.48	0.48
77:S6:23:G:H2'	77:S6:24:C:C6	2.48	0.48
3:L5:2753:G:OP1	28:LZ:133:LYS:NZ	2.36	0.48
17:LI:36:LEU:HD11	17:LI:69:ARG:NE	2.27	0.48
51:SF:40:ALA:HB3	51:SF:67:PRO:HA	1.95	0.48
53:SI:6:ASP:OD2	53:SI:9:HIS:ND1	2.47	0.48
75:S2:1536:G:H2'	75:S2:1537:A:H8	1.78	0.48
3:L5:987:C:H2'	3:L5:988:C:C6	2.48	0.48
3:L5:1604:G:H2'	3:L5:1605:G:C8	2.49	0.48
22:LT:103:ASP:OD1	22:LT:103:ASP:N	2.47	0.48
38:Li:84:LYS:O	38:Li:88:GLU:HG3	2.14	0.48
54:SK:66:HIS:CG	79:SD:76:ARG:NH2	2.82	0.48
62:Sc:24:GLN:HG2	75:S2:1683:C:C2	2.49	0.48
64:SC:142:LYS:HG2	64:SC:153:GLY:HA3	1.95	0.48
69:SW:76:SER:HB2	75:S2:1158:G:H5''	1.96	0.48
75:S2:632:C:C2	75:S2:633:C:C5	3.01	0.48
3:L5:2893:U:OP1	53:SI:205:ARG:NH2	2.46	0.48
3:L5:3911:C:H2'	3:L5:3912:U:H6	1.78	0.48
3:L5:4523:A2M:H5''	3:L5:4524:G:H5'	1.95	0.48
3:L5:4743:G:H2'	3:L5:4744:A:C8	2.48	0.48
3:L5:5006:U:H4'	3:L5:5007:A:H5'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LY:84:ARG:HB2	26:LY:84:ARG:CZ	2.43	0.48
68:SO:16:SER:OG	68:SO:17:LEU:N	2.46	0.48
69:SW:111:MET:HE2	69:SW:111:MET:HB3	1.78	0.48
75:S2:1459:G:N2	75:S2:1466:G:H22	2.10	0.48
3:L5:724:C:OP1	6:LC:350:ARG:NE	2.46	0.48
3:L5:1094:G:H2'	3:L5:1095:A:C8	2.48	0.48
3:L5:1094:G:H2'	3:L5:1095:A:H8	1.78	0.48
3:L5:2520:C:H2'	3:L5:2521:G:C8	2.48	0.48
3:L5:3717:A:OP2	3:L5:3735:G:N2	2.43	0.48
3:L5:3917:A:H2'	3:L5:3918:G:H8	1.77	0.48
18:LD:77:ALA:O	18:LD:108:ARG:NH1	2.46	0.48
20:LR:63:CYS:O	20:LR:67:THR:HG23	2.13	0.48
48:SA:18:PHE:CZ	48:SA:177:MET:HE1	2.49	0.48
49:SB:26:SER:O	49:SB:51:ARG:NH2	2.46	0.48
57:SS:22:GLY:HA2	57:SS:56:ALA:HB3	1.96	0.48
58:ST:36:THR:O	58:ST:36:THR:OG1	2.31	0.48
66:SJ:6:SER:HB2	66:SJ:8:VAL:HG12	1.94	0.48
70:SY:53:ASP:C	70:SY:53:ASP:OD2	2.57	0.48
75:S2:107:A:H2'	75:S2:108:G:C8	2.49	0.48
75:S2:982:G:H2'	75:S2:983:A:H8	1.79	0.48
76:mR:6:C:H2'	76:mR:7:G:C8	2.49	0.48
77:S6:3:C:H2'	77:S6:4:G:H8	1.79	0.48
3:L5:735:G:C5'	14:LM:70:GLN:HE21	2.26	0.48
3:L5:2639:U:O2'	3:L5:2694:G:O6	2.30	0.48
3:L5:3938:G:N2	3:L5:4171:C:OP2	2.46	0.48
3:L5:4761:G:H2'	3:L5:4762:A:H8	1.78	0.48
64:SC:206:SER:OG	64:SC:207:ALA:N	2.44	0.48
75:S2:1461:G:H21	75:S2:1464:C:H5	1.61	0.48
75:S2:1733:U:H2'	75:S2:1734:G:O4'	2.14	0.48
3:L5:2848:G:O2'	3:L5:3838:U:O4	2.26	0.48
9:LE:153:LEU:HD11	9:LE:195:ILE:HG13	1.94	0.48
25:LX:104:ALA:O	25:LX:134:LYS:NZ	2.36	0.48
48:SA:120:ARG:NH1	64:SC:266:TYR:O	2.46	0.48
51:SF:169:ILE:HG13	75:S2:1535:U:N3	2.29	0.48
75:S2:464:A:H3'	75:S2:465:A:H8	1.79	0.48
75:S2:1277:C:H2'	75:S2:1278:A:H8	1.78	0.48
75:S2:1801:A:H2'	75:S2:1802:C:C6	2.48	0.48
3:L5:272:U:H2'	3:L5:273:U:C6	2.49	0.48
3:L5:655:C:H2'	3:L5:656:C:C6	2.49	0.48
3:L5:4459:U:H2'	3:L5:4460:U:C6	2.49	0.48
17:LI:146:GLU:H	17:LI:146:GLU:CD	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:SV:15:ARG:HH21	64:SC:84:PHE:HA	1.79	0.48
75:S2:1388:A:H61	79:SD:161:GLY:HA3	1.78	0.48
75:S2:1407:U:O2'	75:S2:1443:C:N3	2.47	0.48
2:L8:30:U:H2'	2:L8:31:G:H8	1.78	0.47
3:L5:212:A:H2'	3:L5:213:G:H8	1.79	0.47
3:L5:1727:U:H4'	32:LF:127:LYS:HG2	1.96	0.47
3:L5:3610:A:H2'	3:L5:3611:A:H8	1.79	0.47
3:L5:3722:G:H2'	3:L5:3723:A2M:H8	1.95	0.47
3:L5:4373:G:N7	44:Lo:61:LYS:NZ	2.58	0.47
4:LA:29:LEU:H	4:LA:123:ARG:HB3	1.77	0.47
10:LG:165:GLU:OE2	16:LN:26:ARG:NH2	2.46	0.47
49:SB:193:ILE:O	49:SB:197:ILE:HG12	2.14	0.47
51:SF:152:TRP:O	51:SF:156:THR:HG22	2.14	0.47
58:ST:38:LYS:NZ	58:ST:43:LYS:O	2.33	0.47
65:SG:10:THR:HA	65:SG:128:THR:HB	1.96	0.47
65:SG:174:PRO:O	75:S2:77:A:O2'	2.32	0.47
66:SJ:151:LEU:HA	66:SJ:154:GLN:HE22	1.78	0.47
75:S2:508:A:H3'	75:S2:509:G:H8	1.79	0.47
78:Sg:153:CYS:SG	78:Sg:198:VAL:HG22	2.54	0.47
3:L5:4928:C:H4'	14:LM:121:ARG:NH2	2.29	0.47
19:LQ:20:SER:O	19:LQ:26:ARG:NH1	2.47	0.47
19:LQ:88:ASP:OD1	19:LQ:112:ARG:NH1	2.40	0.47
23:LP:110:ASP:OD2	23:LP:110:ASP:C	2.57	0.47
72:Sb:33:MET:HE2	72:Sb:48:SER:HA	1.96	0.47
73:Se:39:ASN:HA	73:Se:43:VAL:HB	1.95	0.47
78:Sg:82:SER:OG	78:Sg:83:TRP:N	2.46	0.47
2:L8:8:U:H2'	2:L8:9:A:C8	2.48	0.47
3:L5:691:C:H2'	3:L5:692:A:C8	2.49	0.47
3:L5:1479:G:H2'	3:L5:1480:C:C6	2.49	0.47
3:L5:1669:A:H4'	3:L5:1685:G:N2	2.29	0.47
3:L5:4088:C:H2'	3:L5:4089:G:C8	2.49	0.47
49:SB:63:LYS:HB2	49:SB:63:LYS:HE3	1.70	0.47
55:SL:13:GLN:HB2	55:SL:16:ILE:HG22	1.97	0.47
75:S2:1004:U:H2'	75:S2:1005:G:H8	1.78	0.47
75:S2:1281:G:H2'	75:S2:1282:A:O4'	2.15	0.47
75:S2:1593:C:H2'	75:S2:1594:A:H8	1.78	0.47
78:Sg:6:THR:OG1	78:Sg:313:THR:OG1	2.25	0.47
3:L5:4860:G:H5'	11:LO:169:ARG:HD3	1.95	0.47
3:L5:4910:G:N2	11:LO:106:ASP:O	2.47	0.47
17:LI:47:PRO:HG2	17:LI:142:LEU:CD1	2.43	0.47
28:LZ:84:ARG:NH2	37:Lg:102:ILE:HD11	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:S2:528:A:H2'	75:S2:529:A:C8	2.49	0.47
2:L8:144:U:H2'	2:L8:145:C:C6	2.50	0.47
3:L5:226:G:N7	6:LC:184:TYR:OH	2.40	0.47
3:L5:2411:C:H2'	3:L5:2412:A:C8	2.50	0.47
3:L5:4239:A:H2'	3:L5:4240:G:C8	2.49	0.47
11:LO:183:LYS:HB2	11:LO:183:LYS:HE2	1.62	0.47
49:SB:131:ASP:OD1	49:SB:131:ASP:N	2.30	0.47
64:SC:102:LEU:HB3	64:SC:130:ILE:HD11	1.96	0.47
75:S2:1124:C:O2'	81:SR:126:MET:O	2.31	0.47
75:S2:1792:G:H2'	75:S2:1793:A:H8	1.80	0.47
77:S6:8:4SU:OP1	77:S6:8:4SU:H6	2.13	0.47
3:L5:3727:A:H2'	3:L5:3728:A:C8	2.50	0.47
3:L5:4976:U:N3	5:LB:342:LYS:O	2.47	0.47
7:LJ:23:ASN:HB3	7:LJ:129:ASP:HB2	1.96	0.47
13:LV:135:ASN:OD1	13:LV:135:ASN:N	2.37	0.47
53:SI:76:THR:OG1	53:SI:77:ARG:N	2.48	0.47
3:L5:382:G:N1	3:L5:385:A:OP2	2.37	0.47
3:L5:487:G:H2'	3:L5:488:G:C8	2.50	0.47
3:L5:1552:G:O2'	3:L5:1574:G:N2	2.35	0.47
3:L5:2607:C:H2'	3:L5:2608:G:H8	1.79	0.47
3:L5:3615:G:O2'	3:L5:3616:U:OP1	2.31	0.47
3:L5:3664:G:H2'	3:L5:3665:G:H8	1.79	0.47
3:L5:4195:G:O2'	3:L5:4442:PSU:OP1	2.26	0.47
3:L5:4319:C:H5''	44:Lo:18:HIS:HB2	1.96	0.47
3:L5:4907:G:H22	3:L5:4914:C:H5	1.62	0.47
9:LE:62:MET:HE3	9:LE:62:MET:HB3	1.83	0.47
25:LX:64:SER:OG	30:Lh:82:ASP:OD2	2.28	0.47
28:LZ:133:LYS:HB3	28:LZ:133:LYS:HE2	1.65	0.47
35:Le:8:VAL:HG12	35:Le:10:PRO:HD3	1.96	0.47
39:Lj:22:CYS:SG	39:Lj:24:SER:OG	2.73	0.47
42:Lm:97:ARG:HB2	42:Lm:120:ASN:HB3	1.97	0.47
46:Pt:1:C:H2'	46:Pt:2:G:H8	1.79	0.47
48:SA:94:THR:HG23	48:SA:186:ARG:HH22	1.78	0.47
54:SK:3:MET:O	54:SK:8:ARG:NH2	2.47	0.47
75:S2:1454:A:OP1	81:SR:49:LYS:NZ	2.39	0.47
75:S2:1554:C:H1'	75:S2:1555:U:H5	1.80	0.47
3:L5:4578:G:H2'	3:L5:4579:PSU:C6	2.49	0.47
5:LB:54:THR:HG22	5:LB:55:HIS:H	1.80	0.47
20:LR:105:LEU:HD22	20:LR:135:LYS:HG2	1.97	0.47
71:SZ:77:LEU:HD12	71:SZ:79:ILE:HD11	1.96	0.47
74:Sa:52:ASP:OD1	74:Sa:52:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:162:A:H2'	3:L5:163:A:H8	1.80	0.47
3:L5:981:C:H5'	3:L5:982:U:H5''	1.96	0.47
3:L5:3893:C:H2'	3:L5:3894:A:C8	2.50	0.47
51:SF:140:ASP:N	51:SF:140:ASP:OD1	2.47	0.47
64:SC:88:ILE:HG22	64:SC:160:LEU:HD23	1.97	0.47
75:S2:553:U:H2'	75:S2:554:A:C4	2.49	0.47
20:LR:148:ASP:CA	20:LR:151:ARG:HH21	2.27	0.47
33:Lc:34:THR:HG23	33:Lc:95:ALA:HB2	1.97	0.47
38:Li:23:LYS:HE2	38:Li:23:LYS:HB2	1.64	0.47
53:SI:113:TYR:HD2	53:SI:121:LEU:HD22	1.80	0.47
56:SQ:142:GLN:HB3	75:S2:1527:C:H5'	1.97	0.47
62:Sc:31:ARG:HH21	62:Sc:43:ILE:HD11	1.79	0.47
75:S2:388:U:H2'	75:S2:389:A:H8	1.79	0.47
75:S2:1101:U:H2'	75:S2:1102:G:H8	1.80	0.47
75:S2:1438:A:H2'	75:S2:1439:A:C8	2.50	0.47
75:S2:1643:U:H2'	75:S2:1644:C:C6	2.50	0.47
82:Sf:140:TYR:HA	82:Sf:147:THR:HA	1.96	0.47
2:L8:87:G:OP1	30:Lh:7:ARG:NH2	2.35	0.46
3:L5:325:U:H2'	3:L5:326:C:C6	2.51	0.46
3:L5:2744:A:H2'	3:L5:2745:A:C8	2.50	0.46
3:L5:3661:G:H4'	3:L5:3662:A:H5'	1.97	0.46
3:L5:4750:G:H2'	3:L5:4751:G:H8	1.80	0.46
40:Lk:14:THR:HA	40:Lk:17:ARG:HG3	1.98	0.46
75:S2:1403:C:H5'	75:S2:1405:A:H62	1.79	0.46
3:L5:478:G:H2'	3:L5:479:G:C8	2.50	0.46
9:LE:161:ARG:NH2	14:LM:106:ASP:OD2	2.38	0.46
28:LZ:3:LYS:NZ	33:Lc:40:GLN:O	2.47	0.46
51:SF:100:ILE:O	51:SF:104:THR:OG1	2.32	0.46
53:SI:65:PHE:O	53:SI:109:TYR:OH	2.28	0.46
57:SS:25:LYS:HZ2	75:S2:1597:C:H5'	1.81	0.46
66:SJ:142:VAL:HG12	66:SJ:144:ILE:H	1.80	0.46
67:SN:4:MET:HE3	75:S2:924:G:H5'	1.95	0.46
75:S2:1476:A:H2'	75:S2:1477:U:H4'	1.96	0.46
3:L5:2899:C:OP1	20:LR:108:ARG:NH2	2.48	0.46
3:L5:3610:A:H2'	3:L5:3611:A:C8	2.50	0.46
3:L5:3720:G:H22	3:L5:3733:A:H2	1.62	0.46
3:L5:3861:A:H2'	3:L5:3862:A:C8	2.50	0.46
11:LO:121:PRO:HA	11:LO:124:LEU:HD12	1.97	0.46
36:Lf:15:LYS:HG2	36:Lf:22:ARG:HB2	1.98	0.46
46:Pt:21:H2U:H2'	46:Pt:21:H2U:O2	2.15	0.46
47:L7:57:C:H2'	47:L7:58:A:H8	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SI:110:ARG:O	53:SI:114:GLU:HG2	2.16	0.46
78:Sg:34:ALA:HB1	78:Sg:66:VAL:HB	1.97	0.46
80:SM:34:GLY:HA2	80:SM:35:ILE:HA	1.62	0.46
3:L5:269:G:H2'	3:L5:270:U:H6	1.81	0.46
3:L5:959:G:C8	9:LE:123:ARG:HB2	2.51	0.46
21:LS:30:MET:HE2	21:LS:32:ILE:HD11	1.98	0.46
45:Lp:28:LYS:HE3	45:Lp:29:ILE:HG13	1.97	0.46
51:SF:135:ARG:NH1	77:S6:32:G:O2'	2.48	0.46
54:SK:41:PRO:HD2	54:SK:44:HIS:HB2	1.98	0.46
75:S2:454:U:H2'	75:S2:455:A:H8	1.80	0.46
75:S2:1297:U:O2'	75:S2:1298:G:N2	2.48	0.46
79:SD:204:LEU:O	79:SD:206:ASP:N	2.37	0.46
14:LM:70:GLN:HA	14:LM:73:VAL:HG12	1.98	0.46
21:LS:69:GLU:OE2	21:LS:70:LYS:N	2.49	0.46
33:Lc:28:VAL:HG11	33:Lc:37:MET:HE3	1.97	0.46
50:SE:16:LYS:NZ	75:S2:812:A:H5'	2.22	0.46
58:ST:96:SER:OG	75:S2:1568:C:OP1	2.25	0.46
75:S2:223:C:H2'	75:S2:224:A:C8	2.51	0.46
75:S2:1636:G:H5'	75:S2:1637:A:H5'	1.97	0.46
81:SR:43:SER:HB3	81:SR:46:LEU:HB2	1.97	0.46
3:L5:481:G:H2'	3:L5:482:G:H8	1.81	0.46
3:L5:2262:G:OP2	29:Lr:98:ARG:NH2	2.36	0.46
3:L5:2695:A:H4'	3:L5:2696:A:H5'	1.96	0.46
3:L5:4761:G:H2'	3:L5:4762:A:C8	2.50	0.46
3:L5:4929:C:H1'	14:LM:118:MET:HE2	1.98	0.46
14:LM:86:TRP:O	14:LM:89:THR:OG1	2.33	0.46
18:LD:172:SER:O	18:LD:172:SER:OG	2.26	0.46
44:Lo:24:THR:HG22	44:Lo:69:ARG:HB3	1.97	0.46
54:SK:24:LYS:O	54:SK:42:ASN:ND2	2.41	0.46
57:SS:136:THR:N	75:S2:1520:G:OP1	2.49	0.46
79:SD:162:ASP:OD2	79:SD:165:ASN:ND2	2.39	0.46
3:L5:1443:A:H2	3:L5:2102:G:H22	1.62	0.46
3:L5:1835:G:OP2	3:L5:1835:G:N2	2.37	0.46
3:L5:5057:C:H2'	3:L5:5058:A:C8	2.50	0.46
4:LA:206:PRO:HG3	4:LA:213:GLY:HA3	1.97	0.46
26:LY:82:ILE:HG22	26:LY:83:GLU:H	1.81	0.46
64:SC:183:LYS:HE2	69:SW:95:PRO:HA	1.98	0.46
66:SJ:111:GLN:NE2	66:SJ:123:ILE:O	2.40	0.46
70:SY:27:VAL:HB	70:SY:69:THR:HB	1.97	0.46
75:S2:941:C:H2'	75:S2:942:G:C8	2.51	0.46
3:L5:126:C:H2'	3:L5:127:G:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:224:U:O2	6:LC:219:LYS:NZ	2.36	0.46
3:L5:267:G:H2'	3:L5:268:G:H8	1.80	0.46
3:L5:279:A:N7	16:LN:12:ARG:NH1	2.63	0.46
3:L5:408:A:H4'	3:L5:409:G:H3'	1.97	0.46
3:L5:2894:A:H2'	3:L5:2895:A:H8	1.81	0.46
3:L5:3765:G:H21	3:L5:3766:A:N6	2.14	0.46
3:L5:4522:G:O2'	3:L5:4525:C:OP2	2.27	0.46
20:LR:99:MET:HB3	20:LR:99:MET:HE3	1.81	0.46
45:Lp:24:LYS:HA	45:Lp:24:LYS:HD3	1.70	0.46
3:L5:4227:OMU:HM23	3:L5:4227:OMU:H1'	1.65	0.46
4:LA:225:ILE:HD12	4:LA:225:ILE:HA	1.83	0.46
11:LO:170:LYS:HB3	11:LO:170:LYS:HE2	1.58	0.46
21:LS:47:PHE:HE1	21:LS:125:GLN:HG2	1.81	0.46
48:SA:32:PHE:O	48:SA:35:GLU:OE2	2.34	0.46
53:SI:4:SER:HB3	53:SI:24:LYS:HD3	1.97	0.46
58:ST:33:TRP:HB2	58:ST:36:THR:HG23	1.97	0.46
60:SV:56:CYS:SG	60:SV:57:GLY:N	2.89	0.46
3:L5:165:A:H2'	3:L5:166:C:C6	2.51	0.46
3:L5:2045:G:OP1	11:LO:63:ASN:ND2	2.49	0.46
3:L5:2517:A:N3	3:L5:2539:C:O2'	2.48	0.46
8:LH:137:SER:HB3	8:LH:143:GLU:HB3	1.98	0.46
56:SQ:110:ASP:HA	56:SQ:113:ILE:HG13	1.97	0.46
67:SN:87:ASP:HB2	67:SN:125:LEU:HD21	1.98	0.46
75:S2:293:C:O2'	75:S2:294:U:H3'	2.15	0.46
75:S2:1310:U:O2'	75:S2:1311:C:H5'	2.14	0.46
75:S2:1621:U:OP2	75:S2:1623:A:O2'	2.31	0.46
82:Sf:142:GLY:O	82:Sf:144:CYS:N	2.49	0.46
3:L5:176:G:H2'	3:L5:177:G:C8	2.51	0.45
3:L5:371:A:N3	3:L5:1531:U:O2'	2.48	0.45
25:LX:81:LEU:HD22	25:LX:83:THR:HG23	1.97	0.45
29:Lr:92:SER:O	29:Lr:96:MET:HG3	2.16	0.45
48:SA:154:LEU:HD23	48:SA:154:LEU:HA	1.82	0.45
49:SB:44:ILE:C	49:SB:44:ILE:CD1	2.89	0.45
49:SB:46:LYS:HB2	49:SB:46:LYS:HE3	1.71	0.45
52:SH:74:LYS:HE2	52:SH:74:LYS:HB2	1.85	0.45
64:SC:194:ARG:NH2	75:S2:1155:U:OP2	2.35	0.45
3:L5:2418:A:N1	3:L5:2429:A:O2'	2.43	0.45
3:L5:2710:C:H41	20:LR:46:LYS:NZ	2.15	0.45
3:L5:3896:C:O2'	5:LB:268:ARG:NH1	2.44	0.45
4:LA:112:ILE:HD12	45:Lp:79:VAL:HG22	1.96	0.45
8:LH:95:VAL:HG22	42:Lm:82:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LD:40:ASP:OD1	18:LD:40:ASP:N	2.49	0.45
39:Lj:31:LYS:HB3	39:Lj:33:THR:HG22	1.99	0.45
50:SE:55:ALA:HB1	50:SE:60:GLU:HB2	1.99	0.45
50:SE:189:LEU:H	50:SE:245:ARG:NH2	2.14	0.45
53:SI:54:LYS:NZ	75:S2:381:C:OP2	2.35	0.45
53:SI:86:SER:OG	53:SI:87:ASN:N	2.48	0.45
54:SK:64:TRP:NE1	63:Sd:23:VAL:HG13	2.31	0.45
56:SQ:51:LEU:HD21	56:SQ:81:ILE:HG12	1.96	0.45
3:L5:732:A:H2'	3:L5:733:A:O4'	2.16	0.45
3:L5:1447:C:H2'	3:L5:1448:G:H8	1.81	0.45
3:L5:2448:G:H2'	3:L5:2449:A:C8	2.51	0.45
3:L5:3910:C:H2'	3:L5:3911:C:C6	2.51	0.45
7:LJ:118:LYS:HE2	57:SS:10:GLN:HA	1.98	0.45
23:LP:94:MET:HG2	23:LP:148:MET:HE3	1.97	0.45
27:LW:3:VAL:HG11	27:LW:12:LYS:HE2	1.98	0.45
54:SK:66:HIS:CG	79:SD:76:ARG:HH22	2.34	0.45
70:SY:44:LEU:HD23	70:SY:44:LEU:HA	1.85	0.45
75:S2:432:G:H2'	75:S2:433:A:C8	2.52	0.45
3:L5:162:A:H2'	3:L5:163:A:C8	2.51	0.45
3:L5:676:C:H2'	3:L5:677:G:H8	1.81	0.45
16:LN:64:ILE:HD11	16:LN:106:ALA:HB2	1.98	0.45
50:SE:108:ARG:NH2	75:S2:846:G:OP2	2.50	0.45
53:SI:29:LEU:HD12	53:SI:29:LEU:O	2.17	0.45
54:SK:79:LEU:HD12	54:SK:79:LEU:HA	1.85	0.45
58:ST:25:SER:O	58:ST:25:SER:OG	2.28	0.45
78:Sg:130:LYS:HD2	78:Sg:138:CYS:SG	2.57	0.45
3:L5:269:G:H2'	3:L5:270:U:C6	2.52	0.45
3:L5:673:C:H2'	3:L5:674:G:H8	1.80	0.45
3:L5:2835:A:O2'	5:LB:228:TYR:O	2.32	0.45
3:L5:2894:A:H2'	3:L5:2895:A:C8	2.51	0.45
10:LG:99:ALA:HA	10:LG:204:PHE:HZ	1.82	0.45
20:LR:96:MET:SD	20:LR:100:ARG:NH2	2.89	0.45
23:LP:110:ASP:OD2	23:LP:110:ASP:O	2.34	0.45
26:LY:2:LYS:HB3	26:LY:2:LYS:HE3	1.57	0.45
32:LF:200:ARG:HD3	32:LF:203:GLU:OE1	2.16	0.45
33:Lc:78:ASN:N	33:Lc:78:ASN:OD1	2.48	0.45
57:SS:28:PHE:O	57:SS:31:THR:OG1	2.30	0.45
75:S2:573:U:N3	75:S2:576:A:OP2	2.38	0.45
78:Sg:40:ILE:HB	78:Sg:59:LEU:HB2	1.98	0.45
3:L5:983:C:H2'	3:L5:984:C:C6	2.52	0.45
3:L5:4688:C:H2'	3:L5:4689:PSU:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:LA:137:ILE:HD11	4:LA:149:LYS:HB2	1.99	0.45
9:LE:170:SER:OG	9:LE:214:ASP:OD2	2.32	0.45
46:Pt:20:G:H4'	46:Pt:21:H2U:OP2	2.16	0.45
71:SZ:46:ASN:HB3	71:SZ:80:ARG:HA	1.99	0.45
75:S2:1568:C:H2'	75:S2:1569:A:C8	2.51	0.45
75:S2:1729:U:O2	75:S2:1805:G:N2	2.37	0.45
3:L5:1557:C:H2'	3:L5:1558:A:H8	1.82	0.45
3:L5:2463:G:H2'	3:L5:2464:C:H6	1.82	0.45
3:L5:2540:C:H2'	3:L5:2541:G:H8	1.82	0.45
8:LH:36:ARG:HB3	8:LH:80:MET:HE1	1.98	0.45
46:Pt:21:H2U:OP2	46:Pt:21:H2U:H61	2.16	0.45
48:SA:36:GLN:H	48:SA:36:GLN:HG3	1.62	0.45
3:L5:1468:C:H2'	3:L5:1469:C:H6	1.81	0.45
3:L5:1558:A:H2'	3:L5:1559:G:C8	2.52	0.45
3:L5:3669:G:H21	3:L5:3672:G:H21	1.65	0.45
3:L5:4728:U:OP2	5:LB:132:LYS:NZ	2.42	0.45
53:SI:177:SER:OG	53:SI:178:ARG:N	2.49	0.45
54:SK:14:LEU:HD22	54:SK:35:LEU:HD13	1.99	0.45
75:S2:1317:C:H2'	75:S2:1318:G:H8	1.80	0.45
3:L5:1097:C:H2'	3:L5:1098:G:C8	2.52	0.45
3:L5:2693:G:H2'	3:L5:2694:G:N2	2.32	0.45
3:L5:2809:G:O2'	3:L5:4644:G:OP1	2.32	0.45
3:L5:4749:C:H2'	3:L5:4750:G:O4'	2.16	0.45
56:SQ:117:ARG:HA	56:SQ:117:ARG:HE	1.80	0.45
69:SW:36:ARG:HD2	69:SW:36:ARG:HA	1.77	0.45
3:L5:921:C:H2'	3:L5:922:C:H6	1.82	0.45
3:L5:1390:G:N2	3:L5:1393:G:OP2	2.41	0.45
3:L5:3848:U:H2'	3:L5:3849:A:C8	2.52	0.45
35:Le:81:ASN:OD1	35:Le:81:ASN:N	2.49	0.45
75:S2:1144:A:H2'	75:S2:1145:A:C8	2.52	0.45
75:S2:1215:C:O2'	75:S2:1645:C:OP2	2.33	0.45
3:L5:142:G:H2'	3:L5:144:G:H8	1.81	0.44
3:L5:291:U:O2'	16:LN:182:HIS:NE2	2.48	0.44
3:L5:1577:G:O2'	3:L5:1612:G:H4'	2.17	0.44
3:L5:3899:OMG:HM23	3:L5:3899:OMG:H1'	1.78	0.44
3:L5:4899:G:H2'	3:L5:4901:G:C8	2.53	0.44
78:Sg:206:LEU:HD12	78:Sg:218:LEU:HG	1.99	0.44
78:Sg:294:ASP:O	78:Sg:296:GLN:NE2	2.48	0.44
3:L5:124:C:OP1	16:LN:144:ARG:NH1	2.50	0.44
3:L5:3707:U:H2'	3:L5:3708:C:C6	2.52	0.44
3:L5:3870:C:H2'	3:L5:3871:A:H8	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:3893:C:H2'	3:L5:3894:A:H8	1.82	0.44
3:L5:4128:A:H1'	10:LG:35:ARG:HB2	2.00	0.44
3:L5:4188:U:H2'	3:L5:4189:U:C6	2.53	0.44
4:LA:98:ILE:HA	4:LA:166:VAL:HG12	1.99	0.44
4:LA:103:PRO:HA	4:LA:162:ASN:O	2.17	0.44
8:LH:20:LEU:HD21	8:LH:45:LEU:HB3	1.99	0.44
20:LR:148:ASP:N	20:LR:151:ARG:NH2	2.65	0.44
30:Lh:87:LYS:HB3	30:Lh:91:MET:HE2	1.98	0.44
66:SJ:149:VAL:HG23	66:SJ:153:SER:HB2	1.98	0.44
3:L5:679:C:H2'	3:L5:680:G:C8	2.53	0.44
3:L5:1076:C:H2'	3:L5:1077:C:C6	2.52	0.44
3:L5:1088:C:H2'	3:L5:1089:G:H8	1.82	0.44
3:L5:2474:G:OP2	25:LX:48:ARG:NH2	2.40	0.44
3:L5:3855:C:H2'	3:L5:3856:A:H8	1.82	0.44
3:L5:4088:C:H2'	3:L5:4089:G:H8	1.82	0.44
48:SA:200:ASP:OD1	48:SA:200:ASP:N	2.49	0.44
49:SB:171:ILE:CG2	49:SB:196:ASP:OD1	2.65	0.44
51:SF:91:ARG:HA	51:SF:94:LYS:HB3	2.00	0.44
57:SS:133:GLY:HA3	75:S2:1623:A:O5'	2.18	0.44
64:SC:183:LYS:HG3	69:SW:95:PRO:O	2.18	0.44
67:SN:99:ARG:NH1	67:SN:119:GLU:OE1	2.50	0.44
75:S2:1101:U:H2'	75:S2:1102:G:C8	2.52	0.44
75:S2:1471:C:H3'	75:S2:1472:C:H5''	1.99	0.44
3:L5:2407:G:OP2	3:L5:2407:G:N2	2.36	0.44
3:L5:5066:U:H2'	3:L5:5067:U:C6	2.51	0.44
66:SJ:78:LEU:HD21	66:SJ:94:LEU:HD23	1.99	0.44
75:S2:960:U:O2'	75:S2:962:A:N7	2.41	0.44
75:S2:1217:A:H2'	75:S2:1218:C:C6	2.53	0.44
81:SR:6:THR:O	81:SR:10:LYS:HG3	2.17	0.44
3:L5:3723:A2M:H2'	3:L5:3724:A2M:H8	1.98	0.44
3:L5:4699:U:H1'	3:L5:4700:A:H5''	1.99	0.44
3:L5:4723:A:H2'	3:L5:4724:A:C8	2.53	0.44
8:LH:1:MET:HE2	8:LH:1:MET:HB3	1.75	0.44
11:LO:54:TYR:CE1	11:LO:145:VAL:HG11	2.52	0.44
12:LL:164:GLU:OE1	12:LL:164:GLU:N	2.36	0.44
28:LZ:83:THR:HG23	37:Lg:95:PHE:CZ	2.52	0.44
46:Pt:24:C:H2'	46:Pt:25:U:C6	2.52	0.44
49:SB:118:GLN:O	75:S2:988:C:O2'	2.34	0.44
50:SE:127:ARG:HD3	50:SE:142:HIS:HA	1.99	0.44
64:SC:201:GLY:N	64:SC:221:ASP:OD1	2.47	0.44
66:SJ:26:ASP:OD1	66:SJ:27:GLN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:Sg:219:TRP:CE3	78:Sg:226:HIS:HB2	2.52	0.44
3:L5:659:G:H2'	3:L5:660:A:H8	1.82	0.44
3:L5:911:U:H2'	3:L5:912:G:O4'	2.17	0.44
3:L5:1445:U:H2'	3:L5:1446:C:H6	1.83	0.44
3:L5:1558:A:H2'	3:L5:1559:G:H8	1.82	0.44
5:LB:366:LYS:HE3	5:LB:366:LYS:HB3	1.72	0.44
18:LD:211:LEU:HD22	18:LD:211:LEU:HA	1.80	0.44
38:Li:55:ARG:O	38:Li:59:GLU:HG3	2.18	0.44
47:L7:92:C:H2'	47:L7:93:G:H8	1.82	0.44
48:SA:155:ARG:NH2	75:S2:1137:U:O2'	2.49	0.44
49:SB:28:LYS:HB3	49:SB:48:LEU:HD22	1.97	0.44
54:SK:24:LYS:HD3	54:SK:66:HIS:NE2	2.33	0.44
58:ST:14:PHE:HA	58:ST:138:VAL:HG21	1.98	0.44
61:SX:101:LEU:HB3	61:SX:124:LYS:HB2	1.99	0.44
75:S2:12:U:H2'	75:S2:13:C:C6	2.53	0.44
75:S2:217:A:H1'	75:S2:309:G:N2	2.32	0.44
75:S2:1232:U:H2'	75:S2:1233:G:H8	1.82	0.44
77:S6:74:A:H8	77:S6:74:A:OP2	2.01	0.44
79:SD:23:GLU:O	79:SD:26:THR:HB	2.18	0.44
3:L5:445:U:H2'	3:L5:446:C:O4'	2.18	0.44
3:L5:656:C:H2'	3:L5:657:C:C6	2.52	0.44
3:L5:2386:U:H2'	3:L5:2387:G:H8	1.82	0.44
5:LB:116:ARG:HB3	5:LB:177:LYS:HG3	2.00	0.44
9:LE:281:ILE:HG23	9:LE:286:LEU:HD13	1.99	0.44
13:LV:60:MET:HE3	13:LV:60:MET:HB2	1.81	0.44
18:LD:241:LYS:HD2	18:LD:241:LYS:HA	1.83	0.44
32:LF:226:HIS:ND1	32:LF:228:VAL:HG22	2.33	0.44
49:SB:192:SER:HA	49:SB:195:LYS:HD3	2.00	0.44
56:SQ:24:HIS:CD2	75:S2:1409:A:H4'	2.53	0.44
75:S2:980:A:H2'	75:S2:981:A:H8	1.81	0.44
75:S2:1533:A:OP1	75:S2:1636:G:O2'	2.31	0.44
3:L5:735:G:P	14:LM:70:GLN:NE2	2.90	0.44
34:Ld:26:THR:OG1	34:Ld:85:ARG:NH1	2.51	0.44
56:SQ:97:GLN:HG2	56:SQ:105:LYS:HZ3	1.82	0.44
64:SC:156:ILE:HG13	64:SC:157:LEU:N	2.33	0.44
64:SC:230:THR:OG1	75:S2:5:U:OP2	2.34	0.44
75:S2:674:C:H2'	75:S2:675:U:C6	2.53	0.44
75:S2:1120:U:C2	75:S2:1121:G:C8	3.06	0.44
75:S2:1277:C:H2'	75:S2:1278:A:C8	2.53	0.44
79:SD:135:GLU:OE1	79:SD:157:MET:SD	2.76	0.44
3:L5:1741:G:O6	47:L7:103:A:O2'	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LJ:40:LEU:O	7:LJ:44:THR:HG22	2.18	0.44
8:LH:124:ARG:H	8:LH:124:ARG:HG2	1.69	0.44
13:LV:92:ASP:OD1	13:LV:94:VAL:HG12	2.17	0.44
18:LD:205:ALA:HB2	18:LD:236:MET:HE3	2.00	0.44
22:LT:94:GLU:OE1	22:LT:94:GLU:N	2.50	0.44
29:Lr:75:THR:O	29:Lr:75:THR:OG1	2.31	0.44
39:Lj:67:LEU:HD12	39:Lj:67:LEU:HA	1.83	0.44
75:S2:454:U:H2'	75:S2:455:A:C8	2.53	0.44
75:S2:952:G:H2'	75:S2:953:C:C6	2.52	0.44
75:S2:982:G:H2'	75:S2:983:A:C8	2.52	0.44
77:S6:47:G7M:H2'	77:S6:47:G7M:H8	1.65	0.44
3:L5:5038:A:OP1	27:LW:61:LYS:NZ	2.42	0.43
12:LL:204:GLU:HA	12:LL:207:VAL:HB	2.00	0.43
14:LM:24:LEU:HD11	14:LM:86:TRP:CD1	2.53	0.43
21:LS:2:LYS:HE3	21:LS:2:LYS:HB2	1.83	0.43
26:LY:77:LYS:HB2	26:LY:79:VAL:HG22	2.00	0.43
31:Lb:63:LYS:HE3	31:Lb:63:LYS:HB3	1.81	0.43
34:Ld:20:VAL:HG22	34:Ld:91:LYS:HA	2.00	0.43
38:Li:22:SER:OG	38:Li:23:LYS:N	2.51	0.43
50:SE:64:ILE:HD11	70:SY:18:LEU:HD22	1.98	0.43
53:SI:57:ALA:HB1	53:SI:60:LEU:HD13	2.00	0.43
61:SX:54:LYS:HE3	61:SX:94:ILE:HG22	1.99	0.43
64:SC:73:MET:HE3	64:SC:73:MET:O	2.18	0.43
75:S2:496:C:H2'	75:S2:497:C:H6	1.82	0.43
75:S2:649:U:H2'	75:S2:650:A:H8	1.82	0.43
78:Sg:219:TRP:HA	78:Sg:226:HIS:HA	1.98	0.43
3:L5:280:G:OP2	16:LN:44:ARG:NH2	2.35	0.43
3:L5:1326:A2M:H2'	3:L5:1327:C:C6	2.53	0.43
3:L5:2556:G:H2'	3:L5:2557:G:C8	2.53	0.43
5:LB:224:LYS:HG2	5:LB:340:THR:HG23	2.00	0.43
8:LH:93:ARG:HH21	8:LH:140:GLN:HG2	1.82	0.43
24:LU:26:THR:O	24:LU:30:GLU:OE2	2.36	0.43
36:Lf:39:THR:HG21	36:Lf:77:ALA:HB2	2.00	0.43
44:Lo:54:PRO:O	85:Lo:202:C:O2'	2.27	0.43
49:SB:26:SER:HA	68:SO:17:LEU:HD21	1.98	0.43
53:SI:98:LYS:HB3	75:S2:377:G:H5'	2.00	0.43
54:SK:32:HIS:HD2	54:SK:34:GLU:H	1.65	0.43
58:ST:62:ARG:NH1	75:S2:1542:C:OP1	2.51	0.43
75:S2:907:G:H2'	75:S2:908:A:C8	2.54	0.43
2:L8:153:C:H2'	2:L8:154:G:H8	1.82	0.43
3:L5:163:A:H2'	3:L5:164:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:212:A:H2'	3:L5:213:G:C8	2.53	0.43
3:L5:987:C:H2'	3:L5:988:C:H6	1.83	0.43
3:L5:1662:C:H2'	3:L5:1663:C:C6	2.53	0.43
3:L5:3736:A:H2'	3:L5:3737:A:C8	2.52	0.43
3:L5:4080:C:H2'	3:L5:4081:G:H8	1.81	0.43
3:L5:4220:6MZ:H9	3:L5:4222:G:C4	2.53	0.43
4:LA:83:HIS:HB3	45:Lp:64:VAL:HG22	2.01	0.43
24:LU:40:GLU:OE2	24:LU:65:ARG:NE	2.51	0.43
49:SB:171:ILE:HG23	49:SB:196:ASP:OD1	2.18	0.43
51:SF:52:SER:OG	56:SQ:117:ARG:NH1	2.52	0.43
62:Sc:13:ARG:HG3	62:Sc:35:MET:HG2	2.00	0.43
75:S2:1221:G:O2'	75:S2:1676:U:O2	2.34	0.43
78:Sg:247:TRP:HB3	78:Sg:258:ILE:HD11	1.99	0.43
79:SD:163:PRO:O	79:SD:167:TYR:HB2	2.18	0.43
3:L5:1076:C:H2'	3:L5:1077:C:H6	1.84	0.43
3:L5:4578:G:H2'	3:L5:4579:PSU:H6	1.82	0.43
10:LG:100:HIS:O	10:LG:100:HIS:ND1	2.45	0.43
17:LI:52:MET:HB2	17:LI:152:LEU:HD22	2.00	0.43
51:SF:83:ASN:HD22	51:SF:83:ASN:HA	1.60	0.43
55:SL:114:SER:HG	55:SL:116:CYS:HG	1.53	0.43
78:Sg:32:LEU:HD13	78:Sg:32:LEU:HA	1.65	0.43
81:SR:105:MET:O	81:SR:109:LEU:HG	2.18	0.43
3:L5:3944:OMG:HM23	3:L5:3944:OMG:H1'	1.87	0.43
3:L5:4538:G:H2'	3:L5:4539:U:C6	2.54	0.43
3:L5:4750:G:H2'	3:L5:4751:G:C8	2.53	0.43
4:LA:247:ARG:HB3	75:S2:1069:U:H4'	2.00	0.43
17:LI:182:GLU:OE2	17:LI:182:GLU:HA	2.19	0.43
19:LQ:125:GLN:O	19:LQ:129:ASP:OD2	2.35	0.43
24:LU:80:LYS:HG2	24:LU:110:TYR:CE2	2.53	0.43
50:SE:6:LYS:HE3	50:SE:6:LYS:HB3	1.93	0.43
75:S2:1839:U:H2'	75:S2:1840:U:C6	2.53	0.43
3:L5:265:C:H4'	30:Lh:112:ARG:HH12	1.84	0.43
3:L5:960:A:H8	9:LE:126:LEU:HD23	1.84	0.43
3:L5:3861:A:H2'	3:L5:3862:A:H8	1.82	0.43
3:L5:4089:G:H2'	3:L5:4090:G:C8	2.53	0.43
3:L5:4320:G:H2'	3:L5:4321:U:C6	2.54	0.43
3:L5:4637:OMG:HM23	3:L5:4637:OMG:H1'	1.75	0.43
3:L5:4934:A:H2'	3:L5:4935:C:C6	2.53	0.43
9:LE:46:ARG:HB3	9:LE:65:ARG:HH21	1.83	0.43
17:LI:66:GLU:OE2	17:LI:66:GLU:HA	2.19	0.43
25:LX:155:ILE:H	25:LX:155:ILE:HG13	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Li:44:ILE:HD13	38:Li:44:ILE:HA	1.91	0.43
50:SE:24:THR:O	50:SE:24:THR:OG1	2.35	0.43
60:SV:41:LYS:O	60:SV:43:THR:N	2.49	0.43
73:Se:24:LYS:HE3	73:Se:24:LYS:HB3	1.80	0.43
3:L5:659:G:H2'	3:L5:660:A:C8	2.54	0.43
3:L5:1195:G:H2'	3:L5:1196:G:C8	2.54	0.43
3:L5:1419:G:C6	15:La:116:LYS:HE2	2.54	0.43
3:L5:4239:A:H2'	3:L5:4240:G:H8	1.83	0.43
3:L5:4344:U:H2'	3:L5:4345:C:C6	2.53	0.43
3:L5:4645:C:OP2	20:LR:62:ARG:NH1	2.52	0.43
10:LG:156:VAL:HB	10:LG:202:VAL:HG13	1.99	0.43
12:LL:42:LYS:O	12:LL:46:ILE:HG13	2.18	0.43
18:LD:64:ILE:HD12	18:LD:109:LEU:HD22	2.01	0.43
20:LR:82:LYS:HA	20:LR:82:LYS:HD2	1.87	0.43
25:LX:63:LYS:HE3	25:LX:63:LYS:HB3	1.77	0.43
26:LY:118:ILE:HG22	26:LY:122:LYS:HD2	2.01	0.43
49:SB:120:MET:HE1	75:S2:987:A:N1	2.33	0.43
64:SC:273:LEU:HD23	64:SC:273:LEU:HA	1.89	0.43
79:SD:170:THR:HA	79:SD:186:VAL:O	2.19	0.43
79:SD:192:TRP:HD1	79:SD:200:PRO:O	2.02	0.43
3:L5:142:G:H2'	3:L5:144:G:C8	2.54	0.43
3:L5:1084:C:H2'	3:L5:1085:C:H6	1.84	0.43
4:LA:53:GLY:O	4:LA:192:LYS:NZ	2.41	0.43
17:LI:36:LEU:HD12	17:LI:73:ASN:HB2	2.01	0.43
17:LI:43:VAL:HG21	17:LI:197:VAL:HG23	1.99	0.43
33:Lc:35:LEU:HD23	33:Lc:35:LEU:HA	1.89	0.43
46:Pt:42:C:O2'	75:S2:1639:G:H8	2.02	0.43
50:SE:247:THR:OG1	50:SE:250:GLU:OE1	2.35	0.43
62:Sc:20:ARG:NH1	75:S2:1680:G:O2'	2.51	0.43
66:SJ:121:LYS:NZ	66:SJ:121:LYS:CB	2.70	0.43
75:S2:1007:C:H2'	75:S2:1008:A:C8	2.54	0.43
21:LS:85:ASP:HA	21:LS:90:THR:HA	2.00	0.43
22:LT:79:GLN:HE22	31:Lb:21:ILE:HD13	1.82	0.43
24:LU:28:PRO:HG3	24:LU:100:LEU:HD21	2.00	0.43
49:SB:71:LEU:HD12	49:SB:71:LEU:HA	1.84	0.43
55:SL:135:SER:OG	55:SL:136:LYS:N	2.50	0.43
66:SJ:79:ARG:HH22	75:S2:819:G:H5''	1.83	0.43
75:S2:929:G:H2'	75:S2:930:C:O4'	2.19	0.43
77:S6:24:C:H2'	77:S6:25:U:C6	2.54	0.43
78:Sg:100:ARG:HH21	78:Sg:102:VAL:HG21	1.84	0.43
78:Sg:304:ASP:OD1	78:Sg:306:LEU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:SD:172:VAL:HG22	79:SD:185:LYS:HG2	2.01	0.43
2:L8:30:U:H2'	2:L8:31:G:C8	2.52	0.43
3:L5:956:A:N6	3:L5:1283:G:H2'	2.33	0.43
3:L5:1772:C:H2'	3:L5:1773:U:H6	1.84	0.43
9:LE:178:PRO:HD2	9:LE:181:LEU:HD12	2.01	0.43
18:LD:83:LEU:HB3	18:LD:88:VAL:HB	2.01	0.43
45:Lp:28:LYS:HE2	45:Lp:28:LYS:HB3	1.67	0.43
49:SB:62:LEU:HD11	49:SB:91:VAL:HG11	1.99	0.43
53:SI:184:ARG:NH2	75:S2:218:U:O2	2.47	0.43
54:SK:62:PHE:HA	54:SK:66:HIS:O	2.19	0.43
57:SS:132:ARG:HD3	75:S2:1623:A:N6	2.34	0.43
61:SX:119:ARG:NH2	75:S2:1192:U:OP2	2.52	0.43
70:SY:68:LYS:HD2	70:SY:68:LYS:HA	1.84	0.43
70:SY:79:LEU:HD23	70:SY:79:LEU:HA	1.65	0.43
75:S2:1331:C:H1'	75:S2:1489:A:C5	2.54	0.43
75:S2:1845:A:H2'	75:S2:1846:G:C8	2.53	0.43
77:S6:14:A:H3'	77:S6:15:G:H8	1.83	0.43
77:S6:24:C:H2'	77:S6:25:U:H6	1.84	0.43
2:L8:83:C:H4'	2:L8:84:A:C5	2.53	0.42
2:L8:141:C:H2'	2:L8:142:U:C6	2.54	0.42
3:L5:27:C:O3'	3:L5:60:G:N2	2.51	0.42
3:L5:709:C:OP1	36:Lf:46:ARG:NH2	2.52	0.42
3:L5:717:U:H2'	3:L5:718:C:C6	2.53	0.42
3:L5:919:C:H2'	3:L5:920:C:H6	1.84	0.42
3:L5:4192:A:H2'	3:L5:4193:C:H6	1.83	0.42
3:L5:4237:C:H2'	3:L5:4238:G:H8	1.84	0.42
9:LE:48:PRO:HD2	9:LE:57:TYR:HE1	1.84	0.42
28:LZ:46:ILE:HG23	28:LZ:68:ILE:HG23	2.01	0.42
31:Lb:50:ASN:HD22	31:Lb:50:ASN:C	2.27	0.42
32:LF:47:ARG:HA	32:LF:47:ARG:HD2	1.86	0.42
49:SB:88:THR:HA	49:SB:98:THR:HA	2.01	0.42
57:SS:14:ARG:NH1	57:SS:17:ASN:OD1	2.47	0.42
70:SY:89:HIS:CD2	75:S2:574:A:H5''	2.54	0.42
70:SY:118:ARG:HA	70:SY:118:ARG:HD2	1.92	0.42
75:S2:1189:A:H2'	75:S2:1190:A:H8	1.83	0.42
75:S2:1270:G:O2'	75:S2:1301:A:N7	2.47	0.42
77:S6:62:C:H2'	77:S6:63:C:C6	2.54	0.42
2:L8:90:C:H2'	2:L8:91:A:C8	2.54	0.42
3:L5:2588:C:OP1	3:L5:2768:C:O2'	2.26	0.42
3:L5:3924:C:H2'	3:L5:3925:OMU:H6	2.01	0.42
3:L5:4208:U:H2'	3:L5:4209:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:4474:A:H5''	42:Lm:125:LYS:HG3	2.00	0.42
3:L5:4710:C:H2'	3:L5:4711:C:H6	1.84	0.42
4:LA:136:VAL:HA	4:LA:148:VAL:HG12	2.01	0.42
6:LC:302:LEU:HD22	19:LQ:38:ARG:HB3	2.01	0.42
8:LH:76:HIS:O	8:LH:80:MET:HG3	2.20	0.42
10:LG:34:LYS:NZ	10:LG:34:LYS:HB3	2.34	0.42
75:S2:1307:U:H2'	75:S2:1308:U:H6	1.84	0.42
3:L5:223:G:H4'	3:L5:225:G:N7	2.34	0.42
3:L5:1084:C:H2'	3:L5:1085:C:C6	2.54	0.42
3:L5:1382:G:H2'	3:L5:1383:G:H8	1.84	0.42
3:L5:2336:G:H2'	3:L5:2337:C:H6	1.83	0.42
3:L5:2720:C:H2'	3:L5:2721:G:O4'	2.19	0.42
3:L5:2727:C:H2'	3:L5:2728:U:C6	2.54	0.42
9:LE:174:LEU:HD11	9:LE:186:LEU:HD22	2.01	0.42
48:SA:76:VAL:HG12	48:SA:123:VAL:HB	2.01	0.42
55:SL:40:ILE:HG12	55:SL:62:PHE:HE1	1.84	0.42
75:S2:553:U:H2'	75:S2:554:A:C8	2.54	0.42
75:S2:656:G:H21	75:S2:663:C:H5''	1.84	0.42
75:S2:1593:C:H2'	75:S2:1594:A:C8	2.54	0.42
75:S2:1736:G:H2'	75:S2:1737:G:C8	2.54	0.42
75:S2:1856:C:H2'	75:S2:1857:G:C8	2.54	0.42
3:L5:653:U:H2'	3:L5:654:C:C6	2.54	0.42
3:L5:1494:U:H2'	3:L5:1495:G:H8	1.84	0.42
3:L5:1564:A:H2'	3:L5:1565:A:C8	2.54	0.42
3:L5:1662:C:H2'	3:L5:1663:C:H6	1.84	0.42
3:L5:1756:U:O2'	3:L5:1757:U:O5'	2.30	0.42
3:L5:2063:G:H2'	3:L5:2064:G:C8	2.54	0.42
3:L5:2633:U:H2'	3:L5:2634:C:H6	1.83	0.42
3:L5:4642:U:H2'	3:L5:4643:G:H8	1.84	0.42
3:L5:4710:C:H2'	3:L5:4711:C:C6	2.54	0.42
3:L5:4760:G:H2'	3:L5:4761:G:O4'	2.18	0.42
11:LO:23:VAL:HG13	11:LO:33:VAL:HG21	2.01	0.42
16:LN:68:ARG:NH1	16:LN:123:GLU:OE2	2.51	0.42
18:LD:197:LYS:HB3	18:LD:202:GLN:HB2	2.01	0.42
32:LF:214:SER:OG	32:LF:215:SER:N	2.51	0.42
3:L5:152:U:OP2	16:LN:49:ARG:NH2	2.34	0.42
3:L5:497:G:H22	3:L5:656:C:H42	1.67	0.42
3:L5:2758:G:O2'	3:L5:2765:A:N3	2.40	0.42
4:LA:247:ARG:NH2	75:S2:1069:U:O2'	2.52	0.42
12:LL:169:ILE:HG21	12:LL:174:LYS:HE3	2.01	0.42
20:LR:126:LYS:HE2	20:LR:126:LYS:HB3	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LY:112:ASP:OD1	26:LY:113:LYS:N	2.49	0.42
28:LZ:93:LYS:HB3	28:LZ:93:LYS:HE3	1.72	0.42
50:SE:189:LEU:HD23	50:SE:189:LEU:HA	1.80	0.42
60:SV:16:LYS:HB3	60:SV:16:LYS:HE3	1.91	0.42
75:S2:1447:G:H2'	75:S2:1448:A:C8	2.54	0.42
3:L5:2864:A:H2'	3:L5:2865:U:C6	2.55	0.42
3:L5:4965:U:H5''	5:LB:128:LYS:HZ1	1.85	0.42
13:LV:87:SER:HA	13:LV:97:TYR:HB3	2.01	0.42
22:LT:18:PRO:HG2	22:LT:21:LYS:HB2	2.01	0.42
24:LU:106:SER:H	24:LU:109:SER:HB3	1.83	0.42
26:LY:83:GLU:OE2	26:LY:84:ARG:NH1	2.53	0.42
28:LZ:89:ILE:HD13	28:LZ:89:ILE:HA	1.90	0.42
33:Lc:33:GLN:O	33:Lc:37:MET:HE2	2.19	0.42
50:SE:36:HIS:ND1	50:SE:85:GLY:HA3	2.35	0.42
71:SZ:88:LEU:HD13	71:SZ:88:LEU:HA	1.88	0.42
75:S2:96:C:H2'	75:S2:97:U:C6	2.55	0.42
2:L8:19:C:H2'	2:L8:20:A:C8	2.55	0.42
3:L5:4070:U:H2'	3:L5:4071:U:C6	2.55	0.42
11:LO:140:ARG:O	11:LO:144:GLU:HG3	2.19	0.42
25:LX:123:LYS:HG2	25:LX:139:ARG:HB3	2.02	0.42
46:Pt:72:C:H2'	46:Pt:73:A:C8	2.55	0.42
47:L7:58:A:H2'	47:L7:59:G:H8	1.84	0.42
49:SB:56:LYS:HB2	49:SB:56:LYS:HE2	1.71	0.42
49:SB:179:ASN:HD22	49:SB:183:GLU:HG2	1.84	0.42
49:SB:222:LYS:HE3	49:SB:222:LYS:HB3	1.88	0.42
50:SE:60:GLU:O	50:SE:64:ILE:HD13	2.19	0.42
52:SH:119:SER:OG	52:SH:120:ARG:NH1	2.52	0.42
56:SQ:10:VAL:HG21	56:SQ:95:TYR:HB2	2.02	0.42
61:SX:129:SER:O	61:SX:133:LEU:HD23	2.20	0.42
66:SJ:116:LYS:HD2	66:SJ:116:LYS:HA	1.74	0.42
67:SN:88:LEU:HD12	67:SN:88:LEU:HA	1.78	0.42
75:S2:607:U:O2'	75:S2:630:U:O4'	2.35	0.42
75:S2:1204:A:O2'	75:S2:1700:C:OP2	2.37	0.42
75:S2:1435:C:H2'	75:S2:1438:A:C8	2.55	0.42
2:L8:93:C:O2'	2:L8:94:G:H8	2.02	0.42
3:L5:483:G:N2	3:L5:488:G:O6	2.53	0.42
3:L5:1441:C:H2'	3:L5:1442:C:C6	2.55	0.42
3:L5:2845:A:H61	3:L5:3843:C:H42	1.68	0.42
3:L5:4093:G:H2'	3:L5:4094:G:C8	2.55	0.42
3:L5:4238:G:H2'	3:L5:4239:A:C8	2.53	0.42
9:LE:264:ILE:HD11	9:LE:267:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LS:163:HIS:CE1	21:LS:166:ARG:HH21	2.37	0.42
46:Pt:15:G:OP2	46:Pt:16:C:N4	2.53	0.42
56:SQ:12:VAL:HG11	56:SQ:91:ALA:HA	2.01	0.42
65:SG:190:ARG:HH22	75:S2:333:G:H3'	1.84	0.42
75:S2:948:C:H2'	75:S2:949:G:H8	1.84	0.42
75:S2:1562:C:H2'	75:S2:1563:G:C8	2.53	0.42
3:L5:2651:C:O2'	3:L5:2653:C:OP1	2.28	0.42
6:LC:84:THR:O	6:LC:87:SER:OG	2.37	0.42
28:LZ:47:ASP:N	28:LZ:69:LYS:O	2.41	0.42
33:Lc:37:MET:HE2	33:Lc:37:MET:HB2	1.96	0.42
49:SB:36:PRO:HD2	49:SB:39:PHE:HE2	1.85	0.42
51:SF:78:MET:SD	51:SF:159:ARG:HD3	2.60	0.42
60:SV:67:ASP:OD2	60:SV:67:ASP:C	2.62	0.42
62:Sc:12:ALA:HB1	62:Sc:32:VAL:HB	2.01	0.42
64:SC:206:SER:OG	64:SC:210:PRO:HG2	2.19	0.42
75:S2:465:A:H5'	75:S2:466:G:C8	2.55	0.42
75:S2:925:G:H1	75:S2:1017:U:H3	1.68	0.42
81:SR:58:MET:HE3	81:SR:58:MET:HB3	1.84	0.42
3:L5:4627:U:H4'	5:LB:373:LYS:HD2	2.01	0.42
4:LA:132:ASN:HD22	4:LA:132:ASN:HA	1.73	0.42
19:LQ:119:LYS:HE3	19:LQ:119:LYS:HB3	1.83	0.42
29:Lr:28:GLU:OE2	29:Lr:31:ASN:ND2	2.45	0.42
44:Lo:33:LEU:HA	44:Lo:38:LYS:HG2	2.01	0.42
53:SI:186:ASP:OD1	53:SI:186:ASP:N	2.53	0.42
63:Sd:50:ILE:HG23	63:Sd:52:PHE:HD1	1.85	0.42
75:S2:874:G:H2'	75:S2:875:A:H8	1.84	0.42
75:S2:1189:A:H2'	75:S2:1190:A:C8	2.55	0.42
75:S2:1750:C:C4	75:S2:1751:C:H1'	2.54	0.42
78:Sg:248:LEU:HD13	78:Sg:248:LEU:HA	1.93	0.42
2:L8:8:U:H2'	2:L8:9:A:H8	1.85	0.41
3:L5:153:G:H2'	3:L5:154:G:H8	1.85	0.41
3:L5:1417:C:H2'	3:L5:1418:C:C6	2.55	0.41
3:L5:1751:A:H2'	3:L5:1752:G:C8	2.55	0.41
3:L5:1824:G:H2'	3:L5:1825:A:C8	2.55	0.41
3:L5:1847:C:H2'	3:L5:1848:C:C6	2.55	0.41
3:L5:2607:C:H2'	3:L5:2608:G:C8	2.55	0.41
3:L5:4263:C:H2'	3:L5:4264:G:O4'	2.20	0.41
7:LJ:78:LYS:HE3	7:LJ:82:ILE:HD11	2.02	0.41
11:LO:165:LYS:HE3	11:LO:169:ARG:HH12	1.85	0.41
17:LI:47:PRO:CG	17:LI:142:LEU:CD1	2.98	0.41
29:Lr:90:LEU:HD22	29:Lr:111:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:SE:92:ILE:HG22	50:SE:94:LYS:H	1.85	0.41
52:SH:69:LEU:O	52:SH:73:GLN:HG2	2.20	0.41
63:Sd:42:CYS:SG	75:S2:1495:G:N2	2.87	0.41
67:SN:54:LEU:HB3	67:SN:60:VAL:HG13	2.02	0.41
70:SY:88:LYS:HB3	70:SY:97:TYR:CE2	2.55	0.41
70:SY:89:HIS:NE2	70:SY:90:ARG:HD2	2.34	0.41
75:S2:1387:G:H2'	75:S2:1388:A:O4'	2.20	0.41
3:L5:478:G:OP1	29:Lr:66:ARG:NH1	2.53	0.41
3:L5:1340:OMC:H1'	3:L5:1340:OMC:HM23	1.84	0.41
3:L5:3910:C:H2'	3:L5:3911:C:H6	1.85	0.41
5:LB:389:MET:HB3	5:LB:389:MET:HE3	1.84	0.41
12:LL:194:ILE:HD12	12:LL:194:ILE:HA	1.86	0.41
28:LZ:14:LEU:HD11	28:LZ:81:MET:HB2	2.01	0.41
47:L7:58:A:H2'	47:L7:59:G:C8	2.56	0.41
56:SQ:85:ARG:HA	56:SQ:88:ILE:HG12	2.02	0.41
68:SO:60:MET:HB3	75:S2:956:G:O5'	2.19	0.41
69:SW:30:CYS:HB2	69:SW:61:ILE:HG13	2.02	0.41
69:SW:64:ASN:OD1	69:SW:64:ASN:N	2.52	0.41
75:S2:367:U:H4'	75:S2:371:A:C8	2.55	0.41
75:S2:1398:G:H1'	78:Sg:63:SER:OG	2.20	0.41
75:S2:1681:U:H2'	75:S2:1682:C:C6	2.55	0.41
75:S2:1743:G:H21	75:S2:1791:A:H62	1.68	0.41
75:S2:1797:U:H2'	75:S2:1798:C:C6	2.55	0.41
3:L5:664:G:H2'	3:L5:665:C:C6	2.55	0.41
3:L5:2685:C:H2'	3:L5:2686:G:O4'	2.20	0.41
3:L5:3723:A2M:OP2	38:Li:68:ARG:HD3	2.20	0.41
9:LE:264:ILE:HG13	9:LE:267:LEU:HB2	2.01	0.41
11:LO:127:VAL:HG12	11:LO:128:ARG:HD2	2.02	0.41
44:Lo:23:VAL:HG22	44:Lo:70:LEU:HD12	2.02	0.41
3:L5:2071:A:H2'	3:L5:2072:C:H6	1.85	0.41
3:L5:3777:G:N2	3:L5:3816:A:OP2	2.36	0.41
7:LJ:40:LEU:HD12	7:LJ:70:VAL:HG13	2.02	0.41
7:LJ:106:GLY:HA3	7:LJ:131:TYR:HD1	1.86	0.41
18:LD:104:LEU:HB2	18:LD:247:ILE:HD12	2.02	0.41
18:LD:125:VAL:HG11	18:LD:199:ILE:HG21	2.02	0.41
19:LQ:63:LEU:HD12	19:LQ:63:LEU:HA	1.91	0.41
20:LR:122:SER:O	20:LR:126:LYS:HG3	2.20	0.41
33:Lc:45:LEU:HD23	33:Lc:96:ILE:HD13	2.02	0.41
37:Lg:33:LEU:HD23	37:Lg:33:LEU:HA	1.88	0.41
44:Lo:23:VAL:HG12	44:Lo:93:LEU:HD11	2.03	0.41
50:SE:62:LYS:HG2	50:SE:63:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:SG:13:GLN:HE22	75:S2:153:G:H21	1.69	0.41
74:Sa:79:ILE:HD11	75:S2:1864:U:H5'	2.01	0.41
75:S2:848:U:H2'	75:S2:849:A:C8	2.47	0.41
75:S2:1667:U:H2'	75:S2:1668:U:C6	2.54	0.41
78:Sg:31:ILE:C	78:Sg:32:LEU:HD22	2.44	0.41
78:Sg:76:GLN:CD	78:Sg:76:GLN:H	2.29	0.41
3:L5:1088:C:H2'	3:L5:1089:G:C8	2.56	0.41
3:L5:1883:G:O2'	35:Le:48:ARG:O	2.30	0.41
3:L5:2864:A:H2'	3:L5:2865:U:H6	1.86	0.41
3:L5:4921:C:H2'	3:L5:4922:C:C6	2.55	0.41
48:SA:198:MET:HE3	81:SR:89:SER:HB2	2.02	0.41
53:SI:29:LEU:C	53:SI:29:LEU:CD1	2.87	0.41
75:S2:115:U:H2'	75:S2:116:U:C6	2.55	0.41
75:S2:429:C:O2'	75:S2:811:A:N1	2.49	0.41
75:S2:1533:A:H2	75:S2:1536:G:N3	2.18	0.41
77:S6:57:C:H2'	77:S6:58:A:O4'	2.20	0.41
3:L5:272:U:H2'	3:L5:273:U:H6	1.86	0.41
3:L5:2079:G:H2'	3:L5:2080:U:C6	2.56	0.41
3:L5:2804:OMC:H2'	3:L5:2805:C:H6	1.86	0.41
3:L5:3736:A:H2'	3:L5:3737:A:H8	1.86	0.41
3:L5:4070:U:H2'	3:L5:4071:U:H6	1.86	0.41
3:L5:4111:U:H2'	3:L5:4112:C:H6	1.85	0.41
3:L5:4965:U:H5''	5:LB:128:LYS:NZ	2.36	0.41
56:SQ:112:LEU:HD23	56:SQ:112:LEU:HA	1.83	0.41
58:ST:88:MET:HE1	75:S2:1665:G:C6	2.55	0.41
73:Se:36:MET:HE3	73:Se:36:MET:HB2	1.77	0.41
75:S2:1690:U:H2'	75:S2:1691:U:C6	2.56	0.41
78:Sg:155:ARG:HD3	78:Sg:155:ARG:HA	1.94	0.41
3:L5:2640:G:H2'	3:L5:2641:A:C8	2.56	0.41
10:LG:170:LEU:HD23	10:LG:170:LEU:HA	1.89	0.41
15:La:36:GLY:HA3	15:La:40:HIS:CE1	2.56	0.41
19:LQ:79:THR:HB	19:LQ:136:THR:HG22	2.03	0.41
49:SB:31:TYR:HB2	49:SB:47:THR:HG23	2.01	0.41
50:SE:124:CYS:HB3	50:SE:141:THR:HB	2.03	0.41
52:SH:149:ASP:OD1	52:SH:149:ASP:N	2.53	0.41
53:SI:117:TYR:OH	53:SI:155:ASN:O	2.30	0.41
55:SL:82:MET:HE3	75:S2:372:U:O2'	2.21	0.41
56:SQ:8:GLN:HB3	56:SQ:95:TYR:HE1	1.86	0.41
56:SQ:113:ILE:HD12	56:SQ:114:GLN:N	2.35	0.41
66:SJ:131:ARG:NH1	66:SJ:143:ASN:O	2.47	0.41
68:SO:137:SER:O	68:SO:137:SER:OG	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:SW:75:ILE:HG13	69:SW:125:ILE:HD13	2.02	0.41
71:SZ:110:THR:OG1	71:SZ:111:ARG:N	2.54	0.41
75:S2:85:A:H2'	75:S2:86:C:H6	1.84	0.41
3:L5:2870:A:H2'	3:L5:2871:A:C8	2.56	0.41
6:LC:140:LYS:HE2	6:LC:140:LYS:HB3	1.83	0.41
8:LH:40:HIS:CD2	8:LH:40:HIS:H	2.39	0.41
25:LX:148:ASP:OD1	25:LX:148:ASP:N	2.38	0.41
33:Lc:20:LEU:HD23	33:Lc:102:SER:HA	2.03	0.41
49:SB:137:LEU:HD11	49:SB:176:VAL:HG21	2.03	0.41
52:SH:93:VAL:HG21	52:SH:133:LEU:HD12	2.02	0.41
57:SS:142:ARG:NH2	75:S2:1522:A:O3'	2.54	0.41
75:S2:496:C:H2'	75:S2:497:C:C6	2.55	0.41
75:S2:1174:U:H2'	75:S2:1175:G:C8	2.55	0.41
3:L5:506:C:H2'	3:L5:507:G:H8	1.86	0.41
3:L5:676:C:H2'	3:L5:677:G:C8	2.55	0.41
3:L5:976:G:H1'	3:L5:977:C:H5'	2.03	0.41
3:L5:1617:G:H1'	3:L5:2513:A:N6	2.35	0.41
3:L5:1683:U:H2'	3:L5:1684:A:C8	2.56	0.41
3:L5:1779:U:H2'	3:L5:1780:A:C8	2.55	0.41
3:L5:2407:G:O6	41:Ll:2:SER:N	2.54	0.41
3:L5:2422:OMC:HM23	3:L5:2422:OMC:H1'	1.70	0.41
3:L5:2781:G:O2'	41:Ll:3:SER:O	2.39	0.41
3:L5:2846:G:O2'	13:LV:19:GLY:O	2.37	0.41
3:L5:3602:C:H2'	3:L5:3603:G:C8	2.55	0.41
3:L5:3690:U:H2'	3:L5:3691:G:O4'	2.20	0.41
3:L5:4318:C:H1'	3:L5:4319:C:H5'	2.03	0.41
3:L5:4771:C:H2'	3:L5:4772:C:C6	2.56	0.41
7:LJ:113:ILE:H	7:LJ:113:ILE:HG13	1.59	0.41
8:LH:7:ASN:OD1	8:LH:7:ASN:N	2.54	0.41
14:LM:26:ALA:HB2	14:LM:77:TRP:HZ3	1.85	0.41
15:La:100:ILE:HD11	15:La:125:LYS:HG3	2.02	0.41
16:LN:99:GLN:O	16:LN:103:GLU:HG3	2.21	0.41
18:LD:107:ARG:NH1	18:LD:169:GLY:O	2.50	0.41
22:LT:53:PRO:HB3	22:LT:91:VAL:HG11	2.03	0.41
23:LP:6:LEU:HD12	23:LP:116:HIS:CD2	2.56	0.41
25:LX:81:LEU:HD23	25:LX:81:LEU:HA	1.91	0.41
26:LY:47:MET:HE1	26:LY:119:LEU:HG	2.02	0.41
46:Pt:54:G:H2'	46:Pt:55:U:C6	2.56	0.41
46:Pt:54:G:H2'	46:Pt:55:U:H6	1.85	0.41
49:SB:44:ILE:CD1	49:SB:44:ILE:O	2.68	0.41
50:SE:98:ASN:ND2	50:SE:116:PRO:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:SI:57:ALA:HB2	53:SI:183:GLY:HA2	2.03	0.41
53:SI:61:ASP:OD2	53:SI:62:VAL:HG22	2.21	0.41
54:SK:65:ARG:HE	54:SK:65:ARG:HB3	1.59	0.41
56:SQ:14:GLY:HA3	56:SQ:86:GLN:HG2	2.01	0.41
64:SC:199:PRO:HD2	64:SC:202:THR:HG21	2.02	0.41
66:SJ:38:ARG:HG3	73:Se:31:ARG:HB2	2.02	0.41
67:SN:46:THR:O	67:SN:50:ILE:HG12	2.21	0.41
69:SW:104:LEU:HD23	69:SW:125:ILE:HA	2.02	0.41
72:Sb:20:LYS:HG2	72:Sb:21:LYS:N	2.36	0.41
75:S2:28:U:H2'	75:S2:29:G:H8	1.86	0.41
75:S2:96:C:H2'	75:S2:97:U:H6	1.85	0.41
75:S2:106:C:H2'	75:S2:107:A:C8	2.56	0.41
75:S2:1013:U:OP1	75:S2:1129:G:O2'	2.38	0.41
75:S2:1606:G:O2'	75:S2:1607:A:H8	2.04	0.41
79:SD:10:LYS:HB3	79:SD:10:LYS:HE3	1.90	0.41
79:SD:23:GLU:HA	79:SD:26:THR:HB	2.02	0.41
3:L5:461:G:H2'	3:L5:462:G:C8	2.57	0.41
3:L5:511:C:H2'	3:L5:512:U:C6	2.56	0.41
3:L5:950:G:H2'	3:L5:951:G:H8	1.84	0.41
3:L5:1739:G:H2'	3:L5:1740:C:C6	2.56	0.41
3:L5:1751:A:H2'	3:L5:1752:G:H8	1.85	0.41
3:L5:2497:C:H2'	3:L5:2498:C:H6	1.85	0.41
3:L5:3917:A:H2'	3:L5:3918:G:C8	2.54	0.41
3:L5:4591:U:H2'	3:L5:4592:C:C6	2.56	0.41
26:LY:38:LEU:HD22	26:LY:42:TYR:HE2	1.85	0.41
35:Le:102:ASN:OD1	35:Le:102:ASN:N	2.52	0.41
51:SF:61:PHE:HA	62:Sc:51:ARG:NH1	2.35	0.41
75:S2:340:C:H2'	75:S2:341:C:O4'	2.21	0.41
75:S2:1348:G:H22	75:S2:1381:G:H22	1.68	0.41
75:S2:1465:A:H2'	75:S2:1466:G:C8	2.56	0.41
77:S6:45:A:H3'	77:S6:46:G:C8	2.56	0.41
78:Sg:51:ASN:HD21	78:Sg:54:ILE:HG12	1.85	0.41
3:L5:694:C:H2'	3:L5:695:G:H8	1.86	0.40
17:LI:99:ILE:HG22	17:LI:123:GLN:HB2	2.03	0.40
24:LU:105:ASN:ND2	24:LU:111:GLU:OE2	2.35	0.40
26:LY:117:LYS:HA	26:LY:117:LYS:HD3	1.85	0.40
49:SB:144:LYS:HE2	49:SB:144:LYS:HB3	1.77	0.40
58:ST:74:SER:OG	75:S2:1587:G:N1	2.54	0.40
61:SX:95:GLU:HG2	61:SX:98:ASP:OD2	2.21	0.40
70:SY:57:VAL:HB	70:SY:60:PHE:CZ	2.56	0.40
76:mR:7:G:O2'	76:mR:9:U:O2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L5:1241:C:H2'	3:L5:1242:G:C8	2.51	0.40
3:L5:1306:C:H2'	3:L5:1307:A:H8	1.86	0.40
3:L5:1577:G:H5'	3:L5:1578:U:H5''	2.02	0.40
3:L5:2634:C:H2'	3:L5:2635:U:C6	2.56	0.40
3:L5:4378:A:OP1	89:L5:5201:HOH:O	2.22	0.40
3:L5:4618:OMG:HM23	3:L5:4618:OMG:H1'	1.86	0.40
3:L5:4862:G:H2'	3:L5:4863:G:C8	2.57	0.40
12:LL:89:LYS:HE2	12:LL:89:LYS:HB3	1.73	0.40
34:Ld:54:MET:HG3	34:Ld:60:PRO:HA	2.02	0.40
34:Ld:91:LYS:HE3	34:Ld:91:LYS:HB3	1.82	0.40
46:Pt:47:G7M:H8	46:Pt:47:G7M:H2'	1.67	0.40
48:SA:90:PHE:HD1	48:SA:179:ALA:HB2	1.86	0.40
57:SS:38:ARG:HH12	75:S2:1603:G:H4'	1.86	0.40
58:ST:28:LEU:HG	58:ST:29:LYS:H	1.86	0.40
64:SC:200:ARG:HA	64:SC:221:ASP:OD1	2.21	0.40
66:SJ:52:LYS:HB2	66:SJ:52:LYS:HE3	1.89	0.40
75:S2:176:U:H2'	75:S2:177:G:C8	2.56	0.40
75:S2:910:G:H2'	75:S2:911:C:C6	2.56	0.40
78:Sg:236:ILE:HD13	78:Sg:236:ILE:HA	1.88	0.40
82:Sf:105:TYR:O	82:Sf:117:LEU:N	2.53	0.40
2:L8:144:U:H2'	2:L8:145:C:H6	1.85	0.40
3:L5:1645:C:H2'	3:L5:1646:A:C8	2.57	0.40
3:L5:4460:U:H2'	3:L5:4461:C:H6	1.87	0.40
3:L5:4928:C:H2'	14:LM:118:MET:HE1	2.03	0.40
5:LB:77:THR:HG21	5:LB:337:VAL:HG22	2.02	0.40
22:LT:27:LEU:HD23	22:LT:27:LEU:HA	1.81	0.40
45:Lp:83:ILE:HA	45:Lp:86:LEU:HB2	2.03	0.40
48:SA:82:THR:O	48:SA:82:THR:OG1	2.38	0.40
54:SK:32:HIS:CD2	54:SK:34:GLU:H	2.38	0.40
57:SS:33:ILE:H	57:SS:33:ILE:HG13	1.75	0.40
57:SS:130:ARG:NH1	75:S2:1230:C:OP1	2.34	0.40
59:SU:72:GLU:OE1	59:SU:73:GLY:N	2.54	0.40
65:SG:133:LEU:O	75:S2:168:C:O2'	2.32	0.40
65:SG:135:PRO:HB2	65:SG:141:ILE:HG13	2.02	0.40
72:Sb:24:LEU:HD12	72:Sb:24:LEU:HA	1.82	0.40
75:S2:5:U:H2'	75:S2:6:G:H8	1.86	0.40
2:L8:17:A:H1'	3:L5:418:A:C2	2.57	0.40
3:L5:2376:A:H2'	3:L5:2377:C:C6	2.57	0.40
3:L5:4237:C:H2'	3:L5:4238:G:C8	2.56	0.40
3:L5:4320:G:OP1	44:Lo:9:ARG:NH2	2.54	0.40
7:LJ:94:LEU:HD23	7:LJ:94:LEU:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LN:9:GLU:HB2	38:Li:44:ILE:HG13	2.03	0.40
18:LD:200:MET:HE3	18:LD:200:MET:HB3	1.75	0.40
20:LR:78:ILE:HD13	20:LR:78:ILE:HA	1.96	0.40
43:Ln:1:MET:HG3	75:S2:1706:G:H5'	2.03	0.40
51:SF:113:VAL:O	51:SF:117:ILE:HG12	2.21	0.40
75:S2:375:U:H2'	75:S2:376:A:C8	2.56	0.40
75:S2:1692:U:H2'	75:S2:1693:G:C8	2.57	0.40
3:L5:398:A2M:HM'3	3:L5:398:A2M:H1'	1.82	0.40
3:L5:739:G:OP2	14:LM:71:LYS:NZ	2.46	0.40
3:L5:1207:C:H2'	3:L5:1208:G:H8	1.87	0.40
3:L5:1268:G:H2'	31:Lb:107:ARG:HH22	1.87	0.40
3:L5:1317:U:H2'	3:L5:1318:C:C6	2.56	0.40
3:L5:1445:U:H2'	3:L5:1446:C:C6	2.56	0.40
3:L5:2664:G:H4'	3:L5:2677:G:H4'	2.04	0.40
3:L5:4523:A2M:H1'	3:L5:4523:A2M:HM'3	1.87	0.40
3:L5:4884:G:N7	9:LE:272:ARG:NH2	2.69	0.40
3:L5:5004:C:H2'	3:L5:5005:G:O4'	2.22	0.40
34:Ld:55:LYS:HE3	34:Ld:55:LYS:HB3	1.81	0.40
49:SB:199:LYS:HE3	49:SB:199:LYS:HB3	1.98	0.40
51:SF:124:ASP:OD2	62:Sc:47:LYS:NZ	2.36	0.40
66:SJ:146:SER:OG	75:S2:522:A:OP1	2.34	0.40
68:SO:98:ARG:HG3	68:SO:132:VAL:HG13	2.04	0.40
75:S2:1177:U:H2'	75:S2:1178:U:C6	2.57	0.40
81:SR:132:ARG:HD3	81:SR:132:ARG:HA	1.90	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	SP	127/145 (88%)	118 (93%)	9 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	LA	248/252 (98%)	238 (96%)	10 (4%)	0	100	100
5	LB	392/396 (99%)	386 (98%)	6 (2%)	0	100	100
6	LC	363/427 (85%)	356 (98%)	7 (2%)	0	100	100
7	LJ	166/178 (93%)	160 (96%)	6 (4%)	0	100	100
8	LH	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
9	LE	202/288 (70%)	193 (96%)	9 (4%)	0	100	100
10	LG	227/266 (85%)	221 (97%)	6 (3%)	0	100	100
11	LO	197/203 (97%)	194 (98%)	3 (2%)	0	100	100
12	LL	204/211 (97%)	198 (97%)	6 (3%)	0	100	100
13	LV	130/140 (93%)	129 (99%)	1 (1%)	0	100	100
14	LM	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
15	La	145/148 (98%)	140 (97%)	5 (3%)	0	100	100
16	LN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
17	LI	199/214 (93%)	195 (98%)	4 (2%)	0	100	100
18	LD	291/297 (98%)	284 (98%)	7 (2%)	0	100	100
19	LQ	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
20	LR	173/196 (88%)	171 (99%)	2 (1%)	0	100	100
21	LS	174/176 (99%)	168 (97%)	6 (3%)	0	100	100
22	LT	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
23	LP	151/154 (98%)	146 (97%)	5 (3%)	0	100	100
24	LU	97/128 (76%)	93 (96%)	4 (4%)	0	100	100
25	LX	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
26	LY	128/145 (88%)	125 (98%)	3 (2%)	0	100	100
27	LW	59/157 (38%)	57 (97%)	2 (3%)	0	100	100
28	LZ	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
29	Lr	120/137 (88%)	115 (96%)	5 (4%)	0	100	100
30	Lh	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
31	Lb	86/159 (54%)	84 (98%)	2 (2%)	0	100	100
32	LF	223/248 (90%)	220 (99%)	3 (1%)	0	100	100
33	Lc	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
34	Ld	105/125 (84%)	99 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	Le	126/129 (98%)	126 (100%)	0	0	100	100
36	Lf	107/110 (97%)	107 (100%)	0	0	100	100
37	Lg	106/109 (97%)	103 (97%)	3 (3%)	0	100	100
38	Li	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
39	Lj	84/87 (97%)	84 (100%)	0	0	100	100
40	Lk	66/70 (94%)	65 (98%)	1 (2%)	0	100	100
41	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
42	Lm	48/128 (38%)	48 (100%)	0	0	100	100
43	Ln	23/25 (92%)	23 (100%)	0	0	100	100
44	Lo	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
45	Lp	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
48	SA	215/295 (73%)	194 (90%)	21 (10%)	0	100	100
49	SB	212/264 (80%)	197 (93%)	15 (7%)	0	100	100
50	SE	256/263 (97%)	238 (93%)	18 (7%)	0	100	100
51	SF	178/204 (87%)	154 (86%)	24 (14%)	0	100	100
52	SH	174/194 (90%)	167 (96%)	7 (4%)	0	100	100
53	SI	182/208 (88%)	168 (92%)	13 (7%)	1 (0%)	24	60
54	SK	93/165 (56%)	80 (86%)	13 (14%)	0	100	100
55	SL	134/158 (85%)	129 (96%)	5 (4%)	0	100	100
56	SQ	138/146 (94%)	122 (88%)	16 (12%)	0	100	100
57	SS	139/152 (91%)	121 (87%)	18 (13%)	0	100	100
58	ST	139/145 (96%)	134 (96%)	5 (4%)	0	100	100
59	SU	93/119 (78%)	88 (95%)	5 (5%)	0	100	100
60	SV	82/83 (99%)	79 (96%)	3 (4%)	0	100	100
61	SX	138/143 (96%)	127 (92%)	11 (8%)	0	100	100
62	Sc	58/69 (84%)	49 (84%)	9 (16%)	0	100	100
63	Sd	50/56 (89%)	44 (88%)	6 (12%)	0	100	100
64	SC	214/293 (73%)	199 (93%)	15 (7%)	0	100	100
65	SG	220/249 (88%)	211 (96%)	9 (4%)	0	100	100
66	SJ	176/194 (91%)	168 (96%)	8 (4%)	0	100	100
67	SN	148/151 (98%)	142 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	SO	134/151 (89%)	114 (85%)	20 (15%)	0	100	100
69	SW	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
70	SY	122/133 (92%)	115 (94%)	7 (6%)	0	100	100
71	SZ	70/125 (56%)	60 (86%)	10 (14%)	0	100	100
72	Sb	77/84 (92%)	66 (86%)	11 (14%)	0	100	100
73	Se	45/133 (34%)	44 (98%)	1 (2%)	0	100	100
74	Sa	104/115 (90%)	103 (99%)	1 (1%)	0	100	100
78	Sg	305/317 (96%)	254 (83%)	42 (14%)	9 (3%)	3	19
79	SD	217/243 (89%)	198 (91%)	19 (9%)	0	100	100
80	SM	102/132 (77%)	89 (87%)	13 (13%)	0	100	100
81	SR	129/135 (96%)	115 (89%)	13 (10%)	1 (1%)	16	50
82	Sf	37/156 (24%)	28 (76%)	6 (16%)	3 (8%)	1	3
All	All	10940/12614 (87%)	10372 (95%)	554 (5%)	14 (0%)	49	80

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
78	Sg	139	LYS
81	SR	131	PRO
82	Sf	121	CYS
82	Sf	122	PRO
78	Sg	51	ASN
78	Sg	142	VAL
82	Sf	143	LYS
78	Sg	135	LEU
78	Sg	215	GLN
78	Sg	246	TYR
78	Sg	4	GLN
78	Sg	73	SER
78	Sg	204	GLY
53	SI	186	ASP

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	SP	47/130 (36%)	46 (98%)	1 (2%)	47	75
4	LA	184/193 (95%)	181 (98%)	3 (2%)	55	79
5	LB	192/344 (56%)	191 (100%)	1 (0%)	81	89
6	LC	285/348 (82%)	285 (100%)	0	100	100
7	LJ	101/149 (68%)	98 (97%)	3 (3%)	36	69
8	LH	143/171 (84%)	143 (100%)	0	100	100
9	LE	158/252 (63%)	155 (98%)	3 (2%)	50	76
10	LG	152/223 (68%)	148 (97%)	4 (3%)	40	72
11	LO	162/174 (93%)	160 (99%)	2 (1%)	63	82
12	LL	148/177 (84%)	147 (99%)	1 (1%)	76	86
13	LV	90/107 (84%)	88 (98%)	2 (2%)	45	74
14	LM	107/116 (92%)	106 (99%)	1 (1%)	70	85
15	La	114/120 (95%)	114 (100%)	0	100	100
16	LN	170/172 (99%)	169 (99%)	1 (1%)	78	88
17	LI	163/181 (90%)	163 (100%)	0	100	100
18	LD	205/250 (82%)	197 (96%)	8 (4%)	28	62
19	LQ	160/165 (97%)	154 (96%)	6 (4%)	29	63
20	LR	137/175 (78%)	133 (97%)	4 (3%)	37	70
21	LS	154/157 (98%)	151 (98%)	3 (2%)	50	76
22	LT	119/140 (85%)	117 (98%)	2 (2%)	53	78
23	LP	134/135 (99%)	130 (97%)	4 (3%)	36	69
24	LU	81/115 (70%)	79 (98%)	2 (2%)	42	72
25	LX	102/133 (77%)	100 (98%)	2 (2%)	48	76
26	LY	114/135 (84%)	113 (99%)	1 (1%)	70	85
27	LW	54/126 (43%)	53 (98%)	1 (2%)	50	76
28	LZ	112/118 (95%)	105 (94%)	7 (6%)	16	48
29	Lr	104/120 (87%)	100 (96%)	4 (4%)	29	63
30	Lh	93/110 (84%)	91 (98%)	2 (2%)	45	74
31	Lb	63/125 (50%)	61 (97%)	2 (3%)	34	67
32	LF	166/215 (77%)	165 (99%)	1 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	Lc	76/97 (78%)	72 (95%)	4 (5%)	20	54
34	Ld	95/110 (86%)	90 (95%)	5 (5%)	20	54
35	Le	112/115 (97%)	111 (99%)	1 (1%)	70	85
36	Lf	84/89 (94%)	82 (98%)	2 (2%)	43	73
37	Lg	86/94 (92%)	86 (100%)	0	100	100
38	Li	70/89 (79%)	67 (96%)	3 (4%)	26	60
39	Lj	70/74 (95%)	68 (97%)	2 (3%)	37	70
40	Lk	58/65 (89%)	52 (90%)	6 (10%)	7	28
41	Ll	45/48 (94%)	44 (98%)	1 (2%)	45	74
42	Lm	41/115 (36%)	40 (98%)	1 (2%)	43	73
43	Ln	24/24 (100%)	22 (92%)	2 (8%)	10	37
44	Lo	88/93 (95%)	85 (97%)	3 (3%)	32	66
45	Lp	70/72 (97%)	65 (93%)	5 (7%)	13	43
48	SA	157/243 (65%)	146 (93%)	11 (7%)	14	44
49	SB	187/231 (81%)	171 (91%)	16 (9%)	10	36
50	SE	182/225 (81%)	175 (96%)	7 (4%)	29	63
51	SF	123/170 (72%)	120 (98%)	3 (2%)	43	73
52	SH	86/174 (49%)	82 (95%)	4 (5%)	23	58
53	SI	139/180 (77%)	131 (94%)	8 (6%)	18	51
54	SK	55/136 (40%)	53 (96%)	2 (4%)	31	65
55	SL	108/142 (76%)	102 (94%)	6 (6%)	19	52
56	SQ	90/121 (74%)	84 (93%)	6 (7%)	15	46
57	SS	65/132 (49%)	63 (97%)	2 (3%)	35	68
58	ST	84/115 (73%)	80 (95%)	4 (5%)	23	57
59	SU	2/107 (2%)	2 (100%)	0	100	100
60	SV	53/67 (79%)	50 (94%)	3 (6%)	18	52
61	SX	104/115 (90%)	98 (94%)	6 (6%)	18	51
62	Sc	44/62 (71%)	41 (93%)	3 (7%)	14	45
63	Sd	43/49 (88%)	41 (95%)	2 (5%)	23	58
64	SC	164/225 (73%)	154 (94%)	10 (6%)	17	49
65	SG	63/218 (29%)	61 (97%)	2 (3%)	34	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
66	SJ	144/168 (86%)	138 (96%)	6 (4%)	26	61
67	SN	118/131 (90%)	112 (95%)	6 (5%)	21	55
68	SO	101/119 (85%)	93 (92%)	8 (8%)	11	39
69	SW	108/113 (96%)	103 (95%)	5 (5%)	24	58
70	SY	96/115 (84%)	92 (96%)	4 (4%)	26	61
71	SZ	34/103 (33%)	32 (94%)	2 (6%)	18	50
72	Sb	37/76 (49%)	37 (100%)	0	100	100
73	Se	38/104 (36%)	37 (97%)	1 (3%)	40	72
74	Sa	82/98 (84%)	79 (96%)	3 (4%)	30	64
78	Sg	163/275 (59%)	154 (94%)	9 (6%)	19	53
79	SD	109/202 (54%)	108 (99%)	1 (1%)	70	85
80	SM	7/108 (6%)	6 (86%)	1 (14%)	3	16
81	SR	59/122 (48%)	58 (98%)	1 (2%)	53	78
All	All	7778/10607 (73%)	7530 (97%)	248 (3%)	35	67

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	SP	85	ILE
4	LA	32	VAL
4	LA	82	ILE
4	LA	104	VAL
5	LB	232	THR
7	LJ	52	LYS
7	LJ	113	ILE
7	LJ	114	ASP
9	LE	51	VAL
9	LE	121	VAL
9	LE	137	VAL
10	LG	154	LEU
10	LG	162	ASP
10	LG	198	THR
10	LG	215	LEU
11	LO	132	THR
11	LO	173	GLN
12	LL	70	VAL
13	LV	101	ASN

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Mol	Chain	Res	Type
13	LV	135	ASN
14	LM	84	THR
16	LN	131	GLU
18	LD	6	VAL
18	LD	7	VAL
18	LD	36	LEU
18	LD	124	GLU
18	LD	167	VAL
18	LD	211	LEU
18	LD	239	MET
18	LD	267	ASN
19	LQ	3	VAL
19	LQ	5	ILE
19	LQ	42	THR
19	LQ	82	VAL
19	LQ	137	VAL
19	LQ	183	SER
20	LR	40	GLN
20	LR	57	VAL
20	LR	111	GLU
20	LR	116	ASP
21	LS	12	VAL
21	LS	90	THR
21	LS	102	THR
22	LT	68	THR
22	LT	90	ASN
23	LP	57	CYS
23	LP	79	THR
23	LP	100	SER
23	LP	108	ASP
24	LU	63	ILE
24	LU	102	VAL
25	LX	148	ASP
25	LX	152	LYS
26	LY	95	VAL
27	LW	52	THR
28	LZ	11	VAL
28	LZ	35	ASP
28	LZ	53	VAL
28	LZ	77	TYR
28	LZ	78	ASN
28	LZ	87	VAL

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Mol	Chain	Res	Type
28	LZ	96	VAL
29	Lr	27	THR
29	Lr	43	LEU
29	Lr	49	VAL
29	Lr	78	VAL
30	Lh	21	LEU
30	Lh	116	LEU
31	Lb	8	THR
31	Lb	50	ASN
32	LF	101	VAL
33	Lc	10	SER
33	Lc	71	VAL
33	Lc	77	ASN
33	Lc	92	CYS
34	Ld	33	ILE
34	Ld	59	THR
34	Ld	96	GLU
34	Ld	104	THR
34	Ld	106	VAL
35	Le	13	VAL
36	Lf	25	THR
36	Lf	59	THR
38	Li	12	ASN
38	Li	21	VAL
38	Li	34	THR
39	Lj	13	ASN
39	Lj	83	THR
40	Lk	8	ILE
40	Lk	12	LEU
40	Lk	13	LEU
40	Lk	27	LYS
40	Lk	36	VAL
40	Lk	48	THR
41	Ll	25	GLN
42	Lm	127	VAL
43	Ln	4	LYS
43	Ln	24	SER
44	Lo	93	LEU
44	Lo	103	VAL
44	Lo	104	ILE
45	Lp	5	THR
45	Lp	16	THR

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Mol	Chain	Res	Type
45	Lp	28	LYS
45	Lp	85[A]	ARG
45	Lp	85[B]	ARG
48	SA	35	GLU
48	SA	36	GLN
48	SA	37	TYR
48	SA	77	ILE
48	SA	104	THR
48	SA	109	THR
48	SA	111	GLN
48	SA	144	THR
48	SA	157	VAL
48	SA	193	HIS
48	SA	197	VAL
49	SB	22	VAL
49	SB	38	MET
49	SB	47	THR
49	SB	59	SER
49	SB	95	ASN
49	SB	112	SER
49	SB	127	VAL
49	SB	129	THR
49	SB	131	ASP
49	SB	139	CYS
49	SB	173	THR
49	SB	180	ASP
49	SB	196	ASP
49	SB	203	SER
49	SB	208	HIS
49	SB	215	VAL
50	SE	33	THR
50	SE	76	VAL
50	SE	87	MET
50	SE	126	VAL
50	SE	139	LEU
50	SE	184	THR
50	SE	223	SER
51	SF	28	VAL
51	SF	66	CYS
51	SF	73	THR
52	SH	45	ILE
52	SH	71	SER

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Mol	Chain	Res	Type
52	SH	105	THR
52	SH	149	ASP
53	SI	3	ILE
53	SI	46	VAL
53	SI	76	THR
53	SI	79	ILE
53	SI	95	THR
53	SI	99	ASN
53	SI	170	LYS
53	SI	195	LEU
54	SK	43	LEU
54	SK	58	VAL
55	SL	54	THR
55	SL	72	ILE
55	SL	80	MET
55	SL	85	THR
55	SL	114	SER
55	SL	127	THR
56	SQ	10	VAL
56	SQ	12	VAL
56	SQ	20	THR
56	SQ	72	VAL
56	SQ	86	GLN
56	SQ	127	CYS
57	SS	125	HIS
57	SS	131	VAL
58	ST	6	VAL
58	ST	34	VAL
58	ST	36	THR
58	ST	64	LEU
60	SV	22[A]	ARG
60	SV	22[B]	ARG
60	SV	76	ASP
61	SX	57	VAL
61	SX	91	LEU
61	SX	105	PHE
61	SX	112	VAL
61	SX	122	VAL
61	SX	128	VAL
62	Sc	21	THR
62	Sc	41	SER
62	Sc	50	VAL

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Mol	Chain	Res	Type
63	Sd	9	SER
63	Sd	49	ASP
64	SC	64	THR
64	SC	106	VAL
64	SC	156	ILE
64	SC	167	ARG
64	SC	190	SER
64	SC	205	VAL
64	SC	206	SER
64	SC	213	LEU
64	SC	222	CYS
64	SC	247	THR
65	SG	35	GLU
65	SG	129	VAL
66	SJ	3	VAL
66	SJ	8	VAL
66	SJ	59	GLU
66	SJ	97	ILE
66	SJ	141	VAL
66	SJ	149	VAL
67	SN	26	LEU
67	SN	29	THR
67	SN	31	ASP
67	SN	60	VAL
67	SN	87	ASP
67	SN	145	THR
68	SO	36	SER
68	SO	45	THR
68	SO	54	CYS
68	SO	62	VAL
68	SO	88	LEU
68	SO	107	THR
68	SO	114	SER
68	SO	124	MET
69	SW	2	VAL
69	SW	30	CYS
69	SW	40	VAL
69	SW	64	ASN
69	SW	83	LEU
70	SY	24	VAL
70	SY	35	VAL
70	SY	50	THR

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Mol	Chain	Res	Type
70	SY	94	HIS
71	SZ	54	THR
71	SZ	100	VAL
73	Se	45	VAL
74	Sa	18	VAL
74	Sa	30	VAL
74	Sa	42	ARG
78	Sg	10	THR
78	Sg	69	VAL
78	Sg	113	PHE
78	Sg	129	ILE
78	Sg	134	THR
78	Sg	166	VAL
78	Sg	186	THR
78	Sg	192	THR
78	Sg	305	ASN
79	SD	10	LYS
80	SM	109	VAL
81	SR	22	THR

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

Mol	Chain	Res	Type
4	LA	38	HIS
4	LA	97	ASN
5	LB	184	GLN
6	LC	50	GLN
6	LC	61	GLN
6	LC	310	HIS
6	LC	329	ASN
7	LJ	46	GLN
8	LH	169	ASN
8	LH	188	GLN
10	LG	64	GLN
10	LG	82	GLN
10	LG	85	GLN
11	LO	50	ASN
11	LO	90	HIS
12	LL	159	ASN
14	LM	70	GLN
15	La	34	ASN
15	La	60	HIS

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Mol	Chain	Res	Type
15	La	66	ASN
15	La	120	GLN
16	LN	8	GLN
16	LN	156	HIS
17	LI	73	ASN
17	LI	143	GLN
18	LD	191	ASN
19	LQ	7	HIS
20	LR	34	ASN
20	LR	141	HIS
22	LT	69	GLN
23	LP	10	ASN
23	LP	34	GLN
23	LP	56	GLN
23	LP	75	GLN
23	LP	97	ASN
26	LY	56	GLN
27	LW	30	GLN
29	Lr	21	ASN
30	Lh	108	GLN
31	Lb	12	GLN
31	Lb	17	HIS
32	LF	192	HIS
32	LF	206	ASN
33	Lc	15	ASN
34	Ld	28	ASN
34	Ld	93	ASN
35	Le	23	HIS
36	Lf	80	ASN
36	Lf	99	HIS
37	Lg	3	GLN
38	Li	15	HIS
42	Lm	109	ASN
42	Lm	120	ASN
44	Lo	45	GLN
44	Lo	102	GLN
45	Lp	33	GLN
48	SA	50	ASN
48	SA	113	GLN
48	SA	132	GLN
49	SB	92	GLN
49	SB	101	HIS

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Mol	Chain	Res	Type
49	SB	118	GLN
49	SB	124	HIS
49	SB	160	GLN
49	SB	232	HIS
50	SE	67	GLN
55	SL	11	GLN
56	SQ	86	GLN
57	SS	19	ASN
60	SV	21	ASN
60	SV	29	HIS
60	SV	35	ASN
68	SO	26	ASN
70	SY	124	ASN
71	SZ	46	ASN
74	Sa	72	HIS
78	Sg	62	HIS
78	Sg	147	HIS
78	Sg	191	HIS
78	Sg	237	ASN
81	SR	31	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	L8	148/156 (94%)	14 (9%)	0
3	L5	3322/5069 (65%)	465 (13%)	5 (0%)
46	Pt	74/77 (96%)	8 (10%)	0
47	L7	118/120 (98%)	17 (14%)	0
75	S2	1544/1868 (82%)	362 (23%)	7 (0%)
76	mR	13/27 (48%)	8 (61%)	0
77	S6	70/74 (94%)	21 (30%)	1 (1%)
All	All	5289/7391 (71%)	895 (16%)	13 (0%)

All (895) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	L8	23	C
2	L8	25	G
2	L8	34	U
2	L8	35	C
2	L8	39	G

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Mol	Chain	Res	Type
2	L8	59	A
2	L8	63	U
2	L8	87	G
2	L8	103	A
2	L8	105	C
2	L8	110	U
2	L8	111	U
2	L8	114	G
2	L8	126	C
3	L5	39	A
3	L5	42	A
3	L5	48	G
3	L5	56	A
3	L5	59	A
3	L5	64	A
3	L5	65	A
3	L5	66	A
3	L5	71	C
3	L5	85	G
3	L5	91	G
3	L5	98	A
3	L5	109	G
3	L5	119	G
3	L5	146	G
3	L5	159	C
3	L5	176	G
3	L5	179	G
3	L5	181	C
3	L5	200	U
3	L5	209	U
3	L5	233	U
3	L5	234	G
3	L5	235	A
3	L5	236	G
3	L5	256	G
3	L5	258	G
3	L5	259	C
3	L5	261	G
3	L5	262	G
3	L5	266	C
3	L5	280	G
3	L5	297	U

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Mol	Chain	Res	Type
3	L5	306	A
3	L5	310	G
3	L5	315	G
3	L5	316	U
3	L5	340	C
3	L5	350	C
3	L5	361	C
3	L5	362	A
3	L5	373	G
3	L5	387	G
3	L5	410	A
3	L5	411	G
3	L5	412	G
3	L5	413	G
3	L5	414	C
3	L5	432	U
3	L5	440	U
3	L5	452	A
3	L5	454	U
3	L5	464	G
3	L5	483	G
3	L5	496	G
3	L5	510	U
3	L5	648	G
3	L5	656	C
3	L5	658	C
3	L5	659	G
3	L5	660	A
3	L5	662	C
3	L5	669	C
3	L5	731	G
3	L5	740	G
3	L5	742	G
3	L5	747	A
3	L5	759	G
3	L5	913	U
3	L5	915	A
3	L5	916	C
3	L5	917	A
3	L5	932	A
3	L5	933	G
3	L5	935	A

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Mol	Chain	Res	Type
3	L5	944	A
3	L5	945	U
3	L5	956	A
3	L5	959	G
3	L5	960	A
3	L5	961	G
3	L5	976	G
3	L5	977	C
3	L5	978	G
3	L5	1068	G
3	L5	1071	C
3	L5	1180	C
3	L5	1200	G
3	L5	1211	G
3	L5	1214	C
3	L5	1218	G
3	L5	1241	C
3	L5	1266	G
3	L5	1280	C
3	L5	1282	G
3	L5	1283	G
3	L5	1284	G
3	L5	1285	U
3	L5	1287	G
3	L5	1326	A2M
3	L5	1337	A
3	L5	1354	A
3	L5	1358	G
3	L5	1359	G
3	L5	1366	G
3	L5	1378	C
3	L5	1379	C
3	L5	1381	U
3	L5	1387	A
3	L5	1394	G
3	L5	1397	A
3	L5	1398	A
3	L5	1399	G
3	L5	1413	C
3	L5	1414	C
3	L5	1420	A
3	L5	1439	C

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Mol	Chain	Res	Type
3	L5	1444	G
3	L5	1445	U
3	L5	1476	C
3	L5	1481	C
3	L5	1483	C
3	L5	1498	G
3	L5	1502	G
3	L5	1523	A
3	L5	1534	A2M
3	L5	1547	A
3	L5	1549	G
3	L5	1562	G
3	L5	1566	C
3	L5	1567	U
3	L5	1570	G
3	L5	1571	G
3	L5	1573	G
3	L5	1574	G
3	L5	1578	U
3	L5	1586	G
3	L5	1591	U
3	L5	1596	U
3	L5	1612	G
3	L5	1613	A
3	L5	1614	C
3	L5	1624	G
3	L5	1625	G
3	L5	1631	A
3	L5	1633	G
3	L5	1634	A
3	L5	1640	C
3	L5	1641	G
3	L5	1654	G
3	L5	1661	C
3	L5	1670	G
3	L5	1676	C
3	L5	1677	U
3	L5	1678	C
3	L5	1691	G
3	L5	1697	G
3	L5	1720	C
3	L5	1755	C

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Mol	Chain	Res	Type
3	L5	1756	U
3	L5	1757	U
3	L5	1759	G
3	L5	1760	G
3	L5	1761	G
3	L5	1787	A
3	L5	1794	A
3	L5	1804	A
3	L5	1805	A
3	L5	1811	G
3	L5	1815	G
3	L5	1820	C
3	L5	1833	G
3	L5	1836	G
3	L5	1837	A
3	L5	1842	G
3	L5	1843	A
3	L5	1846	G
3	L5	1855	G
3	L5	1869	G
3	L5	1897	A
3	L5	1919	G
3	L5	1921	C
3	L5	1922	G
3	L5	1931	C
3	L5	1932	A
3	L5	1948	G
3	L5	1951	G
3	L5	1961	G
3	L5	1962	A
3	L5	2020	U
3	L5	2021	G
3	L5	2022	C
3	L5	2023	C
3	L5	2024	G
3	L5	2025	A
3	L5	2026	A
3	L5	2044	U
3	L5	2046	G
3	L5	2048	U
3	L5	2055	G
3	L5	2056	G

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Mol	Chain	Res	Type
3	L5	2069	A
3	L5	2071	A
3	L5	2084	C
3	L5	2085	G
3	L5	2100	A
3	L5	2102	G
3	L5	2103	G
3	L5	2260	C
3	L5	2261	G
3	L5	2289	C
3	L5	2300	A
3	L5	2301	G
3	L5	2306	G
3	L5	2313	A
3	L5	2316	G
3	L5	2331	G
3	L5	2332	A
3	L5	2348	G
3	L5	2351	OMC
3	L5	2357	G
3	L5	2360	A
3	L5	2364	OMG
3	L5	2395	A
3	L5	2396	A
3	L5	2397	G
3	L5	2398	U
3	L5	2417	A
3	L5	2421	G
3	L5	2425	U
3	L5	2447	U
3	L5	2450	G
3	L5	2453	A
3	L5	2470	C
3	L5	2471	G
3	L5	2474	G
3	L5	2494	U
3	L5	2506	G
3	L5	2513	A
3	L5	2519	U
3	L5	2529	A
3	L5	2554	U
3	L5	2555	G

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Mol	Chain	Res	Type
3	L5	2559	G
3	L5	2569	G
3	L5	2570	U
3	L5	2575	U
3	L5	2583	C
3	L5	2587	A
3	L5	2601	A
3	L5	2627	C
3	L5	2653	C
3	L5	2662	G
3	L5	2669	C
3	L5	2681	G
3	L5	2687	U
3	L5	2694	G
3	L5	2695	A
3	L5	2696	A
3	L5	2703	G
3	L5	2710	C
3	L5	2711	G
3	L5	2721	G
3	L5	2724	G
3	L5	2726	G
3	L5	2732	G
3	L5	2743	A
3	L5	2759	G
3	L5	2760	G
3	L5	2764	A
3	L5	2769	U
3	L5	2770	C
3	L5	2788	U
3	L5	2790	U
3	L5	2798	A
3	L5	2814	C
3	L5	2815	A2M
3	L5	2826	U
3	L5	2827	G
3	L5	2829	U
3	L5	2855	G
3	L5	3616	U
3	L5	3618	C
3	L5	3626	G
3	L5	3630	A

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Mol	Chain	Res	Type
3	L5	3635	A
3	L5	3646	A
3	L5	3648	A
3	L5	3662	A
3	L5	3664	G
3	L5	3673	C
3	L5	3691	G
3	L5	3692	A
3	L5	3710	G
3	L5	3711	A
3	L5	3729	PSU
3	L5	3736	A
3	L5	3748	A
3	L5	3750	G
3	L5	3753	G
3	L5	3760	A
3	L5	3761	C
3	L5	3776	G
3	L5	3777	G
3	L5	3783	A
3	L5	3784	A
3	L5	3785	A
3	L5	3786	U
3	L5	3787	G
3	L5	3788	C
3	L5	3807	A
3	L5	3811	G
3	L5	3812	C
3	L5	3814	U
3	L5	3816	A
3	L5	3817	A
3	L5	3818	U
3	L5	3819	G
3	L5	3838	U
3	L5	3840	U
3	L5	3844	PSU
3	L5	3877	A
3	L5	3878	C
3	L5	3879	G
3	L5	3897	G
3	L5	3901	A
3	L5	3906	A

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Mol	Chain	Res	Type
3	L5	3907	G
3	L5	3908	A
3	L5	3915	U
3	L5	3926	C
3	L5	3939	G
3	L5	3948	C
3	L5	3949	A
3	L5	4068	U
3	L5	4076	G
3	L5	4084	G
3	L5	4096	C
3	L5	4097	G
3	L5	4098	A
3	L5	4099	G
3	L5	4119	C
3	L5	4122	G
3	L5	4127	A
3	L5	4162	C
3	L5	4163	U
3	L5	4170	A
3	L5	4183	G
3	L5	4184	G
3	L5	4191	G
3	L5	4203	A
3	L5	4212	A
3	L5	4225	G
3	L5	4229	U
3	L5	4233	A
3	L5	4251	A
3	L5	4254	G
3	L5	4266	G
3	L5	4268	A
3	L5	4273	A
3	L5	4280	A
3	L5	4281	A
3	L5	4282	A
3	L5	4291	G
3	L5	4295	U
3	L5	4297	G
3	L5	4305	G
3	L5	4306	OMU
3	L5	4314	C

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Mol	Chain	Res	Type
3	L5	4318	C
3	L5	4319	C
3	L5	4320	G
3	L5	4322	G
3	L5	4323	A
3	L5	4324	A
3	L5	4329	G
3	L5	4330	G
3	L5	4332	C
3	L5	4339	A
3	L5	4373	G
3	L5	4377	G
3	L5	4378	A
3	L5	4379	A
3	L5	4380	A
3	L5	4387	C
3	L5	4393	G
3	L5	4394	A
3	L5	4405	G
3	L5	4415	A
3	L5	4420	PSU
3	L5	4421	C
3	L5	4422	A
3	L5	4426	C
3	L5	4448	G
3	L5	4449	A
3	L5	4464	A
3	L5	4465	U
3	L5	4488	A
3	L5	4499	OMG
3	L5	4512	U
3	L5	4513	A
3	L5	4519	C
3	L5	4524	G
3	L5	4548	A
3	L5	4560	C
3	L5	4567	G
3	L5	4569	PSU
3	L5	4575	G
3	L5	4581	G
3	L5	4590	A2M
3	L5	4600	G

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Mol	Chain	Res	Type
3	L5	4608	G
3	L5	4610	A
3	L5	4636	PSU
3	L5	4637	OMG
3	L5	4656	A
3	L5	4657	U
3	L5	4670	C
3	L5	4672	A
3	L5	4691	A
3	L5	4700	A
3	L5	4708	A
3	L5	4709	U
3	L5	4721	G
3	L5	4741	C
3	L5	4742	G
3	L5	4750	G
3	L5	4754	G
3	L5	4757	C
3	L5	4759	C
3	L5	4761	G
3	L5	4765	G
3	L5	4775	C
3	L5	4776	G
3	L5	4860	G
3	L5	4870	G
3	L5	4871	C
3	L5	4874	A
3	L5	4877	G
3	L5	4882	U
3	L5	4883	C
3	L5	4895	C
3	L5	4906	C
3	L5	4908	G
3	L5	4910	G
3	L5	4913	G
3	L5	4914	C
3	L5	4915	G
3	L5	4921	C
3	L5	4923	C
3	L5	4928	C
3	L5	4937	C
3	L5	4943	A

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Mol	Chain	Res	Type
3	L5	4955	A
3	L5	4959	U
3	L5	4976	U
3	L5	4979	A
3	L5	4994	G
3	L5	5013	C
3	L5	5014	A
3	L5	5017	G
3	L5	5034	A
3	L5	5041	G
3	L5	5050	C
3	L5	5069	U
46	Pt	16	C
46	Pt	18	C
46	Pt	19	G
46	Pt	20	G
46	Pt	21	H2U
46	Pt	22	A
46	Pt	61	U
46	Pt	77	A
47	L7	2	U
47	L7	4	U
47	L7	5	A
47	L7	7	G
47	L7	16	A
47	L7	17	C
47	L7	33	U
47	L7	41	G
47	L7	53	U
47	L7	54	A
47	L7	63	C
47	L7	64	G
47	L7	66	G
47	L7	100	A
47	L7	110	G
47	L7	111	C
47	L7	117	G
75	S2	2	A
75	S2	4	C
75	S2	17	C
75	S2	26	U
75	S2	33	G

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Mol	Chain	Res	Type
75	S2	41	G
75	S2	42	A
75	S2	44	U
75	S2	45	A
75	S2	46	A
75	S2	56	G
75	S2	64	A
75	S2	65	C
75	S2	78	C
75	S2	79	A
75	S2	103	A
75	S2	113	G
75	S2	115	U
75	S2	126	G
75	S2	154	U
75	S2	155	G
75	S2	161	U
75	S2	162	C
75	S2	163	U
75	S2	170	A
75	S2	171	A
75	S2	173	A
75	S2	190	G
75	S2	215	G
75	S2	217	A
75	S2	291	G
75	S2	293	C
75	S2	294	U
75	S2	295	C
75	S2	306	C
75	S2	312	G
75	S2	313	A
75	S2	314	U
75	S2	333	G
75	S2	335	G
75	S2	336	A
75	S2	340	C
75	S2	347	G
75	S2	360	A
75	S2	362	C
75	S2	364	A
75	S2	370	G

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Mol	Chain	Res	Type
75	S2	381	C
75	S2	385	G
75	S2	386	C
75	S2	387	C
75	S2	400	C
75	S2	407	G
75	S2	408	A
75	S2	409	C
75	S2	413	G
75	S2	417	C
75	S2	418	A
75	S2	434	G
75	S2	435	A
75	S2	447	A
75	S2	448	A
75	S2	449	A
75	S2	450	C
75	S2	452	G
75	S2	465	A
75	S2	466	G
75	S2	471	G
75	S2	472	C
75	S2	473	A
75	S2	474	G
75	S2	482	G
75	S2	487	U
75	S2	488	U
75	S2	489	A
75	S2	492	C
75	S2	493	A
75	S2	495	U
75	S2	500	A
75	S2	502	C
75	S2	503	C
75	S2	516	A
75	S2	517	C
75	S2	525	A
75	S2	530	U
75	S2	533	A
75	S2	535	G
75	S2	536	A
75	S2	537	C

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Mol	Chain	Res	Type
75	S2	550	C
75	S2	554	A
75	S2	555	A
75	S2	556	U
75	S2	557	U
75	S2	559	G
75	S2	563	G
75	S2	583	C
75	S2	587	A
75	S2	588	G
75	S2	589	G
75	S2	590	A
75	S2	591	U
75	S2	592	C
75	S2	593	C
75	S2	594	A
75	S2	595	U
75	S2	596	U
75	S2	598	G
75	S2	604	A
75	S2	605	A
75	S2	606	G
75	S2	607	U
75	S2	614	C
75	S2	617	G
75	S2	621	C
75	S2	626	G
75	S2	627	U
75	S2	628	A
75	S2	638	C
75	S2	643	A
75	S2	644	G
75	S2	645	C
75	S2	655	A
75	S2	656	G
75	S2	660	C
75	S2	668	A
75	S2	669	A
75	S2	670	A
75	S2	671	A
75	S2	672	A
75	S2	673	G

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Mol	Chain	Res	Type
75	S2	684	G
75	S2	688	U
75	S2	811	A
75	S2	821	G
75	S2	822	U
75	S2	830	A
75	S2	831	G
75	S2	842	C
75	S2	847	A
75	S2	852	G
75	S2	869	A
75	S2	870	A
75	S2	878	G
75	S2	908	A
75	S2	909	G
75	S2	913	A
75	S2	918	U
75	S2	920	A
75	S2	922	A
75	S2	933	G
75	S2	934	G
75	S2	938	A
75	S2	943	U
75	S2	959	G
75	S2	960	U
75	S2	963	A
75	S2	970	G
75	S2	971	G
75	S2	972	A
75	S2	981	A
75	S2	990	A
75	S2	992	A
75	S2	997	A
75	S2	999	G
75	S2	1001	A
75	S2	1002	U
75	S2	1017	U
75	S2	1023	A
75	S2	1027	A
75	S2	1028	A
75	S2	1061	U
75	S2	1062	A

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Mol	Chain	Res	Type
75	S2	1083	A
75	S2	1084	A
75	S2	1085	C
75	S2	1087	A
75	S2	1097	G
75	S2	1109	C
75	S2	1115	U
75	S2	1117	C
75	S2	1118	C
75	S2	1121	G
75	S2	1126	G
75	S2	1130	G
75	S2	1133	A
75	S2	1138	C
75	S2	1149	A
75	S2	1153	C
75	S2	1154	U
75	S2	1157	G
75	S2	1172	U
75	S2	1181	A
75	S2	1195	A
75	S2	1207	G
75	S2	1208	A
75	S2	1212	G
75	S2	1215	C
75	S2	1216	C
75	S2	1217	A
75	S2	1221	G
75	S2	1224	G
75	S2	1242	U
75	S2	1243	U
75	S2	1251	A
75	S2	1253	A
75	S2	1256	G
75	S2	1257	G
75	S2	1259	A
75	S2	1265	A
75	S2	1270	G
75	S2	1271	C
75	S2	1274	G
75	S2	1275	G
75	S2	1276	A

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Mol	Chain	Res	Type
75	S2	1277	C
75	S2	1280	G
75	S2	1282	A
75	S2	1292	C
75	S2	1293	A
75	S2	1294	G
75	S2	1298	G
75	S2	1301	A
75	S2	1302	G
75	S2	1303	C
75	S2	1307	U
75	S2	1308	U
75	S2	1309	C
75	S2	1311	C
75	S2	1312	G
75	S2	1313	A
75	S2	1314	U
75	S2	1317	C
75	S2	1331	C
75	S2	1332	A
75	S2	1341	C
75	S2	1342	U
75	S2	1343	U
75	S2	1371	U
75	S2	1372	U
75	S2	1373	C
75	S2	1378	A
75	S2	1396	A
75	S2	1397	U
75	S2	1401	A
75	S2	1402	A
75	S2	1403	C
75	S2	1405	A
75	S2	1407	U
75	S2	1409	A
75	S2	1410	C
75	S2	1414	A
75	S2	1415	C
75	S2	1420	G
75	S2	1429	G
75	S2	1430	C
75	S2	1431	G

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Mol	Chain	Res	Type
75	S2	1439	A
75	S2	1442	U
75	S2	1447	G
75	S2	1454	A
75	S2	1462	U
75	S2	1463	U
75	S2	1466	G
75	S2	1467	C
75	S2	1469	A
75	S2	1472	C
75	S2	1475	G
75	S2	1476	A
75	S2	1477	U
75	S2	1478	U
75	S2	1480	A
75	S2	1489	A
75	S2	1490	G
75	S2	1494	U
75	S2	1495	G
75	S2	1498	A
75	S2	1506	A
75	S2	1507	G
75	S2	1509	U
75	S2	1510	G
75	S2	1512	C
75	S2	1513	C
75	S2	1521	C
75	S2	1522	A
75	S2	1531	A
75	S2	1533	A
75	S2	1536	G
75	S2	1543	U
75	S2	1546	G
75	S2	1548	G
75	S2	1551	U
75	S2	1552	G
75	S2	1554	C
75	S2	1555	U
75	S2	1556	A
75	S2	1560	U
75	S2	1567	G
75	S2	1570	G

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Mol	Chain	Res	Type
75	S2	1575	G
75	S2	1578	U
75	S2	1579	A
75	S2	1580	A
75	S2	1585	U
75	S2	1586	U
75	S2	1588	A
75	S2	1589	A
75	S2	1599	U
75	S2	1600	G
75	S2	1601	A
75	S2	1604	G
75	S2	1621	U
75	S2	1623	A
75	S2	1634	A
75	S2	1636	G
75	S2	1638	G
75	S2	1639	G
75	S2	1640	A
75	S2	1648	G
75	S2	1654	G
75	S2	1665	G
75	S2	1671	G
75	S2	1680	G
75	S2	1686	G
75	S2	1695	A
75	S2	1699	A
75	S2	1715	A
75	S2	1719	A
75	S2	1721	U
75	S2	1722	G
75	S2	1744	G
75	S2	1745	A
75	S2	1746	U
75	S2	1749	G
75	S2	1751	C
75	S2	1752	C
75	S2	1753	C
75	S2	1754	G
75	S2	1777	G
75	S2	1780	G
75	S2	1781	A

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Mol	Chain	Res	Type
75	S2	1782	G
75	S2	1783	C
75	S2	1798	C
75	S2	1813	A
75	S2	1824	A
75	S2	1825	A
75	S2	1826	G
75	S2	1829	G
75	S2	1831	A
75	S2	1835	A
75	S2	1838	U
75	S2	1849	G
75	S2	1850	A
75	S2	1851	A
75	S2	1852	C
75	S2	1861	G
75	S2	1862	G
75	S2	1863	A
75	S2	1865	C
75	S2	1868	U
75	S2	1869	A
76	mR	8	C
76	mR	9	U
76	mR	10	A
76	mR	11	G
76	mR	12	C
76	mR	13	G
76	mR	16	A
76	mR	17	A
77	S6	6	G
77	S6	8	4SU
77	S6	9	G
77	S6	11	A
77	S6	16	C
77	S6	19	G
77	S6	20	G
77	S6	21	H2U
77	S6	22	A
77	S6	23	G
77	S6	24	C
77	S6	30	G
77	S6	36	A

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Mol	Chain	Res	Type
77	S6	45	A
77	S6	47	G7M
77	S6	53	G
77	S6	60	A
77	S6	62	C
77	S6	66	C
77	S6	70	C
77	S6	74	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	934	C
3	L5	1070	G
3	L5	1633	G
3	L5	3615	G
3	L5	4699	U
75	S2	417	C
75	S2	465	A
75	S2	604	A
75	S2	980	A
75	S2	1293	A
75	S2	1395	C
75	S2	1679	A
77	S6	59	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4403	3	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
3	A2M	L5	1326	3	22,25,26	3.93	10 (45%)	31,36,39	3.74	15 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UR3	L5	4530	3	19,22,23	2.78	8 (42%)	26,32,35	1.29	2 (7%)
3	A2M	L5	2363	3	22,25,26	3.94	11 (50%)	31,36,39	3.78	14 (45%)
3	PSU	L5	3715	3	18,21,22	1.03	1 (5%)	22,30,33	1.70	4 (18%)
3	PSU	L5	4552	3	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
3	PSU	L5	4579	3	18,21,22	1.04	1 (5%)	22,30,33	1.72	4 (18%)
3	PSU	L5	4689	3	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)
3	PSU	L5	4296	3	18,21,22	1.05	1 (5%)	22,30,33	1.69	4 (18%)
3	PSU	L5	4442	3	18,21,22	1.09	1 (5%)	22,30,33	1.79	5 (22%)
3	PSU	L5	4972	3	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
5	HIC	LB	245	5	10,11,12	0.57	0	8,14,16	0.62	0
44	MLZ	Lo	53	44	8,9,10	0.77	0	4,9,11	0.62	0
3	OMC	L5	2422	3	19,22,23	0.59	0	26,31,34	0.78	1 (3%)
77	PSU	S6	56	77	18,21,22	1.06	1 (5%)	22,30,33	1.71	3 (13%)
3	A2M	L5	3825	3	22,25,26	3.94	10 (45%)	31,36,39	3.63	14 (45%)
3	A2M	L5	3723	3	22,25,26	3.93	10 (45%)	31,36,39	3.72	15 (48%)
3	PSU	L5	4431	3	18,21,22	1.05	1 (5%)	22,30,33	1.72	4 (18%)
3	OMG	L5	3792	3	23,26,27	0.50	0	33,38,41	0.49	0
42	M3L	Lm	98	42	10,11,12	0.42	0	9,14,16	0.37	0
3	A2M	L5	3718	3	22,25,26	3.91	10 (45%)	31,36,39	3.69	15 (48%)
3	OMC	L5	3701	3	19,22,23	0.56	0	26,31,34	0.55	0
3	OMC	L5	3887	3	19,22,23	0.54	0	26,31,34	0.71	0
3	A2M	L5	4571	3	22,25,26	3.90	10 (45%)	31,36,39	3.68	14 (45%)
3	6MZ	L5	4220	3	22,25,26	2.69	4 (18%)	30,36,39	3.58	12 (40%)
3	OMC	L5	4456	3	19,22,23	0.58	0	26,31,34	0.79	1 (3%)
3	PSU	L5	3734	3	18,21,22	1.04	1 (5%)	22,30,33	1.73	4 (18%)
46	G7M	Pt	47	46	23,26,27	2.77	8 (34%)	35,39,42	2.33	10 (28%)
3	OMC	L5	3869	3	19,22,23	0.55	0	26,31,34	0.66	0
3	A2M	L5	2815	3	22,25,26	3.95	10 (45%)	31,36,39	3.85	16 (51%)
3	OMG	L5	4228	3	23,26,27	0.49	0	33,38,41	0.54	0
3	PSU	L5	4532	3	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
3	OMU	L5	4227	3	19,22,23	3.02	8 (42%)	26,31,34	1.73	4 (15%)
3	1MA	L5	1322	3	21,25,26	0.50	0	31,37,40	0.75	1 (3%)
46	4SU	Pt	8	46	18,21,22	3.76	8 (44%)	26,30,33	2.23	4 (15%)
3	OMG	L5	1316	3	23,26,27	0.51	0	33,38,41	0.52	0
3	A2M	L5	4523	3	22,25,26	3.90	11 (50%)	31,36,39	3.68	14 (45%)
3	PSU	L5	4423	3	18,21,22	1.09	1 (5%)	22,30,33	1.73	4 (18%)
3	OMC	L5	4536	3	19,22,23	0.55	0	26,31,34	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4500	3	18,21,22	1.12	1 (5%)	22,30,33	1.79	4 (18%)
77	H2U	S6	21	77	18,21,22	0.48	0	21,30,33	1.00	1 (4%)
3	PSU	L5	3762	3	18,21,22	1.04	1 (5%)	22,30,33	1.66	4 (18%)
3	PSU	L5	4628	3	18,21,22	1.05	1 (5%)	22,30,33	1.81	4 (18%)
3	OMG	L5	2424	3	23,26,27	0.50	0	33,38,41	0.44	0
3	PSU	L5	1792	3	18,21,22	1.04	1 (5%)	22,30,33	1.61	4 (18%)
4	V5N	LA	216	4	9,11,12	2.67	2 (22%)	9,14,16	1.21	0
3	OMG	L5	3899	3	23,26,27	0.51	0	33,38,41	0.51	0
3	PSU	L5	4521	3	18,21,22	1.06	1 (5%)	22,30,33	1.79	4 (18%)
3	OMG	L5	4623	3	23,26,27	0.50	0	33,38,41	0.52	0
3	PSU	L5	3764	3	18,21,22	1.04	1 (5%)	22,30,33	1.67	4 (18%)
3	PSU	L5	3758	3	18,21,22	1.04	1 (5%)	22,30,33	1.71	4 (18%)
3	OMC	L5	2365	3	19,22,23	0.53	0	26,31,34	0.64	0
3	OMG	L5	4196	3,46	23,26,27	0.49	0	33,38,41	0.50	0
3	PSU	L5	4531	3	18,21,22	1.06	1 (5%)	22,30,33	1.88	5 (22%)
3	OMU	L5	3925	3	19,22,23	3.01	8 (42%)	26,31,34	1.70	5 (19%)
3	OMG	L5	2876	3	23,26,27	0.55	0	33,38,41	0.48	0
3	PSU	L5	4457	3	18,21,22	1.05	1 (5%)	22,30,33	1.76	5 (22%)
3	OMG	L5	4370	3	23,26,27	0.50	0	33,38,41	0.55	0
15	V5N	La	39	15	9,11,12	2.63	2 (22%)	9,14,16	1.19	1 (11%)
3	A2M	L5	2401	3	22,25,26	3.92	11 (50%)	31,36,39	3.74	16 (51%)
3	OMG	L5	4499	3	23,26,27	0.50	0	33,38,41	0.45	0
3	PSU	L5	4299	3	18,21,22	1.06	1 (5%)	22,30,33	1.73	4 (18%)
46	PSU	Pt	56	46	18,21,22	1.07	1 (5%)	22,30,33	1.75	4 (18%)
3	OMC	L5	1340	3	19,22,23	0.53	0	26,31,34	0.64	0
31	MLZ	Lb	5	31	8,9,10	0.79	0	4,9,11	0.64	0
3	PSU	L5	5001	3	18,21,22	1.08	1 (5%)	22,30,33	1.74	4 (18%)
3	PSU	L5	4353	3	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
3	PSU	L5	4569	3	18,21,22	1.08	1 (5%)	22,30,33	1.70	4 (18%)
3	OMG	L5	3944	3	23,26,27	0.50	0	33,38,41	0.60	0
3	OMU	L5	4498	3	19,22,23	3.02	8 (42%)	26,31,34	1.71	5 (19%)
3	5MC	L5	4447	3	18,22,23	0.72	0	26,32,35	0.73	0
3	A2M	L5	1871	3	22,25,26	3.93	10 (45%)	31,36,39	3.69	15 (48%)
3	5MC	L5	3782	3	18,22,23	0.57	0	26,32,35	0.68	0
3	PSU	L5	4420	3	18,21,22	1.04	1 (5%)	22,30,33	1.59	4 (18%)
3	PSU	L5	5010	3	18,21,22	1.06	1 (5%)	22,30,33	1.71	4 (18%)
3	OMU	L5	4306	3	19,22,23	2.98	8 (42%)	26,31,34	1.72	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	3844	3	18,21,22	1.02	1 (5%)	22,30,33	1.74	4 (18%)
3	A2M	L5	3867	3	22,25,26	3.94	10 (45%)	31,36,39	3.77	15 (48%)
77	4SU	S6	8	77	18,21,22	3.78	8 (44%)	26,30,33	2.20	5 (19%)
3	OMG	L5	2364	3	23,26,27	0.49	0	33,38,41	0.46	0
3	PSU	L5	4636	3	18,21,22	1.06	1 (5%)	22,30,33	1.84	5 (22%)
3	PSU	L5	3729	3	18,21,22	1.09	1 (5%)	22,30,33	1.68	4 (18%)
3	PSU	L5	3851	3	18,21,22	1.04	1 (5%)	22,30,33	1.70	4 (18%)
3	PSU	L5	4576	3	18,21,22	1.05	1 (5%)	22,30,33	1.75	4 (18%)
3	A2M	L5	398	3	22,25,26	3.90	10 (45%)	31,36,39	3.66	13 (41%)
3	OMG	L5	4392	3	23,26,27	0.51	0	33,38,41	0.45	0
3	OMC	L5	3808	3	19,22,23	0.60	0	26,31,34	0.86	2 (7%)
3	OMG	L5	4637	3	23,26,27	0.51	0	33,38,41	0.49	0
3	OMG	L5	4494	3	23,26,27	0.51	0	33,38,41	0.49	0
3	PSU	L5	1860	3	18,21,22	1.07	1 (5%)	22,30,33	1.71	4 (18%)
3	PSU	L5	3853	3	18,21,22	1.03	1 (5%)	22,30,33	1.72	4 (18%)
3	PSU	L5	3770	3	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
3	A2M	L5	1524	3	22,25,26	3.98	10 (45%)	31,36,39	3.97	14 (45%)
3	PSU	L5	4361	3	18,21,22	1.03	1 (5%)	22,30,33	1.68	4 (18%)
3	OMC	L5	3841	3	19,22,23	0.53	0	26,31,34	0.71	1 (3%)
3	PSU	L5	4673	3	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
77	G7M	S6	47	77	23,26,27	2.78	8 (34%)	35,39,42	2.29	10 (28%)
3	PSU	L5	4493	3	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)
3	OMG	L5	4618	3	23,26,27	0.50	0	33,38,41	0.53	0
3	A2M	L5	1534	3,84	22,25,26	3.93	10 (45%)	31,36,39	3.77	14 (45%)
3	PSU	L5	1781	3	18,21,22	1.04	1 (5%)	22,30,33	1.63	4 (18%)
3	OMC	L5	1881	3	19,22,23	0.57	0	26,31,34	0.65	0
3	OMC	L5	2351	3	19,22,23	0.58	0	26,31,34	1.07	2 (7%)
3	OMC	L5	2804	3	19,22,23	0.55	0	26,31,34	0.62	0
3	OMG	L5	3627	3	23,26,27	0.50	0	33,38,41	0.60	0
3	PSU	L5	3768	3	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
3	A2M	L5	3724	3	22,25,26	3.93	10 (45%)	31,36,39	3.71	14 (45%)
3	PSU	L5	3920	3	18,21,22	1.03	1 (5%)	22,30,33	1.75	4 (18%)
3	A2M	L5	4590	3	22,25,26	3.94	9 (40%)	31,36,39	3.80	16 (51%)
46	H2U	Pt	21	46	18,21,22	0.59	0	21,30,33	1.54	4 (19%)
3	OMG	L5	3744	3	23,26,27	0.49	0	33,38,41	0.49	0
3	A2M	L5	3830	3	22,25,26	3.94	10 (45%)	31,36,39	3.70	13 (41%)
3	OMG	L5	1522	3	23,26,27	0.52	0	33,38,41	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PSU	L5	4471	3	18,21,22	1.05	1 (5%)	22,30,33	1.63	4 (18%)
3	A2M	L5	400	3	22,25,26	3.91	10 (45%)	31,36,39	3.71	15 (48%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1326	3	-	2/9/27/28	0/3/3/3
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2363	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4579	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4972	3	-	0/7/25/26	0/2/2/2
5	HIC	LB	245	5	-	0/5/6/8	0/1/1/1
44	MLZ	Lo	53	44	-	5/7/8/10	-
3	OMC	L5	2422	3	-	1/9/27/28	0/2/2/2
77	PSU	S6	56	77	-	0/7/25/26	0/2/2/2
3	A2M	L5	3825	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	3723	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4431	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
42	M3L	Lm	98	42	-	1/9/10/12	-
3	A2M	L5	3718	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	3701	3	-	4/9/27/28	0/2/2/2
3	OMC	L5	3887	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	4571	3	-	1/9/27/28	0/3/3/3
3	6MZ	L5	4220	3	-	2/9/27/28	0/3/3/3
3	OMC	L5	4456	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3734	3	-	0/7/25/26	0/2/2/2
46	G7M	Pt	47	46	-	0/7/25/26	0/3/3/3
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	2815	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4532	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMU	L5	4227	3	-	1/9/27/28	0/2/2/2
3	1MA	L5	1322	3	-	0/7/25/26	0/3/3/3
46	4SU	Pt	8	46	-	0/7/25/26	0/2/2/2
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	4523	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4423	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4500	3	-	3/7/25/26	0/2/2/2
77	H2U	S6	21	77	-	1/7/38/39	0/2/2/2
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
4	V5N	LA	216	4	-	3/9/10/12	0/1/1/1
3	OMG	L5	3899	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4521	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4623	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3764	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2365	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4196	3,46	-	0/9/27/28	0/3/3/3
3	PSU	L5	4531	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	3925	3	-	2/9/27/28	0/2/2/2
3	OMG	L5	2876	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4457	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4370	3	-	1/9/27/28	0/3/3/3
15	V5N	La	39	15	-	0/9/10/12	0/1/1/1
3	A2M	L5	2401	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4499	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	0/7/25/26	0/2/2/2
46	PSU	Pt	56	46	-	0/7/25/26	0/2/2/2
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
31	MLZ	Lb	5	31	-	0/7/8/10	-
3	PSU	L5	5001	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4569	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	3944	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	4498	3	-	0/9/27/28	0/2/2/2
3	5MC	L5	4447	3	-	4/7/25/26	0/2/2/2
3	A2M	L5	1871	3	-	0/9/27/28	0/3/3/3
3	5MC	L5	3782	3	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4420	3	-	5/7/25/26	0/2/2/2
3	PSU	L5	5010	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4306	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	3844	3	-	3/7/25/26	0/2/2/2
3	A2M	L5	3867	3	-	3/9/27/28	0/3/3/3
77	4SU	S6	8	77	-	3/7/25/26	0/2/2/2
3	OMG	L5	2364	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4636	3	-	3/7/25/26	0/2/2/2
3	PSU	L5	3729	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	3851	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4576	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	3/9/27/28	0/3/3/3
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4637	3	-	3/9/27/28	0/3/3/3
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1860	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3853	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	2/9/27/28	0/2/2/2
3	PSU	L5	4673	3	-	0/7/25/26	0/2/2/2
77	G7M	S6	47	77	-	3/7/25/26	0/3/3/3
3	PSU	L5	4493	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4618	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1534	3,84	-	2/9/27/28	0/3/3/3
3	PSU	L5	1781	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	1881	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	2351	3	-	2/9/27/28	0/2/2/2
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	3627	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3724	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	3920	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	4590	3	-	1/9/27/28	0/3/3/3
46	H2U	Pt	21	46	-	3/7/38/39	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3830	3	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4471	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	1/9/27/28	0/3/3/3

All (306) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3830	A2M	C3'-C2'	-12.74	1.24	1.52
3	L5	1524	A2M	C3'-C2'	-12.68	1.24	1.52
3	L5	4590	A2M	C3'-C2'	-12.67	1.24	1.52
3	L5	3825	A2M	C3'-C2'	-12.67	1.24	1.52
3	L5	3867	A2M	C3'-C2'	-12.66	1.24	1.52
3	L5	1534	A2M	C3'-C2'	-12.64	1.24	1.52
3	L5	1871	A2M	C3'-C2'	-12.61	1.24	1.52
3	L5	2363	A2M	C3'-C2'	-12.58	1.24	1.52
3	L5	3724	A2M	C3'-C2'	-12.54	1.25	1.52
3	L5	1326	A2M	C3'-C2'	-12.53	1.25	1.52
3	L5	2815	A2M	C3'-C2'	-12.52	1.25	1.52
3	L5	398	A2M	C3'-C2'	-12.52	1.25	1.52
3	L5	400	A2M	C3'-C2'	-12.51	1.25	1.52
3	L5	3723	A2M	C3'-C2'	-12.50	1.25	1.52
3	L5	3718	A2M	C3'-C2'	-12.48	1.25	1.52
3	L5	2401	A2M	C3'-C2'	-12.46	1.25	1.52
3	L5	4571	A2M	C3'-C2'	-12.45	1.25	1.52
3	L5	4523	A2M	C3'-C2'	-12.38	1.25	1.52
3	L5	4220	6MZ	C6-N6	11.31	1.46	1.34
77	S6	8	4SU	C4-N3	8.25	1.46	1.37
46	Pt	8	4SU	C4-N3	8.09	1.46	1.37
3	L5	4530	UR3	C2-N1	7.33	1.49	1.38
77	S6	8	4SU	C2-N3	7.17	1.50	1.38
3	L5	4227	OMU	C2-N1	7.14	1.49	1.38
46	Pt	8	4SU	C2-N3	7.07	1.50	1.38
3	L5	3925	OMU	C2-N1	7.05	1.49	1.38
3	L5	4498	OMU	C2-N1	7.04	1.49	1.38
77	S6	8	4SU	C2-N1	6.87	1.49	1.38
3	L5	4306	OMU	C2-N1	6.78	1.49	1.38
46	Pt	8	4SU	C2-N1	6.78	1.49	1.38
3	L5	4306	OMU	C2-N3	6.76	1.50	1.38
3	L5	3925	OMU	C2-N3	6.74	1.50	1.38
77	S6	47	G7M	C4-N3	6.74	1.50	1.34
3	L5	4227	OMU	C2-N3	6.73	1.50	1.38
3	L5	4498	OMU	C2-N3	6.72	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1524	A2M	O4'-C4'	-6.72	1.30	1.45
46	Pt	47	G7M	C4-N3	6.69	1.50	1.34
3	L5	1326	A2M	O4'-C4'	-6.63	1.30	1.45
3	L5	3867	A2M	O4'-C4'	-6.63	1.30	1.45
3	L5	2815	A2M	O4'-C4'	-6.59	1.30	1.45
3	L5	2363	A2M	O4'-C4'	-6.55	1.30	1.45
3	L5	3825	A2M	O4'-C4'	-6.52	1.30	1.45
3	L5	4523	A2M	O4'-C4'	-6.50	1.30	1.45
3	L5	3723	A2M	O4'-C4'	-6.49	1.30	1.45
4	LA	216	V5N	CG-ND1	-6.48	1.31	1.37
3	L5	400	A2M	O4'-C4'	-6.48	1.30	1.45
3	L5	2401	A2M	O4'-C4'	-6.48	1.30	1.45
3	L5	4590	A2M	O4'-C4'	-6.44	1.30	1.45
3	L5	3724	A2M	O4'-C4'	-6.42	1.30	1.45
3	L5	4571	A2M	O4'-C4'	-6.37	1.30	1.45
3	L5	398	A2M	O4'-C4'	-6.36	1.30	1.45
3	L5	1871	A2M	O4'-C4'	-6.35	1.30	1.45
15	La	39	V5N	CG-ND1	-6.35	1.31	1.37
3	L5	3830	A2M	O4'-C4'	-6.33	1.30	1.45
3	L5	3718	A2M	O4'-C4'	-6.32	1.30	1.45
3	L5	1534	A2M	O4'-C4'	-6.32	1.30	1.45
3	L5	4530	UR3	C6-C5	6.11	1.49	1.35
46	Pt	47	G7M	C2-N2	5.87	1.48	1.34
77	S6	47	G7M	C2-N2	5.83	1.48	1.34
46	Pt	8	4SU	C6-C5	5.76	1.48	1.35
77	S6	8	4SU	C6-C5	5.72	1.48	1.35
3	L5	4498	OMU	C6-C5	5.69	1.48	1.35
3	L5	4227	OMU	C6-C5	5.65	1.48	1.35
3	L5	4306	OMU	C6-C5	5.63	1.48	1.35
3	L5	3925	OMU	C6-C5	5.58	1.48	1.35
46	Pt	47	G7M	C2-N3	5.52	1.46	1.33
77	S6	47	G7M	C2-N3	5.48	1.46	1.33
3	L5	1524	A2M	C6-N6	5.41	1.47	1.34
3	L5	4571	A2M	C6-N6	5.40	1.47	1.34
3	L5	1534	A2M	C3'-C4'	5.39	1.66	1.53
3	L5	3723	A2M	C6-N6	5.39	1.47	1.34
3	L5	3724	A2M	C6-N6	5.38	1.47	1.34
3	L5	400	A2M	C6-N6	5.38	1.47	1.34
3	L5	4523	A2M	C6-N6	5.37	1.47	1.34
3	L5	2815	A2M	C6-N6	5.37	1.47	1.34
3	L5	2363	A2M	C6-N6	5.37	1.47	1.34
3	L5	3867	A2M	C6-N6	5.36	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3718	A2M	C6-N6	5.36	1.47	1.34
3	L5	1871	A2M	C6-N6	5.36	1.47	1.34
3	L5	3830	A2M	C6-N6	5.36	1.47	1.34
3	L5	1534	A2M	C6-N6	5.35	1.47	1.34
3	L5	2401	A2M	C6-N6	5.35	1.47	1.34
3	L5	4590	A2M	C6-N6	5.34	1.47	1.34
3	L5	1326	A2M	C6-N6	5.34	1.47	1.34
3	L5	398	A2M	C6-N6	5.33	1.47	1.34
3	L5	3825	A2M	C6-N6	5.33	1.47	1.34
3	L5	4571	A2M	C3'-C4'	5.27	1.66	1.53
3	L5	3718	A2M	C3'-C4'	5.26	1.66	1.53
3	L5	3723	A2M	C3'-C4'	5.24	1.66	1.53
3	L5	3830	A2M	C3'-C4'	5.24	1.66	1.53
3	L5	4523	A2M	C3'-C4'	5.22	1.66	1.53
3	L5	3724	A2M	C3'-C4'	5.22	1.66	1.53
3	L5	2363	A2M	C3'-C4'	5.22	1.66	1.53
3	L5	3825	A2M	C3'-C4'	5.20	1.66	1.53
3	L5	1326	A2M	C3'-C4'	5.20	1.66	1.53
3	L5	1871	A2M	C3'-C4'	5.16	1.66	1.53
3	L5	3867	A2M	C3'-C4'	5.12	1.66	1.53
3	L5	2815	A2M	C3'-C4'	5.12	1.66	1.53
3	L5	2401	A2M	C3'-C4'	5.11	1.66	1.53
3	L5	400	A2M	C3'-C4'	5.09	1.66	1.53
3	L5	398	A2M	C3'-C4'	5.08	1.66	1.53
3	L5	4590	A2M	C3'-C4'	5.08	1.66	1.53
3	L5	1524	A2M	C3'-C4'	5.00	1.65	1.53
3	L5	4530	UR3	C2-N3	4.96	1.48	1.39
3	L5	1524	A2M	C1'-N9	-4.91	1.32	1.46
46	Pt	8	4SU	C5-C4	4.84	1.48	1.42
77	S6	8	4SU	C4-S4	-4.63	1.59	1.68
77	S6	8	4SU	C5-C4	4.62	1.48	1.42
3	L5	4590	A2M	O4'-C1'	4.56	1.52	1.42
46	Pt	8	4SU	C4-S4	-4.56	1.59	1.68
3	L5	2815	A2M	C1'-N9	-4.54	1.33	1.46
3	L5	1534	A2M	C1'-N9	-4.53	1.33	1.46
3	L5	3724	A2M	O4'-C1'	4.52	1.52	1.42
3	L5	3830	A2M	O4'-C1'	4.50	1.52	1.42
3	L5	398	A2M	O4'-C1'	4.49	1.52	1.42
3	L5	1871	A2M	O4'-C1'	4.48	1.52	1.42
3	L5	3718	A2M	O4'-C1'	4.47	1.52	1.42
3	L5	4590	A2M	C1'-N9	-4.47	1.33	1.46
3	L5	2401	A2M	C1'-N9	-4.46	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	2815	A2M	O4'-C1'	4.44	1.52	1.42
3	L5	4571	A2M	O4'-C1'	4.43	1.52	1.42
3	L5	2401	A2M	O4'-C1'	4.41	1.52	1.42
3	L5	3723	A2M	C1'-N9	-4.40	1.33	1.46
3	L5	1871	A2M	C1'-N9	-4.40	1.33	1.46
3	L5	3723	A2M	O4'-C1'	4.40	1.52	1.42
3	L5	2363	A2M	O4'-C1'	4.40	1.52	1.42
3	L5	3867	A2M	O4'-C1'	4.39	1.52	1.42
3	L5	3867	A2M	C1'-N9	-4.37	1.33	1.46
3	L5	3825	A2M	O4'-C1'	4.35	1.52	1.42
3	L5	2363	A2M	C1'-N9	-4.34	1.34	1.46
3	L5	400	A2M	O4'-C1'	4.33	1.52	1.42
3	L5	1326	A2M	C1'-N9	-4.32	1.34	1.46
3	L5	4523	A2M	C1'-N9	-4.32	1.34	1.46
3	L5	4523	A2M	O4'-C1'	4.31	1.52	1.42
3	L5	3825	A2M	C1'-N9	-4.31	1.34	1.46
3	L5	1326	A2M	O4'-C1'	4.30	1.52	1.42
3	L5	400	A2M	C1'-N9	-4.30	1.34	1.46
3	L5	1534	A2M	O4'-C1'	4.28	1.52	1.42
3	L5	3724	A2M	C1'-N9	-4.26	1.34	1.46
3	L5	3830	A2M	C1'-N9	-4.26	1.34	1.46
3	L5	4571	A2M	C1'-N9	-4.24	1.34	1.46
3	L5	3718	A2M	C1'-N9	-4.22	1.34	1.46
3	L5	398	A2M	C1'-N9	-4.17	1.34	1.46
3	L5	1524	A2M	O4'-C1'	4.16	1.51	1.42
77	S6	47	G7M	C5-C6	4.15	1.55	1.43
46	Pt	47	G7M	C5-C6	4.10	1.54	1.43
4	LA	216	V5N	CD2-NE2	-4.08	1.31	1.37
3	L5	3925	OMU	C4-N3	4.07	1.45	1.38
3	L5	4498	OMU	C4-N3	4.04	1.45	1.38
3	L5	4306	OMU	C4-N3	4.03	1.45	1.38
3	L5	4227	OMU	C4-N3	4.03	1.45	1.38
15	La	39	V5N	CD2-NE2	-3.99	1.31	1.37
77	S6	47	G7M	C5-N7	-3.84	1.34	1.39
46	Pt	47	G7M	C5-N7	-3.80	1.34	1.39
3	L5	4500	PSU	C6-C5	3.64	1.39	1.35
77	S6	47	G7M	C2-N1	3.61	1.46	1.37
46	Pt	47	G7M	C2-N1	3.54	1.46	1.37
3	L5	4420	PSU	C6-C5	3.52	1.39	1.35
46	Pt	56	PSU	C6-C5	3.51	1.39	1.35
3	L5	1792	PSU	C6-C5	3.50	1.39	1.35
3	L5	4423	PSU	C6-C5	3.50	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	S6	56	PSU	C6-C5	3.48	1.39	1.35
3	L5	4532	PSU	C6-C5	3.48	1.39	1.35
3	L5	4569	PSU	C6-C5	3.48	1.39	1.35
3	L5	1781	PSU	C6-C5	3.45	1.39	1.35
3	L5	3762	PSU	C6-C5	3.45	1.39	1.35
3	L5	5010	PSU	C6-C5	3.44	1.39	1.35
3	L5	4972	PSU	C6-C5	3.44	1.39	1.35
3	L5	3729	PSU	C6-C5	3.44	1.39	1.35
3	L5	3770	PSU	C6-C5	3.42	1.39	1.35
3	L5	4471	PSU	C6-C5	3.42	1.39	1.35
3	L5	4552	PSU	C6-C5	3.40	1.39	1.35
3	L5	5001	PSU	C6-C5	3.40	1.39	1.35
3	L5	1860	PSU	C6-C5	3.40	1.39	1.35
3	L5	3734	PSU	C6-C5	3.37	1.39	1.35
3	L5	3764	PSU	C6-C5	3.37	1.39	1.35
3	L5	4442	PSU	C6-C5	3.37	1.39	1.35
3	L5	4296	PSU	C6-C5	3.36	1.39	1.35
3	L5	4299	PSU	C6-C5	3.36	1.39	1.35
3	L5	3715	PSU	C6-C5	3.35	1.39	1.35
3	L5	4521	PSU	C6-C5	3.34	1.39	1.35
3	L5	4353	PSU	C6-C5	3.33	1.39	1.35
3	L5	3844	PSU	C6-C5	3.32	1.39	1.35
3	L5	4431	PSU	C6-C5	3.32	1.39	1.35
3	L5	4493	PSU	C6-C5	3.31	1.39	1.35
3	L5	4628	PSU	C6-C5	3.31	1.39	1.35
3	L5	4579	PSU	C6-C5	3.30	1.39	1.35
3	L5	4673	PSU	C6-C5	3.30	1.39	1.35
3	L5	3768	PSU	C6-C5	3.30	1.39	1.35
3	L5	4636	PSU	C6-C5	3.29	1.39	1.35
3	L5	3851	PSU	C6-C5	3.29	1.39	1.35
3	L5	3853	PSU	C6-C5	3.28	1.39	1.35
3	L5	4361	PSU	C6-C5	3.26	1.39	1.35
3	L5	3758	PSU	C6-C5	3.26	1.39	1.35
3	L5	4689	PSU	C6-C5	3.26	1.39	1.35
3	L5	4531	PSU	C6-C5	3.26	1.39	1.35
3	L5	4457	PSU	C6-C5	3.25	1.39	1.35
3	L5	4576	PSU	C6-C5	3.22	1.39	1.35
3	L5	3920	PSU	C6-C5	3.20	1.39	1.35
3	L5	4403	PSU	C6-C5	3.19	1.39	1.35
46	Pt	8	4SU	C6-N1	3.10	1.45	1.38
3	L5	4530	UR3	C6-N1	3.08	1.45	1.38
3	L5	3724	A2M	O2'-C2'	3.05	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	398	A2M	O2'-C2'	3.04	1.50	1.42
46	Pt	47	G7M	O6-C6	-3.03	1.17	1.23
3	L5	4227	OMU	O4-C4	-2.99	1.18	1.24
3	L5	1326	A2M	O2'-C2'	2.98	1.50	1.42
3	L5	3723	A2M	O2'-C2'	2.98	1.50	1.42
77	S6	47	G7M	O6-C6	-2.98	1.17	1.23
77	S6	8	4SU	C6-N1	2.98	1.45	1.38
3	L5	3830	A2M	O2'-C2'	2.97	1.50	1.42
3	L5	2363	A2M	O2'-C2'	2.97	1.50	1.42
3	L5	400	A2M	O2'-C2'	2.96	1.50	1.42
3	L5	4571	A2M	O2'-C2'	2.96	1.50	1.42
3	L5	4590	A2M	O2'-C2'	2.96	1.50	1.42
3	L5	3925	OMU	O4-C4	-2.96	1.18	1.24
3	L5	1871	A2M	O2'-C2'	2.94	1.50	1.42
3	L5	2401	A2M	O2'-C2'	2.94	1.50	1.42
3	L5	4523	A2M	C2'-C1'	2.93	1.60	1.53
3	L5	3718	A2M	O2'-C2'	2.93	1.50	1.42
3	L5	4523	A2M	O2'-C2'	2.93	1.50	1.42
3	L5	4306	OMU	O4-C4	-2.92	1.18	1.24
3	L5	3825	A2M	O2'-C2'	2.91	1.50	1.42
3	L5	1534	A2M	O2'-C2'	2.91	1.50	1.42
3	L5	3718	A2M	C2'-C1'	2.90	1.60	1.53
3	L5	1524	A2M	O2'-C2'	2.90	1.50	1.42
3	L5	4498	OMU	O4-C4	-2.89	1.18	1.24
3	L5	398	A2M	C2'-C1'	2.88	1.60	1.53
3	L5	400	A2M	C2'-C1'	2.88	1.60	1.53
3	L5	2815	A2M	O2'-C2'	2.87	1.50	1.42
3	L5	3723	A2M	C2'-C1'	2.86	1.60	1.53
3	L5	3724	A2M	C2'-C1'	2.85	1.60	1.53
3	L5	4220	6MZ	C5-C4	-2.84	1.33	1.39
3	L5	4498	OMU	C6-N1	2.84	1.44	1.38
3	L5	4306	OMU	C6-N1	2.83	1.44	1.38
3	L5	3867	A2M	O2'-C2'	2.82	1.49	1.42
3	L5	4571	A2M	C2'-C1'	2.81	1.60	1.53
3	L5	2401	A2M	C2'-C1'	2.80	1.60	1.53
3	L5	2815	A2M	C2'-C1'	2.80	1.60	1.53
3	L5	4227	OMU	C6-N1	2.79	1.44	1.38
3	L5	3925	OMU	C6-N1	2.77	1.44	1.38
3	L5	4590	A2M	C2'-C1'	2.75	1.60	1.53
3	L5	3825	A2M	C2'-C1'	2.75	1.60	1.53
3	L5	3867	A2M	C2'-C1'	2.75	1.60	1.53
3	L5	3830	A2M	C2'-C1'	2.74	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1524	A2M	C2'-C1'	2.73	1.60	1.53
3	L5	4220	6MZ	C5-N7	-2.72	1.33	1.39
3	L5	1871	A2M	C2'-C1'	2.72	1.60	1.53
3	L5	2815	A2M	C5-C4	-2.71	1.34	1.39
3	L5	3830	A2M	C5-C4	-2.70	1.34	1.39
77	S6	47	G7M	C6-N1	2.70	1.43	1.38
3	L5	1326	A2M	C2'-C1'	2.70	1.60	1.53
3	L5	2363	A2M	C2'-C1'	2.69	1.60	1.53
3	L5	1871	A2M	C5-C4	-2.68	1.34	1.39
3	L5	1524	A2M	C5-C4	-2.68	1.34	1.39
3	L5	1326	A2M	C5-C4	-2.68	1.34	1.39
3	L5	4590	A2M	C5-C4	-2.68	1.34	1.39
3	L5	2401	A2M	C5-C4	-2.67	1.34	1.39
3	L5	2363	A2M	C5-C4	-2.67	1.34	1.39
46	Pt	47	G7M	C6-N1	2.64	1.43	1.38
3	L5	1534	A2M	C5-C4	-2.63	1.34	1.39
3	L5	3825	A2M	C5-C4	-2.62	1.34	1.39
3	L5	4523	A2M	C5-C4	-2.60	1.34	1.39
3	L5	400	A2M	C5-C4	-2.60	1.34	1.39
3	L5	3723	A2M	C5-C4	-2.60	1.34	1.39
3	L5	3867	A2M	C5-C4	-2.56	1.34	1.39
3	L5	3718	A2M	C5-C4	-2.55	1.34	1.39
3	L5	4571	A2M	C5-C4	-2.54	1.34	1.39
3	L5	3724	A2M	C5-C4	-2.54	1.34	1.39
3	L5	398	A2M	C5-C4	-2.54	1.34	1.39
3	L5	1534	A2M	C2'-C1'	2.43	1.59	1.53
3	L5	4498	OMU	C5-C4	2.41	1.49	1.43
3	L5	4306	OMU	C5-C4	2.35	1.48	1.43
3	L5	3925	OMU	O2-C2	-2.34	1.18	1.23
3	L5	4498	OMU	O2-C2	-2.33	1.18	1.23
3	L5	4227	OMU	C5-C4	2.33	1.48	1.43
3	L5	4530	UR3	C5-C4	2.28	1.49	1.43
3	L5	3925	OMU	C5-C4	2.28	1.48	1.43
3	L5	3718	A2M	C5-N7	-2.26	1.34	1.39
3	L5	4227	OMU	O2-C2	-2.26	1.18	1.23
3	L5	4306	OMU	O2-C2	-2.23	1.19	1.23
3	L5	4530	UR3	C4-N3	2.21	1.45	1.40
3	L5	4530	UR3	O2-C2	-2.19	1.18	1.22
3	L5	400	A2M	C5-N7	-2.18	1.34	1.39
3	L5	3867	A2M	C5-N7	-2.17	1.34	1.39
3	L5	1326	A2M	C5-N7	-2.17	1.34	1.39
3	L5	4530	UR3	O4-C4	-2.16	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	4571	A2M	C5-N7	-2.13	1.35	1.39
3	L5	398	A2M	C5-N7	-2.11	1.35	1.39
3	L5	1871	A2M	C5-N7	-2.11	1.35	1.39
3	L5	3830	A2M	C5-N7	-2.11	1.35	1.39
3	L5	1534	A2M	C5-N7	-2.10	1.35	1.39
3	L5	3724	A2M	C5-N7	-2.10	1.35	1.39
3	L5	2363	A2M	C5-N7	-2.09	1.35	1.39
3	L5	3825	A2M	C5-N7	-2.09	1.35	1.39
46	Pt	8	4SU	O2-C2	-2.09	1.19	1.23
3	L5	4523	A2M	C5-N7	-2.07	1.35	1.39
3	L5	2401	A2M	C5-N7	-2.07	1.35	1.39
3	L5	2815	A2M	O3'-C3'	2.06	1.47	1.43
3	L5	4523	A2M	O3'-C3'	2.06	1.47	1.43
3	L5	2401	A2M	O3'-C3'	2.06	1.47	1.43
3	L5	3723	A2M	C5-N7	-2.05	1.35	1.39
77	S6	8	4SU	O2-C2	-2.04	1.19	1.23
3	L5	4220	6MZ	C8-N9	-2.04	1.33	1.37
3	L5	2363	A2M	O3'-C3'	2.01	1.47	1.43
3	L5	1524	A2M	C5-N7	-2.01	1.35	1.39

All (517) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1524	A2M	C1'-N9-C8	-12.74	98.36	127.14
3	L5	1534	A2M	C1'-N9-C8	-11.48	101.21	127.14
3	L5	3867	A2M	C1'-N9-C8	-11.42	101.36	127.14
3	L5	4220	6MZ	C1'-N9-C8	-11.39	101.42	127.14
3	L5	2815	A2M	C1'-N9-C8	-11.31	101.59	127.14
3	L5	2363	A2M	C1'-N9-C8	-11.27	101.68	127.14
3	L5	1326	A2M	C1'-N9-C8	-11.26	101.72	127.14
3	L5	4590	A2M	C1'-N9-C8	-11.06	102.16	127.14
3	L5	3723	A2M	C1'-N9-C8	-11.05	102.18	127.14
3	L5	3724	A2M	C1'-N9-C8	-11.00	102.30	127.14
3	L5	400	A2M	C1'-N9-C8	-10.98	102.34	127.14
3	L5	1524	A2M	C4-N9-C1'	10.97	152.72	126.59
3	L5	2401	A2M	C1'-N9-C8	-10.96	102.38	127.14
3	L5	4571	A2M	C1'-N9-C8	-10.88	102.57	127.14
3	L5	3718	A2M	C1'-N9-C8	-10.87	102.60	127.14
3	L5	4523	A2M	C1'-N9-C8	-10.78	102.80	127.14
3	L5	3830	A2M	C1'-N9-C8	-10.74	102.89	127.14
3	L5	398	A2M	C1'-N9-C8	-10.69	103.00	127.14
3	L5	3825	A2M	C1'-N9-C8	-10.59	103.23	127.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4220	6MZ	C4-N9-C1'	10.44	151.47	126.59
3	L5	1871	A2M	C1'-N9-C8	-10.44	103.57	127.14
3	L5	3867	A2M	C4-N9-C1'	10.23	150.96	126.59
3	L5	1534	A2M	C4-N9-C1'	10.09	150.64	126.59
3	L5	2363	A2M	C4-N9-C1'	10.08	150.61	126.59
3	L5	1326	A2M	C4-N9-C1'	10.04	150.52	126.59
3	L5	3718	A2M	C4-N9-C1'	9.95	150.31	126.59
3	L5	2815	A2M	C4-N9-C1'	9.94	150.27	126.59
3	L5	400	A2M	C4-N9-C1'	9.89	150.16	126.59
3	L5	3724	A2M	C4-N9-C1'	9.85	150.07	126.59
3	L5	4571	A2M	C4-N9-C1'	9.84	150.04	126.59
3	L5	3723	A2M	C4-N9-C1'	9.80	149.95	126.59
3	L5	4590	A2M	C4-N9-C1'	9.74	149.79	126.59
3	L5	3830	A2M	C4-N9-C1'	9.70	149.70	126.59
3	L5	398	A2M	C4-N9-C1'	9.67	149.63	126.59
3	L5	2401	A2M	C4-N9-C1'	9.67	149.63	126.59
3	L5	4523	A2M	C4-N9-C1'	9.64	149.57	126.59
3	L5	3825	A2M	C4-N9-C1'	9.49	149.22	126.59
3	L5	1871	A2M	C4-N9-C1'	9.29	148.72	126.59
46	Pt	8	4SU	C4-N3-C2	-7.73	119.83	127.34
77	S6	8	4SU	C4-N3-C2	-7.25	120.29	127.34
46	Pt	47	G7M	CN7-N7-C5	6.25	134.53	126.77
3	L5	2815	A2M	N6-C6-N1	-6.09	105.01	118.35
3	L5	4590	A2M	N6-C6-N1	-6.05	105.09	118.35
3	L5	2363	A2M	N6-C6-N1	-6.04	105.13	118.35
3	L5	3830	A2M	N6-C6-N1	-6.03	105.15	118.35
3	L5	1534	A2M	N6-C6-N1	-6.02	105.18	118.35
77	S6	47	G7M	CN7-N7-C5	6.00	134.22	126.77
3	L5	2401	A2M	N6-C6-N1	-5.99	105.23	118.35
3	L5	1871	A2M	N6-C6-N1	-5.97	105.27	118.35
3	L5	3825	A2M	N6-C6-N1	-5.91	105.41	118.35
3	L5	3867	A2M	N6-C6-N1	-5.90	105.43	118.35
3	L5	3724	A2M	N6-C6-N1	-5.90	105.43	118.35
3	L5	1524	A2M	N6-C6-N1	-5.89	105.46	118.35
3	L5	398	A2M	N6-C6-N1	-5.87	105.50	118.35
3	L5	3718	A2M	N6-C6-N1	-5.86	105.51	118.35
3	L5	1326	A2M	N6-C6-N1	-5.85	105.53	118.35
3	L5	400	A2M	N6-C6-N1	-5.85	105.54	118.35
3	L5	4571	A2M	N6-C6-N1	-5.83	105.58	118.35
3	L5	3723	A2M	N6-C6-N1	-5.73	105.80	118.35
3	L5	4523	A2M	N6-C6-N1	-5.73	105.80	118.35
3	L5	2815	A2M	N3-C2-N1	-5.59	119.86	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1871	A2M	N3-C2-N1	-5.56	119.90	128.60
46	Pt	8	4SU	C5-C4-N3	5.53	119.82	114.69
3	L5	2401	A2M	N3-C2-N1	-5.52	119.96	128.60
3	L5	3724	A2M	N3-C2-N1	-5.52	119.97	128.60
3	L5	4523	A2M	N3-C2-N1	-5.49	120.01	128.60
3	L5	398	A2M	N3-C2-N1	-5.49	120.01	128.60
3	L5	3723	A2M	N3-C2-N1	-5.46	120.06	128.60
3	L5	4590	A2M	N3-C2-N1	-5.44	120.09	128.60
3	L5	4571	A2M	N3-C2-N1	-5.44	120.09	128.60
3	L5	2363	A2M	N3-C2-N1	-5.43	120.11	128.60
3	L5	400	A2M	N3-C2-N1	-5.41	120.14	128.60
3	L5	3830	A2M	N3-C2-N1	-5.41	120.14	128.60
3	L5	4220	6MZ	C5-C4-N3	-5.40	119.70	126.75
3	L5	1534	A2M	N3-C2-N1	-5.39	120.17	128.60
77	S6	8	4SU	C5-C4-N3	5.38	119.68	114.69
3	L5	1326	A2M	N3-C2-N1	-5.38	120.18	128.60
3	L5	3718	A2M	C5-C4-N3	-5.37	119.75	126.75
3	L5	3867	A2M	C5-C4-N3	-5.32	119.80	126.75
3	L5	4498	OMU	C4-N3-C2	-5.32	119.57	126.58
3	L5	3825	A2M	N3-C2-N1	-5.31	120.30	128.60
3	L5	3830	A2M	C5-C4-N3	-5.30	119.83	126.75
3	L5	2363	A2M	C5-C4-N3	-5.30	119.83	126.75
3	L5	4227	OMU	C4-N3-C2	-5.30	119.59	126.58
3	L5	4220	6MZ	N1-C2-N3	-5.29	120.33	128.60
3	L5	2815	A2M	C5-C6-N6	5.27	134.91	123.43
3	L5	4571	A2M	C5-C4-N3	-5.27	119.88	126.75
3	L5	1524	A2M	N3-C2-N1	-5.26	120.37	128.60
3	L5	1871	A2M	C5-C6-N6	5.24	134.83	123.43
3	L5	4306	OMU	C4-N3-C2	-5.23	119.69	126.58
3	L5	1326	A2M	C5-C4-N3	-5.22	119.93	126.75
3	L5	3830	A2M	C5-C6-N6	5.18	134.71	123.43
3	L5	4590	A2M	C5-C4-N3	-5.18	119.99	126.75
3	L5	1534	A2M	C5-C6-N6	5.18	134.69	123.43
3	L5	4590	A2M	C5-C6-N6	5.17	134.69	123.43
3	L5	398	A2M	C5-C4-N3	-5.17	120.00	126.75
3	L5	400	A2M	C5-C4-N3	-5.17	120.01	126.75
3	L5	2401	A2M	C5-C6-N6	5.16	134.66	123.43
3	L5	3724	A2M	C5-C4-N3	-5.15	120.03	126.75
3	L5	3724	A2M	C5-C6-N6	5.15	134.64	123.43
3	L5	3825	A2M	C5-C6-N6	5.15	134.64	123.43
3	L5	2815	A2M	C5-C4-N3	-5.15	120.03	126.75
3	L5	3867	A2M	C5-C6-N6	5.15	134.63	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3718	A2M	C5-C6-N6	5.15	134.63	123.43
3	L5	400	A2M	C5-C6-N6	5.15	134.63	123.43
3	L5	2363	A2M	C5-C6-N6	5.14	134.62	123.43
3	L5	1524	A2M	C5-C6-N6	5.14	134.60	123.43
3	L5	3867	A2M	N3-C2-N1	-5.12	120.59	128.60
3	L5	4523	A2M	C5-C4-N3	-5.10	120.09	126.75
3	L5	1326	A2M	C5-C6-N6	5.10	134.53	123.43
3	L5	1534	A2M	C5-C4-N3	-5.10	120.10	126.75
3	L5	3718	A2M	N3-C2-N1	-5.09	120.64	128.60
3	L5	398	A2M	C5-C6-N6	5.09	134.50	123.43
3	L5	3925	OMU	C4-N3-C2	-5.07	119.89	126.58
3	L5	4571	A2M	C5-C6-N6	5.06	134.43	123.43
3	L5	3723	A2M	C5-C4-N3	-5.04	120.18	126.75
3	L5	2401	A2M	C5-C4-N3	-5.03	120.19	126.75
3	L5	3825	A2M	C5-C4-N3	-5.03	120.19	126.75
3	L5	3723	A2M	C5-C6-N6	5.01	134.34	123.43
3	L5	4523	A2M	C5-C6-N6	4.96	134.23	123.43
3	L5	1524	A2M	C5-C4-N3	-4.95	120.29	126.75
3	L5	1871	A2M	C5-C4-N3	-4.91	120.35	126.75
3	L5	4531	PSU	C4-N3-C2	-4.82	119.39	126.34
3	L5	4636	PSU	C4-N3-C2	-4.81	119.41	126.34
3	L5	4531	PSU	N1-C2-N3	4.75	120.52	115.13
3	L5	4220	6MZ	C4-C5-C6	4.73	120.48	116.81
46	Pt	47	G7M	CN7-N7-C8	-4.73	117.53	124.84
3	L5	4530	UR3	C4-N3-C2	-4.71	120.13	124.56
3	L5	1524	A2M	N9-C8-N7	-4.69	107.50	113.91
77	S6	47	G7M	CN7-N7-C8	-4.68	117.62	124.84
3	L5	4521	PSU	C4-N3-C2	-4.67	119.61	126.34
3	L5	4628	PSU	N1-C2-N3	4.63	120.38	115.13
3	L5	4457	PSU	C4-N3-C2	-4.63	119.67	126.34
3	L5	4628	PSU	C4-N3-C2	-4.61	119.70	126.34
3	L5	4353	PSU	C4-N3-C2	-4.59	119.73	126.34
3	L5	4403	PSU	C4-N3-C2	-4.58	119.74	126.34
3	L5	4576	PSU	C4-N3-C2	-4.58	119.74	126.34
3	L5	3920	PSU	C4-N3-C2	-4.58	119.74	126.34
3	L5	5001	PSU	C4-N3-C2	-4.58	119.75	126.34
3	L5	4636	PSU	N1-C2-N3	4.55	120.29	115.13
3	L5	4500	PSU	C4-N3-C2	-4.55	119.78	126.34
46	Pt	56	PSU	C4-N3-C2	-4.54	119.79	126.34
77	S6	56	PSU	C4-N3-C2	-4.54	119.79	126.34
3	L5	4431	PSU	C4-N3-C2	-4.53	119.81	126.34
3	L5	4500	PSU	N1-C2-N3	4.52	120.25	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3734	PSU	C4-N3-C2	-4.52	119.83	126.34
3	L5	4299	PSU	C4-N3-C2	-4.52	119.83	126.34
3	L5	4442	PSU	C4-N3-C2	-4.51	119.83	126.34
3	L5	4353	PSU	N1-C2-N3	4.51	120.24	115.13
3	L5	3758	PSU	C4-N3-C2	-4.51	119.84	126.34
3	L5	3768	PSU	C4-N3-C2	-4.51	119.85	126.34
3	L5	3844	PSU	N1-C2-N3	4.50	120.22	115.13
3	L5	4569	PSU	C4-N3-C2	-4.50	119.86	126.34
3	L5	4552	PSU	C4-N3-C2	-4.49	119.86	126.34
3	L5	4673	PSU	N1-C2-N3	4.49	120.22	115.13
3	L5	4521	PSU	N1-C2-N3	4.49	120.22	115.13
3	L5	3851	PSU	C4-N3-C2	-4.48	119.88	126.34
3	L5	3853	PSU	N1-C2-N3	4.48	120.21	115.13
3	L5	4972	PSU	C4-N3-C2	-4.48	119.89	126.34
3	L5	1860	PSU	C4-N3-C2	-4.48	119.89	126.34
3	L5	4972	PSU	N1-C2-N3	4.47	120.19	115.13
3	L5	4457	PSU	N1-C2-N3	4.47	120.19	115.13
46	Pt	56	PSU	N1-C2-N3	4.46	120.19	115.13
3	L5	4299	PSU	N1-C2-N3	4.45	120.17	115.13
3	L5	4423	PSU	C4-N3-C2	-4.45	119.93	126.34
3	L5	2815	A2M	N9-C8-N7	-4.44	107.83	113.91
3	L5	3844	PSU	C4-N3-C2	-4.44	119.94	126.34
3	L5	4361	PSU	C4-N3-C2	-4.44	119.94	126.34
3	L5	1871	A2M	O4'-C1'-N9	4.44	116.81	108.06
3	L5	4423	PSU	N1-C2-N3	4.44	120.16	115.13
3	L5	4442	PSU	N1-C2-N3	4.43	120.15	115.13
3	L5	4493	PSU	N1-C2-N3	4.43	120.15	115.13
3	L5	4579	PSU	C4-N3-C2	-4.43	119.95	126.34
3	L5	4532	PSU	N1-C2-N3	4.43	120.14	115.13
77	S6	47	G7M	C2-N3-C4	4.42	120.18	112.30
3	L5	4673	PSU	C4-N3-C2	-4.42	119.97	126.34
3	L5	4296	PSU	N1-C2-N3	4.42	120.14	115.13
3	L5	4552	PSU	N1-C2-N3	4.41	120.13	115.13
3	L5	5001	PSU	N1-C2-N3	4.41	120.13	115.13
3	L5	3770	PSU	C4-N3-C2	-4.41	119.99	126.34
3	L5	3715	PSU	C4-N3-C2	-4.41	119.99	126.34
3	L5	4689	PSU	C4-N3-C2	-4.40	120.00	126.34
3	L5	4579	PSU	N1-C2-N3	4.40	120.11	115.13
3	L5	3768	PSU	N1-C2-N3	4.40	120.11	115.13
46	Pt	47	G7M	C2-N3-C4	4.40	120.13	112.30
3	L5	3715	PSU	N1-C2-N3	4.39	120.11	115.13
3	L5	4493	PSU	C4-N3-C2	-4.39	120.01	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	5010	PSU	C4-N3-C2	-4.39	120.01	126.34
3	L5	5010	PSU	N1-C2-N3	4.39	120.10	115.13
3	L5	3770	PSU	N1-C2-N3	4.39	120.10	115.13
3	L5	4576	PSU	N1-C2-N3	4.38	120.09	115.13
3	L5	3853	PSU	C4-N3-C2	-4.37	120.04	126.34
3	L5	3734	PSU	N1-C2-N3	4.37	120.08	115.13
3	L5	3920	PSU	N1-C2-N3	4.37	120.08	115.13
3	L5	4431	PSU	N1-C2-N3	4.37	120.08	115.13
3	L5	4590	A2M	N9-C8-N7	-4.37	107.94	113.91
3	L5	4569	PSU	N1-C2-N3	4.36	120.08	115.13
3	L5	4689	PSU	N1-C2-N3	4.36	120.08	115.13
3	L5	4532	PSU	C4-N3-C2	-4.34	120.08	126.34
3	L5	3762	PSU	N1-C2-N3	4.34	120.04	115.13
3	L5	3764	PSU	N1-C2-N3	4.34	120.04	115.13
3	L5	3851	PSU	N1-C2-N3	4.32	120.03	115.13
3	L5	2401	A2M	N9-C8-N7	-4.31	108.01	113.91
3	L5	4296	PSU	C4-N3-C2	-4.31	120.13	126.34
3	L5	3764	PSU	C4-N3-C2	-4.31	120.13	126.34
3	L5	1860	PSU	N1-C2-N3	4.30	120.01	115.13
3	L5	1534	A2M	N9-C8-N7	-4.30	108.04	113.91
3	L5	4403	PSU	N1-C2-N3	4.28	119.98	115.13
3	L5	3758	PSU	N1-C2-N3	4.27	119.96	115.13
3	L5	4361	PSU	N1-C2-N3	4.26	119.96	115.13
3	L5	1781	PSU	N1-C2-N3	4.26	119.96	115.13
3	L5	3729	PSU	N1-C2-N3	4.25	119.94	115.13
3	L5	1781	PSU	C4-N3-C2	-4.25	120.22	126.34
3	L5	4471	PSU	C4-N3-C2	-4.24	120.24	126.34
3	L5	1792	PSU	N1-C2-N3	4.21	119.90	115.13
3	L5	398	A2M	O4'-C1'-N9	4.19	116.31	108.06
3	L5	3729	PSU	C4-N3-C2	-4.18	120.32	126.34
3	L5	4471	PSU	N1-C2-N3	4.18	119.86	115.13
3	L5	1871	A2M	N9-C8-N7	-4.16	108.22	113.91
77	S6	56	PSU	N1-C2-N3	4.15	119.83	115.13
3	L5	3723	A2M	N9-C8-N7	-4.15	108.24	113.91
3	L5	3762	PSU	C4-N3-C2	-4.15	120.36	126.34
46	Pt	47	G7M	C1'-N9-C8	-4.14	112.75	126.74
3	L5	3830	A2M	O4'-C1'-N9	4.11	116.15	108.06
46	Pt	47	G7M	C1'-N9-C4	4.10	138.69	126.50
3	L5	1326	A2M	N9-C8-N7	-4.10	108.31	113.91
77	S6	47	G7M	C5-C4-N3	-4.10	120.29	128.15
3	L5	4420	PSU	N1-C2-N3	4.10	119.77	115.13
3	L5	2363	A2M	N9-C8-N7	-4.07	108.35	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
77	S6	8	4SU	C5-C4-S4	-4.06	119.23	124.47
46	Pt	47	G7M	C5-C4-N3	-4.06	120.36	128.15
3	L5	4590	A2M	O4'-C1'-N9	4.06	116.06	108.06
3	L5	1792	PSU	C4-N3-C2	-4.05	120.50	126.34
3	L5	3718	A2M	O4'-C1'-N9	4.05	116.03	108.06
3	L5	3724	A2M	N9-C8-N7	-4.04	108.39	113.91
3	L5	3825	A2M	N9-C8-N7	-4.02	108.42	113.91
3	L5	2401	A2M	O4'-C1'-N9	4.01	115.96	108.06
3	L5	4498	OMU	N3-C2-N1	4.00	120.20	114.89
3	L5	3825	A2M	O4'-C1'-N9	4.00	115.94	108.06
3	L5	4523	A2M	O4'-C1'-N9	3.99	115.92	108.06
3	L5	3830	A2M	N9-C8-N7	-3.99	108.46	113.91
3	L5	3867	A2M	N9-C8-N7	-3.99	108.46	113.91
3	L5	4523	A2M	N9-C8-N7	-3.98	108.47	113.91
77	S6	47	G7M	C1'-N9-C4	3.98	138.33	126.50
77	S6	47	G7M	C1'-N9-C8	-3.97	113.32	126.74
3	L5	400	A2M	N9-C8-N7	-3.97	108.49	113.91
46	Pt	47	G7M	C5-C6-N1	3.95	120.04	111.79
3	L5	3723	A2M	O4'-C1'-N9	3.94	115.83	108.06
77	S6	47	G7M	C5-C6-N1	3.89	119.92	111.79
3	L5	398	A2M	N9-C8-N7	-3.87	108.62	113.91
3	L5	4571	A2M	N9-C8-N7	-3.84	108.67	113.91
3	L5	4420	PSU	C4-N3-C2	-3.83	120.82	126.34
46	Pt	21	H2U	O2-C2-N1	3.83	127.91	123.11
3	L5	2363	A2M	O4'-C1'-N9	3.80	115.55	108.06
3	L5	3724	A2M	O4'-C1'-N9	3.80	115.54	108.06
3	L5	4227	OMU	N3-C2-N1	3.78	119.91	114.89
3	L5	4306	OMU	N3-C2-N1	3.77	119.90	114.89
3	L5	4571	A2M	O4'-C1'-N9	3.75	115.45	108.06
46	Pt	8	4SU	N3-C2-N1	3.73	119.84	114.89
3	L5	4220	6MZ	N9-C8-N7	-3.71	108.83	113.91
3	L5	3925	OMU	N3-C2-N1	3.71	119.81	114.89
3	L5	400	A2M	O4'-C1'-N9	3.70	115.36	108.06
46	Pt	21	H2U	C5-C4-N3	-3.68	112.51	116.65
3	L5	3718	A2M	N9-C8-N7	-3.66	108.90	113.91
3	L5	2815	A2M	C2-N3-C4	3.66	120.40	111.75
3	L5	3830	A2M	C2-N3-C4	3.64	120.34	111.75
46	Pt	8	4SU	C5-C4-S4	-3.63	119.79	124.47
3	L5	4590	A2M	C2-N3-C4	3.63	120.32	111.75
3	L5	2363	A2M	C2-N3-C4	3.62	120.31	111.75
3	L5	4571	A2M	C2-N3-C4	3.59	120.24	111.75
3	L5	3724	A2M	C2-N3-C4	3.58	120.22	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	2401	A2M	C2-N3-C4	3.58	120.20	111.75
3	L5	398	A2M	C2-N3-C4	3.58	120.20	111.75
46	Pt	47	G7M	O6-C6-C5	-3.57	120.00	128.06
3	L5	4523	A2M	C2-N3-C4	3.57	120.18	111.75
3	L5	1326	A2M	C2-N3-C4	3.55	120.15	111.75
3	L5	1534	A2M	C2-N3-C4	3.54	120.11	111.75
3	L5	2815	A2M	O4'-C1'-N9	3.54	115.03	108.06
3	L5	1871	A2M	C2'-C1'-N9	-3.54	107.58	113.53
3	L5	3867	A2M	O4'-C1'-N9	3.53	115.02	108.06
3	L5	1871	A2M	C2-N3-C4	3.53	120.09	111.75
3	L5	400	A2M	C2-N3-C4	3.53	120.08	111.75
3	L5	3723	A2M	C2-N3-C4	3.50	120.03	111.75
77	S6	8	4SU	N3-C2-N1	3.50	119.53	114.89
3	L5	3867	A2M	C2-N3-C4	3.48	119.98	111.75
3	L5	3825	A2M	C2-N3-C4	3.48	119.97	111.75
77	S6	47	G7M	O6-C6-C5	-3.48	120.22	128.06
3	L5	3718	A2M	C2-N3-C4	3.47	119.94	111.75
3	L5	4220	6MZ	C2-N3-C4	3.46	119.94	111.75
3	L5	1326	A2M	O4'-C1'-N9	3.46	114.89	108.06
3	L5	1524	A2M	C2-N3-C4	3.45	119.89	111.75
3	L5	4227	OMU	C5-C4-N3	3.39	119.91	114.84
3	L5	4306	OMU	C5-C4-N3	3.32	119.81	114.84
3	L5	3925	OMU	C5-C4-N3	3.29	119.76	114.84
3	L5	2351	OMC	C1'-N1-C2	3.28	125.73	118.42
3	L5	4498	OMU	C5-C4-N3	3.28	119.74	114.84
3	L5	2815	A2M	C5-N7-C8	3.20	108.06	103.51
3	L5	1524	A2M	C5-N7-C8	3.14	107.97	103.51
3	L5	1524	A2M	N3-C4-N9	3.12	132.22	127.08
3	L5	4590	A2M	C5-N7-C8	3.09	107.91	103.51
3	L5	2815	A2M	C2'-C1'-N9	-3.09	108.32	113.53
46	Pt	47	G7M	C2-N1-C6	-3.09	119.47	125.10
3	L5	4590	A2M	C4'-O4'-C1'	-3.07	102.70	109.47
3	L5	2401	A2M	C5-N7-C8	3.07	107.86	103.51
77	S6	47	G7M	C2-N1-C6	-3.06	119.52	125.10
3	L5	1534	A2M	C5-N7-C8	3.06	107.85	103.51
3	L5	3867	A2M	N3-C4-N9	3.01	132.05	127.08
77	S6	21	H2U	C5-C4-N3	-3.01	113.27	116.65
3	L5	2363	A2M	C5-N7-C8	3.00	107.78	103.51
3	L5	1326	A2M	C5-N7-C8	2.98	107.75	103.51
3	L5	1871	A2M	C5-N7-C8	2.95	107.71	103.51
3	L5	4220	6MZ	C5-N7-C8	2.95	107.70	103.51
3	L5	3830	A2M	C5-N7-C8	2.95	107.70	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3925	OMU	O4-C4-C5	-2.94	119.99	125.16
3	L5	1524	A2M	C4-N9-C8	2.94	108.92	105.73
3	L5	3723	A2M	C5-N7-C8	2.94	107.68	103.51
3	L5	3724	A2M	C5-N7-C8	2.94	107.68	103.51
46	Pt	47	G7M	N9-C4-N3	2.94	131.84	125.94
3	L5	3867	A2M	C5-N7-C8	2.93	107.67	103.51
3	L5	4220	6MZ	N3-C4-N9	2.93	131.91	127.08
3	L5	1326	A2M	N3-C4-N9	2.92	131.90	127.08
3	L5	2363	A2M	N3-C4-N9	2.92	131.89	127.08
3	L5	400	A2M	C5-N7-C8	2.91	107.65	103.51
3	L5	4227	OMU	O4-C4-C5	-2.91	120.04	125.16
3	L5	1534	A2M	N3-C4-N9	2.90	131.86	127.08
3	L5	3825	A2M	C5-N7-C8	2.89	107.62	103.51
3	L5	4523	A2M	C4'-O4'-C1'	-2.89	103.10	109.47
3	L5	4628	PSU	O2-C2-N1	-2.88	119.62	122.79
3	L5	4571	A2M	N3-C4-N9	2.87	131.80	127.08
3	L5	398	A2M	C5-N7-C8	2.86	107.57	103.51
3	L5	4531	PSU	C6-C5-C4	2.86	120.20	118.20
3	L5	3867	A2M	C4'-O4'-C1'	-2.85	103.19	109.47
3	L5	4571	A2M	C5-N7-C8	2.85	107.55	103.51
3	L5	4523	A2M	C5-N7-C8	2.84	107.55	103.51
77	S6	47	G7M	N9-C4-N3	2.83	131.62	125.94
3	L5	4523	A2M	N3-C4-N9	2.82	131.72	127.08
3	L5	3718	A2M	C5-N7-C8	2.81	107.50	103.51
3	L5	4590	A2M	N3-C4-N9	2.81	131.71	127.08
3	L5	4306	OMU	O4-C4-C5	-2.80	120.23	125.16
3	L5	2815	A2M	N3-C4-N9	2.80	131.70	127.08
3	L5	3830	A2M	N3-C4-N9	2.80	131.69	127.08
3	L5	3718	A2M	N3-C4-N9	2.79	131.69	127.08
3	L5	3770	PSU	O2-C2-N1	-2.79	119.72	122.79
3	L5	400	A2M	N3-C4-N9	2.79	131.68	127.08
3	L5	3724	A2M	N3-C4-N9	2.79	131.68	127.08
3	L5	4689	PSU	O2-C2-N1	-2.78	119.73	122.79
3	L5	3723	A2M	N3-C4-N9	2.78	131.66	127.08
3	L5	4500	PSU	O2-C2-N1	-2.77	119.74	122.79
3	L5	2401	A2M	C2'-C1'-N9	-2.77	108.87	113.53
3	L5	398	A2M	N3-C4-N9	2.77	131.64	127.08
3	L5	2401	A2M	N3-C4-N9	2.75	131.62	127.08
3	L5	4423	PSU	O2-C2-N1	-2.75	119.76	122.79
3	L5	3762	PSU	O2-C2-N1	-2.75	119.77	122.79
3	L5	4673	PSU	O2-C2-N1	-2.73	119.78	122.79
3	L5	4498	OMU	O4-C4-C5	-2.71	120.39	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3808	OMC	C1'-N1-C2	2.70	124.45	118.42
3	L5	4531	PSU	O2-C2-N1	-2.68	119.84	122.79
3	L5	3729	PSU	O2-C2-N1	-2.65	119.87	122.79
46	Pt	56	PSU	O2-C2-N1	-2.65	119.87	122.79
3	L5	4353	PSU	O2-C2-N1	-2.64	119.88	122.79
3	L5	4576	PSU	O2-C2-N1	-2.64	119.89	122.79
46	Pt	21	H2U	O2-C2-N3	-2.63	116.60	121.50
3	L5	3715	PSU	O2-C2-N1	-2.63	119.90	122.79
3	L5	2815	A2M	C4'-O4'-C1'	-2.62	103.70	109.47
3	L5	4442	PSU	O2-C2-N1	-2.61	119.92	122.79
3	L5	5010	PSU	O2-C2-N1	-2.60	119.92	122.79
3	L5	3825	A2M	N3-C4-N9	2.60	131.37	127.08
3	L5	4689	PSU	C6-N1-C2	-2.60	120.03	122.68
3	L5	3764	PSU	O2-C2-N1	-2.59	119.93	122.79
3	L5	3853	PSU	O2-C2-N1	-2.59	119.94	122.79
3	L5	4972	PSU	O2-C2-N1	-2.59	119.94	122.79
3	L5	3762	PSU	C6-N1-C2	-2.59	120.04	122.68
3	L5	3734	PSU	O2-C2-N1	-2.57	119.96	122.79
3	L5	4420	PSU	O2-C2-N1	-2.56	119.97	122.79
3	L5	4299	PSU	O2-C2-N1	-2.55	119.99	122.79
3	L5	4521	PSU	O2-C2-N1	-2.54	119.99	122.79
3	L5	1871	A2M	N3-C4-N9	2.54	131.26	127.08
3	L5	4532	PSU	O2-C2-N1	-2.53	120.00	122.79
3	L5	1326	A2M	C4'-O4'-C1'	-2.53	103.89	109.47
3	L5	2351	OMC	C1'-N1-C6	-2.53	115.32	120.84
3	L5	4590	A2M	C2'-C1'-N9	-2.53	109.27	113.53
3	L5	3768	PSU	O2-C2-N1	-2.52	120.01	122.79
3	L5	3758	PSU	O2-C2-N1	-2.52	120.02	122.79
3	L5	4673	PSU	C6-N1-C2	-2.52	120.11	122.68
3	L5	4296	PSU	O2-C2-N1	-2.51	120.02	122.79
3	L5	3729	PSU	C6-N1-C2	-2.51	120.11	122.68
3	L5	4493	PSU	O2-C2-N1	-2.51	120.03	122.79
3	L5	3844	PSU	O2-C2-N1	-2.50	120.03	122.79
3	L5	4552	PSU	O2-C2-N1	-2.50	120.03	122.79
3	L5	1781	PSU	O2-C2-N1	-2.50	120.04	122.79
3	L5	4579	PSU	O2-C2-N1	-2.49	120.05	122.79
3	L5	4471	PSU	O2-C2-N1	-2.49	120.05	122.79
3	L5	4457	PSU	O2-C2-N1	-2.48	120.06	122.79
3	L5	4420	PSU	C6-N1-C2	-2.48	120.15	122.68
3	L5	3723	A2M	C4'-O4'-C1'	-2.48	104.01	109.47
3	L5	4403	PSU	O2-C2-N1	-2.47	120.07	122.79
3	L5	4431	PSU	O2-C2-N1	-2.45	120.09	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	5001	PSU	O2-C2-N1	-2.45	120.09	122.79
3	L5	1860	PSU	O2-C2-N1	-2.45	120.10	122.79
3	L5	3853	PSU	C6-N1-C2	-2.44	120.19	122.68
3	L5	3851	PSU	O2-C2-N1	-2.44	120.11	122.79
3	L5	1792	PSU	O2-C2-N1	-2.43	120.12	122.79
77	S6	56	PSU	O2-C2-N1	-2.42	120.13	122.79
3	L5	4569	PSU	O2-C2-N1	-2.41	120.14	122.79
3	L5	3724	A2M	C4'-O4'-C1'	-2.41	104.17	109.47
3	L5	3718	A2M	C5-C4-N9	2.39	108.57	105.78
3	L5	2815	A2M	C4-C5-N7	-2.39	107.70	110.62
77	S6	8	4SU	C1'-N1-C2	2.39	121.89	117.57
3	L5	1792	PSU	C6-N1-C2	-2.39	120.24	122.68
3	L5	3920	PSU	O2-C2-N1	-2.38	120.17	122.79
3	L5	4296	PSU	C6-N1-C2	-2.38	120.25	122.68
3	L5	4423	PSU	C6-N1-C2	-2.37	120.26	122.68
3	L5	4442	PSU	O4'-C1'-C2'	2.36	108.47	105.14
3	L5	4628	PSU	C6-N1-C2	-2.36	120.27	122.68
3	L5	1534	A2M	O4'-C1'-C2'	-2.35	102.44	106.57
3	L5	3723	A2M	C2'-C1'-N9	-2.35	109.58	113.53
3	L5	3768	PSU	C6-N1-C2	-2.34	120.29	122.68
3	L5	4636	PSU	O2-C2-N1	-2.34	120.22	122.79
3	L5	4500	PSU	C6-N1-C2	-2.34	120.30	122.68
3	L5	4361	PSU	O2-C2-N1	-2.33	120.23	122.79
3	L5	4493	PSU	C6-N1-C2	-2.33	120.30	122.68
3	L5	5010	PSU	C6-N1-C2	-2.33	120.30	122.68
3	L5	4532	PSU	C6-N1-C2	-2.32	120.31	122.68
3	L5	3764	PSU	C6-N1-C2	-2.32	120.31	122.68
3	L5	3830	A2M	C5-C4-N9	2.32	108.48	105.78
3	L5	4590	A2M	C4-C5-N7	-2.31	107.80	110.62
3	L5	3925	OMU	C1'-N1-C2	2.31	121.75	117.57
3	L5	4579	PSU	C6-N1-C2	-2.30	120.33	122.68
3	L5	3825	A2M	C5-C4-N9	2.28	108.44	105.78
3	L5	2363	A2M	C4'-O4'-C1'	-2.28	104.44	109.47
3	L5	3770	PSU	C6-N1-C2	-2.27	120.36	122.68
3	L5	2401	A2M	C4'-O4'-C1'	-2.26	104.48	109.47
3	L5	4353	PSU	C6-N1-C2	-2.26	120.38	122.68
3	L5	4220	6MZ	C5-C4-N9	2.24	108.39	105.78
3	L5	1524	A2M	C2'-C1'-N9	-2.24	109.76	113.53
3	L5	2363	A2M	C4-C5-N7	-2.24	107.89	110.62
46	Pt	21	H2U	C4-N3-C2	2.24	127.65	125.79
3	L5	1871	A2M	C5-C4-N9	2.24	108.39	105.78
3	L5	4456	OMC	C1'-N1-C2	2.24	123.41	118.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3718	A2M	C6-C5-C4	2.23	120.19	117.18
3	L5	3715	PSU	C6-N1-C2	-2.23	120.40	122.68
3	L5	4442	PSU	C6-N1-C2	-2.23	120.41	122.68
3	L5	2422	OMC	C1'-N1-C2	2.23	123.39	118.42
3	L5	4299	PSU	C6-N1-C2	-2.22	120.41	122.68
3	L5	2815	A2M	C4-N9-C8	2.22	108.14	105.73
3	L5	4306	OMU	O2-C2-N1	-2.21	119.84	122.79
3	L5	398	A2M	C5-C4-N9	2.21	108.36	105.78
3	L5	1524	A2M	C4'-O4'-C1'	-2.21	104.59	109.47
3	L5	4636	PSU	C6-C5-C4	2.21	119.74	118.20
3	L5	3844	PSU	C6-N1-C2	-2.20	120.43	122.68
3	L5	3718	A2M	C4-C5-N7	-2.20	107.94	110.62
3	L5	2401	A2M	C4-C5-N7	-2.20	107.94	110.62
3	L5	1534	A2M	C4-N9-C8	2.19	108.11	105.73
3	L5	3830	A2M	C4-C5-N7	-2.19	107.95	110.62
3	L5	4403	PSU	O4'-C1'-C2'	2.18	108.22	105.14
3	L5	4571	A2M	C5-C4-N9	2.18	108.32	105.78
3	L5	1534	A2M	C4-C5-N7	-2.18	107.97	110.62
3	L5	3825	A2M	C4-C5-N7	-2.18	107.97	110.62
3	L5	400	A2M	C5-C4-N9	2.17	108.31	105.78
3	L5	400	A2M	C4'-O4'-C1'	-2.17	104.69	109.47
3	L5	4590	A2M	C5-C4-N9	2.17	108.30	105.78
3	L5	1871	A2M	C4-C5-N7	-2.16	107.98	110.62
3	L5	4220	6MZ	C4-C5-N7	-2.16	107.98	110.62
3	L5	3724	A2M	C5-C4-N9	2.16	108.30	105.78
3	L5	4457	PSU	C6-N1-C2	-2.16	120.47	122.68
3	L5	5001	PSU	C6-N1-C2	-2.16	120.48	122.68
3	L5	4531	PSU	C6-N1-C2	-2.15	120.48	122.68
3	L5	4569	PSU	C6-N1-C2	-2.15	120.48	122.68
15	La	39	V5N	O-C-CA	-2.15	119.14	124.78
3	L5	3724	A2M	C4-C5-N7	-2.15	108.00	110.62
3	L5	2363	A2M	C5-C4-N9	2.15	108.28	105.78
3	L5	1322	1MA	N1-C6-N6	2.14	125.22	119.77
3	L5	4590	A2M	C4-N9-C8	2.14	108.05	105.73
3	L5	4552	PSU	C6-N1-C2	-2.14	120.49	122.68
3	L5	4471	PSU	C6-N1-C2	-2.14	120.50	122.68
3	L5	2815	A2M	C5-C4-N9	2.14	108.27	105.78
46	Pt	56	PSU	C6-N1-C2	-2.14	120.50	122.68
3	L5	3867	A2M	C6-C5-C4	2.13	120.05	117.18
3	L5	1326	A2M	C4-C5-N7	-2.13	108.03	110.62
3	L5	4972	PSU	C6-N1-C2	-2.12	120.51	122.68
3	L5	1781	PSU	C6-N1-C2	-2.11	120.52	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	400	A2M	C4-C5-N7	-2.11	108.04	110.62
3	L5	3718	A2M	C2'-C1'-N9	-2.11	109.97	113.53
3	L5	4530	UR3	C6-N1-C2	-2.11	119.90	121.79
3	L5	3723	A2M	C4-C5-N7	-2.11	108.05	110.62
3	L5	3867	A2M	C4-C5-N7	-2.11	108.05	110.62
3	L5	4431	PSU	C6-N1-C2	-2.10	120.53	122.68
3	L5	4521	PSU	C6-N1-C2	-2.10	120.54	122.68
3	L5	4361	PSU	C6-N1-C2	-2.09	120.54	122.68
3	L5	2401	A2M	C4-N9-C8	2.09	107.99	105.73
3	L5	4576	PSU	C6-N1-C2	-2.09	120.55	122.68
3	L5	4571	A2M	C4-C5-N7	-2.08	108.08	110.62
3	L5	1860	PSU	C6-N1-C2	-2.08	120.56	122.68
3	L5	398	A2M	C4-C5-N7	-2.08	108.09	110.62
3	L5	3808	OMC	C1'-N1-C6	-2.07	116.32	120.84
3	L5	4498	OMU	O2-C2-N1	-2.07	120.03	122.79
3	L5	2401	A2M	C5-C4-N9	2.07	108.19	105.78
3	L5	3758	PSU	C6-N1-C2	-2.07	120.57	122.68
3	L5	4636	PSU	O4'-C1'-C2'	2.07	108.06	105.14
3	L5	4523	A2M	C5-C4-N9	2.06	108.18	105.78
3	L5	3825	A2M	C4'-O4'-C1'	-2.06	104.93	109.47
3	L5	1534	A2M	O4'-C1'-N9	2.06	112.12	108.06
3	L5	3851	PSU	C6-N1-C2	-2.06	120.58	122.68
3	L5	3734	PSU	C6-N1-C2	-2.06	120.58	122.68
3	L5	1326	A2M	C5-C4-N9	2.05	108.17	105.78
3	L5	1524	A2M	C4-C5-N7	-2.05	108.12	110.62
3	L5	3723	A2M	C5-C4-N9	2.04	108.16	105.78
3	L5	3867	A2M	C5-C4-N9	2.04	108.15	105.78
3	L5	3920	PSU	C6-N1-C2	-2.03	120.60	122.68
3	L5	1326	A2M	C6-C5-C4	2.03	119.92	117.18
3	L5	4220	6MZ	C9-N6-C6	2.02	124.61	122.87
3	L5	3841	OMC	C1'-N1-C2	2.02	122.92	118.42
3	L5	4457	PSU	O4'-C1'-C2'	2.02	107.99	105.14
3	L5	1871	A2M	C4'-O4'-C1'	-2.02	105.03	109.47
3	L5	400	A2M	C6-C5-C4	2.01	119.89	117.18
3	L5	4523	A2M	C4-C5-N7	-2.01	108.17	110.62
3	L5	4571	A2M	C6-C5-C4	2.00	119.87	117.18

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	LA	216	V5N	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
4	LA	216	V5N	C-CA-CB-CG
44	Lo	53	MLZ	N-CA-CB-CG
44	Lo	53	MLZ	C-CA-CB-CG
3	L5	398	A2M	C1'-C2'-O2'-CM'
3	L5	400	A2M	C1'-C2'-O2'-CM'
3	L5	1326	A2M	C1'-C2'-O2'-CM'
3	L5	2422	OMC	C1'-C2'-O2'-CM2
3	L5	3701	OMC	C2'-C1'-N1-C2
3	L5	3701	OMC	C2'-C1'-N1-C6
3	L5	3723	A2M	C1'-C2'-O2'-CM'
3	L5	3724	A2M	C1'-C2'-O2'-CM'
3	L5	3825	A2M	C1'-C2'-O2'-CM'
3	L5	3867	A2M	C1'-C2'-O2'-CM'
3	L5	3899	OMG	C1'-C2'-O2'-CM2
3	L5	4220	6MZ	C5-C6-N6-C9
3	L5	4220	6MZ	N1-C6-N6-C9
3	L5	4227	OMU	C1'-C2'-O2'-CM2
3	L5	4306	OMU	C1'-C2'-O2'-CM2
3	L5	4420	PSU	C2'-C1'-C5-C4
3	L5	4420	PSU	C2'-C1'-C5-C6
3	L5	4420	PSU	C3'-C4'-C5'-O5'
3	L5	4523	A2M	C1'-C2'-O2'-CM'
3	L5	4569	PSU	C3'-C4'-C5'-O5'
3	L5	4569	PSU	O4'-C4'-C5'-O5'
3	L5	4571	A2M	C1'-C2'-O2'-CM'
3	L5	4636	PSU	C2'-C1'-C5-C6
3	L5	4636	PSU	O4'-C1'-C5-C6
3	L5	4637	OMG	C1'-C2'-O2'-CM2
77	S6	47	G7M	O4'-C4'-C5'-O5'
77	S6	47	G7M	C3'-C4'-C5'-O5'
3	L5	4590	A2M	C4'-C5'-O5'-P
3	L5	398	A2M	O4'-C4'-C5'-O5'
3	L5	2364	OMG	O4'-C4'-C5'-O5'
3	L5	2364	OMG	C3'-C4'-C5'-O5'
3	L5	3729	PSU	O4'-C4'-C5'-O5'
3	L5	4420	PSU	O4'-C4'-C5'-O5'
3	L5	4637	OMG	O4'-C4'-C5'-O5'
3	L5	3844	PSU	O4'-C4'-C5'-O5'
44	Lo	53	MLZ	CA-CB-CG-CD
46	Pt	21	H2U	C2'-C1'-N1-C2
3	L5	3729	PSU	C3'-C4'-C5'-O5'
3	L5	3925	OMU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	L5	4637	OMG	C3'-C4'-C5'-O5'
46	Pt	21	H2U	C2'-C1'-N1-C6
46	Pt	21	H2U	C4'-C5'-O5'-P
3	L5	3925	OMU	O4'-C4'-C5'-O5'
44	Lo	53	MLZ	CG-CD-CE-NZ
3	L5	4447	5MC	C2'-C1'-N1-C6
3	L5	2876	OMG	C1'-C2'-O2'-CM2
3	L5	3718	A2M	C1'-C2'-O2'-CM'
77	S6	47	G7M	C4'-C5'-O5'-P
3	L5	2876	OMG	C3'-C2'-O2'-CM2
3	L5	4500	PSU	C4'-C5'-O5'-P
42	Lm	98	M3L	N-CA-CB-CG
3	L5	3841	OMC	O4'-C4'-C5'-O5'
3	L5	3844	PSU	C3'-C4'-C5'-O5'
3	L5	3701	OMC	O4'-C1'-N1-C6
3	L5	4447	5MC	O4'-C1'-N1-C6
3	L5	2363	A2M	O4'-C4'-C5'-O5'
3	L5	4523	A2M	O4'-C4'-C5'-O5'
77	S6	8	4SU	C3'-C4'-C5'-O5'
3	L5	2815	A2M	C4'-C5'-O5'-P
3	L5	4420	PSU	C4'-C5'-O5'-P
3	L5	4370	OMG	C3'-C2'-O2'-CM2
4	LA	216	V5N	C-CA-CB-O2
3	L5	3701	OMC	O4'-C1'-N1-C2
3	L5	1326	A2M	C4'-C5'-O5'-P
3	L5	3844	PSU	C4'-C5'-O5'-P
3	L5	398	A2M	C3'-C4'-C5'-O5'
3	L5	1534	A2M	C4'-C5'-O5'-P
3	L5	1524	A2M	C3'-C4'-C5'-O5'
3	L5	4447	5MC	O4'-C1'-N1-C2
3	L5	4500	PSU	O4'-C1'-C5-C4
3	L5	2351	OMC	O4'-C4'-C5'-O5'
3	L5	4447	5MC	C2'-C1'-N1-C2
3	L5	3782	5MC	O4'-C4'-C5'-O5'
3	L5	3867	A2M	C3'-C4'-C5'-O5'
3	L5	3867	A2M	C4'-C5'-O5'-P
3	L5	4296	PSU	C3'-C4'-C5'-O5'
77	S6	8	4SU	O4'-C4'-C5'-O5'
3	L5	2351	OMC	C2'-C1'-N1-C2
3	L5	4500	PSU	O4'-C1'-C5-C6
3	L5	1534	A2M	O4'-C4'-C5'-O5'
3	L5	4636	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
77	S6	21	H2U	C3'-C4'-C5'-O5'
44	Lo	53	MLZ	CD-CE-NZ-CM
3	L5	3841	OMC	C3'-C4'-C5'-O5'
77	S6	8	4SU	C4'-C5'-O5'-P

There are no ring outliers.

28 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	1326	A2M	2	0
3	L5	4579	PSU	2	0
3	L5	4689	PSU	1	0
3	L5	4442	PSU	1	0
3	L5	2422	OMC	1	0
3	L5	3723	A2M	3	0
3	L5	4431	PSU	1	0
3	L5	3718	A2M	3	0
3	L5	4220	6MZ	1	0
46	Pt	47	G7M	1	0
3	L5	4227	OMU	2	0
3	L5	4523	A2M	2	0
77	S6	21	H2U	1	0
3	L5	3899	OMG	1	0
3	L5	3925	OMU	1	0
3	L5	1340	OMC	1	0
3	L5	3944	OMG	1	0
3	L5	1871	A2M	1	0
3	L5	4420	PSU	1	0
77	S6	8	4SU	2	0
3	L5	398	A2M	1	0
3	L5	4637	OMG	1	0
77	S6	47	G7M	2	0
3	L5	4618	OMG	2	0
3	L5	2351	OMC	1	0
3	L5	2804	OMC	1	0
3	L5	3724	A2M	1	0
46	Pt	21	H2U	3	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 106 ligands modelled in this entry, 103 are monoatomic - leaving 3 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
85	C	Lo	202	-	18,21,22	0.45	0	26,30,33	1.32	3 (11%)
88	HYG	S2	1901	-	35,39,39	3.11	11 (31%)	43,60,60	1.88	9 (20%)
85	C	L5	5102	-	18,21,22	0.43	0	26,30,33	0.51	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
85	C	Lo	202	-	-	4/7/25/26	0/2/2/2
88	HYG	S2	1901	-	-	5/12/87/87	0/4/4/4
85	C	L5	5102	-	-	1/7/25/26	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	S2	1901	HYG	O29-C12	11.06	1.61	1.43
88	S2	1901	HYG	O14-C13	6.54	1.58	1.41
88	S2	1901	HYG	O22-C17	6.54	1.53	1.43
88	S2	1901	HYG	O28-C23	5.92	1.47	1.40
88	S2	1901	HYG	C16-C15	4.52	1.62	1.53
88	S2	1901	HYG	C17-C12	-4.24	1.44	1.53
88	S2	1901	HYG	O28-C27	2.97	1.48	1.44
88	S2	1901	HYG	C25-C24	-2.97	1.48	1.53
88	S2	1901	HYG	O18-C13	-2.59	1.34	1.41
88	S2	1901	HYG	O30-C24	2.43	1.47	1.42
88	S2	1901	HYG	O31-C25	2.13	1.48	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	S2	1901	HYG	O29-C12-C13	5.41	125.05	110.86
88	S2	1901	HYG	O22-C17-C16	4.92	123.19	111.22
88	S2	1901	HYG	O28-C27-C26	4.32	114.66	108.52
85	Lo	202	C	C1'-N1-C2	4.13	127.65	118.42
88	S2	1901	HYG	O14-C15-C16	3.50	116.04	109.69
85	Lo	202	C	C1'-N1-C6	-3.02	114.26	120.84
88	S2	1901	HYG	C23-O28-C27	2.90	117.52	112.00
88	S2	1901	HYG	O22-C17-C12	2.87	108.17	103.58
85	Lo	202	C	O2-C2-N3	-2.66	118.01	122.33
88	S2	1901	HYG	C13-O18-C6	-2.60	111.52	117.96
88	S2	1901	HYG	O29-C12-C17	2.46	107.51	103.58
88	S2	1901	HYG	C19-C15-C16	-2.32	107.58	113.00

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	S2	1901	HYG	O28-C27-C33-C34
88	S2	1901	HYG	C27-C33-C34-O35
88	S2	1901	HYG	N36-C33-C34-O35
88	S2	1901	HYG	O14-C13-O18-C6
85	Lo	202	C	O4'-C1'-N1-C6
85	L5	5102	C	O4'-C4'-C5'-O5'
88	S2	1901	HYG	C26-C27-C33-C34
85	Lo	202	C	C4'-C5'-O5'-P
85	Lo	202	C	C2'-C1'-N1-C2
85	Lo	202	C	O4'-C1'-N1-C2

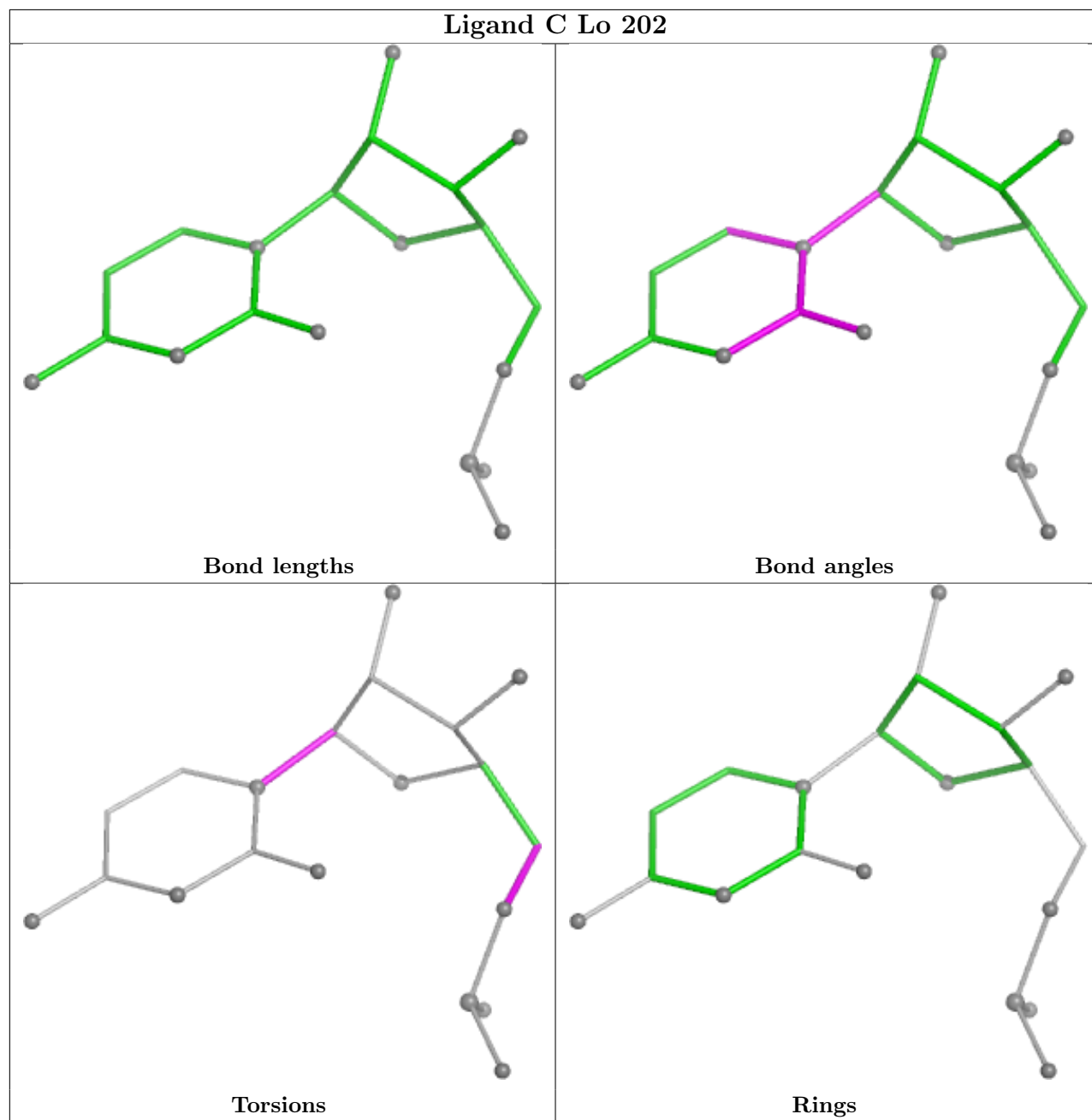
There are no ring outliers.

1 monomer is involved in 1 short contact:

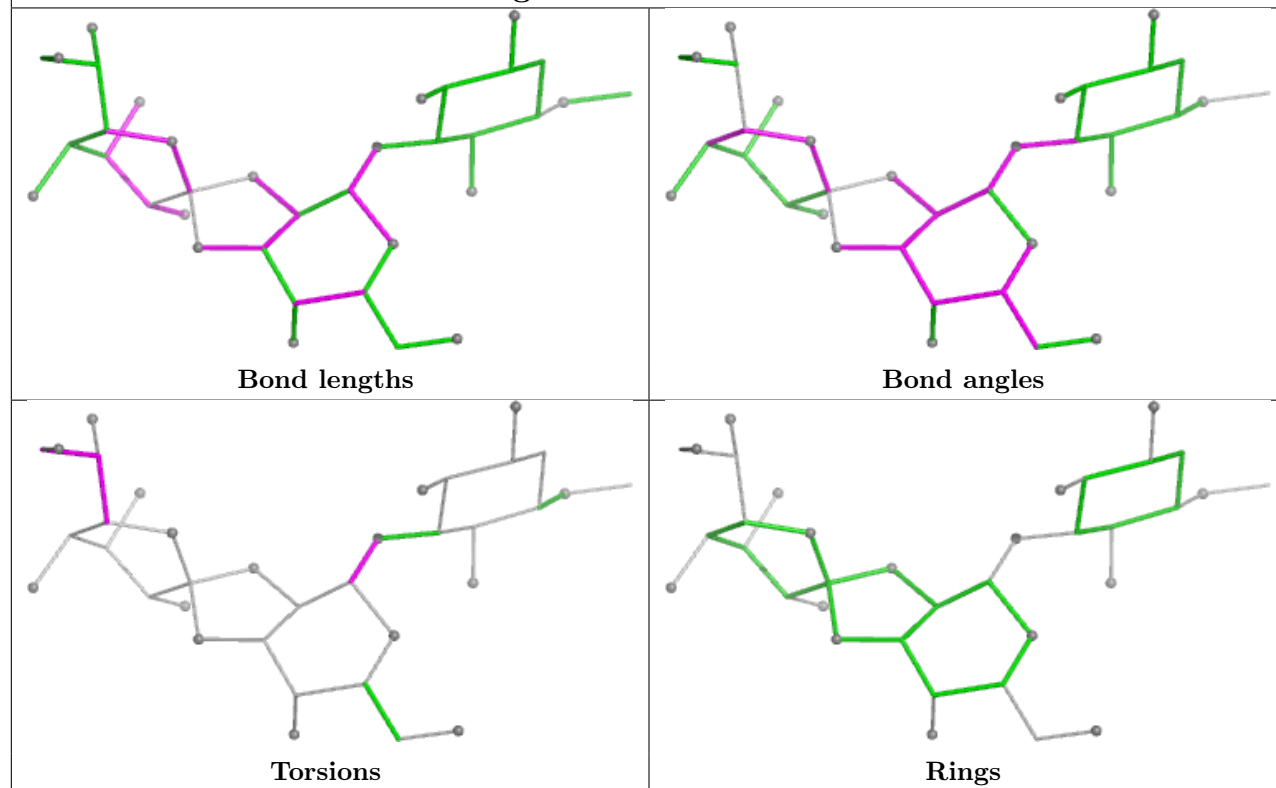
Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	Lo	202	C	1	0

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

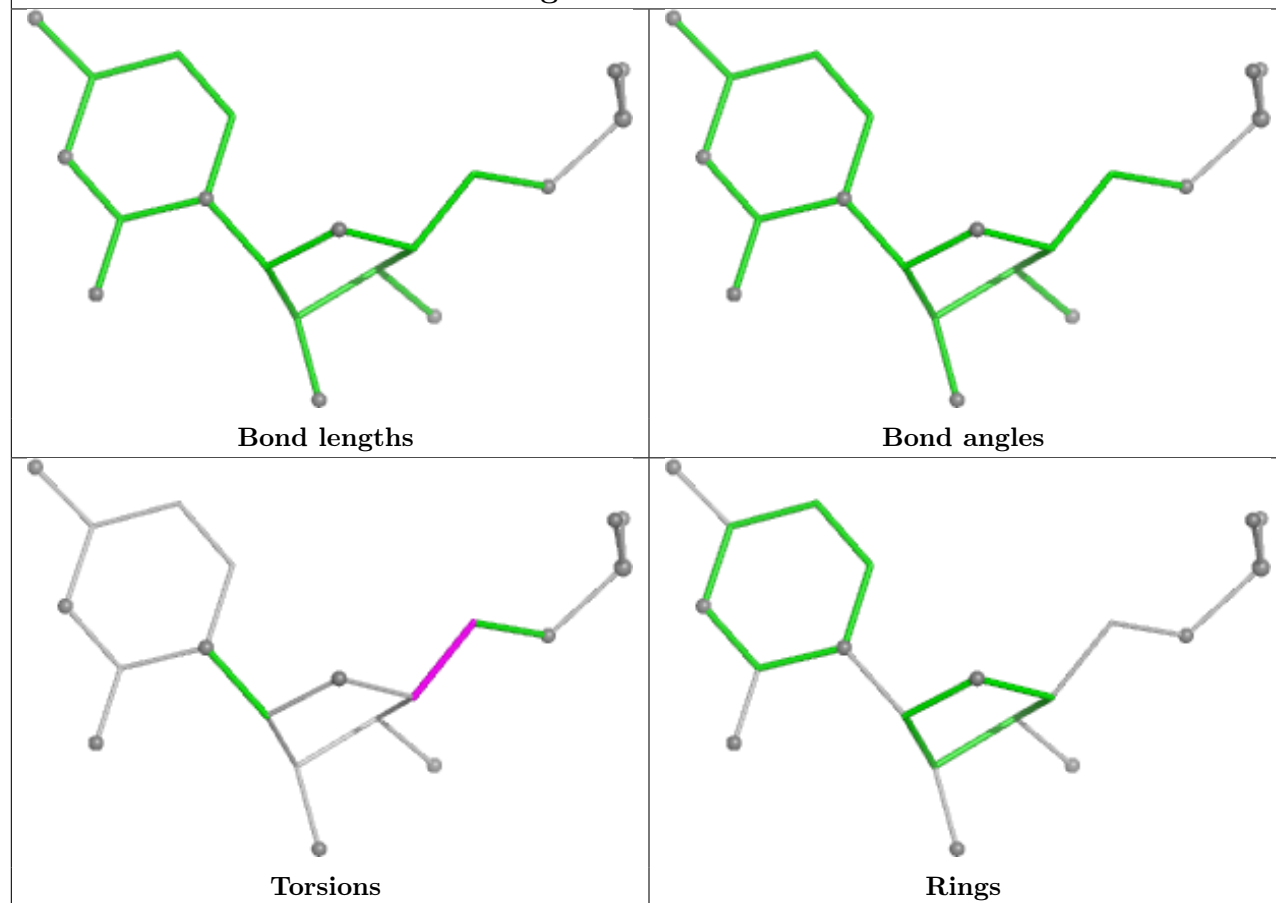
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand HYG S2 1901



Ligand C L5 5102



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
77	S6	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S6	47:G7M	O3'	49:C	P	4.81

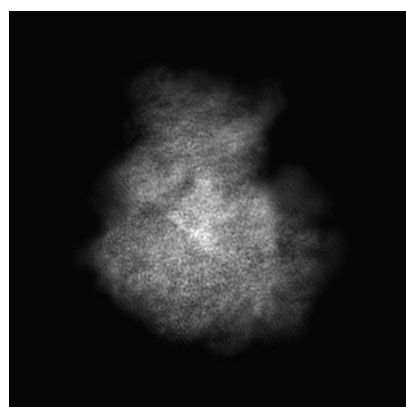
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54265. These allow visual inspection of the internal detail of the map and identification of artifacts.

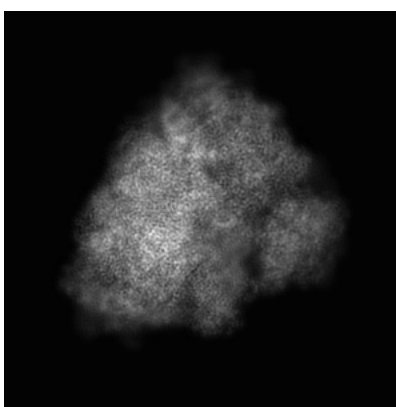
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

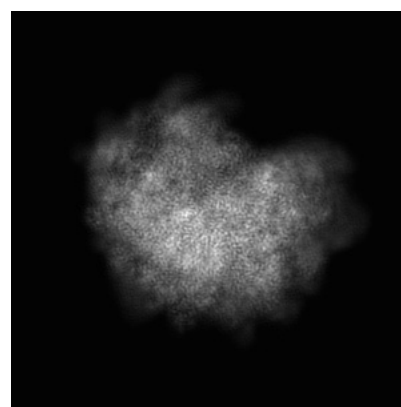
6.1.1 Primary map



X



Y

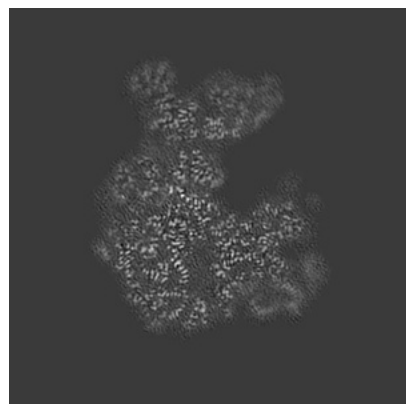


Z

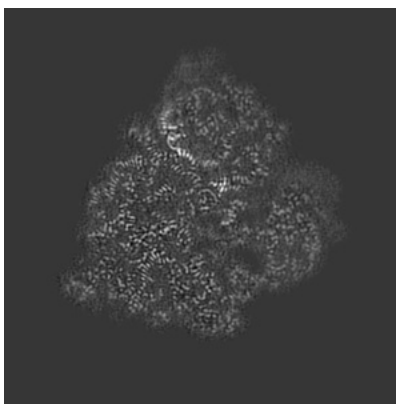
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

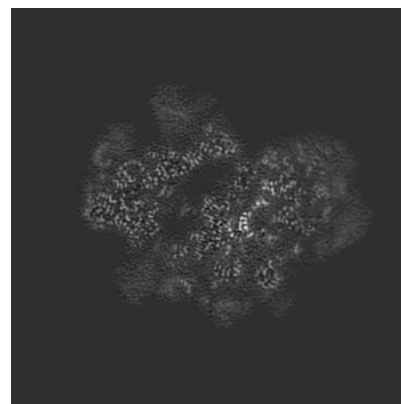
6.2.1 Primary map



X Index: 240



Y Index: 240

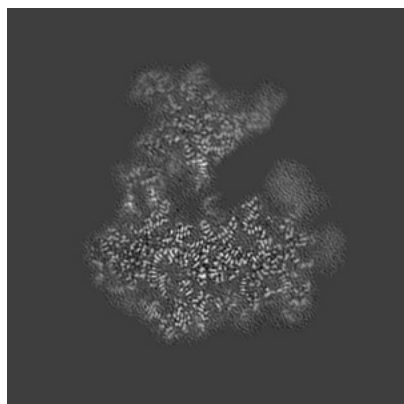


Z Index: 240

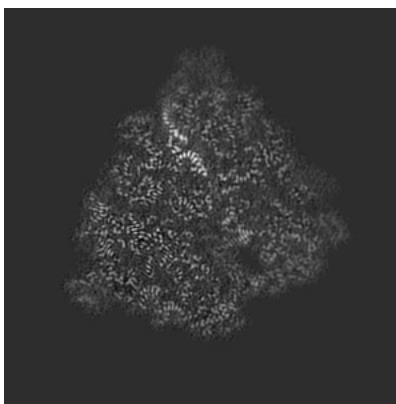
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

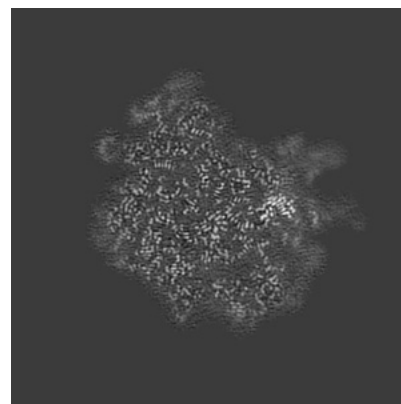
6.3.1 Primary map



X Index: 210



Y Index: 233

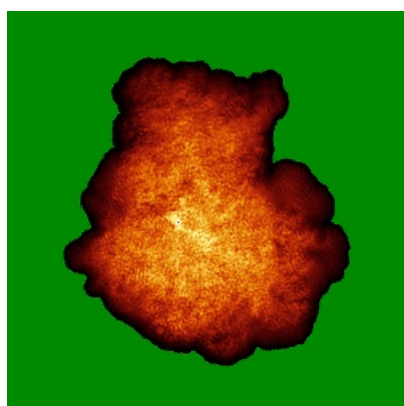


Z Index: 205

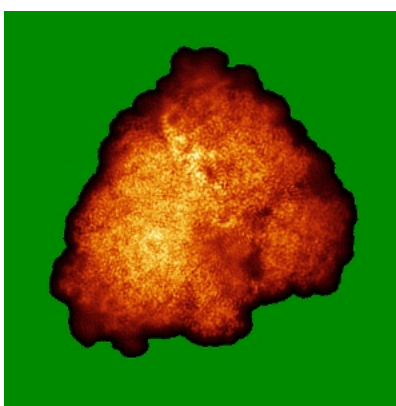
The images above show the largest variance slices of the map in three orthogonal directions.

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

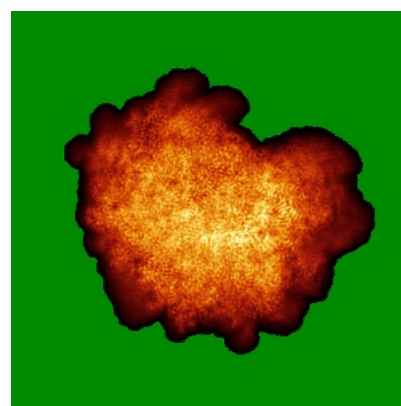
6.4.1 Primary map



X



Y

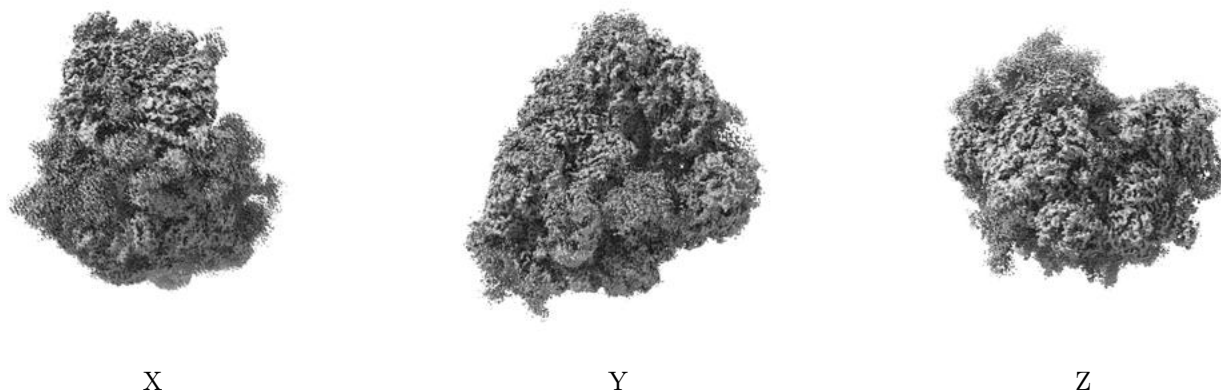


Z

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 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

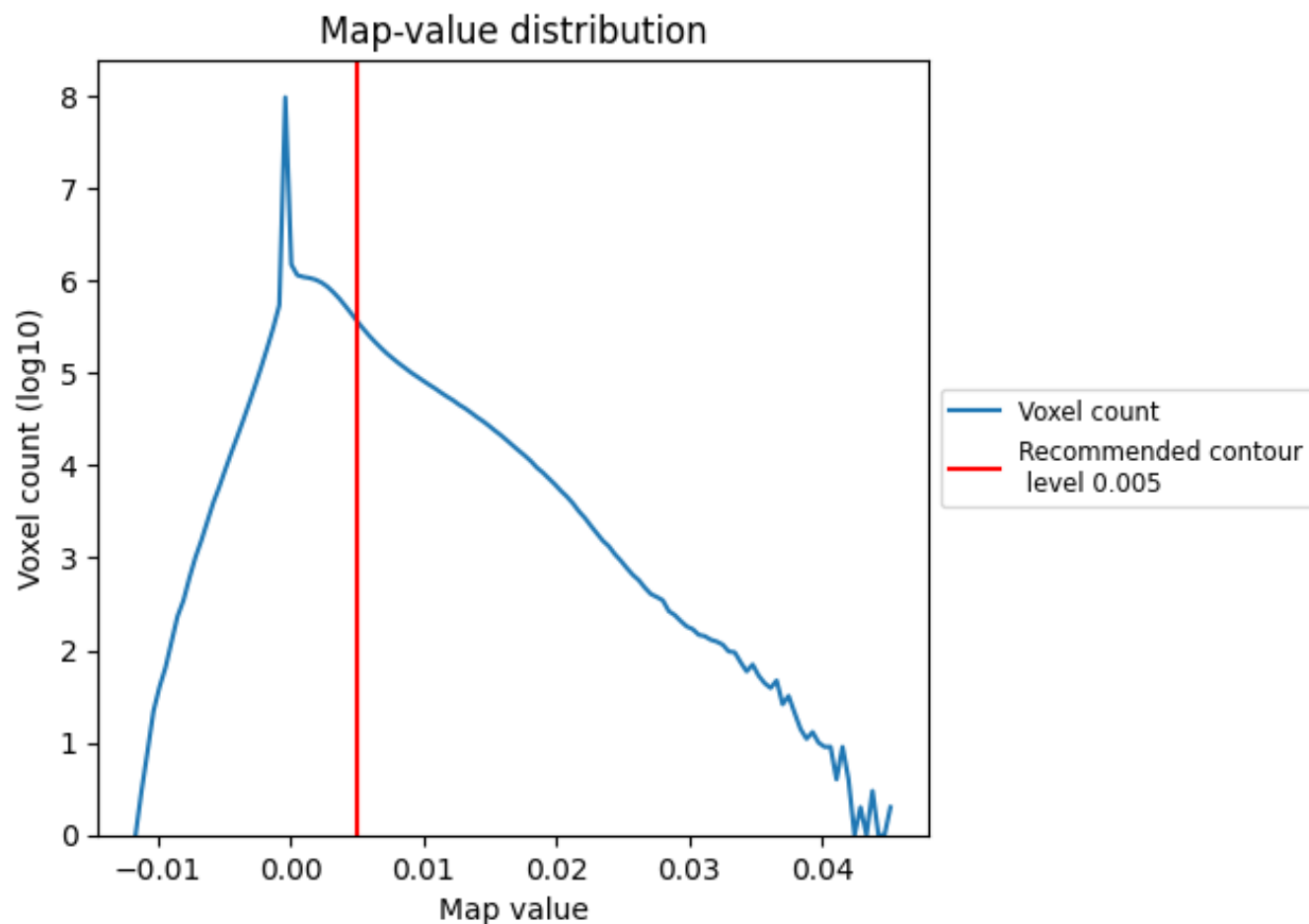
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

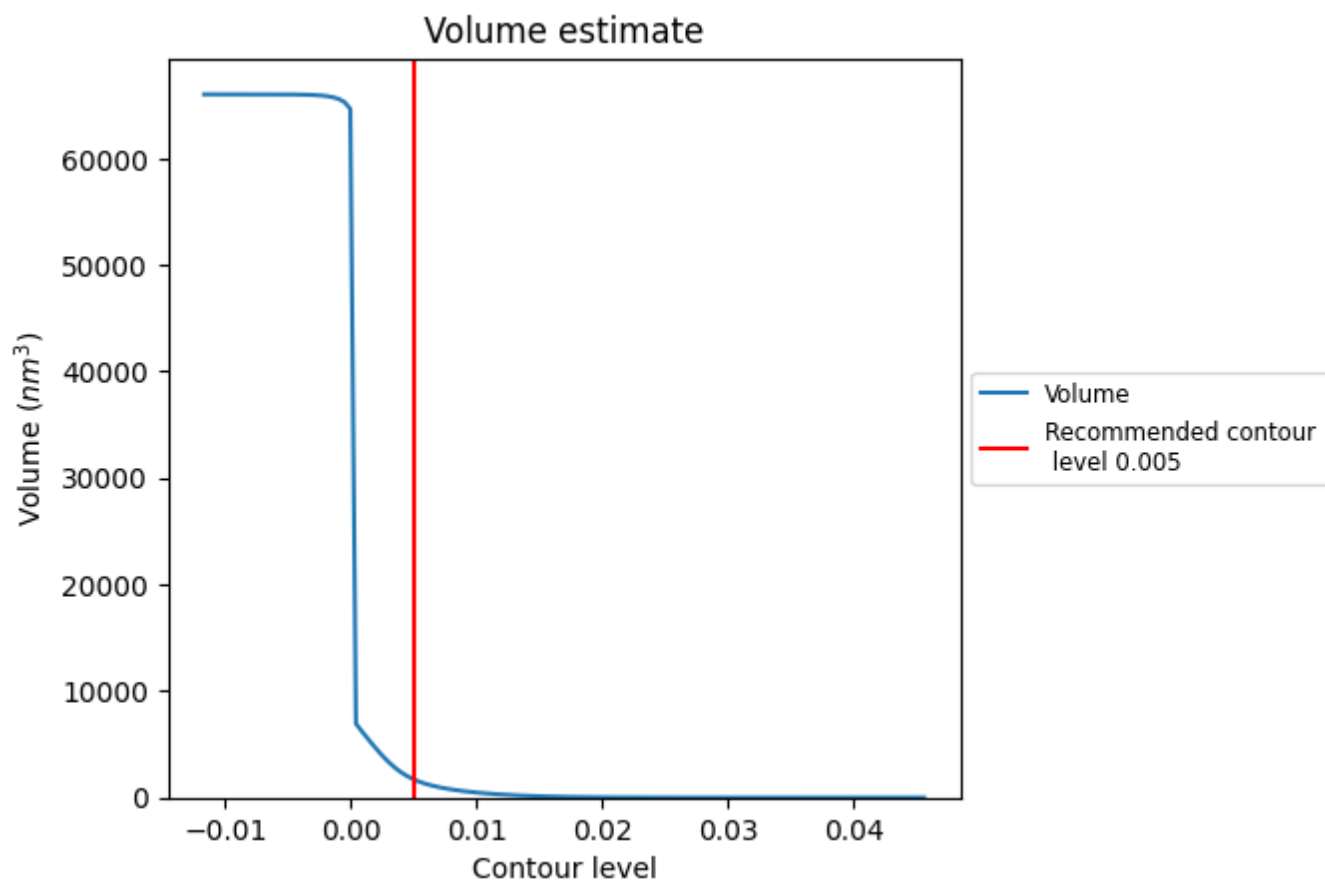
This section contains the results of statistical analysis of the map.

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.

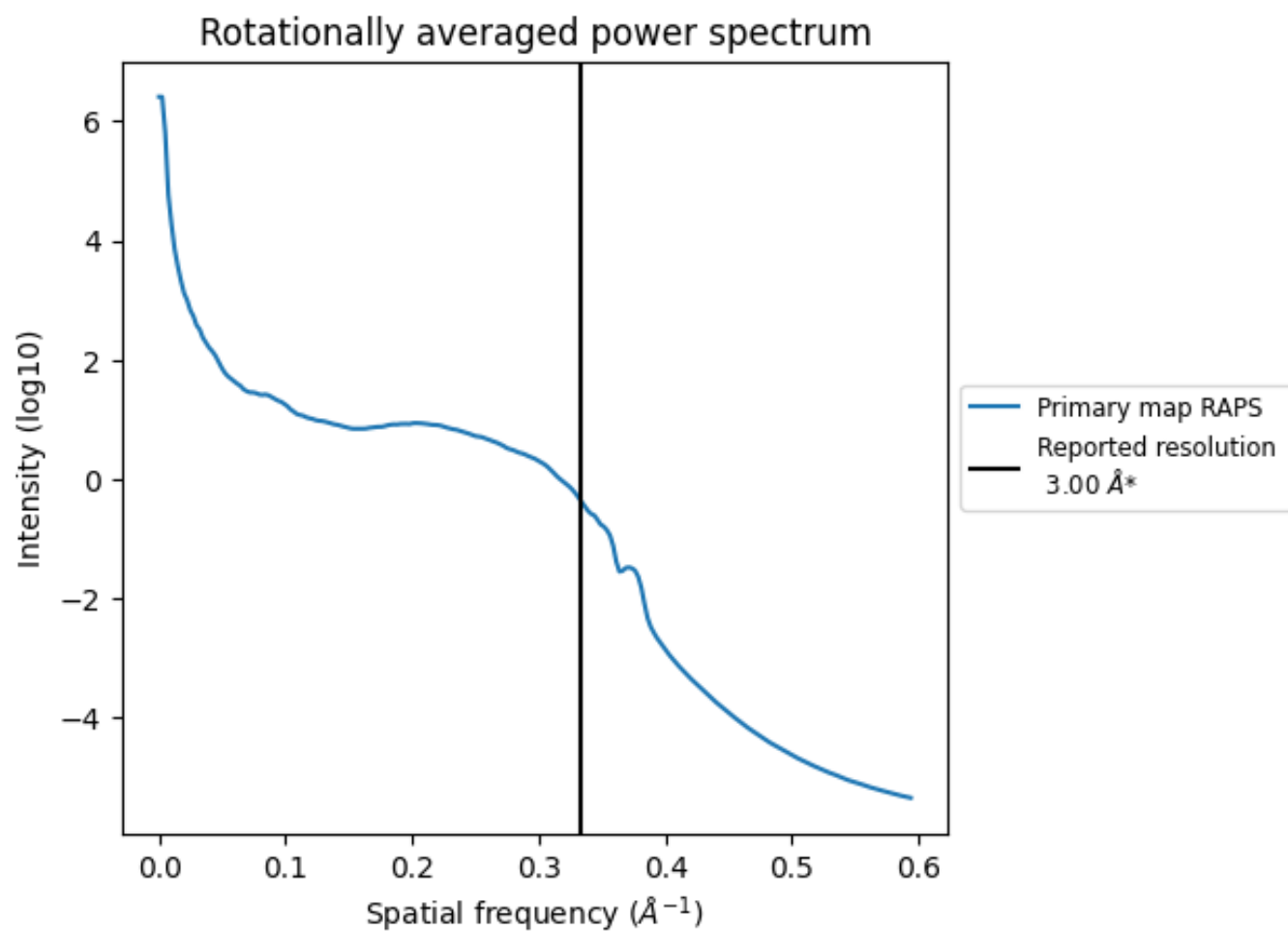
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1714 nm^3 ; this corresponds to an approximate mass of 1549 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 0.333 Å⁻¹

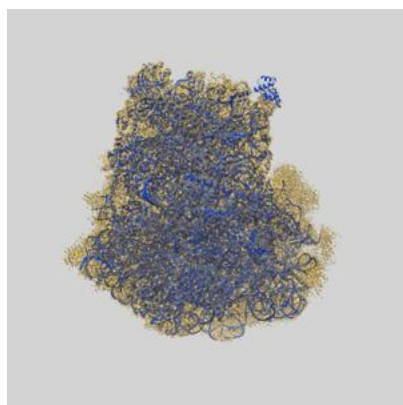
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

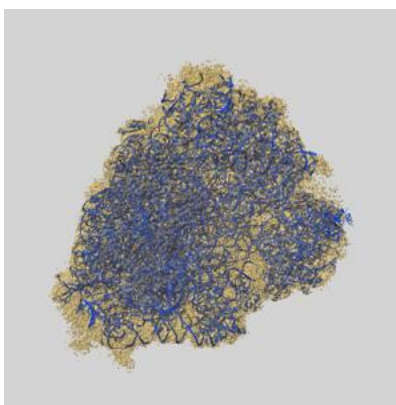
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54265 and PDB model 9RU7. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

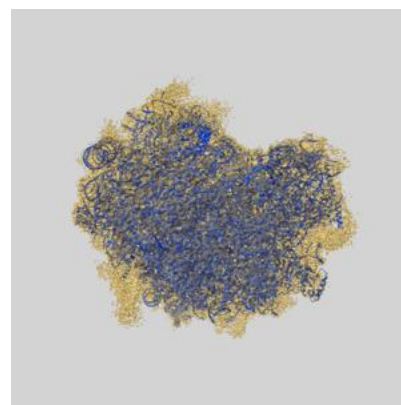
9.1 Map-model overlay [i](#)



X



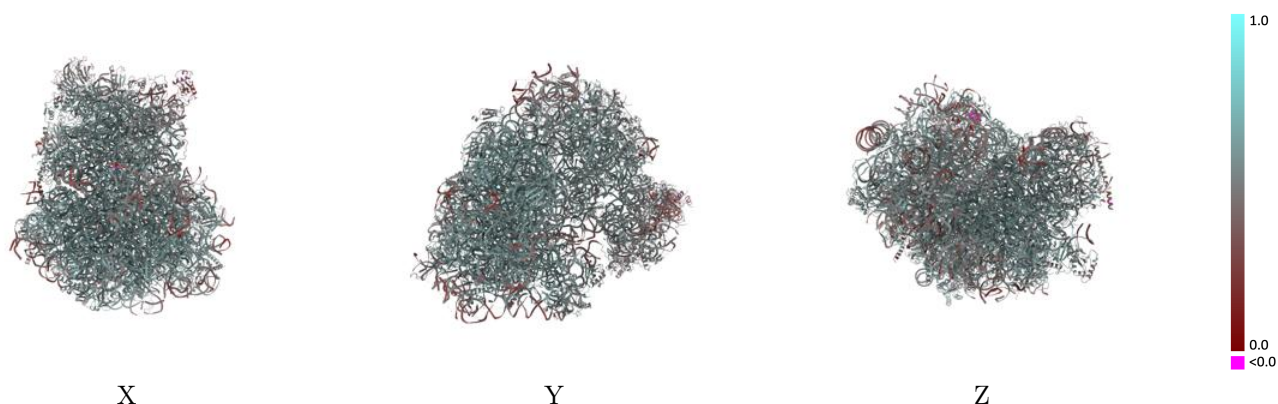
Y



Z

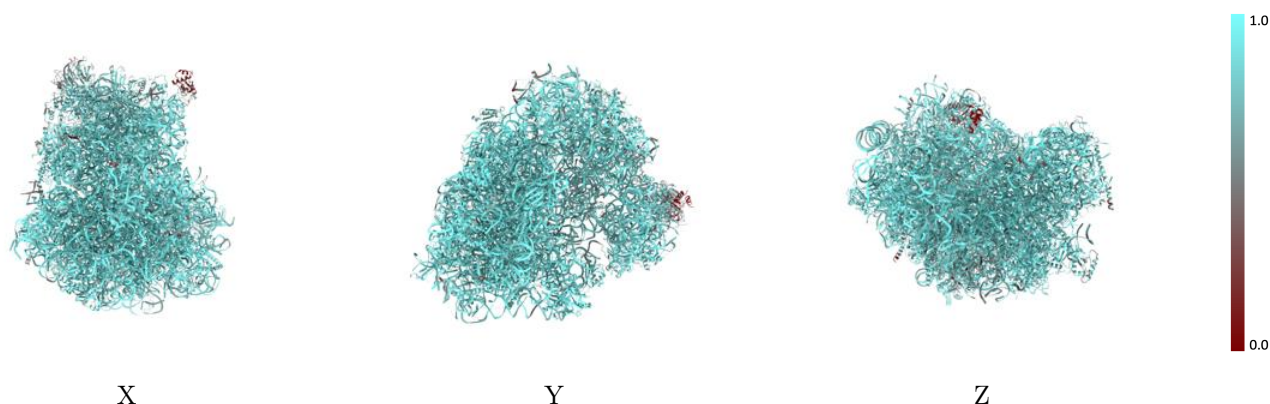
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



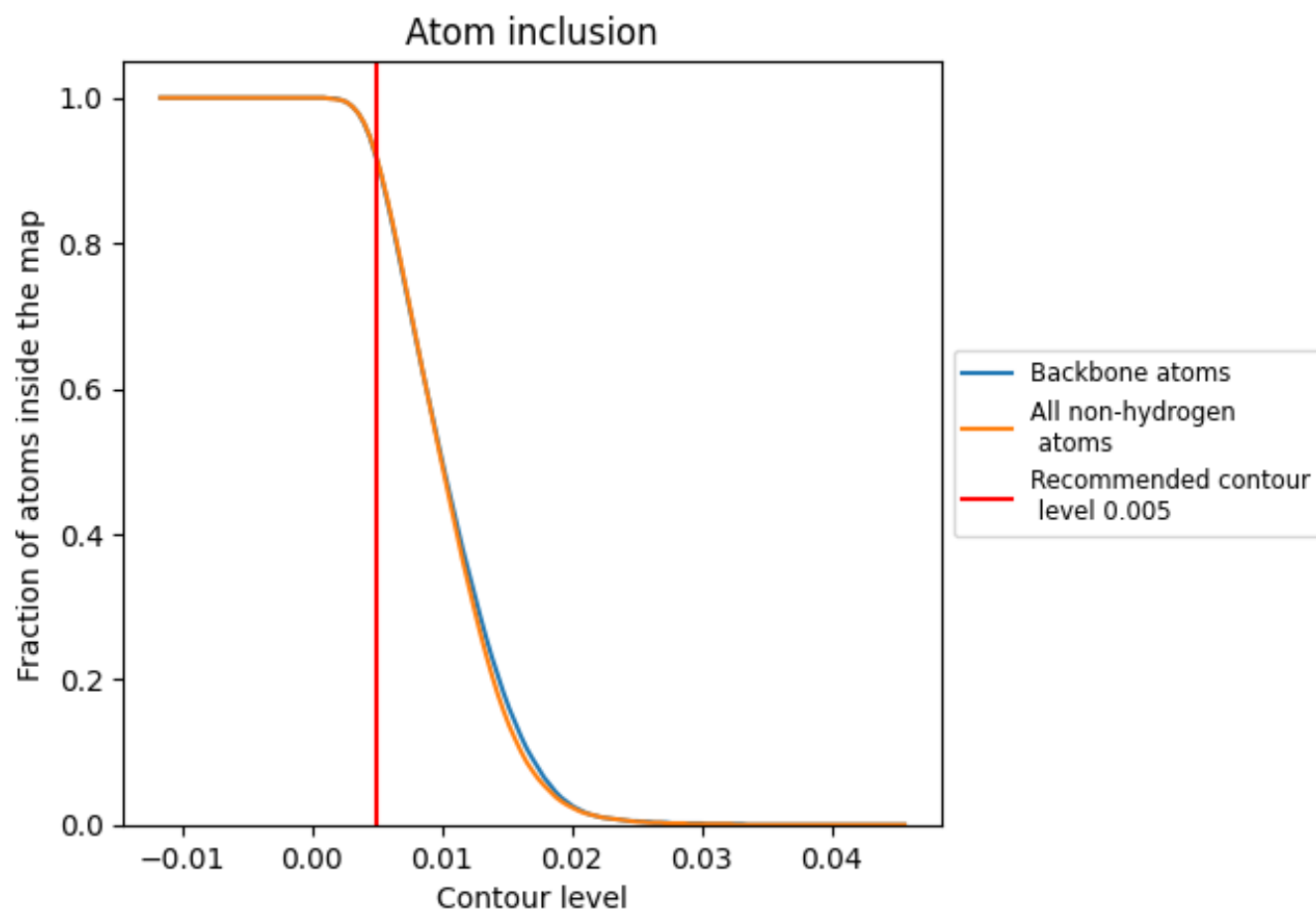
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 92% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.5400
L5	 0.9470	 0.5450
L7	 0.9750	 0.5630
L8	 0.9580	 0.5540
LA	 0.9650	 0.5940
LB	 0.9750	 0.5980
LC	 0.9160	 0.5790
LD	 0.9130	 0.5560
LE	 0.8960	 0.5550
LF	 0.9350	 0.5830
LG	 0.8820	 0.5440
LH	 0.9270	 0.5710
LI	 0.9240	 0.5770
LJ	 0.9180	 0.5420
LL	 0.8900	 0.5640
LM	 0.9300	 0.5680
LN	 0.9650	 0.6030
LO	 0.9370	 0.5860
LP	 0.9250	 0.5920
LQ	 0.9430	 0.5940
LR	 0.9420	 0.5700
LS	 0.9360	 0.5920
LT	 0.9170	 0.5730
LU	 0.8190	 0.5140
LV	 0.9470	 0.5880
LW	 0.9820	 0.5840
LX	 0.8980	 0.5720
LY	 0.8970	 0.5730
LZ	 0.9260	 0.5550
La	 0.9450	 0.5950
Lb	 0.8840	 0.5500
Lc	 0.9740	 0.5560
Ld	 0.8940	 0.5690
Le	 0.9250	 0.5940
Lf	 0.9520	 0.6080



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Chain	Atom inclusion	Q-score
Lg	 0.9640	 0.5840
Lh	 0.8950	 0.5640
Li	 0.9130	 0.5660
Lj	 0.9740	 0.6020
Lk	 0.8300	 0.5240
Ll	 0.9470	 0.5820
Lm	 0.9490	 0.5800
Ln	 0.9500	 0.5720
Lo	 0.8960	 0.5760
Lp	 0.9800	 0.5780
Lr	 0.9210	 0.5820
Pt	 0.7710	 0.4530
S2	 0.9410	 0.5170
S6	 0.7340	 0.2550
SA	 0.8070	 0.5400
SB	 0.8670	 0.5320
SC	 0.8490	 0.5540
SD	 0.7700	 0.5060
SE	 0.8520	 0.5280
SF	 0.8410	 0.5020
SG	 0.7970	 0.4640
SH	 0.7400	 0.5060
SI	 0.9260	 0.5370
SJ	 0.8550	 0.5180
SK	 0.8090	 0.4600
SL	 0.9150	 0.5630
SM	 0.2490	 0.2880
SN	 0.9200	 0.5520
SO	 0.8640	 0.5270
SP	 0.8820	 0.4830
SQ	 0.8390	 0.5210
SR	 0.7660	 0.5160
SS	 0.9140	 0.5020
ST	 0.8580	 0.4930
SU	 0.8320	 0.5010
SV	 0.7840	 0.5400
SW	 0.8930	 0.5640
SX	 0.8840	 0.5540
SY	 0.7990	 0.4940
SZ	 0.8420	 0.4810
Sa	 0.8680	 0.5450
Sb	 0.8710	 0.5610

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Chain	Atom inclusion	Q-score
Sc	 0.8120	 0.5020
Sd	 0.9110	 0.5400
Se	 0.8280	 0.5230
Sf	 0.5580	 0.3090
Sg	 0.6510	 0.4570
mR	 0.4510	 0.3870